



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:23 AM GMT

PDB ID : 3ABL
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (15-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 : 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

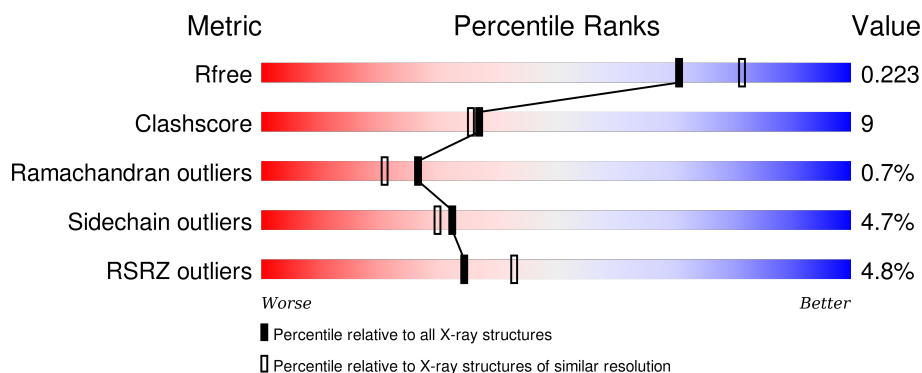
1 Overall quality at a glance

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))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 ≥ 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>76%</div> <div>21%</div> <div>.</div> </div>
1	N	514	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	B	227	<div> <div>75%</div> <div>21%</div> <div>..</div> </div>
2	O	227	<div> <div>3%</div> <div>71%</div> <div>23%</div> <div>5%</div> </div>
3	C	261	<div> <div>81%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PER	A	520	-	-	-	X
18	HEA	A	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	TGL	A	521	-	-	-	X
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1521	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	Q	1523	-	-	-	X
20	PGV	A	522	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	C	267	-	-	-	X
20	PGV	N	1266	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1267	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	PSC	B	230	-	-	-	X
22	PSC	O	1230	-	-	-	X
23	CHD	C	271	X	-	-	X
23	CHD	J	60	X	-	-	X
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	X
24	DMU	C	272	X	-	-	X
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	X
24	DMU	Z	1526	X	-	-	-
26	CDL	C	270	-	-	-	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	-	X
26	CDL	T	1269	-	-	X	-
28	PEK	G	264	-	-	-	X
28	PEK	P	1265	-	-	-	X
28	PEK	T	263	-	-	X	-

2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32244 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			

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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			

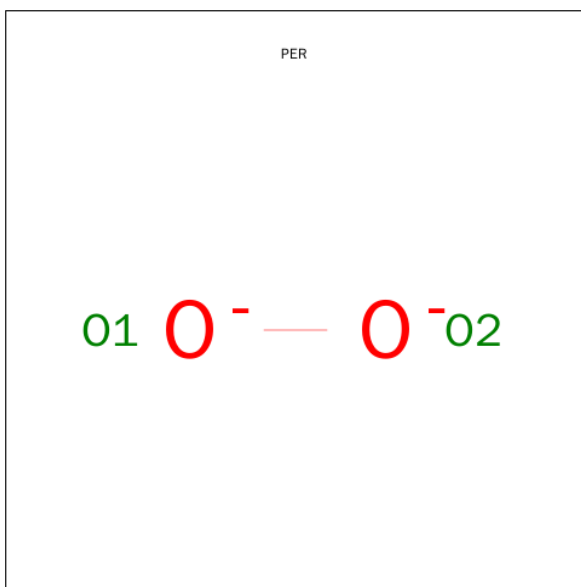
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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).

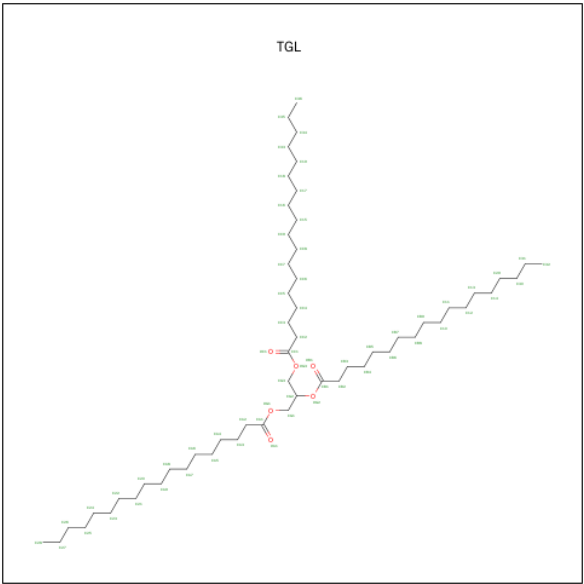
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



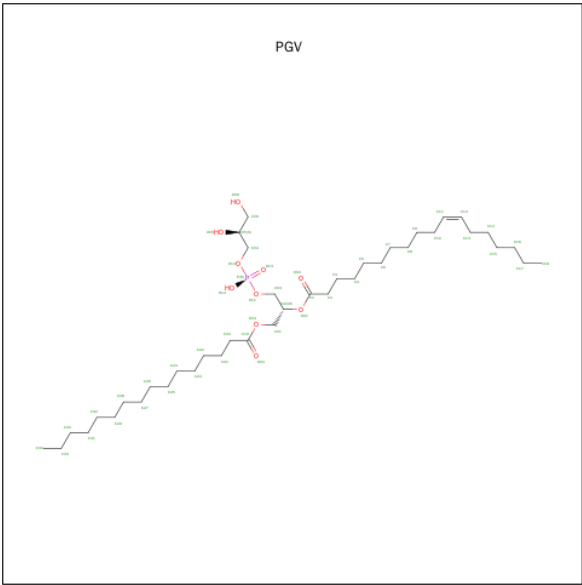
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- 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	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	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).



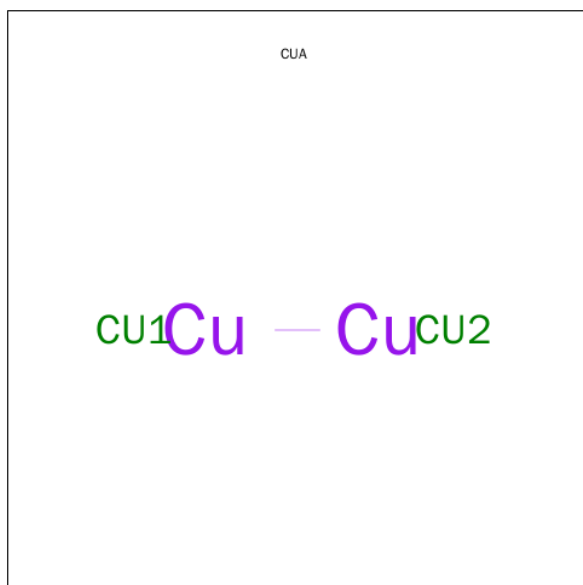
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

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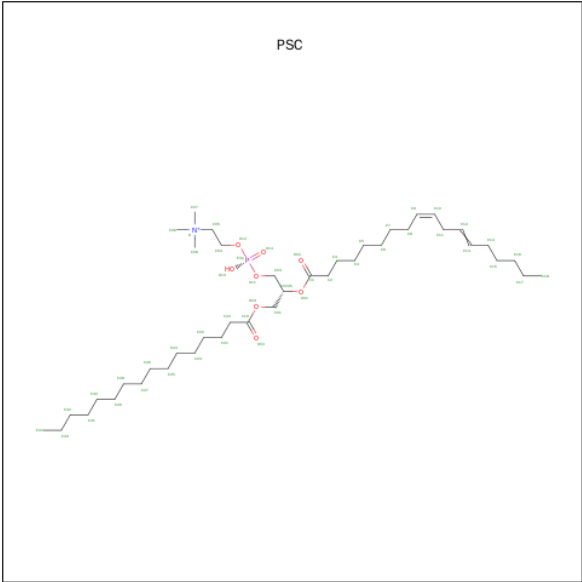
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



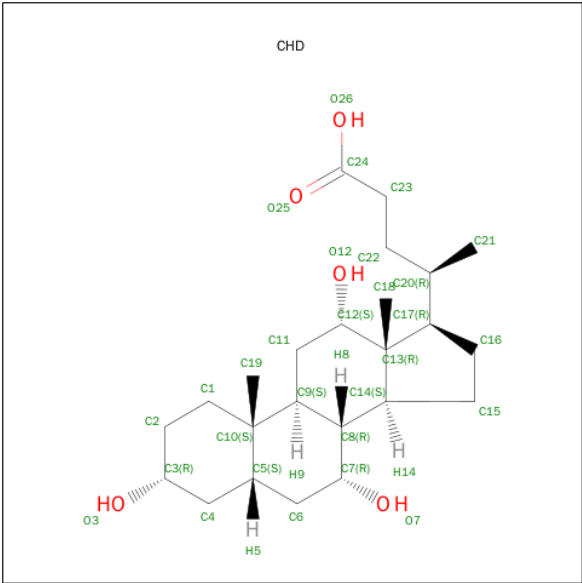
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- 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: C₄₂H₈₁NO₈P).



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

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



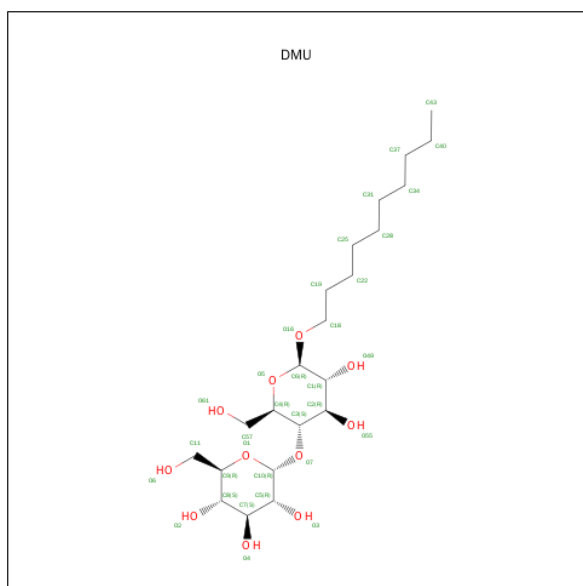
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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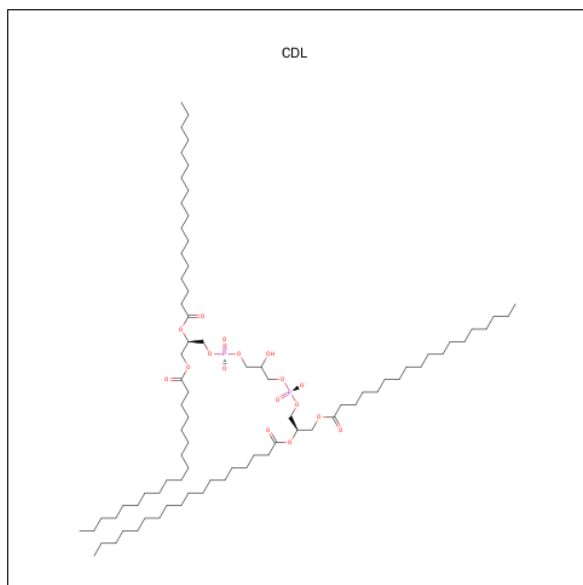
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0
			29	24	5		

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



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

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



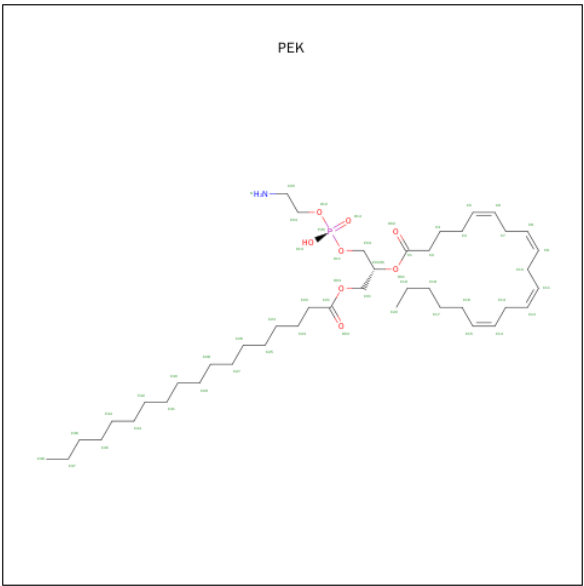
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O P 100 81 17 2	0	0
26	G	1	Total C O P 100 81 17 2	0	0
26	P	1	Total C O P 100 81 17 2	0	0
26	T	1	Total C O P 100 81 17 2	0	0

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

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

- Molecule 28 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
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

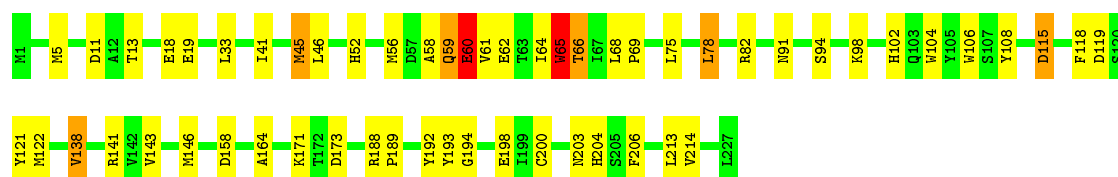
- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	219	Total	O	0	0
			219	219		
29	B	139	Total	O	0	0
			139	139		
29	C	105	Total	O	0	0
			105	105		
29	D	110	Total	O	0	0
			110	110		
29	E	68	Total	O	0	0
			68	68		

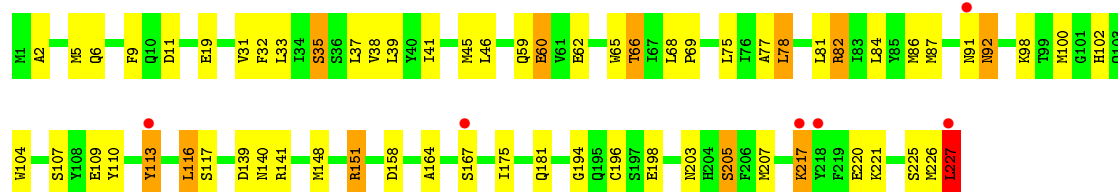
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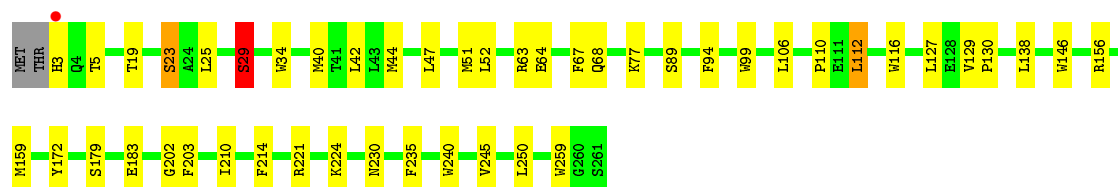
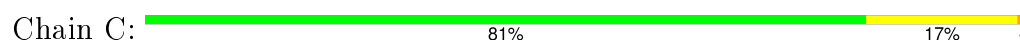
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	76	Total 76	O 76	0	0
29	G	45	Total 45	O 45	0	0
29	H	48	Total 48	O 48	0	0
29	I	35	Total 35	O 35	0	0
29	J	21	Total 21	O 21	0	0
29	K	22	Total 22	O 22	0	0
29	L	27	Total 27	O 27	0	0
29	M	18	Total 18	O 18	0	0
29	N	204	Total 204	O 204	0	0
29	O	109	Total 109	O 109	0	0
29	P	106	Total 106	O 106	0	0
29	Q	67	Total 67	O 67	0	0
29	R	52	Total 52	O 52	0	0
29	S	69	Total 69	O 69	0	0
29	T	48	Total 48	O 48	0	0
29	U	38	Total 38	O 38	0	0
29	V	19	Total 19	O 19	0	0
29	W	16	Total 16	O 16	0	0
29	X	16	Total 16	O 16	0	0
29	Y	17	Total 17	O 17	0	0
29	Z	14	Total 14	O 14	0	0



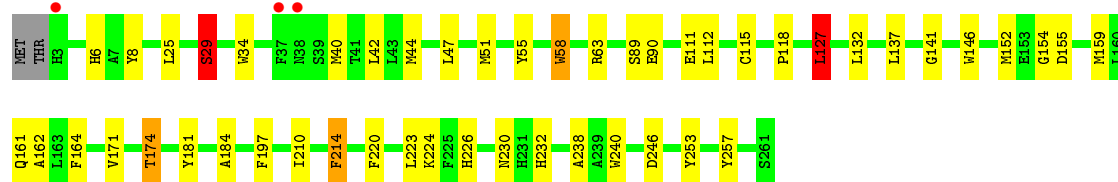
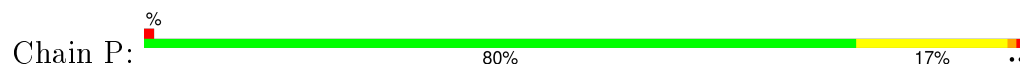
• Molecule 2: Cytochrome c oxidase subunit 2



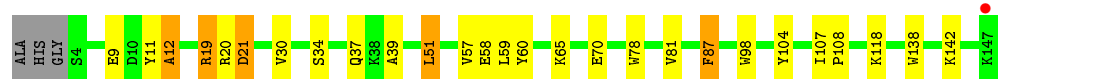
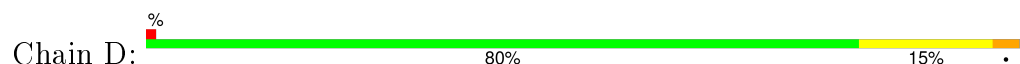
• Molecule 3: Cytochrome c oxidase subunit 3



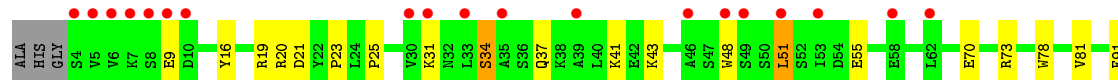
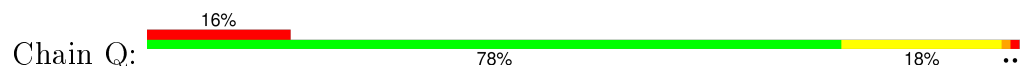
• Molecule 3: Cytochrome c oxidase subunit 3

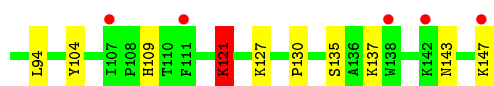


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

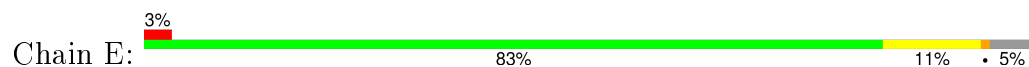


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

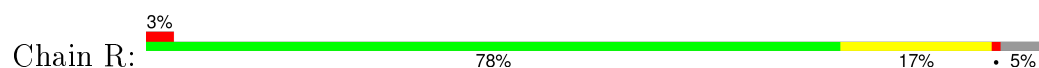




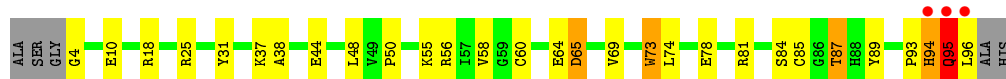
- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A



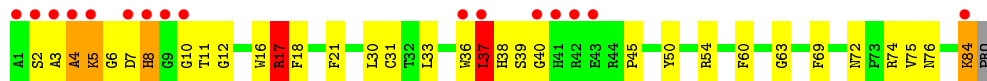
- Molecule 6: Cytochrome c oxidase subunit 5B



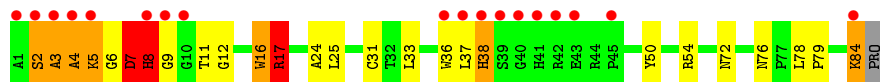
- Molecule 6: Cytochrome c oxidase subunit 5B



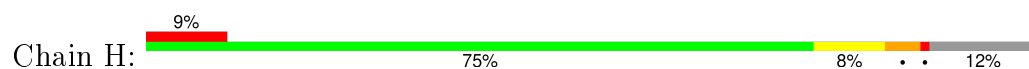
- Molecule 7: Cytochrome c oxidase subunit 6A2

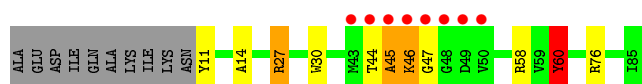


- Molecule 7: Cytochrome c oxidase subunit 6A2

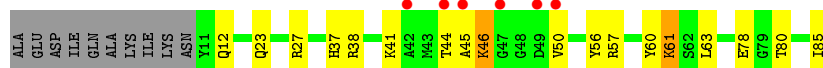


- Molecule 8: Cytochrome c oxidase subunit 6B1

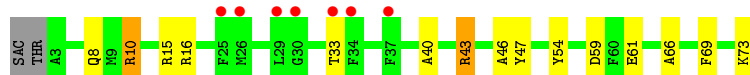




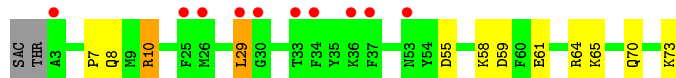
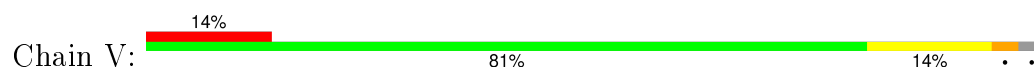
- Molecule 8: Cytochrome c oxidase subunit 6B1



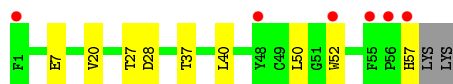
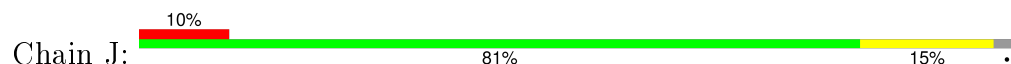
- Molecule 9: Cytochrome c oxidase subunit 6C



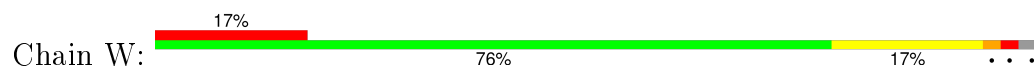
- Molecule 9: Cytochrome c oxidase subunit 6C



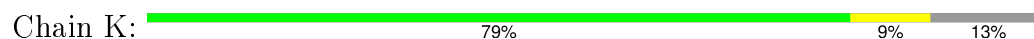
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



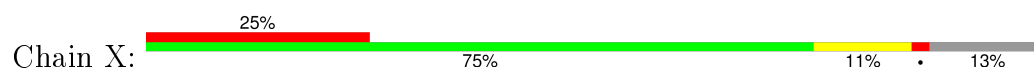
- Molecule 10: Cytochrome c oxidase polypeptide 7A1

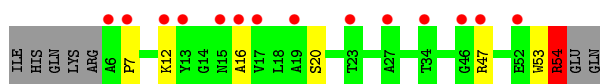


- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B

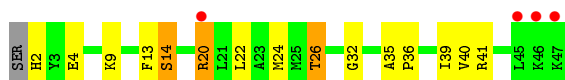




- Molecule 12: Cytochrome c oxidase subunit 7C



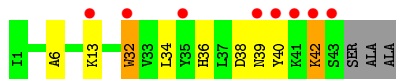
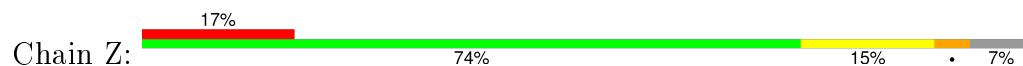
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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	184.14Å 207.51Å 178.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 38.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.10) 98.6 (38.32-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.176 , 0.210 0.193 , 0.223	Depositor DCC
R_{free} test set	13838 reflections (3.68%)	DCC
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 62.3	EDS
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 389450 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32244	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.72	46/4156 (1.1%)	1.25	23/5678 (0.4%)
1	N	1.55	27/4156 (0.6%)	1.16	20/5678 (0.4%)
2	B	1.61	18/1860 (1.0%)	1.29	13/2534 (0.5%)
2	O	1.36	7/1860 (0.4%)	1.11	5/2534 (0.2%)
3	C	1.52	12/2197 (0.5%)	1.04	3/3005 (0.1%)
3	P	1.53	18/2197 (0.8%)	1.07	6/3005 (0.2%)
4	D	1.67	20/1229 (1.6%)	1.24	8/1658 (0.5%)
4	Q	1.27	3/1229 (0.2%)	1.06	3/1658 (0.2%)
5	E	1.51	6/860 (0.7%)	1.17	4/1167 (0.3%)
5	R	1.27	3/860 (0.3%)	0.99	0/1167
6	F	1.57	9/733 (1.2%)	1.23	4/996 (0.4%)
6	S	1.34	2/733 (0.3%)	1.17	3/996 (0.3%)
7	G	1.44	5/690 (0.7%)	1.23	2/937 (0.2%)
7	T	1.48	5/690 (0.7%)	1.29	6/937 (0.6%)
8	H	1.51	5/648 (0.8%)	1.09	2/877 (0.2%)
8	U	1.28	2/648 (0.3%)	1.03	1/877 (0.1%)
9	I	1.53	6/598 (1.0%)	1.20	5/792 (0.6%)
9	V	1.24	0/598	1.04	2/792 (0.3%)
10	J	1.33	1/462 (0.2%)	0.99	1/625 (0.2%)
10	W	1.26	1/462 (0.2%)	1.09	3/625 (0.5%)
11	K	1.48	2/398 (0.5%)	1.06	1/546 (0.2%)
11	X	1.15	0/398	0.98	1/546 (0.2%)
12	L	1.57	4/393 (1.0%)	1.16	2/526 (0.4%)
12	Y	1.40	3/393 (0.8%)	0.98	0/526
13	M	1.54	3/345 (0.9%)	1.12	2/470 (0.4%)
13	Z	1.20	1/345 (0.3%)	0.98	0/470
All	All	1.51	209/29138 (0.7%)	1.15	120/39622 (0.3%)

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

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	S	0	1
All	All	0	2

The worst 5 of 209 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	60	CYS	CB-SG	10.42	2.00	1.82
3	P	29	SER	CB-OG	-9.66	1.29	1.42
4	D	39	ALA	CA-CB	8.57	1.70	1.52
1	N	139	ALA	CA-CB	8.38	1.70	1.52
7	G	36	TRP	CB-CG	8.16	1.65	1.50

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	17	ARG	NE-CZ-NH2	-15.09	112.76	120.30
7	T	17	ARG	NE-CZ-NH2	-14.08	113.26	120.30
4	D	19	ARG	NE-CZ-NH1	-12.84	113.88	120.30
4	Q	20	ARG	NE-CZ-NH2	-12.82	113.89	120.30
5	E	90	ARG	NE-CZ-NH2	-12.63	113.99	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	S	93	PRO	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	61	0
1	N	4027	0	4001	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1824	0	1833	27	0
2	O	1824	0	1833	41	0
3	C	2110	0	2027	29	0
3	P	2110	0	2027	28	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	17	0
5	E	842	0	838	4	0
5	R	842	0	838	10	0
6	F	717	0	700	16	0
6	S	717	0	700	20	0
7	G	675	0	643	34	0
7	T	675	0	643	43	0
8	H	628	0	580	5	0
8	U	628	0	580	5	0
9	I	585	0	597	10	0
9	V	585	0	597	12	0
10	J	451	0	446	5	0
10	W	451	0	446	7	0
11	K	384	0	366	1	0
11	X	384	0	366	6	0
12	L	380	0	380	11	0
12	Y	380	0	380	13	0
13	M	335	0	352	2	0
13	Z	335	0	352	5	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	0	0
17	N	1	0	0	0	0
18	A	120	0	108	12	0
18	N	120	0	108	9	0
19	A	63	0	110	6	0
19	D	63	0	110	15	0
19	L	63	0	110	16	0
19	N	126	0	220	20	0
19	Q	63	0	110	5	0
20	A	102	0	152	10	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	P	102	0	152	8	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	18	0
22	O	52	0	80	12	0
23	B	29	0	37	1	0
23	C	58	0	71	5	0
23	J	29	0	36	3	0
23	O	29	0	36	2	0
23	P	58	0	71	6	0
23	W	29	0	36	4	0
24	C	33	0	37	5	0
24	M	33	0	39	1	0
24	P	33	0	40	2	0
24	Z	33	0	39	1	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	13	0
26	G	100	0	156	24	0
26	P	100	0	156	16	0
26	T	100	0	156	23	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	20	0
28	P	106	0	154	14	0
28	T	53	0	77	21	0
29	A	219	0	0	6	0
29	B	139	0	0	3	0
29	C	105	0	0	2	0
29	D	110	0	0	0	0
29	E	68	0	0	0	0
29	F	76	0	0	3	0
29	G	45	0	0	7	0
29	H	48	0	0	1	0
29	I	35	0	0	1	0
29	J	21	0	0	1	0
29	K	22	0	0	0	0
29	L	27	0	0	1	0
29	M	18	0	0	0	0
29	N	204	0	0	2	0
29	O	109	0	0	0	0
29	P	106	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Q	67	0	0	3	0
29	R	52	0	0	0	0
29	S	69	0	0	4	0
29	T	48	0	0	4	0
29	U	38	0	0	3	0
29	V	19	0	0	0	0
29	W	16	0	0	0	0
29	X	16	0	0	0	0
29	Y	17	0	0	1	0
29	Z	14	0	0	0	0
All	All	32244	0	31064	577	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 577 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:CG1	1:A:75:ILE:CD1	1.74	1.62
3:P:174:THR:CB	3:P:174:THR:CG2	1.74	1.60
28:G:265:PEK:H383	26:G:269:CDL:C27	1.62	1.29
28:P:1265:PEK:H383	26:T:1269:CDL:C27	1.64	1.25
7:T:2:SER:OG	28:T:263:PEK:H302	1.33	1.23

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%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	484 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	39	37
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	39	37
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	39	37
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	26	21
5	E	102/109 (94%)	99 (97%)	3 (3%)	0	100	100
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	88 (97%)	1 (1%)	2 (2%)	8	3
6	S	91/98 (93%)	86 (94%)	3 (3%)	2 (2%)	8	3
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1	0
8	H	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	6	2
8	U	73/85 (86%)	66 (90%)	4 (6%)	3 (4%)	3	1
9	I	69/73 (94%)	68 (99%)	1 (1%)	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%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	43 (92%)	4 (8%)	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%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3478/3614 (96%)	3316 (95%)	136 (4%)	26 (1%)	26	21

5 of 26 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%)	416 (98%)	10 (2%)	58	62
1	N	426/426 (100%)	412 (97%)	14 (3%)	45	47
2	B	210/210 (100%)	199 (95%)	11 (5%)	29	25
2	O	210/210 (100%)	192 (91%)	18 (9%)	13	9
3	C	224/226 (99%)	217 (97%)	7 (3%)	47	50
3	P	224/226 (99%)	219 (98%)	5 (2%)	60	64
4	D	128/129 (99%)	127 (99%)	1 (1%)	86	91
4	Q	128/129 (99%)	121 (94%)	7 (6%)	27	23
5	E	91/95 (96%)	89 (98%)	2 (2%)	60	64
5	R	91/95 (96%)	89 (98%)	2 (2%)	60	64
6	F	79/81 (98%)	72 (91%)	7 (9%)	12	8
6	S	79/81 (98%)	72 (91%)	7 (9%)	12	8
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	3
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	8
8	H	67/75 (89%)	65 (97%)	2 (3%)	48	51
8	U	67/75 (89%)	60 (90%)	7 (10%)	9	5
9	I	56/57 (98%)	53 (95%)	3 (5%)	27	24
9	V	56/57 (98%)	53 (95%)	3 (5%)	27	24
10	J	48/50 (96%)	47 (98%)	1 (2%)	61	66
10	W	48/50 (96%)	46 (96%)	2 (4%)	36	35
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	58
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	26
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	58
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16	12
13	M	37/38 (97%)	30 (81%)	7 (19%)	2	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3022/3082 (98%)	2881 (95%)	141 (5%)	32 30

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	109	PHE
2	O	65	TRP
10	W	4	ARG
1	N	138	HIS
1	N	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	99	ASN
2	O	22	HIS
9	V	70	GLN
1	N	178	GLN
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 ⓘ

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	8,9,10	1.38	2 (25%)	6,9,11	5.63	4 (66%)
2	FME	B	1	2	8,9,10	2.14	2 (25%)	6,9,11	6.80	4 (66%)

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	1.98	3 (37%)	7,14,16	2.39	2 (28%)
1	FME	N	1	1	8,9,10	0.78	0	6,9,11	5.56	4 (66%)
2	FME	O	1	2	8,9,10	1.18	1 (12%)	6,9,11	6.97	4 (66%)
7	TPO	T	11	7	8,10,11	1.99	3 (37%)	7,14,16	1.75	3 (42%)

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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.87	1.10	1.22
1	A	1	FME	CB-CA	-2.57	1.48	1.53
2	O	1	FME	O1-CN	-2.47	1.15	1.22
1	A	1	FME	O1-CN	-2.42	1.15	1.22
7	T	11	TPO	O-C	2.13	1.29	1.19

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-15.94	98.31	122.82
2	B	1	FME	CA-N-CN	-14.83	100.01	122.82
1	A	1	FME	CA-N-CN	-13.10	102.67	122.82
1	N	1	FME	CA-N-CN	-12.51	103.58	122.82
2	B	1	FME	CG-CB-CA	-5.03	98.30	113.06

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	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, 2 are unknown and 8 are monoatomic - 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	40,67,67	1.56	8 (20%)	41,103,103	2.84	14 (34%)
18	HEA	A	516	1,15	40,67,67	1.52	9 (22%)	41,103,103	2.82	16 (39%)
15	PER	A	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.40	7 (11%)	65,65,65	2.40	14 (21%)
20	PGV	A	522	-	50,50,50	1.10	1 (2%)	51,56,56	1.43	7 (13%)
20	PGV	A	524	-	50,50,50	1.17	2 (4%)	51,56,56	1.52	7 (13%)
23	CHD	B	1086	-	29,32,32	1.82	7 (24%)	48,51,51	5.23	35 (72%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	230	-	51,51,51	1.36	3 (5%)	55,59,59	1.29	5 (9%)
20	PGV	C	267	-	50,50,50	0.94	3 (6%)	51,56,56	1.50	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	C	268	-	50,50,50	1.21	2 (4%)	51,56,56	1.42	5 (9%)
26	CDL	C	270	-	99,99,99	1.38	12 (12%)	101,111,111	1.63	17 (16%)
23	CHD	C	271	-	29,32,32	0.77	1 (3%)	48,51,51	5.02	32 (66%)
24	DMU	C	272	-	34,34,34	1.18	1 (2%)	45,45,45	3.42	23 (51%)
23	CHD	C	525	-	29,32,32	1.65	7 (24%)	48,51,51	5.17	38 (79%)
19	TGL	D	523	-	62,62,62	1.56	7 (11%)	65,65,65	1.78	12 (18%)
28	PEK	G	1263	-	51,52,52	1.16	2 (3%)	52,57,57	1.34	6 (11%)
28	PEK	G	264	-	51,52,52	0.91	2 (3%)	52,57,57	2.19	11 (21%)
28	PEK	G	265	-	51,52,52	1.15	2 (3%)	52,57,57	1.15	4 (7%)
26	CDL	G	269	-	99,99,99	1.36	12 (12%)	101,111,111	1.32	13 (12%)
23	CHD	J	60	-	29,32,32	0.70	0	48,51,51	4.86	36 (75%)
19	TGL	L	522	-	62,62,62	1.43	7 (11%)	65,65,65	1.86	13 (20%)
24	DMU	M	526	-	34,34,34	0.88	2 (5%)	45,45,45	3.23	26 (57%)
20	PGV	N	1266	-	50,50,50	0.87	2 (4%)	51,56,56	1.65	10 (19%)
19	TGL	N	1521	-	62,62,62	1.30	6 (9%)	65,65,65	1.68	11 (16%)
19	TGL	N	1522	-	62,62,62	1.46	7 (11%)	65,65,65	1.55	10 (15%)
20	PGV	N	1524	-	50,50,50	1.15	2 (4%)	51,56,56	1.31	5 (9%)
18	HEA	N	515	1	40,67,67	1.33	6 (15%)	41,103,103	3.16	17 (41%)
18	HEA	N	516	1,15	40,67,67	1.38	6 (15%)	41,103,103	1.97	10 (24%)
15	PER	N	520	18,14	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	O	1230	-	51,51,51	1.22	3 (5%)	55,59,59	1.30	5 (9%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.58	6 (20%)	48,51,51	5.86	31 (64%)
28	PEK	P	1264	-	51,52,52	1.04	4 (7%)	52,57,57	1.69	8 (15%)
28	PEK	P	1265	-	51,52,52	1.20	2 (3%)	52,57,57	1.33	5 (9%)
20	PGV	P	1267	-	50,50,50	0.91	3 (6%)	51,56,56	1.55	11 (21%)
20	PGV	P	1268	-	50,50,50	1.18	2 (4%)	51,56,56	1.44	5 (9%)
26	CDL	P	1270	-	99,99,99	1.32	13 (13%)	101,111,111	1.44	13 (12%)
23	CHD	P	1271	-	29,32,32	0.82	1 (3%)	48,51,51	5.22	35 (72%)
24	DMU	P	1272	-	34,34,34	1.22	3 (8%)	45,45,45	3.21	22 (48%)
23	CHD	P	1525	-	29,32,32	1.29	5 (17%)	48,51,51	5.51	38 (79%)
19	TGL	Q	1523	-	62,62,62	1.37	6 (9%)	65,65,65	1.42	10 (15%)
26	CDL	T	1269	-	99,99,99	1.30	12 (12%)	101,111,111	1.52	15 (14%)
28	PEK	T	263	-	51,52,52	1.29	3 (5%)	52,57,57	1.41	6 (11%)
23	CHD	W	1060	-	29,32,32	0.84	1 (3%)	48,51,51	4.93	36 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	Z	1526	-	34,34,34	1.00	2 (5%)	45,45,45	3.34	25 (55%)

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
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
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	-	1/1/12/12	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
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
28	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
28	PEK	G	264	-	-	0/56/56/56	0/0/0/0
28	PEK	G	265	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	1/110/110/110	0/0/0/0
23	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
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
19	TGL	N	1522	-	-	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	2/2/7/16	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
22	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	1/1/12/12	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
28	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	-	1/1/12/12	0/7/74/74	0/4/4/4
24	DMU	P	1272	-	5/5/10/10	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
28	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1060	-	2/2/12/12	0/7/74/74	0/4/4/4
24	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 192 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C1D-ND	-4.51	1.30	1.36
23	B	1086	CHD	C8-C7	-4.13	1.46	1.53
18	N	515	HEA	C1A-NA	-3.59	1.31	1.36
23	C	525	CHD	C13-C12	-3.59	1.48	1.54
28	P	1264	PEK	O03-C01	-3.55	1.37	1.45

The worst 5 of 672 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C19-C10-C9	-11.70	93.64	111.18
23	B	1086	CHD	C18-C13-C12	-11.13	98.23	109.09
23	O	229	CHD	C18-C13-C12	-10.91	98.45	109.09
23	O	229	CHD	C19-C10-C9	-10.85	94.91	111.18
23	P	1271	CHD	C18-C13-C12	-9.88	99.46	109.09

5 of 39 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	W	1060	CHD	C17
23	W	1060	CHD	C9
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB

All (3) 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
26	G	269	CDL	PB2-OB2-CB2-C1

There are no ring outliers.

44 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	515	HEA	7	0
18	A	516	HEA	5	0
15	A	520	PER	1	0
19	A	521	TGL	6	0
20	A	522	PGV	2	0
20	A	524	PGV	8	0
23	B	1086	CHD	1	0
22	B	230	PSC	18	0
20	C	267	PGV	5	0
20	C	268	PGV	1	0
26	C	270	CDL	13	0
23	C	271	CHD	3	0
24	C	272	DMU	5	0
23	C	525	CHD	2	0
19	D	523	TGL	15	0
28	G	1263	PEK	7	0
28	G	264	PEK	6	0
28	G	265	PEK	7	0
26	G	269	CDL	24	0
23	J	60	CHD	3	0
19	L	522	TGL	16	0
24	M	526	DMU	1	0
20	N	1266	PGV	1	0
19	N	1521	TGL	9	0
19	N	1522	TGL	11	0
20	N	1524	PGV	6	0
18	N	515	HEA	8	0
18	N	516	HEA	1	0
15	N	520	PER	1	0
22	O	1230	PSC	12	0
23	O	229	CHD	2	0
28	P	1264	PEK	6	0
28	P	1265	PEK	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	1267	PGV	5	0
20	P	1268	PGV	3	0
26	P	1270	CDL	16	0
23	P	1271	CHD	3	0
24	P	1272	DMU	2	0
23	P	1525	CHD	3	0
19	Q	1523	TGL	5	0
26	T	1269	CDL	23	0
28	T	263	PEK	21	0
23	W	1060	CHD	4	0
24	Z	1526	DMU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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%)	-0.09	3 (0%) 90 92	20, 25, 32, 63	0
1	N	513/514 (99%)	-0.17	3 (0%) 90 92	24, 31, 38, 63	0
2	B	226/227 (99%)	-0.51	0 100 100	21, 29, 49, 77	0
2	O	226/227 (99%)	-0.22	6 (2%) 58 65	28, 37, 56, 77	0
3	C	259/261 (99%)	-0.63	1 (0%) 93 94	22, 28, 40, 63	0
3	P	259/261 (99%)	-0.49	3 (1%) 81 85	25, 32, 43, 63	0
4	D	144/147 (97%)	-0.52	1 (0%) 89 91	25, 31, 48, 64	0
4	Q	144/147 (97%)	0.80	24 (16%) 2 3	33, 44, 67, 108	0
5	E	104/109 (95%)	-0.53	3 (2%) 55 63	26, 31, 51, 65	0
5	R	104/109 (95%)	-0.09	3 (2%) 55 63	31, 38, 58, 74	0
6	F	93/98 (94%)	-0.13	3 (3%) 51 60	23, 34, 52, 94	0
6	S	93/98 (94%)	0.24	4 (4%) 39 48	29, 38, 59, 91	0
7	G	83/85 (97%)	0.39	16 (19%) 2 2	25, 35, 94, 102	0
7	T	83/85 (97%)	0.59	18 (21%) 1 1	27, 38, 93, 100	0
8	H	75/85 (88%)	-0.08	8 (10%) 8 11	28, 36, 69, 75	0
8	U	75/85 (88%)	0.20	6 (8%) 15 21	32, 41, 72, 76	0
9	I	71/73 (97%)	0.24	7 (9%) 9 13	28, 38, 65, 70	0
9	V	71/73 (97%)	0.68	10 (14%) 4 5	30, 48, 65, 75	0
10	J	57/59 (96%)	-0.12	6 (10%) 8 11	28, 37, 57, 70	0
10	W	57/59 (96%)	0.59	10 (17%) 2 3	33, 42, 62, 79	0
11	K	49/56 (87%)	-0.22	0 100 100	28, 35, 47, 55	0
11	X	49/56 (87%)	1.48	14 (28%) 1 1	38, 45, 60, 71	0
12	L	46/47 (97%)	-0.38	3 (6%) 22 29	26, 31, 51, 75	0
12	Y	46/47 (97%)	0.11	4 (8%) 13 17	33, 39, 60, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.04	6 (13%) 4 5	27, 30, 65, 89	0
13	Z	43/46 (93%)	0.63	8 (18%) 2 2	35, 39, 77, 95	0
All	All	3526/3614 (97%)	-0.10	170 (4%) 34 43	20, 33, 58, 108	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	18.1
4	Q	5	VAL	12.6
4	Q	4	SER	10.7
6	F	96	LEU	9.4
4	Q	8	SER	9.1

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
7	TPO	G	11	11/12	0.53	0.34	-	68,74,91,92	0
2	FME	O	1	10/11	0.96	0.11	-	36,37,46,55	0
1	FME	N	1	10/11	0.91	0.20	-	48,54,69,70	0
2	FME	B	1	10/11	0.97	0.14	-	27,29,39,57	0
1	FME	A	1	10/11	0.91	0.16	-	42,48,68,76	0
7	TPO	T	11	11/12	0.38	0.35	-	70,77,97,98	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
23	CHD	W	1060	29/29	0.52	0.46	9.65	107,109,111,111	0
20	PGV	A	524	51/51	0.77	0.23	9.05	33,71,98,101	0
24	DMU	C	272	33/33	0.30	0.36	7.60	70,99,105,105	0
26	CDL	C	270	100/100	0.77	0.24	6.10	43,84,127,129	0
23	CHD	J	60	29/29	0.67	0.41	5.67	99,100,106,106	0
19	TGL	N	1522	63/63	0.59	0.31	5.58	45,73,89,92	0
26	CDL	P	1270	100/100	0.72	0.27	5.26	43,87,117,123	0
19	TGL	L	522	63/63	0.71	0.26	4.62	36,66,84,86	0
24	DMU	P	1272	33/33	0.47	0.40	4.43	89,103,109,111	0
15	PER	A	520	2/2	0.99	0.21	3.87	16,16,16,19	0
22	PSC	O	1230	52/52	0.66	0.30	3.85	41,93,121,122	0
19	TGL	D	523	63/63	0.76	0.19	3.48	41,69,96,98	0
19	TGL	A	521	63/63	0.81	0.21	3.47	47,71,92,98	0
19	TGL	N	1521	63/63	0.74	0.23	3.22	53,75,92,94	0
20	PGV	N	1266	51/51	0.96	0.21	3.21	28,41,63,64	0
22	PSC	B	230	52/52	0.68	0.28	2.94	39,96,121,123	0
20	PGV	A	522	51/51	0.97	0.18	2.59	25,37,63,68	0
20	PGV	C	267	51/51	0.96	0.17	2.58	20,31,74,77	0
19	TGL	Q	1523	63/63	0.67	0.20	2.48	53,78,92,94	0
28	PEK	G	264	53/53	0.96	0.18	2.48	23,43,71,73	0
26	CDL	G	269	100/100	0.66	0.26	2.46	62,86,114,116	0
20	PGV	N	1524	51/51	0.76	0.22	2.46	43,72,104,106	0
23	CHD	C	271	29/29	0.85	0.23	2.36	59,69,71,72	0
28	PEK	P	1265	53/53	0.59	0.30	2.30	42,86,105,108	0
20	PGV	P	1267	51/51	0.96	0.17	2.17	21,37,76,85	0
20	PGV	P	1268	51/51	0.73	0.23	2.04	64,97,112,113	0
28	PEK	G	265	53/53	0.49	0.27	1.90	45,91,106,111	0
15	PER	N	520	2/2	0.97	0.13	1.79	20,20,20,27	0
23	CHD	P	1271	29/29	0.88	0.21	1.68	68,74,77,78	0
20	PGV	C	268	51/51	0.72	0.19	1.60	59,88,104,105	0
24	DMU	Z	1526	33/33	0.77	0.20	1.50	42,51,63,65	0
28	PEK	P	1264	53/53	0.95	0.17	1.50	26,47,80,82	0
26	CDL	T	1269	100/100	0.69	0.22	1.46	52,85,111,116	0
28	PEK	T	263	53/53	0.54	0.30	1.28	48,93,126,127	0
28	PEK	G	1263	53/53	0.58	0.32	1.22	50,107,128,129	0
24	DMU	M	526	33/33	0.85	0.14	0.69	35,44,55,60	0
18	HEA	N	515	60/60	0.97	0.15	0.67	22,28,54,56	0
18	HEA	A	515	60/60	0.98	0.15	0.15	16,23,46,47	0
18	HEA	N	516	60/60	0.98	0.12	-0.05	23,28,35,38	0
21	CUA	B	228	2/2	1.00	0.10	-0.07	23,23,23,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CHD	C	525	29/29	0.95	0.08	-0.27	24,32,36,43	0
23	CHD	B	1086	29/29	0.96	0.08	-0.34	23,28,35,44	0
16	MG	A	518	1/1	0.98	0.12	-0.43	21,21,21,21	0
18	HEA	A	516	60/60	0.99	0.11	-0.49	13,22,29,32	0
17	NA	A	519	1/1	0.98	0.07	-0.55	25,25,25,25	0
23	CHD	P	1525	29/29	0.94	0.09	-0.57	25,33,39,39	0
27	ZN	F	99	1/1	1.00	0.07	-0.58	30,30,30,30	0
23	CHD	O	229	29/29	0.96	0.07	-0.62	21,25,34,39	0
27	ZN	S	99	1/1	0.99	0.06	-1.14	34,34,34,34	0
16	MG	N	1518	1/1	0.91	0.09	-1.46	29,29,29,29	0
21	CUA	O	228	2/2	0.97	0.07	-1.54	31,31,31,32	0
17	NA	N	1519	1/1	0.95	0.06	-1.91	30,30,30,30	0
14	CU	N	517	1/1	1.00	0.13	-	30,30,30,30	0
14	CU	A	517	1/1	0.99	0.11	-	24,24,24,24	0
25	UNX	C	262	1/1	0.68	0.27	-	39,39,39,39	0
25	UNX	P	1262	1/1	0.76	0.33	-	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.