wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 01:55 AM GMT

PDB ID	:	2EIJ
Title	:	Bovine heart cytochrome C oxidase in the fully reduced state
Authors	:	Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2007-03-13
Resolution	:	1.90 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 (i) symbol.

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

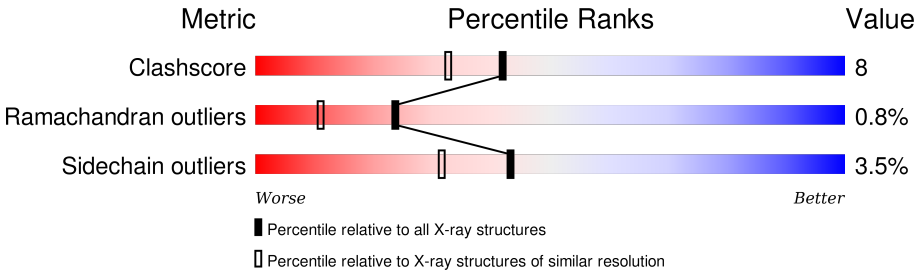
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	88% 11% •
1	N	514	82% 17% •
2	B	227	84% 15% •
2	O	227	73% 25% •
3	C	261	89% 11% •
3	P	261	87% 11% ••
4	D	147	89% 9% •

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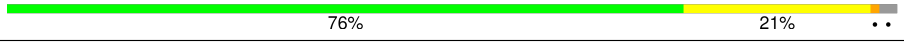
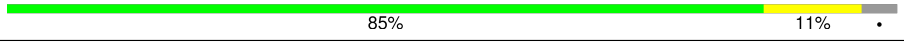
Mol	Chain	Length	Quality of chain
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
22	CHD	C	271	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
23	DMU	C	272	X	-	-	-
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	-
23	DMU	Z	1526	X	-	-	-

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 32488 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

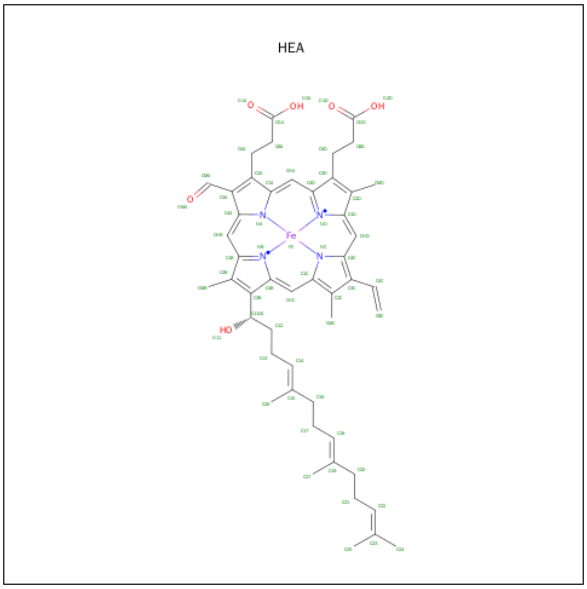
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

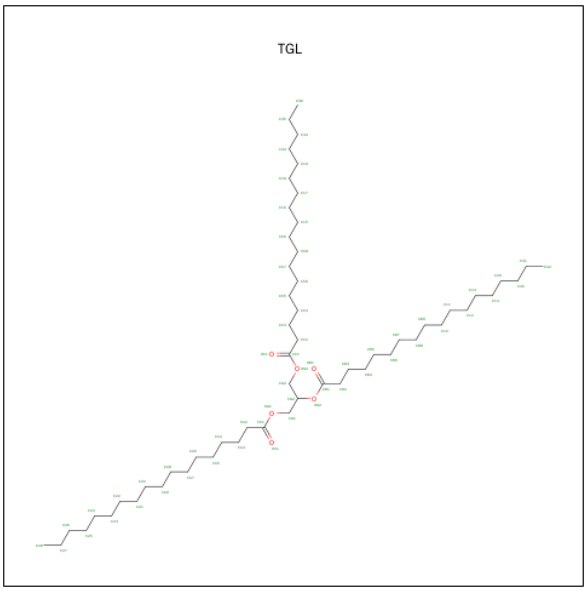
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Na 1 1	0	0
16	N	1	Total Na 1 1	0	0

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



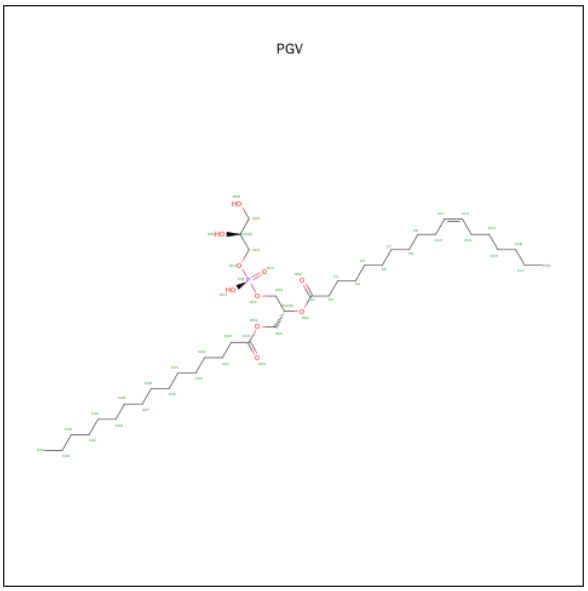
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	A	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0
17	N	1	Total C Fe N O 60 49 1 4 6	0	0

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



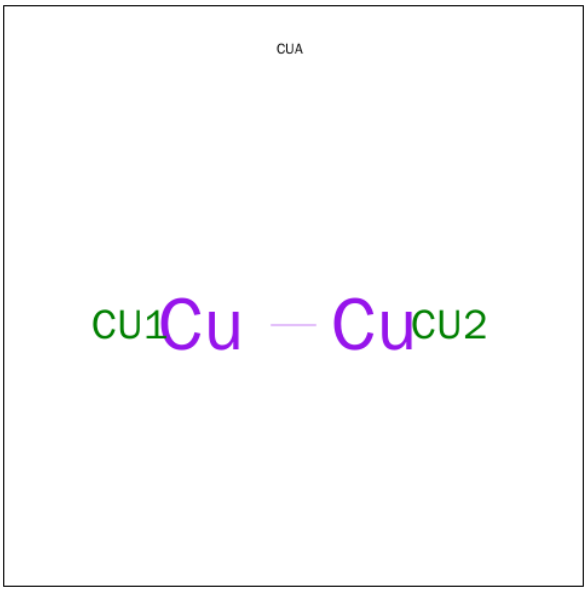
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 63 57 6	0	0
18	B	1	Total C O 63 57 6	0	0
18	L	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0
18	N	1	Total C O 63 57 6	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



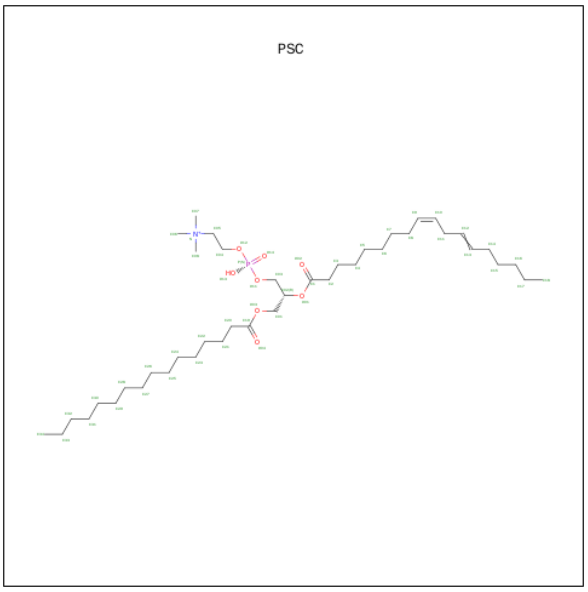
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

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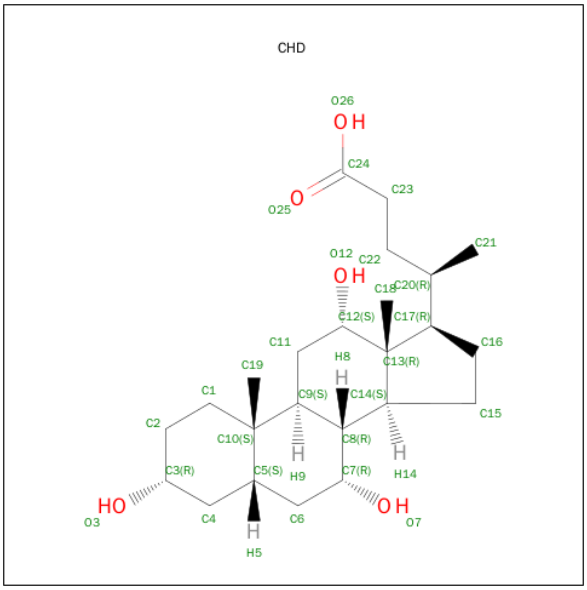
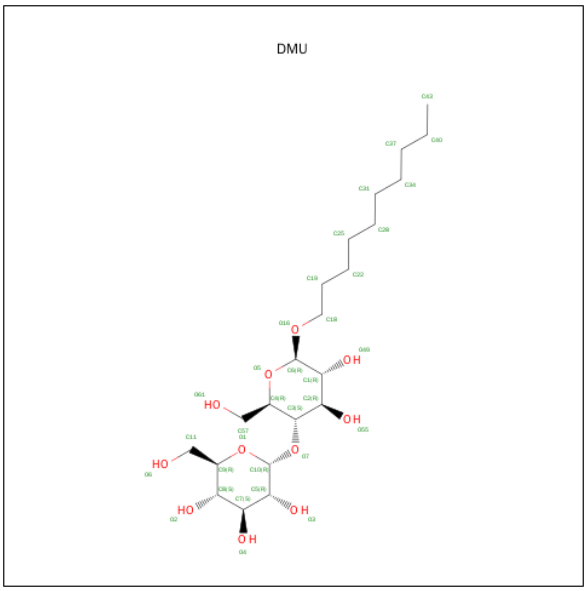
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

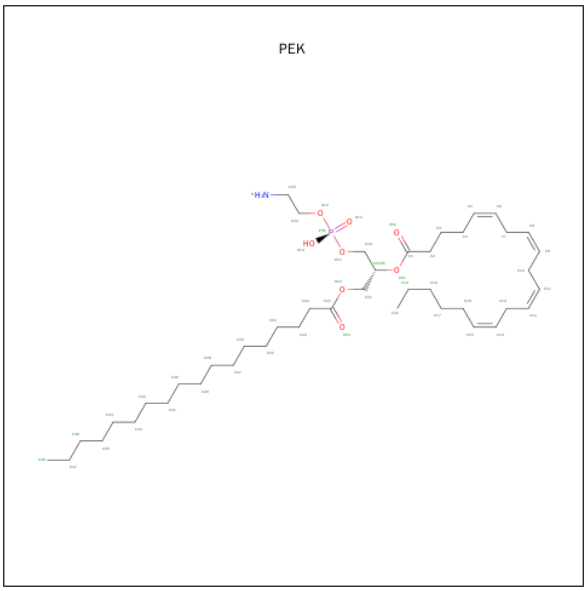


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 33 22 11	0	0
23	M	1	Total C O 33 22 11	0	0
23	P	1	Total C O 33 22 11	0	0
23	Z	1	Total C O 33 22 11	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

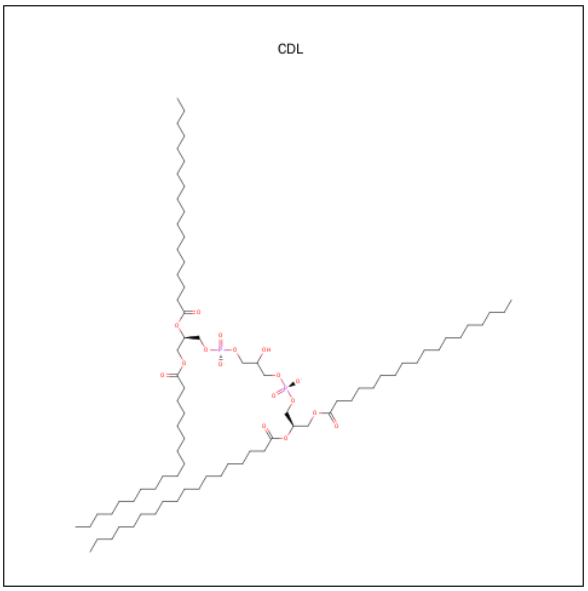
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total Zn 1 1	0	0
24	C	1	Total Zn 1 1	0	0
24	F	1	Total Zn 1 1	0	0
24	S	1	Total Zn 1 1	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O P 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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	237	Total O 237 237	0	0
27	B	145	Total O 145 145	0	0
27	C	110	Total O 110 110	0	0
27	D	94	Total O 94 94	0	0
27	E	60	Total O 60 60	0	0
27	F	72	Total O 72 72	0	0
27	G	44	Total O 44 44	0	0
27	H	50	Total O 50 50	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	38	Total O 38 38	0	0
27	J	23	Total O 23 23	0	0
27	K	22	Total O 22 22	0	0
27	L	27	Total O 27 27	0	0
27	M	24	Total O 24 24	0	0
27	N	218	Total O 218 218	0	0
27	O	122	Total O 122 122	0	0
27	P	112	Total O 112 112	0	0
27	Q	53	Total O 53 53	0	0
27	R	45	Total O 45 45	0	0
27	S	76	Total O 76 76	0	0
27	T	42	Total O 42 42	0	0
27	U	46	Total O 46 46	0	0
27	V	25	Total O 25 25	0	0
27	W	18	Total O 18 18	0	0
27	X	21	Total O 21 21	0	0
27	Y	17	Total O 17 17	0	0
27	Z	15	Total O 15 15	0	0

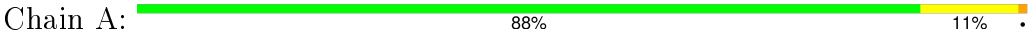
3 Residue-property plots (i)

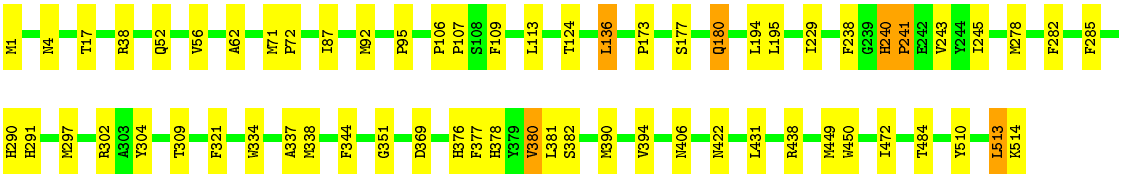
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Cytochrome c oxidase subunit 1

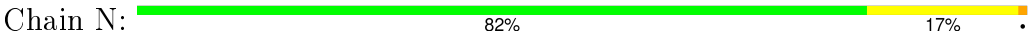
Chain A:

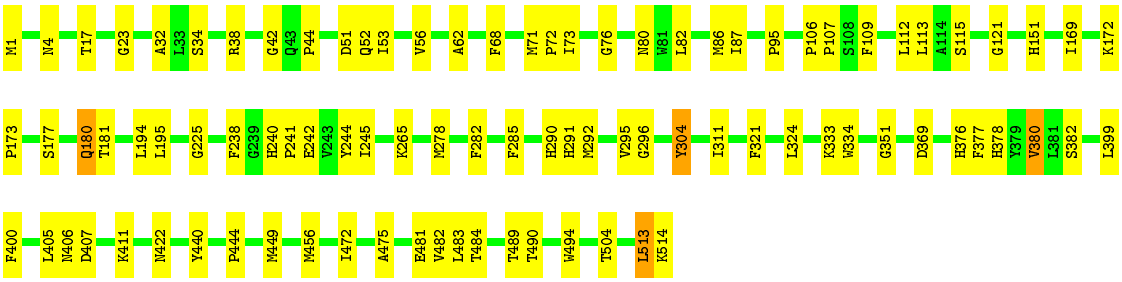




• Molecule 1: Cytochrome c oxidase subunit 1

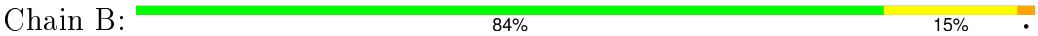
Chain N:

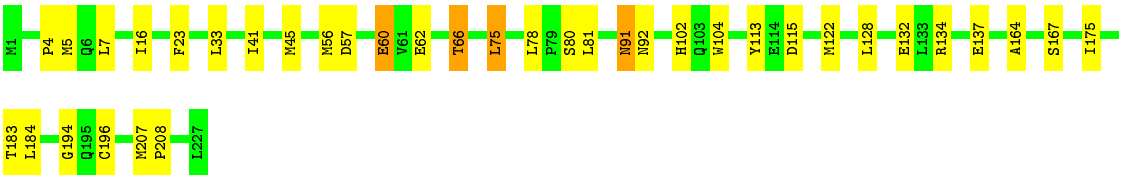




• Molecule 2: Cytochrome c oxidase subunit 2

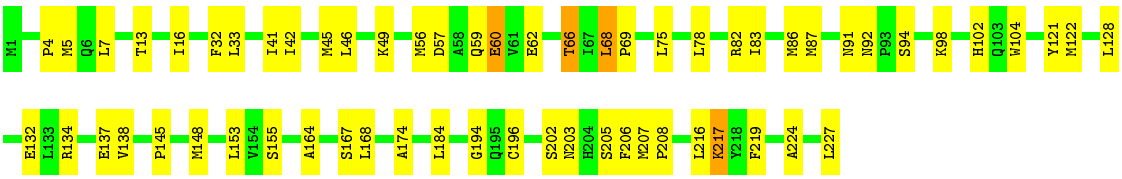
Chain B:





• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:

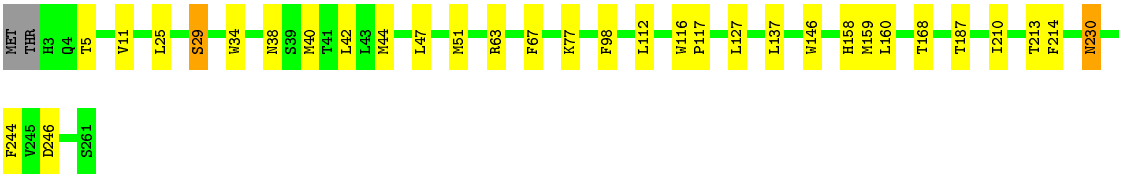


• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:

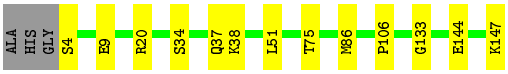
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:



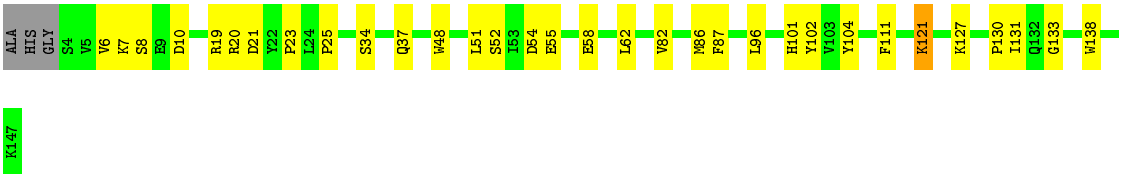
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:



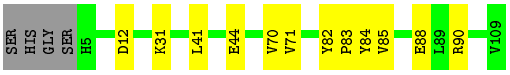
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:



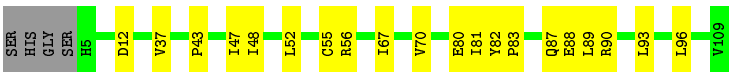
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:



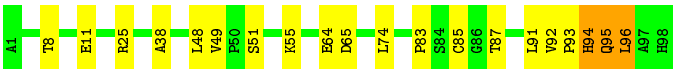
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:



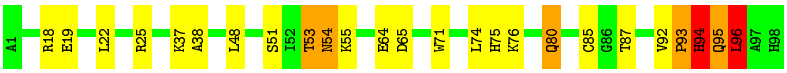
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:



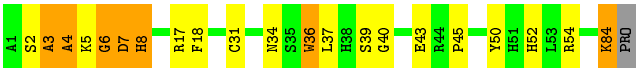
• Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:



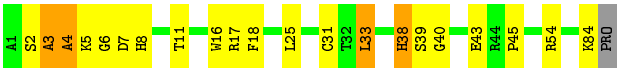
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:



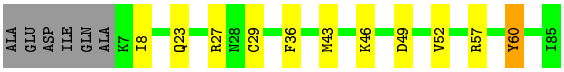
• Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:



• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:

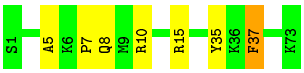


• Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:

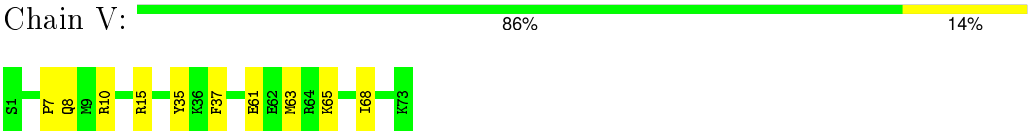
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:



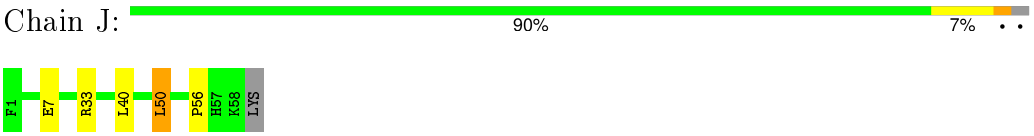
• Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:



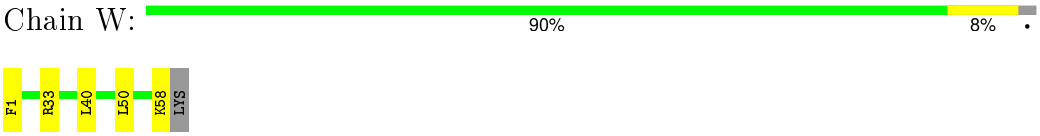
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:



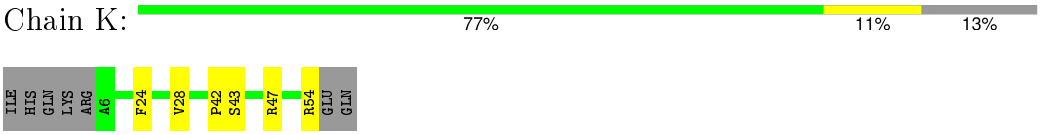
• Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:



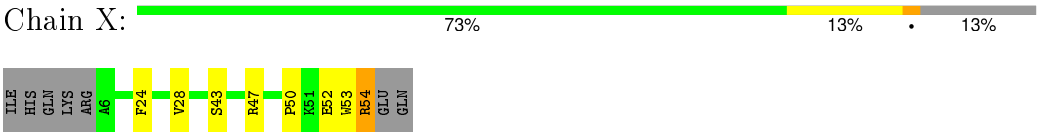
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:



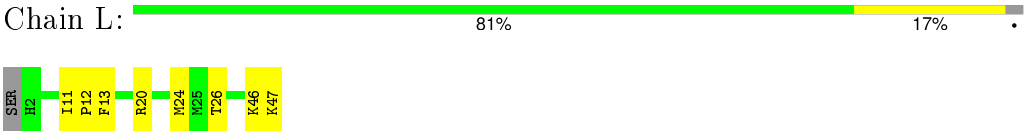
• Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:



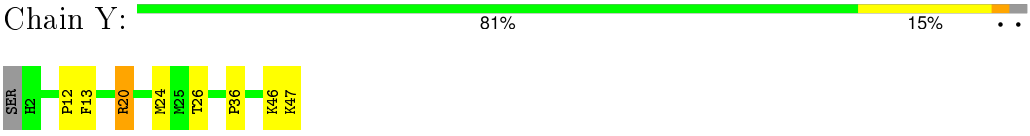
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:



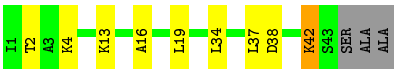
• Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:



• Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	183.06Å 206.58Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32488	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.52	0/4156	0.69	2/5678 (0.0%)
1	N	0.52	0/4156	0.66	0/5678
2	B	0.51	0/1860	0.77	1/2534 (0.0%)
2	O	0.52	0/1860	0.79	1/2534 (0.0%)
3	C	0.53	0/2197	0.59	0/3005
3	P	0.51	0/2197	0.62	1/3005 (0.0%)
4	D	0.51	0/1229	0.67	1/1658 (0.1%)
4	Q	0.54	0/1229	0.67	1/1658 (0.1%)
5	E	0.53	0/871	0.67	0/1182
5	R	0.54	0/871	0.70	0/1182
6	F	0.50	0/765	0.82	2/1038 (0.2%)
6	S	0.49	0/765	0.81	2/1038 (0.2%)
7	G	0.51	0/690	0.71	1/937 (0.1%)
7	T	0.55	0/690	0.72	1/937 (0.1%)
8	H	0.49	0/682	0.68	0/921
8	U	0.48	0/682	0.69	0/921
9	I	0.52	0/605	0.61	0/802
9	V	0.49	0/605	0.60	0/802
10	J	0.46	0/471	0.63	0/636
10	W	0.48	0/471	0.65	0/636
11	K	0.53	0/398	0.68	0/546
11	X	0.50	0/398	0.66	0/546
12	L	0.51	0/393	0.59	0/526
12	Y	0.54	0/393	0.60	0/526
13	M	0.50	0/345	0.65	0/470
13	Z	0.47	0/345	0.60	0/470
All	All	0.52	0/29324	0.68	13/39866 (0.0%)

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

of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	3
8	U	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	33	LEU	CA-CB-CG	6.53	130.31	115.30
6	S	94	HIS	N-CA-C	6.39	128.27	111.00
4	D	133	GLY	N-CA-C	6.33	128.93	113.10
6	F	94	HIS	N-CA-C	6.21	127.75	111.00
4	Q	133	GLY	N-CA-C	5.94	127.94	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
1	N	244	TYR	Sidechain
1	N	304	TYR	Sidechain
8	U	11	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	57	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	20	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	21	0
3	P	2110	0	2027	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1195	0	1183	11	0
4	Q	1195	0	1183	23	0
5	E	852	0	845	7	0
5	R	852	0	845	12	0
6	F	748	0	728	12	0
6	S	748	0	728	21	0
7	G	675	0	644	26	0
7	T	675	0	644	20	0
8	H	662	0	623	6	0
8	U	662	0	623	9	0
9	I	601	0	613	4	0
9	V	601	0	613	7	0
10	J	460	0	459	5	0
10	W	460	0	459	5	0
11	K	384	0	366	3	0
11	X	384	0	366	10	0
12	L	380	0	380	12	0
12	Y	380	0	380	8	0
13	M	335	0	352	7	0
13	Z	335	0	352	8	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	6	0
17	N	120	0	108	5	0
18	A	63	0	110	4	0
18	B	63	0	110	7	0
18	L	63	0	110	20	0
18	N	189	0	330	27	0
19	A	51	0	76	7	0
19	C	153	0	228	6	0
19	N	102	0	152	8	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	52	0	80	11	0
21	O	52	0	80	15	0
22	B	29	0	39	1	0
22	C	58	0	78	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	1	0
22	W	29	0	39	4	0
23	C	33	0	36	3	0
23	M	33	0	36	0	0
23	P	33	0	36	8	0
23	Z	33	0	36	0	0
24	C	1	0	0	0	0
24	F	1	0	0	0	0
24	P	1	0	0	0	0
24	S	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	10	0
25	P	106	0	154	13	0
25	T	53	0	77	6	0
26	C	100	0	156	11	0
26	G	100	0	156	18	0
26	P	100	0	156	15	0
26	T	100	0	156	19	0
27	A	237	0	0	3	0
27	B	145	0	0	1	0
27	C	110	0	0	1	0
27	D	94	0	0	3	0
27	E	60	0	0	0	0
27	F	72	0	0	1	0
27	G	44	0	0	2	0
27	H	50	0	0	2	0
27	I	38	0	0	2	0
27	J	23	0	0	1	0
27	K	22	0	0	1	0
27	L	27	0	0	0	0
27	M	24	0	0	1	0
27	N	218	0	0	5	0
27	O	122	0	0	3	0
27	P	112	0	0	4	0
27	Q	53	0	0	1	0
27	R	45	0	0	0	0
27	S	76	0	0	6	0
27	T	42	0	0	1	0
27	U	46	0	0	2	0
27	V	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	W	18	0	0	0	0
27	X	21	0	0	2	0
27	Y	17	0	0	0	0
27	Z	15	0	0	1	0
All	All	32488	0	31294	523	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 8.

The worst 5 of 523 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:HD2	7:G:84:LYS:H	1.18	1.05
7:T:84:LYS:H	7:T:84:LYS:HD2	1.20	1.02
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
10:W:33:ARG:HG2	22:W:1060:CHD:H152	1.40	1.00
21:B:230:PSC:H343	21:B:230:PSC:H142	1.44	0.99

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%)	499 (98%)	13 (2%)	0	100 100
1	N	512/514 (100%)	501 (98%)	11 (2%)	0	100 100
2	B	225/227 (99%)	213 (95%)	10 (4%)	2 (1%)	21 9
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	21 9
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100 100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	39 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	1
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	7	1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	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%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3359 (96%)	116 (3%)	29 (1%)	24	11

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS

5.3.2 Protein sidechains (i)

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%)	417 (98%)	9 (2%)	61	55
1	N	426/426 (100%)	416 (98%)	10 (2%)	58	51
2	B	210/210 (100%)	200 (95%)	10 (5%)	31	19
2	O	210/210 (100%)	199 (95%)	11 (5%)	29	17
3	C	224/226 (99%)	218 (97%)	6 (3%)	52	43
3	P	224/226 (99%)	220 (98%)	4 (2%)	66	61
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	66
4	Q	128/129 (99%)	124 (97%)	4 (3%)	47	37
5	E	92/95 (97%)	90 (98%)	2 (2%)	60	53
5	R	92/95 (97%)	90 (98%)	2 (2%)	60	53
6	F	81/81 (100%)	79 (98%)	2 (2%)	55	47
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	7
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	7
7	T	67/68 (98%)	62 (92%)	5 (8%)	17	7
8	H	71/75 (95%)	69 (97%)	2 (3%)	51	41
8	U	71/75 (95%)	68 (96%)	3 (4%)	36	24
9	I	57/57 (100%)	54 (95%)	3 (5%)	28	16
9	V	57/57 (100%)	55 (96%)	2 (4%)	43	31
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	57
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	57
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	45
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	17
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	45
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29	17
13	M	37/38 (97%)	32 (86%)	5 (14%)	5	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	3
All	All	3040/3082 (99%)	2935 (96%)	105 (4%)	43	31

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	38	ASP
1	N	513	LEU
11	X	47	ARG
13	M	42	LYS
1	N	241	PRO

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

Mol	Chain	Res	Type
10	J	29	ASN
1	N	178	GLN
6	S	94	HIS
1	N	80	ASN
1	N	180	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	FME	A	1	1	8,9,10	0.58	0	6,9,11	1.47	2 (33%)
2	FME	B	1	2	8,9,10	0.77	0	6,9,11	1.72	1 (16%)
7	TPO	G	11	7	8,10,11	1.68	1 (12%)	7,14,16	0.97	0
9	SAC	I	1	9	7,8,9	2.36	2 (28%)	7,9,11	2.05	2 (28%)
1	FME	N	1	1	8,9,10	0.73	0	6,9,11	1.95	2 (33%)
2	FME	O	1	2	8,9,10	0.65	0	6,9,11	1.51	1 (16%)
7	TPO	T	11	7	8,10,11	1.24	1 (12%)	7,14,16	0.99	0
9	SAC	V	1	9	7,8,9	2.70	2 (28%)	7,9,11	2.19	4 (57%)

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.29	1.58	1.54
7	G	11	TPO	CB-CA	3.72	1.60	1.54
9	I	1	SAC	CA-N	3.75	1.51	1.46
9	V	1	SAC	CA-N	4.67	1.53	1.46
9	I	1	SAC	OAC-C1A	4.82	1.34	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	1	FME	CA-N-CN	-4.06	116.57	122.82
2	B	1	FME	CA-N-CN	-3.66	117.20	122.82
2	O	1	FME	CA-N-CN	-3.36	117.65	122.82
9	V	1	SAC	CA-N-C1A	-3.14	110.72	121.37
9	I	1	SAC	CA-N-C1A	-2.97	111.30	121.37

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	N	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 10 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	HEA	A	515	1	40,67,67	1.28	5 (12%)	41,103,103	1.72	8 (19%)
17	HEA	A	516	1	40,67,67	1.59	6 (15%)	41,103,103	1.49	8 (19%)
18	TGL	A	523	-	62,62,62	0.71	0	65,65,65	1.28	7 (10%)
19	PGV	A	524	-	50,50,50	1.07	3 (6%)	51,56,56	0.92	4 (7%)
22	CHD	B	1086	-	29,32,32	0.68	0	48,51,51	1.76	14 (29%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	PSC	B	230	-	51,51,51	1.21	3 (5%)	55,59,59	0.99	1 (1%)
18	TGL	B	521	-	62,62,62	0.69	0	65,65,65	1.54	9 (13%)
25	PEK	C	264	-	51,52,52	1.40	4 (7%)	52,57,57	1.03	3 (5%)
25	PEK	C	265	-	51,52,52	1.63	9 (17%)	52,57,57	1.13	5 (9%)
19	PGV	C	266	-	50,50,50	0.88	2 (4%)	51,56,56	0.77	2 (3%)
19	PGV	C	267	-	50,50,50	0.81	1 (2%)	51,56,56	0.88	2 (3%)
19	PGV	C	268	-	50,50,50	1.14	3 (6%)	51,56,56	0.79	1 (1%)
26	CDL	C	270	-	99,99,99	0.80	2 (2%)	101,111,111	0.90	4 (3%)
22	CHD	C	271	-	29,32,32	0.85	0	48,51,51	3.65	22 (45%)
23	DMU	C	272	-	34,34,34	2.69	11 (32%)	45,45,45	4.33	19 (42%)
22	CHD	C	525	-	29,32,32	0.76	0	48,51,51	1.55	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	PEK	G	1263	-	51,52,52	1.80	8 (15%)	52,57,57	1.14	4 (7%)
26	CDL	G	269	-	99,99,99	0.97	5 (5%)	101,111,111	0.94	7 (6%)
22	CHD	J	60	-	29,32,32	1.04	1 (3%)	48,51,51	3.48	30 (62%)
18	TGL	L	522	-	62,62,62	1.07	5 (8%)	65,65,65	1.66	12 (18%)
23	DMU	M	526	-	34,34,34	3.21	8 (23%)	45,45,45	4.36	20 (44%)
19	PGV	N	1266	-	50,50,50	0.93	3 (6%)	51,56,56	0.85	3 (5%)
18	TGL	N	1521	-	62,62,62	0.74	1 (1%)	65,65,65	1.49	9 (13%)
18	TGL	N	1522	-	62,62,62	1.12	4 (6%)	65,65,65	1.63	11 (16%)
18	TGL	N	1523	-	62,62,62	0.76	2 (3%)	65,65,65	1.28	6 (9%)
19	PGV	N	1524	-	50,50,50	1.06	4 (8%)	51,56,56	0.91	5 (9%)
17	HEA	N	515	1	40,67,67	1.31	5 (12%)	41,103,103	1.79	10 (24%)
17	HEA	N	516	1	40,67,67	1.46	6 (15%)	41,103,103	1.49	9 (21%)
21	PSC	O	1230	-	51,51,51	1.20	3 (5%)	55,59,59	0.99	1 (1%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	0.68	1 (3%)	48,51,51	1.82	14 (29%)
25	PEK	P	1264	-	51,52,52	1.41	5 (9%)	52,57,57	1.05	3 (5%)
25	PEK	P	1265	-	51,52,52	1.64	10 (19%)	52,57,57	1.12	5 (9%)
19	PGV	P	1267	-	50,50,50	0.87	2 (4%)	51,56,56	0.83	2 (3%)
19	PGV	P	1268	-	50,50,50	1.14	2 (4%)	51,56,56	0.81	2 (3%)
26	CDL	P	1270	-	99,99,99	0.83	3 (3%)	101,111,111	0.87	4 (3%)
22	CHD	P	1271	-	29,32,32	0.79	0	48,51,51	3.65	23 (47%)
23	DMU	P	1272	-	34,34,34	2.81	11 (32%)	45,45,45	4.37	19 (42%)
22	CHD	P	1525	-	29,32,32	0.78	1 (3%)	48,51,51	1.49	9 (18%)
26	CDL	T	1269	-	99,99,99	0.96	5 (5%)	101,111,111	0.96	7 (6%)
25	PEK	T	263	-	51,52,52	1.84	10 (19%)	52,57,57	1.14	4 (7%)
22	CHD	W	1060	-	29,32,32	1.15	3 (10%)	48,51,51	3.49	29 (60%)
23	DMU	Z	1526	-	34,34,34	3.13	8 (23%)	45,45,45	4.31	20 (44%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	TGL	A	523	-	-	0/65/65/65	0/0/0/0
19	PGV	A	524	-	-	2/55/55/55	0/0/0/0
22	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	PSC	B	230	-	-	0/55/55/55	0/0/0/0
18	TGL	B	521	-	-	0/65/65/65	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
25	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	266	-	-	0/55/55/55	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	C	272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
22	CHD	J	60	-	5/5/12/12	0/7/74/74	0/4/4/4
18	TGL	L	522	-	-	0/65/65/65	0/0/0/0
23	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
17	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
21	PSC	O	1230	-	-	0/55/55/55	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
19	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
23	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

The worst 5 of 165 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	526	DMU	O7-C3	-8.55	1.22	1.43
23	Z	1526	DMU	O7-C3	-8.05	1.23	1.43
23	M	526	DMU	O16-C6	-6.96	1.27	1.40
23	Z	1526	DMU	O16-C6	-6.84	1.27	1.40
23	M	526	DMU	O16-C18	-6.80	1.23	1.42

The worst 5 of 384 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	1271	CHD	C17-C13-C12	-9.14	109.58	117.68
22	C	271	CHD	C17-C13-C12	-8.87	109.82	117.68
22	C	271	CHD	C19-C10-C9	-7.60	99.79	111.18
23	M	526	DMU	C8-C7-C5	-7.45	96.90	110.79
23	Z	1526	DMU	C8-C7-C5	-7.36	97.06	110.79

5 of 54 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
17	A	516	HEA	ND
17	A	516	HEA	NA

All (4) torsion outliers are listed below:

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

There are no ring outliers.

36 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	515	HEA	2	0
17	A	516	HEA	4	0
18	A	523	TGL	4	0
19	A	524	PGV	7	0
22	B	1086	CHD	1	0
21	B	230	PSC	11	0
18	B	521	TGL	7	0
25	C	264	PEK	4	0
25	C	265	PEK	7	0
19	C	267	PGV	5	0
19	C	268	PGV	1	0
26	C	270	CDL	11	0
22	C	271	CHD	3	0
23	C	272	DMU	3	0
25	G	1263	PEK	10	0
26	G	269	CDL	18	0
22	J	60	CHD	2	0
18	L	522	TGL	20	0
18	N	1521	TGL	9	0
18	N	1522	TGL	14	0
18	N	1523	TGL	4	0
19	N	1524	PGV	8	0
17	N	515	HEA	3	0
17	N	516	HEA	2	0
21	O	1230	PSC	15	0
22	O	229	CHD	1	0
25	P	1264	PEK	6	0
25	P	1265	PEK	7	0
19	P	1267	PGV	5	0
19	P	1268	PGV	1	0
26	P	1270	CDL	15	0
22	P	1271	CHD	1	0
23	P	1272	DMU	8	0
26	T	1269	CDL	19	0
25	T	263	PEK	6	0
22	W	1060	CHD	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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