



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2017 – 02:44 PM EDT

PDB ID : 5WAU
Title : Crystal Structure of CO-bound Cytochrome c Oxidase determined by Synchrotron X-Ray Crystallography at 100 K
Authors : Fromme, R.; Ishigami, I.; Yeh, S.Y.; Zatsepin, N.; Grant, T.; Fromme, P.; Rousseau, D.
Deposited on : unknown
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

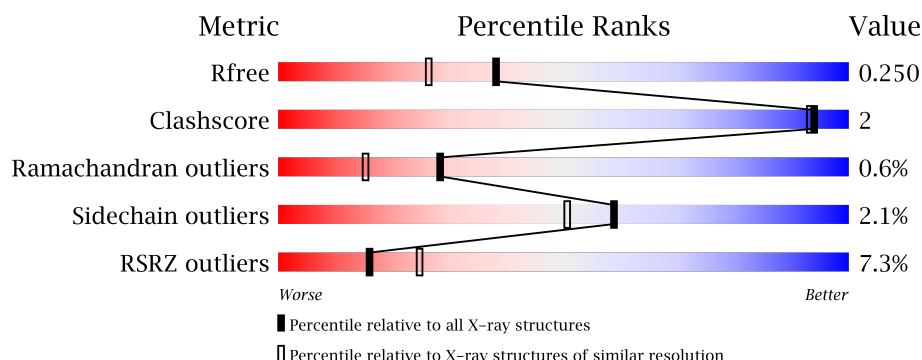
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
1	a	514	<div> <div>2%</div> <div> <div></div> <div>98%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
2	b	227	<div> <div>5%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
3	C	261	<div> <div></div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	c	261	
4	D	147	
4	d	147	
5	E	109	
5	e	109	
6	F	98	
6	f	98	
7	G	85	
7	g	85	
8	H	85	
8	h	85	
9	I	73	
9	i	73	
10	J	59	
10	j	59	
11	K	56	
11	k	56	
12	L	47	
12	l	47	
13	M	46	
13	m	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	a	601	X	-	-	-
14	HEA	a	602	X	-	-	-
16	MG	a	604	-	-	-	X
18	PGV	A	606	-	-	-	X
18	PGV	C	303	-	-	-	X
18	PGV	a	606	-	-	-	X
18	PGV	a	607	-	-	-	X
18	PGV	c	306	-	-	-	X
19	TGL	A	608	-	-	-	X
19	TGL	A	609	-	-	-	X
19	TGL	D	201	-	-	-	X
19	TGL	b	302	-	-	-	X
19	TGL	d	201	-	-	-	X
19	TGL	l	101	-	-	-	X
20	CMO	a	608	-	-	-	X
23	CHD	J	101	-	-	-	X
23	CHD	j	101	-	-	-	X
24	PEK	C	302	-	-	-	X
24	PEK	C	307	-	-	-	X
24	PEK	G	101	-	-	-	X
24	PEK	c	304	-	-	-	X
24	PEK	c	305	-	-	-	X
25	CDL	C	305	-	-	-	X
25	CDL	G	102	-	-	-	X
25	CDL	c	307	-	-	-	X
25	CDL	g	101	-	-	-	X
26	DMU	C	308	-	-	-	X
26	DMU	c	309	-	-	-	X
26	DMU	m	101	-	-	-	X
27	PSC	E	201	-	-	-	X
27	PSC	b	303	-	-	-	X
29	SAC	I	101	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32575 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	a	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	226	Total	C	N	O	S	0	0	0
			1814	1179	280	338	17			
2	b	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	c	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

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

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	i	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

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

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

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

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

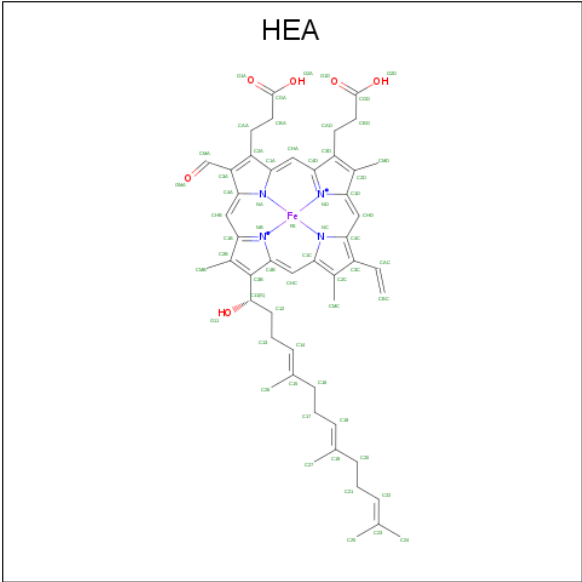
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

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

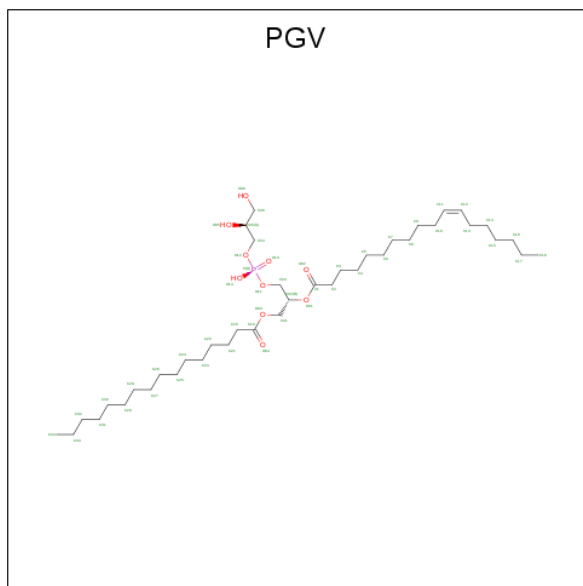
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

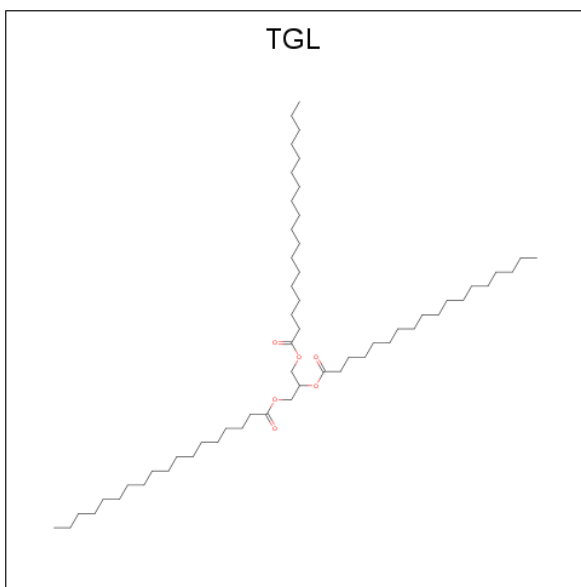
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	a	1	Total Na 1 1	0	0

- Molecule 18 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).



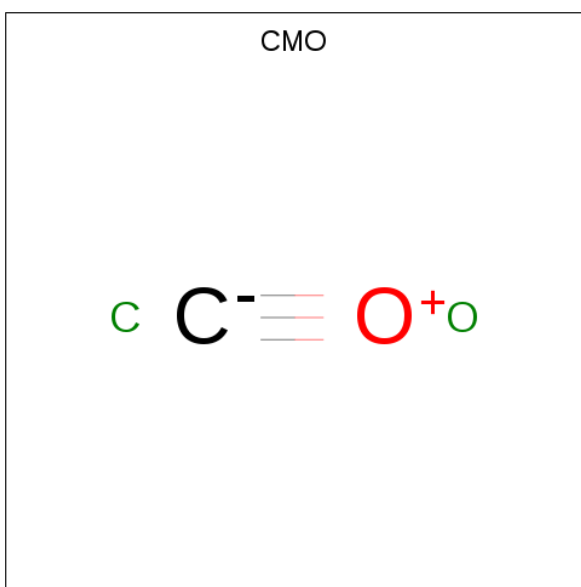
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	a	1	Total C O P 51 40 10 1	0	0
18	a	1	Total C O P 51 40 10 1	0	0
18	c	1	Total C O P 51 40 10 1	0	0
18	c	1	Total C O P 51 40 10 1	0	0

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



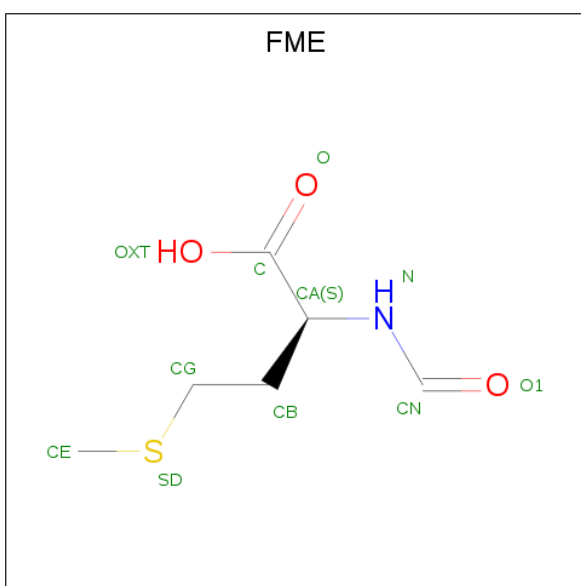
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	b	1	Total	C	O	0	0
			63	57	6		
19	d	1	Total	C	O	0	0
			63	57	6		
19	l	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



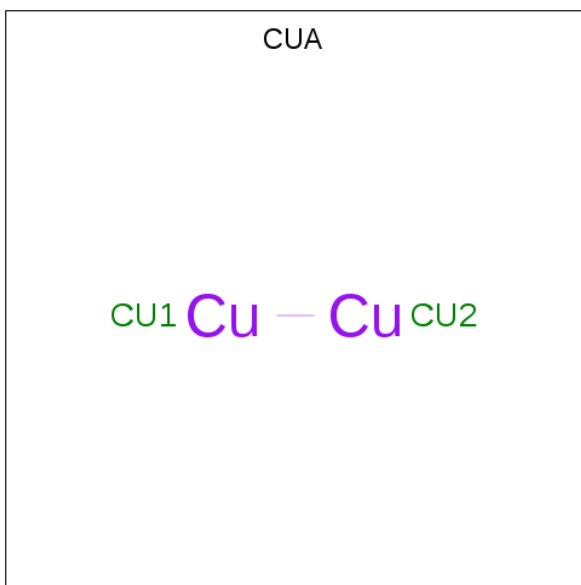
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			2	1	1		
20	a	1	Total	C	O	0	0
			2	1	1		

- Molecule 21 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



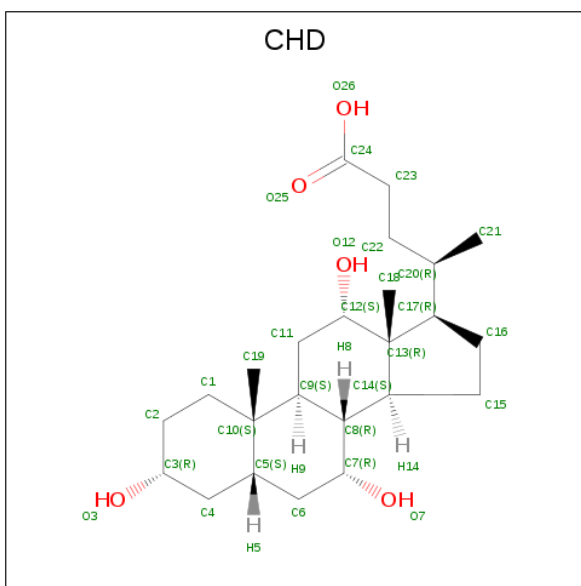
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	S	0	0
			10	6	1	2	1		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

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



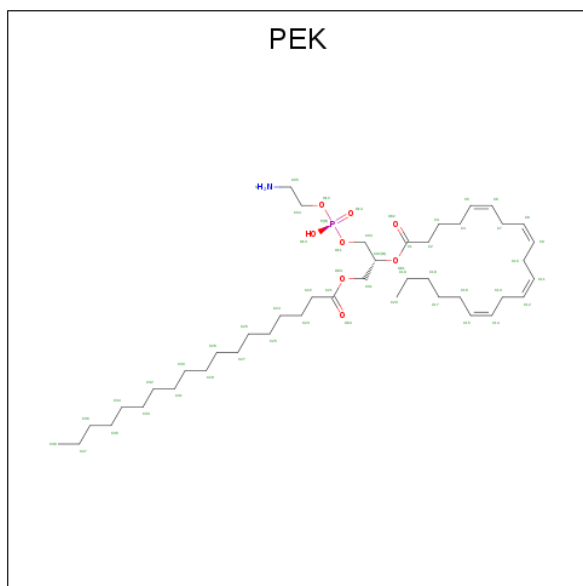
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		
23	G	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	c	1	Total	C	O	0	0
			29	24	5		
23	c	1	Total	C	O	0	0
			29	24	5		
23	j	1	Total	C	O	0	0
			29	24	5		

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



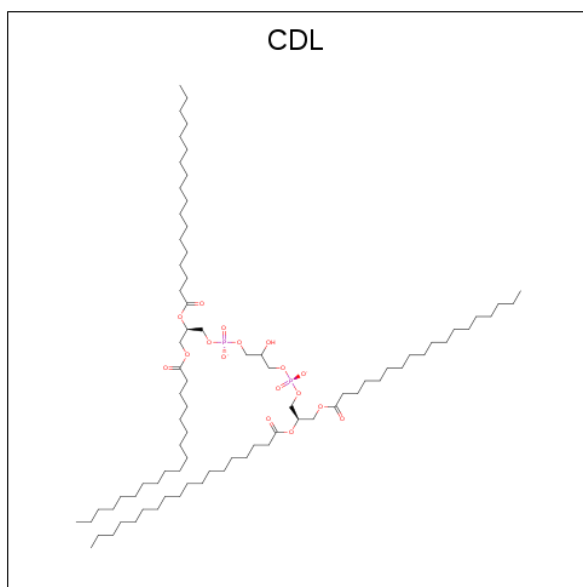
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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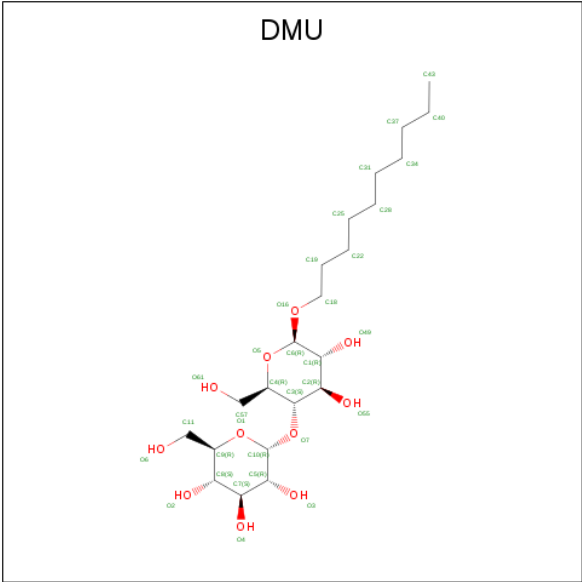
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	c	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



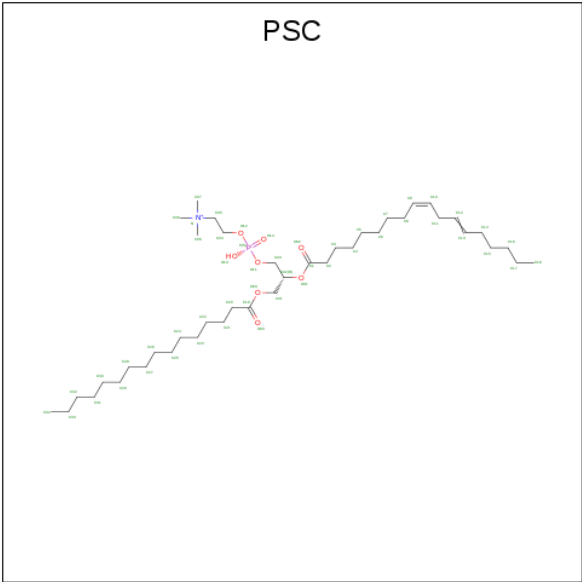
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	O	P		0	0
			100	81	17	2			
25	G	1	Total	C	O	P		0	0
			100	81	17	2			
25	c	1	Total	C	O	P		0	0
			100	81	17	2			
25	g	1	Total	C	O	P		0	0
			100	81	17	2			

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	M	1	Total	C	O	0	0
			33	22	11		
26	c	1	Total	C	O	0	0
			33	22	11		
26	m	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 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).

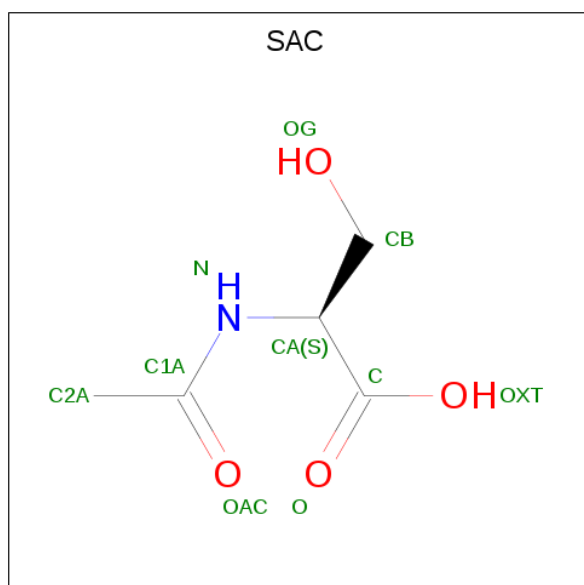


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
27	b	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	I	1	Total	C	N	O	0	0
			9	5	1	3		
29	i	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	243	Total	O	0	0
			243	243		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	180	Total 180	O 180	0	0
30	C	122	Total 122	O 122	0	0
30	D	125	Total 125	O 125	0	0
30	E	100	Total 100	O 100	0	0
30	F	104	Total 104	O 104	0	0
30	G	57	Total 57	O 57	0	0
30	H	57	Total 57	O 57	0	0
30	I	33	Total 33	O 33	0	0
30	J	36	Total 36	O 36	0	0
30	K	41	Total 41	O 41	0	0
30	L	47	Total 47	O 47	0	0
30	M	29	Total 29	O 29	0	0
30	a	187	Total 187	O 187	0	0
30	b	109	Total 109	O 109	0	0
30	c	96	Total 96	O 96	0	0
30	d	37	Total 37	O 37	0	0
30	e	56	Total 56	O 56	0	0
30	f	62	Total 62	O 62	0	0
30	g	27	Total 27	O 27	0	0
30	h	36	Total 36	O 36	0	0
30	i	23	Total 23	O 23	0	0

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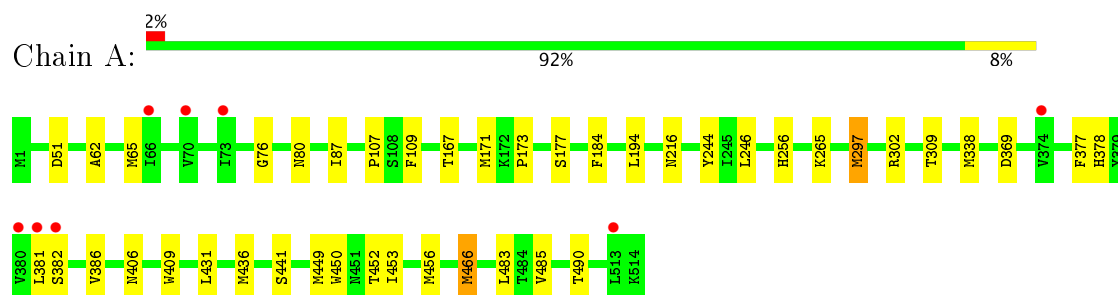
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	j	14	Total 14	O 14	0	0
30	k	7	Total 7	O 7	0	0
30	l	8	Total 8	O 8	0	0
30	m	5	Total 5	O 5	0	0

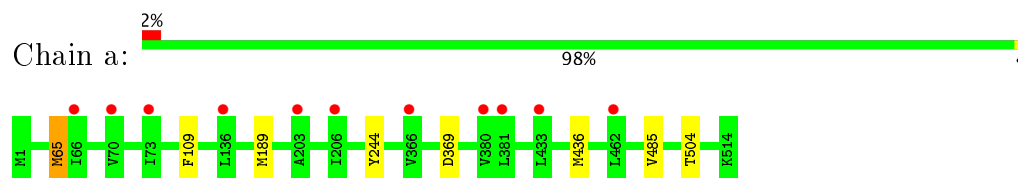
3 Residue-property plots [i](#)

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

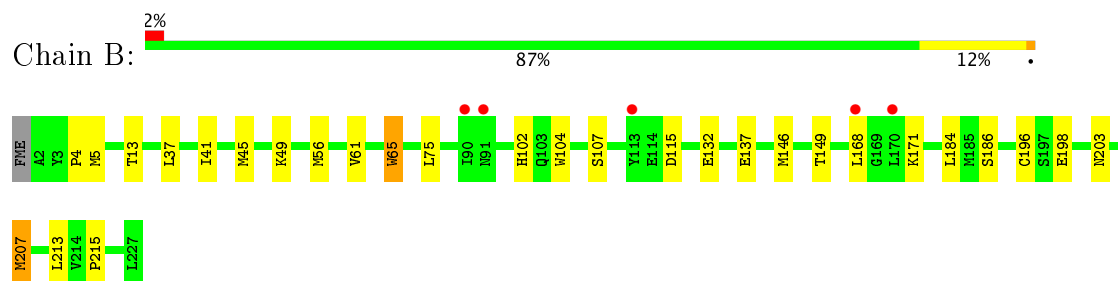
- Molecule 1: Cytochrome c oxidase subunit 1



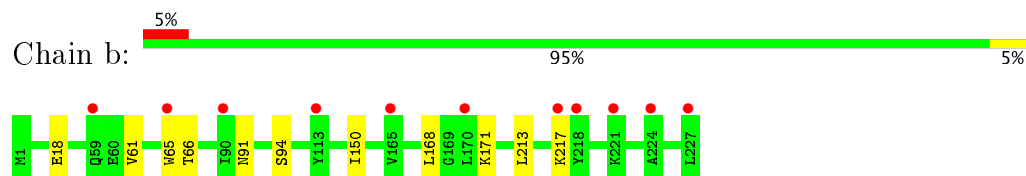
- Molecule 1: Cytochrome c oxidase subunit 1



- Molecule 2: Cytochrome c oxidase subunit 2

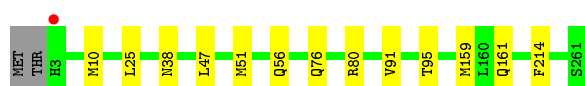


- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3

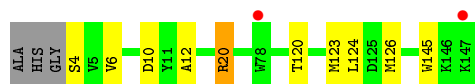




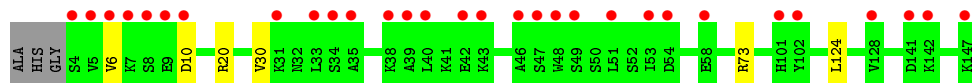
- Molecule 3: Cytochrome c oxidase subunit 3



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



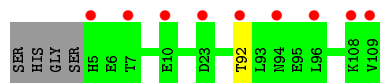
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



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



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

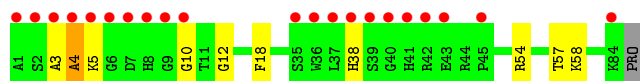
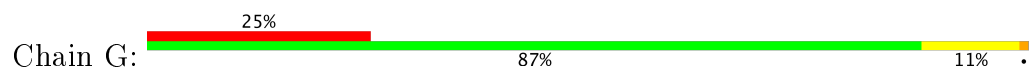


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

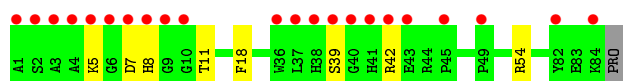
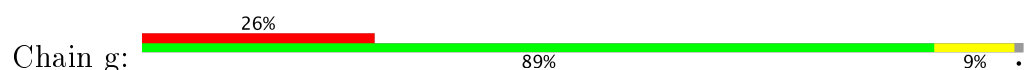




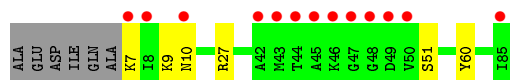
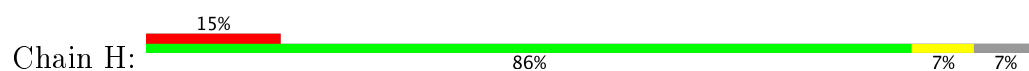
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



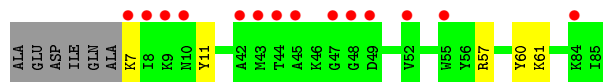
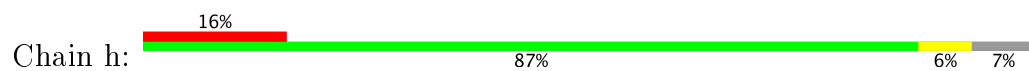
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



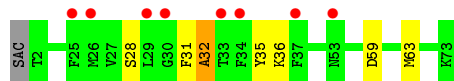
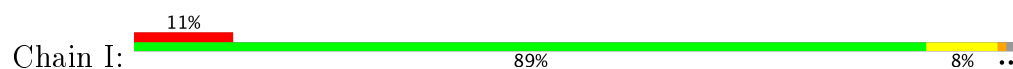
- Molecule 8: Cytochrome c oxidase subunit 6B1



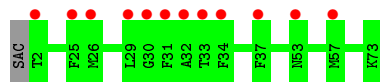
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 9: Cytochrome c oxidase subunit 6C

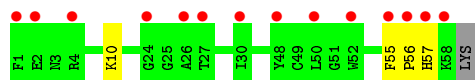
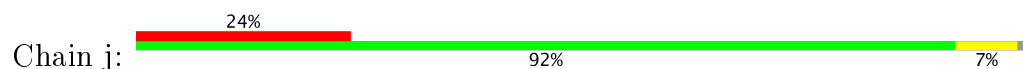


- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

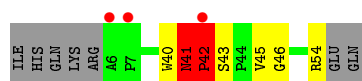
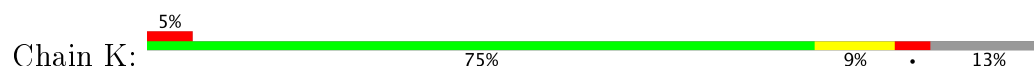




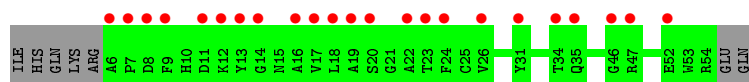
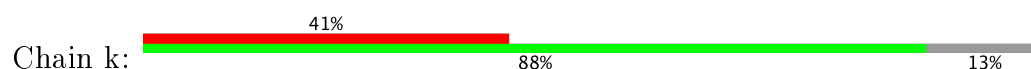
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



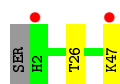
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



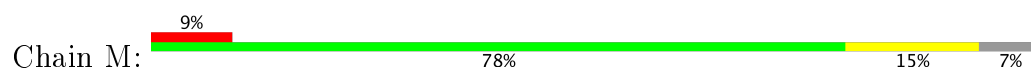
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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

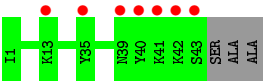


- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	177.92Å 182.56Å 208.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.95 38.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.3 (39.00-1.95) 94.3 (38.64-1.95)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.217 , 0.244 0.225 , 0.250	Depositor DCC
R_{free} test set	23097 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32575	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CMO, 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	0.68	2/5678 (0.0%)
1	a	0.49	1/4156 (0.0%)	0.66	2/5678 (0.0%)
2	B	0.53	1/1860 (0.1%)	0.77	1/2534 (0.0%)
2	b	0.46	0/1860	0.71	0/2534
3	C	0.45	0/2197	0.62	0/3005
3	c	0.46	0/2197	0.59	0/3005
4	D	0.46	0/1229	0.64	2/1658 (0.1%)
4	d	0.44	0/1229	0.66	1/1658 (0.1%)
5	E	0.46	0/871	0.65	0/1182
5	e	0.42	0/871	0.66	0/1182
6	F	0.51	0/765	0.72	0/1038
6	f	0.43	0/765	0.66	0/1038
7	G	0.48	0/690	0.71	0/937
7	g	0.50	0/690	0.67	0/937
8	H	0.48	0/682	0.72	0/921
8	h	0.44	0/682	0.66	0/921
9	I	0.45	0/605	0.69	0/802
9	i	0.45	0/605	0.66	0/802
10	J	0.43	0/471	0.58	0/636
10	j	0.47	0/471	0.65	0/636
11	K	0.52	0/398	0.83	2/546 (0.4%)
11	k	0.41	0/398	0.57	0/546
12	L	0.48	0/393	0.63	0/526
12	l	0.47	0/393	0.61	0/526
13	M	0.48	0/345	0.63	0/470
13	m	0.43	0/345	0.52	0/470
All	All	0.48	2/29324 (0.0%)	0.67	10/39866 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	g	0	1
10	j	0	1
11	K	0	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	5.24	1.33	1.23
1	a	244	TYR	CE2-CZ	5.23	1.45	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	207	MET	CG-SD-CE	-6.29	90.14	100.20
4	D	20	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	466	MET	CG-SD-CE	-5.85	90.85	100.20
1	a	244	TYR	CZ-CE2-CD2	-5.80	114.58	119.80
1	a	65	MET	CG-SD-CE	5.78	109.44	100.20
11	K	41	ASN	CB-CA-C	5.39	121.19	110.40
1	A	244	TYR	CZ-CE2-CD2	-5.27	115.06	119.80
4	D	20	ARG	NE-CZ-NH1	5.25	122.93	120.30
11	K	41	ASN	C-N-CD	5.08	139.07	128.40
4	d	20	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	K	41	ASN	Peptide
11	K	42	PRO	Peptide
11	K	46	GLY	Peptide
7	g	11	TPO	Peptide
10	j	55	PHE	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	40	0
1	a	4027	0	4001	0	0
2	B	1814	0	1822	21	0
2	b	1824	0	1833	0	0
3	C	2110	0	2027	8	0
3	c	2110	0	2027	0	0
4	D	1195	0	1183	10	0
4	d	1195	0	1183	0	0
5	E	852	0	845	1	0
5	e	852	0	845	0	0
6	F	748	0	728	4	0
6	f	748	0	728	0	0
7	G	675	0	643	4	0
7	g	675	0	643	0	0
8	H	662	0	623	1	0
8	h	662	0	623	0	0
9	I	592	0	604	6	0
9	i	592	0	604	0	0
10	J	460	0	459	2	0
10	j	460	0	459	0	0
11	K	384	0	366	11	0
11	k	384	0	366	0	0
12	L	380	0	380	1	0
12	l	380	0	380	0	0
13	M	335	0	352	10	0
13	m	335	0	352	0	0
14	A	120	0	108	6	0
14	a	120	0	108	0	0
15	A	1	0	0	0	0
15	a	1	0	0	0	0
16	A	1	0	0	0	0
16	a	1	0	0	0	0
17	A	1	0	0	0	0
17	a	1	0	0	0	0
18	A	102	0	152	1	0
18	C	102	0	152	0	0
18	a	102	0	152	0	0
18	c	102	0	152	0	0
19	A	126	0	220	0	0
19	D	63	0	110	0	0
19	b	63	0	110	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	d	63	0	110	0	0
19	l	63	0	110	0	0
20	A	2	0	0	0	0
20	a	2	0	0	0	0
21	B	10	0	10	0	0
22	B	2	0	0	0	0
22	b	2	0	0	0	0
23	B	29	0	39	0	0
23	C	58	0	78	0	0
23	G	29	0	39	0	0
23	J	29	0	39	0	0
23	c	58	0	78	0	0
23	j	29	0	39	0	0
24	C	106	0	154	0	0
24	G	53	0	77	1	0
24	c	159	0	231	0	0
25	C	100	0	156	0	0
25	G	100	0	156	0	0
25	c	100	0	156	0	0
25	g	100	0	156	0	0
26	C	33	0	42	0	0
26	M	33	0	42	0	0
26	c	33	0	42	0	0
26	m	33	0	42	0	0
27	E	52	0	80	0	0
27	b	52	0	80	0	0
28	F	1	0	0	0	0
28	f	1	0	0	0	0
29	I	9	0	8	0	0
29	i	9	0	8	0	0
30	A	243	0	0	3	0
30	B	180	0	0	1	0
30	C	122	0	0	1	0
30	D	125	0	0	0	0
30	E	100	0	0	0	0
30	F	104	0	0	0	0
30	G	57	0	0	0	0
30	H	57	0	0	1	0
30	I	33	0	0	1	0
30	J	36	0	0	0	0
30	K	41	0	0	1	0
30	L	47	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	M	29	0	0	0	0
30	a	187	0	0	0	0
30	b	109	0	0	0	0
30	c	96	0	0	0	0
30	d	37	0	0	0	0
30	e	56	0	0	0	0
30	f	62	0	0	0	0
30	g	27	0	0	0	0
30	h	36	0	0	0	0
30	i	23	0	0	0	0
30	j	14	0	0	0	0
30	k	7	0	0	0	0
30	l	8	0	0	0	0
30	m	5	0	0	0	0
All	All	32575	0	31313	94	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 2.

All (94) 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)
2:B:4:PRO:HB3	11:K:42:PRO:CG	1.99	0.92
1:A:466:MET:CE	13:M:26:PHE:HB2	2.10	0.82
2:B:56:MET:SD	30:B:433:HOH:O	60.84	0.78
1:A:171:MET:SD	30:A:863:HOH:O	17.10	0.78
2:B:4:PRO:HB3	11:K:42:PRO:HG2	1.69	0.72
4:D:120:THR:O	4:D:123:MET:O	5.02	0.72
6:F:75:HIS:H	6:F:80:GLN:HE22	1.40	0.68
11:K:54:ARG:C	30:K:102:HOH:O	2.34	0.66
2:B:4:PRO:HB3	11:K:42:PRO:HG3	1.80	0.63
1:A:51:ASP:OD2	1:A:441:SER:OG	2.17	0.62
1:A:377:PHE:O	1:A:381:LEU:HB2	2.01	0.60
2:B:186:SER:HB3	2:B:213:LEU:HD22	5.10	0.59
1:A:466:MET:HE2	13:M:26:PHE:HB2	1.81	0.59
2:B:4:PRO:CB	11:K:42:PRO:HG2	2.32	0.59
3:C:91:VAL:O	3:C:95:THR:HG23	2.02	0.59
9:I:28:SER:O	9:I:31:PHE:O	2.21	0.59
1:A:382:SER:O	1:A:386:VAL:HB	2.05	0.57
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.98	0.57
1:A:167:THR:HG23	1:A:171:MET:HE3	4.90	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:MET:HA	9:I:63:MET:HE3	4.54	0.56
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.92	0.55
1:A:449:MET:HE2	2:B:5:MET:HG2	1.88	0.54
1:A:216:ASN:HD21	7:G:58:LYS:H	3.08	0.54
1:A:431:LEU:HD13	1:A:436:MET:HE2	4.52	0.54
1:A:167:THR:HG23	1:A:171:MET:CE	4.09	0.54
9:I:31:PHE:O	9:I:32:ALA:HB3	2.09	0.53
1:A:409:TRP:HE1	13:M:15:GLN:HE22	1.55	0.53
1:A:453:ILE:HA	1:A:456:MET:HE2	1.91	0.53
2:B:13:THR:HB	2:B:168:LEU:HD12	5.08	0.53
4:D:123:MET:O	4:D:124:LEU:HB2	4.64	0.53
2:B:149:THR:O	2:B:184:LEU:O	4.89	0.53
2:B:102:HIS:HE1	2:B:107:SER:OG	1.92	0.52
1:A:177:SER:HA	7:G:10:GLY:HA3	38.88	0.52
1:A:452:THR:O	1:A:456:MET:HE2	3.61	0.52
1:A:466:MET:HE3	13:M:26:PHE:HB2	1.90	0.52
1:A:406:ASN:HD21	18:A:606:PGV:H32	4.01	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.51
1:A:466:MET:CE	13:M:26:PHE:CB	2.84	0.51
1:A:184:PHE:H	1:A:256:HIS:HE1	1.58	0.51
1:A:246:LEU:HD13	1:A:381:LEU:HD21	1.92	0.51
2:B:4:PRO:CB	11:K:42:PRO:CG	2.81	0.51
3:C:161:GLN:HE21	24:G:101:PEK:H42	1.76	0.51
2:B:146:MET:HE3	2:B:215:PRO:N	5.67	0.50
9:I:31:PHE:O	9:I:32:ALA:CB	2.60	0.50
1:A:466:MET:HE3	13:M:26:PHE:CB	2.42	0.49
1:A:87:ILE:O	1:A:173:PRO:HD3	2.13	0.49
2:B:49:LYS:O	4:D:20:ARG:NH2	2.40	0.49
4:D:123:MET:O	4:D:124:LEU:CB	4.25	0.48
6:F:85:CYS:SG	6:F:87:THR:HG23	2.54	0.48
1:A:297:MET:CG	1:A:302:ARG:HG3	2.43	0.48
1:A:485:VAL:HG23	13:M:1:ILE:HD12	3.95	0.48
2:B:104:TRP:HD1	2:B:207:MET:CE	2.27	0.47
6:F:54:ASN:HD22	6:F:54:ASN:C	4.65	0.47
1:A:194:LEU:CD2	7:G:4:ALA:HB1	44.71	0.47
1:A:184:PHE:H	1:A:256:HIS:CE1	2.33	0.47
1:A:65:MET:HA	1:A:65:MET:HE2	4.78	0.46
4:D:6:VAL:HG13	4:D:10:ASP:CB	4.04	0.46
2:B:41:ILE:O	2:B:45:MET:HG2	2.26	0.46
1:A:256:HIS:HD2	30:A:732:HOH:O	1.98	0.46
13:M:28:LEU:HB2	13:M:29:PRO:HD3	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.98	0.46
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.97	0.45
11:K:41:ASN:HB3	11:K:42:PRO:CD	2.47	0.45
11:K:41:ASN:HB3	11:K:42:PRO:HD3	1.98	0.45
8:H:27:ARG:NH1	30:H:102:HOH:O	17.60	0.45
9:I:59:ASP:O	9:I:63:MET:HG3	2.67	0.45
1:A:76:GLY:O	1:A:80:ASN:HB2	2.19	0.45
3:C:76:GLN:O	3:C:80:ARG:HG3	2.16	0.45
1:A:309:THR:CG2	14:A:602:HEA:HMB2	2.52	0.45
11:K:40:TRP:O	11:K:42:PRO:HD3	2.17	0.44
4:D:6:VAL:HG13	4:D:10:ASP:HB2	3.23	0.44
1:A:409:TRP:HE1	13:M:15:GLN:NE2	2.16	0.44
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.08	0.44
30:A:707:HOH:O	3:C:10:MET:HE1	6.86	0.43
3:C:56:GLN:NE2	10:J:31:LEU:HB3	3.87	0.43
3:C:47:LEU:O	3:C:51:MET:HG2	2.27	0.43
1:A:381:LEU:HG	14:A:602:HEA:HAC	2.01	0.42
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	2.06	0.42
9:I:35:TYR:N	30:I:201:HOH:O	2.40	0.42
1:A:216:ASN:ND2	7:G:57:THR:H	3.87	0.42
5:E:66:ARG:O	5:E:70:VAL:HG13	2.19	0.41
2:B:4:PRO:HB3	11:K:42:PRO:CB	2.50	0.41
4:D:145:TRP:CG	11:K:45:VAL:O	2.73	0.41
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.02	0.41
3:C:76:GLN:NE2	30:C:404:HOH:O	17.09	0.41
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.09	0.41
2:B:61:VAL:CG1	2:B:65:TRP:CZ3	3.04	0.41
1:A:483:LEU:HD22	4:D:6:VAL:HB	3.52	0.41
4:D:12:ALA:HA	6:F:73:TRP:CD1	2.96	0.41
2:B:13:THR:HB	2:B:168:LEU:CD1	4.55	0.41
1:A:378:HIS:O	1:A:382:SER:HB3	2.21	0.40
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.03	0.40
10:J:30:ILE:O	10:J:34:VAL:HG23	2.61	0.40
12:L:26:THR:HG21	13:M:21:VAL:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	a	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
2	B	224/227 (99%)	217 (97%)	7 (3%)	0	100	100
2	b	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	20	9
3	C	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	38	25
3	c	257/261 (98%)	250 (97%)	6 (2%)	1 (0%)	38	25
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	d	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	25	13
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	e	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	5	0
6	f	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	18	7
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	4	0
7	g	81/85 (95%)	72 (89%)	8 (10%)	1 (1%)	15	5
8	H	77/85 (91%)	69 (90%)	6 (8%)	2 (3%)	6	1
8	h	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	14	4
9	I	70/73 (96%)	68 (97%)	1 (1%)	1 (1%)	13	4
9	i	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	j	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	10	2
11	K	47/56 (84%)	43 (92%)	1 (2%)	3 (6%)	1	0
11	k	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	l	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3501/3614 (97%)	3369 (96%)	111 (3%)	21 (1%)	28	15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	38	ASN
6	F	95	GLN
6	F	96	LEU
11	K	41	ASN
11	K	42	PRO
11	K	43	SER
3	c	38	ASN
4	d	124	LEU
7	G	4	ALA
7	G	12	GLY
8	H	51	SER
9	I	32	ALA
8	h	11	TYR
2	b	91	ASN
10	j	56	PRO
2	b	150	ILE
6	f	2	SER
7	g	8	HIS
6	F	97	ALA
7	G	3	ALA
8	H	10	ASN

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%)	422 (99%)	4 (1%)	82	81
1	a	426/426 (100%)	419 (98%)	7 (2%)	68	63
2	B	210/210 (100%)	205 (98%)	5 (2%)	54	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	210/210 (100%)	201 (96%)	9 (4%)	33	19
3	C	224/226 (99%)	222 (99%)	2 (1%)	82	81
3	c	224/226 (99%)	221 (99%)	3 (1%)	73	69
4	D	128/129 (99%)	127 (99%)	1 (1%)	85	83
4	d	128/129 (99%)	124 (97%)	4 (3%)	45	32
5	E	92/95 (97%)	92 (100%)	0	100	100
5	e	92/95 (97%)	91 (99%)	1 (1%)	78	75
6	F	81/81 (100%)	80 (99%)	1 (1%)	75	72
6	f	81/81 (100%)	78 (96%)	3 (4%)	39	25
7	G	67/68 (98%)	63 (94%)	4 (6%)	22	9
7	g	67/68 (98%)	61 (91%)	6 (9%)	11	3
8	H	71/75 (95%)	68 (96%)	3 (4%)	34	20
8	h	71/75 (95%)	67 (94%)	4 (6%)	25	11
9	I	57/57 (100%)	56 (98%)	1 (2%)	64	57
9	i	57/57 (100%)	57 (100%)	0	100	100
10	J	49/50 (98%)	49 (100%)	0	100	100
10	j	49/50 (98%)	47 (96%)	2 (4%)	35	21
11	K	39/46 (85%)	39 (100%)	0	100	100
11	k	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	51	40
12	l	39/40 (98%)	38 (97%)	1 (3%)	51	40
13	M	37/38 (97%)	36 (97%)	1 (3%)	50	39
13	m	37/38 (97%)	37 (100%)	0	100	100
All	All	3040/3082 (99%)	2977 (98%)	63 (2%)	59	50

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	297	MET
1	A	338	MET
1	A	369	ASP
2	B	37	LEU
2	B	65	TRP

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Mol	Chain	Res	Type
2	B	75	LEU
2	B	115	ASP
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
4	D	4	SER
6	F	95	GLN
7	G	5	LYS
7	G	18	PHE
7	G	38	HIS
7	G	54	ARG
8	H	7	LYS
8	H	9	LYS
8	H	60	TYR
9	I	36	LYS
12	L	47	LYS
13	M	38	ASP
1	a	65	MET
1	a	109	PHE
1	a	189	MET
1	a	369	ASP
1	a	436	MET
1	a	485	VAL
1	a	504	THR
2	b	18	GLU
2	b	61	VAL
2	b	65	TRP
2	b	66	THR
2	b	94	SER
2	b	168	LEU
2	b	171	LYS
2	b	213	LEU
2	b	217	LYS
3	c	38	ASN
3	c	159	MET
3	c	214	PHE
4	d	6	VAL
4	d	10	ASP
4	d	30	VAL
4	d	73	ARG
5	e	92	THR
6	f	43	LYS

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Mol	Chain	Res	Type
6	f	54	ASN
6	f	96	LEU
7	g	5	LYS
7	g	7	ASP
7	g	18	PHE
7	g	39	SER
7	g	42	ARG
7	g	54	ARG
8	h	7	LYS
8	h	57	ARG
8	h	60	TYR
8	h	61	LYS
10	j	10	LYS
10	j	57	HIS
12	l	2	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	256	HIS
1	A	422	ASN
2	B	52	HIS
2	B	102	HIS
4	D	37	GLN
4	D	76	ASN
6	F	80	GLN
10	J	9	GLN
13	M	15	GLN
1	a	216	ASN
2	b	10	GLN
2	b	59	GLN
2	b	103	GLN
3	c	56	GLN
3	c	76	GLN
6	f	54	ASN
13	m	15	GLN
13	m	39	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	FME	A	1	1	9,9,10	0.67	0	7,9,11	2.71	2 (28%)
7	TPO	G	11	7	9,10,11	1.39	1 (11%)	10,14,16	1.12	1 (10%)
1	FME	a	1	1	9,9,10	0.50	0	7,9,11	1.79	2 (28%)
2	FME	b	1	2	9,9,10	0.70	0	7,9,11	2.31	2 (28%)
7	TPO	g	11	7	9,10,11	1.29	2 (22%)	10,14,16	1.69	1 (10%)

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
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
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	-	1/8/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	11	TPO	P-OG1	2.04	1.63	1.59
7	g	11	TPO	CA-C	2.14	1.53	1.50
7	G	11	TPO	P-OG1	3.10	1.65	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CA-N-CN	-6.68	112.55	122.82
2	b	1	FME	CA-N-CN	-4.54	115.84	122.82
1	a	1	FME	CA-N-CN	-3.81	116.96	122.82
2	b	1	FME	CB-CA-C	-3.02	106.67	111.65
1	A	1	FME	O-C-CA	-2.32	119.74	125.15
7	G	11	TPO	CG2-CB-CA	-2.24	109.06	113.22
1	a	1	FME	O-C-CA	-2.24	119.94	125.15
7	g	11	TPO	C-CA-N	4.66	119.27	109.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	g	11	TPO	OG1-CB-CA-N
1	A	1	FME	O1-CN-N-CA
1	a	1	FME	O1-CN-N-CA
2	b	1	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 8 are monoatomic - leaving 49 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	HEA	A	601	1	44,67,67	2.08	6 (13%)	37,103,103	2.47	16 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	602	1,20	44,67,67	2.21	8 (18%)	37,103,103	2.36	7 (18%)
18	PGV	A	606	-	50,50,50	1.02	2 (4%)	51,56,56	0.97	3 (5%)
18	PGV	A	607	-	50,50,50	0.85	2 (4%)	51,56,56	0.88	2 (3%)
19	TGL	A	608	-	62,62,62	1.09	3 (4%)	65,65,65	1.02	4 (6%)
19	TGL	A	609	-	62,62,62	1.03	3 (4%)	65,65,65	1.02	5 (7%)
20	CMO	A	610	15,14	0,1,1	0.00	-	0,0,0	0.00	-
21	FME	B	301	2	9,9,10	0.89	0	7,9,11	3.69	3 (42%)
22	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	B	303	-	29,32,32	0.64	0	47,51,51	1.23	7 (14%)
23	CHD	C	301	-	29,32,32	0.55	0	47,51,51	1.14	5 (10%)
24	PEK	C	302	-	52,52,52	0.84	2 (3%)	54,57,57	0.99	4 (7%)
18	PGV	C	303	-	50,50,50	0.83	2 (4%)	51,56,56	0.82	1 (1%)
18	PGV	C	304	-	50,50,50	1.06	2 (4%)	51,56,56	1.06	4 (7%)
25	CDL	C	305	-	99,99,99	0.98	4 (4%)	101,111,111	1.05	7 (6%)
23	CHD	C	306	-	29,32,32	0.44	0	47,51,51	1.27	5 (10%)
24	PEK	C	307	-	52,52,52	1.01	2 (3%)	54,57,57	0.92	3 (5%)
26	DMU	C	308	-	34,34,34	0.72	1 (2%)	45,45,45	1.33	6 (13%)
19	TGL	D	201	-	62,62,62	1.09	3 (4%)	65,65,65	0.99	5 (7%)
27	PSC	E	201	-	51,51,51	1.03	2 (3%)	56,59,59	1.91	10 (17%)
24	PEK	G	101	-	52,52,52	1.00	2 (3%)	54,57,57	1.22	5 (9%)
25	CDL	G	102	-	99,99,99	1.02	4 (4%)	101,111,111	0.99	7 (6%)
23	CHD	G	103	-	29,32,32	0.61	0	47,51,51	1.07	3 (6%)
29	SAC	I	101	9	8,8,9	1.54	1 (12%)	6,9,11	1.45	1 (16%)
23	CHD	J	101	-	29,32,32	0.56	0	47,51,51	2.16	16 (34%)
26	DMU	M	101	-	34,34,34	0.53	1 (2%)	45,45,45	0.78	1 (2%)
14	HEA	a	601	1	44,67,67	2.43	10 (22%)	37,103,103	2.37	12 (32%)
14	HEA	a	602	1,20	44,67,67	2.65	8 (18%)	37,103,103	2.48	10 (27%)
18	PGV	a	606	-	50,50,50	1.05	2 (4%)	51,56,56	1.24	6 (11%)
18	PGV	a	607	-	50,50,50	0.83	2 (4%)	51,56,56	0.78	2 (3%)
20	CMO	a	608	15,14	0,1,1	0.00	-	0,0,0	0.00	-
22	CUA	b	301	2	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	b	302	-	62,62,62	1.03	3 (4%)	65,65,65	0.99	3 (4%)
27	PSC	b	303	-	51,51,51	1.02	2 (3%)	56,59,59	1.86	11 (19%)
24	PEK	c	301	-	52,52,52	0.98	2 (3%)	54,57,57	0.97	3 (5%)
18	PGV	c	302	-	50,50,50	1.04	2 (4%)	51,56,56	1.29	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	c	303	-	29,32,32	0.52	0	47,51,51	1.07	3 (6%)
24	PEK	c	304	-	52,52,52	0.88	2 (3%)	54,57,57	0.87	3 (5%)
24	PEK	c	305	-	52,52,52	0.98	2 (3%)	54,57,57	0.98	3 (5%)
18	PGV	c	306	-	50,50,50	0.88	2 (4%)	51,56,56	0.84	1 (1%)
25	CDL	c	307	-	99,99,99	0.99	4 (4%)	101,111,111	1.07	6 (5%)
23	CHD	c	308	-	29,32,32	0.41	0	47,51,51	1.04	3 (6%)
26	DMU	c	309	-	34,34,34	0.98	2 (5%)	45,45,45	1.50	7 (15%)
19	TGL	d	201	-	62,62,62	1.09	3 (4%)	65,65,65	1.18	8 (12%)
25	CDL	g	101	-	99,99,99	0.99	4 (4%)	101,111,111	1.08	7 (6%)
29	SAC	i	101	9	8,8,9	1.69	2 (25%)	6,9,11	1.05	1 (16%)
23	CHD	j	101	-	29,32,32	0.48	0	47,51,51	1.45	11 (23%)
19	TGL	l	101	-	62,62,62	1.11	3 (4%)	65,65,65	1.16	5 (7%)
26	DMU	m	101	-	34,34,34	0.49	0	45,45,45	1.00	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1,20	2/2/7/16	0/24/76/76	0/0/8/8
18	PGV	A	606	-	-	0/55/55/55	0/0/0/0
18	PGV	A	607	-	-	0/55/55/55	0/0/0/0
19	TGL	A	608	-	-	0/65/65/65	0/0/0/0
19	TGL	A	609	-	-	0/65/65/65	0/0/0/0
20	CMO	A	610	15,14	-	0/0/0/0	0/0/0/0
21	FME	B	301	2	-	1/6/9/11	0/0/0/0
22	CUA	B	302	2	-	0/0/0/0	0/0/0/0
23	CHD	B	303	-	-	0/7/74/74	0/4/4/4
23	CHD	C	301	-	-	0/7/74/74	0/4/4/4
24	PEK	C	302	-	-	0/56/56/56	0/0/0/0
18	PGV	C	303	-	-	0/55/55/55	0/0/0/0
18	PGV	C	304	-	-	0/55/55/55	0/0/0/0
25	CDL	C	305	-	-	0/110/110/110	0/0/0/0
23	CHD	C	306	-	-	0/7/74/74	0/4/4/4
24	PEK	C	307	-	-	0/56/56/56	0/0/0/0
26	DMU	C	308	-	-	0/19/59/59	0/2/2/2
19	TGL	D	201	-	-	0/65/65/65	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PSC	E	201	-	-	0/55/55/55	0/0/0/0
24	PEK	G	101	-	-	0/56/56/56	0/0/0/0
25	CDL	G	102	-	-	0/110/110/110	0/0/0/0
23	CHD	G	103	-	-	0/7/74/74	0/4/4/4
29	SAC	I	101	9	-	1/6/8/10	0/0/0/0
23	CHD	J	101	-	-	0/7/74/74	0/4/4/4
26	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	HEA	a	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	a	602	1,20	2/2/7/16	0/24/76/76	0/0/8/8
18	PGV	a	606	-	-	2/55/55/55	0/0/0/0
18	PGV	a	607	-	-	0/55/55/55	0/0/0/0
20	CMO	a	608	15,14	-	0/0/0/0	0/0/0/0
22	CUA	b	301	2	-	0/0/0/0	0/0/0/0
19	TGL	b	302	-	-	0/65/65/65	0/0/0/0
27	PSC	b	303	-	-	0/55/55/55	0/0/0/0
24	PEK	c	301	-	-	0/56/56/56	0/0/0/0
18	PGV	c	302	-	-	0/55/55/55	0/0/0/0
23	CHD	c	303	-	-	0/7/74/74	0/4/4/4
24	PEK	c	304	-	-	0/56/56/56	0/0/0/0
24	PEK	c	305	-	-	0/56/56/56	0/0/0/0
18	PGV	c	306	-	-	0/55/55/55	0/0/0/0
25	CDL	c	307	-	-	1/110/110/110	0/0/0/0
23	CHD	c	308	-	-	0/7/74/74	0/4/4/4
26	DMU	c	309	-	-	0/19/59/59	0/2/2/2
19	TGL	d	201	-	-	0/65/65/65	0/0/0/0
25	CDL	g	101	-	-	0/110/110/110	0/0/0/0
29	SAC	i	101	9	-	0/6/8/10	0/0/0/0
23	CHD	j	101	-	-	0/7/74/74	0/4/4/4
19	TGL	l	101	-	-	0/65/65/65	0/0/0/0
26	DMU	m	101	-	-	0/19/59/59	0/2/2/2

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4D-ND	-2.35	1.31	1.36
14	a	602	HEA	C1B-NB	-2.23	1.31	1.36
14	A	602	HEA	C1B-NB	-2.21	1.31	1.36
14	a	601	HEA	C1D-ND	-2.18	1.34	1.36
14	a	601	HEA	C4D-CHA	2.14	1.45	1.40
26	M	101	DMU	O16-C6	2.21	1.44	1.40
29	i	101	SAC	CA-C	2.22	1.53	1.50
14	a	602	HEA	C3D-C2D	2.27	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	601	HEA	C1C-CHC	2.35	1.46	1.40
14	a	601	HEA	C1B-CHB	2.40	1.46	1.40
14	A	601	HEA	C4C-CHD	2.44	1.46	1.40
14	A	602	HEA	C1C-CHC	2.48	1.46	1.40
26	C	308	DMU	O16-C6	2.49	1.44	1.40
14	a	602	HEA	C4C-CHD	2.63	1.47	1.40
26	c	309	DMU	O16-C6	2.72	1.44	1.40
14	a	601	HEA	C3D-C2D	2.87	1.46	1.37
14	A	602	HEA	C3D-C2D	2.88	1.46	1.37
14	A	601	HEA	C3A-C2A	2.94	1.44	1.40
14	a	601	HEA	C4C-CHD	3.03	1.48	1.40
14	a	602	HEA	C1C-CHC	3.04	1.48	1.40
14	A	601	HEA	C3D-C2D	3.18	1.47	1.37
18	A	607	PGV	O01-C1	3.25	1.43	1.34
24	c	304	PEK	O01-C1	3.40	1.44	1.34
24	C	302	PEK	O01-C1	3.46	1.44	1.34
18	a	607	PGV	O01-C1	3.49	1.44	1.34
18	C	303	PGV	O01-C1	3.60	1.44	1.34
18	A	607	PGV	O03-C19	3.60	1.43	1.33
18	C	303	PGV	O03-C19	3.66	1.44	1.33
18	a	607	PGV	O03-C19	3.70	1.44	1.33
24	C	302	PEK	O03-C21	3.76	1.44	1.33
18	c	306	PGV	O03-C19	3.79	1.44	1.33
26	c	309	DMU	O5-C6	3.84	1.51	1.41
18	A	606	PGV	O01-C1	3.97	1.45	1.34
18	c	306	PGV	O01-C1	3.99	1.45	1.34
29	i	101	SAC	CA-N	4.01	1.52	1.46
25	G	102	CDL	OA6-CA5	4.09	1.46	1.34
25	C	305	CDL	OB6-CB5	4.10	1.46	1.34
19	A	608	TGL	OG2-CB1	4.12	1.46	1.34
29	I	101	SAC	CA-N	4.12	1.52	1.46
24	c	301	PEK	O01-C1	4.16	1.46	1.34
19	A	609	TGL	OG3-CC1	4.19	1.45	1.33
19	A	609	TGL	OG2-CB1	4.20	1.46	1.34
25	g	101	CDL	OA6-CA5	4.22	1.46	1.34
19	b	302	TGL	OG3-CC1	4.22	1.45	1.33
24	c	304	PEK	O03-C21	4.29	1.46	1.33
25	C	305	CDL	OB8-CB7	4.30	1.46	1.33
27	E	201	PSC	O03-C19	4.32	1.46	1.33
25	c	307	CDL	OB8-CB7	4.33	1.46	1.33
19	b	302	TGL	OG2-CB1	4.33	1.46	1.34
19	d	201	TGL	OG3-CC1	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	303	PSC	O03-C19	4.36	1.46	1.33
25	C	305	CDL	OA6-CA5	4.37	1.47	1.34
25	g	101	CDL	OB6-CB5	4.38	1.47	1.34
19	b	302	TGL	OG1-CA1	4.39	1.46	1.33
25	c	307	CDL	OB6-CB5	4.40	1.47	1.34
25	C	305	CDL	OA8-CA7	4.40	1.46	1.33
19	A	609	TGL	OG1-CA1	4.40	1.46	1.33
25	g	101	CDL	OA8-CA7	4.41	1.46	1.33
19	D	201	TGL	OG3-CC1	4.43	1.46	1.33
25	g	101	CDL	OB8-CB7	4.43	1.46	1.33
24	c	305	PEK	O01-C1	4.43	1.47	1.34
18	C	304	PGV	O01-C1	4.43	1.47	1.34
24	G	101	PEK	O03-C21	4.44	1.46	1.33
25	c	307	CDL	OA8-CA7	4.45	1.46	1.33
19	d	201	TGL	OG1-CA1	4.46	1.46	1.33
24	C	307	PEK	O01-C1	4.47	1.47	1.34
19	D	201	TGL	OG2-CB1	4.47	1.47	1.34
24	G	101	PEK	O01-C1	4.48	1.47	1.34
18	c	302	PGV	O03-C19	4.49	1.46	1.33
24	c	305	PEK	O03-C21	4.49	1.46	1.33
19	l	101	TGL	OG1-CA1	4.50	1.46	1.33
25	G	102	CDL	OB6-CB5	4.50	1.47	1.34
19	A	608	TGL	OG3-CC1	4.51	1.46	1.33
14	a	601	HEA	C3A-C2A	4.53	1.46	1.40
25	c	307	CDL	OA6-CA5	4.53	1.47	1.34
19	d	201	TGL	OG2-CB1	4.54	1.47	1.34
25	G	102	CDL	OA8-CA7	4.54	1.46	1.33
19	D	201	TGL	OG1-CA1	4.54	1.46	1.33
24	c	301	PEK	O03-C21	4.60	1.46	1.33
18	c	302	PGV	O01-C1	4.61	1.47	1.34
24	C	307	PEK	O03-C21	4.62	1.47	1.33
27	E	201	PSC	O01-C1	4.66	1.47	1.34
19	l	101	TGL	OG2-CB1	4.67	1.47	1.34
25	G	102	CDL	OB8-CB7	4.72	1.47	1.33
18	a	606	PGV	O03-C19	4.73	1.47	1.33
18	A	606	PGV	O03-C19	4.74	1.47	1.33
18	a	606	PGV	O01-C1	4.77	1.48	1.34
14	A	602	HEA	C3A-C2A	4.77	1.46	1.40
27	b	303	PSC	O01-C1	4.78	1.48	1.34
19	l	101	TGL	OG3-CC1	4.80	1.47	1.33
19	A	608	TGL	OG1-CA1	4.82	1.47	1.33
18	C	304	PGV	O03-C19	4.83	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	a	601	HEA	C3C-C2C	4.97	1.46	1.40
14	a	602	HEA	C3C-C2C	5.09	1.47	1.40
14	A	601	HEA	C3C-C2C	5.09	1.47	1.40
14	A	602	HEA	C3C-C2C	5.10	1.47	1.40
14	a	602	HEA	C3A-C2A	5.45	1.47	1.40
14	A	602	HEA	C1A-NA	5.87	1.43	1.36
14	A	601	HEA	C4A-NA	6.01	1.43	1.36
14	a	601	HEA	C4A-NA	7.04	1.45	1.36
14	A	601	HEA	C1A-NA	8.46	1.46	1.36
14	A	602	HEA	C4A-NA	9.12	1.47	1.36
14	a	602	HEA	C1A-NA	9.17	1.47	1.36
14	a	601	HEA	C1A-NA	10.29	1.48	1.36
14	a	602	HEA	C4A-NA	10.82	1.49	1.36

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	301	FME	CA-N-CN	-8.81	109.27	122.82
14	a	602	HEA	C4B-C3B-C2B	-8.18	101.15	106.87
14	A	602	HEA	C4B-C3B-C2B	-7.76	101.45	106.87
14	a	602	HEA	CAD-CBD-CGD	-7.10	100.53	112.66
27	E	201	PSC	C08-N-C06	-6.69	92.04	108.98
27	b	303	PSC	C08-N-C06	-6.58	92.32	108.98
14	a	601	HEA	C1B-C2B-C3B	-6.55	102.44	107.00
27	E	201	PSC	C08-N-C07	-6.50	92.52	108.98
14	a	601	HEA	C4B-C3B-C2B	-6.39	102.41	106.87
27	b	303	PSC	C08-N-C07	-6.36	92.88	108.98
14	A	601	HEA	C1B-C2B-C3B	-6.21	102.67	107.00
14	A	602	HEA	C1B-C2B-C3B	-5.42	103.22	107.00
14	A	601	HEA	C4B-C3B-C2B	-5.27	103.19	106.87
14	A	602	HEA	CAD-CBD-CGD	-5.04	104.05	112.66
27	E	201	PSC	C08-N-C05	-4.32	93.33	109.93
14	A	601	HEA	C13-C12-C11	-4.28	107.98	114.46
14	a	602	HEA	C1B-C2B-C3B	-4.18	104.09	107.00
23	J	101	CHD	C6-C5-C4	-3.70	106.92	111.13
23	C	306	CHD	C21-C20-C22	-3.69	104.53	110.35
14	a	601	HEA	C13-C12-C11	-3.56	109.07	114.46
27	b	303	PSC	C08-N-C05	-3.46	96.66	109.93
23	J	101	CHD	C21-C20-C17	-3.37	107.67	112.95
18	c	302	PGV	O03-C19-O04	-3.24	115.51	123.55
14	A	602	HEA	CBA-CAA-C2A	-3.23	106.31	112.47
14	a	602	HEA	CBA-CAA-C2A	-3.20	106.36	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	309	DMU	C18-O16-C6	-3.18	108.41	113.87
23	B	303	CHD	C19-C10-C1	-3.04	103.24	108.24
23	C	306	CHD	C19-C10-C1	-2.81	103.62	108.24
14	A	602	HEA	C13-C12-C11	-2.81	110.20	114.46
25	C	305	CDL	OA6-CA5-OA7	-2.80	116.69	123.68
24	G	101	PEK	O03-C21-O04	-2.78	116.64	123.55
14	a	601	HEA	CAA-CBA-CGA	-2.77	107.93	112.66
23	J	101	CHD	C17-C13-C14	-2.75	97.28	100.08
14	A	601	HEA	C17-C18-C19	-2.74	120.80	127.68
14	A	601	HEA	CAA-CBA-CGA	-2.71	108.02	112.66
25	C	305	CDL	OB8-CB7-OB9	-2.70	116.84	123.55
23	J	101	CHD	O7-C7-C6	-2.66	103.58	110.02
23	j	101	CHD	C23-C22-C20	-2.66	111.14	114.72
18	A	607	PGV	O03-C19-O04	-2.65	116.98	123.55
23	j	101	CHD	C6-C5-C4	-2.64	108.13	111.13
23	c	308	CHD	C6-C5-C4	-2.59	108.18	111.13
14	A	601	HEA	OMA-CMA-C3A	-2.59	119.12	125.08
23	j	101	CHD	C5-C6-C7	-2.56	111.60	114.44
14	A	601	HEA	O11-C11-C3B	-2.55	104.48	111.83
23	c	303	CHD	C19-C10-C1	-2.54	104.06	108.24
21	B	301	FME	O1-CN-N	-2.50	118.22	125.20
18	A	606	PGV	O03-C19-O04	-2.50	117.34	123.55
23	G	103	CHD	C19-C10-C1	-2.45	104.21	108.24
19	d	201	TGL	OG2-CB1-OB1	-2.44	117.58	123.68
23	J	101	CHD	C19-C10-C1	-2.42	104.27	108.24
23	j	101	CHD	O7-C7-C6	-2.40	104.21	110.02
23	B	303	CHD	O3-C3-C4	-2.38	105.13	109.87
14	a	602	HEA	OMA-CMA-C3A	-2.36	119.66	125.08
19	A	608	TGL	OG1-CA1-OA1	-2.36	117.70	123.55
25	G	102	CDL	OA6-CA5-OA7	-2.35	117.80	123.68
25	g	101	CDL	OA8-CA7-OA9	-2.35	117.71	123.55
23	C	301	CHD	C19-C10-C1	-2.35	104.38	108.24
23	C	306	CHD	C6-C5-C4	-2.34	108.48	111.13
23	B	303	CHD	C14-C13-C12	-2.34	105.17	107.39
14	A	601	HEA	CAD-CBD-CGD	-2.33	108.67	112.66
23	c	308	CHD	C19-C10-C1	-2.32	104.44	108.24
19	D	201	TGL	OG2-CB1-OB1	-2.27	118.01	123.68
21	B	301	FME	CB-CA-C	-2.27	107.91	111.65
25	C	305	CDL	OA8-CA7-OA9	-2.27	117.92	123.55
23	j	101	CHD	C19-C10-C5	-2.27	106.39	110.30
26	C	308	DMU	C2-C3-C4	-2.26	106.07	110.88
29	i	101	SAC	O-C-CA	-2.26	119.89	125.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	E	201	PSC	O03-C19-O04	-2.25	117.96	123.55
19	d	201	TGL	OG3-CC1-OC1	-2.24	117.99	123.55
24	G	101	PEK	O01-C1-O02	-2.23	118.11	123.68
25	c	307	CDL	OB8-CB7-OB9	-2.23	118.01	123.55
27	E	201	PSC	O01-C1-O02	-2.21	118.15	123.68
26	m	101	DMU	O1-C10-C5	-2.20	106.04	110.30
24	C	302	PEK	O03-C21-O04	-2.20	118.08	123.55
14	a	601	HEA	OMA-CMA-C3A	-2.20	120.03	125.08
25	G	102	CDL	OB6-CB5-OB7	-2.19	118.22	123.68
24	c	305	PEK	O03-C21-O04	-2.18	118.13	123.55
14	a	601	HEA	CMB-C2B-C1B	-2.18	125.11	128.46
24	C	302	PEK	O01-C1-O02	-2.18	118.23	123.68
26	c	309	DMU	O7-C10-O1	-2.18	105.41	110.70
25	c	307	CDL	OA6-CA5-OA7	-2.17	118.26	123.68
14	A	601	HEA	CMB-C2B-C1B	-2.17	125.13	128.46
19	A	609	TGL	OG2-CB1-OB1	-2.16	118.29	123.68
14	A	601	HEA	CMC-C2C-C1C	-2.16	125.15	128.46
25	g	101	CDL	OB6-CB5-OB7	-2.14	118.35	123.68
14	A	601	HEA	CBA-CAA-C2A	-2.13	108.40	112.47
18	c	302	PGV	O01-C1-O02	-2.12	118.38	123.68
23	J	101	CHD	C18-C13-C12	-2.11	106.93	109.08
24	c	304	PEK	O01-C1-O02	-2.10	118.43	123.68
23	J	101	CHD	C19-C10-C5	-2.09	106.70	110.30
18	C	304	PGV	O03-C19-O04	-2.09	118.37	123.55
18	a	606	PGV	O01-C1-O02	-2.06	118.53	123.68
23	C	301	CHD	C9-C8-C7	-2.05	109.51	111.92
19	l	101	TGL	OG1-CA1-OA1	-2.05	118.46	123.55
23	j	101	CHD	C21-C20-C22	-2.05	107.12	110.35
27	b	303	PSC	C21-C20-C19	-2.03	106.18	113.58
18	a	606	PGV	O03-C19-O04	-2.02	118.53	123.55
19	d	201	TGL	OG1-CA1-OA1	-2.01	118.56	123.55
26	M	101	DMU	O1-C9-C11	2.02	111.25	106.41
14	a	601	HEA	C25-C23-C24	2.02	119.32	114.60
25	G	102	CDL	CA6-OA8-CA7	2.03	123.23	117.13
23	J	101	CHD	C9-C10-C5	2.05	111.59	108.63
23	C	301	CHD	C18-C13-C12	2.08	111.19	109.08
24	G	101	PEK	C2-C3-C4	2.10	117.04	113.29
14	a	602	HEA	C25-C23-C24	2.10	119.51	114.60
23	c	303	CHD	C6-C7-C8	2.10	113.74	111.50
23	B	303	CHD	C11-C12-C13	2.11	113.41	111.22
23	j	101	CHD	C13-C17-C20	2.11	122.06	119.49
23	B	303	CHD	C1-C10-C9	2.12	114.77	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	303	PGV	O01-C1-C2	2.12	115.96	111.55
23	c	308	CHD	C11-C12-C13	2.13	113.43	111.22
14	a	602	HEA	C27-C19-C20	2.14	119.00	115.29
23	C	306	CHD	C21-C20-C17	2.15	116.31	112.95
25	g	101	CDL	OB8-CB6-CB4	2.16	114.08	108.66
26	m	101	DMU	O7-C10-C5	2.17	113.01	108.11
14	a	601	HEA	CMD-C2D-C3D	2.19	129.07	124.94
19	A	609	TGL	OG1-CA1-CA2	2.19	118.29	111.90
18	c	302	PGV	O03-C01-C02	2.20	114.19	108.66
23	C	301	CHD	C21-C20-C17	2.20	116.40	112.95
23	C	306	CHD	C18-C13-C12	2.21	111.32	109.08
23	J	101	CHD	C13-C14-C8	2.22	117.64	114.77
19	D	201	TGL	OG3-CC1-CC2	2.24	118.41	111.90
19	A	609	TGL	OG3-CC1-CC2	2.25	118.44	111.90
18	a	606	PGV	O03-C01-C02	2.25	114.31	108.66
14	A	601	HEA	C25-C23-C24	2.31	119.99	114.60
23	c	303	CHD	C18-C13-C12	2.32	111.43	109.08
27	b	303	PSC	O01-C02-C01	2.32	116.86	108.44
23	B	303	CHD	C6-C7-C8	2.34	113.99	111.50
18	a	607	PGV	O03-C19-C20	2.36	118.78	111.90
27	E	201	PSC	C06-N-C05	2.38	119.06	109.93
14	a	602	HEA	CMB-C2B-C3B	2.38	129.49	124.92
23	j	101	CHD	O7-C7-C8	2.42	114.72	109.33
18	a	606	PGV	C01-O03-C19	2.43	124.43	117.13
23	G	103	CHD	C11-C12-C13	2.43	113.74	111.22
27	b	303	PSC	C01-O03-C19	2.43	124.44	117.13
26	C	308	DMU	O7-C3-C2	2.43	113.04	107.19
26	C	308	DMU	O5-C6-C1	2.43	114.99	110.30
23	J	101	CHD	C11-C12-C13	2.44	113.75	111.22
19	D	201	TGL	CG3-OG3-CC1	2.45	124.50	117.13
26	c	309	DMU	C10-C5-C7	2.45	114.53	109.98
23	j	101	CHD	C9-C10-C5	2.45	112.17	108.63
23	C	301	CHD	C6-C7-C8	2.46	114.11	111.50
23	j	101	CHD	C10-C9-C8	2.49	114.55	111.87
24	C	307	PEK	O03-C21-C22	2.50	119.16	111.90
19	d	201	TGL	OG2-CG2-CG1	2.52	117.59	108.44
24	c	301	PEK	C01-O03-C21	2.53	124.73	117.13
18	a	607	PGV	O01-C1-C2	2.53	116.81	111.55
24	c	301	PEK	O03-C21-C22	2.57	119.37	111.90
29	I	101	SAC	CB-CA-N	2.60	116.65	110.60
26	m	101	DMU	C7-C8-C9	2.61	114.82	110.22
19	d	201	TGL	CG2-OG2-CB1	2.63	124.09	117.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	303	PSC	C02-O01-C1	2.64	124.12	117.88
27	E	201	PSC	C07-N-C05	2.65	120.10	109.93
19	A	609	TGL	CG3-OG3-CC1	2.70	125.25	117.13
24	C	307	PEK	C01-O03-C21	2.71	125.27	117.13
23	J	101	CHD	C5-C4-C3	2.72	116.87	112.87
24	C	302	PEK	O01-C1-C2	2.74	117.25	111.55
19	l	101	TGL	OG3-CC1-CC2	2.82	120.10	111.90
26	C	308	DMU	C10-O1-C9	2.83	119.05	113.72
27	E	201	PSC	O03-C19-C20	2.83	120.14	111.90
25	G	102	CDL	OA8-CA7-C31	2.84	120.15	111.90
23	G	103	CHD	C22-C20-C17	2.84	116.23	110.26
19	d	201	TGL	OG1-CA1-CA2	2.87	120.24	111.90
18	c	302	PGV	C01-O03-C19	2.90	125.85	117.13
24	c	304	PEK	O01-C1-C2	2.91	117.59	111.55
19	b	302	TGL	OG3-CC1-CC2	2.94	120.47	111.90
18	c	306	PGV	O01-C1-C2	2.96	117.70	111.55
27	b	303	PSC	O03-C19-C20	2.97	120.53	111.90
25	c	307	CDL	OA8-CA7-C31	2.97	120.55	111.90
19	l	101	TGL	CG3-OG3-CC1	3.02	126.22	117.13
26	m	101	DMU	O1-C9-C8	3.03	115.23	109.66
19	l	101	TGL	OG1-CA1-CA2	3.04	120.75	111.90
18	A	607	PGV	O03-C19-C20	3.04	120.75	111.90
26	C	308	DMU	C6-C1-C2	3.05	115.65	109.98
23	j	101	CHD	C21-C20-C17	3.07	117.75	112.95
25	c	307	CDL	OB8-CB7-C71	3.09	120.89	111.90
23	B	303	CHD	C17-C13-C14	3.10	103.24	100.08
27	b	303	PSC	O01-C1-C2	3.10	117.99	111.55
19	b	302	TGL	OG1-CA1-CA2	3.10	120.93	111.90
19	D	201	TGL	OG1-CA1-CA2	3.13	121.00	111.90
24	c	305	PEK	O03-C21-C22	3.13	121.01	111.90
19	A	608	TGL	OG3-CC1-CC2	3.18	121.14	111.90
14	a	601	HEA	C26-C15-C16	3.20	120.84	115.29
24	c	304	PEK	O03-C21-C22	3.21	121.25	111.90
19	A	608	TGL	OG1-CA1-CA2	3.23	121.29	111.90
26	c	309	DMU	O1-C10-C5	3.24	116.54	110.30
18	a	606	PGV	O03-C19-C20	3.27	121.41	111.90
18	C	304	PGV	O03-C01-C02	3.28	116.89	108.66
25	g	101	CDL	OB8-CB7-C71	3.28	121.45	111.90
25	C	305	CDL	OB8-CB7-C71	3.29	121.47	111.90
25	G	102	CDL	OB8-CB7-C71	3.35	121.64	111.90
25	C	305	CDL	OA8-CA7-C31	3.36	121.67	111.90
18	A	606	PGV	O01-C1-C2	3.36	118.53	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	608	TGL	OG2-CB1-CB2	3.39	118.59	111.55
23	J	101	CHD	C6-C5-C10	3.50	116.48	112.66
25	g	101	CDL	OA8-CA7-C31	3.53	122.17	111.90
19	d	201	TGL	OG3-CC1-CC2	3.55	122.22	111.90
25	C	305	CDL	OB6-CB5-C51	3.56	118.94	111.55
18	C	304	PGV	O01-C1-C2	3.60	119.03	111.55
14	A	601	HEA	C3C-C4C-NC	3.64	113.91	109.21
18	A	606	PGV	O03-C19-C20	3.65	122.51	111.90
26	c	309	DMU	C10-O1-C9	3.71	120.70	113.72
14	A	601	HEA	C26-C15-C16	3.72	121.74	115.29
24	C	307	PEK	O01-C1-C2	3.75	119.34	111.55
14	a	602	HEA	C3C-C4C-NC	3.77	114.08	109.21
24	G	101	PEK	O03-C21-C22	3.78	122.90	111.90
14	A	601	HEA	CMB-C2B-C3B	3.78	132.18	124.92
26	C	308	DMU	C6-O5-C4	3.80	120.88	113.72
26	c	309	DMU	O5-C6-C1	3.84	117.70	110.30
14	a	601	HEA	CMC-C2C-C3C	3.91	132.14	124.89
14	a	601	HEA	CMB-C2B-C3B	3.91	132.43	124.92
24	c	301	PEK	O01-C1-C2	3.92	119.69	111.55
27	b	303	PSC	C07-N-C05	3.94	125.03	109.93
14	A	602	HEA	C3C-C4C-NC	3.95	114.32	109.21
18	c	302	PGV	O03-C19-C20	3.96	123.42	111.90
25	G	102	CDL	OA6-CA5-C11	4.00	119.85	111.55
24	c	305	PEK	O01-C1-C2	4.00	119.86	111.55
27	b	303	PSC	C07-N-C06	4.02	119.15	108.98
25	g	101	CDL	OA6-CA5-C11	4.10	120.07	111.55
19	D	201	TGL	OG2-CB1-CB2	4.14	120.16	111.55
19	A	609	TGL	OG2-CB1-CB2	4.19	120.25	111.55
18	C	304	PGV	O03-C19-C20	4.22	124.17	111.90
14	a	601	HEA	C3C-C4C-NC	4.25	114.70	109.21
25	G	102	CDL	OB6-CB5-C51	4.27	120.41	111.55
24	C	302	PEK	O03-C21-C22	4.29	124.39	111.90
19	b	302	TGL	OG2-CB1-CB2	4.32	120.53	111.55
23	J	101	CHD	C5-C6-C7	4.33	119.23	114.44
26	c	309	DMU	O16-C6-C1	4.42	115.45	108.23
27	E	201	PSC	C07-N-C06	4.43	120.20	108.98
14	A	602	HEA	CMC-C2C-C3C	4.43	133.12	124.89
14	a	602	HEA	CMC-C2C-C3C	4.43	133.12	124.89
19	d	201	TGL	OG2-CB1-CB2	4.48	120.85	111.55
25	c	307	CDL	OB6-CB5-C51	4.50	120.89	111.55
25	C	305	CDL	OA6-CA5-C11	4.78	121.47	111.55
27	E	201	PSC	O01-C1-C2	4.82	121.55	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	101	CHD	C13-C17-C20	4.95	125.50	119.49
23	J	101	CHD	C22-C20-C17	5.26	121.30	110.26
25	g	101	CDL	OB6-CB5-C51	5.27	122.49	111.55
23	J	101	CHD	C6-C7-C8	5.28	117.11	111.50
19	l	101	TGL	OG2-CB1-CB2	5.37	122.69	111.55
24	G	101	PEK	O01-C1-C2	5.45	122.87	111.55
14	A	601	HEA	CMC-C2C-C3C	5.46	135.03	124.89
18	c	302	PGV	O01-C1-C2	5.46	122.90	111.55
25	c	307	CDL	OA6-CA5-C11	5.61	123.19	111.55
18	a	606	PGV	O01-C1-C2	5.97	123.95	111.55

All (8) chirality outliers are listed below:

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

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	I	101	SAC	CB-CA-N-C1A
25	c	307	CDL	CA4-OA6-CA5-C11
18	a	606	PGV	C02-O01-C1-O02
18	a	606	PGV	C02-O01-C1-C2
21	B	301	FME	O1-CN-N-CA

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	2	0
14	A	602	HEA	4	0
18	A	606	PGV	1	0
24	G	101	PEK	1	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 ⓘ

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%)	0.23	8 (1%) 72 80	21, 27, 36, 72	0
1	a	513/514 (99%)	0.38	11 (2%) 64 73	27, 39, 52, 76	0
2	B	226/227 (99%)	0.01	5 (2%) 62 72	23, 34, 55, 89	0
2	b	226/227 (99%)	0.42	11 (4%) 30 41	35, 45, 70, 104	0
3	C	259/261 (99%)	-0.21	1 (0%) 92 95	26, 32, 44, 79	0
3	c	259/261 (99%)	-0.06	4 (1%) 74 82	30, 39, 55, 79	0
4	D	144/147 (97%)	-0.07	2 (1%) 75 83	29, 37, 53, 77	0
4	d	144/147 (97%)	1.36	30 (20%) 1 1	46, 58, 90, 147	0
5	E	105/109 (96%)	-0.00	3 (2%) 52 62	32, 40, 60, 107	0
5	e	105/109 (96%)	0.64	9 (8%) 11 17	39, 51, 70, 105	0
6	F	98/98 (100%)	0.86	9 (9%) 10 16	27, 38, 87, 129	0
6	f	98/98 (100%)	1.15	13 (13%) 4 6	34, 48, 103, 143	0
7	G	83/85 (97%)	1.08	21 (25%) 1 0	30, 40, 106, 141	0
7	g	83/85 (97%)	1.21	22 (26%) 1 0	32, 49, 103, 118	0
8	H	79/85 (92%)	0.75	13 (16%) 2 2	29, 42, 89, 120	0
8	h	79/85 (92%)	1.06	14 (17%) 2 2	40, 52, 97, 116	0
9	I	72/73 (98%)	0.43	8 (11%) 6 9	32, 45, 63, 75	0
9	i	72/73 (98%)	0.98	12 (16%) 2 2	37, 54, 73, 90	0
10	J	58/59 (98%)	0.45	6 (10%) 7 12	30, 42, 64, 110	0
10	j	58/59 (98%)	1.24	14 (24%) 1 0	42, 53, 77, 130	0
11	K	49/56 (87%)	0.49	3 (6%) 22 31	31, 41, 58, 73	0
11	k	49/56 (87%)	1.91	23 (46%) 0 0	53, 60, 79, 91	0
12	L	46/47 (97%)	0.01	2 (4%) 36 47	28, 34, 54, 88	0
12	l	46/47 (97%)	0.55	4 (8%) 11 17	44, 52, 72, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.25	4 (9%) 9 15	31, 35, 62, 88	0
13	m	43/46 (93%)	1.22	7 (16%) 2 3	47, 57, 87, 117	0
All	All	3550/3614 (98%)	0.43	259 (7%) 16 25	21, 40, 73, 147	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	f	97	ALA	17.8
4	d	4	SER	17.5
6	f	96	LEU	17.1
6	F	96	LEU	15.6
4	d	5	VAL	14.8
4	d	7	LYS	13.8
10	j	57	HIS	12.6
13	m	43	SER	11.6
4	d	6	VAL	11.5
6	F	97	ALA	11.5
6	f	98	HIS	10.6
7	G	2	SER	10.4
6	F	98	HIS	10.4
6	F	2	SER	10.0
5	e	109	VAL	9.9
6	F	1	ALA	9.7
8	h	8	ILE	9.7
7	G	3	ALA	8.9
6	F	94	HIS	8.4
6	f	1	ALA	8.0
5	E	5	HIS	7.5
10	J	57	HIS	7.5
7	g	1	ALA	7.3
8	H	45	ALA	7.3
10	J	58	LYS	7.2
4	d	33	LEU	7.2
6	f	94	HIS	7.0
13	m	42	LYS	7.0
7	g	3	ALA	7.0
11	k	7	PRO	6.8
7	G	10	GLY	6.6
12	l	47	LYS	6.6
7	G	36	TRP	6.4
13	M	43	SER	6.4

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Mol	Chain	Res	Type	RSRZ
7	g	41	HIS	6.4
7	g	10	GLY	6.2
8	h	45	ALA	6.2
9	I	37	PHE	6.2
4	d	147	LYS	6.1
9	i	37	PHE	6.0
7	g	36	TRP	5.9
5	e	5	HIS	5.9
6	F	95	GLN	5.8
2	b	227	LEU	5.8
7	G	1	ALA	5.7
7	G	40	GLY	5.7
6	f	95	GLN	5.6
8	H	8	ILE	5.6
2	b	113	TYR	5.5
7	G	9	GLY	5.5
7	G	5	LYS	5.5
8	H	47	GLY	5.3
4	d	8	SER	5.3
8	h	44	THR	5.3
11	k	13	TYR	5.3
7	g	40	GLY	5.2
7	g	5	LYS	5.2
10	j	52	TRP	5.2
8	h	10	ASN	5.2
10	J	1	PHE	5.1
7	g	84	LYS	4.9
10	j	48	TYR	4.9
6	f	2	SER	4.9
2	b	90	ILE	4.9
7	G	41	HIS	4.9
4	D	147	LYS	4.8
10	J	56	PRO	4.7
13	m	41	LYS	4.7
11	k	23	THR	4.6
8	h	7	LYS	4.5
9	i	2	THR	4.5
11	k	6	ALA	4.4
5	E	109	VAL	4.4
7	G	39	SER	4.4
4	d	51	LEU	4.4
4	d	48	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
7	G	43	GLU	4.4
8	H	50	VAL	4.3
7	G	42	ARG	4.3
7	g	8	HIS	4.3
7	G	84	LYS	4.2
7	g	2	SER	4.2
11	K	7	PRO	4.2
7	G	37	LEU	4.1
8	h	48	GLY	4.1
3	c	3	HIS	4.1
4	d	39	ALA	4.0
10	J	52	TRP	4.0
8	h	9	LYS	4.0
7	g	4	ALA	4.0
3	C	3	HIS	3.9
9	i	26	MET	3.9
7	g	42	ARG	3.9
7	G	6	GLY	3.9
10	j	30	ILE	3.9
10	j	1	PHE	3.8
11	K	42	PRO	3.8
9	i	25	PHE	3.8
5	e	96	LEU	3.8
5	e	108	LYS	3.8
11	k	12	LYS	3.8
4	d	46	ALA	3.7
2	B	90	ILE	3.7
4	d	58	GLU	3.7
11	k	19	ALA	3.6
8	H	48	GLY	3.6
13	M	42	LYS	3.5
1	a	381	LEU	3.5
9	I	34	PHE	3.5
9	i	34	PHE	3.4
2	b	218	TYR	3.4
4	d	128	VAL	3.4
8	H	44	THR	3.4
11	k	18	LEU	3.4
7	g	39	SER	3.4
11	K	6	ALA	3.4
8	H	10	ASN	3.3
10	j	56	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	b	224	ALA	3.3
9	I	30	GLY	3.3
8	H	85	ILE	3.3
2	b	170	LEU	3.3
10	J	55	PHE	3.3
6	F	22	LEU	3.3
10	j	27	THR	3.3
13	m	40	TYR	3.3
8	H	42	ALA	3.2
2	b	221	LYS	3.2
11	k	47	ARG	3.2
5	e	92	THR	3.2
11	k	16	ALA	3.2
13	M	39	ASN	3.2
9	I	29	LEU	3.2
3	c	37	PHE	3.2
8	h	42	ALA	3.2
9	I	25	PHE	3.2
11	k	26	VAL	3.2
9	I	33	THR	3.1
9	i	33	THR	3.1
7	G	45	PRO	3.1
13	m	39	ASN	3.1
12	L	2	HIS	3.1
12	L	47	LYS	3.1
1	A	381	LEU	3.0
6	f	27	GLY	3.0
1	A	70	VAL	3.0
1	a	366	VAL	3.0
11	k	9	PHE	3.0
7	G	7	ASP	3.0
7	g	82	TYR	3.0
9	I	26	MET	3.0
4	d	34	SER	3.0
10	j	55	PHE	3.0
4	d	49	SER	3.0
8	H	46	LYS	2.9
13	M	40	TYR	2.9
10	j	26	ALA	2.9
4	d	10	ASP	2.9
13	m	35	TYR	2.9
7	g	43	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	170	LEU	2.9
6	f	22	LEU	2.9
8	h	49	ASP	2.9
4	d	102	TYR	2.9
8	h	52	VAL	2.8
13	m	13	LYS	2.8
9	I	53	ASN	2.8
10	j	24	GLY	2.8
11	k	20	SER	2.8
4	d	40	LEU	2.8
7	g	45	PRO	2.7
11	k	17	VAL	2.7
4	d	142	LYS	2.7
9	i	31	PHE	2.7
4	d	101	HIS	2.7
9	i	30	GLY	2.7
7	g	7	ASP	2.7
7	g	6	GLY	2.7
1	a	73	ILE	2.6
11	k	8	ASP	2.6
8	H	43	MET	2.6
8	h	55	TRP	2.6
4	d	9	GLU	2.6
4	d	35	ALA	2.6
8	h	47	GLY	2.6
11	k	34	THR	2.6
6	f	44	GLU	2.6
7	G	4	ALA	2.6
8	H	7	LYS	2.6
9	i	29	LEU	2.6
10	j	4	ARG	2.6
4	d	53	ILE	2.6
1	A	73	ILE	2.5
5	e	7	THR	2.5
12	l	38	PHE	2.5
3	c	38	ASN	2.5
11	k	46	GLY	2.5
7	g	38	HIS	2.5
2	b	217	LYS	2.5
6	f	93	PRO	2.4
1	A	513	LEU	2.4
4	d	43	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
7	G	8	HIS	2.4
9	i	57	MET	2.4
1	a	70	VAL	2.4
4	D	78	TRP	2.4
7	g	37	LEU	2.4
11	k	31	TYR	2.4
1	A	66	ILE	2.4
2	b	165	VAL	2.4
5	e	94	ASN	2.4
6	f	43	LYS	2.4
4	d	141	ASP	2.4
10	j	58	LYS	2.4
1	a	433	LEU	2.3
1	a	203	ALA	2.3
2	b	65	TRP	2.3
10	j	2	GLU	2.3
12	l	20	ARG	2.3
4	d	38	LYS	2.3
9	i	53	ASN	2.3
8	h	84	LYS	2.3
12	l	45	LEU	2.3
2	b	59	GLN	2.3
2	B	113	TYR	2.3
7	G	35	SER	2.3
2	B	168	LEU	2.2
1	A	382	SER	2.2
7	G	38	HIS	2.2
5	E	9	GLU	2.2
10	j	50	LEU	2.2
11	k	22	ALA	2.2
11	k	35	GLN	2.2
1	A	380	VAL	2.2
1	a	462	LEU	2.2
5	e	10	GLU	2.2
2	B	91	ASN	2.1
9	i	32	ALA	2.1
11	k	24	PHE	2.1
1	a	380	VAL	2.1
8	h	43	MET	2.1
1	a	66	ILE	2.1
4	d	42	GLU	2.1
11	k	52	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	31	LYS	2.1
7	g	49	PRO	2.1
1	a	136	LEU	2.1
4	d	54	ASP	2.1
6	F	3	GLY	2.1
8	H	49	ASP	2.1
1	a	206	ILE	2.1
7	g	9	GLY	2.1
3	c	33	MET	2.0
11	k	11	ASP	2.0
5	e	23	ASP	2.0
4	d	47	SER	2.0
1	A	374	VAL	2.0
6	f	25	ARG	2.0
11	k	14	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FME	b	1	10/11	0.96	0.16	-	45,47,58,59	0
7	TPO	G	11	11/12	0.57	0.31	-	64,95,111,114	0
7	TPO	g	11	11/12	0.30	0.46	-	88,116,130,131	0
1	FME	A	1	10/11	0.90	0.23	-	39,49,82,85	0
1	FME	a	1	10/11	0.92	0.21	-	55,69,82,85	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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
19	TGL	l	101	63/63	0.45	0.36	9.08	63,80,110,114	0
25	CDL	C	305	100/100	0.60	0.33	8.10	53,87,111,114	0
20	CMO	a	608	2/2	0.89	0.24	7.93	65,65,65,69	0
19	TGL	A	608	63/63	0.67	0.30	7.24	55,79,96,100	0
26	DMU	C	308	33/33	0.30	0.41	6.92	70,94,111,112	0
27	PSC	b	303	52/52	0.51	0.38	5.44	53,96,136,144	0
19	TGL	b	302	63/63	0.57	0.33	5.28	68,86,96,97	0
19	TGL	D	201	63/63	0.61	0.30	5.20	61,78,87,94	0
18	PGV	a	606	51/51	0.43	0.43	5.14	62,89,129,134	0
24	PEK	G	101	53/53	0.55	0.33	5.02	61,84,119,130	0
19	TGL	A	609	63/63	0.59	0.30	4.92	50,68,89,94	0
25	CDL	c	307	100/100	0.56	0.34	4.90	62,96,126,135	0
18	PGV	A	606	51/51	0.65	0.34	4.74	48,77,123,129	0
26	DMU	c	309	33/33	0.27	0.37	4.59	100,119,130,133	0
19	TGL	d	201	63/63	0.57	0.27	4.05	67,81,103,111	0
23	CHD	J	101	29/29	0.75	0.32	3.78	64,70,84,86	0
23	CHD	j	101	29/29	0.79	0.33	3.53	86,90,99,103	0
24	PEK	C	302	53/53	0.95	0.22	3.25	31,53,83,89	0
18	PGV	a	607	51/51	0.96	0.20	3.18	32,48,74,83	0
24	PEK	c	304	53/53	0.94	0.22	2.97	41,63,99,101	0
16	MG	a	604	1/1	0.70	0.21	2.89	47,47,47,47	0
24	PEK	c	305	53/53	0.51	0.34	2.89	63,90,111,120	0
18	PGV	c	306	51/51	0.94	0.19	2.85	32,46,82,85	0
25	CDL	G	102	100/100	0.60	0.34	2.70	62,96,130,139	0
25	CDL	g	101	100/100	0.61	0.30	2.58	66,102,140,149	0
27	PSC	E	201	52/52	0.67	0.34	2.47	53,101,160,171	0
29	SAC	I	101	9/10	0.85	0.23	2.41	64,68,76,79	0
24	PEK	C	307	53/53	0.44	0.41	2.30	59,86,146,157	0
18	PGV	C	303	51/51	0.96	0.17	2.21	27,39,70,76	0
26	DMU	m	101	33/33	0.76	0.25	2.18	70,81,91,94	0
18	PGV	A	607	51/51	0.96	0.18	1.87	25,42,65,69	0
26	DMU	M	101	33/33	0.84	0.19	1.55	39,48,58,63	0
23	CHD	c	308	29/29	0.90	0.20	1.42	59,62,68,69	0
21	FME	B	301	10/11	0.94	0.16	1.27	30,33,43,46	0
18	PGV	c	302	51/51	0.55	0.31	1.07	63,84,114,117	0
18	PGV	C	304	51/51	0.65	0.24	0.98	64,90,105,109	0
24	PEK	c	301	53/53	0.61	0.31	0.97	58,93,150,158	0
14	HEA	a	601	60/60	0.96	0.18	0.88	32,37,55,62	0
23	CHD	C	306	29/29	0.91	0.19	0.83	50,54,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	HEA	a	602	60/60	0.96	0.16	0.80	29,32,40,43	0
20	CMO	A	610	2/2	0.97	0.15	0.63	46,46,46,46	0
23	CHD	B	303	29/29	0.95	0.12	0.41	31,32,36,41	0
14	HEA	A	602	60/60	0.97	0.14	0.16	22,24,33,35	0
14	HEA	A	601	60/60	0.98	0.15	-0.12	21,23,45,50	0
17	NA	A	605	1/1	0.93	0.10	-0.18	28,28,28,28	0
23	CHD	G	103	29/29	0.95	0.09	-0.39	32,35,38,41	0
23	CHD	c	303	29/29	0.96	0.08	-0.84	34,36,40,41	0
23	CHD	C	301	29/29	0.96	0.06	-1.06	31,34,36,38	0
22	CUA	b	301	2/2	0.94	0.07	-1.24	36,36,36,38	0
22	CUA	B	302	2/2	0.98	0.06	-1.73	24,24,24,24	0
28	ZN	f	101	1/1	0.99	0.06	-1.81	41,41,41,41	0
28	ZN	F	101	1/1	0.99	0.04	-2.11	33,33,33,33	0
16	MG	A	604	1/1	0.97	0.09	-2.18	27,27,27,27	0
17	NA	a	605	1/1	0.90	0.06	-3.17	48,48,48,48	0
15	CU	a	603	1/1	0.99	0.10	-	34,34,34,34	0
29	SAC	i	101	9/10	0.60	0.48	-	100,104,108,108	0
15	CU	A	603	1/1	1.00	0.07	-	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.