



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:50 AM GMT

PDB ID : 2DYR
Title : Bovine heart cytochrome C oxidase at the fully oxidized state
Authors : Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2006-09-16
Resolution : 1.80 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

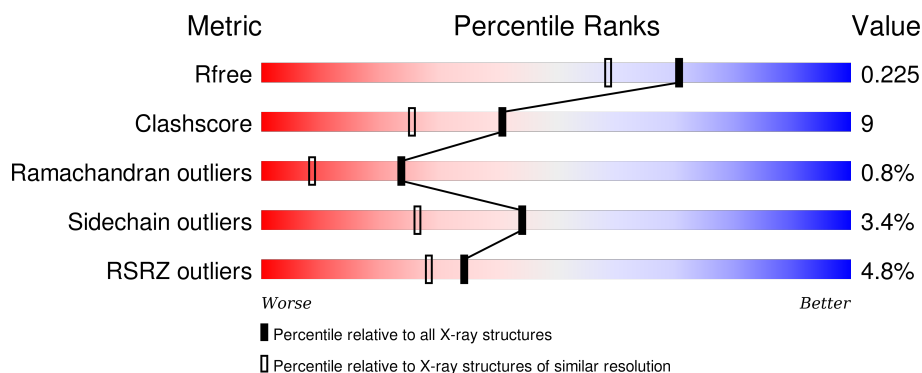
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



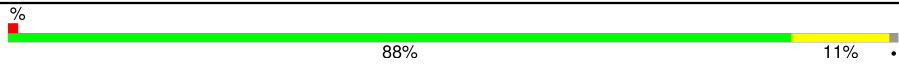
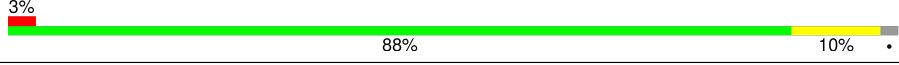
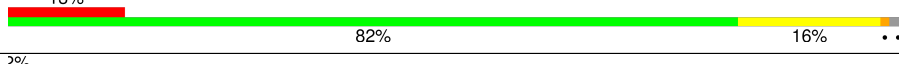


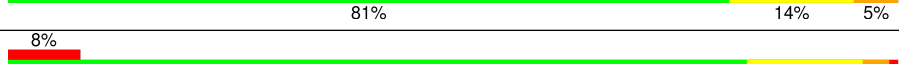
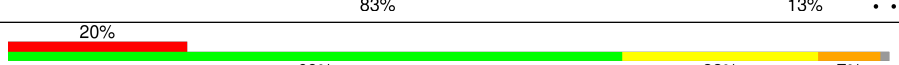
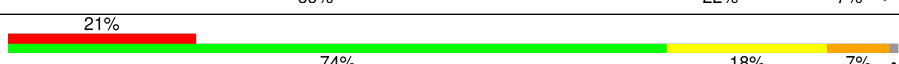
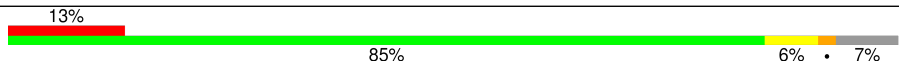
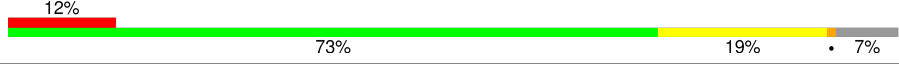

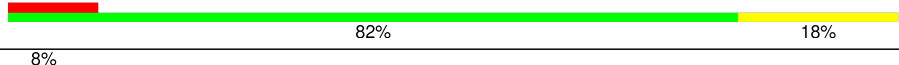
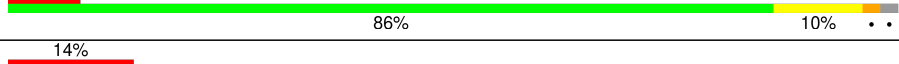
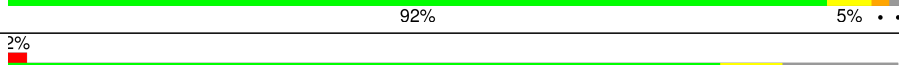
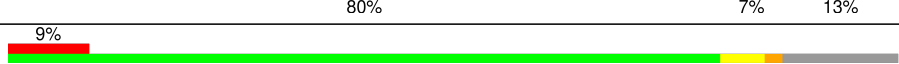





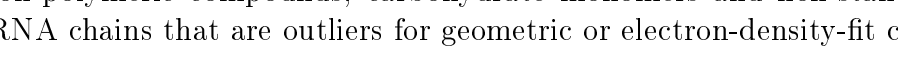
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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>87%</div> <div>13%</div> </div>
1	N	514	<div> <div>84%</div> <div>16%</div> </div>
2	B	227	<div> <div>2%</div> <div>81%</div> <div>17%</div> </div>
2	O	227	<div> <div>4%</div> <div>75%</div> <div>23%</div> </div>
3	C	261	<div> <div>90%</div> <div>10%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
18	PGV	A	524	-	-	-	X
18	PGV	C	268	-	-	-	X
18	PGV	P	1268	-	-	-	X
18	PGV	Z	1524	-	-	-	X
20	TGL	B	521	-	-	-	X
20	TGL	D	523	-	-	-	X
20	TGL	L	522	-	-	X	X
20	TGL	N	1521	-	-	-	X
20	TGL	N	1522	-	-	-	X
20	TGL	Q	1523	-	-	-	X
21	PSC	B	230	-	-	-	X
21	PSC	O	1230	-	-	-	X
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	X
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	X
23	DMU	C	272	X	-	-	X
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	X
23	DMU	Z	1526	X	-	-	X
26	CDL	C	270	-	-	-	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	-	X
26	CDL	T	1269	-	-	X	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32735 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

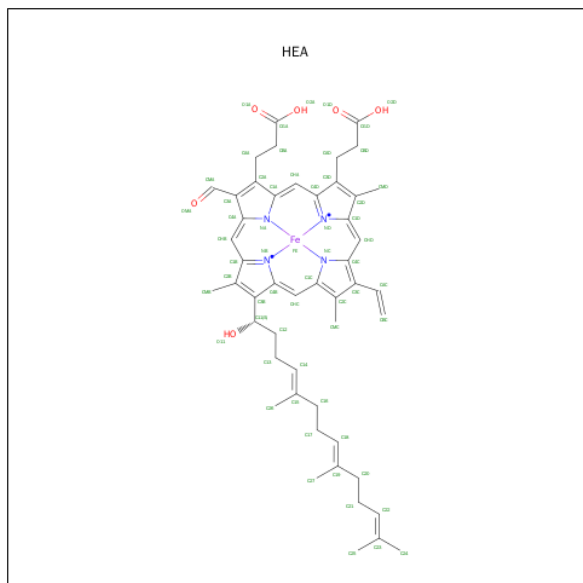
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

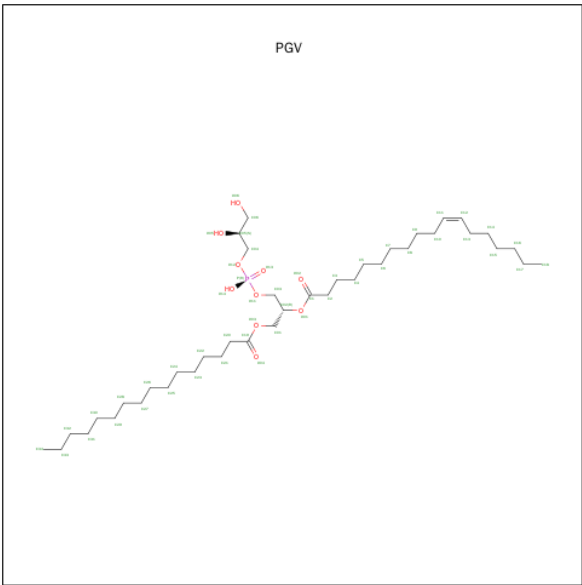
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



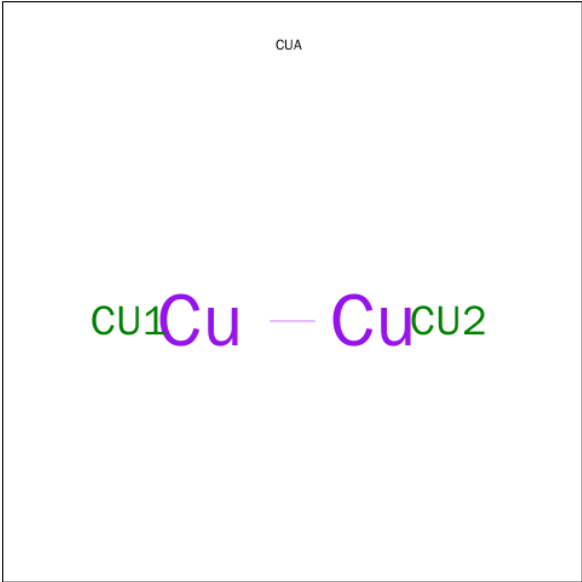
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- 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).



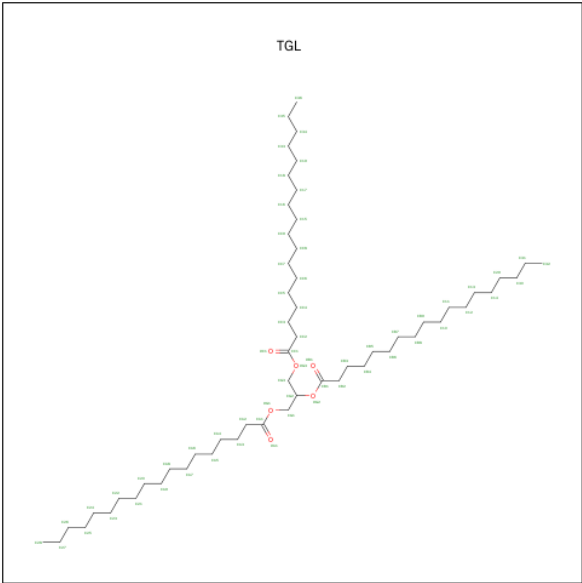
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



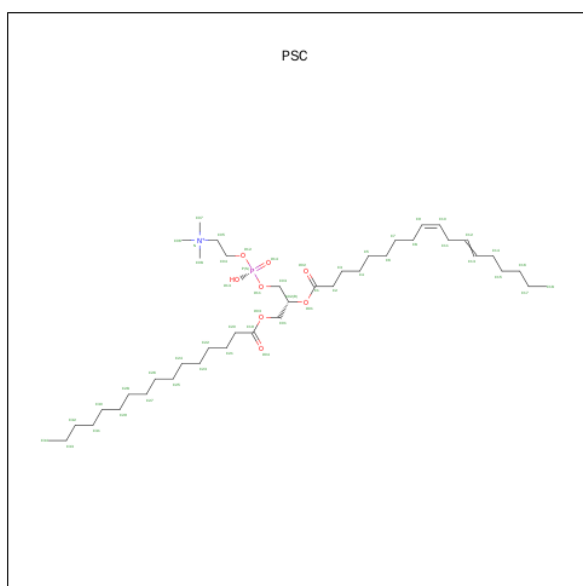
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		

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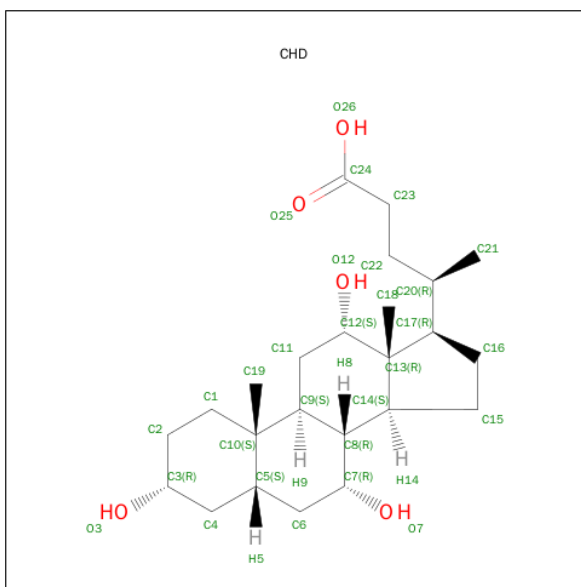
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		

- 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: $C_{42}H_{81}NO_8P$).



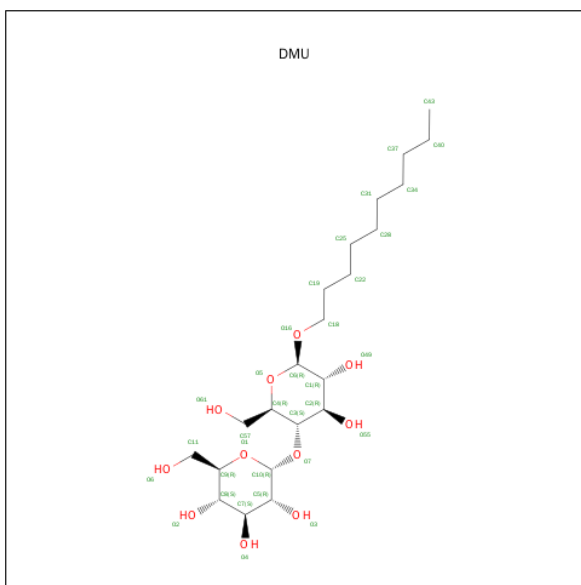
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

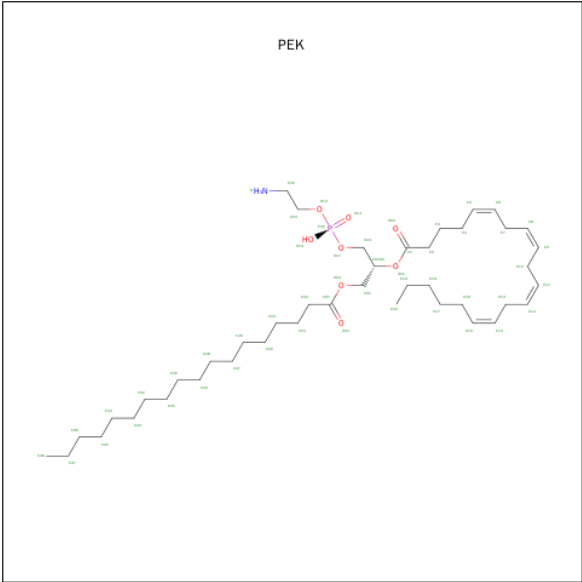


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 33 22 11	0	0
23	M	1	Total C O 33 22 11	0	0
23	P	1	Total C O 33 22 11	0	0
23	Z	1	Total C O 33 22 11	0	0

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

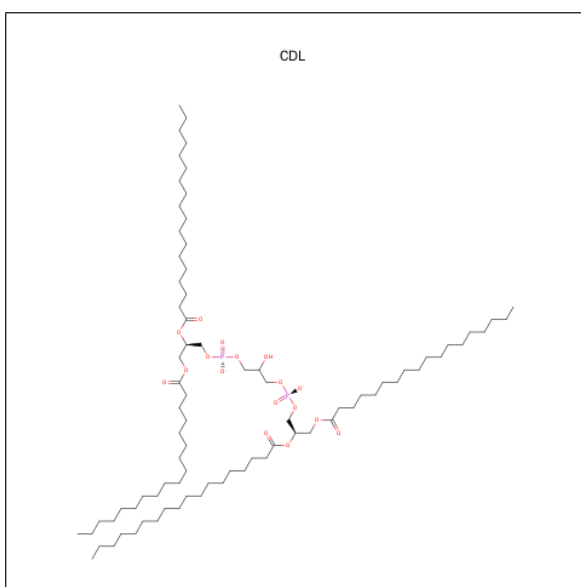
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- 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: C₄₃H₇₈NO₈P).



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: C₈₁H₁₅₆O₁₇P₂).



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

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

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	243	Total	O	0	0
			243	243		
28	B	186	Total	O	0	0
			186	186		
28	C	127	Total	O	0	0
			127	127		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	109	Total 109	O 109	0	0
28	E	67	Total 67	O 67	0	0
28	F	85	Total 85	O 85	0	0
28	G	57	Total 57	O 57	0	0
28	H	66	Total 66	O 66	0	0
28	I	58	Total 58	O 58	0	0
28	J	21	Total 21	O 21	0	0
28	K	38	Total 38	O 38	0	0
28	L	22	Total 22	O 22	0	0
28	M	27	Total 27	O 27	0	0
28	N	212	Total 212	O 212	0	0
28	O	152	Total 152	O 152	0	0
28	P	120	Total 120	O 120	0	0
28	Q	75	Total 75	O 75	0	0
28	R	32	Total 32	O 32	0	0
28	S	53	Total 53	O 53	0	0
28	T	59	Total 59	O 59	0	0
28	U	62	Total 62	O 62	0	0
28	V	33	Total 33	O 33	0	0
28	W	18	Total 18	O 18	0	0
28	X	29	Total 29	O 29	0	0

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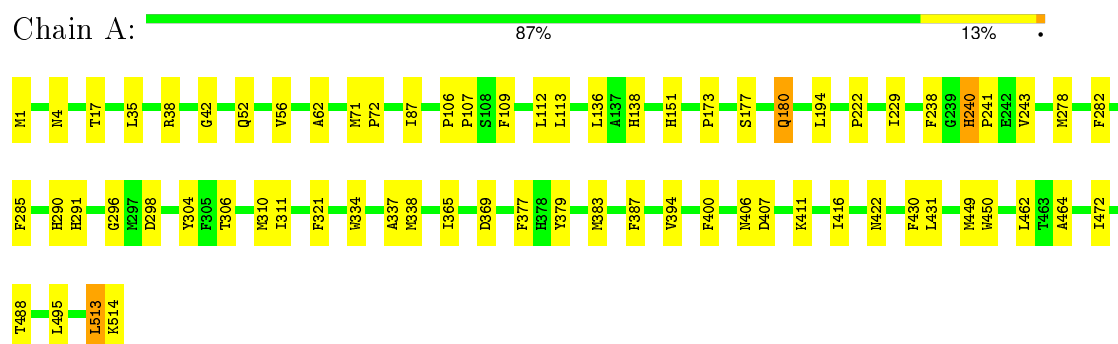
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	Y	31	Total	O	0	0
			31	31		
28	Z	21	Total	O	0	0
			21	21		

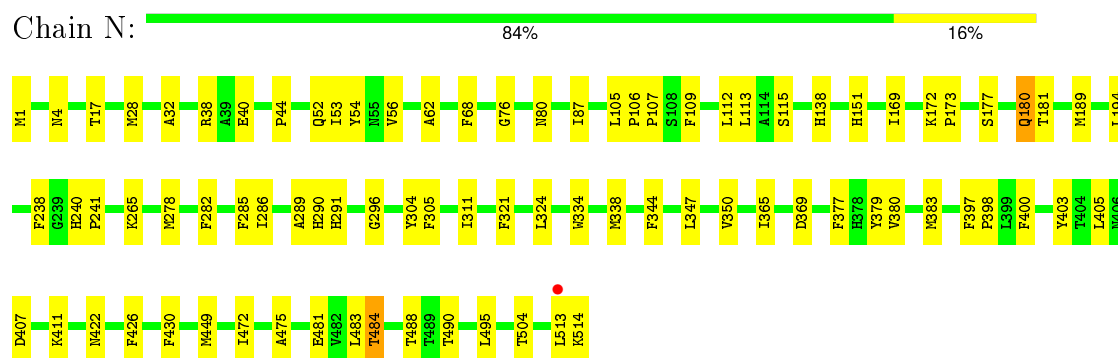
3 Residue-property plots

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

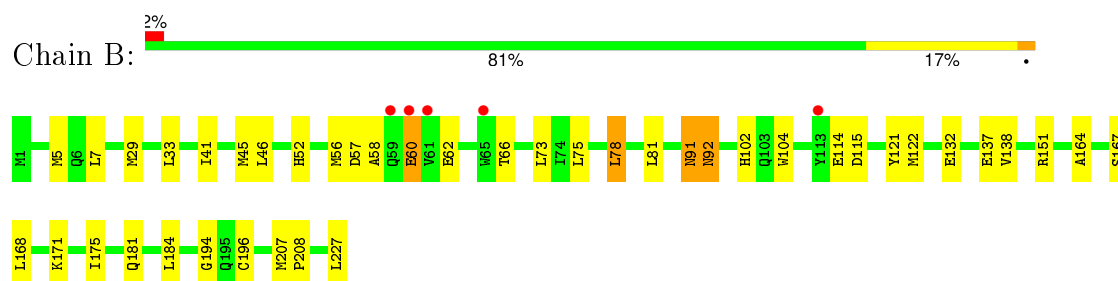
• Molecule 1: Cytochrome c oxidase subunit 1



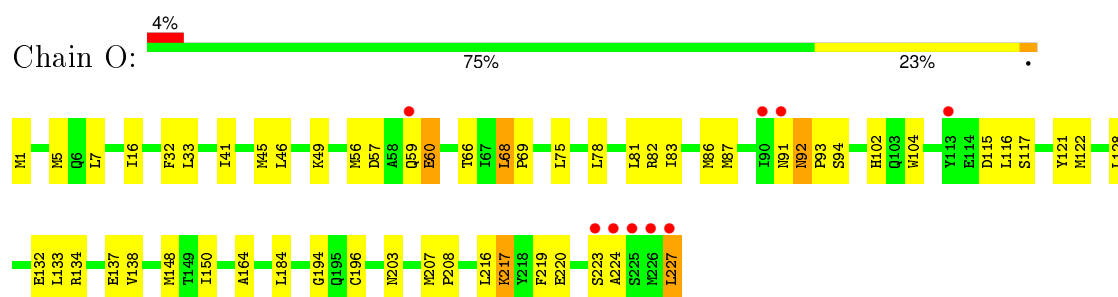
• Molecule 1: Cytochrome c oxidase subunit 1



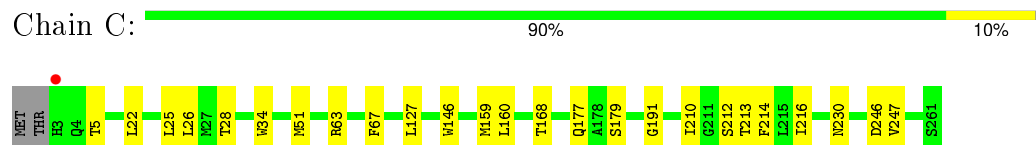
• Molecule 2: Cytochrome c oxidase subunit 2



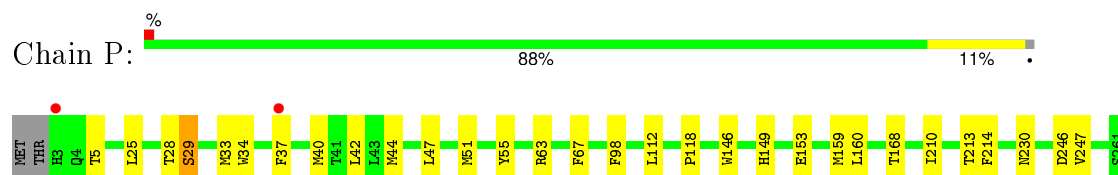
• Molecule 2: Cytochrome c oxidase subunit 2



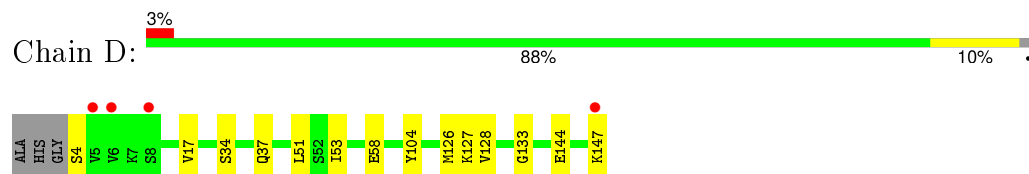
- Molecule 3: Cytochrome c oxidase subunit 3



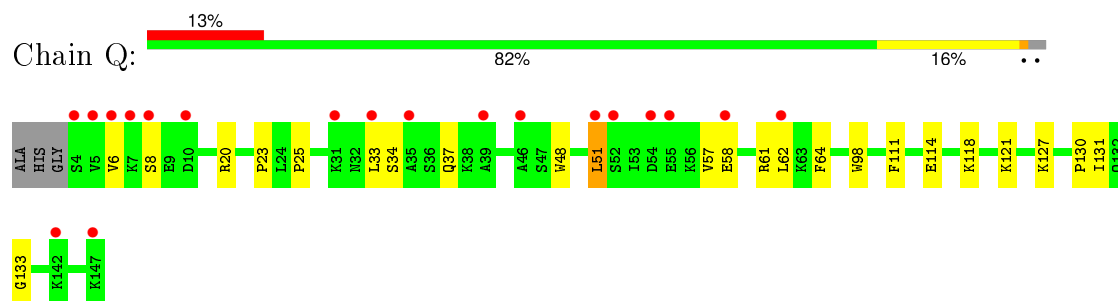
- Molecule 3: Cytochrome c oxidase subunit 3



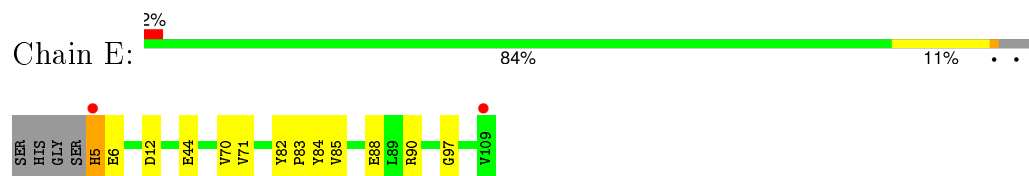
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



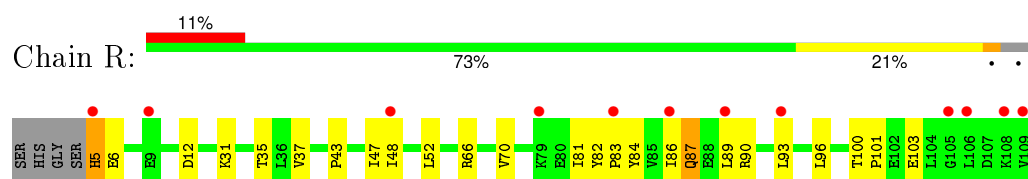
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



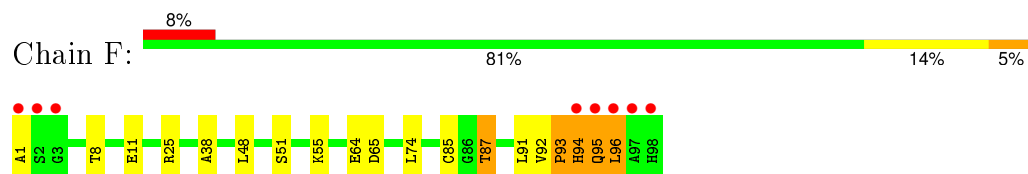
- Molecule 5: Cytochrome c oxidase polypeptide Va



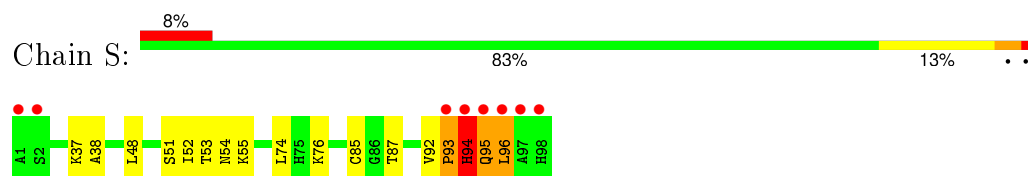
- Molecule 5: Cytochrome c oxidase polypeptide Va



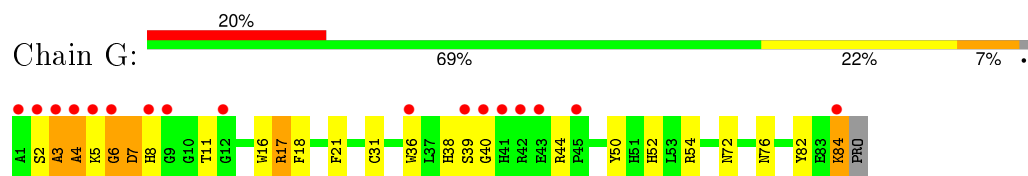
- Molecule 6: Cytochrome c oxidase polypeptide Vb



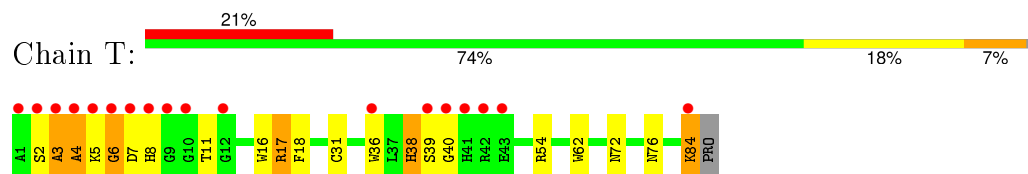
- Molecule 6: Cytochrome c oxidase polypeptide Vb



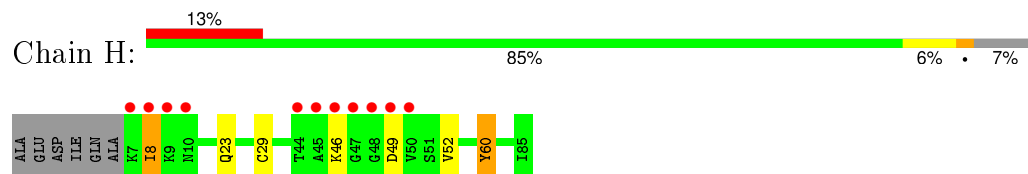
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



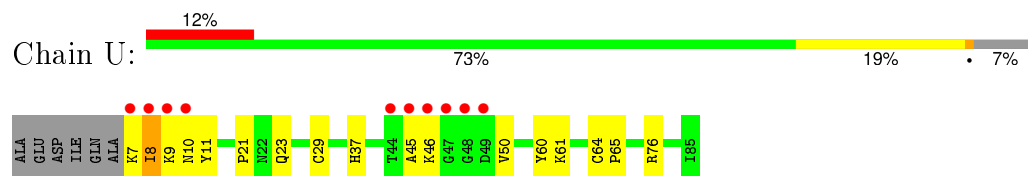
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



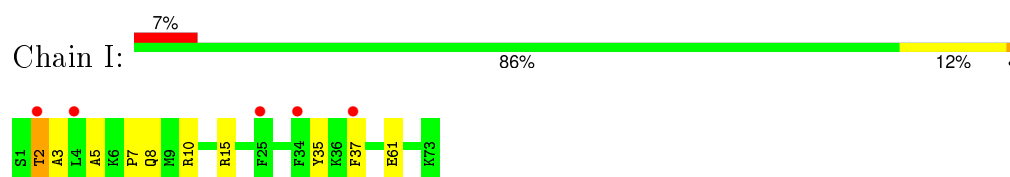
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



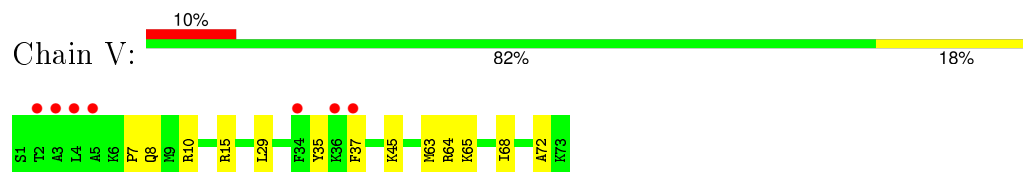
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



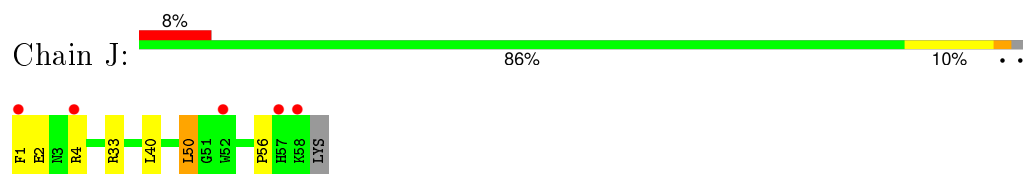
- Molecule 9: Cytochrome c oxidase polypeptide VIc



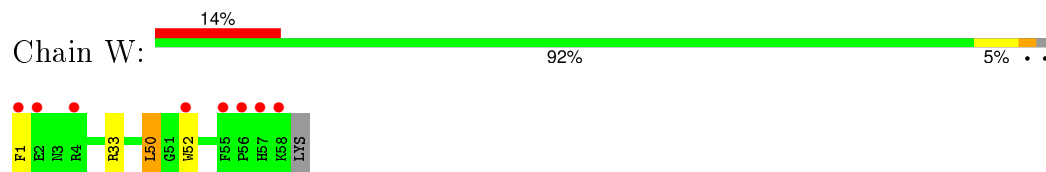
- Molecule 9: Cytochrome c oxidase polypeptide VIc



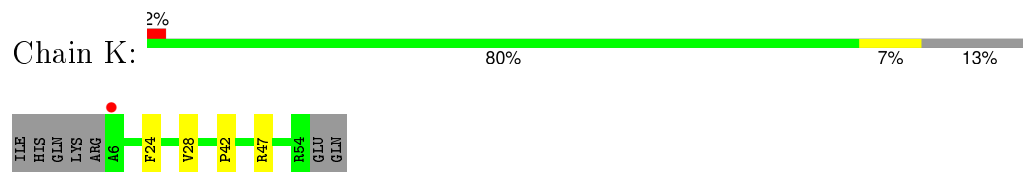
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



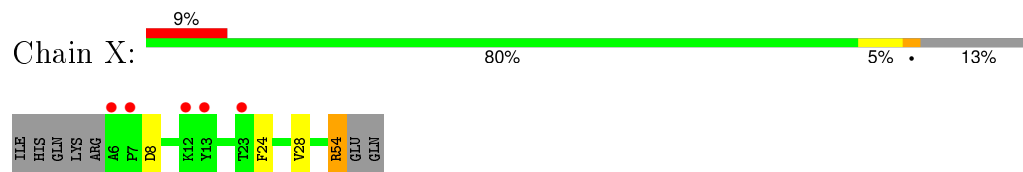
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



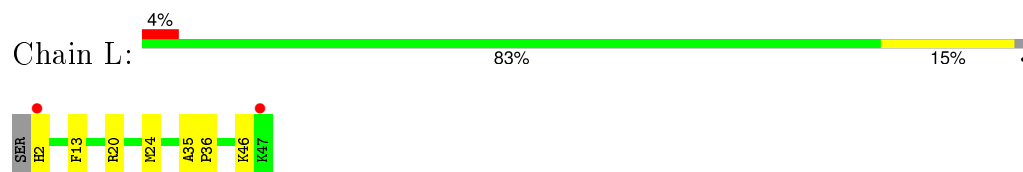
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



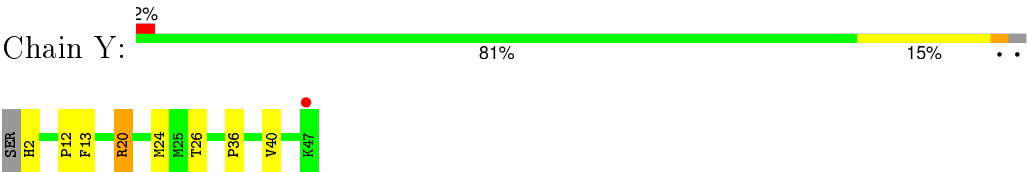
- Molecule 11: Cytochrome c oxidase polypeptide VIIb



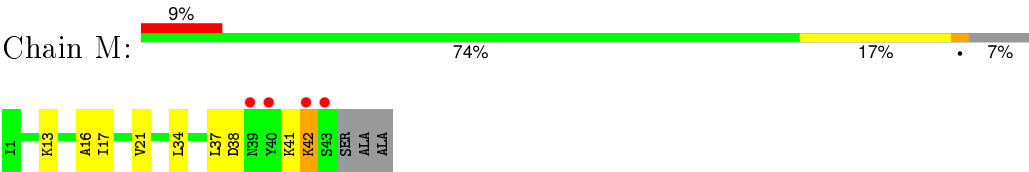
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



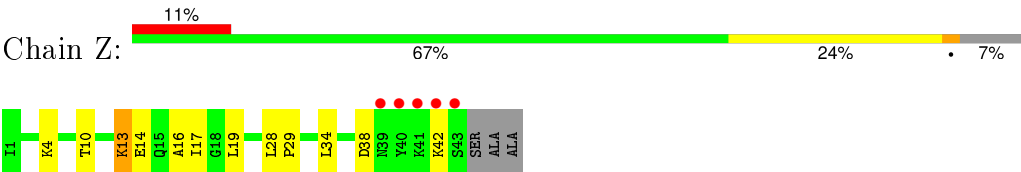
- Molecule 12: Cytochrome c oxidase polypeptide VIIc



● Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



● Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 68.19 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 98.9 (68.19-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 1.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.202 , 0.227 0.202 , 0.225	Depositor DCC
R_{free} test set	22930 reflections (3.92%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.0	EDS
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 608996 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32735	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/4156	0.67	0/5678
1	N	0.48	0/4156	0.65	0/5678
2	B	0.48	0/1860	0.76	0/2534
2	O	0.50	0/1860	0.79	1/2534 (0.0%)
3	C	0.51	0/2197	0.58	0/3005
3	P	0.48	0/2197	0.61	0/3005
4	D	0.47	0/1229	0.66	1/1658 (0.1%)
4	Q	0.50	0/1229	0.65	1/1658 (0.1%)
5	E	0.50	0/871	0.66	0/1182
5	R	0.48	0/871	0.68	0/1182
6	F	0.47	0/765	0.83	3/1038 (0.3%)
6	S	0.47	0/765	0.87	3/1038 (0.3%)
7	G	0.51	0/690	0.70	1/937 (0.1%)
7	T	0.53	0/690	0.70	1/937 (0.1%)
8	H	0.47	0/682	0.68	0/921
8	U	0.48	0/682	0.67	0/921
9	I	0.52	0/605	0.59	0/802
9	V	0.51	0/605	0.62	0/802
10	J	0.45	0/471	0.60	0/636
10	W	0.46	0/471	0.63	0/636
11	K	0.48	0/398	0.66	0/546
11	X	0.47	0/398	0.65	0/546
12	L	0.48	0/393	0.55	0/526
12	Y	0.53	0/393	0.57	0/526
13	M	0.46	0/345	0.62	0/470
13	Z	0.45	0/345	0.62	0/470
All	All	0.49	0/29324	0.67	11/39866 (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	1
8	U	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	7.74	131.91	111.00
6	F	94	HIS	N-CA-C	7.14	130.29	111.00
4	D	133	GLY	N-CA-C	5.67	127.28	113.10
2	O	227	LEU	CA-CB-CG	5.64	128.28	115.30
4	Q	133	GLY	N-CA-C	5.61	127.12	113.10
6	F	93	PRO	N-CA-C	5.47	126.31	112.10
6	S	54	ASN	CB-CA-C	-5.35	99.69	110.40
7	G	6	GLY	N-CA-C	5.29	126.33	113.10
7	T	6	GLY	N-CA-C	5.26	126.25	113.10
6	F	95	GLN	N-CA-C	5.07	124.70	111.00
6	S	93	PRO	N-CA-C	5.01	125.12	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4027	0	4001	74	0
2	B	1824	0	1833	28	0
2	O	1824	0	1833	39	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	29	0
4	D	1195	0	1183	10	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0
5	R	852	0	845	15	0
6	F	748	0	728	12	0
6	S	748	0	728	15	0
7	G	675	0	644	26	0
7	T	675	0	644	28	0
8	H	662	0	623	4	0
8	U	662	0	623	9	0
9	I	601	0	613	6	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	4	0
11	K	384	0	366	3	0
11	X	384	0	366	6	0
12	L	380	0	380	14	0
12	Y	380	0	380	9	0
13	M	335	0	352	6	0
13	Z	335	0	352	6	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	3	0
17	N	120	0	108	4	0
18	A	102	0	152	7	0
18	C	102	0	152	7	0
18	N	51	0	76	2	0
18	P	102	0	152	8	0
18	Z	51	0	76	4	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	10	0
20	D	63	0	110	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	L	63	0	110	23	0
20	N	126	0	220	30	0
20	Q	63	0	110	6	0
21	B	52	0	80	13	0
21	O	52	0	80	12	0
22	B	29	0	39	0	0
22	C	58	0	78	2	0
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	2	0
22	W	29	0	39	2	0
23	C	33	0	36	2	0
23	M	33	0	36	0	0
23	P	33	0	36	7	0
23	Z	33	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	7	0
25	P	106	0	154	12	0
25	T	53	0	77	8	0
26	C	100	0	156	16	0
26	G	100	0	156	21	0
26	P	100	0	156	13	0
26	T	100	0	156	21	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	243	0	0	4	0
28	B	186	0	0	4	0
28	C	127	0	0	2	0
28	D	109	0	0	4	0
28	E	67	0	0	0	0
28	F	85	0	0	1	0
28	G	57	0	0	2	0
28	H	66	0	0	1	0
28	I	58	0	0	3	0
28	J	21	0	0	1	0
28	K	38	0	0	0	0
28	L	22	0	0	2	0
28	M	27	0	0	2	0
28	N	212	0	0	3	0
28	O	152	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	P	120	0	0	3	0
28	Q	75	0	0	3	0
28	R	32	0	0	0	0
28	S	53	0	0	1	0
28	T	59	0	0	2	0
28	U	62	0	0	3	0
28	V	33	0	0	2	0
28	W	18	0	0	0	0
28	X	29	0	0	1	0
28	Y	31	0	0	2	0
28	Z	21	0	0	2	0
All	All	32735	0	31294	534	0

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

All (534) 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	1.17	1.05
7:T:84:LYS:H	7:T:84:LYS:HD2	1.19	1.02
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.24	1.01
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
21:B:230:PSC:H343	21:B:230:PSC:H142	1.42	1.01
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.21	0.98
7:T:72:ASN:H	7:T:76:ASN:HD22	1.16	0.94
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.93
26:P:1270:CDL:H191	26:P:1270:CDL:H642	1.51	0.92
26:C:270:CDL:H191	26:C:270:CDL:H642	1.51	0.91
7:G:72:ASN:H	7:G:76:ASN:HD22	1.19	0.90
10:W:33:ARG:HG2	22:W:1060:CHD:H152	1.53	0.90
26:G:269:CDL:H541	26:G:269:CDL:H231	1.53	0.90
2:O:224:ALA:O	2:O:227:LEU:HG	1.72	0.89
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.53	0.89
20:B:521:TGL:H281	20:B:521:TGL:H102	1.55	0.88
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.55	0.88
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.56	0.88
20:N:1521:TGL:H281	20:N:1521:TGL:H102	1.54	0.88
6:F:85:CYS:SG	6:F:87:THR:HG23	2.14	0.87
25:C:264:PEK:H102	25:C:264:PEK:H161	1.57	0.86
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.16	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:472:ILE:HG21	20:N:1522:TGL:HA92	1.58	0.85
7:G:5:LYS:HB3	1:N:278:MET:SD	2.16	0.85
1:A:472:ILE:HG21	20:L:522:TGL:HA92	1.59	0.84
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.59	0.84
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.58	0.83
2:O:41:ILE:HD13	21:O:1230:PSC:H342	1.60	0.83
6:S:53:THR:HA	6:S:94:HIS:CE1	2.14	0.83
12:L:20:ARG:HH22	20:L:522:TGL:HC61	1.45	0.82
28:C:4863:HOH:O	6:F:1:ALA:HB2	1.79	0.81
7:G:31:CYS:SG	26:G:269:CDL:H532	2.21	0.80
12:L:24:MET:SD	20:L:522:TGL:H162	2.21	0.80
20:L:522:TGL:HC62	20:L:522:TGL:HC22	1.64	0.80
21:O:1230:PSC:H071	9:V:10:ARG:HE	1.47	0.80
1:A:278:MET:SD	7:T:5:LYS:HB3	2.22	0.79
20:N:1521:TGL:C28	20:N:1521:TGL:H102	2.12	0.79
7:T:84:LYS:CD	7:T:84:LYS:H	1.95	0.79
26:G:269:CDL:H622	18:P:1268:PGV:H152	1.64	0.78
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.66	0.77
20:B:521:TGL:C28	20:B:521:TGL:H102	2.15	0.77
4:D:34:SER:H	4:D:37:GLN:NE2	1.84	0.76
20:N:1522:TGL:HC62	20:N:1522:TGL:HC22	1.66	0.76
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.68	0.76
1:N:321:PHE:CD2	21:O:1230:PSC:H341	2.20	0.75
20:B:521:TGL:H241	20:B:521:TGL:H201	1.69	0.74
3:P:246:ASP:HB2	28:P:4502:HOH:O	1.87	0.74
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.37	0.73
20:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.69	0.73
12:L:13:PHE:HA	20:L:522:TGL:HC31	1.70	0.73
20:N:1521:TGL:H201	20:N:1521:TGL:H241	1.68	0.73
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.70	0.73
26:G:269:CDL:H522	26:G:269:CDL:H202	1.70	0.72
3:P:34:TRP:CZ2	23:P:1272:DMU:H29	2.25	0.72
20:N:1522:TGL:H202	20:N:1522:TGL:H242	1.72	0.71
12:L:20:ARG:HH12	20:L:522:TGL:HC61	1.55	0.71
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.70
20:L:522:TGL:H242	20:L:522:TGL:H202	1.72	0.70
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.73	0.70
1:N:334:TRP:CZ3	20:Q:1523:TGL:HA51	2.27	0.70
2:B:41:ILE:HD13	21:B:230:PSC:H342	1.74	0.70
18:C:268:PGV:H152	26:T:1269:CDL:H622	1.74	0.69
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:PHE:CD2	21:B:230:PSC:H341	2.27	0.69
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.39	0.69
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.75	0.69
18:Z:1524:PGV:H321	18:Z:1524:PGV:H152	1.74	0.69
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.75	0.68
1:N:449:MET:SD	2:O:5:MET:HG2	2.33	0.68
21:B:230:PSC:C07	9:I:10:ARG:HH21	2.06	0.67
10:J:33:ARG:HG2	22:J:60:CHD:H152	1.77	0.67
4:Q:114:GLU:HG2	28:Q:4443:HOH:O	1.95	0.67
1:N:1:FME:HCN	1:N:4:ASN:H	1.60	0.67
7:G:72:ASN:H	7:G:76:ASN:ND2	1.93	0.67
18:A:524:PGV:H152	18:A:524:PGV:H321	1.77	0.67
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.76	0.66
18:P:1267:PGV:H12	18:P:1267:PGV:H161	1.76	0.66
6:S:52:ILE:O	6:S:94:HIS:NE2	2.29	0.66
6:S:85:CYS:SG	6:S:87:THR:HG23	2.35	0.66
5:R:89:LEU:O	5:R:93:LEU:HG	1.95	0.66
21:O:1230:PSC:C07	9:V:10:ARG:HE	2.08	0.66
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.26	0.66
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.78	0.66
12:L:20:ARG:NH2	20:L:522:TGL:HC61	2.11	0.65
4:Q:58:GLU:O	4:Q:62:LEU:HG	1.96	0.65
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.77	0.65
13:Z:19:LEU:HD23	18:Z:1524:PGV:H322	1.78	0.65
1:A:334:TRP:CZ3	20:D:523:TGL:HA51	2.31	0.65
26:C:270:CDL:C19	26:C:270:CDL:H642	2.25	0.65
1:A:472:ILE:HG21	20:L:522:TGL:CA9	2.26	0.64
18:C:267:PGV:H12	18:C:267:PGV:H161	1.77	0.64
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.62	0.64
26:P:1270:CDL:H112	28:P:5001:HOH:O	1.97	0.64
26:G:269:CDL:C23	26:G:269:CDL:H541	2.26	0.64
7:G:84:LYS:N	7:G:84:LYS:HD2	2.01	0.64
7:G:84:LYS:H	7:G:84:LYS:CD	2.00	0.64
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.80	0.64
3:C:34:TRP:CZ2	23:C:272:DMU:H29	2.33	0.64
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.62	0.63
18:C:267:PGV:H182	26:C:270:CDL:H673	1.79	0.63
1:N:472:ILE:HG21	20:N:1522:TGL:CA9	2.26	0.63
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.81	0.62
1:N:472:ILE:HD13	20:N:1522:TGL:HA91	1.80	0.62
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:1268:PGV:H062	28:U:4465:HOH:O	1.99	0.62
26:G:269:CDL:H172	26:G:269:CDL:H511	1.80	0.62
6:S:52:ILE:O	6:S:94:HIS:CE1	2.52	0.62
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.82	0.62
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.35	0.61
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.65	0.61
2:B:92:ASN:HB3	28:B:5097:HOH:O	1.99	0.61
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.81	0.61
21:B:230:PSC:H072	9:I:10:ARG:HH21	1.65	0.61
3:P:210:ILE:HG23	18:P:1267:PGV:H102	1.82	0.61
20:B:521:TGL:HC22	28:I:2381:HOH:O	2.00	0.61
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.28	0.60
26:G:269:CDL:C54	26:G:269:CDL:H231	2.30	0.60
1:A:17:THR:OG1	20:L:522:TGL:H281	2.01	0.60
18:C:267:PGV:H172	26:C:270:CDL:H662	1.82	0.60
20:N:1521:TGL:H161	2:O:7:LEU:HD11	1.84	0.60
20:N:1521:TGL:HC92	28:O:4466:HOH:O	2.02	0.60
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.83	0.60
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.67	0.60
9:V:65:LYS:O	11:X:54:ARG:NH1	2.34	0.60
1:A:282:PHE:HA	7:T:4:ALA:CB	2.32	0.59
1:N:113:LEU:CD1	20:N:1522:TGL:H292	2.32	0.59
7:T:17:ARG:HD2	28:T:3307:HOH:O	2.02	0.59
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.02	0.59
3:P:34:TRP:HZ2	23:P:1272:DMU:H29	1.67	0.59
12:L:20:ARG:NH1	20:L:522:TGL:HC61	2.18	0.59
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.02	0.59
6:F:92:VAL:O	6:F:92:VAL:HG23	2.03	0.58
21:B:230:PSC:H21	21:B:230:PSC:H222	1.85	0.58
6:F:25:ARG:HD2	28:F:4173:HOH:O	2.03	0.58
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.32	0.58
1:A:430:PHE:HE1	20:B:521:TGL:HB21	1.69	0.58
20:N:1522:TGL:H162	12:Y:24:MET:SD	2.43	0.58
20:B:521:TGL:HA82	20:B:521:TGL:H222	1.86	0.58
3:C:210:ILE:HG23	18:C:267:PGV:H102	1.86	0.58
12:L:20:ARG:HH22	20:L:522:TGL:CC6	2.16	0.58
8:U:50:VAL:HG21	28:U:5105:HOH:O	2.04	0.58
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.68	0.57
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.87	0.57
6:S:53:THR:HA	6:S:94:HIS:HE1	1.65	0.57
18:A:525:PGV:H182	3:C:28:THR:HG22	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:1230:PSC:H222	21:O:1230:PSC:H21	1.85	0.57
2:O:41:ILE:CD1	21:O:1230:PSC:H342	2.34	0.57
25:C:265:PEK:C38	26:G:269:CDL:H273	2.35	0.57
7:G:17:ARG:HD2	28:G:2307:HOH:O	2.04	0.57
1:N:112:LEU:HG	28:N:3073:HOH:O	2.04	0.57
20:Q:1523:TGL:HC21	20:Q:1523:TGL:HG11	1.85	0.56
1:A:1:FME:HE2	1:A:1:FME:HA	1.85	0.56
1:A:321:PHE:CZ	21:B:230:PSC:H171	2.40	0.56
12:Y:20:ARG:NH1	28:Y:4492:HOH:O	2.39	0.56
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.86	0.56
6:S:76:LYS:HE3	6:S:93:PRO:HG3	1.87	0.56
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.88	0.56
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.69	0.56
9:I:5:ALA:O	9:I:7:PRO:HD3	2.04	0.56
1:N:321:PHE:CZ	21:O:1230:PSC:H171	2.41	0.56
20:N:1521:TGL:H222	20:N:1521:TGL:HA82	1.87	0.56
1:A:1:FME:HCN	1:A:4:ASN:H	1.70	0.56
26:C:270:CDL:H431	28:J:5157:HOH:O	2.05	0.56
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.87	0.56
6:F:93:PRO:HB2	6:F:94:HIS:ND1	2.21	0.56
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.88	0.55
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.89	0.55
7:T:84:LYS:N	7:T:84:LYS:HD2	2.05	0.55
1:A:113:LEU:CD1	20:L:522:TGL:H292	2.37	0.55
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.05	0.55
7:T:72:ASN:N	7:T:76:ASN:HD22	1.97	0.55
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.72	0.55
26:G:269:CDL:H212	1:N:311:ILE:HD12	1.89	0.55
18:A:524:PGV:H062	28:M:2158:HOH:O	2.05	0.55
18:A:524:PGV:H311	13:M:16:ALA:HA	1.88	0.55
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.88	0.55
2:O:57:ASP:H	21:O:1230:PSC:H201	1.72	0.55
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.37	0.54
1:N:87:ILE:O	1:N:173:PRO:HD3	2.07	0.54
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.54
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.90	0.54
20:L:522:TGL:HC21	20:L:522:TGL:OA1	2.06	0.54
20:D:523:TGL:HC21	20:D:523:TGL:HG11	1.90	0.54
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.42	0.54
21:B:230:PSC:H12	21:B:230:PSC:H322	1.89	0.54
25:C:265:PEK:H383	26:G:269:CDL:H273	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.41	0.54
1:N:430:PHE:HE1	20:N:1521:TGL:HB21	1.73	0.54
3:C:34:TRP:HZ2	23:C:272:DMU:H29	1.71	0.54
4:D:58:GLU:HG3	28:D:4047:HOH:O	2.07	0.54
2:B:56:MET:HG2	21:B:230:PSC:H211	1.88	0.54
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.43	0.54
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.43	0.54
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.42	0.54
13:Z:16:ALA:HA	18:Z:1524:PGV:H311	1.90	0.54
26:T:1269:CDL:HA62	26:T:1269:CDL:H322	1.90	0.54
17:A:515:HEA:HMC1	17:A:515:HEA:HBC1	1.89	0.54
2:O:59:GLN:O	2:O:59:GLN:HG3	2.08	0.54
18:P:1267:PGV:H182	26:P:1270:CDL:H673	1.88	0.54
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.37	0.54
18:N:1266:PGV:H182	3:P:28:THR:HG22	1.90	0.54
20:N:1522:TGL:HC21	20:N:1522:TGL:OA1	2.09	0.53
9:V:15:ARG:HD2	28:V:4894:HOH:O	2.08	0.53
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.91	0.53
3:C:213:THR:HG23	26:C:270:CDL:H762	1.90	0.53
1:A:407:ASP:O	1:A:411:LYS:HG3	2.09	0.53
5:E:84:TYR:O	5:E:88:GLU:HG2	2.09	0.53
18:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.53
1:A:406:ASN:HD21	18:A:524:PGV:C2	2.21	0.53
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.23	0.53
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.91	0.53
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.90	0.52
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.91	0.52
6:S:51:SER:O	6:S:94:HIS:N	2.42	0.52
21:O:1230:PSC:H322	21:O:1230:PSC:H12	1.91	0.52
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.44	0.52
25:C:264:PEK:H102	25:C:264:PEK:C16	2.36	0.52
28:A:4756:HOH:O	8:H:23:GLN:HG3	2.08	0.52
7:G:3:ALA:O	7:G:4:ALA:HB2	2.10	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.90	0.52
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.75	0.52
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.74	0.52
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.57	0.52
20:N:1521:TGL:HC22	28:Q:3381:HOH:O	2.09	0.52
1:N:28:MET:HE2	17:N:515:HEA:H271	1.92	0.52
1:A:472:ILE:HD13	20:L:522:TGL:HA91	1.92	0.51
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:40:LEU:HD12	22:J:60:CHD:H183	1.90	0.51
20:N:1522:TGL:H202	20:N:1522:TGL:C24	2.40	0.51
1:N:488:THR:HB	1:N:495:LEU:HD13	1.92	0.51
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.92	0.51
20:N:1521:TGL:HB91	2:O:32:PHE:HE2	1.75	0.51
6:F:64:GLU:O	6:F:65:ASP:HB2	2.11	0.51
1:N:347:LEU:HD13	1:N:383:MET:SD	2.49	0.51
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.10	0.51
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.10	0.51
8:H:49:ASP:O	8:H:52:VAL:HG22	2.11	0.51
10:W:1:PHE:HD1	10:W:1:PHE:H1	1.55	0.51
7:T:72:ASN:H	7:T:76:ASN:ND2	1.98	0.51
7:G:2:SER:O	25:G:1263:PEK:H322	2.10	0.51
1:A:136:LEU:HB2	28:A:4733:HOH:O	2.11	0.51
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.93	0.50
1:N:400:PHE:HB3	20:N:1522:TGL:H283	1.93	0.50
6:S:52:ILE:O	6:S:94:HIS:CD2	2.64	0.50
1:N:407:ASP:O	1:N:411:LYS:HG3	2.12	0.50
12:L:24:MET:HG3	28:L:5077:HOH:O	2.11	0.50
3:C:51:MET:SD	26:C:270:CDL:C62	3.00	0.50
1:A:87:ILE:O	1:A:173:PRO:HD3	2.11	0.50
12:Y:2:HIS:N	28:Y:5165:HOH:O	2.45	0.50
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.92	0.50
28:B:4821:HOH:O	25:P:1265:PEK:H031	2.11	0.50
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.42	0.50
1:N:52:GLN:O	1:N:56:VAL:HG23	2.12	0.50
4:D:127:LYS:HD2	28:I:2389:HOH:O	2.11	0.49
7:G:2:SER:OG	25:G:1263:PEK:H301	2.12	0.49
20:L:522:TGL:C24	20:L:522:TGL:H202	2.39	0.49
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
1:A:488:THR:HB	1:A:495:LEU:HD13	1.94	0.49
7:T:3:ALA:O	7:T:4:ALA:HB2	2.12	0.49
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.49
1:A:1:FME:CE	1:A:1:FME:HA	2.42	0.49
5:R:48:ILE:O	5:R:52:LEU:HG	2.12	0.49
13:M:42:LYS:HA	13:M:42:LYS:CE	2.42	0.49
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.60	0.49
3:P:34:TRP:CE2	23:P:1272:DMU:H29	2.46	0.49
1:A:449:MET:SD	2:B:5:MET:HG2	2.53	0.49
18:P:1268:PGV:H101	28:P:4808:HOH:O	2.13	0.49
1:A:379:TYR:O	1:A:383:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:365:ILE:HD11	28:N:4705:HOH:O	2.12	0.49
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.93	0.49
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.78	0.48
4:D:17:VAL:HG12	28:D:4051:HOH:O	2.13	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
1:N:484:THR:HB	28:Z:5071:HOH:O	2.13	0.48
3:C:51:MET:SD	26:C:270:CDL:H622	2.53	0.48
1:N:17:THR:OG1	20:N:1522:TGL:H281	2.13	0.48
2:B:58:ALA:O	2:B:62:GLU:HG3	2.13	0.48
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.48
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.94	0.48
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.29	0.48
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.94	0.48
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.44	0.48
6:F:51:SER:O	6:F:94:HIS:N	2.46	0.48
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.49	0.48
2:O:1:FME:SD	2:O:133:LEU:CD1	3.02	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
25:C:265:PEK:H383	26:G:269:CDL:C27	2.44	0.48
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.95	0.48
6:S:52:ILE:C	6:S:94:HIS:CE1	2.88	0.47
1:N:379:TYR:O	1:N:383:MET:HB2	2.14	0.47
20:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.95	0.47
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.96	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.12	0.47
2:O:220:GLU:O	2:O:223:SER:HB2	2.14	0.47
3:P:34:TRP:NE1	23:P:1272:DMU:H29	2.30	0.47
2:B:114:GLU:HB3	28:B:4063:HOH:O	2.13	0.47
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.96	0.47
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.63	0.47
6:S:92:VAL:HG23	6:S:92:VAL:O	2.14	0.47
2:O:56:MET:HG2	21:O:1230:PSC:H211	1.97	0.47
4:D:34:SER:N	4:D:37:GLN:HE21	1.96	0.47
7:G:5:LYS:CD	1:N:278:MET:HB3	2.44	0.47
18:Z:1524:PGV:H062	28:Z:3158:HOH:O	2.15	0.47
1:A:383:MET:O	1:A:387:PHE:HB2	2.15	0.47
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.47
1:A:222:PRO:HD2	28:B:4914:HOH:O	2.15	0.47
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.97	0.47
1:A:52:GLN:O	1:A:56:VAL:HG23	2.15	0.47
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:HD21	18:A:524:PGV:H21	1.80	0.46
10:W:50:LEU:HD22	10:W:50:LEU:O	2.16	0.46
25:C:264:PEK:H32	25:C:264:PEK:H71	1.98	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.46
22:P:1271:CHD:H12A	22:P:1271:CHD:H112	1.68	0.46
1:A:365:ILE:HD11	28:H:4750:HOH:O	2.16	0.46
1:A:311:ILE:HD12	26:T:1269:CDL:H212	1.98	0.46
1:A:278:MET:HB3	7:T:5:LYS:HD3	1.98	0.46
25:G:1263:PEK:H132	3:P:247:VAL:HG11	1.97	0.46
1:N:28:MET:CE	17:N:515:HEA:H271	2.46	0.46
2:O:216:LEU:O	2:O:219:PHE:HB3	2.16	0.46
18:P:1267:PGV:H12	18:P:1267:PGV:C16	2.43	0.46
6:F:55:LYS:HA	6:F:74:LEU:O	2.15	0.46
6:S:55:LYS:HA	6:S:74:LEU:O	2.15	0.46
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.33	0.46
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.97	0.46
26:G:269:CDL:H221	1:N:286:ILE:CD1	2.46	0.46
7:T:2:SER:OG	25:T:263:PEK:H301	2.15	0.46
7:T:38:HIS:CE1	26:T:1269:CDL:H111	2.51	0.46
6:S:87:THR:HG21	28:S:3337:HOH:O	2.16	0.46
26:C:270:CDL:H162	26:C:270:CDL:H352	1.97	0.46
7:G:4:ALA:CB	1:N:282:PHE:HA	2.46	0.46
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.98	0.46
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.98	0.46
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.46
26:T:1269:CDL:H382	28:T:5116:HOH:O	2.15	0.46
1:A:422:ASN:HB3	20:B:521:TGL:H242	1.98	0.46
9:I:5:ALA:N	28:I:4913:HOH:O	2.36	0.46
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.14	0.46
7:G:7:ASP:O	1:N:169:ILE:HD12	2.16	0.45
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.16	0.45
2:B:52:HIS:HE1	21:B:230:PSC:H02	1.80	0.45
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.81	0.45
2:O:46:LEU:HD12	20:Q:1523:TGL:H271	1.97	0.45
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.98	0.45
3:C:177:GLN:OE1	3:C:177:GLN:HA	2.17	0.45
18:C:267:PGV:H12	18:C:267:PGV:C16	2.44	0.45
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.46	0.45
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.81	0.45
1:A:240:HIS:O	1:A:243:VAL:HG22	2.16	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:1522:TGL:HB31	20:N:1522:TGL:HB61	1.80	0.45
1:A:113:LEU:HD12	20:L:522:TGL:H292	1.98	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.45
1:N:54:TYR:HB2	28:N:3111:HOH:O	2.15	0.45
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.45
21:B:230:PSC:H042	21:B:230:PSC:H062	1.81	0.45
26:P:1270:CDL:H352	26:P:1270:CDL:H162	1.99	0.45
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.52	0.45
2:B:7:LEU:HD11	20:B:521:TGL:H161	1.99	0.45
20:D:523:TGL:H242	20:D:523:TGL:H212	1.66	0.45
2:O:1:FME:SD	2:O:133:LEU:HD11	2.57	0.45
3:C:246:ASP:HB2	28:C:4590:HOH:O	2.17	0.45
3:P:25:LEU:O	3:P:29:SER:HB2	2.17	0.45
1:N:177:SER:H	1:N:180:GLN:NE2	2.15	0.45
10:J:50:LEU:HD22	10:J:50:LEU:O	2.17	0.45
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.99	0.45
23:P:1272:DMU:H25	25:P:1264:PEK:H341	1.99	0.45
1:A:513:LEU:HD22	1:A:513:LEU:HA	1.79	0.45
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.79	0.45
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.38	0.45
28:O:4738:HOH:O	8:U:61:LYS:HD3	2.17	0.45
7:T:84:LYS:N	7:T:84:LYS:CD	2.73	0.44
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.32	0.44
3:P:34:TRP:HE1	23:P:1272:DMU:H29	1.82	0.44
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.98	0.44
5:E:71:VAL:HG11	5:E:85:VAL:HG11	2.00	0.44
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.99	0.44
1:N:350:VAL:HG13	20:N:1521:TGL:HB81	1.99	0.44
12:L:20:ARG:CZ	20:L:522:TGL:HC61	2.47	0.44
2:O:83:ILE:O	2:O:87:MET:HG3	2.18	0.44
20:Q:1523:TGL:H212	20:Q:1523:TGL:H242	1.67	0.44
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.32	0.44
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.99	0.44
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.00	0.44
26:C:270:CDL:H672	26:C:270:CDL:H641	1.85	0.44
25:P:1265:PEK:H383	26:T:1269:CDL:C27	2.47	0.44
11:X:8:ASP:HB2	28:X:5081:HOH:O	2.17	0.44
2:O:102:HIS:O	2:O:104:TRP:HA	2.18	0.44
22:W:1060:CHD:H161	22:W:1060:CHD:H212	1.76	0.44
3:C:191:GLY:HA3	28:G:2161:HOH:O	2.17	0.44
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:344:PHE:C	1:N:344:PHE:CD1	2.90	0.44
5:R:31:LYS:HE2	5:R:35:THR:OG1	2.17	0.44
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.53	0.44
2:O:56:MET:HA	21:O:1230:PSC:H202	1.99	0.44
7:T:31:CYS:HG	26:T:1269:CDL:H532	1.80	0.44
9:V:45:LYS:HB3	28:V:5052:HOH:O	2.17	0.44
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.31	0.44
20:B:521:TGL:H201	20:B:521:TGL:C24	2.45	0.43
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.83	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.00	0.43
2:B:227:LEU:HA	2:B:227:LEU:HD23	1.76	0.43
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.00	0.43
5:E:5:HIS:HB3	5:E:6:GLU:H	1.56	0.43
2:B:41:ILE:O	2:B:45:MET:HG2	2.18	0.43
5:R:100:THR:HB	5:R:101:PRO:HD2	2.00	0.43
8:U:7:LYS:O	8:U:8:ILE:HG22	2.17	0.43
4:Q:98:TRP:CD2	23:Z:1526:DMU:H10	2.53	0.43
7:T:2:SER:O	25:T:263:PEK:H322	2.18	0.43
7:G:44:ARG:HD2	7:G:82:TYR:CE1	2.52	0.43
20:L:522:TGL:HB31	20:L:522:TGL:HB61	1.79	0.43
2:B:91:ASN:HD22	2:B:92:ASN:N	2.17	0.43
2:O:116:LEU:HD12	2:O:117:SER:N	2.34	0.43
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.19	0.43
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.01	0.43
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.54	0.43
11:X:24:PHE:O	11:X:28:VAL:HG12	2.19	0.43
13:M:17:ILE:O	13:M:21:VAL:HG23	2.18	0.43
26:C:270:CDL:H202	26:C:270:CDL:H171	1.79	0.43
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.01	0.43
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.49	0.43
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.34	0.43
3:C:168:THR:CG2	25:C:265:PEK:H14	2.49	0.43
1:N:449:MET:SD	2:O:5:MET:CG	3.06	0.43
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	2.01	0.43
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.43
3:P:40:MET:O	3:P:44:MET:HG2	2.19	0.43
20:N:1522:TGL:H272	20:N:1522:TGL:H231	2.00	0.42
5:R:82:TYR:N	5:R:83:PRO:CD	2.82	0.42
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.83	0.42
3:C:51:MET:HB3	26:C:270:CDL:H622	2.00	0.42
26:G:269:CDL:H571	26:G:269:CDL:H601	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:522:TGL:HD22	20:L:522:TGL:H231	2.01	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.86	0.42
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.19	0.42
12:Y:20:ARG:HB3	12:Y:20:ARG:NH1	2.34	0.42
20:D:523:TGL:HC31	28:D:4745:HOH:O	2.18	0.42
1:A:298:ASP:HB3	28:A:2387:HOH:O	2.20	0.42
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.48	0.42
1:N:177:SER:H	1:N:180:GLN:HE21	1.67	0.42
3:P:149:HIS:O	3:P:153:GLU:HG3	2.19	0.42
3:P:51:MET:SD	26:P:1270:CDL:C62	3.07	0.42
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.55	0.42
2:B:29:MET:HB2	9:I:35:TYR:CE2	2.55	0.42
2:O:121:TYR:O	2:O:138:VAL:HA	2.19	0.42
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.19	0.42
1:N:112:LEU:HD23	1:N:112:LEU:C	2.39	0.42
3:C:210:ILE:HD13	18:C:267:PGV:H301	2.02	0.42
25:P:1264:PEK:H32	25:P:1264:PEK:H71	2.01	0.42
12:L:20:ARG:HH22	20:L:522:TGL:HC32	1.85	0.42
1:A:306:THR:O	1:A:310:MET:HG3	2.20	0.42
23:P:1272:DMU:H30	7:T:62:TRP:HB3	2.01	0.42
1:N:400:PHE:HB3	20:N:1522:TGL:C28	2.50	0.42
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.84	0.42
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.20	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
21:B:230:PSC:H221	21:B:230:PSC:H251	1.77	0.42
1:N:426:PHE:CZ	20:N:1521:TGL:HA62	2.55	0.42
1:A:400:PHE:HB3	20:L:522:TGL:H283	2.02	0.42
1:N:169:ILE:HD11	1:N:189:MET:SD	2.59	0.42
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.20	0.42
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.82	0.42
8:U:9:LYS:HB3	8:U:10:ASN:H	1.57	0.41
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.54	0.41
22:C:271:CHD:H12A	22:C:271:CHD:H112	1.67	0.41
9:V:64:ARG:HD3	9:V:72:ALA:HB1	2.01	0.41
1:N:422:ASN:HB3	20:N:1521:TGL:H242	2.02	0.41
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.35	0.41
3:C:212:SER:O	3:C:216:ILE:HG13	2.21	0.41
2:O:1:FME:SD	2:O:133:LEU:HD13	2.61	0.41
13:M:41:LYS:NZ	28:M:5113:HOH:O	2.53	0.41
5:R:84:TYR:O	5:R:87:GLN:HB3	2.21	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:LEU:HG	26:G:269:CDL:OB3	2.20	0.41
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.34	0.41
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.02	0.41
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.50	0.41
28:D:4059:HOH:O	5:E:97:GLY:HA2	2.20	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.97	0.41
25:G:1263:PEK:H182	3:P:98:PHE:CD2	2.56	0.41
1:A:406:ASN:HD21	18:A:524:PGV:H22	1.84	0.41
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.41
1:N:398:PRO:HA	1:N:403:TYR:O	2.20	0.41
26:G:269:CDL:H732	26:G:269:CDL:H762	1.98	0.41
1:N:430:PHE:CE1	20:N:1521:TGL:HB21	2.54	0.41
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.56	0.41
4:Q:64:PHE:CE1	5:R:66:ARG:HB2	2.56	0.41
22:O:229:CHD:H212	22:O:229:CHD:H12	2.02	0.41
26:C:270:CDL:H602	26:C:270:CDL:H572	1.91	0.41
2:B:57:ASP:H	21:B:230:PSC:H201	1.86	0.41
3:C:168:THR:HG22	25:C:265:PEK:H14	2.03	0.41
4:Q:118:LYS:HE3	28:Q:4443:HOH:O	2.21	0.41
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.03	0.41
1:A:416:ILE:HG22	1:A:464:ALA:HB2	2.02	0.41
3:C:22:LEU:O	3:C:26:LEU:HG	2.21	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.93	0.41
1:N:105:LEU:HD23	1:N:105:LEU:HA	1.88	0.41
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.02	0.41
2:B:102:HIS:O	2:B:104:TRP:HA	2.21	0.41
9:V:35:TYR:C	9:V:37:PHE:H	2.25	0.41
1:A:112:LEU:HG	28:A:2073:HOH:O	2.19	0.41
25:T:263:PEK:H312	25:T:263:PEK:H282	1.84	0.40
12:L:20:ARG:HH12	20:L:522:TGL:CC6	2.30	0.40
20:D:523:TGL:HC22	20:D:523:TGL:HC51	1.93	0.40
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.20	0.40
8:U:50:VAL:HG12	8:U:50:VAL:O	2.21	0.40
1:N:172:LYS:HB2	1:N:172:LYS:HE2	1.92	0.40
5:R:100:THR:OG1	5:R:103:GLU:HG3	2.21	0.40
4:D:53:ILE:HA	4:D:53:ILE:HD13	1.88	0.40
2:B:121:TYR:O	2:B:138:VAL:HA	2.21	0.40
26:C:270:CDL:H602	26:C:270:CDL:H632	1.69	0.40
3:P:47:LEU:O	3:P:51:MET:HG2	2.21	0.40
20:Q:1523:TGL:CC2	20:Q:1523:TGL:HG11	2.49	0.40
8:U:45:ALA:HB2	28:U:5144:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:HG23	9:I:3:ALA:O	2.21	0.40
7:T:2:SER:O	7:T:3:ALA:HB3	2.21	0.40
20:N:1521:TGL:H201	20:N:1521:TGL:C24	2.44	0.40
6:S:53:THR:CA	6:S:94:HIS:CE1	2.96	0.40
12:L:46:LYS:HG3	28:L:4932:HOH:O	2.22	0.40
18:N:1266:PGV:H251	18:N:1266:PGV:H42	2.04	0.40
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.02	0.40
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.56	0.40
3:C:247:VAL:HG11	25:T:263:PEK:H132	2.02	0.40
1:A:430:PHE:CE1	20:B:521:TGL:HB21	2.52	0.40
20:Q:1523:TGL:HC22	20:Q:1523:TGL:HC51	1.92	0.40
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.87	0.40
2:O:59:GLN:O	2:O:59:GLN:CG	2.69	0.40
1:A:310:MET:HB3	2:B:73:LEU:HD22	2.03	0.40
1:N:397:PHE:HB3	1:N:398:PRO:HD3	2.03	0.40
5:R:5:HIS:HB3	5:R:6:GLU:H	1.57	0.40
2:O:150:ILE:HD12	2:O:184:LEU:HD22	2.04	0.40
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	2.03	0.40
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.02	0.40
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.20	0.40

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%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	21	7
2	O	225/227 (99%)	208 (92%)	15 (7%)	2 (1%)	21	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
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%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	5 (5%)	2 (2%)	9	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	0
7	G	81/85 (95%)	67 (83%)	7 (9%)	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%)	66 (93%)	5 (7%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	127 (4%)	27 (1%)	24	8

All (27) 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
6	S	95	GLN
7	T	4	ALA

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Mol	Chain	Res	Type
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	60	GLU
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
2	O	60	GLU
7	T	3	ALA
8	U	8	ILE
8	H	46	LYS
7	T	40	GLY
6	F	96	LEU
7	G	6	GLY
6	S	96	LEU
7	T	6	GLY
8	U	46	LYS
2	O	92	ASN
2	B	92	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%)	417 (98%)	9 (2%)	61	47
1	N	426/426 (100%)	414 (97%)	12 (3%)	51	35
2	B	210/210 (100%)	201 (96%)	9 (4%)	35	17
2	O	210/210 (100%)	199 (95%)	11 (5%)	29	12
3	C	224/226 (99%)	220 (98%)	4 (2%)	66	54
3	P	224/226 (99%)	219 (98%)	5 (2%)	60	45
4	D	128/129 (99%)	126 (98%)	2 (2%)	70	59
4	Q	128/129 (99%)	125 (98%)	3 (2%)	58	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	27
5	R	92/95 (97%)	89 (97%)	3 (3%)	45	27
6	F	81/81 (100%)	79 (98%)	2 (2%)	55	39
6	S	81/81 (100%)	78 (96%)	3 (4%)	41	23
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	5
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	3
8	H	71/75 (95%)	68 (96%)	3 (4%)	36	18
8	U	71/75 (95%)	68 (96%)	3 (4%)	36	18
9	I	57/57 (100%)	52 (91%)	5 (9%)	12	3
9	V	57/57 (100%)	55 (96%)	2 (4%)	43	25
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	49
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	49
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	54	37
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	37
12	Y	39/40 (98%)	37 (95%)	2 (5%)	29	12
13	M	37/38 (97%)	33 (89%)	4 (11%)	8	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	2
All	All	3040/3082 (99%)	2936 (97%)	104 (3%)	44	26

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	241	PRO
1	A	338	MET
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU

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Mol	Chain	Res	Type
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
9	I	2	THR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
12	L	2	HIS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO

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Mol	Chain	Res	Type
1	N	338	MET
1	N	369	ASP
1	N	484	THR
1	N	504	THR
1	N	513	LEU
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	148	MET
2	O	217	LYS
3	P	29	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	51	LEU
4	Q	121	LYS
5	R	5	HIS
5	R	87	GLN
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	95	GLN
7	T	17	ARG
7	T	18	PHE
7	T	36	TRP
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	21	PRO
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	29	LEU
10	W	50	LEU

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Mol	Chain	Res	Type
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	76	ASN
9	I	8	GLN
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
7	T	76	ASN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	FME	A	1	1	8,9,10	0.60	0	6,9,11	1.34	1 (16%)
2	FME	B	1	2	8,9,10	0.79	0	6,9,11	1.94	1 (16%)
7	TPO	G	11	7	8,10,11	1.58	1 (12%)	7,14,16	1.04	0
9	SAC	I	1	9	7,8,9	2.50	2 (28%)	7,9,11	2.05	2 (28%)
1	FME	N	1	1	8,9,10	0.68	0	6,9,11	1.80	2 (33%)
2	FME	O	1	2	8,9,10	0.60	0	6,9,11	1.32	1 (16%)
7	TPO	T	11	7	8,10,11	1.33	1 (12%)	7,14,16	1.07	1 (14%)
9	SAC	V	1	9	7,8,9	2.69	2 (28%)	7,9,11	2.18	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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	CB-CA	2.94	1.59	1.54
7	G	11	TPO	CB-CA	3.51	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	4.05	1.52	1.46
9	V	1	SAC	CA-N	4.49	1.52	1.46
9	I	1	SAC	OAC-C1A	5.01	1.34	1.23
9	V	1	SAC	OAC-C1A	5.15	1.35	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-4.41	116.05	122.82
1	N	1	FME	CA-N-CN	-3.73	117.09	122.82
9	V	1	SAC	CA-N-C1A	-3.18	110.59	121.37
9	I	1	SAC	CA-N-C1A	-2.77	111.98	121.37
2	O	1	FME	CA-N-CN	-2.69	118.68	122.82
1	A	1	FME	CA-N-CN	-2.43	119.08	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.25	117.94	122.06
1	N	1	FME	O-C-CA	-2.25	119.51	125.44
7	T	11	TPO	O-C-CA	-2.01	120.12	125.44
9	V	1	SAC	C2A-C1A-N	2.54	120.97	116.11
9	V	1	SAC	CB-CA-N	2.74	116.60	110.60
9	I	1	SAC	CB-CA-N	3.55	118.37	110.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 2 are unknown and 8 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	1.19	3 (7%)	41,103,103	1.59	8 (19%)
17	HEA	A	516	1	40,67,67	1.53	6 (15%)	41,103,103	1.34	8 (19%)
18	PGV	A	524	-	50,50,50	1.06	3 (6%)	51,56,56	0.89	1 (1%)
18	PGV	A	525	-	50,50,50	0.89	2 (4%)	51,56,56	0.78	2 (3%)
22	CHD	B	1086	-	29,32,32	0.63	0	48,51,51	1.77	14 (29%)
19	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	PSC	B	230	-	51,51,51	1.18	3 (5%)	55,59,59	0.94	1 (1%)
20	TGL	B	521	-	62,62,62	0.67	0	65,65,65	1.49	11 (16%)
25	PEK	C	264	-	51,52,52	1.43	4 (7%)	52,57,57	1.08	3 (5%)
25	PEK	C	265	-	51,52,52	1.63	9 (17%)	52,57,57	1.11	5 (9%)
18	PGV	C	267	-	50,50,50	0.83	1 (2%)	51,56,56	0.86	2 (3%)
18	PGV	C	268	-	50,50,50	1.21	3 (6%)	51,56,56	0.78	1 (1%)
26	CDL	C	270	-	99,99,99	0.78	3 (3%)	101,111,111	0.94	5 (4%)
22	CHD	C	271	-	29,32,32	0.74	0	48,51,51	3.62	21 (43%)
23	DMU	C	272	-	34,34,34	2.96	8 (23%)	45,45,45	4.18	19 (42%)
22	CHD	C	525	-	29,32,32	0.76	1 (3%)	48,51,51	1.64	10 (20%)
20	TGL	D	523	-	62,62,62	0.76	1 (1%)	65,65,65	1.37	8 (12%)
25	PEK	G	1263	-	51,52,52	1.84	11 (21%)	52,57,57	1.15	3 (5%)
26	CDL	G	269	-	99,99,99	0.92	5 (5%)	101,111,111	0.94	6 (5%)
22	CHD	J	60	-	29,32,32	0.81	1 (3%)	48,51,51	3.21	25 (52%)
20	TGL	L	522	-	62,62,62	1.10	4 (6%)	65,65,65	1.69	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	DMU	M	526	-	34,34,34	3.19	8 (23%)	45,45,45	4.31	19 (42%)
18	PGV	N	1266	-	50,50,50	0.93	2 (4%)	51,56,56	0.83	3 (5%)
20	TGL	N	1521	-	62,62,62	0.70	2 (3%)	65,65,65	1.47	10 (15%)
20	TGL	N	1522	-	62,62,62	1.13	5 (8%)	65,65,65	1.67	12 (18%)
17	HEA	N	515	1	40,67,67	1.26	6 (15%)	41,103,103	1.56	9 (21%)
17	HEA	N	516	1	40,67,67	1.37	6 (15%)	41,103,103	1.39	8 (19%)
21	PSC	O	1230	-	51,51,51	1.14	3 (5%)	55,59,59	0.94	1 (1%)
19	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	229	-	29,32,32	0.74	0	48,51,51	1.81	13 (27%)
25	PEK	P	1264	-	51,52,52	1.42	4 (7%)	52,57,57	1.12	3 (5%)
25	PEK	P	1265	-	51,52,52	1.66	11 (21%)	52,57,57	1.09	5 (9%)
18	PGV	P	1267	-	50,50,50	0.84	1 (2%)	51,56,56	0.86	1 (1%)
18	PGV	P	1268	-	50,50,50	1.24	3 (6%)	51,56,56	0.80	1 (1%)
26	CDL	P	1270	-	99,99,99	0.81	3 (3%)	101,111,111	0.92	5 (4%)
22	CHD	P	1271	-	29,32,32	0.72	0	48,51,51	3.56	21 (43%)
23	DMU	P	1272	-	34,34,34	2.97	8 (23%)	45,45,45	4.17	19 (42%)
22	CHD	P	1525	-	29,32,32	0.76	0	48,51,51	1.57	8 (16%)
20	TGL	Q	1523	-	62,62,62	0.79	2 (3%)	65,65,65	1.34	8 (12%)
26	CDL	T	1269	-	99,99,99	0.89	5 (5%)	101,111,111	0.95	6 (5%)
25	PEK	T	263	-	51,52,52	1.85	11 (21%)	52,57,57	1.15	3 (5%)
22	CHD	W	1060	-	29,32,32	0.89	1 (3%)	48,51,51	3.19	25 (52%)
18	PGV	Z	1524	-	50,50,50	1.04	4 (8%)	51,56,56	0.86	2 (3%)
23	DMU	Z	1526	-	34,34,34	3.15	8 (23%)	45,45,45	4.25	19 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
18	PGV	A	524	-	-	2/55/55/55	0/0/0/0
18	PGV	A	525	-	-	0/55/55/55	0/0/0/0
22	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
19	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	PSC	B	230	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	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
18	PGV	C	267	-	-	0/55/55/55	0/0/0/0
18	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
20	TGL	D	523	-	-	0/65/65/65	0/0/0/0
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
20	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
18	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
20	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
20	TGL	N	1522	-	-	0/65/65/65	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
19	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
18	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
18	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
20	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1060	-	5/5/12/12	0/7/74/74	0/4/4/4
18	PGV	Z	1524	-	-	2/55/55/55	0/0/0/0
23	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Z	1526	DMU	O7-C3	-8.34	1.23	1.43
23	M	526	DMU	O7-C3	-8.28	1.23	1.43
23	M	526	DMU	O1-C9	-7.00	1.26	1.44
23	P	1272	DMU	O1-C9	-6.93	1.27	1.44
23	M	526	DMU	O16-C6	-6.92	1.27	1.40
23	P	1272	DMU	O7-C3	-6.89	1.26	1.43
23	Z	1526	DMU	O16-C6	-6.86	1.27	1.40
23	C	272	DMU	O7-C3	-6.85	1.26	1.43
23	Z	1526	DMU	O1-C9	-6.74	1.27	1.44
23	C	272	DMU	O1-C9	-6.63	1.27	1.44
23	C	272	DMU	O16-C6	-6.58	1.28	1.40
23	P	1272	DMU	O16-C6	-6.45	1.28	1.40
23	C	272	DMU	O16-C18	-6.40	1.25	1.42
23	P	1272	DMU	O16-C18	-6.36	1.25	1.42
23	M	526	DMU	O5-C4	-6.33	1.28	1.44
23	Z	1526	DMU	O5-C4	-6.27	1.28	1.44
23	Z	1526	DMU	O7-C10	-6.16	1.24	1.41
23	M	526	DMU	O7-C10	-6.14	1.25	1.41
23	M	526	DMU	O16-C18	-6.08	1.25	1.42
23	Z	1526	DMU	O16-C18	-5.80	1.26	1.42
23	M	526	DMU	O1-C10	-5.79	1.27	1.41
23	Z	1526	DMU	O1-C10	-5.75	1.27	1.41
23	C	272	DMU	O7-C10	-5.30	1.27	1.41
23	P	1272	DMU	O7-C10	-5.26	1.27	1.41
23	C	272	DMU	O5-C4	-5.20	1.31	1.44
23	C	272	DMU	O1-C10	-5.16	1.28	1.41
23	P	1272	DMU	O1-C10	-5.13	1.28	1.41
23	P	1272	DMU	O5-C4	-5.10	1.31	1.44
23	C	272	DMU	O5-C6	-4.76	1.29	1.41
23	P	1272	DMU	O5-C6	-4.63	1.29	1.41
23	M	526	DMU	O5-C6	-4.55	1.30	1.41
23	Z	1526	DMU	O5-C6	-4.32	1.30	1.41
17	A	516	HEA	C3A-C2A	-3.49	1.35	1.40
17	N	515	HEA	C3A-CMA	-3.35	1.38	1.46
17	N	516	HEA	C3A-CMA	-3.19	1.39	1.46
17	A	515	HEA	C3A-CMA	-2.98	1.39	1.46
17	A	516	HEA	C3C-C2C	-2.62	1.36	1.40
17	N	515	HEA	C3A-C2A	-2.53	1.37	1.40
17	A	516	HEA	C3A-CMA	-2.52	1.40	1.46
22	C	525	CHD	C10-C9	-2.04	1.52	1.56
17	N	516	HEA	C3A-C2A	-2.01	1.37	1.40
18	A	525	PGV	C20-C19	2.00	1.56	1.50
18	Z	1524	PGV	C20-C19	2.02	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	523	TGL	OG1-CA1	2.03	1.39	1.33
25	P	1265	PEK	P-O12	2.03	1.68	1.59
17	A	515	HEA	C1A-NA	2.05	1.39	1.36
20	N	1522	TGL	CC2-CC1	2.06	1.56	1.50
26	T	1269	CDL	OA6-CA5	2.06	1.40	1.34
18	C	268	PGV	C04-C05	2.07	1.59	1.51
25	C	265	PEK	P-O11	2.07	1.68	1.59
20	N	1521	TGL	CG3-CG2	2.08	1.56	1.50
18	Z	1524	PGV	C03-C02	2.08	1.56	1.50
20	Q	1523	TGL	CG3-CG2	2.09	1.56	1.50
26	C	270	CDL	OA8-CA7	2.10	1.39	1.33
25	G	1263	PEK	C2-C1	2.11	1.57	1.50
18	A	524	PGV	C20-C19	2.12	1.57	1.50
20	N	1522	TGL	CG3-CG2	2.12	1.56	1.50
17	N	516	HEA	C18-C19	2.13	1.37	1.33
25	P	1265	PEK	O01-C1	2.13	1.40	1.34
26	G	269	CDL	C11-CA5	2.16	1.57	1.50
25	P	1265	PEK	P-O11	2.19	1.69	1.59
17	N	515	HEA	C1A-NA	2.21	1.39	1.36
26	T	1269	CDL	CA6-CA4	2.21	1.57	1.50
17	A	516	HEA	C20-C19	2.21	1.56	1.51
21	O	1230	PSC	C2-C1	2.22	1.57	1.50
26	P	1270	CDL	OA8-CA7	2.25	1.40	1.33
20	Q	1523	TGL	OG2-CB1	2.27	1.41	1.34
25	G	1263	PEK	C22-C21	2.28	1.57	1.50
20	L	522	TGL	CG3-CG2	2.30	1.57	1.50
18	N	1266	PGV	C01-C02	2.30	1.57	1.50
17	N	515	HEA	C1D-ND	2.30	1.39	1.36
25	C	265	PEK	O03-C21	2.31	1.40	1.33
25	T	263	PEK	C22-C21	2.32	1.57	1.50
20	N	1521	TGL	OG2-CB1	2.34	1.41	1.34
25	G	1263	PEK	P-O11	2.35	1.69	1.59
26	T	1269	CDL	C11-CA5	2.37	1.57	1.50
25	G	1263	PEK	O01-C1	2.39	1.41	1.34
18	P	1268	PGV	C2-C1	2.40	1.57	1.50
21	B	230	PSC	C2-C1	2.45	1.58	1.50
26	C	270	CDL	CA3-CA4	2.46	1.57	1.50
25	C	265	PEK	C22-C21	2.49	1.58	1.50
26	G	269	CDL	OA6-CA5	2.51	1.41	1.34
25	C	265	PEK	C01-C02	2.51	1.57	1.50
26	P	1270	CDL	CA3-CA4	2.53	1.57	1.50
17	N	515	HEA	C4B-NB	2.53	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	60	CHD	C13-C17	2.54	1.60	1.55
25	P	1265	PEK	C22-C21	2.54	1.58	1.50
26	T	1269	CDL	CB3-CB4	2.55	1.57	1.50
25	P	1265	PEK	C01-C02	2.55	1.57	1.50
25	T	263	PEK	P-O11	2.58	1.70	1.59
26	G	269	CDL	CA6-CA4	2.60	1.58	1.50
26	C	270	CDL	CA6-CA4	2.71	1.58	1.50
26	G	269	CDL	CB3-CB4	2.74	1.58	1.50
25	P	1265	PEK	O03-C21	2.76	1.41	1.33
17	N	516	HEA	C4B-NB	2.76	1.40	1.36
25	P	1265	PEK	C03-C02	2.76	1.58	1.50
25	T	263	PEK	C2-C1	2.81	1.59	1.50
25	T	263	PEK	O01-C1	2.83	1.42	1.34
18	Z	1524	PGV	O03-C19	2.85	1.41	1.33
17	N	515	HEA	C4A-NA	2.86	1.40	1.36
25	C	265	PEK	C03-C02	2.86	1.58	1.50
20	N	1522	TGL	CG1-CG2	2.89	1.58	1.50
22	W	1060	CHD	C13-C17	2.93	1.60	1.55
20	L	522	TGL	OG1-CA1	2.98	1.42	1.33
26	P	1270	CDL	CA6-CA4	3.01	1.59	1.50
20	L	522	TGL	CG1-CG2	3.14	1.59	1.50
18	C	267	PGV	C12-C11	3.22	1.50	1.31
18	P	1267	PGV	C12-C11	3.24	1.50	1.31
18	A	524	PGV	O03-C19	3.33	1.43	1.33
18	C	268	PGV	O01-C1	3.40	1.44	1.34
17	A	516	HEA	C4B-NB	3.42	1.41	1.36
17	A	515	HEA	C1D-ND	3.52	1.41	1.36
17	N	516	HEA	C1D-ND	3.57	1.41	1.36
17	N	516	HEA	C4A-NA	3.60	1.41	1.36
25	T	263	PEK	C03-C02	3.63	1.61	1.50
26	G	269	CDL	CB6-CB4	3.64	1.61	1.50
25	T	263	PEK	C01-C02	3.70	1.61	1.50
20	N	1522	TGL	OG1-CA1	3.81	1.44	1.33
25	G	1263	PEK	C03-C02	3.82	1.61	1.50
18	A	525	PGV	C12-C11	3.85	1.53	1.31
18	A	524	PGV	C12-C11	3.88	1.54	1.31
18	P	1268	PGV	O01-C1	3.93	1.46	1.34
26	T	1269	CDL	CB6-CB4	3.94	1.61	1.50
18	Z	1524	PGV	C12-C11	3.97	1.54	1.31
25	G	1263	PEK	C01-C02	3.97	1.61	1.50
25	C	265	PEK	C6-C5	3.99	1.54	1.31
18	N	1266	PGV	C12-C11	4.02	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	1263	PEK	C9-C8	4.04	1.55	1.31
25	P	1264	PEK	C6-C5	4.07	1.55	1.31
25	P	1264	PEK	C9-C8	4.07	1.55	1.31
25	T	263	PEK	C9-C8	4.10	1.55	1.31
25	C	264	PEK	C9-C8	4.10	1.55	1.31
25	C	264	PEK	C6-C5	4.10	1.55	1.31
21	B	230	PSC	C13-C12	4.10	1.55	1.31
21	O	1230	PSC	C13-C12	4.13	1.55	1.31
25	G	1263	PEK	O03-C21	4.14	1.45	1.33
25	P	1265	PEK	C6-C5	4.14	1.55	1.31
25	T	263	PEK	C15-C14	4.14	1.55	1.31
21	B	230	PSC	C10-C9	4.20	1.56	1.31
25	G	1263	PEK	C15-C14	4.21	1.56	1.31
25	P	1265	PEK	C9-C8	4.22	1.56	1.31
25	P	1265	PEK	C15-C14	4.22	1.56	1.31
25	T	263	PEK	O03-C21	4.27	1.46	1.33
21	O	1230	PSC	C10-C9	4.27	1.56	1.31
25	C	265	PEK	C15-C14	4.29	1.56	1.31
25	C	265	PEK	C12-C11	4.33	1.56	1.31
25	C	265	PEK	C9-C8	4.35	1.56	1.31
18	C	268	PGV	C12-C11	4.37	1.57	1.31
25	P	1265	PEK	C12-C11	4.39	1.57	1.31
18	P	1268	PGV	C12-C11	4.42	1.57	1.31
25	C	264	PEK	C12-C11	4.51	1.57	1.31
25	G	1263	PEK	C6-C5	4.51	1.57	1.31
25	T	263	PEK	C6-C5	4.52	1.57	1.31
25	P	1264	PEK	C15-C14	4.53	1.57	1.31
25	T	263	PEK	C12-C11	4.54	1.58	1.31
25	P	1264	PEK	C12-C11	4.64	1.58	1.31
25	C	264	PEK	C15-C14	4.65	1.58	1.31
20	L	522	TGL	OG2-CB1	4.66	1.48	1.34
25	G	1263	PEK	C12-C11	4.71	1.58	1.31
20	N	1522	TGL	OG2-CB1	4.76	1.48	1.34
17	A	516	HEA	C1D-ND	4.79	1.43	1.36

All (367) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C17-C13-C12	-9.83	108.97	117.68
22	C	271	CHD	C17-C13-C12	-9.77	109.02	117.68
22	C	271	CHD	C19-C10-C9	-7.72	99.61	111.18
22	P	1271	CHD	C19-C10-C9	-7.14	100.48	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	526	DMU	C8-C7-C5	-6.67	98.34	110.79
23	Z	1526	DMU	C8-C7-C5	-6.45	98.76	110.79
20	B	521	TGL	CG1-OG1-CA1	-5.45	101.61	116.85
20	N	1521	TGL	CG1-OG1-CA1	-5.41	101.72	116.85
22	W	1060	CHD	C15-C14-C8	-5.38	110.50	118.32
22	J	60	CHD	C15-C14-C8	-5.25	110.69	118.32
22	P	1271	CHD	C15-C14-C8	-4.91	111.19	118.32
22	C	271	CHD	C15-C14-C8	-4.85	111.28	118.32
22	C	271	CHD	C19-C10-C1	-4.79	100.14	108.20
20	L	522	TGL	C12-C11-C10	-4.70	90.25	114.53
22	P	1271	CHD	C19-C10-C1	-4.68	100.32	108.20
20	L	522	TGL	CB9-CB8-CB7	-4.68	90.36	114.53
20	N	1522	TGL	CB9-CB8-CB7	-4.67	90.40	114.53
22	J	60	CHD	C18-C13-C14	-4.59	103.98	111.22
20	N	1522	TGL	C12-C11-C10	-4.56	90.97	114.53
22	W	1060	CHD	C18-C13-C14	-4.35	104.36	111.22
17	A	515	HEA	CAD-C3D-C4D	-4.14	122.52	127.01
23	C	272	DMU	C2-C3-C4	-4.11	101.55	110.84
22	C	525	CHD	C14-C13-C12	-4.09	103.73	107.39
23	P	1272	DMU	C2-C3-C4	-3.94	101.93	110.84
20	Q	1523	TGL	CG1-OG1-CA1	-3.90	105.94	116.85
22	J	60	CHD	C17-C13-C12	-3.80	114.31	117.68
22	W	1060	CHD	C17-C13-C12	-3.80	114.31	117.68
17	A	515	HEA	C27-C19-C18	-3.79	116.06	123.50
22	B	1086	CHD	C16-C17-C13	-3.78	99.84	103.60
17	N	515	HEA	C27-C19-C18	-3.75	116.14	123.50
20	D	523	TGL	CG1-OG1-CA1	-3.65	106.63	116.85
22	O	229	CHD	C14-C13-C12	-3.62	104.15	107.39
22	B	1086	CHD	C14-C13-C12	-3.61	104.16	107.39
21	B	230	PSC	C01-O03-C19	-3.56	106.89	116.85
21	O	1230	PSC	C01-O03-C19	-3.48	107.11	116.85
22	P	1525	CHD	C15-C14-C8	-3.47	113.27	118.32
22	O	229	CHD	C16-C17-C13	-3.45	100.17	103.60
22	C	271	CHD	C18-C13-C14	-3.40	105.85	111.22
22	B	1086	CHD	C15-C14-C8	-3.36	113.44	118.32
22	O	229	CHD	C15-C14-C8	-3.31	113.51	118.32
22	B	1086	CHD	C15-C14-C13	-3.27	100.35	103.60
22	B	1086	CHD	O3-C3-C4	-3.23	103.44	109.86
22	C	525	CHD	C15-C14-C8	-3.20	113.67	118.32
17	N	515	HEA	CAD-C3D-C4D	-3.12	123.62	127.01
18	N	1266	PGV	C01-O03-C19	-3.12	108.14	116.85
26	P	1270	CDL	CB6-OB8-CB7	-3.11	108.16	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C19-C10-C9	-3.04	106.62	111.18
22	P	1525	CHD	C14-C13-C12	-3.02	104.68	107.39
22	P	1271	CHD	C18-C13-C14	-2.98	106.52	111.22
26	C	270	CDL	CB6-OB8-CB7	-2.97	108.54	116.85
22	P	1525	CHD	C14-C8-C9	-2.96	105.55	109.62
23	Z	1526	DMU	C2-C3-C4	-2.93	104.21	110.84
17	N	515	HEA	C17-C18-C19	-2.92	121.42	127.76
26	C	270	CDL	OB6-CB5-C51	-2.87	105.29	111.53
18	P	1267	PGV	C9-C10-C11	-2.85	97.48	112.45
22	W	1060	CHD	C19-C10-C9	-2.82	106.95	111.18
18	C	267	PGV	C9-C10-C11	-2.82	97.65	112.45
22	B	1086	CHD	C19-C10-C1	-2.81	103.47	108.20
23	M	526	DMU	C2-C3-C4	-2.71	104.71	110.84
22	O	229	CHD	C15-C14-C13	-2.69	100.93	103.60
17	N	515	HEA	C13-C14-C15	-2.66	121.97	127.76
25	C	264	PEK	O03-C21-C22	-2.66	103.80	111.90
17	A	516	HEA	CAD-C3D-C4D	-2.64	124.14	127.01
17	A	515	HEA	C13-C14-C15	-2.64	122.03	127.76
18	A	525	PGV	C01-O03-C19	-2.64	109.47	116.85
22	C	525	CHD	C14-C8-C9	-2.63	106.00	109.62
25	P	1264	PEK	O03-C21-C22	-2.55	104.12	111.90
17	N	515	HEA	C26-C15-C14	-2.55	118.49	123.50
22	C	525	CHD	C16-C17-C13	-2.55	101.06	103.60
22	O	229	CHD	O3-C3-C4	-2.55	104.79	109.86
17	N	516	HEA	CAA-C2A-C1A	-2.49	124.30	127.01
20	B	521	TGL	CA8-CA7-CA6	-2.49	101.70	114.53
26	P	1270	CDL	OB6-CB5-C51	-2.48	106.14	111.53
25	P	1264	PEK	C3-C2-C1	-2.47	103.91	113.59
17	N	515	HEA	CMB-C2B-C1B	-2.44	124.32	128.36
20	N	1521	TGL	CA8-CA7-CA6	-2.40	102.13	114.53
17	A	515	HEA	C17-C18-C19	-2.40	122.54	127.76
22	W	1060	CHD	C18-C13-C12	-2.39	106.76	109.09
22	O	229	CHD	C19-C10-C1	-2.39	104.19	108.20
22	O	229	CHD	C14-C8-C9	-2.38	106.35	109.62
22	B	1086	CHD	C14-C8-C9	-2.38	106.35	109.62
17	N	516	HEA	CAD-C3D-C4D	-2.35	124.46	127.01
25	C	264	PEK	C3-C2-C1	-2.32	104.49	113.59
26	C	270	CDL	C52-C51-CB5	-2.30	104.57	113.59
17	N	516	HEA	CMB-C2B-C1B	-2.23	124.67	128.36
18	A	525	PGV	O01-C1-C2	-2.23	106.67	111.53
26	T	1269	CDL	OB8-CB7-C71	-2.22	105.15	111.90
22	J	60	CHD	C19-C10-C1	-2.20	104.50	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	267	PGV	O01-C1-C2	-2.19	106.77	111.53
26	G	269	CDL	OB8-CB7-C71	-2.18	105.24	111.90
26	P	1270	CDL	C52-C51-CB5	-2.18	105.01	113.59
20	B	521	TGL	CA3-CA2-CA1	-2.18	105.02	113.59
22	C	525	CHD	C15-C14-C13	-2.18	101.43	103.60
18	N	1266	PGV	O01-C1-C2	-2.14	106.87	111.53
20	N	1521	TGL	CA6-CA5-CA4	-2.14	103.50	114.53
17	A	515	HEA	CMB-C2B-C1B	-2.13	124.83	128.36
20	N	1521	TGL	CA3-CA2-CA1	-2.11	105.31	113.59
20	B	521	TGL	CA6-CA5-CA4	-2.10	103.69	114.53
17	A	516	HEA	CMC-C2C-C1C	-2.07	124.94	128.36
22	C	525	CHD	C19-C10-C9	-2.06	108.09	111.18
25	C	265	PEK	C14-C13-C12	-2.05	105.19	112.00
20	B	521	TGL	CB9-CB8-CB7	-2.05	103.95	114.53
25	P	1265	PEK	C14-C13-C12	-2.04	105.22	112.00
22	W	1060	CHD	C19-C10-C5	-2.01	106.70	110.25
17	A	516	HEA	C3C-C4C-NC	2.00	111.80	109.21
25	C	265	PEK	P-O12-C04	2.02	133.06	121.50
18	Z	1524	PGV	O01-C02-C03	2.03	115.51	108.36
20	B	521	TGL	C10-CB9-CB8	2.03	125.02	114.53
22	C	271	CHD	C14-C8-C7	2.03	114.56	111.74
22	P	1525	CHD	C9-C11-C12	2.04	116.94	114.36
17	N	515	HEA	CMC-C2C-C3C	2.04	129.08	125.09
22	J	60	CHD	C6-C5-C4	2.04	113.33	111.05
22	W	1060	CHD	C9-C11-C12	2.05	116.95	114.36
22	B	1086	CHD	C17-C13-C14	2.07	102.14	100.05
26	P	1270	CDL	OB6-CB5-OB7	2.08	129.25	123.67
20	N	1521	TGL	OG1-CG1-CG2	2.09	114.31	108.69
22	P	1271	CHD	C1-C2-C3	2.09	113.83	110.43
25	P	1265	PEK	P-O12-C04	2.10	133.48	121.50
20	N	1521	TGL	C10-CB9-CB8	2.11	125.42	114.53
22	C	271	CHD	C1-C2-C3	2.11	113.86	110.43
17	A	515	HEA	C20-C19-C18	2.12	125.07	121.05
22	O	229	CHD	C1-C2-C3	2.13	113.89	110.43
20	B	521	TGL	OG2-CG2-CG3	2.14	115.90	108.36
22	P	1525	CHD	C1-C10-C5	2.16	111.35	107.81
22	B	1086	CHD	C5-C6-C7	2.16	116.84	114.44
22	J	60	CHD	C9-C11-C12	2.16	117.09	114.36
20	Q	1523	TGL	CG2-OG2-CB1	2.17	123.09	117.89
26	G	269	CDL	C19-C18-C17	2.17	125.73	114.53
20	L	522	TGL	CC7-CC6-CC5	2.17	125.75	114.53
25	C	264	PEK	O03-C21-O04	2.18	129.13	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	521	TGL	OG1-CG1-CG2	2.19	114.58	108.69
22	P	1271	CHD	C11-C12-C13	2.19	113.42	111.20
25	P	1265	PEK	O03-C01-C02	2.21	114.65	108.69
26	T	1269	CDL	C19-C18-C17	2.22	125.97	114.53
22	P	1525	CHD	C1-C2-C3	2.23	114.05	110.43
20	Q	1523	TGL	CB4-CB3-CB2	2.24	121.50	113.29
22	O	229	CHD	C9-C11-C12	2.24	117.19	114.36
25	C	265	PEK	O03-C01-C02	2.25	114.75	108.69
20	N	1521	TGL	OG2-CG2-CG3	2.26	116.32	108.36
26	G	269	CDL	OB8-CB6-CB4	2.26	114.77	108.69
17	A	515	HEA	C27-C19-C20	2.26	118.86	115.41
25	T	263	PEK	C14-C13-C12	2.27	119.54	112.00
20	D	523	TGL	CB4-CB3-CB2	2.27	121.60	113.29
26	C	270	CDL	OB6-CB5-OB7	2.28	129.78	123.67
17	A	515	HEA	C4B-C3B-C11	2.28	129.49	127.01
20	L	522	TGL	C13-C12-C11	2.28	126.33	114.53
22	B	1086	CHD	C5-C4-C3	2.29	116.32	112.91
20	N	1522	TGL	C20-CA9-CA8	2.29	126.37	114.53
25	P	1264	PEK	O03-C21-O04	2.29	129.41	123.49
20	L	522	TGL	C20-CA9-CA8	2.30	126.41	114.53
17	N	516	HEA	C26-C15-C16	2.30	118.92	115.41
20	Q	1523	TGL	CB3-CB2-CB1	2.31	122.67	113.59
20	N	1522	TGL	OG1-CG1-CG2	2.31	114.91	108.69
20	D	523	TGL	CG2-OG2-CB1	2.32	123.47	117.89
17	N	515	HEA	C20-C19-C18	2.33	125.47	121.05
18	N	1266	PGV	O03-C01-C02	2.35	115.00	108.69
26	T	1269	CDL	OB8-CB6-CB4	2.37	115.07	108.69
25	G	1263	PEK	C14-C13-C12	2.37	119.89	112.00
22	W	1060	CHD	C1-C2-C3	2.38	114.29	110.43
20	L	522	TGL	OG1-CG1-CG2	2.38	115.10	108.69
20	Q	1523	TGL	OG2-CG2-CG1	2.39	116.77	108.36
25	P	1265	PEK	C24-C23-C22	2.41	122.13	113.29
17	N	516	HEA	C21-C20-C19	2.41	120.57	112.71
17	A	516	HEA	C21-C20-C19	2.41	120.58	112.71
26	T	1269	CDL	C20-C19-C18	2.42	127.01	114.53
23	P	1272	DMU	C10-O7-C3	2.43	124.34	118.01
23	C	272	DMU	C10-O7-C3	2.43	124.36	118.01
17	A	516	HEA	CMC-C2C-C3C	2.44	129.85	125.09
20	N	1522	TGL	C13-C12-C11	2.46	127.24	114.53
22	W	1060	CHD	C14-C8-C7	2.46	115.16	111.74
22	J	60	CHD	C1-C2-C3	2.47	114.43	110.43
20	D	523	TGL	OG2-CG2-CG1	2.48	117.08	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C14-C8-C7	2.48	115.19	111.74
26	P	1270	CDL	OA8-CA6-CA4	2.49	115.39	108.69
20	N	1521	TGL	CG3-CG2-CG1	2.49	117.90	112.07
26	G	269	CDL	C20-C19-C18	2.50	127.43	114.53
22	P	1271	CHD	C16-C15-C14	2.50	110.16	105.12
22	P	1271	CHD	O12-C12-C13	2.50	115.17	111.11
22	B	1086	CHD	C9-C11-C12	2.51	117.53	114.36
23	M	526	DMU	O7-C10-O1	2.53	117.09	110.68
20	D	523	TGL	CB3-CB2-CB1	2.54	123.59	113.59
17	N	516	HEA	C3C-C4C-NC	2.55	112.50	109.21
20	L	522	TGL	C10-CB9-CB8	2.55	127.72	114.53
20	D	523	TGL	OG2-CG2-CG3	2.56	117.36	108.36
22	O	229	CHD	C1-C10-C5	2.59	112.06	107.81
20	N	1522	TGL	C10-CB9-CB8	2.59	127.89	114.53
20	N	1522	TGL	CC4-CC3-CC2	2.60	122.82	113.29
17	A	516	HEA	CBD-CAD-C3D	2.61	117.20	112.53
18	C	268	PGV	O03-C01-C02	2.62	115.75	108.69
17	N	515	HEA	C4B-C3B-C11	2.62	129.86	127.01
22	C	271	CHD	C16-C15-C14	2.63	110.42	105.12
25	C	265	PEK	C24-C23-C22	2.64	122.96	113.29
26	G	269	CDL	C23-C22-C21	2.64	128.19	114.53
23	Z	1526	DMU	C10-O7-C3	2.65	124.93	118.01
22	W	1060	CHD	C4-C5-C10	2.66	115.59	112.66
18	P	1268	PGV	O03-C01-C02	2.66	115.86	108.69
20	L	522	TGL	CC4-CC3-CC2	2.67	123.07	113.29
26	C	270	CDL	OA8-CA6-CA4	2.67	115.88	108.69
22	P	1271	CHD	C15-C16-C17	2.67	110.51	105.12
22	C	525	CHD	C2-C1-C10	2.68	117.62	112.84
20	B	521	TGL	CG3-CG2-CG1	2.69	118.36	112.07
22	B	1086	CHD	C1-C10-C5	2.69	112.22	107.81
26	T	1269	CDL	C23-C22-C21	2.70	128.48	114.53
22	C	271	CHD	C15-C16-C17	2.71	110.58	105.12
22	W	1060	CHD	C15-C16-C17	2.71	110.59	105.12
23	C	272	DMU	O1-C10-C5	2.72	115.85	110.28
22	B	1086	CHD	C1-C2-C3	2.72	114.84	110.43
22	J	60	CHD	C4-C5-C10	2.74	115.67	112.66
22	C	271	CHD	O12-C12-C13	2.76	115.59	111.11
22	J	60	CHD	C15-C16-C17	2.79	110.75	105.12
22	C	525	CHD	C10-C9-C8	2.80	114.95	111.88
22	P	1271	CHD	C6-C5-C10	2.80	115.74	112.66
22	J	60	CHD	C16-C15-C14	2.82	110.80	105.12
20	N	1522	TGL	CG2-OG2-CB1	2.83	124.68	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	271	CHD	C6-C5-C10	2.85	115.80	112.66
22	W	1060	CHD	C16-C15-C14	2.86	110.89	105.12
20	Q	1523	TGL	OG2-CG2-CG3	2.88	118.52	108.36
17	N	516	HEA	C4B-C3B-C11	2.88	130.14	127.01
26	T	1269	CDL	C22-C21-C20	2.89	129.44	114.53
20	L	522	TGL	CG2-OG2-CB1	2.90	124.85	117.89
26	G	269	CDL	C22-C21-C20	2.91	129.53	114.53
20	Q	1523	TGL	OG1-CG1-CG2	2.92	116.56	108.69
23	P	1272	DMU	O1-C10-C5	2.93	116.29	110.28
22	J	60	CHD	C14-C13-C12	2.93	110.02	107.39
22	C	525	CHD	C5-C6-C7	2.94	117.71	114.44
22	B	1086	CHD	C10-C9-C8	2.94	115.11	111.88
22	P	1525	CHD	C5-C6-C7	2.95	117.72	114.44
17	A	516	HEA	C4B-C3B-C11	2.96	130.22	127.01
23	P	1272	DMU	C8-C7-C5	2.96	116.32	110.79
23	C	272	DMU	C8-C7-C5	2.97	116.34	110.79
22	W	1060	CHD	C14-C13-C12	2.98	110.06	107.39
17	A	516	HEA	C27-C19-C20	3.01	120.00	115.41
22	W	1060	CHD	C11-C9-C10	3.04	116.95	113.79
22	C	271	CHD	C5-C6-C7	3.05	117.84	114.44
22	C	271	CHD	C5-C4-C3	3.05	117.46	112.91
20	B	521	TGL	CG3-OG3-CC1	3.08	125.47	116.85
20	N	1521	TGL	CG3-OG3-CC1	3.10	125.51	116.85
23	Z	1526	DMU	O7-C10-O1	3.11	118.55	110.68
17	N	516	HEA	C27-C19-C20	3.14	120.20	115.41
22	J	60	CHD	C11-C9-C10	3.15	117.07	113.79
22	J	60	CHD	C5-C4-C3	3.16	117.62	112.91
18	Z	1524	PGV	C02-O01-C1	3.20	125.58	117.89
22	J	60	CHD	C2-C1-C10	3.32	118.77	112.84
20	L	522	TGL	C11-C10-CB9	3.33	131.71	114.53
23	M	526	DMU	C10-O7-C3	3.35	126.76	118.01
22	W	1060	CHD	C5-C4-C3	3.39	117.96	112.91
22	P	1271	CHD	C5-C4-C3	3.39	117.96	112.91
22	P	1271	CHD	C5-C6-C7	3.40	118.23	114.44
23	P	1272	DMU	O5-C6-O16	3.43	118.32	110.05
18	A	524	PGV	C02-O01-C1	3.44	126.14	117.89
20	D	523	TGL	OG1-CG1-CG2	3.45	117.97	108.69
22	O	229	CHD	C5-C4-C3	3.46	118.06	112.91
20	N	1522	TGL	C11-C10-CB9	3.47	132.47	114.53
20	N	1522	TGL	CC3-CC2-CC1	3.50	127.34	113.59
23	C	272	DMU	O5-C6-O16	3.51	118.51	110.05
22	C	271	CHD	C1-C10-C9	3.53	117.14	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1060	CHD	C2-C1-C10	3.53	119.14	112.84
22	P	1271	CHD	C1-C10-C9	3.54	117.15	111.45
20	L	522	TGL	C16-C15-CC9	3.67	133.48	114.53
20	L	522	TGL	CC3-CC2-CC1	3.67	128.02	113.59
20	N	1522	TGL	C16-C15-CC9	3.70	133.62	114.53
22	P	1271	CHD	C4-C3-C2	3.71	115.25	110.52
22	O	229	CHD	C5-C6-C7	3.74	118.61	114.44
25	T	263	PEK	C02-O01-C1	3.74	126.86	117.89
22	O	229	CHD	C10-C9-C8	3.86	116.12	111.88
25	P	1265	PEK	C11-C10-C9	3.92	125.04	112.00
25	C	265	PEK	C11-C10-C9	3.92	125.05	112.00
25	G	1263	PEK	C02-O01-C1	3.93	127.32	117.89
22	J	60	CHD	C5-C6-C7	3.94	118.83	114.44
20	N	1522	TGL	C15-CC9-CC8	4.03	135.36	114.53
20	L	522	TGL	C15-CC9-CC8	4.09	135.65	114.53
22	P	1271	CHD	C4-C5-C10	4.11	117.18	112.66
22	C	271	CHD	C4-C3-C2	4.12	115.77	110.52
23	C	272	DMU	O5-C6-C1	4.14	118.77	110.28
22	W	1060	CHD	C5-C6-C7	4.14	119.05	114.44
23	C	272	DMU	C10-O1-C9	4.19	121.88	113.75
22	J	60	CHD	C11-C12-C13	4.21	115.47	111.20
23	M	526	DMU	O7-C3-C4	4.22	120.40	109.32
23	P	1272	DMU	C10-O1-C9	4.22	121.94	113.75
25	G	1263	PEK	O03-C01-C02	4.24	120.11	108.69
20	N	1521	TGL	CG2-OG2-CB1	4.24	128.07	117.89
23	P	1272	DMU	O5-C6-C1	4.24	118.99	110.28
25	T	263	PEK	O03-C01-C02	4.27	120.19	108.69
20	B	521	TGL	CG2-OG2-CB1	4.30	128.21	117.89
22	W	1060	CHD	C1-C10-C5	4.40	115.04	107.81
22	W	1060	CHD	C11-C12-C13	4.40	115.67	111.20
23	P	1272	DMU	O7-C10-O1	4.43	121.89	110.68
23	Z	1526	DMU	O7-C10-C5	4.46	118.97	108.10
22	C	271	CHD	C4-C5-C10	4.52	117.63	112.66
20	Q	1523	TGL	CG3-OG3-CC1	4.54	129.54	116.85
23	C	272	DMU	O7-C10-O1	4.54	122.18	110.68
22	C	525	CHD	C13-C17-C20	4.55	125.04	119.50
22	P	1271	CHD	C14-C13-C12	4.57	111.48	107.39
22	J	60	CHD	C1-C10-C5	4.67	115.49	107.81
23	M	526	DMU	O7-C10-C5	4.72	119.59	108.10
23	Z	1526	DMU	O7-C3-C4	4.82	121.98	109.32
20	D	523	TGL	CG3-OG3-CC1	4.83	130.36	116.85
22	C	271	CHD	C14-C13-C12	4.89	111.77	107.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1060	CHD	C4-C3-C2	5.00	116.90	110.52
22	P	1525	CHD	C13-C17-C20	5.05	125.65	119.50
23	M	526	DMU	O5-C6-O16	5.12	122.39	110.05
23	Z	1526	DMU	O16-C6-C1	5.15	114.55	108.04
22	J	60	CHD	C4-C3-C2	5.27	117.24	110.52
22	J	60	CHD	C9-C8-C7	5.34	118.23	111.92
23	P	1272	DMU	O7-C10-C5	5.34	121.11	108.10
23	Z	1526	DMU	O5-C6-C1	5.35	121.25	110.28
22	W	1060	CHD	C9-C8-C7	5.35	118.25	111.92
23	C	272	DMU	O7-C10-C5	5.41	121.28	108.10
23	C	272	DMU	O7-C3-C2	5.42	121.15	107.17
22	C	271	CHD	C1-C10-C5	5.47	116.79	107.81
23	M	526	DMU	O5-C6-C1	5.47	121.50	110.28
23	C	272	DMU	O5-C4-C57	5.48	120.21	106.36
22	P	1271	CHD	C1-C10-C5	5.49	116.84	107.81
23	P	1272	DMU	O5-C4-C57	5.50	120.25	106.36
23	P	1272	DMU	O7-C3-C2	5.50	121.37	107.17
22	J	60	CHD	C6-C5-C10	5.51	118.73	112.66
22	W	1060	CHD	C6-C5-C10	5.57	118.80	112.66
22	P	1271	CHD	C9-C8-C7	5.59	118.53	111.92
23	C	272	DMU	C18-O16-C6	5.60	123.73	113.94
23	Z	1526	DMU	C18-O16-C6	5.63	123.79	113.94
22	C	271	CHD	C9-C8-C7	5.68	118.63	111.92
23	C	272	DMU	O1-C9-C8	5.73	120.44	109.68
23	Z	1526	DMU	O5-C6-O16	5.78	123.97	110.05
23	P	1272	DMU	C18-O16-C6	6.01	124.44	113.94
22	W	1060	CHD	C10-C9-C8	6.11	118.58	111.88
23	P	1272	DMU	O1-C9-C8	6.12	121.18	109.68
22	J	60	CHD	C10-C9-C8	6.13	118.60	111.88
23	M	526	DMU	C18-O16-C6	6.15	124.69	113.94
23	M	526	DMU	O16-C6-C1	6.18	115.85	108.04
23	Z	1526	DMU	O5-C4-C57	6.59	123.02	106.36
23	Z	1526	DMU	O7-C3-C2	6.66	124.35	107.17
22	J	60	CHD	C13-C17-C20	6.75	127.72	119.50
23	M	526	DMU	O1-C9-C11	6.86	123.70	106.36
23	M	526	DMU	O5-C4-C57	6.87	123.72	106.36
23	Z	1526	DMU	C7-C8-C9	6.91	122.25	110.20
22	W	1060	CHD	C13-C17-C20	6.98	128.00	119.50
23	Z	1526	DMU	O1-C9-C8	6.99	122.80	109.68
23	M	526	DMU	C7-C8-C9	7.02	122.44	110.20
23	M	526	DMU	O7-C3-C2	7.10	125.48	107.17
23	M	526	DMU	O5-C4-C3	7.18	124.92	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	1526	DMU	O1-C9-C11	7.22	124.61	106.36
23	M	526	DMU	O1-C9-C8	7.38	123.54	109.68
23	Z	1526	DMU	O5-C4-C3	7.55	125.69	109.75
23	P	1272	DMU	O7-C3-C4	7.64	129.39	109.32
23	P	1272	DMU	O1-C9-C11	7.66	125.70	106.36
23	C	272	DMU	O7-C3-C4	7.84	129.92	109.32
23	C	272	DMU	O1-C9-C11	8.02	126.62	106.36
23	Z	1526	DMU	C6-O5-C4	8.07	129.41	113.75
23	M	526	DMU	C6-O5-C4	8.20	129.67	113.75
23	P	1272	DMU	O5-C4-C3	8.34	127.36	109.75
23	C	272	DMU	O5-C4-C3	8.35	127.38	109.75
23	P	1272	DMU	C6-O5-C4	8.52	130.29	113.75
23	C	272	DMU	C6-O5-C4	8.76	130.74	113.75
22	W	1060	CHD	C17-C13-C14	9.14	109.29	100.05
22	J	60	CHD	C17-C13-C14	9.48	109.63	100.05
22	C	271	CHD	C10-C9-C8	9.51	122.32	111.88
23	Z	1526	DMU	C10-C5-C7	9.92	129.53	109.97
22	P	1271	CHD	C10-C9-C8	9.95	122.80	111.88
22	P	1271	CHD	C17-C13-C14	9.96	110.12	100.05
23	M	526	DMU	C1-C2-C3	10.04	131.64	109.60
23	M	526	DMU	C10-C5-C7	10.06	129.80	109.97
23	Z	1526	DMU	C1-C2-C3	10.11	131.80	109.60
23	P	1272	DMU	C1-C2-C3	10.36	132.34	109.60
22	C	271	CHD	C17-C13-C14	10.47	110.64	100.05
23	C	272	DMU	C1-C2-C3	10.48	132.62	109.60
23	C	272	DMU	O16-C6-C1	11.07	122.02	108.04
23	P	1272	DMU	O16-C6-C1	11.18	122.16	108.04

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	M	526	DMU	C4
23	M	526	DMU	C5
23	M	526	DMU	C6
23	M	526	DMU	C2
23	M	526	DMU	C9
22	J	60	CHD	C12
22	J	60	CHD	C8
22	J	60	CHD	C9
22	J	60	CHD	C14
22	J	60	CHD	C17
23	C	272	DMU	C5

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Mol	Chain	Res	Type	Atom
23	C	272	DMU	C6
23	C	272	DMU	C9
23	C	272	DMU	C4
23	C	272	DMU	C2
23	C	272	DMU	C10
23	P	1272	DMU	C5
23	P	1272	DMU	C6
23	P	1272	DMU	C9
23	P	1272	DMU	C4
23	P	1272	DMU	C2
23	P	1272	DMU	C10
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
22	P	1271	CHD	C12
22	P	1271	CHD	C8
22	P	1271	CHD	C3
22	P	1271	CHD	C9
22	P	1271	CHD	C14
23	Z	1526	DMU	C4
23	Z	1526	DMU	C5
23	Z	1526	DMU	C6
23	Z	1526	DMU	C2
23	Z	1526	DMU	C9
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB
22	W	1060	CHD	C12
22	W	1060	CHD	C8
22	W	1060	CHD	C9
22	W	1060	CHD	C14
22	W	1060	CHD	C17
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB
22	C	271	CHD	C12
22	C	271	CHD	C8
22	C	271	CHD	C3
22	C	271	CHD	C9
22	C	271	CHD	C14
17	N	516	HEA	ND
17	N	516	HEA	NA

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Mol	Chain	Res	Type	Atom
17	N	516	HEA	NB

All (4) torsion outliers are listed below:

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

There are no ring outliers.

37 monomers are involved in 249 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	515	HEA	2	0
17	A	516	HEA	1	0
18	A	524	PGV	6	0
18	A	525	PGV	1	0
21	B	230	PSC	13	0
20	B	521	TGL	10	0
25	C	264	PEK	5	0
25	C	265	PEK	6	0
18	C	267	PGV	6	0
18	C	268	PGV	1	0
26	C	270	CDL	16	0
22	C	271	CHD	2	0
23	C	272	DMU	2	0
20	D	523	TGL	5	0
25	G	1263	PEK	7	0
26	G	269	CDL	21	0
22	J	60	CHD	2	0
20	L	522	TGL	23	0
18	N	1266	PGV	2	0
20	N	1521	TGL	14	0
20	N	1522	TGL	16	0
17	N	515	HEA	4	0
21	O	1230	PSC	12	0
22	O	229	CHD	1	0
25	P	1264	PEK	6	0
25	P	1265	PEK	6	0
18	P	1267	PGV	5	0
18	P	1268	PGV	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	P	1270	CDL	13	0
22	P	1271	CHD	2	0
23	P	1272	DMU	7	0
20	Q	1523	TGL	6	0
26	T	1269	CDL	21	0
25	T	263	PEK	8	0
22	W	1060	CHD	2	0
18	Z	1524	PGV	4	0
23	Z	1526	DMU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.19	0 100 100	16, 22, 31, 72	0
1	N	513/514 (99%)	-0.24	1 (0%) 95 93	17, 24, 34, 66	0
2	B	226/227 (99%)	-0.47	5 (2%) 65 60	18, 29, 52, 90	0
2	O	226/227 (99%)	-0.18	9 (3%) 42 36	22, 32, 61, 84	0
3	C	259/261 (99%)	-0.50	1 (0%) 93 91	19, 25, 39, 70	0
3	P	259/261 (99%)	-0.44	2 (0%) 87 85	19, 26, 40, 74	0
4	D	144/147 (97%)	-0.30	4 (2%) 56 51	21, 31, 57, 86	0
4	Q	144/147 (97%)	1.04	19 (13%) 4 3	28, 42, 65, 100	0
5	E	105/109 (96%)	-0.01	2 (1%) 70 66	22, 31, 59, 101	0
5	R	105/109 (96%)	0.81	12 (11%) 7 5	25, 39, 71, 102	0
6	F	98/98 (100%)	0.26	8 (8%) 14 11	20, 32, 88, 110	0
6	S	98/98 (100%)	0.27	8 (8%) 14 11	20, 31, 93, 106	0
7	G	83/85 (97%)	0.83	17 (20%) 1 1	23, 34, 99, 107	0
7	T	83/85 (97%)	0.88	18 (21%) 1 1	23, 36, 102, 109	0
8	H	79/85 (92%)	0.25	11 (13%) 4 3	23, 35, 90, 108	0
8	U	79/85 (92%)	0.42	10 (12%) 5 4	27, 39, 91, 110	0
9	I	72/73 (98%)	0.35	5 (6%) 20 16	25, 44, 65, 85	0
9	V	72/73 (98%)	0.66	7 (9%) 10 7	24, 49, 68, 94	0
10	J	58/59 (98%)	0.38	5 (8%) 13 10	26, 36, 73, 99	0
10	W	58/59 (98%)	0.47	8 (13%) 4 3	26, 38, 75, 106	0
11	K	49/56 (87%)	-0.13	1 (2%) 68 64	27, 36, 50, 66	0
11	X	49/56 (87%)	0.84	5 (10%) 9 6	35, 41, 60, 76	0
12	L	46/47 (97%)	-0.36	2 (4%) 39 32	22, 28, 52, 87	0
12	Y	46/47 (97%)	-0.28	1 (2%) 65 60	26, 34, 65, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.07	4 (9%) 11 8	23, 28, 75, 103	0
13	Z	43/46 (93%)	0.35	5 (11%) 6 5	31, 36, 80, 106	0
All	All	3550/3614 (98%)	-0.01	170 (4%) 34 28	16, 29, 64, 110	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	26.1
4	Q	6	VAL	25.0
4	Q	4	SER	19.3
6	S	97	ALA	17.2
6	F	96	LEU	12.2
6	F	98	HIS	12.1
6	S	94	HIS	12.0
6	F	1	ALA	11.9
6	F	97	ALA	9.8
10	W	58	LYS	9.5
6	F	2	SER	9.0
6	S	98	HIS	9.0
13	Z	43	SER	8.9
9	V	3	ALA	8.9
4	Q	8	SER	8.9
7	G	1	ALA	8.6
6	S	1	ALA	8.5
5	R	5	HIS	8.3
8	U	7	LYS	8.2
5	R	109	VAL	7.9
6	S	96	LEU	7.7
8	U	8	ILE	7.6
6	F	95	GLN	7.5
7	T	1	ALA	7.4
7	T	3	ALA	7.4
10	J	58	LYS	7.3
7	T	42	ARG	7.1
7	T	5	LYS	7.1
10	J	1	PHE	7.1
7	T	4	ALA	7.0
7	G	5	LYS	6.7
5	R	79	LYS	6.6
7	T	36	TRP	6.3
7	G	4	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
10	W	1	PHE	6.3
9	I	37	PHE	6.2
9	V	2	THR	6.2
2	O	226	MET	6.2
7	T	2	SER	6.1
8	H	7	LYS	6.0
8	U	44	THR	6.0
7	G	3	ALA	6.0
5	E	5	HIS	6.0
2	O	227	LEU	6.0
7	G	2	SER	5.9
7	T	8	HIS	5.8
10	W	57	HIS	5.8
11	X	6	ALA	5.6
6	S	2	SER	5.6
13	M	43	SER	5.5
4	Q	35	ALA	5.4
9	V	5	ALA	5.3
2	O	113	TYR	5.1
6	F	94	HIS	4.9
9	V	37	PHE	4.8
4	Q	7	LYS	4.8
8	H	47	GLY	4.8
8	U	48	GLY	4.7
7	T	39	SER	4.6
13	Z	42	LYS	4.6
7	T	84	LYS	4.5
8	H	8	ILE	4.5
7	G	42	ARG	4.5
4	Q	147	LYS	4.4
7	T	6	GLY	4.4
8	H	46	LYS	4.4
4	Q	58	GLU	4.4
5	R	108	LYS	4.3
7	G	36	TRP	4.3
4	Q	51	LEU	4.3
8	H	45	ALA	4.3
8	H	44	THR	4.3
7	G	6	GLY	4.2
12	Y	47	LYS	4.2
4	D	6	VAL	4.1
8	U	9	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
7	T	9	GLY	4.0
13	Z	41	LYS	3.9
6	S	95	GLN	3.9
1	N	513	LEU	3.8
8	U	46	LYS	3.8
12	L	2	HIS	3.8
8	U	47	GLY	3.7
11	X	7	PRO	3.7
2	O	59	GLN	3.7
3	P	3	HIS	3.6
11	X	13	TYR	3.6
7	G	84	LYS	3.5
2	O	91	ASN	3.5
7	G	8	HIS	3.5
2	B	59	GLN	3.4
4	Q	33	LEU	3.4
7	G	39	SER	3.4
8	H	48	GLY	3.3
4	Q	39	ALA	3.2
9	I	2	THR	3.2
9	V	4	LEU	3.2
4	D	5	VAL	3.2
10	J	57	HIS	3.2
5	E	109	VAL	3.1
7	T	10	GLY	3.1
13	M	40	TYR	3.1
13	M	39	ASN	3.1
7	G	41	HIS	3.1
6	F	3	GLY	3.0
13	Z	40	TYR	3.0
7	G	40	GLY	3.0
7	T	40	GLY	3.0
10	W	55	PHE	2.9
5	R	86	ILE	2.9
8	U	45	ALA	2.9
11	K	6	ALA	2.9
5	R	9	GLU	2.8
8	U	10	ASN	2.8
8	H	9	LYS	2.8
9	I	4	LEU	2.8
2	O	90	ILE	2.8
10	W	52	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
5	R	83	PRO	2.7
4	Q	46	ALA	2.7
7	T	41	HIS	2.6
8	H	10	ASN	2.6
2	O	223	SER	2.5
10	J	4	ARG	2.5
4	D	147	LYS	2.5
12	L	47	LYS	2.5
10	J	52	TRP	2.5
5	R	105	GLY	2.5
4	Q	10	ASP	2.5
9	V	36	LYS	2.5
7	G	9	GLY	2.5
8	H	49	ASP	2.5
5	R	89	LEU	2.5
5	R	93	LEU	2.5
5	R	106	LEU	2.5
8	H	50	VAL	2.4
7	G	12	GLY	2.4
7	G	45	PRO	2.4
7	T	43	GLU	2.4
13	M	42	LYS	2.4
6	S	93	PRO	2.4
2	B	65	TRP	2.3
7	G	43	GLU	2.3
13	Z	39	ASN	2.3
7	T	7	ASP	2.3
2	O	224	ALA	2.3
2	B	60	GLU	2.3
10	W	56	PRO	2.2
10	W	2	GLU	2.2
11	X	23	THR	2.2
9	I	25	PHE	2.2
5	R	48	ILE	2.2
3	C	3	HIS	2.2
10	W	4	ARG	2.2
11	X	12	LYS	2.2
4	Q	52	SER	2.1
4	Q	55	GLU	2.1
3	P	37	PHE	2.1
9	I	34	PHE	2.1
9	V	34	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	Q	62	LEU	2.1
7	T	12	GLY	2.1
4	Q	31	LYS	2.0
4	Q	142	LYS	2.0
8	U	49	ASP	2.1
2	B	61	VAL	2.0
2	O	225	SER	2.0
4	D	8	SER	2.0
2	B	113	TYR	2.0
4	Q	54	ASP	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	O	1	10/11	0.93	0.15	-	37,38,47,53	0
7	TPO	T	11	11/12	0.53	0.31	-	76,84,110,112	0
2	FME	B	1	10/11	0.93	0.14	-	23,31,39,50	0
9	SAC	I	1	9/10	0.69	0.39	-	93,97,99,99	0
1	FME	N	1	10/11	0.90	0.16	-	39,43,65,69	0
9	SAC	V	1	9/10	0.51	0.49	-	99,100,104,104	0
1	FME	A	1	10/11	0.83	0.15	-	40,45,66,72	0
7	TPO	G	11	11/12	0.38	0.37	-	77,85,107,108	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
23	DMU	C	272	33/33	0.58	0.39	15.12	71,97,102,104	0
18	PGV	A	524	51/51	0.74	0.26	11.05	35,71,101,104	0
26	CDL	P	1270	100/100	0.67	0.37	9.51	42,88,101,105	0
20	TGL	L	522	63/63	0.71	0.30	9.41	34,65,79,81	0
20	TGL	N	1522	63/63	0.63	0.32	8.88	42,67,79,82	0
20	TGL	N	1521	63/63	0.78	0.24	8.00	49,67,84,86	0
26	CDL	C	270	100/100	0.73	0.38	7.76	44,87,100,106	0
22	CHD	W	1060	29/29	0.64	0.40	7.71	98,104,106,108	0
22	CHD	J	60	29/29	0.73	0.37	7.68	98,104,107,109	0
23	DMU	P	1272	33/33	0.56	0.39	7.25	73,96,104,105	0
20	TGL	B	521	63/63	0.80	0.23	7.23	49,64,85,90	0
18	PGV	Z	1524	51/51	0.78	0.27	6.79	38,71,101,104	0
20	TGL	D	523	63/63	0.74	0.23	5.39	47,65,79,82	0
20	TGL	Q	1523	63/63	0.67	0.23	3.64	45,70,80,84	0
26	CDL	G	269	100/100	0.59	0.32	3.59	61,83,101,105	0
18	PGV	C	268	51/51	0.62	0.39	2.85	65,84,103,106	0
21	PSC	B	230	52/52	0.61	0.35	2.80	48,84,113,116	0
26	CDL	T	1269	100/100	0.59	0.32	2.64	54,84,97,105	0
18	PGV	P	1268	51/51	0.69	0.37	2.30	65,84,104,106	0
23	DMU	Z	1526	33/33	0.89	0.19	2.15	40,49,61,64	0
21	PSC	O	1230	52/52	0.59	0.34	2.13	48,80,111,116	0
18	PGV	P	1267	51/51	0.96	0.12	1.91	23,34,59,61	0
22	CHD	P	1271	29/29	0.78	0.28	1.74	89,95,98,101	0
25	PEK	P	1264	53/53	0.95	0.13	1.65	25,44,68,72	0
25	PEK	G	1263	53/53	0.61	0.39	1.58	46,83,99,101	0
18	PGV	C	267	51/51	0.97	0.10	1.40	20,34,58,62	0
25	PEK	T	263	53/53	0.50	0.40	1.38	45,83,100,103	0
25	PEK	P	1265	53/53	0.52	0.33	1.37	46,89,107,109	0
22	CHD	C	271	29/29	0.76	0.26	1.32	87,95,96,97	0
15	MG	A	518	1/1	0.99	0.10	1.12	20,20,20,20	0
25	PEK	C	264	53/53	0.96	0.12	1.10	10,44,70,73	0
23	DMU	M	526	33/33	0.92	0.12	1.03	32,42,55,58	0
15	MG	N	1518	1/1	0.96	0.10	1.03	26,26,26,26	0
25	PEK	C	265	53/53	0.51	0.29	0.99	44,88,103,104	0
19	CUA	B	228	2/2	0.99	0.08	0.95	19,19,19,22	0
18	PGV	A	525	51/51	0.97	0.11	0.85	21,36,56,63	0
22	CHD	C	525	29/29	0.97	0.12	0.81	21,27,30,33	0
18	PGV	N	1266	51/51	0.97	0.11	0.74	20,38,55,64	0
17	HEA	N	515	60/60	0.98	0.11	0.49	18,24,41,43	0
17	HEA	A	515	60/60	0.99	0.11	0.44	12,20,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CHD	P	1525	29/29	0.96	0.10	0.24	20,27,31,34	0
17	HEA	N	516	60/60	0.99	0.10	-0.18	17,20,29,31	0
17	HEA	A	516	60/60	0.99	0.10	-0.25	15,18,29,29	0
19	CUA	O	228	2/2	0.98	0.08	-0.44	26,26,26,27	0
22	CHD	O	229	29/29	0.98	0.07	-0.46	19,22,28,32	0
22	CHD	B	1086	29/29	0.97	0.07	-0.48	20,24,30,37	0
27	ZN	S	99	1/1	0.99	0.06	-0.69	27,27,27,27	0
16	NA	N	1519	1/1	0.93	0.07	-0.71	30,30,30,30	0
27	ZN	F	99	1/1	0.99	0.06	-1.06	25,25,25,25	0
16	NA	A	519	1/1	0.96	0.06	-1.33	27,27,27,27	0
24	UNX	C	262	1/1	0.86	0.27	-	47,47,47,47	0
14	CU	A	517	1/1	1.00	0.09	-	20,20,20,20	0
24	UNX	P	1262	1/1	0.90	0.44	-	43,43,43,43	0
14	CU	N	517	1/1	1.00	0.09	-	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.