



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:45 AM GMT

PDB ID : 2DYS
Title : Bovine heart cytochrome C oxidase modified by DCCD
Authors : Shinzawa-Itoh, K.; Aoyama, H.; Muramoto, K.; Kurauchi, T.; Mizushima, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2006-09-16
Resolution : 2.20 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

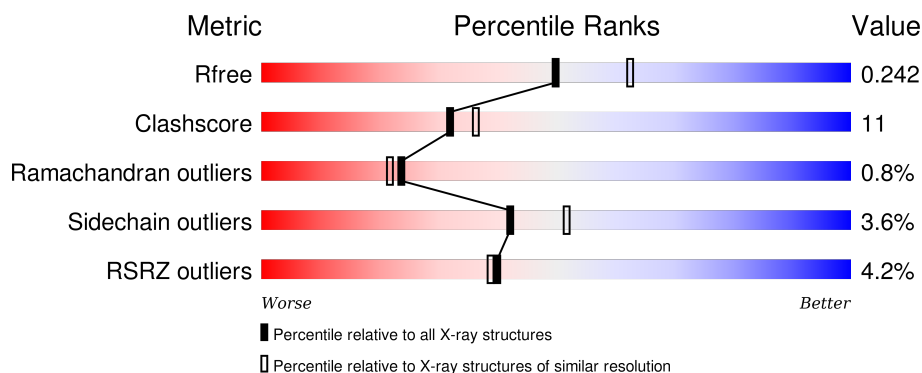
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.







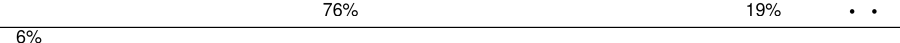



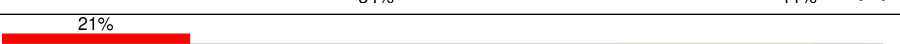
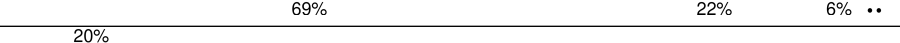




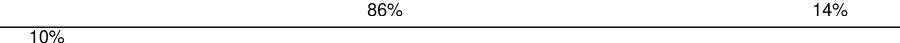




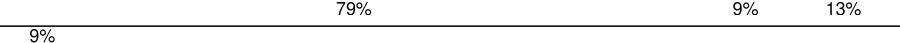

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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>84%</div> <div>15%</div> </div>
1	N	514	<div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	B	227	<div> <div>74%</div> <div>24%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
3	C	261	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MG	A	602	-	-	-	X
15	MG	N	602	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	NA	A	603	-	-	-	X
16	NA	N	603	-	-	-	X
17	HEA	A	604	X	-	-	-
17	HEA	A	605	X	-	-	-
17	HEA	N	604	X	-	-	-
17	HEA	N	605	X	-	-	-
18	PGV	A	606	-	-	-	X
18	PGV	A	607	-	-	-	X
18	PGV	C	308	-	-	-	X
18	PGV	N	608	-	-	-	X
18	PGV	P	308	-	-	-	X
20	TGL	B	302	-	-	-	X
20	TGL	D	201	-	-	-	X
20	TGL	L	101	-	-	X	X
20	TGL	N	606	-	-	-	X
20	TGL	N	607	-	-	-	X
20	TGL	O	303	-	-	-	X
21	PSC	B	303	-	-	X	X
21	PSC	O	304	-	-	X	X
22	CHD	C	310	X	-	-	-
22	CHD	J	101	X	-	-	X
22	CHD	P	310	X	-	-	X
22	CHD	W	101	X	-	-	X
23	DCW	C	301	-	-	X	-
24	DMU	C	302	X	-	-	X
24	DMU	M	101	X	-	-	-
24	DMU	P	302	X	-	-	X
24	DMU	Z	101	X	-	-	X
26	PEK	G	102	-	-	-	X
26	PEK	T	101	-	-	-	X
27	CDL	C	309	-	-	-	X
27	CDL	G	101	-	-	-	X
27	CDL	P	309	-	-	-	X
27	CDL	T	102	-	-	X	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32170 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
			2109	1412	336	349	12			
3	P	259	Total	C	N	O	S	0	0	0
			2109	1412	336	349	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		

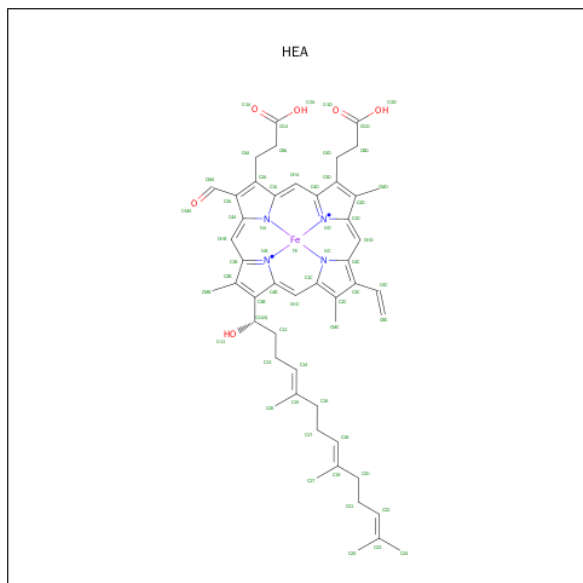
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

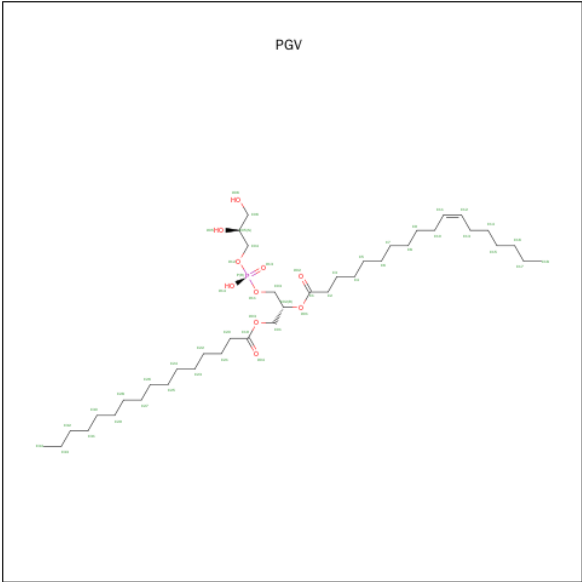
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

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



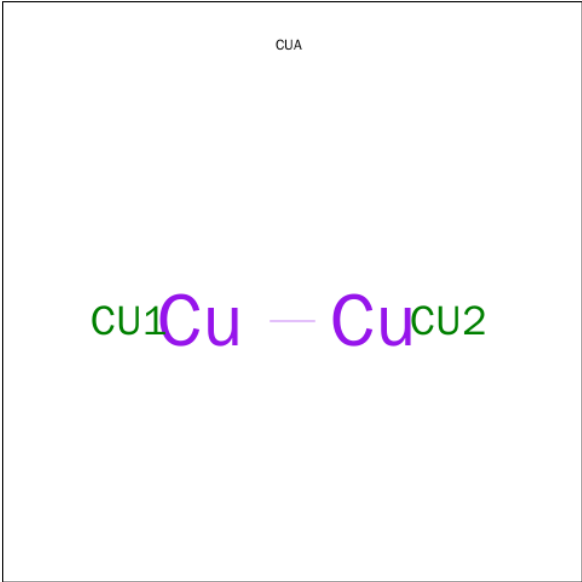
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- 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).



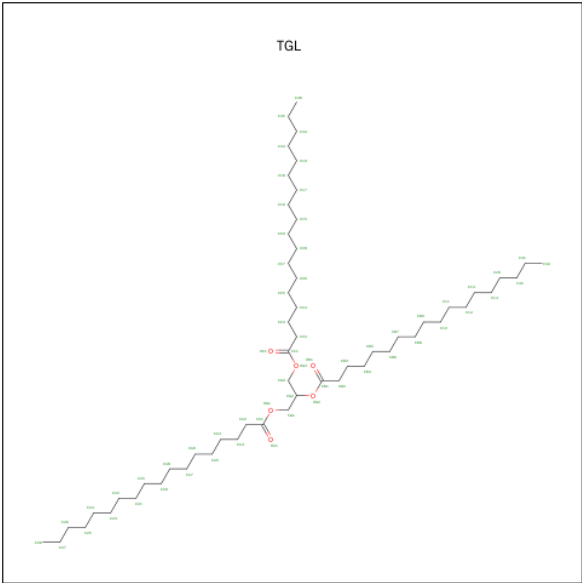
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- 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).



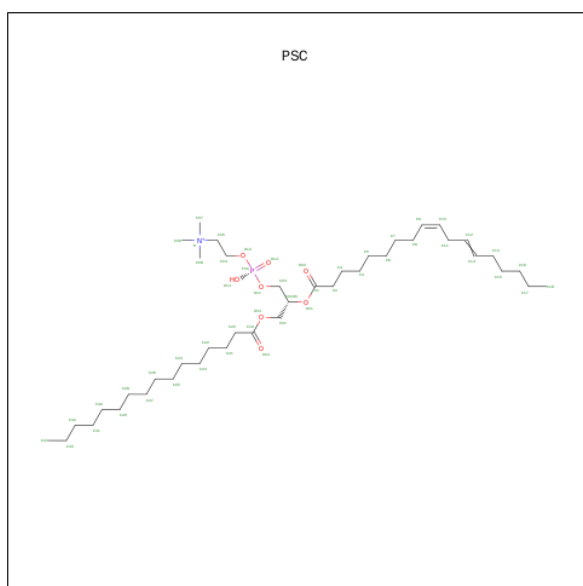
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		

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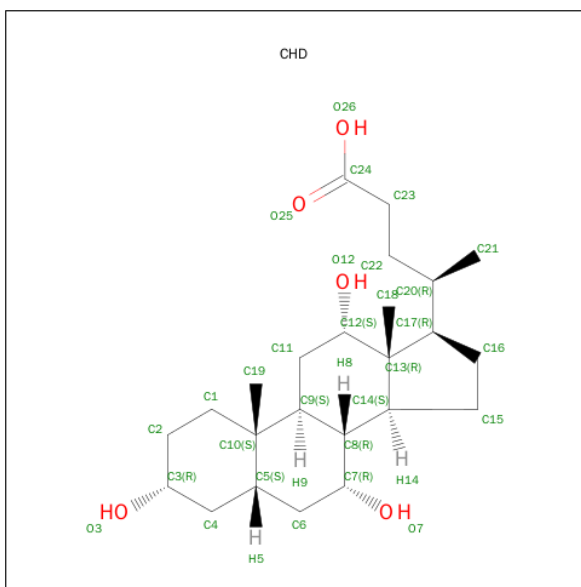
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	O	1	Total	C	O	0	0
			63	57	6		

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



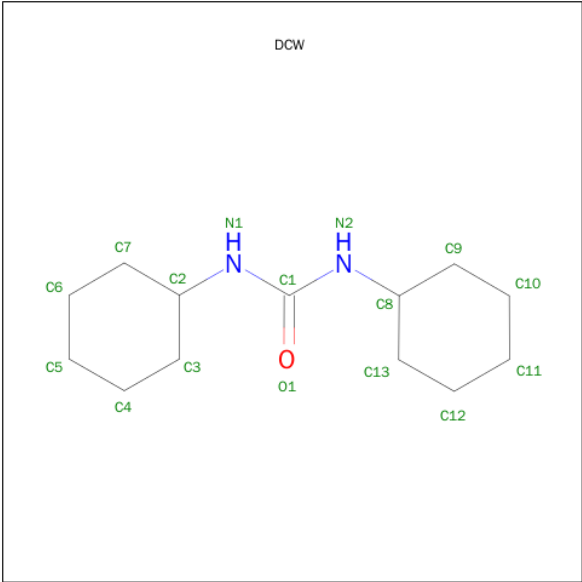
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



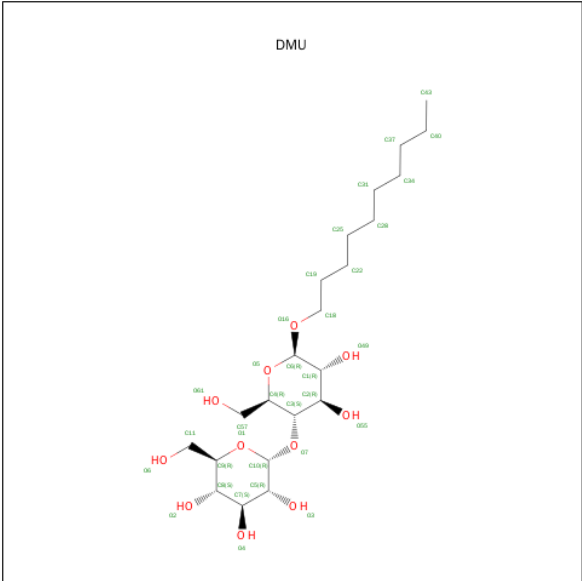
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is DICYCLOHEXYLUREA (three-letter code: DCW) (formula: $C_{13}H_{24}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	C	1	Total	C	N	O	0	0
			16	13	2	1		
23	P	1	Total	C	N	O	0	0
			16	13	2	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		

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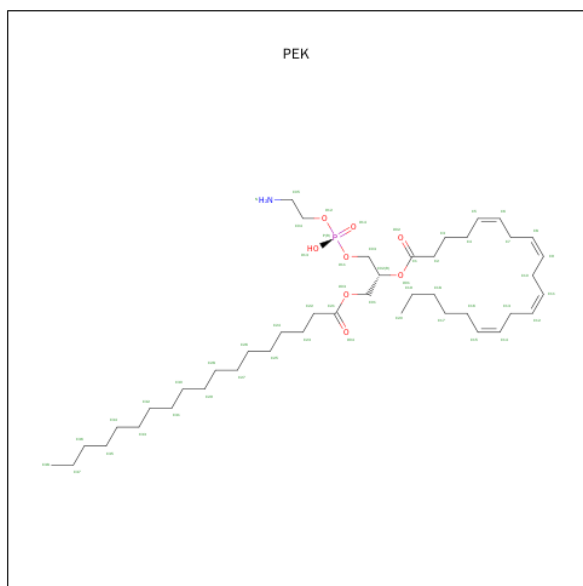
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

- Molecule 26 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).



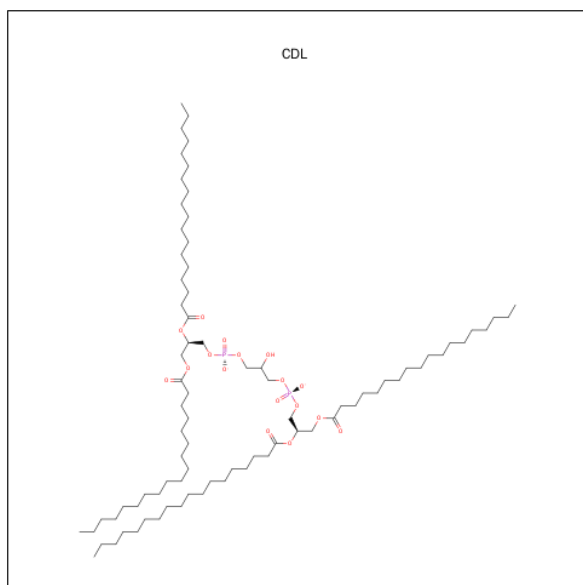
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	199	Total O 199 199	0	0
29	B	119	Total O 119 119	0	0
29	C	82	Total O 82 82	0	0
29	D	79	Total O 79 79	0	0
29	E	58	Total O 58 58	0	0
29	F	64	Total O 64 64	0	0
29	G	35	Total O 35 35	0	0
29	H	39	Total O 39 39	0	0
29	I	29	Total O 29 29	0	0
29	J	14	Total O 14 14	0	0
29	K	21	Total O 21 21	0	0
29	L	17	Total O 17 17	0	0
29	M	14	Total O 14 14	0	0
29	N	176	Total O 176 176	0	0
29	O	103	Total O 103 103	0	0
29	P	74	Total O 74 74	0	0
29	Q	46	Total O 46 46	0	0
29	R	41	Total O 41 41	0	0
29	S	56	Total O 56 56	0	0
29	T	30	Total O 30 30	0	0
29	U	39	Total O 39 39	0	0

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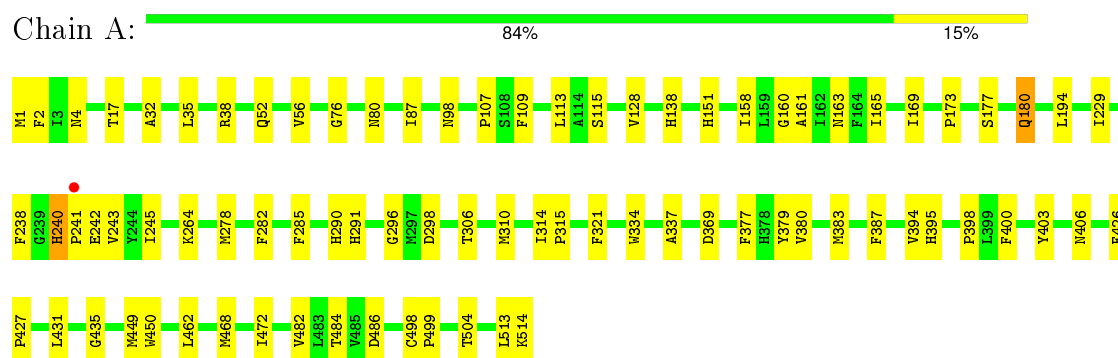
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	V	19	Total 19	O 19	0	0
29	W	14	Total 14	O 14	0	0
29	X	17	Total 17	O 17	0	0
29	Y	13	Total 13	O 13	0	0
29	Z	10	Total 10	O 10	0	0

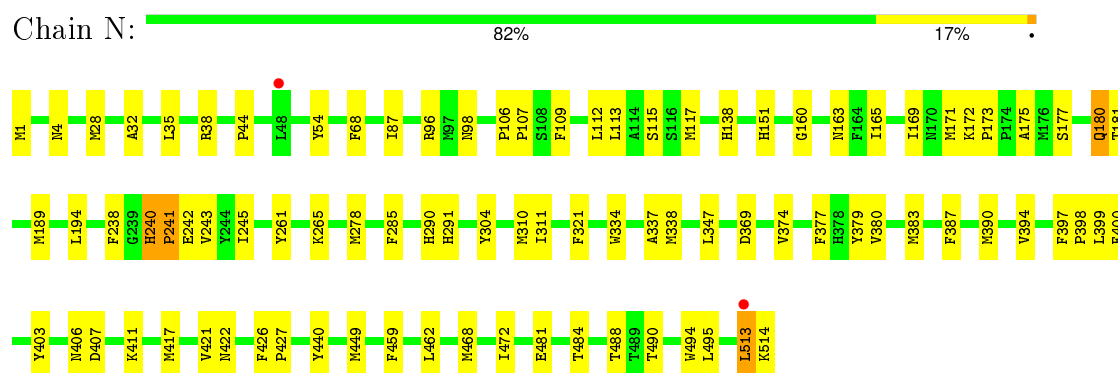
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

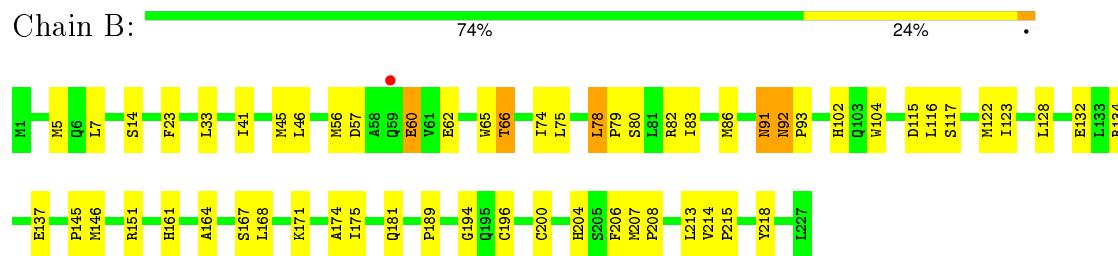
• Molecule 1: Cytochrome c oxidase subunit 1



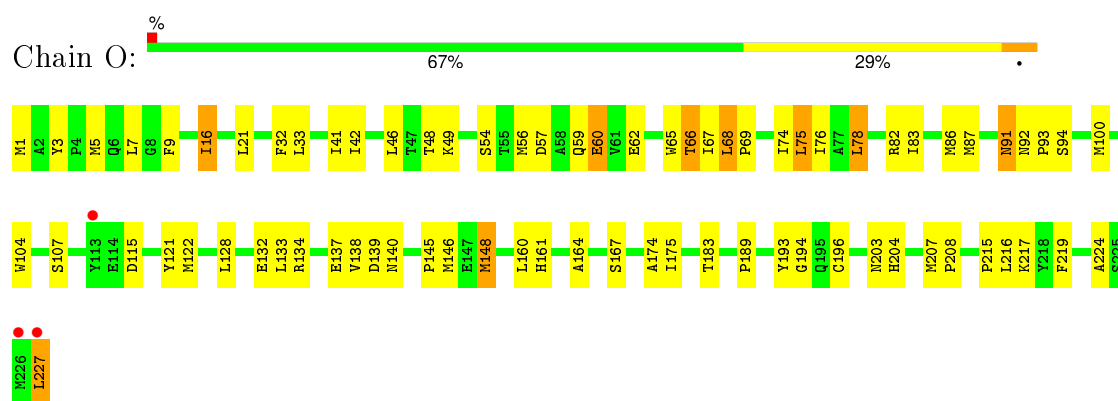
• Molecule 1: Cytochrome c oxidase subunit 1



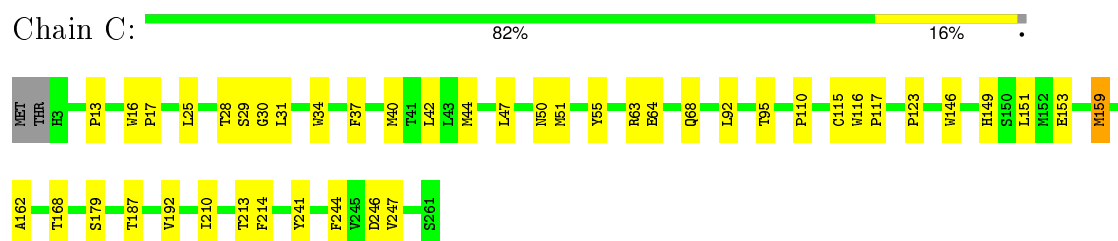
• Molecule 2: Cytochrome c oxidase subunit 2



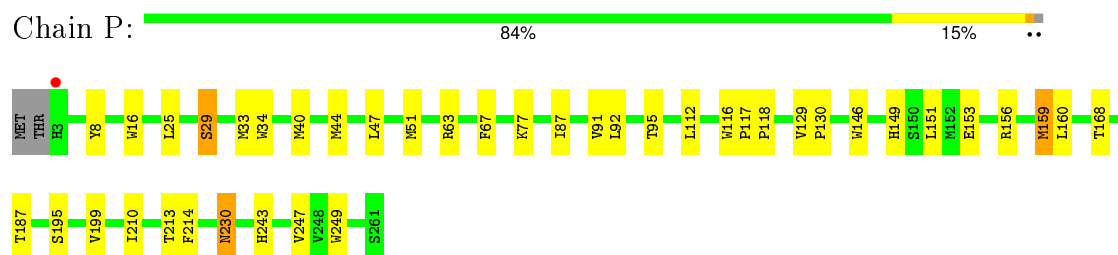
• Molecule 2: Cytochrome c oxidase subunit 2



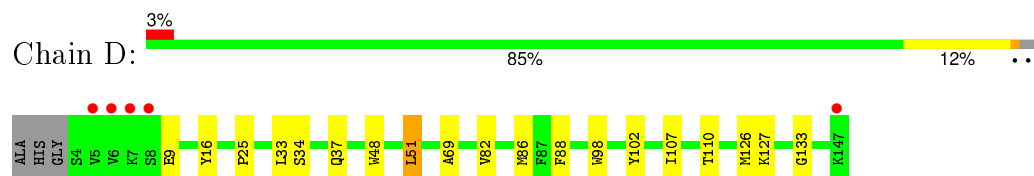
- Molecule 3: Cytochrome c oxidase subunit 3



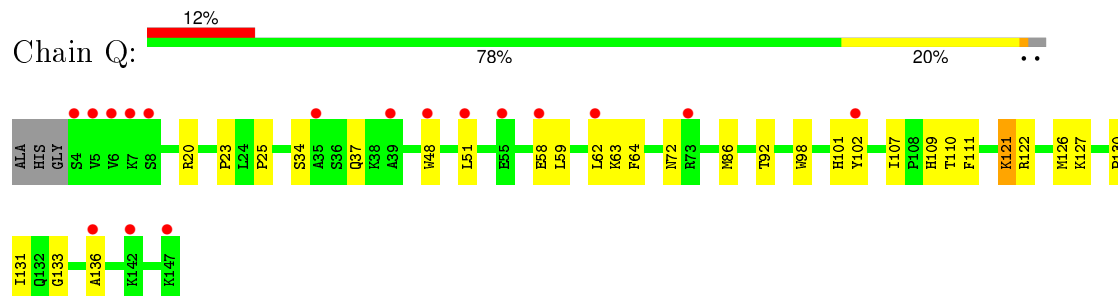
- Molecule 3: Cytochrome c oxidase subunit 3



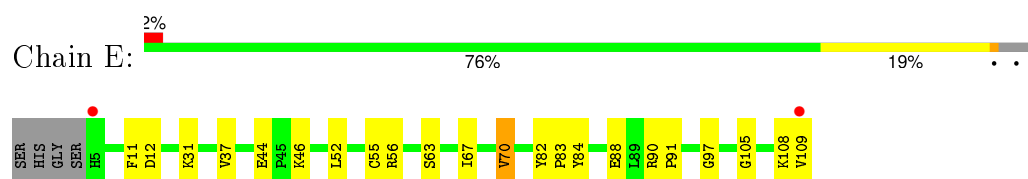
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



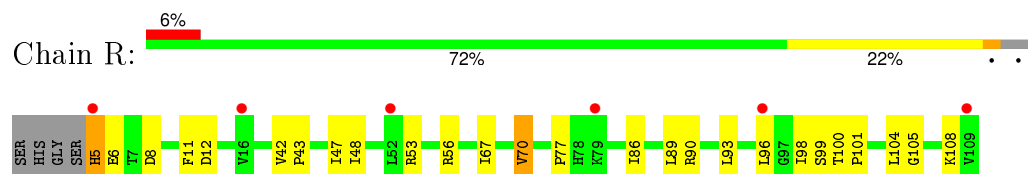
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



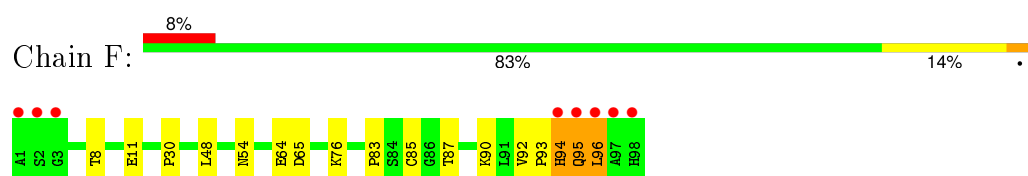
- Molecule 5: Cytochrome c oxidase polypeptide Va



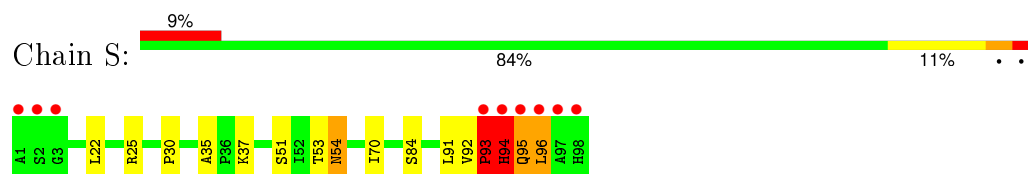
- Molecule 5: Cytochrome c oxidase polypeptide Va



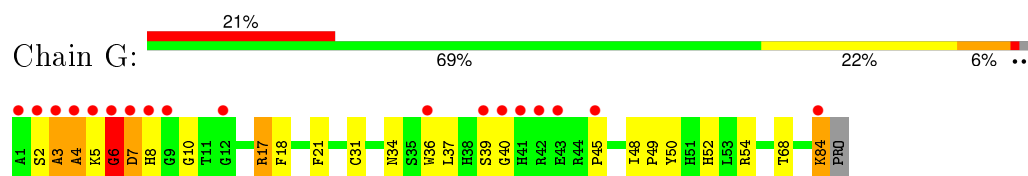
- Molecule 6: Cytochrome c oxidase polypeptide Vb



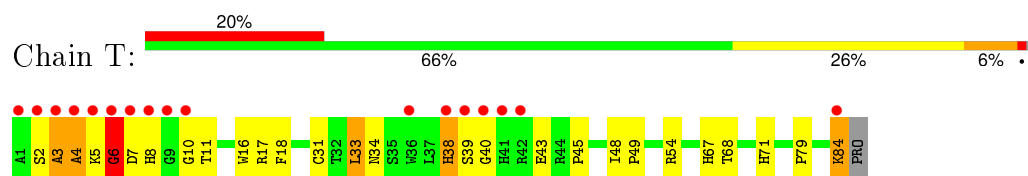
- Molecule 6: Cytochrome c oxidase polypeptide Vb



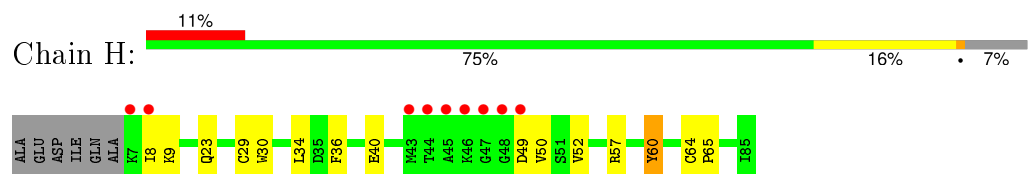
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



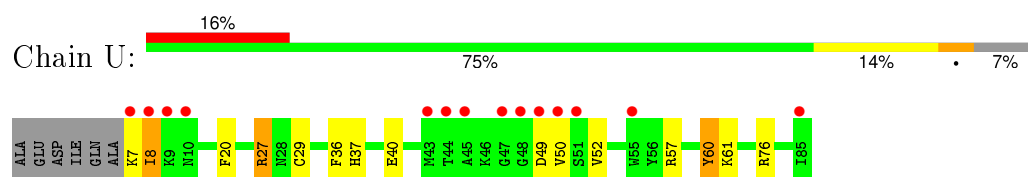
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



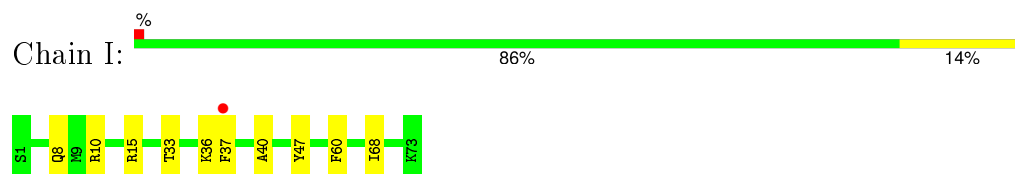
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



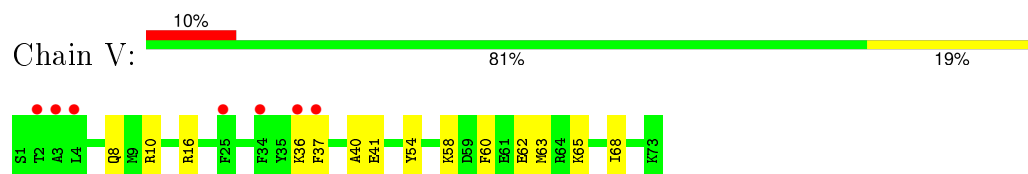
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



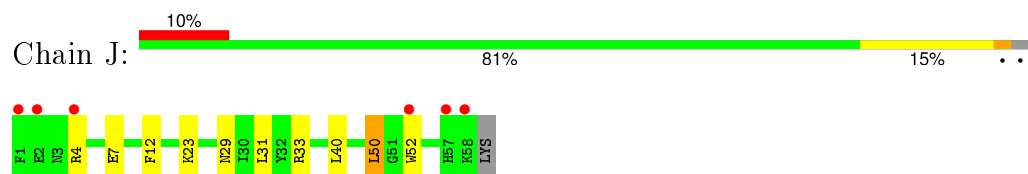
- Molecule 9: Cytochrome c oxidase polypeptide VIc



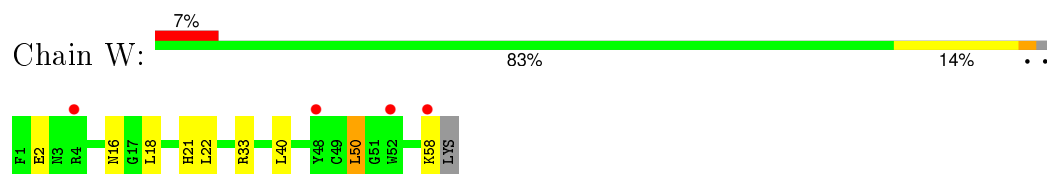
- Molecule 9: Cytochrome c oxidase polypeptide VIc



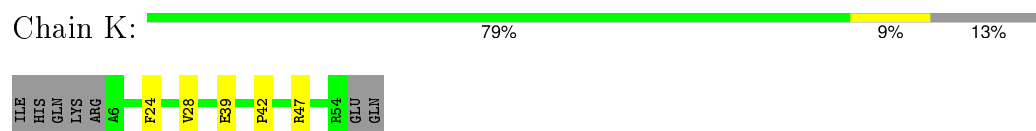
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



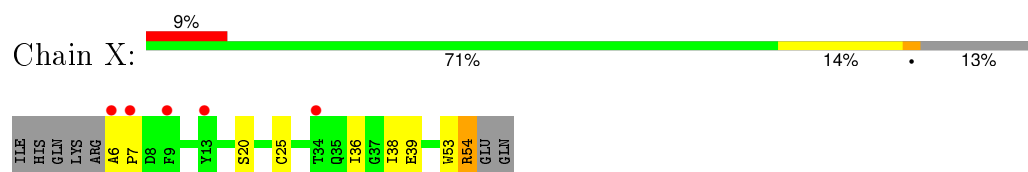
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart




- Molecule 11: Cytochrome c oxidase polypeptide VIIb



- Molecule 11: Cytochrome c oxidase polypeptide VIIb




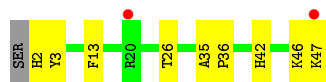
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  81% 17%



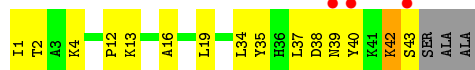
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  4% 79% 19%



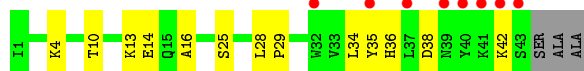
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  7% 61% 30% 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  17% 65% 28% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.13Å 207.23Å 178.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 58.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 99.3 (58.85-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.242 0.206 , 0.242	Depositor DCC
R_{free} test set	16858 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.0	EDS
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 340546 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32170	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, DCW, 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	0.59	0/4156	0.72	1/5678 (0.0%)
1	N	0.55	0/4156	0.69	0/5678
2	B	0.56	0/1860	0.79	0/2534
2	O	0.55	0/1860	0.80	1/2534 (0.0%)
3	C	0.59	0/2196	0.64	0/3003
3	P	0.56	0/2196	0.64	0/3003
4	D	0.59	0/1229	0.73	2/1658 (0.1%)
4	Q	0.59	0/1229	0.69	1/1658 (0.1%)
5	E	0.53	0/871	0.69	0/1182
5	R	0.54	0/871	0.71	1/1182 (0.1%)
6	F	0.54	0/765	0.84	2/1038 (0.2%)
6	S	0.54	0/765	0.85	2/1038 (0.2%)
7	G	0.61	0/690	0.76	1/937 (0.1%)
7	T	0.60	0/690	0.79	2/937 (0.2%)
8	H	0.53	0/682	0.70	0/921
8	U	0.49	0/682	0.68	0/921
9	I	0.56	0/605	0.65	0/802
9	V	0.57	0/605	0.62	0/802
10	J	0.51	0/471	0.67	0/636
10	W	0.51	0/471	0.72	0/636
11	K	0.56	0/398	0.70	0/546
11	X	0.50	0/398	0.68	0/546
12	L	0.59	0/393	0.61	0/526
12	Y	0.52	0/393	0.64	0/526
13	M	0.55	0/345	0.65	0/470
13	Z	0.53	0/345	0.66	0/470
All	All	0.56	0/29322	0.71	13/39862 (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	2
9	I	0	1
All	All	0	4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	33	LEU	CA-CB-CG	6.86	131.08	115.30
6	S	94	HIS	N-CA-C	6.48	128.49	111.00
6	F	94	HIS	N-CA-C	6.21	127.75	111.00
4	D	51	LEU	CA-CB-CG	6.02	129.15	115.30
6	F	93	PRO	N-CA-C	5.85	127.30	112.10
5	R	42	VAL	N-CA-C	-5.42	96.38	111.00
2	O	227	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	435	GLY	N-CA-C	5.36	126.50	113.10
4	Q	133	GLY	N-CA-C	5.33	126.43	113.10
4	D	133	GLY	N-CA-C	5.28	126.30	113.10
7	G	6	GLY	N-CA-C	5.15	125.98	113.10
6	S	93	PRO	N-CA-C	5.15	125.49	112.10
7	T	6	GLY	N-CA-C	5.09	125.84	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
9	I	47	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	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	69	0
1	N	4027	0	4001	72	0
2	B	1824	0	1833	44	0
2	O	1824	0	1833	57	0
3	C	2109	0	2027	40	0
3	P	2109	0	2027	40	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	25	0
5	E	852	0	845	15	0
5	R	852	0	845	16	0
6	F	748	0	728	9	0
6	S	748	0	728	12	0
7	G	675	0	644	24	0
7	T	675	0	644	28	0
8	H	662	0	623	9	0
8	U	662	0	623	12	0
9	I	601	0	613	6	0
9	V	601	0	613	12	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	4	0
11	X	384	0	366	10	0
12	L	380	0	380	13	0
12	Y	380	0	380	9	0
13	M	335	0	352	10	0
13	Z	335	0	352	8	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	5	0
17	N	120	0	108	6	0
18	A	102	0	152	16	0
18	C	102	0	152	9	0
18	N	102	0	152	13	0
18	P	102	0	152	9	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	B	63	0	110	6	0
20	D	63	0	110	6	0
20	L	63	0	110	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	126	0	220	19	0
20	O	63	0	110	7	0
21	B	52	0	80	23	0
21	O	52	0	80	21	0
22	B	29	0	39	1	0
22	C	58	0	77	1	0
22	J	29	0	39	2	0
22	O	29	0	39	0	0
22	P	58	0	78	2	0
22	W	29	0	39	4	0
23	C	16	0	23	9	0
23	P	16	0	23	8	0
24	C	33	0	37	5	0
24	M	33	0	37	1	0
24	P	33	0	37	5	0
24	Z	33	0	37	1	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	106	0	154	18	0
26	G	53	0	77	10	0
26	P	106	0	154	17	0
26	T	53	0	77	8	0
27	C	100	0	156	15	0
27	G	100	0	156	15	0
27	P	100	0	156	14	0
27	T	100	0	156	21	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	199	0	0	6	0
29	B	119	0	0	2	0
29	C	82	0	0	2	0
29	D	79	0	0	2	0
29	E	58	0	0	3	0
29	F	64	0	0	2	0
29	G	35	0	0	1	0
29	H	39	0	0	1	0
29	I	29	0	0	4	0
29	J	14	0	0	1	0
29	K	21	0	0	0	0
29	L	17	0	0	2	0
29	M	14	0	0	1	0
29	N	176	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	O	103	0	0	5	0
29	P	74	0	0	3	0
29	Q	46	0	0	2	0
29	R	41	0	0	1	0
29	S	56	0	0	3	0
29	T	30	0	0	2	0
29	U	39	0	0	0	0
29	V	19	0	0	0	0
29	W	14	0	0	2	0
29	X	17	0	0	0	0
29	Y	13	0	0	0	0
29	Z	10	0	0	1	0
All	All	32170	0	31343	655	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (655) 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)
10:W:33:ARG:HG2	22:W:101:CHD:H152	1.31	1.10
21:B:303:PSC:H343	21:B:303:PSC:H142	1.31	1.07
21:O:304:PSC:H142	21:O:304:PSC:H343	1.28	1.06
7:G:84:LYS:HD2	7:G:84:LYS:H	1.22	1.05
12:L:20:ARG:HH12	20:L:101:TGL:HC61	1.15	1.05
7:T:5:LYS:HB2	26:T:101:PEK:H362	1.39	1.04
20:O:303:TGL:H281	20:O:303:TGL:H102	1.43	1.01
4:D:34:SER:H	4:D:37:GLN:HE21	1.09	1.01
7:T:84:LYS:H	7:T:84:LYS:HD2	1.27	0.98
7:T:31:CYS:SG	27:T:102:CDL:H532	2.04	0.97
7:G:5:LYS:HB2	26:G:102:PEK:H362	1.46	0.97
20:B:302:TGL:H281	20:B:302:TGL:H102	1.45	0.97
3:C:63:ARG:HE	27:C:309:CDL:HA22	1.31	0.93
27:G:101:CDL:H541	27:G:101:CDL:H231	1.54	0.90
20:L:101:TGL:HC62	20:L:101:TGL:HC22	1.54	0.90
18:A:607:PGV:H343	23:C:301:DCW:H41C	1.54	0.89
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.89
20:N:606:TGL:HC22	20:N:606:TGL:HC62	1.54	0.88
7:G:31:CYS:SG	27:G:101:CDL:H532	2.14	0.88
18:N:609:PGV:H321	26:P:305:PEK:H361	1.53	0.87
20:O:303:TGL:C28	20:O:303:TGL:H102	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:20:ARG:NH1	20:L:101:TGL:HC61	1.91	0.85
3:P:63:ARG:HE	27:P:309:CDL:HA22	1.38	0.85
27:C:309:CDL:H191	27:C:309:CDL:H642	1.59	0.84
20:B:302:TGL:H102	20:B:302:TGL:C28	2.07	0.84
26:P:305:PEK:H102	26:P:305:PEK:H161	1.60	0.84
2:O:224:ALA:O	2:O:227:LEU:HG	1.78	0.84
26:C:305:PEK:H161	26:C:305:PEK:H102	1.60	0.84
27:P:309:CDL:H642	27:P:309:CDL:H191	1.59	0.83
20:N:606:TGL:HC31	12:Y:13:PHE:HA	1.62	0.82
10:J:33:ARG:HG2	22:J:101:CHD:H152	1.62	0.82
27:T:102:CDL:H231	27:T:102:CDL:H541	1.60	0.82
7:G:5:LYS:HB3	1:N:278:MET:SD	2.21	0.80
18:A:607:PGV:H321	26:C:305:PEK:H361	1.63	0.79
12:L:13:PHE:HA	20:L:101:TGL:HC31	1.65	0.79
1:N:472:ILE:HG21	20:N:606:TGL:HA92	1.64	0.78
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.67	0.77
1:A:472:ILE:HG21	20:L:101:TGL:HA92	1.67	0.75
7:T:5:LYS:HG3	26:T:101:PEK:H383	1.68	0.75
2:O:57:ASP:H	21:O:304:PSC:H201	1.49	0.75
20:N:607:TGL:HC21	20:N:607:TGL:HG11	1.67	0.75
20:N:606:TGL:H202	20:N:606:TGL:H242	1.69	0.74
27:G:101:CDL:H622	18:P:308:PGV:H152	1.66	0.74
20:L:101:TGL:H242	20:L:101:TGL:H202	1.69	0.74
27:G:101:CDL:H541	27:G:101:CDL:C23	2.19	0.73
20:D:201:TGL:HG11	20:D:201:TGL:HC21	1.69	0.73
1:A:321:PHE:CD2	21:B:303:PSC:H341	2.23	0.73
7:G:84:LYS:H	7:G:84:LYS:CD	1.98	0.73
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.53	0.73
3:P:25:LEU:O	3:P:29:SER:HB2	1.89	0.72
2:B:65:TRP:CZ3	21:B:303:PSC:H331	2.23	0.72
7:G:5:LYS:HG3	26:G:102:PEK:H383	1.71	0.72
21:B:303:PSC:C07	9:I:10:ARG:HH21	2.02	0.71
4:D:34:SER:H	4:D:37:GLN:NE2	1.84	0.71
1:N:113:LEU:CD1	20:N:606:TGL:H292	2.21	0.71
21:O:304:PSC:H222	21:O:304:PSC:H21	1.71	0.71
21:B:303:PSC:H222	21:B:303:PSC:H21	1.73	0.70
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.73	0.70
29:O:500:HOH:O	8:U:61:LYS:HE3	1.91	0.70
1:N:321:PHE:CD2	21:O:304:PSC:H341	2.27	0.69
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.73	0.69
7:T:38:HIS:NE2	27:T:102:CDL:H111	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:TRP:HZ2	24:C:302:DMU:H29	1.57	0.69
21:B:303:PSC:H072	9:I:10:ARG:HH21	1.57	0.69
1:A:113:LEU:CD1	20:L:101:TGL:H292	2.23	0.69
18:C:308:PGV:H152	27:T:102:CDL:H622	1.74	0.69
7:T:84:LYS:H	7:T:84:LYS:CD	2.05	0.69
26:P:305:PEK:H71	26:P:305:PEK:H32	1.73	0.69
20:B:302:TGL:H201	20:B:302:TGL:H241	1.75	0.69
7:T:45:PRO:HD2	29:T:204:HOH:O	1.92	0.68
2:O:56:MET:HA	21:O:304:PSC:C20	2.24	0.68
6:S:94:HIS:CD2	6:S:95:GLN:N	2.61	0.68
1:N:334:TRP:CZ3	20:N:607:TGL:HA51	2.29	0.68
1:A:379:TYR:O	1:A:383:MET:HB2	1.93	0.68
1:N:1:FME:HCN	1:N:4:ASN:H	1.59	0.68
6:S:94:HIS:CG	6:S:95:GLN:H	2.08	0.67
1:N:321:PHE:CZ	21:O:304:PSC:H171	2.30	0.67
26:C:305:PEK:H32	26:C:305:PEK:H71	1.75	0.67
20:O:303:TGL:H201	20:O:303:TGL:H241	1.76	0.66
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.30	0.66
9:V:58:LYS:O	9:V:62:GLU:HG3	1.95	0.66
27:T:102:CDL:C23	27:T:102:CDL:H541	2.24	0.66
1:A:113:LEU:HD12	20:L:101:TGL:H292	1.76	0.66
18:A:607:PGV:H343	23:C:301:DCW:C4	2.24	0.66
12:L:20:ARG:HH22	20:L:101:TGL:HC32	1.61	0.65
20:O:303:TGL:HC92	29:O:486:HOH:O	1.96	0.65
1:A:161:ALA:O	1:A:165:ILE:HG13	1.95	0.65
3:C:51:MET:HB3	27:C:309:CDL:H622	1.77	0.65
3:C:34:TRP:CZ2	24:C:302:DMU:H29	2.31	0.65
20:L:101:TGL:HB91	20:L:101:TGL:H361	1.79	0.64
1:N:417:MET:O	1:N:421:VAL:HG22	1.98	0.64
3:P:187:THR:HB	7:T:68:THR:HG21	1.80	0.64
7:G:45:PRO:HD2	29:G:202:HOH:O	1.97	0.64
1:A:177:SER:H	1:A:180:GLN:NE2	1.95	0.64
2:B:41:ILE:HD13	21:B:303:PSC:H342	1.79	0.64
2:O:41:ILE:CD1	21:O:304:PSC:H342	2.28	0.64
7:T:5:LYS:HD2	26:T:101:PEK:H371	1.78	0.64
27:G:101:CDL:H202	27:G:101:CDL:H522	1.80	0.63
18:C:307:PGV:H172	27:C:309:CDL:H662	1.78	0.63
26:C:306:PEK:C38	27:G:101:CDL:H273	2.28	0.63
5:R:89:LEU:O	5:R:93:LEU:HG	1.99	0.63
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.81	0.63
10:W:58:LYS:HE3	12:Y:47:LYS:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:87:ILE:O	1:N:173:PRO:HD3	1.98	0.62
3:P:210:ILE:HG23	18:P:307:PGV:H102	1.81	0.62
27:T:102:CDL:H172	27:T:102:CDL:H511	1.81	0.62
3:C:40:MET:O	3:C:44:MET:HG2	1.99	0.62
3:P:34:TRP:CZ2	24:P:302:DMU:H29	2.35	0.62
12:L:9:LYS:HG3	29:L:216:HOH:O	1.99	0.62
1:N:35:LEU:HD11	1:N:462:LEU:HD13	1.82	0.62
18:C:307:PGV:H182	27:C:309:CDL:H673	1.82	0.61
7:G:5:LYS:HD2	26:G:102:PEK:H371	1.82	0.61
18:N:608:PGV:H152	18:N:608:PGV:H321	1.81	0.61
26:P:306:PEK:C38	27:T:102:CDL:H273	2.31	0.61
27:G:101:CDL:H172	27:G:101:CDL:H511	1.82	0.61
18:A:606:PGV:H062	29:M:201:HOH:O	2.00	0.61
2:O:56:MET:HG2	21:O:304:PSC:H211	1.83	0.61
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.83	0.61
27:T:102:CDL:H202	27:T:102:CDL:H522	1.83	0.61
12:L:20:ARG:HH12	20:L:101:TGL:CC6	2.03	0.60
1:A:383:MET:O	1:A:387:PHE:HB2	2.00	0.60
2:B:14:SER:HB3	2:B:168:LEU:HD23	1.84	0.60
27:P:309:CDL:H112	29:P:467:HOH:O	2.01	0.60
29:B:2065:HOH:O	7:T:17:ARG:HD3	2.00	0.60
2:O:42:ILE:O	2:O:46:LEU:HG	2.02	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.48	0.60
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.36	0.60
1:A:240:HIS:O	1:A:243:VAL:HG22	2.01	0.60
1:A:484:THR:HB	13:M:2:THR:OG1	2.02	0.60
3:C:210:ILE:HG23	18:C:307:PGV:H102	1.82	0.60
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.38	0.59
23:P:301:DCW:H62C	18:P:307:PGV:H301	1.84	0.59
18:A:606:PGV:H321	18:A:606:PGV:H152	1.85	0.59
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.03	0.59
2:O:91:ASN:HD21	2:O:183:THR:HG21	1.68	0.59
3:C:246:ASP:HB2	29:C:467:HOH:O	2.03	0.59
10:W:33:ARG:HG2	22:W:101:CHD:C15	2.20	0.59
20:N:606:TGL:HB91	20:N:606:TGL:H361	1.83	0.58
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.85	0.58
9:V:65:LYS:O	11:X:54:ARG:NH1	2.34	0.58
2:O:56:MET:HA	21:O:304:PSC:H202	1.84	0.58
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.39	0.58
1:N:379:TYR:O	1:N:383:MET:HB2	2.03	0.58
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:MET:HA	21:B:303:PSC:C20	2.33	0.58
10:J:7:GLU:HG3	29:J:209:HOH:O	2.03	0.58
5:E:84:TYR:O	5:E:88:GLU:HG2	2.04	0.58
10:W:40:LEU:HD12	22:W:101:CHD:H183	1.87	0.57
18:P:307:PGV:H172	27:P:309:CDL:H662	1.86	0.57
1:A:278:MET:SD	7:T:5:LYS:HB3	2.44	0.57
26:C:306:PEK:H383	27:G:101:CDL:H273	1.86	0.57
18:N:609:PGV:H343	23:P:301:DCW:H41C	1.86	0.57
5:E:67:ILE:O	5:E:70:VAL:HG12	2.05	0.57
2:O:59:GLN:O	2:O:59:GLN:HG3	2.05	0.57
1:A:87:ILE:O	1:A:173:PRO:HD3	2.05	0.57
2:O:41:ILE:HD13	21:O:304:PSC:H342	1.87	0.57
1:N:151:HIS:CD2	26:P:305:PEK:H382	2.40	0.57
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.35	0.57
2:O:65:TRP:CZ3	21:O:304:PSC:H331	2.40	0.57
3:P:47:LEU:O	3:P:51:MET:HG2	2.05	0.57
18:N:608:PGV:H062	29:Z:201:HOH:O	2.04	0.56
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.87	0.56
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.88	0.56
18:P:307:PGV:H182	27:P:309:CDL:H673	1.87	0.56
2:O:146:MET:SD	2:O:189:PRO:HB3	2.45	0.56
3:P:149:HIS:O	3:P:153:GLU:HG3	2.05	0.56
18:C:307:PGV:H161	18:C:307:PGV:H12	1.85	0.56
1:N:472:ILE:HG21	20:N:606:TGL:CA9	2.32	0.56
26:P:305:PEK:H102	26:P:305:PEK:C16	2.35	0.56
3:P:213:THR:HG23	27:P:309:CDL:H762	1.87	0.56
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.87	0.56
2:B:65:TRP:HZ3	21:B:303:PSC:H331	1.71	0.56
3:P:160:LEU:HD13	22:P:310:CHD:H181	1.88	0.56
2:B:56:MET:HG2	21:B:303:PSC:H211	1.86	0.56
3:P:168:THR:HG22	26:P:306:PEK:H14	1.86	0.56
27:G:101:CDL:H231	27:G:101:CDL:C54	2.33	0.56
1:A:472:ILE:HG21	20:L:101:TGL:CA9	2.35	0.56
9:V:36:LYS:HA	9:V:40:ALA:HB3	1.87	0.56
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.40	0.56
4:D:9:GLU:HB3	29:D:376:HOH:O	2.05	0.56
12:L:24:MET:SD	20:L:101:TGL:H162	2.46	0.56
6:F:92:VAL:O	6:F:92:VAL:HG23	2.04	0.56
8:U:40:GLU:HG3	8:U:50:VAL:CG1	2.36	0.55
6:S:93:PRO:HB3	29:S:240:HOH:O	2.05	0.55
1:N:98:ASN:HB2	1:N:163:ASN:HD21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:109:HIS:HD2	29:Q:207:HOH:O	1.89	0.55
1:N:165:ILE:O	1:N:169:ILE:HG12	2.06	0.55
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.70	0.55
1:A:17:THR:OG1	20:L:101:TGL:H281	2.07	0.55
1:N:240:HIS:O	1:N:243:VAL:HG22	2.07	0.55
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.36	0.55
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.89	0.55
10:J:12:PHE:O	10:J:23:LYS:HE2	2.07	0.55
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.89	0.55
3:P:67:PHE:HE1	27:P:309:CDL:H1	1.72	0.55
12:L:20:ARG:NH2	20:L:101:TGL:HC32	2.22	0.55
2:B:78:LEU:HD12	27:T:102:CDL:H351	1.89	0.55
18:A:607:PGV:C34	23:C:301:DCW:H41C	2.33	0.55
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.42	0.55
5:E:105:GLY:O	5:E:108:LYS:HG2	2.07	0.54
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.07	0.54
21:O:304:PSC:H071	9:V:10:ARG:HE	1.71	0.54
3:P:51:MET:HB3	27:P:309:CDL:H622	1.90	0.54
7:T:34:ASN:ND2	27:T:102:CDL:H151	2.22	0.54
17:N:604:HEA:HMC1	17:N:604:HEA:HBC1	1.90	0.54
8:H:49:ASP:O	8:H:52:VAL:HG22	2.08	0.54
21:O:304:PSC:C07	9:V:10:ARG:HE	2.21	0.54
2:O:67:ILE:HD11	29:O:488:HOH:O	2.06	0.54
4:D:88:PHE:HZ	13:M:19:LEU:HD21	1.73	0.54
2:B:57:ASP:H	21:B:303:PSC:H201	1.74	0.53
18:P:307:PGV:H12	18:P:307:PGV:H161	1.90	0.53
1:A:282:PHE:HA	7:T:4:ALA:CB	2.38	0.53
1:A:334:TRP:CZ3	20:D:201:TGL:HA51	2.42	0.53
1:N:406:ASN:HD21	18:N:608:PGV:H21	1.72	0.53
20:N:606:TGL:H202	20:N:606:TGL:C24	2.38	0.53
1:N:98:ASN:HB2	1:N:163:ASN:ND2	2.23	0.53
23:C:301:DCW:C10	26:C:305:PEK:H371	2.39	0.53
3:C:213:THR:HG23	27:C:309:CDL:H762	1.90	0.53
2:B:146:MET:SD	2:B:189:PRO:HB3	2.48	0.53
1:A:377:PHE:HA	1:A:380:VAL:HG22	1.88	0.53
7:G:37:LEU:HD21	27:G:101:CDL:H361	1.91	0.53
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.23	0.53
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.91	0.53
21:B:303:PSC:H032	29:E:203:HOH:O	2.09	0.53
24:P:302:DMU:H25	26:P:305:PEK:H322	1.90	0.53
9:I:33:THR:HG22	29:I:126:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:60:TYR:C	8:H:60:TYR:CD1	2.81	0.53
8:U:40:GLU:HG3	8:U:50:VAL:HG11	1.91	0.53
3:P:34:TRP:HZ2	24:P:302:DMU:H29	1.74	0.53
7:G:2:SER:OG	26:G:102:PEK:H301	2.09	0.52
18:N:608:PGV:P	18:N:608:PGV:H061	2.49	0.52
1:N:383:MET:O	1:N:387:PHE:HB2	2.09	0.52
7:T:3:ALA:HB1	26:T:101:PEK:H382	1.91	0.52
7:G:17:ARG:HD2	29:O:401:HOH:O	2.09	0.52
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.74	0.52
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.91	0.52
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.91	0.52
27:C:309:CDL:H642	27:C:309:CDL:C19	2.36	0.52
1:N:449:MET:SD	2:O:5:MET:HG2	2.49	0.52
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.39	0.52
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	1.91	0.52
17:A:604:HEA:HMC1	17:A:604:HEA:HBC1	1.91	0.52
2:B:56:MET:HA	21:B:303:PSC:H202	1.91	0.52
1:N:514:LYS:HE2	29:S:225:HOH:O	2.10	0.52
20:L:101:TGL:H362	29:L:214:HOH:O	2.08	0.52
1:N:406:ASN:HD21	18:N:608:PGV:C2	2.23	0.52
10:W:2:GLU:HA	29:W:213:HOH:O	2.10	0.52
18:N:609:PGV:C32	26:P:305:PEK:H361	2.34	0.51
3:P:187:THR:CB	7:T:68:THR:HG21	2.39	0.51
1:N:175:ALA:CB	1:N:513:LEU:HD23	2.40	0.51
1:A:160:GLY:HA3	29:A:741:HOH:O	2.10	0.51
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.91	0.51
3:C:168:THR:HG22	26:C:306:PEK:H14	1.91	0.51
8:U:49:ASP:O	8:U:52:VAL:HG22	2.11	0.51
2:B:146:MET:HA	2:B:213:LEU:HD12	1.93	0.51
5:R:67:ILE:O	5:R:70:VAL:HG12	2.10	0.51
5:R:99:SER:HB2	5:R:104:LEU:HD21	1.91	0.51
20:L:101:TGL:H202	20:L:101:TGL:C24	2.39	0.51
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.46	0.51
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.43	0.51
7:T:3:ALA:O	7:T:4:ALA:HB2	2.11	0.51
8:U:20:PHE:CE2	8:U:27:ARG:HG2	2.39	0.51
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.93	0.51
6:F:30:PRO:O	6:F:96:LEU:HD11	2.11	0.51
20:B:302:TGL:HC82	29:B:2113:HOH:O	2.10	0.51
5:E:63:SER:O	5:E:67:ILE:HG13	2.11	0.51
2:B:62:GLU:O	2:B:66:THR:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ILE:O	2:B:45:MET:HG2	2.11	0.51
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.41	0.51
20:D:201:TGL:HG11	20:D:201:TGL:CC2	2.39	0.50
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.98	0.50
26:P:306:PEK:H383	27:T:102:CDL:H273	1.92	0.50
6:S:22:LEU:O	6:S:25:ARG:HB3	2.11	0.50
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.92	0.50
10:W:50:LEU:HD22	10:W:50:LEU:O	2.12	0.50
3:C:55:TYR:HE1	27:C:309:CDL:H521	1.77	0.50
1:N:113:LEU:HD13	20:N:606:TGL:H292	1.93	0.50
29:A:883:HOH:O	20:D:201:TGL:HG2	2.12	0.50
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.93	0.50
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.93	0.50
7:T:2:SER:OG	26:T:101:PEK:H301	2.11	0.50
26:C:306:PEK:H231	7:G:21:PHE:CD2	2.46	0.50
1:N:175:ALA:HB1	1:N:513:LEU:HD23	1.94	0.50
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.60	0.50
1:A:98:ASN:HB2	1:A:163:ASN:ND2	2.27	0.50
26:C:305:PEK:C3	26:C:305:PEK:H71	2.42	0.49
4:D:127:LYS:HD2	29:I:108:HOH:O	2.10	0.49
2:O:7:LEU:HD11	20:O:303:TGL:H161	1.92	0.49
8:U:7:LYS:O	8:U:8:ILE:HG22	2.11	0.49
26:C:305:PEK:C16	26:C:305:PEK:H102	2.38	0.49
3:P:210:ILE:HG12	18:P:307:PGV:H132	1.94	0.49
1:N:28:MET:CE	17:N:604:HEA:H271	2.43	0.49
21:B:303:PSC:H073	5:E:11:PHE:CG	2.47	0.49
18:N:609:PGV:H262	18:P:307:PGV:H292	1.94	0.49
26:C:306:PEK:H383	27:G:101:CDL:C27	2.42	0.49
8:H:40:GLU:HG3	8:H:50:VAL:HG13	1.94	0.49
1:N:400:PHE:HB3	20:N:606:TGL:H283	1.95	0.49
2:O:161:HIS:HB2	2:O:174:ALA:HB3	1.93	0.49
5:E:31:LYS:HE3	6:F:83:PRO:O	2.13	0.49
2:B:218:TYR:HE1	29:I:117:HOH:O	1.95	0.49
2:O:1:FME:SD	2:O:133:LEU:CD1	3.01	0.49
2:O:139:ASP:OD2	2:O:140:ASN:N	2.45	0.48
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.48
2:O:62:GLU:O	2:O:66:THR:HB	2.13	0.48
3:C:116:TRP:HA	3:C:117:PRO:C	2.33	0.48
1:N:347:LEU:HD13	1:N:383:MET:SD	2.52	0.48
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.13	0.48
7:G:3:ALA:O	7:G:4:ALA:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:54:TYR:HB2	29:N:768:HOH:O	2.11	0.48
24:C:302:DMU:H25	26:C:305:PEK:H322	1.94	0.48
3:P:187:THR:HG22	26:P:305:PEK:H052	1.94	0.48
29:H:138:HOH:O	8:U:8:ILE:HG21	2.14	0.48
5:E:46:LYS:HG2	29:E:238:HOH:O	2.13	0.48
2:B:102:HIS:O	2:B:104:TRP:HA	2.14	0.48
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.95	0.48
21:O:304:PSC:H62	21:O:304:PSC:H241	1.95	0.48
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.95	0.48
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.31	0.48
23:C:301:DCW:H62C	18:C:307:PGV:H301	1.96	0.48
6:S:22:LEU:HD23	6:S:25:ARG:NH1	2.28	0.48
4:Q:51:LEU:HD21	4:Q:59:LEU:CD1	2.43	0.48
2:B:82:ARG:HG2	2:B:86:MET:HE3	1.94	0.48
3:P:116:TRP:HA	3:P:117:PRO:C	2.32	0.48
9:I:36:LYS:HA	9:I:40:ALA:HB3	1.95	0.48
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.49	0.48
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.73	0.48
2:B:79:PRO:O	2:B:83:ILE:HG13	2.13	0.48
1:A:151:HIS:CD2	26:C:305:PEK:H382	2.49	0.48
20:N:607:TGL:H271	2:O:46:LEU:HD12	1.96	0.48
1:A:298:ASP:HB3	29:A:834:HOH:O	2.13	0.48
3:C:16:TRP:HA	3:C:16:TRP:CE3	2.48	0.48
18:A:607:PGV:H262	18:C:307:PGV:H292	1.96	0.47
1:A:1:FME:HCN	1:A:4:ASN:H	1.79	0.47
20:B:302:TGL:HC22	29:I:107:HOH:O	2.12	0.47
27:P:309:CDL:H642	27:P:309:CDL:C19	2.36	0.47
21:B:303:PSC:H241	21:B:303:PSC:H62	1.96	0.47
18:A:606:PGV:H061	18:A:606:PGV:P	2.54	0.47
5:E:84:TYR:CZ	5:E:88:GLU:HG3	2.49	0.47
1:A:2:PHE:HB3	29:A:890:HOH:O	2.14	0.47
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.14	0.47
5:R:105:GLY:O	5:R:108:LYS:HG2	2.14	0.47
18:N:608:PGV:H311	13:Z:16:ALA:HA	1.97	0.47
2:B:91:ASN:HD22	2:B:92:ASN:N	2.12	0.47
26:P:306:PEK:H383	27:T:102:CDL:C27	2.45	0.47
27:C:309:CDL:H602	27:C:309:CDL:H632	1.67	0.47
27:G:101:CDL:H212	1:N:311:ILE:HD12	1.97	0.47
3:C:168:THR:CG2	26:C:306:PEK:H14	2.45	0.47
3:P:210:ILE:HD13	23:P:301:DCW:H61C	1.94	0.47
1:A:406:ASN:HD21	18:A:606:PGV:C2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:177:SER:H	1:N:180:GLN:NE2	2.13	0.47
3:C:37:PHE:CD1	10:J:52:TRP:HZ3	2.33	0.47
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.96	0.47
1:N:160:GLY:HA3	29:N:740:HOH:O	2.13	0.47
6:S:54:ASN:HD22	6:S:54:ASN:C	2.18	0.47
5:E:37:VAL:HG11	5:E:70:VAL:HG21	1.97	0.47
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.49	0.47
5:R:86:ILE:HD13	5:R:86:ILE:HA	1.68	0.47
1:A:314:ILE:HB	1:A:315:PRO:CD	2.45	0.47
11:K:24:PHE:O	11:K:28:VAL:HG12	2.15	0.47
10:J:29:ASN:H	10:J:29:ASN:HD22	1.63	0.47
1:N:472:ILE:HD13	20:N:606:TGL:HA91	1.96	0.47
22:P:310:CHD:H161	29:P:469:HOH:O	2.14	0.47
1:A:1:FME:HCN	1:A:4:ASN:HB2	1.96	0.47
2:O:83:ILE:O	2:O:87:MET:HG3	2.15	0.47
6:F:85:CYS:SG	6:F:87:THR:HG23	2.55	0.47
1:A:398:PRO:HA	1:A:403:TYR:O	2.15	0.47
1:A:306:THR:O	1:A:310:MET:HG3	2.14	0.47
11:X:36:ILE:HG13	11:X:38:ILE:HG13	1.97	0.46
1:N:398:PRO:HA	1:N:403:TYR:O	2.15	0.46
26:G:102:PEK:H042	3:P:77:LYS:NZ	2.30	0.46
18:C:307:PGV:H182	27:C:309:CDL:C67	2.45	0.46
1:A:35:LEU:HD11	1:A:462:LEU:HB2	1.98	0.46
12:L:41:ARG:HD2	13:M:40:TYR:CZ	2.51	0.46
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.81	0.46
3:P:168:THR:CG2	26:P:306:PEK:H14	2.45	0.46
7:G:2:SER:O	26:G:102:PEK:H322	2.15	0.46
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.50	0.46
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.15	0.46
27:T:102:CDL:H601	27:T:102:CDL:H571	1.45	0.46
3:C:16:TRP:HE3	3:C:16:TRP:HA	1.80	0.46
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.98	0.46
20:N:607:TGL:H242	20:N:607:TGL:H212	1.75	0.46
1:A:128:VAL:HG12	1:A:128:VAL:O	2.16	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
4:Q:98:TRP:CD2	24:Z:101:DMU:H10	2.50	0.46
3:P:195:SER:O	3:P:199:VAL:HG23	2.16	0.46
1:N:407:ASP:O	1:N:411:LYS:HG3	2.15	0.46
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.51	0.46
1:N:113:LEU:HD12	20:N:606:TGL:H292	1.97	0.46
20:N:607:TGL:HG11	20:N:607:TGL:CC2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:LEU:O	3:C:95:THR:HB	2.15	0.46
1:A:400:PHE:HB3	20:L:101:TGL:H283	1.98	0.46
11:X:6:ALA:HA	11:X:7:PRO:HD2	1.86	0.46
6:F:90:LYS:HD2	29:F:244:HOH:O	2.15	0.46
1:A:321:PHE:CE2	21:B:303:PSC:H341	2.51	0.45
20:O:303:TGL:HC22	29:Q:220:HOH:O	2.16	0.45
3:C:55:TYR:CE1	27:C:309:CDL:H521	2.51	0.45
2:O:62:GLU:HB2	29:O:490:HOH:O	2.16	0.45
5:R:5:HIS:HB3	5:R:6:GLU:H	1.63	0.45
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.34	0.45
2:O:217:LYS:HA	2:O:217:LYS:HE2	1.98	0.45
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.99	0.45
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.79	0.45
21:B:303:PSC:C34	21:B:303:PSC:H142	2.23	0.45
10:J:40:LEU:HD12	22:J:101:CHD:H183	1.99	0.45
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.51	0.45
1:N:468:MET:O	1:N:472:ILE:HG13	2.16	0.45
3:C:117:PRO:HG3	3:C:123:PRO:HG2	1.99	0.45
6:F:64:GLU:O	6:F:65:ASP:HB2	2.17	0.45
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.16	0.45
1:N:310:MET:HE1	2:O:76:ILE:HB	1.98	0.45
21:B:303:PSC:H12	21:B:303:PSC:H322	1.99	0.45
21:O:304:PSC:H032	29:R:203:HOH:O	2.17	0.45
12:L:20:ARG:HH22	20:L:101:TGL:CC4	2.29	0.45
13:M:42:LYS:HA	13:M:42:LYS:CE	2.44	0.45
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.97	0.45
1:A:482:VAL:HG22	13:M:1:ILE:HD11	1.98	0.45
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.47	0.45
12:L:20:ARG:HH22	20:L:101:TGL:CC3	2.28	0.45
18:A:606:PGV:H311	13:M:16:ALA:HA	1.98	0.45
3:P:92:LEU:O	3:P:95:THR:HB	2.16	0.45
2:O:216:LEU:O	2:O:219:PHE:HB3	2.17	0.45
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.98	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.45
6:S:70:ILE:HG13	6:S:84:SER:HB3	1.98	0.45
21:B:303:PSC:H221	21:B:303:PSC:H251	1.75	0.45
1:A:165:ILE:O	1:A:169:ILE:HG12	2.16	0.45
4:D:102:TYR:CD1	13:M:35:TYR:HE1	2.35	0.45
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.82	0.45
22:C:310:CHD:H112	22:C:310:CHD:H12A	1.71	0.45
20:N:606:TGL:H272	20:N:606:TGL:H231	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.30	0.45
7:G:7:ASP:O	1:N:169:ILE:HD12	2.16	0.45
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.16	0.45
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.17	0.45
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.52	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.44
23:C:301:DCW:H101	26:C:305:PEK:C37	2.47	0.44
1:N:334:TRP:CZ2	2:O:46:LEU:HB3	2.53	0.44
10:W:16:ASN:ND2	10:W:18:LEU:HD12	2.33	0.44
1:A:264:LYS:HE2	29:A:888:HOH:O	2.15	0.44
2:B:74:ILE:HD11	27:T:102:CDL:H452	1.98	0.44
3:C:247:VAL:HG11	26:T:101:PEK:H132	1.99	0.44
7:T:38:HIS:CD2	27:T:102:CDL:HA21	2.52	0.44
1:A:406:ASN:HD21	18:A:606:PGV:H21	1.82	0.44
5:R:96:LEU:HD12	5:R:98:ILE:HD11	1.98	0.44
3:P:249:TRP:HD1	29:P:419:HOH:O	1.99	0.44
3:P:40:MET:O	3:P:44:MET:HG2	2.17	0.44
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.53	0.44
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.32	0.44
1:N:488:THR:HB	1:N:495:LEU:HD13	1.99	0.44
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.17	0.44
1:A:472:ILE:HD13	20:L:101:TGL:HA91	2.00	0.44
7:T:6:GLY:O	26:T:101:PEK:H311	2.18	0.44
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.32	0.44
8:H:30:TRP:CE2	8:H:34:LEU:HD11	2.51	0.44
18:N:609:PGV:H343	23:P:301:DCW:C4	2.47	0.44
4:Q:122:ARG:HG2	4:Q:126:MET:CE	2.47	0.44
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.99	0.44
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.80	0.44
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.97	0.44
2:O:100:MET:HB2	2:O:107:SER:OG	2.18	0.44
1:A:377:PHE:CD1	17:A:605:HEA:HAD1	2.53	0.44
3:C:30:GLY:HA2	3:C:42:LEU:HB3	2.00	0.44
7:G:84:LYS:HD2	7:G:84:LYS:N	2.07	0.44
3:C:47:LEU:O	3:C:51:MET:HG2	2.18	0.44
12:Y:26:THR:HG23	13:Z:25:SER:HB3	2.00	0.44
1:A:449:MET:SD	2:B:5:MET:HG2	2.57	0.44
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.00	0.44
6:S:30:PRO:O	6:S:96:LEU:HD11	2.18	0.44
1:A:321:PHE:CZ	21:B:303:PSC:H171	2.53	0.43
24:C:302:DMU:H30	24:C:302:DMU:O1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:PHE:CZ	13:M:19:LEU:HD21	2.53	0.43
4:D:98:TRP:CD2	24:M:101:DMU:H10	2.53	0.43
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.18	0.43
5:E:97:GLY:HA2	29:E:258:HOH:O	2.18	0.43
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.82	0.43
3:C:31:LEU:HA	3:C:31:LEU:HD23	1.89	0.43
2:O:121:TYR:O	2:O:138:VAL:HA	2.17	0.43
3:P:210:ILE:CD1	23:P:301:DCW:H52C	2.48	0.43
5:R:53:ARG:O	5:R:56:ARG:HB3	2.18	0.43
6:S:51:SER:HB2	6:S:91:LEU:HD11	2.00	0.43
27:T:102:CDL:HA62	27:T:102:CDL:H322	2.01	0.43
23:C:301:DCW:H101	26:C:305:PEK:H371	2.01	0.43
13:Z:35:TYR:HD2	13:Z:36:HIS:CE1	2.37	0.43
8:H:9:LYS:HE2	8:H:9:LYS:HB2	1.86	0.43
21:O:304:PSC:H073	5:R:11:PHE:CG	2.53	0.43
4:Q:122:ARG:HG2	4:Q:126:MET:HE3	2.00	0.43
2:O:134:ARG:HB2	4:Q:110:THR:HG21	1.99	0.43
2:O:9:PHE:HB2	2:O:21:LEU:HD21	2.00	0.43
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.72	0.43
1:N:513:LEU:HA	1:N:513:LEU:HD22	1.81	0.43
3:C:149:HIS:O	3:C:153:GLU:HG3	2.19	0.43
7:T:48:ILE:HA	7:T:49:PRO:HD3	1.80	0.43
2:O:74:ILE:O	2:O:78:LEU:HD22	2.19	0.43
5:R:100:THR:HB	5:R:101:PRO:HD2	2.00	0.43
2:O:48:THR:HB	9:V:16:ARG:CZ	2.48	0.43
3:P:210:ILE:HD13	23:P:301:DCW:C6	2.49	0.43
27:P:309:CDL:H431	29:W:206:HOH:O	2.19	0.43
4:D:82:VAL:O	4:D:86:MET:HG3	2.18	0.43
4:D:126:MET:HA	9:I:68:ILE:HD13	2.01	0.43
20:L:101:TGL:H272	20:L:101:TGL:H231	2.01	0.43
1:A:282:PHE:HZ	27:T:102:CDL:H761	1.84	0.43
27:T:102:CDL:H231	27:T:102:CDL:C54	2.40	0.43
1:N:400:PHE:HB3	20:N:606:TGL:C28	2.49	0.43
17:A:605:HEA:HAD2	17:A:605:HEA:HHA	1.85	0.43
2:O:1:FME:SD	2:O:133:LEU:HD11	2.58	0.43
1:A:468:MET:HG3	29:A:849:HOH:O	2.18	0.43
4:Q:86:MET:O	11:X:25:CYS:HB2	2.18	0.43
10:J:50:LEU:HD22	10:J:50:LEU:O	2.18	0.43
21:O:304:PSC:O01	21:O:304:PSC:H212	2.19	0.43
27:P:309:CDL:H672	27:P:309:CDL:H641	1.87	0.43
17:N:604:HEA:H271	17:N:604:HEA:H212	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.53	0.43
1:A:426:PHE:HB3	1:A:427:PRO:HD3	2.01	0.43
2:B:41:ILE:CD1	21:B:303:PSC:H342	2.45	0.43
7:T:2:SER:O	26:T:101:PEK:H322	2.19	0.43
7:T:84:LYS:N	7:T:84:LYS:HD2	2.10	0.43
3:C:55:TYR:CD1	27:C:309:CDL:H532	2.54	0.43
3:P:51:MET:SD	27:P:309:CDL:H622	2.59	0.43
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.53	0.43
2:O:1:FME:SD	2:O:133:LEU:HD13	2.59	0.43
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.37	0.43
4:D:69:ALA:O	5:E:109:VAL:HG12	2.18	0.43
3:C:151:LEU:HB2	3:C:159:MET:HG3	2.01	0.43
2:B:200:CYS:SG	2:B:204:HIS:HA	2.58	0.43
7:G:34:ASN:O	7:G:37:LEU:HB3	2.18	0.42
1:A:98:ASN:HB2	1:A:163:ASN:HD21	1.84	0.42
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.42
3:C:51:MET:SD	27:C:309:CDL:H622	2.59	0.42
20:D:201:TGL:HC51	20:D:201:TGL:HC22	1.82	0.42
18:N:608:PGV:H012	29:N:860:HOH:O	2.19	0.42
1:A:1:FME:HA	1:A:1:FME:HE2	2.01	0.42
22:B:304:CHD:H231	22:B:304:CHD:H213	1.82	0.42
1:N:321:PHE:HB3	2:O:65:TRP:CE3	2.54	0.42
1:A:76:GLY:O	1:A:80:ASN:HB2	2.19	0.42
26:G:102:PEK:H132	3:P:247:VAL:HG11	2.00	0.42
27:G:101:CDL:H601	27:G:101:CDL:H571	1.42	0.42
23:P:301:DCW:C10	26:P:305:PEK:H371	2.50	0.42
7:T:31:CYS:SG	27:T:102:CDL:H552	2.60	0.42
2:B:7:LEU:HD11	20:B:302:TGL:H161	2.02	0.42
18:A:607:PGV:H332	24:C:302:DMU:H24	2.01	0.42
24:P:302:DMU:H26	24:P:302:DMU:H18	1.80	0.42
4:Q:126:MET:HA	9:V:68:ILE:HD13	2.01	0.42
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.55	0.42
3:P:87:ILE:O	3:P:91:VAL:HG23	2.19	0.42
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.54	0.42
1:A:52:GLN:O	1:A:56:VAL:HG23	2.20	0.42
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.54	0.42
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.55	0.42
17:N:605:HEA:HAD2	17:N:605:HEA:HHA	1.82	0.42
12:Y:26:THR:HG23	13:Z:25:SER:HB2	2.02	0.42
2:B:134:ARG:HB2	4:D:110:THR:HG21	2.01	0.42
2:O:57:ASP:N	21:O:304:PSC:H201	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:609:PGV:H321	26:P:305:PEK:C36	2.37	0.42
18:A:606:PGV:H301	18:A:606:PGV:H152	2.02	0.42
3:C:241:TYR:O	3:C:244:PHE:HB3	2.19	0.42
1:A:514:LYS:HE2	29:F:226:HOH:O	2.18	0.42
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.02	0.42
26:G:102:PEK:H132	3:P:247:VAL:CG1	2.50	0.42
7:G:5:LYS:CB	26:G:102:PEK:H362	2.34	0.42
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.85	0.42
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.03	0.42
20:L:101:TGL:HB61	20:L:101:TGL:HB31	1.92	0.42
18:A:607:PGV:H182	3:C:28:THR:HG22	2.00	0.42
24:P:302:DMU:H30	24:P:302:DMU:O1	2.19	0.42
26:P:305:PEK:C3	26:P:305:PEK:H71	2.43	0.42
23:P:301:DCW:H62C	18:P:307:PGV:H281	2.02	0.42
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.20	0.42
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.84	0.42
21:O:304:PSC:H073	5:R:11:PHE:CB	2.49	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
4:Q:130:PRO:O	4:Q:136:ALA:HB2	2.20	0.41
1:N:426:PHE:HB3	1:N:427:PRO:HD3	2.01	0.41
1:A:498:CYS:HA	1:A:499:PRO:HA	1.93	0.41
6:S:92:VAL:HG23	6:S:92:VAL:O	2.19	0.41
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.68	0.41
3:P:168:THR:HG21	26:P:306:PEK:H12	2.00	0.41
1:N:422:ASN:HB3	20:O:303:TGL:H242	2.02	0.41
1:A:158:ILE:HD13	23:C:301:DCW:H121	2.01	0.41
2:O:224:ALA:O	2:O:227:LEU:CG	2.59	0.41
2:B:122:MET:SD	2:B:206:PHE:HB3	2.60	0.41
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.20	0.41
2:O:1:FME:CE	2:O:133:LEU:HD13	2.51	0.41
9:V:37:PHE:HA	9:V:41:GLU:HB2	2.02	0.41
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.01	0.41
1:N:261:TYR:CE2	1:N:337:ALA:HB3	2.55	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.81	0.41
3:P:16:TRP:HA	3:P:16:TRP:CE3	2.55	0.41
2:B:78:LEU:CD1	27:T:102:CDL:H351	2.50	0.41
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.84	0.41
21:O:304:PSC:H12	21:O:304:PSC:H322	2.03	0.41
3:P:243:HIS:O	3:P:247:VAL:HG23	2.20	0.41
3:C:187:THR:CB	7:G:68:THR:HG21	2.50	0.41
27:P:309:CDL:H401	27:P:309:CDL:H371	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:309:CDL:H672	27:C:309:CDL:H641	1.90	0.41
18:A:606:PGV:C15	18:A:606:PGV:H321	2.50	0.41
17:A:604:HEA:HHC	17:A:604:HEA:H122	2.03	0.41
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.55	0.41
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.55	0.41
22:W:101:CHD:H12A	22:W:101:CHD:H112	1.83	0.41
26:C:306:PEK:H371	27:G:101:CDL:H261	2.01	0.41
1:A:383:MET:O	1:A:387:PHE:CB	2.68	0.41
1:N:175:ALA:HB2	6:S:35:ALA:HB1	2.03	0.41
1:A:394:VAL:HG23	1:A:395:HIS:N	2.35	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.02	0.41
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.86	0.41
1:N:390:MET:O	1:N:394:VAL:HG13	2.21	0.41
2:O:1:FME:HCN	2:O:193:TYR:HB2	2.03	0.41
5:E:52:LEU:O	5:E:55:CYS:HB2	2.20	0.41
2:B:116:LEU:HD12	2:B:117:SER:N	2.36	0.41
21:O:304:PSC:H073	5:R:11:PHE:HB3	2.03	0.41
1:N:377:PHE:CD1	17:N:605:HEA:HAD1	2.56	0.41
3:C:187:THR:HG22	26:C:305:PEK:H052	2.02	0.41
27:G:101:CDL:HA62	27:G:101:CDL:H322	2.02	0.41
8:U:57:ARG:HH11	8:U:61:LYS:HE2	1.86	0.41
1:A:377:PHE:HA	1:A:380:VAL:CG2	2.51	0.41
8:H:40:GLU:HG3	8:H:50:VAL:CG1	2.51	0.41
7:G:48:ILE:HA	7:G:49:PRO:HD3	1.86	0.41
2:O:75:LEU:HD12	2:O:75:LEU:HA	1.86	0.41
2:B:123:ILE:CG2	2:B:128:LEU:HD23	2.51	0.41
8:H:64:CYS:HA	8:H:65:PRO:HD3	1.97	0.41
2:B:215:PRO:HD3	9:I:60:PHE:CD2	2.56	0.41
4:D:33:LEU:HD22	4:D:37:GLN:HB3	2.03	0.41
1:N:113:LEU:O	1:N:117:MET:HG2	2.20	0.41
1:N:172:LYS:HD2	1:N:181:THR:HG21	2.03	0.41
1:N:169:ILE:HD11	1:N:189:MET:SD	2.61	0.41
1:A:1:FME:HA	1:A:1:FME:CE	2.51	0.41
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.03	0.41
2:O:160:LEU:HD22	2:O:175:ILE:HG12	2.02	0.41
7:T:79:PRO:HD2	29:T:203:HOH:O	2.19	0.41
3:C:115:CYS:HB2	29:C:478:HOH:O	2.20	0.41
20:D:201:TGL:HC61	29:D:364:HOH:O	2.20	0.40
2:B:92:ASN:HA	2:B:93:PRO:HD2	1.93	0.40
3:P:129:VAL:N	3:P:130:PRO:CD	2.84	0.40
3:P:156:ARG:HG3	3:P:156:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:301:DCW:H62C	18:C:307:PGV:H281	2.02	0.40
27:P:309:CDL:HB21	27:P:309:CDL:CB3	2.51	0.40
17:N:604:HEA:H122	17:N:604:HEA:HHC	2.03	0.40
3:C:29:SER:HB2	3:C:42:LEU:HD13	2.02	0.40
3:P:230:ASN:HB2	29:S:217:HOH:O	2.21	0.40
10:W:21:HIS:O	10:W:22:LEU:HD23	2.21	0.40
2:B:56:MET:HA	21:B:303:PSC:H201	2.04	0.40
18:A:607:PGV:H91	3:C:50:ASN:OD1	2.20	0.40
3:C:51:MET:SD	27:C:309:CDL:C62	3.09	0.40
4:D:107:ILE:HD13	11:K:39:GLU:CB	2.51	0.40
4:Q:121:LYS:HG2	11:X:53:TRP:HD1	1.85	0.40
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.56	0.40
27:T:102:CDL:H251	27:T:102:CDL:H222	1.85	0.40
17:A:605:HEA:HMB1	17:A:605:HEA:H11	1.91	0.40
21:B:303:PSC:H212	21:B:303:PSC:O01	2.21	0.40
7:G:6:GLY:O	26:G:102:PEK:H311	2.21	0.40
1:N:459:PHE:HB3	4:Q:92:THR:HG23	2.04	0.40
7:T:67:HIS:HD2	7:T:71:HIS:CD2	2.39	0.40
2:B:145:PRO:HA	2:B:214:VAL:O	2.21	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%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
2	B	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	21	19
2	O	225/227 (99%)	206 (92%)	18 (8%)	1 (0%)	39	42
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	140 (99%)	2 (1%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
6	F	96/98 (98%)	87 (91%)	6 (6%)	3 (3%)	5	2
6	S	96/98 (98%)	87 (91%)	5 (5%)	4 (4%)	3	1
7	G	81/85 (95%)	64 (79%)	9 (11%)	8 (10%)	1	0
7	T	81/85 (95%)	65 (80%)	8 (10%)	8 (10%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15	11
8	U	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	15	11
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	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%)	3329 (95%)	147 (4%)	28 (1%)	24	22

All (28) 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
7	T	7	ASP
7	T	8	HIS

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Mol	Chain	Res	Type
7	T	39	SER
2	B	60	GLU
6	F	94	HIS
6	F	95	GLN
7	G	40	GLY
8	H	8	ILE
2	O	60	GLU
7	T	40	GLY
7	G	3	ALA
6	S	93	PRO
7	T	3	ALA
8	U	8	ILE
7	G	6	GLY
6	F	96	LEU
6	S	96	LEU
7	T	6	GLY
2	B	92	ASN
7	G	10	GLY
7	T	10	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	416 (98%)	10 (2%)	58	71
1	N	426/426 (100%)	414 (97%)	12 (3%)	51	63
2	B	210/210 (100%)	201 (96%)	9 (4%)	35	43
2	O	210/210 (100%)	195 (93%)	15 (7%)	18	19
3	C	224/226 (99%)	217 (97%)	7 (3%)	47	59
3	P	224/226 (99%)	219 (98%)	5 (2%)	60	72
4	D	128/129 (99%)	127 (99%)	1 (1%)	86	93
4	Q	128/129 (99%)	127 (99%)	1 (1%)	86	93
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	92/95 (97%)	88 (96%)	4 (4%)	35	43
6	F	81/81 (100%)	80 (99%)	1 (1%)	78	88
6	S	81/81 (100%)	78 (96%)	3 (4%)	41	50
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	17
7	T	67/68 (98%)	61 (91%)	6 (9%)	12	11
8	H	71/75 (95%)	69 (97%)	2 (3%)	51	63
8	U	71/75 (95%)	68 (96%)	3 (4%)	36	44
9	I	57/57 (100%)	54 (95%)	3 (5%)	28	32
9	V	57/57 (100%)	56 (98%)	1 (2%)	66	79
10	J	49/50 (98%)	47 (96%)	2 (4%)	37	45
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	76
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	34
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	66
12	Y	39/40 (98%)	39 (100%)	0	100	100
13	M	37/38 (97%)	29 (78%)	8 (22%)	1	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	7
All	All	3040/3082 (99%)	2931 (96%)	109 (4%)	42	52

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	115	SER
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	369	ASP
1	A	486	ASP
1	A	504	THR
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	13	PRO
3	C	17	PRO
3	C	110	PRO
3	C	159	MET
3	C	179	SER
3	C	192	VAL
3	C	214	PHE
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
5	E	91	PRO
6	F	48	LEU
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	4	ARG
10	J	50	LEU
12	L	2	HIS
13	M	4	LYS
13	M	12	PRO
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	96	ARG
1	N	109	PHE
1	N	115	SER

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Mol	Chain	Res	Type
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	338	MET
1	N	369	ASP
1	N	484	THR
1	N	513	LEU
2	O	3	TYR
2	O	16	ILE
2	O	32	PHE
2	O	33	LEU
2	O	54	SER
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	167	SER
3	P	29	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	121	LYS
5	R	5	HIS
5	R	70	VAL
5	R	77	PRO
5	R	90	ARG
6	S	37	LYS
6	S	53	THR
6	S	54	ASN
7	T	18	PHE
7	T	33	LEU
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
7	T	84	LYS

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Mol	Chain	Res	Type
8	U	27	ARG
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
10	W	50	LEU
11	X	20	SER
11	X	54	ARG
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 (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	52	HIS
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
3	C	70	HIS
3	C	149	HIS
4	D	37	GLN
4	D	143	ASN
5	E	78	HIS
5	E	94	ASN
7	G	66	ASN
7	G	71	HIS
9	I	8	GLN
10	J	29	ASN
11	K	35	GLN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	52	HIS

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Mol	Chain	Res	Type
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	149	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	94	HIS
7	T	34	ASN
7	T	66	ASN
7	T	71	HIS
9	V	8	GLN
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	0.67	0	6,9,11	1.56	1 (16%)
2	FME	B	1	2	8,9,10	0.91	0	6,9,11	1.38	1 (16%)
7	TPO	G	11	7	8,10,11	1.83	1 (12%)	7,14,16	1.11	1 (14%)
9	SAC	I	1	9	7,8,9	2.48	2 (28%)	7,9,11	2.03	2 (28%)
1	FME	N	1	1	8,9,10	0.74	0	6,9,11	1.29	2 (33%)
2	FME	O	1	2	8,9,10	0.59	0	6,9,11	1.23	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	T	11	7	8,10,11	1.33	1 (12%)	7,14,16	1.06	1 (14%)
9	SAC	V	1	9	7,8,9	2.86	2 (28%)	7,9,11	2.13	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 Torsions 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	2.48	1.58	1.54
9	I	1	SAC	CA-N	3.97	1.52	1.46
7	G	11	TPO	CB-CA	4.33	1.61	1.54
9	I	1	SAC	OAC-C1A	5.01	1.34	1.23
9	V	1	SAC	OAC-C1A	5.08	1.35	1.23
9	V	1	SAC	CA-N	5.21	1.53	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CA-N-CN	-2.97	118.25	122.82
9	I	1	SAC	CA-N-C1A	-2.89	111.56	121.37
9	V	1	SAC	CA-N-C1A	-2.83	111.76	121.37
2	B	1	FME	CA-N-CN	-2.76	118.58	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.54	117.40	122.06
2	O	1	FME	CA-N-CN	-2.37	119.18	122.82
1	N	1	FME	CA-N-CN	-2.21	119.43	122.82
1	N	1	FME	O-C-CA	-2.08	119.95	125.44
7	T	11	TPO	O-C-CA	-2.03	120.07	125.44
7	G	11	TPO	O-C-CA	-2.02	120.09	125.44
9	V	1	SAC	C2A-C1A-N	2.56	121.00	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CB-CA-N	2.64	116.39	110.60
9	I	1	SAC	CB-CA-N	3.38	118.01	110.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	4	0
1	N	1	FME	1	0
2	O	1	FME	5	0
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
17	HEA	A	604	1	40,67,67	1.14	2 (5%)	41,103,103	1.99	13 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	HEA	A	605	1	40,67,67	1.56	8 (20%)	41,103,103	1.46	6 (14%)
18	PGV	A	606	-	50,50,50	1.17	3 (6%)	51,56,56	1.05	4 (7%)
18	PGV	A	607	-	50,50,50	1.01	3 (6%)	51,56,56	1.11	2 (3%)
19	CUA	B	301	2	0,1,1	0.00	-	0,0,0	0.00	-
20	TGL	B	302	-	62,62,62	0.77	2 (3%)	65,65,65	1.67	12 (18%)
21	PSC	B	303	-	51,51,51	1.32	6 (11%)	55,59,59	1.13	1 (1%)
22	CHD	B	304	-	29,32,32	0.85	1 (3%)	48,51,51	1.89	12 (25%)
23	DCW	C	301	3	17,17,17	1.31	2 (11%)	21,21,21	1.00	0
24	DMU	C	302	-	34,34,34	2.70	14 (41%)	45,45,45	4.27	18 (40%)
22	CHD	C	304	-	29,32,32	0.89	2 (6%)	48,51,51	1.96	12 (25%)
26	PEK	C	305	-	51,52,52	1.44	5 (9%)	52,57,57	1.10	3 (5%)
26	PEK	C	306	-	51,52,52	1.68	9 (17%)	52,57,57	1.13	4 (7%)
18	PGV	C	307	-	50,50,50	0.98	3 (6%)	51,56,56	1.02	5 (9%)
18	PGV	C	308	-	50,50,50	1.42	5 (10%)	51,56,56	0.84	2 (3%)
27	CDL	C	309	-	99,99,99	0.88	3 (3%)	101,111,111	0.94	5 (4%)
22	CHD	C	310	-	29,32,32	0.97	1 (3%)	48,51,51	3.52	26 (54%)
20	TGL	D	201	-	62,62,62	0.96	4 (6%)	65,65,65	1.49	11 (16%)
27	CDL	G	101	-	99,99,99	1.15	8 (8%)	101,111,111	0.96	8 (7%)
26	PEK	G	102	-	51,52,52	1.93	12 (23%)	52,57,57	1.21	4 (7%)
22	CHD	J	101	-	29,32,32	0.94	2 (6%)	48,51,51	3.72	25 (52%)
20	TGL	L	101	-	62,62,62	1.28	6 (9%)	65,65,65	1.78	12 (18%)
24	DMU	M	101	-	34,34,34	3.13	8 (23%)	45,45,45	4.27	19 (42%)
17	HEA	N	604	1	40,67,67	1.41	7 (17%)	41,103,103	1.97	12 (29%)
17	HEA	N	605	1	40,67,67	1.52	8 (20%)	41,103,103	1.54	8 (19%)
20	TGL	N	606	-	62,62,62	1.40	6 (9%)	65,65,65	1.75	13 (20%)
20	TGL	N	607	-	62,62,62	0.86	2 (3%)	65,65,65	1.46	10 (15%)
18	PGV	N	608	-	50,50,50	1.21	4 (8%)	51,56,56	1.03	3 (5%)
18	PGV	N	609	-	50,50,50	1.13	5 (10%)	51,56,56	1.17	3 (5%)
19	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	302	-	29,32,32	0.68	0	48,51,51	1.88	14 (29%)
20	TGL	O	303	-	62,62,62	0.85	2 (3%)	65,65,65	1.62	9 (13%)
21	PSC	O	304	-	51,51,51	1.29	4 (7%)	55,59,59	1.14	3 (5%)
23	DCW	P	301	3	17,17,17	1.58	2 (11%)	21,21,21	0.88	0
24	DMU	P	302	-	34,34,34	2.58	13 (38%)	45,45,45	4.37	18 (40%)
22	CHD	P	304	-	29,32,32	0.69	1 (3%)	48,51,51	1.86	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEK	P	305	-	51,52,52	1.54	7 (13%)	52,57,57	1.19	7 (13%)
26	PEK	P	306	-	51,52,52	1.65	8 (15%)	52,57,57	1.14	4 (7%)
18	PGV	P	307	-	50,50,50	0.95	3 (6%)	51,56,56	0.89	2 (3%)
18	PGV	P	308	-	50,50,50	1.41	5 (10%)	51,56,56	0.88	3 (5%)
27	CDL	P	309	-	99,99,99	0.93	5 (5%)	101,111,111	0.95	4 (3%)
22	CHD	P	310	-	29,32,32	0.87	1 (3%)	48,51,51	3.59	26 (54%)
26	PEK	T	101	-	51,52,52	2.07	12 (23%)	52,57,57	1.20	3 (5%)
27	CDL	T	102	-	99,99,99	1.14	10 (10%)	101,111,111	0.99	9 (8%)
22	CHD	W	101	-	29,32,32	1.08	2 (6%)	48,51,51	3.77	25 (52%)
24	DMU	Z	101	-	34,34,34	3.02	10 (29%)	45,45,45	4.19	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	604	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	A	605	1	3/3/7/16	0/24/76/76	0/0/8/8
18	PGV	A	606	-	-	1/55/55/55	0/0/0/0
18	PGV	A	607	-	-	0/55/55/55	0/0/0/0
19	CUA	B	301	2	-	0/0/0/0	0/0/0/0
20	TGL	B	302	-	-	0/65/65/65	0/0/0/0
21	PSC	B	303	-	-	0/55/55/55	0/0/0/0
22	CHD	B	304	-	-	0/7/74/74	0/4/4/4
23	DCW	C	301	3	-	0/8/24/24	0/2/2/2
24	DMU	C	302	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	C	304	-	-	0/7/74/74	0/4/4/4
26	PEK	C	305	-	-	0/56/56/56	0/0/0/0
26	PEK	C	306	-	-	0/56/56/56	0/0/0/0
18	PGV	C	307	-	-	0/55/55/55	0/0/0/0
18	PGV	C	308	-	-	0/55/55/55	0/0/0/0
27	CDL	C	309	-	-	0/110/110/110	0/0/0/0
22	CHD	C	310	-	5/5/12/12	0/7/74/74	0/4/4/4
20	TGL	D	201	-	-	0/65/65/65	0/0/0/0
27	CDL	G	101	-	-	0/110/110/110	0/0/0/0
26	PEK	G	102	-	-	0/56/56/56	0/0/0/0
22	CHD	J	101	-	5/5/12/12	0/7/74/74	0/4/4/4
20	TGL	L	101	-	-	0/65/65/65	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	M	101	-	5/5/10/10	0/19/59/59	0/2/2/2
17	HEA	N	604	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	N	605	1	3/3/7/16	0/24/76/76	0/0/8/8
20	TGL	N	606	-	-	0/65/65/65	0/0/0/0
20	TGL	N	607	-	-	0/65/65/65	0/0/0/0
18	PGV	N	608	-	-	1/55/55/55	0/0/0/0
18	PGV	N	609	-	-	0/55/55/55	0/0/0/0
19	CUA	O	301	2	-	0/0/0/0	0/0/0/0
22	CHD	O	302	-	-	0/7/74/74	0/4/4/4
20	TGL	O	303	-	-	0/65/65/65	0/0/0/0
21	PSC	O	304	-	-	0/55/55/55	0/0/0/0
23	DCW	P	301	3	-	0/8/24/24	0/2/2/2
24	DMU	P	302	-	6/6/10/10	0/19/59/59	0/2/2/2
22	CHD	P	304	-	-	0/7/74/74	0/4/4/4
26	PEK	P	305	-	-	0/56/56/56	0/0/0/0
26	PEK	P	306	-	-	0/56/56/56	0/0/0/0
18	PGV	P	307	-	-	0/55/55/55	0/0/0/0
18	PGV	P	308	-	-	0/55/55/55	0/0/0/0
27	CDL	P	309	-	-	0/110/110/110	0/0/0/0
22	CHD	P	310	-	5/5/12/12	0/7/74/74	0/4/4/4
26	PEK	T	101	-	-	0/56/56/56	0/0/0/0
27	CDL	T	102	-	-	0/110/110/110	0/0/0/0
22	CHD	W	101	-	5/5/12/12	0/7/74/74	0/4/4/4
24	DMU	Z	101	-	5/5/10/10	0/19/59/59	0/2/2/2

All (226) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	101	DMU	O7-C3	-7.71	1.24	1.43
24	Z	101	DMU	O7-C3	-7.22	1.25	1.43
24	M	101	DMU	O16-C6	-6.70	1.28	1.40
24	M	101	DMU	O1-C9	-6.56	1.27	1.44
24	Z	101	DMU	O16-C18	-6.48	1.24	1.42
24	M	101	DMU	O5-C4	-6.43	1.28	1.44
24	Z	101	DMU	O1-C9	-6.26	1.28	1.44
24	P	302	DMU	O16-C18	-6.23	1.25	1.42
24	M	101	DMU	O16-C18	-6.18	1.25	1.42
24	M	101	DMU	O7-C10	-6.15	1.24	1.41
24	Z	101	DMU	O7-C10	-6.12	1.25	1.41
24	C	302	DMU	O16-C18	-6.11	1.25	1.42
24	Z	101	DMU	O5-C4	-6.10	1.29	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	101	DMU	O16-C6	-6.07	1.29	1.40
24	C	302	DMU	O16-C6	-5.90	1.29	1.40
24	P	302	DMU	O16-C6	-5.54	1.30	1.40
24	M	101	DMU	O1-C10	-5.20	1.28	1.41
24	C	302	DMU	O1-C9	-5.13	1.31	1.44
24	C	302	DMU	O7-C3	-5.00	1.31	1.43
24	P	302	DMU	O7-C3	-4.99	1.31	1.43
24	M	101	DMU	O5-C6	-4.89	1.29	1.41
24	Z	101	DMU	O1-C10	-4.79	1.29	1.41
24	P	302	DMU	O1-C9	-4.63	1.32	1.44
24	P	302	DMU	O5-C4	-4.46	1.33	1.44
24	C	302	DMU	O5-C4	-4.41	1.33	1.44
24	Z	101	DMU	O5-C6	-4.35	1.30	1.41
17	A	605	HEA	C3A-C2A	-4.15	1.34	1.40
23	P	301	DCW	C8-N2	-4.09	1.38	1.46
24	C	302	DMU	O7-C10	-4.06	1.30	1.41
24	C	302	DMU	O5-C6	-4.03	1.31	1.41
17	N	605	HEA	C3A-C2A	-3.87	1.35	1.40
24	P	302	DMU	O7-C10	-3.79	1.31	1.41
24	P	302	DMU	O5-C6	-3.77	1.32	1.41
17	N	604	HEA	C3A-CMA	-3.69	1.37	1.46
24	C	302	DMU	O1-C10	-3.60	1.32	1.41
17	A	604	HEA	C3A-CMA	-3.45	1.38	1.46
24	P	302	DMU	O1-C10	-3.28	1.33	1.41
17	A	605	HEA	C3A-CMA	-3.15	1.39	1.46
17	N	605	HEA	C3A-CMA	-3.06	1.39	1.46
22	C	310	CHD	C19-C10	-2.77	1.49	1.54
23	C	301	DCW	C8-N2	-2.65	1.41	1.46
22	P	310	CHD	C19-C10	-2.62	1.49	1.54
26	P	305	PEK	O03-C01	-2.61	1.39	1.45
22	C	304	CHD	C10-C9	-2.56	1.51	1.56
23	P	301	DCW	C1-N2	-2.53	1.29	1.35
22	C	304	CHD	C13-C12	-2.42	1.50	1.54
22	B	304	CHD	C13-C12	-2.38	1.50	1.54
17	N	604	HEA	C3A-C2A	-2.17	1.37	1.40
17	A	605	HEA	C3C-C2C	-2.13	1.37	1.40
26	C	305	PEK	O03-C01	-2.10	1.40	1.45
23	C	301	DCW	C2-N1	-2.09	1.42	1.46
17	N	605	HEA	C3C-C2C	-2.07	1.37	1.40
26	P	305	PEK	O01-C02	-2.02	1.41	1.46
26	G	102	PEK	P-O12	2.01	1.68	1.59
17	N	604	HEA	C17-C18	2.01	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	605	HEA	C1A-NA	2.01	1.39	1.36
21	B	303	PSC	C8-C9	2.02	1.59	1.50
18	C	308	PGV	C04-C05	2.04	1.59	1.51
20	N	606	TGL	CC2-CC1	2.05	1.56	1.50
18	P	308	PGV	O03-C19	2.06	1.39	1.33
18	N	609	PGV	C03-C02	2.08	1.56	1.50
27	T	102	CDL	CB2-C1	2.08	1.59	1.51
17	N	604	HEA	C1A-NA	2.09	1.39	1.36
21	B	303	PSC	P-O12	2.09	1.68	1.59
27	T	102	CDL	CA6-CA4	2.10	1.56	1.50
22	J	101	CHD	C20-C17	2.10	1.58	1.54
26	T	101	PEK	O03-C01	2.10	1.49	1.45
18	P	307	PGV	C01-C02	2.12	1.56	1.50
20	L	101	TGL	CC2-CC1	2.12	1.57	1.50
26	G	102	PEK	O03-C01	2.12	1.49	1.45
27	P	309	CDL	PA1-OA5	2.13	1.68	1.59
18	N	608	PGV	O01-C1	2.15	1.40	1.34
21	O	304	PSC	P-O12	2.15	1.68	1.59
24	Z	101	DMU	C8-C7	2.15	1.58	1.52
26	P	306	PEK	P-O12	2.16	1.68	1.59
26	G	102	PEK	O01-C1	2.16	1.40	1.34
24	Z	101	DMU	C8-C9	2.18	1.57	1.53
18	C	307	PGV	O01-C1	2.19	1.40	1.34
24	P	302	DMU	C10-C5	2.21	1.59	1.52
24	P	302	DMU	C2-C1	2.22	1.58	1.52
27	C	309	CDL	C31-CA7	2.23	1.57	1.50
21	B	303	PSC	C01-C02	2.23	1.57	1.50
27	T	102	CDL	C51-CB5	2.23	1.57	1.50
24	C	302	DMU	C10-C5	2.23	1.59	1.52
22	P	304	CHD	C8-C9	2.25	1.58	1.53
26	G	102	PEK	C2-C1	2.25	1.57	1.50
27	G	101	CDL	C31-CA7	2.26	1.57	1.50
18	P	307	PGV	C20-C19	2.28	1.57	1.50
17	A	604	HEA	C17-C18	2.29	1.57	1.50
27	G	101	CDL	CB3-CB4	2.30	1.57	1.50
27	T	102	CDL	C31-CA7	2.31	1.57	1.50
20	B	302	TGL	CG3-CG2	2.32	1.57	1.50
27	C	309	CDL	CA3-CA4	2.34	1.57	1.50
20	D	201	TGL	CB2-CB1	2.37	1.57	1.50
27	T	102	CDL	OA6-CA5	2.38	1.41	1.34
20	N	606	TGL	CG3-CG2	2.38	1.57	1.50
17	N	605	HEA	C18-C19	2.39	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	306	PEK	P-O11	2.39	1.69	1.59
21	B	303	PSC	C2-C1	2.41	1.57	1.50
17	N	605	HEA	C4B-NB	2.41	1.39	1.36
24	C	302	DMU	C8-C9	2.43	1.58	1.53
17	A	605	HEA	C18-C19	2.47	1.37	1.33
17	A	605	HEA	C4B-NB	2.47	1.40	1.36
24	P	302	DMU	C5-C7	2.47	1.58	1.52
20	B	302	TGL	OG2-CB1	2.48	1.41	1.34
17	N	605	HEA	C17-C18	2.48	1.57	1.50
27	P	309	CDL	C31-CA7	2.48	1.58	1.50
26	C	306	PEK	P-O12	2.51	1.70	1.59
27	T	102	CDL	C71-CB7	2.52	1.58	1.50
18	C	308	PGV	C03-C02	2.52	1.57	1.50
17	N	604	HEA	C4B-NB	2.53	1.40	1.36
27	P	309	CDL	OA8-CA7	2.54	1.41	1.33
20	D	201	TGL	CA2-CA1	2.54	1.58	1.50
18	P	308	PGV	C03-C02	2.54	1.57	1.50
27	T	102	CDL	CB3-CB4	2.55	1.57	1.50
27	G	101	CDL	C51-CB5	2.56	1.58	1.50
18	N	608	PGV	O03-C19	2.57	1.41	1.33
27	G	101	CDL	C71-CB7	2.60	1.58	1.50
26	P	306	PEK	O03-C21	2.61	1.41	1.33
18	A	607	PGV	C03-C02	2.62	1.58	1.50
24	C	302	DMU	C8-C7	2.62	1.59	1.52
22	W	101	CHD	C20-C17	2.66	1.59	1.54
17	A	605	HEA	C16-C15	2.68	1.57	1.51
18	N	609	PGV	C20-C19	2.68	1.58	1.50
24	C	302	DMU	C5-C7	2.69	1.59	1.52
20	O	303	TGL	CG3-CG2	2.69	1.58	1.50
20	L	101	TGL	CB2-CB1	2.70	1.58	1.50
26	T	101	PEK	C22-C21	2.72	1.58	1.50
18	P	308	PGV	C2-C1	2.72	1.58	1.50
26	C	306	PEK	C01-C02	2.72	1.58	1.50
20	N	607	TGL	CA2-CA1	2.73	1.58	1.50
26	C	306	PEK	O03-C21	2.73	1.41	1.33
27	G	101	CDL	CB6-CB4	2.75	1.58	1.50
18	A	607	PGV	C2-C1	2.79	1.59	1.50
27	P	309	CDL	CA3-CA4	2.80	1.58	1.50
26	P	306	PEK	C01-C02	2.83	1.58	1.50
18	C	307	PGV	O03-C19	2.83	1.41	1.33
18	N	609	PGV	C01-C02	2.87	1.58	1.50
20	L	101	TGL	CG3-CG2	2.87	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	306	PEK	C03-C02	2.87	1.58	1.50
26	T	101	PEK	P-O11	2.91	1.72	1.59
18	C	308	PGV	C2-C1	2.92	1.59	1.50
27	T	102	CDL	C11-CA5	2.97	1.59	1.50
26	C	306	PEK	C03-C02	2.98	1.59	1.50
20	N	606	TGL	CB2-CB1	2.98	1.59	1.50
18	A	606	PGV	O03-C19	2.99	1.42	1.33
26	P	305	PEK	C2-C1	2.99	1.59	1.50
27	G	101	CDL	OA6-CA5	2.99	1.43	1.34
20	O	303	TGL	OG2-CB1	3.03	1.43	1.34
18	A	606	PGV	C03-C02	3.04	1.59	1.50
17	A	605	HEA	C3C-CAC	3.05	1.54	1.47
22	J	101	CHD	C13-C17	3.06	1.60	1.55
27	C	309	CDL	CA6-CA4	3.08	1.59	1.50
26	T	101	PEK	O01-C1	3.10	1.43	1.34
24	C	302	DMU	C6-C1	3.11	1.61	1.52
21	O	304	PSC	C2-C1	3.14	1.60	1.50
27	G	101	CDL	OB6-CB5	3.19	1.43	1.34
26	G	102	PEK	P-O11	3.20	1.73	1.59
26	T	101	PEK	C2-C1	3.21	1.60	1.50
26	G	102	PEK	O03-C21	3.26	1.43	1.33
24	P	302	DMU	C3-C4	3.27	1.62	1.52
20	D	201	TGL	OG3-CC1	3.29	1.43	1.33
24	C	302	DMU	C3-C4	3.30	1.62	1.52
18	N	609	PGV	C2-C1	3.32	1.60	1.50
27	G	101	CDL	C11-CA5	3.34	1.60	1.50
20	D	201	TGL	OG1-CA1	3.35	1.43	1.33
27	T	102	CDL	OB6-CB5	3.36	1.44	1.34
20	N	606	TGL	CG1-CG2	3.37	1.60	1.50
27	P	309	CDL	CA6-CA4	3.40	1.60	1.50
18	C	307	PGV	C12-C11	3.43	1.51	1.31
20	N	607	TGL	OG1-CA1	3.43	1.43	1.33
27	T	102	CDL	CB6-CB4	3.50	1.60	1.50
17	A	605	HEA	C1D-ND	3.50	1.41	1.36
24	P	302	DMU	C6-C1	3.51	1.63	1.52
20	L	101	TGL	CG1-CG2	3.57	1.60	1.50
17	N	604	HEA	C4A-NA	3.59	1.41	1.36
18	N	609	PGV	C12-C11	3.63	1.52	1.31
22	W	101	CHD	C13-C17	3.66	1.62	1.55
18	P	307	PGV	C12-C11	3.67	1.52	1.31
18	A	607	PGV	C12-C11	3.74	1.53	1.31
17	N	605	HEA	C1D-ND	3.75	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	101	TGL	OG1-CA1	3.79	1.44	1.33
18	N	608	PGV	C03-C02	3.83	1.61	1.50
17	N	604	HEA	C1D-ND	3.91	1.42	1.36
21	O	304	PSC	C13-C12	3.93	1.54	1.31
26	T	101	PEK	C9-C8	3.96	1.54	1.31
26	C	305	PEK	C9-C8	3.96	1.54	1.31
26	G	102	PEK	C9-C8	3.97	1.54	1.31
26	C	305	PEK	C6-C5	4.00	1.54	1.31
21	B	303	PSC	C13-C12	4.01	1.54	1.31
26	P	306	PEK	C15-C14	4.01	1.54	1.31
26	G	102	PEK	C12-C11	4.05	1.55	1.31
18	A	606	PGV	C12-C11	4.09	1.55	1.31
18	N	608	PGV	C12-C11	4.11	1.55	1.31
26	P	305	PEK	C9-C8	4.13	1.55	1.31
26	C	306	PEK	C15-C14	4.20	1.56	1.31
26	P	306	PEK	C9-C8	4.22	1.56	1.31
26	C	306	PEK	C9-C8	4.22	1.56	1.31
26	P	306	PEK	C6-C5	4.23	1.56	1.31
26	C	306	PEK	C6-C5	4.23	1.56	1.31
26	T	101	PEK	C12-C11	4.40	1.57	1.31
26	T	101	PEK	C6-C5	4.41	1.57	1.31
26	G	102	PEK	C6-C5	4.42	1.57	1.31
26	P	305	PEK	C6-C5	4.47	1.57	1.31
26	C	305	PEK	C12-C11	4.51	1.57	1.31
26	P	305	PEK	C15-C14	4.52	1.57	1.31
26	P	305	PEK	C12-C11	4.52	1.57	1.31
26	C	306	PEK	C12-C11	4.53	1.57	1.31
26	P	306	PEK	C12-C11	4.60	1.58	1.31
21	B	303	PSC	C10-C9	4.60	1.58	1.31
18	C	308	PGV	C12-C11	4.62	1.58	1.31
18	P	308	PGV	O01-C1	4.63	1.48	1.34
26	G	102	PEK	C01-C02	4.65	1.63	1.50
26	C	305	PEK	C15-C14	4.67	1.58	1.31
18	P	308	PGV	C12-C11	4.69	1.58	1.31
26	T	101	PEK	C15-C14	4.71	1.58	1.31
21	O	304	PSC	C10-C9	4.71	1.59	1.31
26	T	101	PEK	C01-C02	4.81	1.64	1.50
18	C	308	PGV	O01-C1	4.82	1.48	1.34
26	G	102	PEK	C15-C14	4.88	1.59	1.31
26	T	101	PEK	O03-C21	4.95	1.48	1.33
26	T	101	PEK	C03-C02	4.95	1.64	1.50
26	G	102	PEK	C03-C02	5.02	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	101	TGL	OG2-CB1	5.03	1.49	1.34
20	N	606	TGL	OG2-CB1	5.31	1.50	1.34
20	N	606	TGL	OG1-CA1	5.43	1.49	1.33

All (411) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	310	CHD	C17-C13-C12	-10.11	108.72	117.68
22	C	310	CHD	C17-C13-C12	-9.52	109.24	117.68
24	M	101	DMU	C8-C7-C5	-7.63	96.55	110.79
24	Z	101	DMU	C8-C7-C5	-7.45	96.89	110.79
22	P	310	CHD	C19-C10-C9	-6.37	101.63	111.18
22	C	310	CHD	C19-C10-C9	-6.31	101.72	111.18
20	O	303	TGL	CG1-OG1-CA1	-5.84	100.51	116.85
22	B	304	CHD	C18-C13-C12	-5.74	103.49	109.09
20	B	302	TGL	CG1-OG1-CA1	-5.70	100.92	116.85
20	L	101	TGL	C12-C11-C10	-5.44	86.46	114.53
17	A	604	HEA	C27-C19-C18	-5.35	113.00	123.50
17	N	604	HEA	C27-C19-C18	-5.30	113.10	123.50
22	W	101	CHD	C17-C13-C12	-5.26	113.02	117.68
22	C	310	CHD	C19-C10-C1	-5.26	99.35	108.20
22	P	310	CHD	C15-C14-C8	-5.25	110.69	118.32
20	N	606	TGL	C12-C11-C10	-5.20	87.67	114.53
22	W	101	CHD	C15-C14-C8	-5.20	110.77	118.32
22	W	101	CHD	C18-C13-C14	-5.08	103.21	111.22
22	J	101	CHD	C15-C14-C8	-5.06	110.97	118.32
22	C	310	CHD	C15-C14-C8	-5.02	111.03	118.32
22	J	101	CHD	C17-C13-C12	-5.01	113.24	117.68
22	J	101	CHD	C18-C13-C14	-4.73	103.76	111.22
22	P	310	CHD	C19-C10-C1	-4.72	100.27	108.20
20	N	606	TGL	CB9-CB8-CB7	-4.60	90.79	114.53
21	B	303	PSC	C01-O03-C19	-4.57	104.06	116.85
22	O	302	CHD	C18-C13-C12	-4.56	104.64	109.09
20	L	101	TGL	CB9-CB8-CB7	-4.54	91.07	114.53
21	O	304	PSC	C01-O03-C19	-4.48	104.32	116.85
17	A	604	HEA	CAD-C3D-C4D	-4.30	122.33	127.01
20	D	201	TGL	CG1-OG1-CA1	-4.29	104.84	116.85
22	P	310	CHD	C6-C5-C4	-3.83	106.77	111.05
20	N	607	TGL	CG1-OG1-CA1	-3.82	106.16	116.85
17	N	604	HEA	CAD-C3D-C4D	-3.79	122.90	127.01
17	A	604	HEA	CAA-C2A-C1A	-3.78	122.91	127.01
17	A	605	HEA	CAD-C3D-C4D	-3.75	122.94	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	310	CHD	C6-C5-C4	-3.75	106.86	111.05
17	N	605	HEA	CAD-C3D-C4D	-3.72	122.97	127.01
22	P	304	CHD	C15-C14-C8	-3.62	113.06	118.32
22	P	304	CHD	C14-C8-C9	-3.60	104.67	109.62
22	C	304	CHD	C14-C8-C9	-3.57	104.71	109.62
22	C	304	CHD	C15-C14-C8	-3.56	113.14	118.32
24	P	302	DMU	C2-C3-C4	-3.53	102.86	110.84
18	A	607	PGV	C01-O03-C19	-3.51	107.04	116.85
22	C	304	CHD	C16-C17-C13	-3.50	100.12	103.60
22	B	304	CHD	C14-C8-C9	-3.48	104.83	109.62
22	B	304	CHD	C15-C14-C8	-3.48	113.27	118.32
22	O	302	CHD	C15-C14-C8	-3.48	113.27	118.32
17	N	605	HEA	CMC-C2C-C1C	-3.46	122.64	128.36
17	N	604	HEA	C17-C18-C19	-3.39	120.40	127.76
18	N	609	PGV	C01-O03-C19	-3.35	107.49	116.85
22	J	101	CHD	C19-C10-C5	-3.34	104.35	110.25
26	P	305	PEK	C3-C2-C1	-3.33	100.49	113.59
22	W	101	CHD	C19-C10-C5	-3.33	104.38	110.25
17	A	605	HEA	CMC-C2C-C1C	-3.32	122.88	128.36
22	C	304	CHD	C14-C13-C12	-3.28	104.45	107.39
24	C	302	DMU	C2-C3-C4	-3.27	103.45	110.84
22	C	304	CHD	C15-C14-C13	-3.22	100.39	103.60
18	C	307	PGV	O01-C1-C2	-3.17	104.64	111.53
26	C	305	PEK	C3-C2-C1	-3.12	101.32	113.59
27	P	309	CDL	CB6-OB8-CB7	-3.12	108.12	116.85
27	C	309	CDL	CB6-OB8-CB7	-3.11	108.14	116.85
22	P	310	CHD	O3-C3-C4	-2.98	103.94	109.86
22	O	302	CHD	C14-C8-C9	-2.93	105.59	109.62
22	C	310	CHD	O3-C3-C4	-2.90	104.10	109.86
22	O	302	CHD	C18-C13-C17	-2.84	106.74	111.22
22	P	310	CHD	C14-C8-C9	-2.79	105.78	109.62
27	T	102	CDL	OB8-CB7-C71	-2.75	103.51	111.90
18	P	307	PGV	O01-C1-C2	-2.62	105.83	111.53
17	A	604	HEA	C17-C18-C19	-2.59	122.14	127.76
27	P	309	CDL	OB6-CB5-C51	-2.57	105.94	111.53
22	B	304	CHD	O3-C3-C4	-2.56	104.76	109.86
18	C	308	PGV	C02-O01-C1	-2.55	111.77	117.89
18	P	308	PGV	C02-O01-C1	-2.54	111.79	117.89
27	G	101	CDL	OB8-CB7-C71	-2.53	104.18	111.90
22	P	304	CHD	C14-C13-C12	-2.52	105.13	107.39
20	B	302	TGL	CA8-CA7-CA6	-2.51	101.56	114.53
17	A	604	HEA	C21-C20-C19	-2.51	104.53	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	302	CHD	O3-C3-C4	-2.51	104.87	109.86
22	P	304	CHD	C13-C14-C8	-2.51	111.51	114.75
20	O	303	TGL	CA8-CA7-CA6	-2.50	101.61	114.53
22	P	304	CHD	C16-C17-C13	-2.48	101.13	103.60
22	C	310	CHD	C14-C8-C9	-2.45	106.25	109.62
20	O	303	TGL	CB7-CB6-CB5	-2.43	101.97	114.53
17	A	604	HEA	CMC-C2C-C1C	-2.42	124.35	128.36
26	C	305	PEK	O03-C21-C22	-2.40	104.60	111.90
18	A	606	PGV	C3-C2-C1	-2.39	104.21	113.59
22	P	310	CHD	C19-C10-C5	-2.36	106.09	110.25
26	P	305	PEK	C02-O01-C1	-2.36	112.24	117.89
27	C	309	CDL	OB6-CB5-C51	-2.34	106.43	111.53
20	B	302	TGL	CB7-CB6-CB5	-2.32	102.57	114.53
21	O	304	PSC	O01-C1-C2	-2.31	106.50	111.53
22	C	304	CHD	C13-C14-C8	-2.28	111.80	114.75
18	C	307	PGV	C9-C10-C11	-2.28	100.51	112.45
22	P	310	CHD	C18-C13-C14	-2.26	107.64	111.22
20	O	303	TGL	CB9-CB8-CB7	-2.25	102.91	114.53
20	B	302	TGL	CB9-CB8-CB7	-2.25	102.93	114.53
18	N	608	PGV	C3-C2-C1	-2.24	104.81	113.59
17	N	604	HEA	CAA-C2A-C1A	-2.22	124.60	127.01
18	P	307	PGV	C9-C10-C11	-2.21	100.87	112.45
22	C	304	CHD	O12-C12-C13	-2.20	107.54	111.11
22	J	101	CHD	C19-C10-C1	-2.20	104.50	108.20
26	P	305	PEK	C24-C23-C22	-2.20	105.23	113.29
17	N	604	HEA	C21-C20-C19	-2.19	105.59	112.71
20	D	201	TGL	OG3-CG3-CG2	-2.17	102.84	108.69
21	O	304	PSC	C07-N-C06	-2.16	103.42	108.98
18	A	606	PGV	C4-C3-C2	-2.16	105.38	113.29
22	O	302	CHD	O12-C12-C13	-2.11	107.69	111.11
27	C	309	CDL	C52-C51-CB5	-2.10	105.34	113.59
22	P	304	CHD	C15-C14-C13	-2.09	101.52	103.60
20	N	607	TGL	CA5-CA4-CA3	-2.08	103.77	114.53
22	C	310	CHD	C19-C10-C5	-2.08	106.59	110.25
22	W	101	CHD	C19-C10-C1	-2.04	104.76	108.20
26	P	305	PEK	O03-C21-C22	-2.03	105.70	111.90
17	N	604	HEA	C13-C14-C15	-2.03	123.36	127.76
18	C	307	PGV	C3-C2-C1	-2.03	105.63	113.59
27	P	309	CDL	C52-C51-CB5	-2.02	105.64	113.59
20	N	607	TGL	OG3-CG3-CG2	-2.01	103.27	108.69
22	B	304	CHD	C16-C17-C13	-2.00	101.60	103.60
20	B	302	TGL	CB6-CB5-CB4	2.01	124.90	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	102	CDL	C79-C78-C77	2.01	124.92	114.53
20	D	201	TGL	C10-CB9-CB8	2.02	124.94	114.53
20	D	201	TGL	C25-C24-C23	2.03	124.99	114.53
22	C	310	CHD	C1-C2-C3	2.03	113.72	110.43
17	A	604	HEA	CBD-CAD-C3D	2.03	116.17	112.53
18	C	307	PGV	O01-C1-O02	2.03	129.12	123.67
20	N	607	TGL	CB4-CB3-CB2	2.03	120.74	113.29
22	P	310	CHD	C11-C12-C13	2.03	113.27	111.20
20	N	606	TGL	CC7-CC6-CC5	2.04	125.07	114.53
20	O	303	TGL	C33-C19-C18	2.04	125.09	114.53
20	D	201	TGL	CB4-CB3-CB2	2.04	120.79	113.29
18	C	308	PGV	O03-C01-C02	2.05	114.20	108.69
20	B	302	TGL	OG1-CG1-CG2	2.05	114.21	108.69
18	P	308	PGV	O01-C02-C03	2.06	115.61	108.36
22	B	304	CHD	C5-C6-C7	2.06	116.73	114.44
26	G	102	PEK	C14-C13-C12	2.06	118.86	112.00
17	N	604	HEA	CBD-CAD-C3D	2.06	116.23	112.53
20	O	303	TGL	OG2-CG2-CG3	2.08	115.70	108.36
22	P	304	CHD	C6-C5-C10	2.09	114.96	112.66
26	P	305	PEK	C2-C3-C4	2.10	117.48	113.30
26	G	102	PEK	C03-C02-C01	2.11	117.00	112.07
22	P	310	CHD	C5-C4-C3	2.12	116.06	112.91
22	O	302	CHD	C1-C10-C5	2.13	111.30	107.81
27	C	309	CDL	CA4-OA6-CA5	2.13	123.00	117.89
27	G	101	CDL	C19-C18-C17	2.14	125.56	114.53
20	N	607	TGL	OG2-CG2-CG1	2.14	115.90	108.36
20	N	606	TGL	C10-CB9-CB8	2.15	125.62	114.53
18	N	609	PGV	C4-C3-C2	2.15	121.17	113.29
22	J	101	CHD	C9-C11-C12	2.15	117.07	114.36
20	B	302	TGL	C33-C19-C18	2.18	125.77	114.53
27	G	101	CDL	C80-C79-C78	2.18	125.79	114.53
26	C	306	PEK	C24-C23-C22	2.19	121.32	113.29
27	G	101	CDL	C83-C82-C81	2.19	125.84	114.53
27	T	102	CDL	C19-C18-C17	2.19	125.85	114.53
22	P	304	CHD	C1-C2-C3	2.19	113.99	110.43
26	C	306	PEK	O03-C01-C02	2.20	114.60	108.69
26	P	305	PEK	O03-C21-O04	2.20	129.16	123.49
27	C	309	CDL	OA8-CA6-CA4	2.20	114.62	108.69
20	B	302	TGL	OG3-CG3-CG2	2.21	114.63	108.69
22	C	310	CHD	C13-C17-C20	2.21	122.19	119.50
27	T	102	CDL	C80-C79-C78	2.21	125.95	114.53
20	N	606	TGL	C20-CA9-CA8	2.22	126.01	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	308	PGV	O03-C01-C02	2.23	114.69	108.69
27	T	102	CDL	OB8-CB6-CB4	2.24	114.72	108.69
20	B	302	TGL	OG2-CG2-CG3	2.24	116.25	108.36
26	P	306	PEK	O03-C01-C02	2.26	114.77	108.69
27	T	102	CDL	C20-C19-C18	2.26	126.21	114.53
27	G	101	CDL	OB8-CB6-CB4	2.27	114.79	108.69
22	W	101	CHD	C14-C8-C9	2.27	112.75	109.62
17	A	604	HEA	C27-C19-C20	2.27	118.88	115.41
17	N	604	HEA	C20-C21-C22	2.28	117.66	111.69
22	C	304	CHD	C17-C13-C14	2.29	102.37	100.05
20	L	101	TGL	CC7-CC6-CC5	2.29	126.36	114.53
22	W	101	CHD	C1-C2-C3	2.32	114.19	110.43
18	C	307	PGV	O03-C01-C02	2.35	115.01	108.69
27	T	102	CDL	C83-C82-C81	2.36	126.74	114.53
26	P	306	PEK	C24-C23-C22	2.36	121.96	113.29
17	A	604	HEA	C20-C21-C22	2.37	117.88	111.69
27	G	101	CDL	C20-C19-C18	2.38	126.80	114.53
27	P	309	CDL	OA8-CA6-CA4	2.38	115.09	108.69
26	T	101	PEK	C03-C02-C01	2.38	117.64	112.07
17	A	605	HEA	C26-C15-C16	2.40	119.07	115.41
27	T	102	CDL	C23-C22-C21	2.40	126.93	114.53
20	L	101	TGL	C13-C12-C11	2.41	126.98	114.53
22	P	310	CHD	C13-C17-C20	2.42	122.44	119.50
17	N	605	HEA	C17-C18-C19	2.43	133.05	127.76
26	P	305	PEK	C11-C10-C9	2.45	120.15	112.00
22	C	310	CHD	C5-C6-C7	2.45	117.17	114.44
22	J	101	CHD	C1-C2-C3	2.46	114.42	110.43
22	C	310	CHD	C6-C5-C10	2.46	115.36	112.66
17	N	605	HEA	C26-C15-C16	2.47	119.18	115.41
22	P	310	CHD	C11-C9-C10	2.48	116.37	113.79
24	P	302	DMU	C10-O7-C3	2.49	124.52	118.01
22	C	310	CHD	C14-C13-C12	2.50	109.63	107.39
17	A	605	HEA	CBD-CAD-C3D	2.50	117.01	112.53
22	O	302	CHD	C2-C1-C10	2.52	117.33	112.84
18	A	606	PGV	O01-C02-C03	2.52	117.24	108.36
22	C	304	CHD	C5-C6-C7	2.53	117.25	114.44
20	L	101	TGL	C20-CA9-CA8	2.53	127.61	114.53
27	G	101	CDL	C22-C21-C20	2.54	127.63	114.53
22	J	101	CHD	C14-C8-C9	2.56	113.15	109.62
22	C	310	CHD	C14-C8-C7	2.58	115.31	111.74
17	A	604	HEA	C16-C17-C18	2.59	118.46	111.69
17	N	604	HEA	C16-C17-C18	2.60	118.50	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C11-C9-C10	2.60	116.49	113.79
17	N	605	HEA	CMC-C2C-C3C	2.60	130.18	125.09
27	G	101	CDL	C23-C22-C21	2.61	127.98	114.53
20	D	201	TGL	CB3-CB2-CB1	2.61	123.84	113.59
20	N	606	TGL	OG1-CG1-CG2	2.61	115.71	108.69
24	C	302	DMU	C10-O7-C3	2.61	124.83	118.01
26	C	305	PEK	C11-C10-C9	2.61	120.69	112.00
22	O	302	CHD	C9-C11-C12	2.61	117.66	114.36
22	W	101	CHD	C5-C4-C3	2.62	116.80	112.91
22	W	101	CHD	C9-C11-C12	2.62	117.67	114.36
22	P	310	CHD	C14-C8-C7	2.63	115.38	111.74
24	Z	101	DMU	O7-C10-C5	2.63	114.50	108.10
17	N	605	HEA	C4B-C3B-C11	2.63	129.87	127.01
22	B	304	CHD	C2-C1-C10	2.64	117.55	112.84
20	N	607	TGL	CB3-CB2-CB1	2.64	123.98	113.59
18	N	608	PGV	C02-O01-C1	2.65	124.24	117.89
22	C	310	CHD	C16-C15-C14	2.68	110.52	105.12
20	N	607	TGL	OG2-CG2-CG3	2.68	117.82	108.36
20	D	201	TGL	OG2-CG2-CG3	2.69	117.85	108.36
26	P	306	PEK	P-O12-C04	2.71	136.98	121.50
22	P	310	CHD	C16-C15-C14	2.71	110.58	105.12
18	N	608	PGV	O01-C02-C03	2.71	117.93	108.36
27	T	102	CDL	C22-C21-C20	2.72	128.55	114.53
17	A	605	HEA	C4B-C3B-C11	2.73	129.97	127.01
26	C	306	PEK	P-O12-C04	2.73	137.07	121.50
20	N	606	TGL	C13-C12-C11	2.76	128.80	114.53
22	C	310	CHD	C11-C12-C13	2.77	114.01	111.20
22	J	101	CHD	C5-C4-C3	2.80	117.08	112.91
22	W	101	CHD	C11-C9-C10	2.81	116.71	113.79
17	N	605	HEA	C3C-C4C-NC	2.82	112.86	109.21
22	O	302	CHD	C1-C2-C3	2.83	115.03	110.43
22	W	101	CHD	C15-C16-C17	2.85	110.86	105.12
17	N	604	HEA	CMC-C2C-C3C	2.85	130.67	125.09
22	P	310	CHD	C5-C6-C7	2.87	117.63	114.44
22	P	310	CHD	C15-C16-C17	2.87	110.91	105.12
22	P	310	CHD	C4-C3-C2	2.89	114.21	110.52
22	C	310	CHD	C15-C16-C17	2.91	110.98	105.12
22	C	310	CHD	C1-C10-C9	2.91	116.14	111.45
22	C	310	CHD	C4-C3-C2	2.91	114.23	110.52
20	O	303	TGL	CG3-CG2-CG1	2.93	118.94	112.07
22	O	302	CHD	C18-C13-C14	2.94	115.85	111.22
20	N	607	TGL	OG1-CG1-CG2	2.94	116.60	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C15-C16-C17	2.96	111.08	105.12
22	B	304	CHD	C5-C4-C3	2.97	117.33	112.91
22	P	310	CHD	C9-C10-C5	2.99	113.10	108.67
22	J	101	CHD	C16-C15-C14	3.00	111.17	105.12
18	A	606	PGV	C02-O01-C1	3.00	125.10	117.89
22	C	310	CHD	C9-C10-C5	3.01	113.13	108.67
22	J	101	CHD	C13-C14-C8	3.03	118.66	114.75
22	O	302	CHD	C5-C4-C3	3.03	117.43	112.91
17	A	604	HEA	CMC-C2C-C3C	3.05	131.06	125.09
22	P	310	CHD	C1-C10-C9	3.05	116.37	111.45
24	Z	101	DMU	C10-O1-C9	3.05	119.67	113.75
20	L	101	TGL	OG1-CG1-CG2	3.07	116.96	108.69
22	C	310	CHD	C11-C9-C10	3.08	117.00	113.79
18	A	607	PGV	O03-C01-C02	3.11	117.05	108.69
20	D	201	TGL	OG2-CG2-CG1	3.11	119.32	108.36
22	B	304	CHD	C1-C2-C3	3.12	115.49	110.43
20	N	606	TGL	CC4-CC3-CC2	3.12	124.73	113.29
17	A	605	HEA	CMC-C2C-C3C	3.12	131.20	125.09
20	B	302	TGL	CG3-OG3-CC1	3.14	125.63	116.85
22	P	304	CHD	C5-C6-C7	3.14	117.94	114.44
20	N	606	TGL	CC3-CC2-CC1	3.15	125.99	113.59
20	L	101	TGL	CC4-CC3-CC2	3.17	124.93	113.29
22	W	101	CHD	C13-C14-C8	3.20	118.87	114.75
17	N	605	HEA	C27-C19-C20	3.20	120.30	115.41
20	B	302	TGL	CG3-CG2-CG1	3.21	119.58	112.07
22	B	304	CHD	C9-C11-C12	3.22	118.42	114.36
20	N	606	TGL	C11-C10-CB9	3.23	131.23	114.53
22	C	310	CHD	C4-C5-C10	3.25	116.23	112.66
24	Z	101	DMU	O5-C6-C1	3.25	116.94	110.28
20	L	101	TGL	CC3-CC2-CC1	3.29	126.52	113.59
22	W	101	CHD	C16-C15-C14	3.30	111.77	105.12
24	M	101	DMU	O7-C10-C5	3.33	116.20	108.10
22	C	304	CHD	C13-C17-C20	3.33	123.56	119.50
20	D	201	TGL	OG1-CG1-CG2	3.34	117.67	108.69
22	O	302	CHD	C5-C6-C7	3.37	118.19	114.44
22	P	310	CHD	C14-C13-C12	3.41	110.44	107.39
20	O	303	TGL	CG3-OG3-CC1	3.42	126.43	116.85
22	P	310	CHD	C4-C5-C10	3.44	116.44	112.66
24	M	101	DMU	O5-C6-C1	3.44	117.34	110.28
20	L	101	TGL	C11-C10-CB9	3.45	132.33	114.53
20	N	606	TGL	CG2-OG2-CB1	3.50	126.30	117.89
24	M	101	DMU	C10-O1-C9	3.53	120.61	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	607	TGL	CG2-OG2-CB1	3.59	126.49	117.89
22	B	304	CHD	C18-C13-C14	3.64	116.96	111.22
26	G	102	PEK	C02-O01-C1	3.65	126.65	117.89
24	M	101	DMU	O7-C10-O1	3.68	119.99	110.68
22	J	101	CHD	C14-C8-C7	3.71	116.88	111.74
20	L	101	TGL	C16-C15-CC9	3.71	133.71	114.53
17	A	604	HEA	C20-C19-C18	3.72	128.11	121.05
22	B	304	CHD	C17-C13-C12	3.73	120.98	117.68
22	C	304	CHD	C1-C10-C5	3.74	113.95	107.81
20	N	606	TGL	C16-C15-CC9	3.75	133.90	114.53
20	L	101	TGL	CG2-OG2-CB1	3.76	126.91	117.89
22	W	101	CHD	C1-C10-C5	3.76	113.99	107.81
24	P	302	DMU	O1-C10-C5	3.78	118.04	110.28
18	N	609	PGV	O03-C01-C02	3.80	118.92	108.69
24	M	101	DMU	O7-C3-C4	3.81	119.32	109.32
20	N	606	TGL	C15-CC9-CC8	3.81	134.22	114.53
22	W	101	CHD	C14-C8-C7	3.82	117.03	111.74
24	C	302	DMU	O7-C10-O1	3.85	120.42	110.68
20	D	201	TGL	CG3-OG3-CC1	3.91	127.78	116.85
22	J	101	CHD	C2-C1-C10	3.92	119.83	112.84
20	L	101	TGL	C15-CC9-CC8	3.92	134.76	114.53
26	T	101	PEK	C02-O01-C1	3.96	127.40	117.89
24	Z	101	DMU	O7-C3-C4	3.97	119.77	109.32
24	C	302	DMU	O1-C10-C5	4.00	118.48	110.28
22	P	304	CHD	C13-C17-C20	4.01	124.38	119.50
22	J	101	CHD	C1-C10-C5	4.04	114.45	107.81
20	D	201	TGL	CG2-OG2-CB1	4.05	127.61	117.89
24	Z	101	DMU	O7-C10-O1	4.08	121.01	110.68
22	W	101	CHD	C2-C1-C10	4.12	120.19	112.84
17	A	604	HEA	C4B-C3B-C11	4.12	131.48	127.01
17	N	604	HEA	C20-C19-C18	4.19	129.00	121.05
26	P	306	PEK	C11-C10-C9	4.22	126.04	112.00
26	T	101	PEK	O03-C01-C02	4.29	120.22	108.69
26	C	306	PEK	C11-C10-C9	4.30	126.30	112.00
24	P	302	DMU	C10-O1-C9	4.30	122.09	113.75
24	P	302	DMU	O7-C10-C5	4.41	118.84	108.10
22	P	304	CHD	C1-C10-C5	4.49	115.19	107.81
22	J	101	CHD	C4-C3-C2	4.53	116.30	110.52
24	P	302	DMU	O7-C10-O1	4.54	122.18	110.68
24	C	302	DMU	C10-O1-C9	4.54	122.57	113.75
24	P	302	DMU	O5-C4-C57	4.66	118.13	106.36
26	G	102	PEK	O03-C01-C02	4.66	121.23	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	101	DMU	C10-O7-C3	4.70	130.29	118.01
22	W	101	CHD	C4-C3-C2	4.76	116.59	110.52
20	N	607	TGL	CG3-OG3-CC1	4.77	130.20	116.85
22	O	302	CHD	C17-C13-C12	4.80	121.93	117.68
22	P	304	CHD	C10-C9-C8	4.81	117.17	111.88
20	O	303	TGL	CG2-OG2-CB1	4.89	129.63	117.89
17	N	604	HEA	C4B-C3B-C11	4.92	132.35	127.01
24	C	302	DMU	O7-C10-C5	4.96	120.18	108.10
24	Z	101	DMU	C18-O16-C6	5.15	122.95	113.94
24	C	302	DMU	O5-C4-C57	5.17	119.41	106.36
24	M	101	DMU	C10-O7-C3	5.21	131.62	118.01
22	P	310	CHD	C1-C10-C5	5.32	116.56	107.81
24	C	302	DMU	C8-C7-C5	5.33	120.74	110.79
22	W	101	CHD	C6-C5-C4	5.40	117.07	111.05
22	J	101	CHD	C6-C5-C4	5.49	117.18	111.05
22	C	310	CHD	C9-C8-C7	5.51	118.43	111.92
22	P	310	CHD	C9-C8-C7	5.56	118.49	111.92
22	C	310	CHD	C1-C10-C5	5.59	116.99	107.81
24	C	302	DMU	O5-C6-C1	5.61	121.78	110.28
24	M	101	DMU	C6-C1-C2	5.62	121.05	109.97
24	P	302	DMU	C8-C7-C5	5.65	121.33	110.79
24	C	302	DMU	O1-C9-C8	5.69	120.36	109.68
24	P	302	DMU	O1-C9-C8	5.70	120.39	109.68
22	J	101	CHD	C5-C6-C7	5.71	120.81	114.44
24	M	101	DMU	O5-C6-O16	5.74	123.89	110.05
24	P	302	DMU	O5-C6-C1	5.74	122.06	110.28
24	Z	101	DMU	C6-C1-C2	5.77	121.34	109.97
22	C	304	CHD	C10-C9-C8	5.81	118.26	111.88
20	B	302	TGL	CG2-OG2-CB1	5.82	131.86	117.89
24	Z	101	DMU	O7-C3-C2	5.91	122.41	107.17
24	C	302	DMU	C18-O16-C6	6.00	124.44	113.94
22	J	101	CHD	C9-C8-C7	6.01	119.02	111.92
24	P	302	DMU	O7-C3-C2	6.16	123.06	107.17
24	M	101	DMU	C18-O16-C6	6.16	124.70	113.94
24	P	302	DMU	C6-O5-C4	6.16	125.71	113.75
22	W	101	CHD	C5-C6-C7	6.18	121.32	114.44
24	P	302	DMU	C18-O16-C6	6.18	124.74	113.94
24	Z	101	DMU	O1-C9-C8	6.20	121.32	109.68
24	C	302	DMU	O7-C3-C2	6.22	123.23	107.17
24	Z	101	DMU	O5-C6-O16	6.23	125.05	110.05
24	M	101	DMU	O1-C9-C8	6.31	121.52	109.68
22	W	101	CHD	C9-C8-C7	6.37	119.45	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	101	DMU	O5-C4-C57	6.39	122.52	106.36
24	M	101	DMU	O7-C3-C2	6.51	123.98	107.17
24	Z	101	DMU	O5-C4-C57	6.53	122.87	106.36
22	W	101	CHD	C11-C12-C13	6.54	117.85	111.20
24	C	302	DMU	O7-C3-C4	6.58	126.60	109.32
22	J	101	CHD	C6-C5-C10	6.63	119.96	112.66
22	W	101	CHD	C6-C5-C10	6.63	119.97	112.66
22	J	101	CHD	C11-C12-C13	6.79	118.10	111.20
24	M	101	DMU	C6-O5-C4	6.91	127.17	113.75
24	C	302	DMU	C6-O5-C4	7.01	127.36	113.75
24	Z	101	DMU	C6-O5-C4	7.04	127.41	113.75
24	P	302	DMU	O7-C3-C4	7.32	128.56	109.32
24	Z	101	DMU	O5-C4-C3	7.39	125.35	109.75
24	M	101	DMU	O5-C4-C3	7.42	125.43	109.75
24	Z	101	DMU	O1-C9-C11	7.74	125.91	106.36
24	M	101	DMU	O1-C9-C11	7.76	125.97	106.36
22	W	101	CHD	C10-C9-C8	7.77	120.41	111.88
24	Z	101	DMU	O16-C6-C1	7.89	118.00	108.04
24	C	302	DMU	O5-C4-C3	8.08	126.82	109.75
22	J	101	CHD	C13-C17-C20	8.11	129.37	119.50
24	C	302	DMU	O1-C9-C11	8.11	126.86	106.36
22	J	101	CHD	C10-C9-C8	8.27	120.96	111.88
22	W	101	CHD	C13-C17-C20	8.32	129.63	119.50
24	M	101	DMU	O16-C6-C1	8.44	118.69	108.04
24	P	302	DMU	O1-C9-C11	8.49	127.82	106.36
24	M	101	DMU	C7-C8-C9	8.60	125.18	110.20
24	Z	101	DMU	C7-C8-C9	8.71	125.38	110.20
24	P	302	DMU	O5-C4-C3	9.10	128.97	109.75
22	C	310	CHD	C10-C9-C8	9.36	122.16	111.88
22	P	310	CHD	C10-C9-C8	9.42	122.22	111.88
24	C	302	DMU	C1-C2-C3	9.75	131.01	109.60
24	P	302	DMU	C1-C2-C3	9.92	131.38	109.60
22	C	310	CHD	C17-C13-C14	10.47	110.63	100.05
22	W	101	CHD	C17-C13-C14	10.51	110.68	100.05
24	Z	101	DMU	C10-C5-C7	10.57	130.80	109.97
22	J	101	CHD	C17-C13-C14	10.59	110.75	100.05
24	M	101	DMU	C10-C5-C7	10.75	131.17	109.97
22	P	310	CHD	C17-C13-C14	10.82	110.98	100.05
24	C	302	DMU	O16-C6-C1	13.70	125.34	108.04
24	P	302	DMU	O16-C6-C1	14.07	125.81	108.04

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	302	DMU	C5
24	C	302	DMU	C6
24	C	302	DMU	C9
24	C	302	DMU	C4
24	C	302	DMU	C2
24	C	302	DMU	C10
22	W	101	CHD	C12
22	W	101	CHD	C8
22	W	101	CHD	C9
22	W	101	CHD	C14
22	W	101	CHD	C17
22	P	310	CHD	C12
22	P	310	CHD	C8
22	P	310	CHD	C3
22	P	310	CHD	C9
22	P	310	CHD	C14
22	C	310	CHD	C12
22	C	310	CHD	C8
22	C	310	CHD	C3
22	C	310	CHD	C9
22	C	310	CHD	C14
17	N	604	HEA	ND
17	N	604	HEA	NA
17	N	604	HEA	NB
24	Z	101	DMU	C2
24	Z	101	DMU	C4
24	Z	101	DMU	C6
24	Z	101	DMU	C5
24	Z	101	DMU	C9
24	P	302	DMU	C5
24	P	302	DMU	C6
24	P	302	DMU	C9
24	P	302	DMU	C4
24	P	302	DMU	C2
24	P	302	DMU	C10
17	N	605	HEA	ND
17	N	605	HEA	NA
17	N	605	HEA	NB
17	A	604	HEA	ND
17	A	604	HEA	NA
17	A	604	HEA	NB
24	M	101	DMU	C2
24	M	101	DMU	C4

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Mol	Chain	Res	Type	Atom
24	M	101	DMU	C6
24	M	101	DMU	C5
24	M	101	DMU	C9
17	A	605	HEA	ND
17	A	605	HEA	NA
17	A	605	HEA	NB
22	J	101	CHD	C12
22	J	101	CHD	C8
22	J	101	CHD	C9
22	J	101	CHD	C14
22	J	101	CHD	C17

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	P-O11-C03-C02
18	N	608	PGV	P-O11-C03-C02

There are no ring outliers.

41 monomers are involved in 284 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	604	HEA	2	0
17	A	605	HEA	3	0
18	A	606	PGV	8	0
18	A	607	PGV	8	0
20	B	302	TGL	6	0
21	B	303	PSC	23	0
22	B	304	CHD	1	0
23	C	301	DCW	9	0
24	C	302	DMU	5	0
26	C	305	PEK	11	0
26	C	306	PEK	7	0
18	C	307	PGV	8	0
18	C	308	PGV	1	0
27	C	309	CDL	15	0
22	C	310	CHD	1	0
20	D	201	TGL	6	0
27	G	101	CDL	15	0
26	G	102	PEK	10	0
22	J	101	CHD	2	0
20	L	101	TGL	23	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	M	101	DMU	1	0
17	N	604	HEA	4	0
17	N	605	HEA	2	0
20	N	606	TGL	14	0
20	N	607	TGL	5	0
18	N	608	PGV	7	0
18	N	609	PGV	6	0
20	O	303	TGL	7	0
21	O	304	PSC	21	0
23	P	301	DCW	8	0
24	P	302	DMU	5	0
26	P	305	PEK	11	0
26	P	306	PEK	6	0
18	P	307	PGV	8	0
18	P	308	PGV	1	0
27	P	309	CDL	14	0
22	P	310	CHD	2	0
26	T	101	PEK	8	0
27	T	102	CDL	21	0
22	W	101	CHD	4	0
24	Z	101	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%)	-0.09	1 (0%) 95 95	16, 25, 36, 67	0
1	N	513/514 (99%)	-0.17	2 (0%) 93 93	20, 32, 45, 70	0
2	B	226/227 (99%)	-0.52	1 (0%) 93 93	16, 31, 65, 95	0
2	O	226/227 (99%)	-0.43	3 (1%) 79 78	27, 41, 71, 96	0
3	C	259/261 (99%)	-0.54	0 100 100	20, 30, 50, 83	0
3	P	259/261 (99%)	-0.55	1 (0%) 93 93	23, 33, 56, 89	0
4	D	144/147 (97%)	-0.41	5 (3%) 48 46	24, 36, 63, 90	0
4	Q	144/147 (97%)	0.80	17 (11%) 6 6	35, 53, 78, 108	0
5	E	105/109 (96%)	-0.10	2 (1%) 70 68	26, 36, 68, 109	0
5	R	105/109 (96%)	0.39	6 (5%) 27 27	32, 45, 70, 111	0
6	F	98/98 (100%)	0.22	8 (8%) 14 14	22, 37, 100, 118	0
6	S	98/98 (100%)	0.49	9 (9%) 11 10	26, 43, 103, 115	0
7	G	83/85 (97%)	0.72	18 (21%) 1 1	23, 39, 103, 112	0
7	T	83/85 (97%)	0.78	17 (20%) 1 1	26, 45, 103, 113	0
8	H	79/85 (92%)	0.17	9 (11%) 7 6	25, 41, 99, 105	0
8	U	79/85 (92%)	0.68	14 (17%) 2 2	32, 48, 99, 109	0
9	I	72/73 (98%)	0.16	1 (1%) 78 77	27, 45, 74, 83	0
9	V	72/73 (98%)	0.50	7 (9%) 10 9	34, 56, 80, 97	0
10	J	58/59 (98%)	0.15	6 (10%) 9 8	27, 41, 79, 106	0
10	W	58/59 (98%)	0.41	4 (6%) 20 19	34, 49, 87, 110	0
11	K	49/56 (87%)	-0.29	0 100 100	29, 41, 57, 74	0
11	X	49/56 (87%)	0.68	5 (10%) 9 8	44, 56, 74, 88	0
12	L	46/47 (97%)	-0.44	0 100 100	21, 32, 55, 92	0
12	Y	46/47 (97%)	-0.29	2 (4%) 39 38	34, 43, 69, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.14	3 (6%) 19 19	23, 32, 97, 108	0
13	Z	43/46 (93%)	0.34	8 (18%) 2 1	39, 47, 101, 112	0
All	All	3550/3614 (98%)	-0.06	149 (4%) 40 39	16, 35, 74, 118	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	18.6
4	Q	6	VAL	15.5
6	S	97	ALA	15.1
6	S	96	LEU	15.1
4	Q	8	SER	11.2
6	F	98	HIS	10.4
6	F	97	ALA	9.2
6	F	96	LEU	8.9
4	Q	7	LYS	8.9
6	S	94	HIS	8.8
5	R	5	HIS	8.6
13	Z	43	SER	8.6
6	S	2	SER	8.6
6	F	1	ALA	8.4
8	U	8	ILE	8.4
8	U	7	LYS	8.3
6	F	95	GLN	7.8
6	F	2	SER	7.4
4	Q	35	ALA	7.4
10	W	58	LYS	7.4
7	T	2	SER	7.1
7	T	3	ALA	7.1
5	E	5	HIS	6.9
6	S	98	HIS	6.8
7	G	1	ALA	6.8
4	Q	4	SER	6.6
9	V	2	THR	6.6
6	S	1	ALA	6.4
7	T	42	ARG	6.4
7	G	40	GLY	6.3
10	J	58	LYS	6.3
7	G	42	ARG	6.1
8	H	45	ALA	6.1
7	T	39	SER	6.0

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Mol	Chain	Res	Type	RSRZ
7	G	2	SER	5.9
8	H	44	THR	5.8
7	G	5	LYS	5.7
7	T	36	TRP	5.7
8	U	44	THR	5.6
7	T	5	LYS	5.3
8	H	46	LYS	5.2
5	R	109	VAL	5.2
7	T	4	ALA	5.0
7	G	9	GLY	5.0
7	G	4	ALA	4.9
8	H	7	LYS	4.8
3	P	3	HIS	4.8
4	Q	147	LYS	4.8
9	I	37	PHE	4.8
8	U	9	LYS	4.7
8	H	47	GLY	4.7
7	G	3	ALA	4.7
2	O	113	TYR	4.7
8	U	45	ALA	4.6
7	G	8	HIS	4.6
7	T	8	HIS	4.6
6	S	93	PRO	4.4
13	Z	39	ASN	4.4
7	T	84	LYS	4.3
6	F	94	HIS	4.3
11	X	6	ALA	4.2
7	T	41	HIS	4.2
10	J	1	PHE	4.2
2	O	227	LEU	4.1
6	S	95	GLN	4.1
4	Q	39	ALA	4.1
8	U	47	GLY	4.1
13	M	40	TYR	4.1
13	Z	37	LEU	4.0
9	V	3	ALA	4.0
13	Z	41	LYS	4.0
11	X	13	TYR	3.9
4	Q	51	LEU	3.7
13	Z	40	TYR	3.7
10	W	48	TYR	3.6
7	T	40	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
8	H	48	GLY	3.5
7	T	1	ALA	3.5
1	N	513	LEU	3.4
7	G	41	HIS	3.3
8	H	43	MET	3.3
13	M	43	SER	3.2
10	J	52	TRP	3.2
10	J	57	HIS	3.1
5	R	79	LYS	3.0
4	D	5	VAL	3.0
12	Y	47	LYS	3.0
7	T	9	GLY	3.0
10	W	52	TRP	3.0
9	V	36	LYS	3.0
8	U	48	GLY	2.9
6	F	3	GLY	2.9
4	Q	62	LEU	2.9
7	G	6	GLY	2.9
4	Q	142	LYS	2.9
4	D	6	VAL	2.8
8	U	50	VAL	2.8
9	V	25	PHE	2.8
7	G	84	LYS	2.8
5	R	52	LEU	2.8
2	O	226	MET	2.8
9	V	37	PHE	2.8
7	T	7	ASP	2.7
7	G	36	TRP	2.7
2	B	59	GLN	2.7
4	Q	58	GLU	2.7
10	J	2	GLU	2.7
11	X	9	PHE	2.6
8	H	8	ILE	2.6
8	U	85	ILE	2.6
4	Q	102	TYR	2.6
6	S	3	GLY	2.6
10	W	4	ARG	2.5
8	U	43	MET	2.5
8	U	51	SER	2.4
12	Y	20	ARG	2.4
7	G	43	GLU	2.4
7	T	10	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
9	V	34	PHE	2.4
1	N	48	LEU	2.4
5	R	96	LEU	2.4
7	G	7	ASP	2.4
4	Q	136	ALA	2.4
13	M	39	ASN	2.3
4	Q	55	GLU	2.3
4	D	147	LYS	2.3
4	D	7	LYS	2.3
4	Q	48	TRP	2.3
5	E	109	VAL	2.3
11	X	7	PRO	2.2
4	D	8	SER	2.2
5	R	16	VAL	2.2
11	X	34	THR	2.2
7	G	45	PRO	2.2
9	V	4	LEU	2.2
1	A	241	PRO	2.2
13	Z	42	LYS	2.1
7	T	6	GLY	2.1
13	Z	35	TYR	2.1
8	U	10	ASN	2.1
7	T	38	HIS	2.1
8	H	49	ASP	2.1
4	Q	73	ARG	2.1
8	U	49	ASP	2.1
10	J	4	ARG	2.1
7	G	39	SER	2.1
8	U	55	TRP	2.0
13	Z	32	TRP	2.0
7	G	12	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FME	O	1	10/11	0.95	0.14	-	40,42,47,54	0
7	TPO	G	11	11/12	0.55	0.32	-	89,96,117,119	0
2	FME	B	1	10/11	0.95	0.13	-	25,33,44,53	0
9	SAC	V	1	9/10	0.49	0.64	-	101,107,109,110	0
1	FME	N	1	10/11	0.92	0.21	-	57,61,85,85	0
7	TPO	T	11	11/12	0.49	0.29	-	87,93,112,113	0
9	SAC	I	1	9/10	0.80	0.27	-	89,93,96,97	0
1	FME	A	1	10/11	0.87	0.14	-	50,60,76,86	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(\AA^2)	Q<0.9
24	DMU	C	302	33/33	0.65	0.41	16.74	88,116,120,120	0
22	CHD	W	101	29/29	0.75	0.34	13.35	89,100,103,108	0
22	CHD	J	101	29/29	0.81	0.37	7.84	91,99,104,107	0
18	PGV	A	606	51/51	0.75	0.30	7.76	32,75,113,120	0
16	NA	A	603	1/1	0.78	0.20	7.50	44,44,44,44	0
24	DMU	P	302	33/33	0.64	0.41	7.32	91,116,120,120	0
20	TGL	D	201	63/63	0.74	0.25	6.46	45,70,82,87	0
27	CDL	P	309	100/100	0.74	0.39	6.00	37,90,108,118	0
20	TGL	O	303	63/63	0.76	0.26	5.61	46,70,91,96	0
27	CDL	C	309	100/100	0.75	0.36	5.60	43,92,103,109	0
20	TGL	L	101	63/63	0.76	0.29	5.09	36,67,81,84	0
18	PGV	N	608	51/51	0.79	0.36	5.00	38,80,114,119	0
20	TGL	N	606	63/63	0.68	0.34	4.88	39,68,86,88	0
15	MG	N	602	1/1	0.94	0.16	4.51	35,35,35,35	0
20	TGL	B	302	63/63	0.82	0.22	4.21	41,67,89,94	0
16	NA	N	603	1/1	0.81	0.19	3.74	50,50,50,50	0
18	PGV	C	308	51/51	0.69	0.39	3.74	61,87,113,116	0
24	DMU	Z	101	33/33	0.82	0.33	3.36	50,72,86,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	MG	A	602	1/1	0.95	0.17	2.88	23,23,23,23	0
20	TGL	N	607	63/63	0.73	0.22	2.79	48,69,85,92	0
27	CDL	T	102	100/100	0.62	0.35	2.74	47,86,112,120	0
27	CDL	G	101	100/100	0.64	0.34	2.73	55,88,111,120	0
21	PSC	B	303	52/52	0.57	0.36	2.52	47,90,120,120	0
21	PSC	O	304	52/52	0.64	0.39	2.43	48,88,120,120	0
18	PGV	P	308	51/51	0.68	0.39	2.43	66,90,112,116	0
22	CHD	P	310	29/29	0.85	0.24	2.42	78,91,94,99	0
18	PGV	A	607	51/51	0.97	0.15	2.07	22,41,66,76	0
18	PGV	N	609	51/51	0.97	0.14	1.95	25,43,64,77	0
24	DMU	M	101	33/33	0.85	0.20	1.93	45,63,80,87	0
26	PEK	P	306	53/53	0.66	0.35	1.80	40,89,110,114	0
18	PGV	P	307	51/51	0.96	0.13	1.79	23,36,68,73	0
26	PEK	T	101	53/53	0.46	0.46	1.71	50,90,115,120	0
26	PEK	G	102	53/53	0.54	0.41	1.60	50,89,115,120	0
18	PGV	C	307	51/51	0.96	0.12	1.40	22,33,65,72	0
22	CHD	C	310	29/29	0.84	0.26	1.35	75,92,97,101	0
26	PEK	C	306	53/53	0.56	0.30	1.16	46,91,115,120	0
26	PEK	P	305	53/53	0.94	0.14	0.88	24,46,73,77	0
17	HEA	N	604	60/60	0.98	0.17	0.81	20,32,50,55	0
19	CUA	B	301	2/2	0.99	0.14	0.69	24,24,24,27	0
17	HEA	A	604	60/60	0.99	0.17	0.64	16,25,49,54	0
26	PEK	C	305	53/53	0.95	0.13	0.59	17,43,71,73	0
28	ZN	F	101	1/1	0.99	0.09	0.54	32,32,32,32	0
17	HEA	N	605	60/60	0.98	0.17	0.51	16,27,34,36	0
17	HEA	A	605	60/60	0.98	0.16	0.39	10,24,31,33	0
23	DCW	P	301	16/16	0.93	0.15	0.34	52,59,70,70	0
23	DCW	C	301	16/16	0.90	0.17	0.19	46,50,53,54	0
22	CHD	C	304	29/29	0.97	0.12	-0.15	25,31,37,39	0
22	CHD	P	304	29/29	0.96	0.12	-0.26	25,32,40,46	0
19	CUA	O	301	2/2	0.98	0.10	-0.38	36,36,36,36	0
22	CHD	O	302	29/29	0.97	0.10	-0.38	17,29,37,40	0
22	CHD	B	304	29/29	0.97	0.08	-0.54	20,27,34,38	0
28	ZN	S	101	1/1	0.99	0.06	-1.12	34,34,34,34	0
25	UNX	P	303	1/1	0.67	0.26	-	50,50,50,50	0
14	CU	A	601	1/1	0.99	0.12	-	23,23,23,23	0
14	CU	N	601	1/1	0.99	0.15	-	28,28,28,28	0
25	UNX	C	303	1/1	0.75	0.39	-	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.