



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2017 – 06:27 PM EST

PDB ID : 5IY5
Title : Electron transfer complex of cytochrome c and cytochrome c oxidase at 2.0 angstrom resolution
Authors : Shimada, S.; Baba, J.; Aoe, S.; Shimada, A.; Yamashita, E.; Tsukihara, T.
Deposited on : 2016-03-24
Resolution : 2.00 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

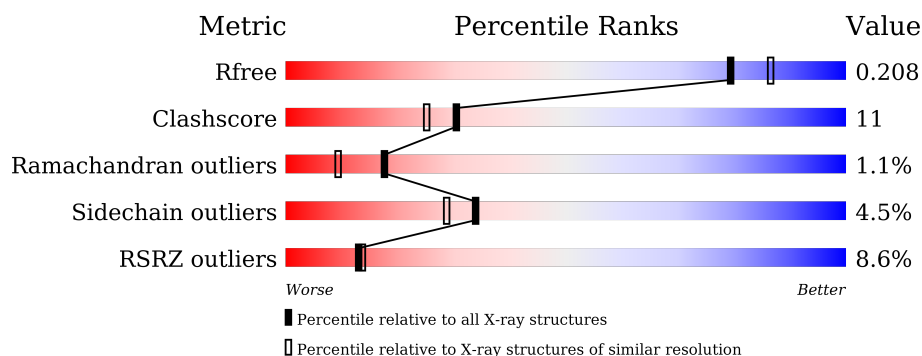
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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>4%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	N	514	<div> <div>5%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
2	B	227	<div> <div>%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
3	C	259	<div> <div>%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
3	P	259	<div> <div>2%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	
14	1	105	
14	2	105	

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
16	MG	A	602	-	-	-	X
16	MG	N	603	-	-	-	X
18	HEA	A	605	X	-	-	-
18	HEA	N	606	X	-	-	-
20	PGV	A	607	-	-	-	X
20	PGV	C	305	-	-	-	X
20	PGV	P	305	-	-	-	X
21	TGL	B	301	-	-	-	X
21	TGL	D	201	-	-	-	X
21	TGL	L	101	-	-	-	X
21	TGL	N	608	-	-	-	X
21	TGL	Q	201	-	-	-	X
23	EDO	N	613	-	-	-	X
24	CHD	J	101	-	-	-	X
24	CHD	P	307	-	-	-	X
24	CHD	W	101	-	-	-	X
26	CDL	C	306	-	-	-	X
26	CDL	G	101	-	-	X	X
26	CDL	P	306	-	-	-	X
26	CDL	T	101	-	-	X	X
27	UNL	C	308	-	-	-	X
27	UNL	C	310	-	-	X	X
27	UNL	J	102	-	-	-	X
27	UNL	L	102	-	-	-	X
27	UNL	N	601	-	-	X	X
27	UNL	N	609	-	-	-	X
27	UNL	N	610	-	-	-	X
27	UNL	P	308	-	-	X	X
27	UNL	P	310	-	-	X	X
27	UNL	Y	101	-	-	-	X
28	PSC	V	101	-	-	X	-
29	ZN	S	101	-	-	X	-
30	DMU	Z	101	-	-	-	X

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 34765 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	11	0
			4084	2731	628	685	40			
1	N	514	Total	C	N	O	S	0	8	0
			4065	2717	627	683	38			

- 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	2	0
			1836	1192	283	343	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	6	0
			2149	1437	343	355	14			
3	P	259	Total	C	N	O	S	0	5	0
			2143	1433	342	354	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	199	218	4			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	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 6B1.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	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 subunit 7A1, mitochondrial.

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

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

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

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

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

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

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

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 a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			
14	2	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ACE	-	acetylation	UNP P00004
2	0	ACE	-	acetylation	UNP P00004

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

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

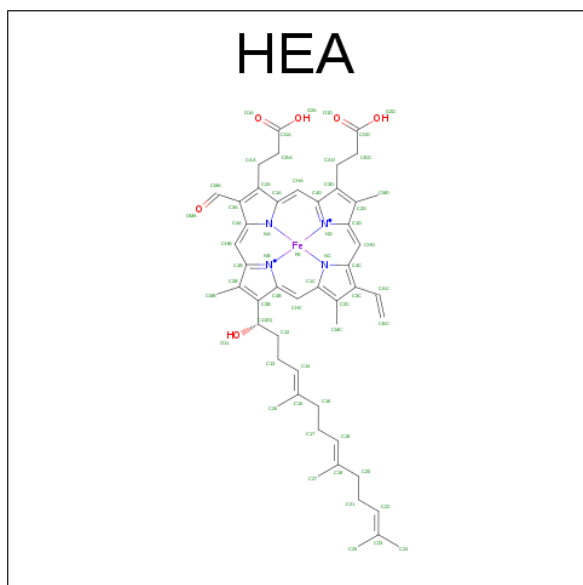
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

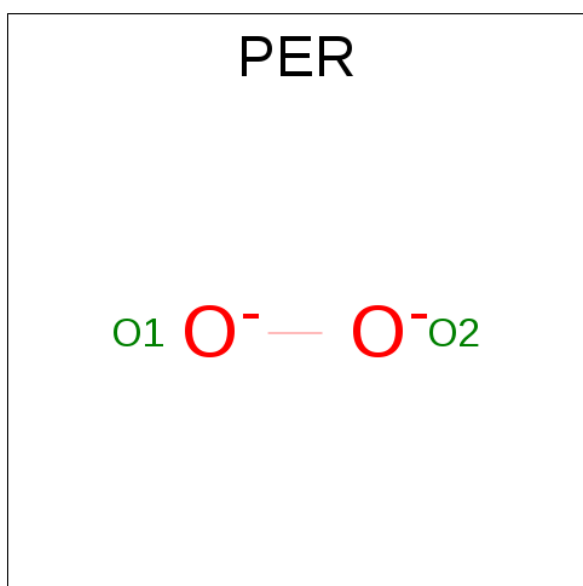
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	1	Total Na 1 1	0	0
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



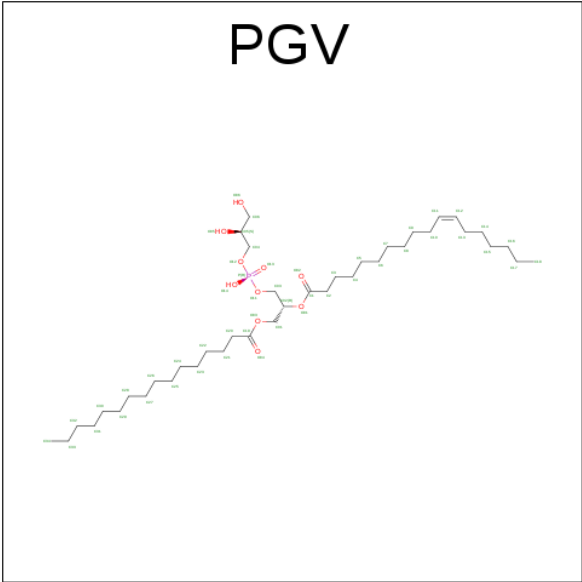
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



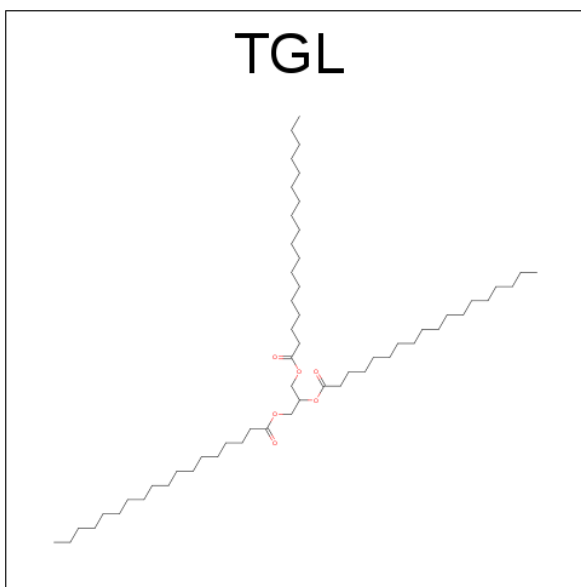
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		
19	N	1	Total	O	0	0
			2	2		

- Molecule 20 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



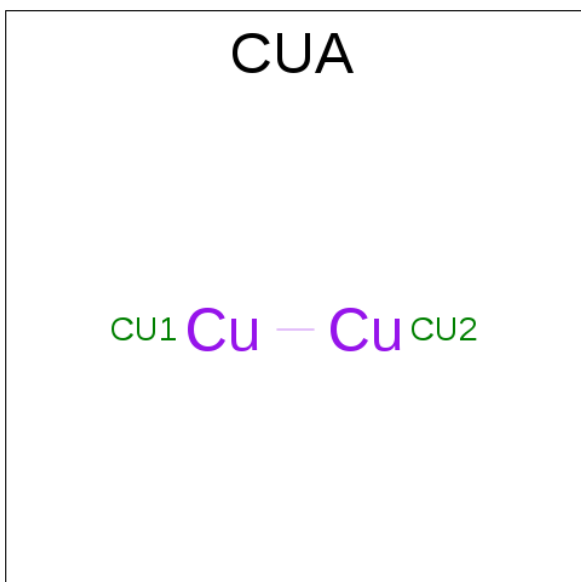
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



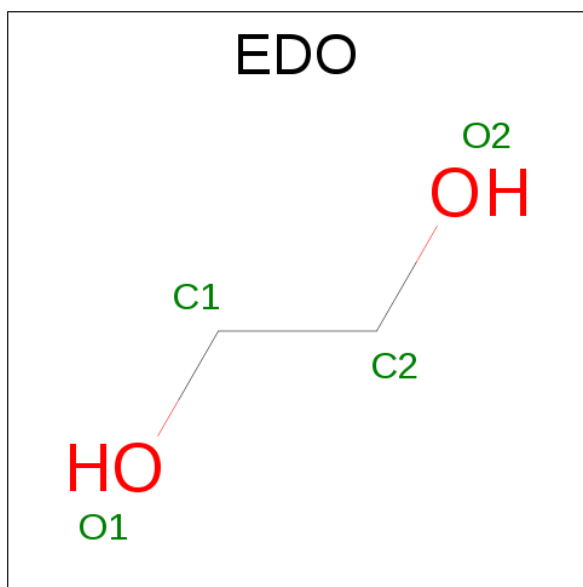
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



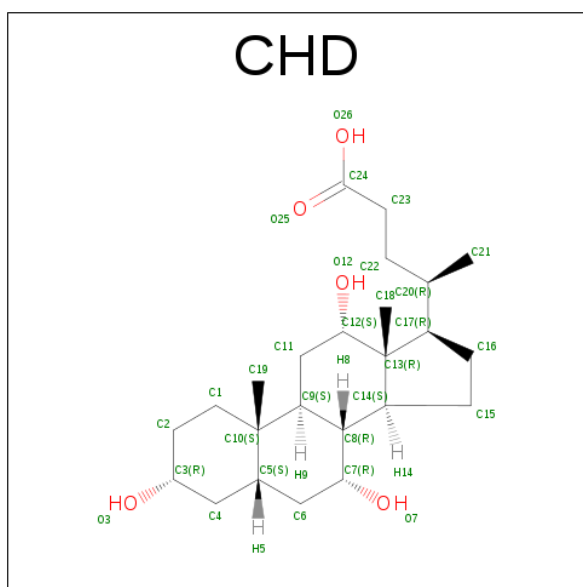
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- Molecule 23 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



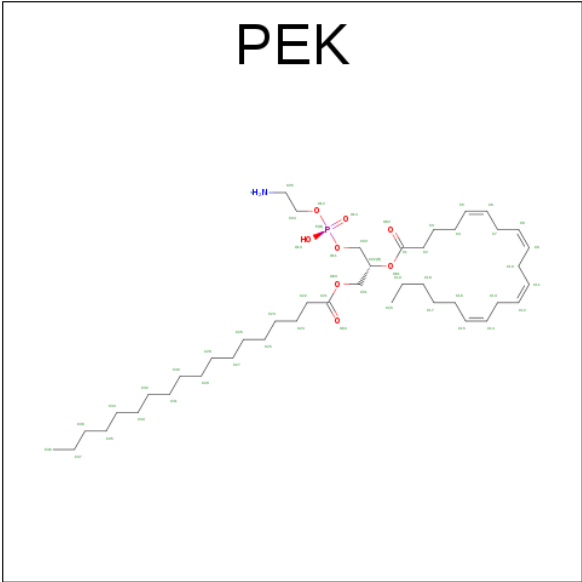
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	F	1	Total C O 4 2 2	0	0
23	G	1	Total C O 4 2 2	0	0
23	I	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	S	1	Total C O 4 2 2	0	0

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



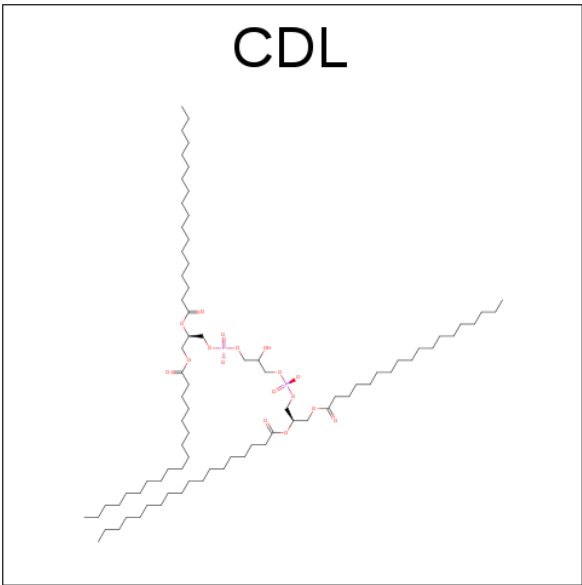
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	J	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	T	1	Total	C	O	0	0
			29	24	5		
24	W	1	Total	C	O	0	0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

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

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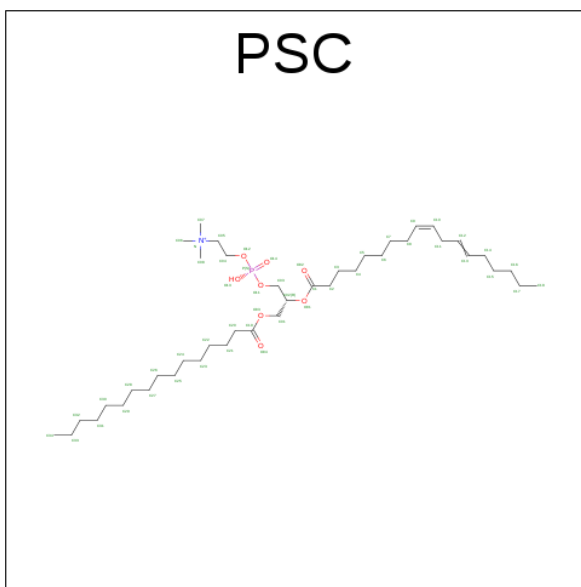
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	P	3	Total	C	0	0
			43	43		
27	J	1	Total	C	0	0
			10	10		
27	C	3	Total	C	0	0
			42	42		
27	W	1	Total	C	0	0
			9	9		
27	T	1	Total	C	0	0
			18	18		
27	N	4	Total	C	0	0
			63	63		
27	Y	1	Total	C	0	0
			10	10		
27	L	1	Total	C	0	0
			10	10		

- Molecule 28 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).

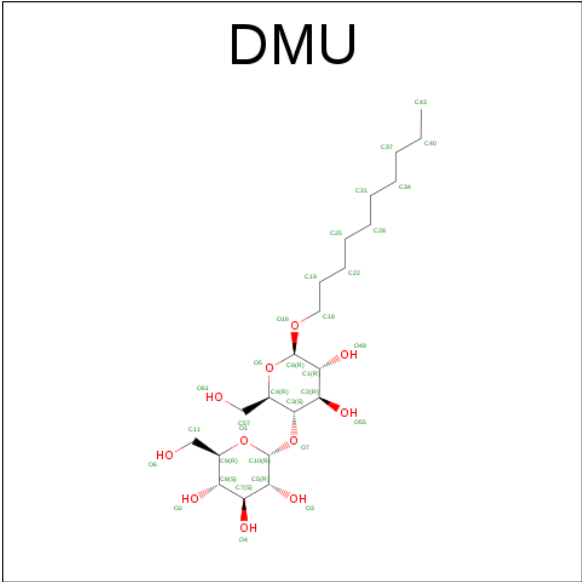


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	V	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

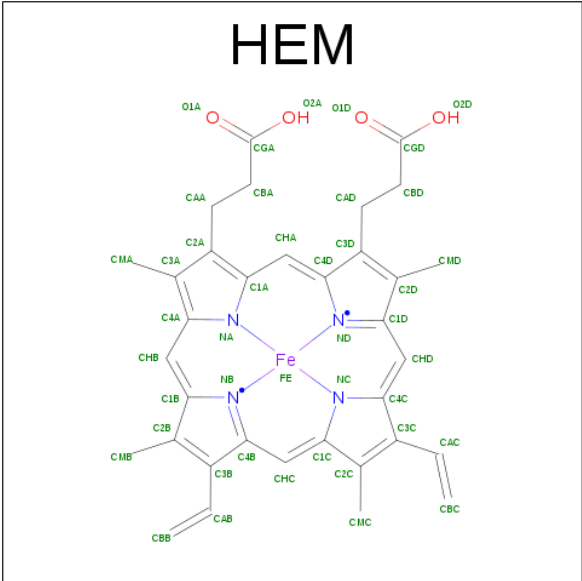
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	S	1	Total	Zn	0	0
			1	1		
29	F	1	Total	Zn	0	0
			1	1		

- Molecule 30 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 32 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	252	Total	O	0	0
			252	252		
32	B	193	Total	O	0	0
			193	193		
32	C	137	Total	O	0	0
			137	137		
32	D	122	Total	O	0	0
			122	122		
32	E	119	Total	O	0	0
			119	119		
32	F	97	Total	O	0	0
			97	97		
32	G	60	Total	O	0	0
			60	60		
32	H	76	Total	O	0	0
			76	76		
32	I	49	Total	O	0	0
			49	49		
32	J	30	Total	O	0	0
			30	30		
32	K	29	Total	O	0	0
			29	29		
32	L	33	Total	O	0	0
			33	33		
32	M	26	Total	O	0	0
			26	26		
32	N	229	Total	O	0	0
			229	229		
32	O	141	Total	O	0	0
			141	141		
32	P	110	Total	O	0	0
			110	110		
32	Q	99	Total	O	0	0
			99	99		
32	R	83	Total	O	0	0
			83	83		

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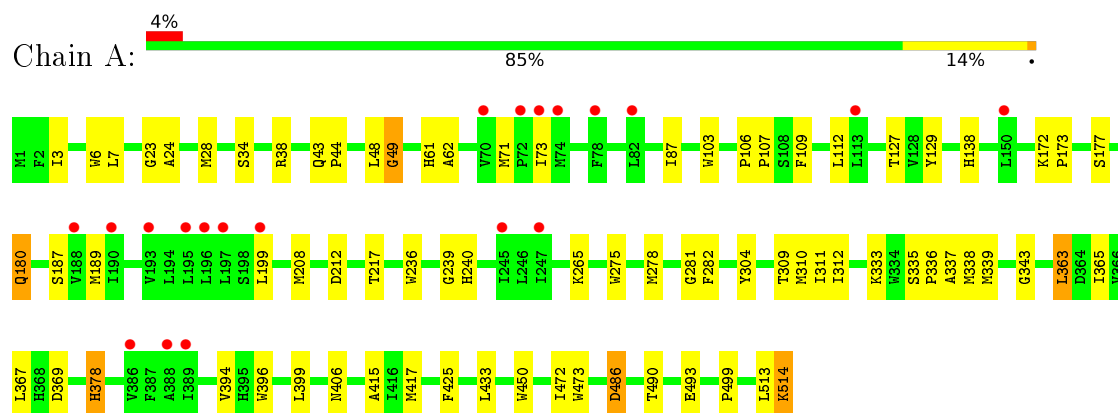
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	S	95	Total 95	O 95	0	0
32	T	41	Total 41	O 41	0	0
32	U	54	Total 54	O 54	0	0
32	V	17	Total 17	O 17	0	0
32	W	10	Total 10	O 10	0	0
32	X	17	Total 17	O 17	0	0
32	Y	21	Total 21	O 21	0	0
32	Z	16	Total 16	O 16	0	0
32	1	53	Total 53	O 53	0	0
32	2	28	Total 28	O 28	0	0

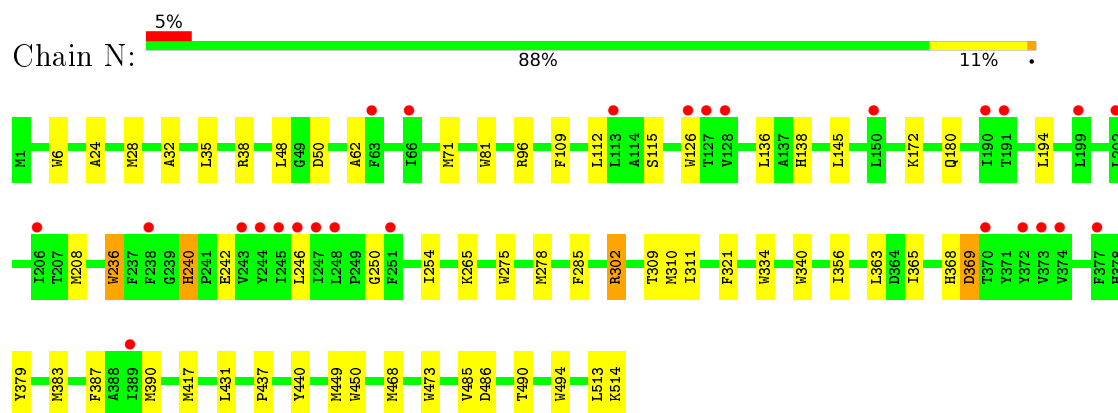
3 Residue-property plots [i](#)

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.

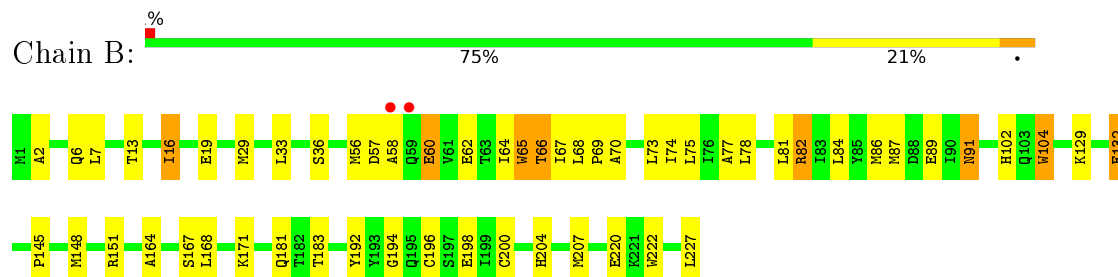
• Molecule 1: Cytochrome c oxidase subunit 1



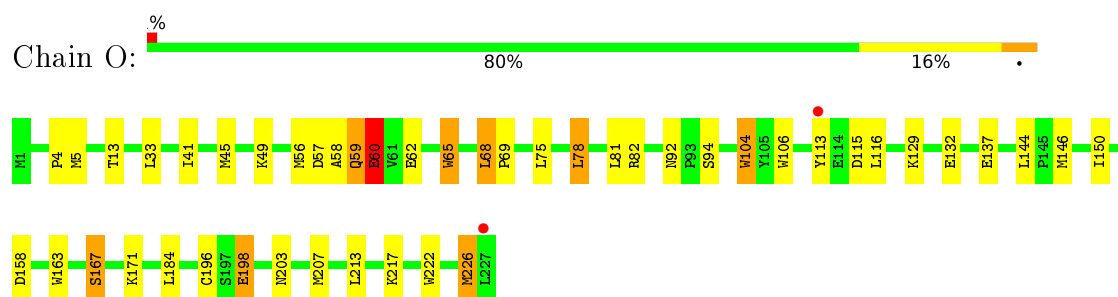
• Molecule 1: Cytochrome c oxidase subunit 1



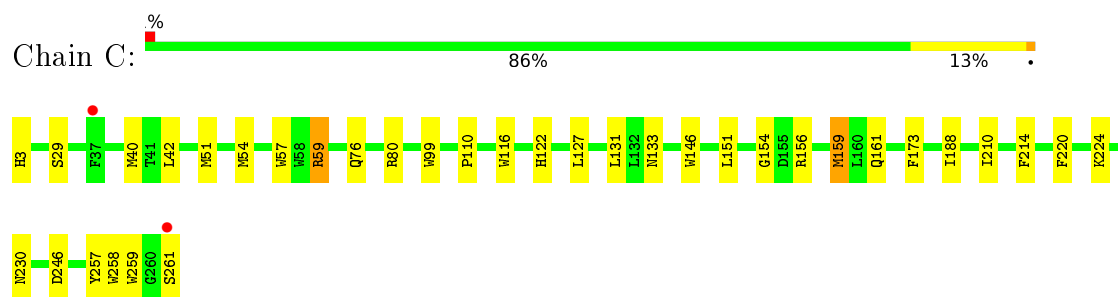
• Molecule 2: Cytochrome c oxidase subunit 2



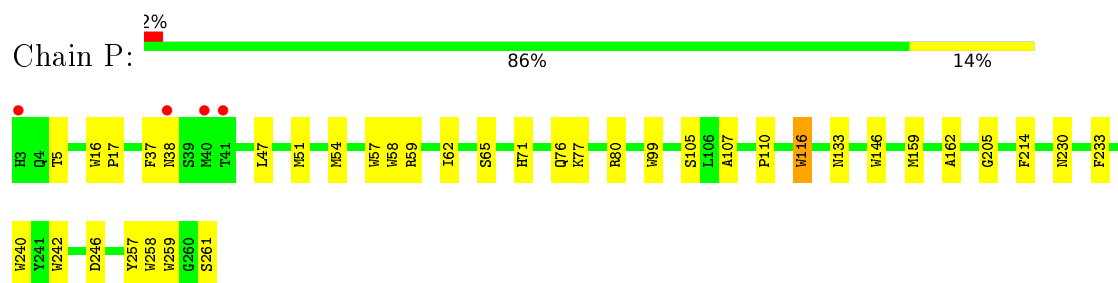
• Molecule 2: Cytochrome c oxidase subunit 2



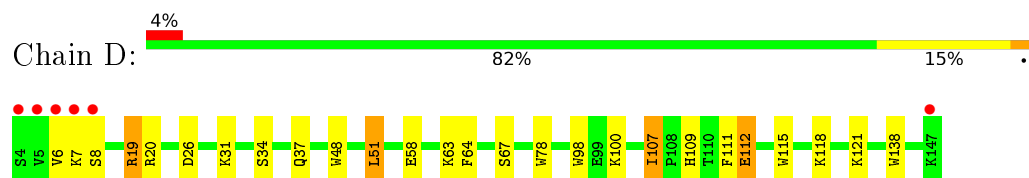
• Molecule 3: Cytochrome c oxidase subunit 3



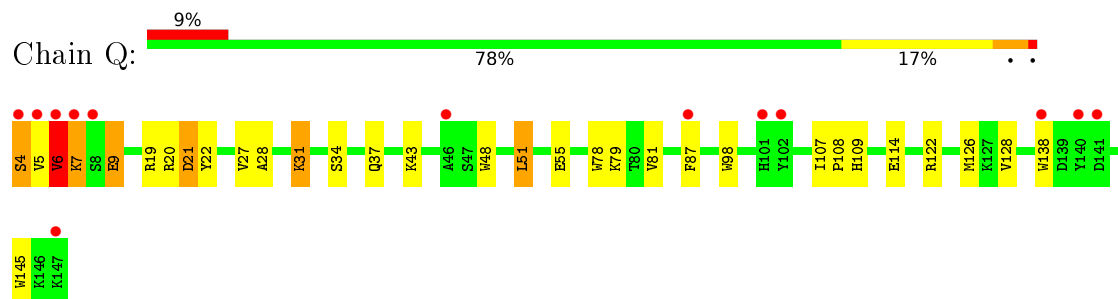
• Molecule 3: Cytochrome c oxidase subunit 3



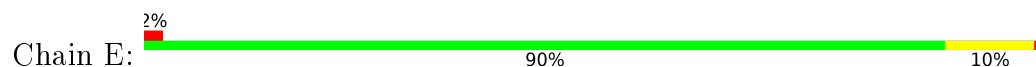
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

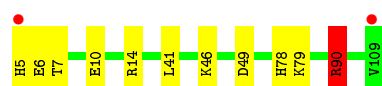


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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

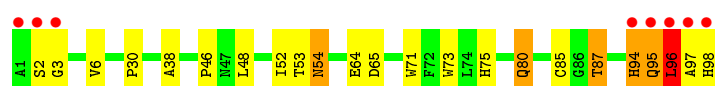




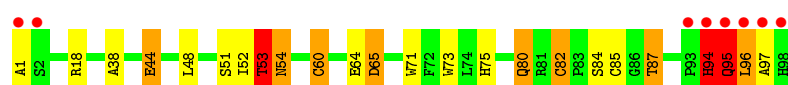
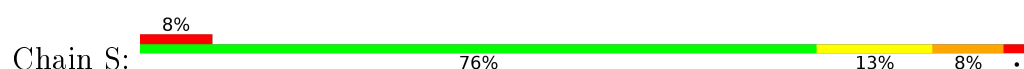
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



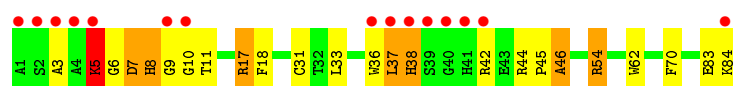
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



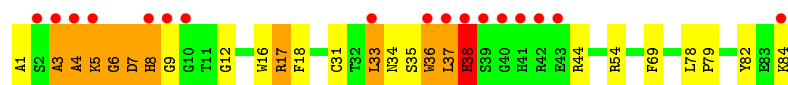
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



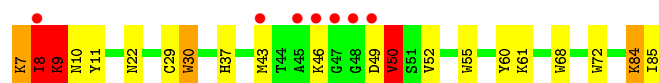
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



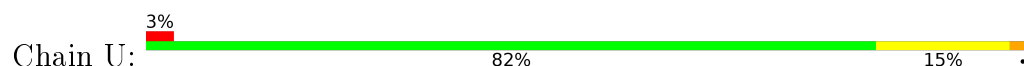
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

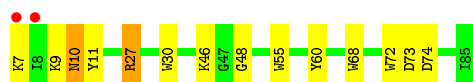


- Molecule 8: Cytochrome c oxidase subunit 6B1

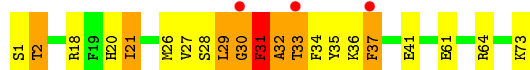


- Molecule 8: Cytochrome c oxidase subunit 6B1

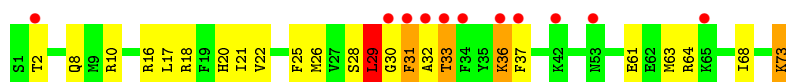




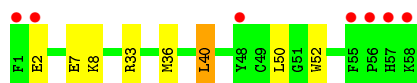
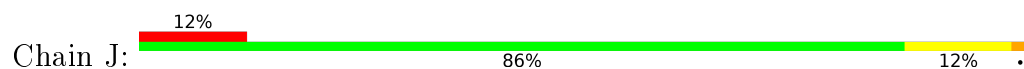
- Molecule 9: Cytochrome c oxidase subunit 6C



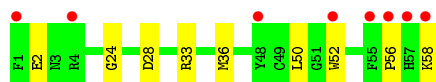
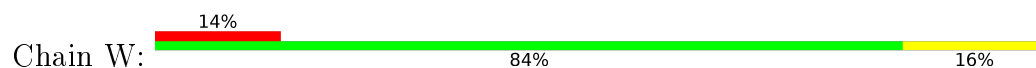
- Molecule 9: Cytochrome c oxidase subunit 6C



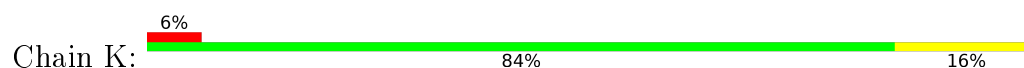
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



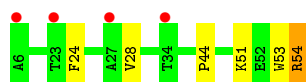
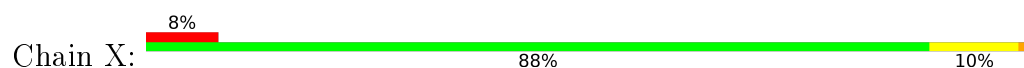
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



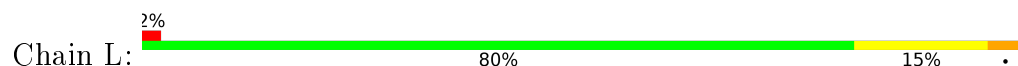
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

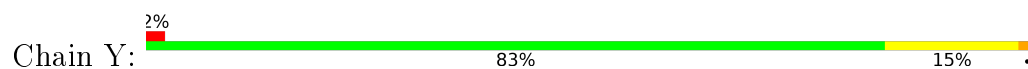


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

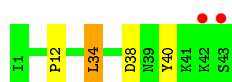




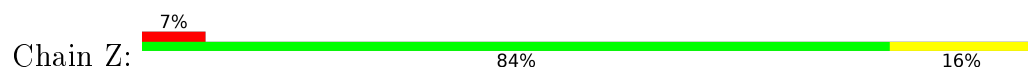
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



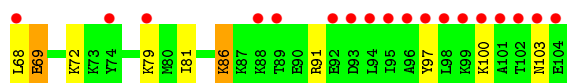
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



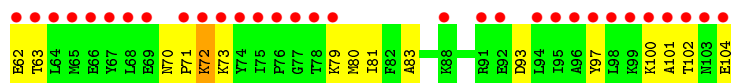
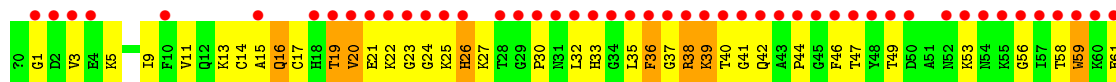
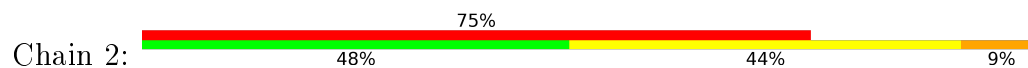
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- Molecule 14: Cytochrome c



- Molecule 14: Cytochrome c



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.29Å 183.87Å 148.93Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 49.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.00) 99.4 (49.35-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.167 , 0.207 0.168 , 0.208	Depositor DCC
R_{free} test set	19990 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34765	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.31	11/4244 (0.3%)	1.04	9/5793 (0.2%)
1	N	1.20	9/4214 (0.2%)	0.94	5/5754 (0.1%)
2	B	1.26	6/1878 (0.3%)	1.09	4/2558 (0.2%)
2	O	0.99	6/1860 (0.3%)	0.96	1/2534 (0.0%)
3	C	1.20	5/2247 (0.2%)	0.87	1/3070 (0.0%)
3	P	1.15	7/2238 (0.3%)	0.86	0/3058
4	D	1.21	7/1229 (0.6%)	1.13	8/1658 (0.5%)
4	Q	1.09	5/1240 (0.4%)	0.97	2/1672 (0.1%)
5	E	1.04	0/871	0.99	5/1182 (0.4%)
5	R	1.01	1/871 (0.1%)	0.89	0/1182
6	F	1.17	3/765 (0.4%)	1.04	2/1038 (0.2%)
6	S	1.15	4/765 (0.5%)	1.15	5/1038 (0.5%)
7	G	1.17	2/690 (0.3%)	1.01	3/937 (0.3%)
7	T	1.20	1/690 (0.1%)	1.09	5/937 (0.5%)
8	H	1.25	7/682 (1.0%)	1.19	4/921 (0.4%)
8	U	1.05	4/682 (0.6%)	0.99	4/921 (0.4%)
9	I	1.09	0/605	1.09	2/802 (0.2%)
9	V	0.86	0/605	0.96	1/802 (0.1%)
10	J	0.96	1/471 (0.2%)	0.88	1/636 (0.2%)
10	W	0.87	1/471 (0.2%)	0.86	0/636
11	K	1.13	1/398 (0.3%)	0.96	0/546
11	X	0.94	1/398 (0.3%)	0.86	0/546
12	L	1.15	0/393	0.90	0/526
12	Y	1.05	0/393	0.95	1/526 (0.2%)
13	M	1.05	0/345	1.01	1/470 (0.2%)
13	Z	1.01	1/345 (0.3%)	1.01	2/470 (0.4%)
14	1	0.73	1/840 (0.1%)	0.78	0/1120
14	2	0.68	1/840 (0.1%)	0.74	0/1120
All	All	1.14	85/31270 (0.3%)	0.98	66/42453 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	S	0	2
8	H	0	2
9	V	0	2
All	All	0	8

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	116	TRP	CD2-CE2	8.38	1.51	1.41
2	B	132	GLU	CD-OE2	8.22	1.34	1.25
6	S	60	CYS	CB-SG	8.20	1.96	1.82
2	B	167	SER	CB-OG	-8.05	1.31	1.42
1	N	236	TRP	CD2-CE2	7.79	1.50	1.41
1	N	275	TRP	CD2-CE2	7.66	1.50	1.41
4	D	115	TRP	CD2-CE2	7.58	1.50	1.41
3	C	116	TRP	CD2-CE2	7.46	1.50	1.41
1	A	396	TRP	CD2-CE2	7.42	1.50	1.41
2	B	65	TRP	CD2-CE2	7.40	1.50	1.41
2	O	106	TRP	CD2-CE2	7.02	1.49	1.41
3	P	242	TRP	CD2-CE2	7.02	1.49	1.41
3	C	99	TRP	CD2-CE2	6.78	1.49	1.41
6	F	73	TRP	CD2-CE2	6.65	1.49	1.41
1	A	473	TRP	CD2-CE2	6.63	1.49	1.41
1	A	49	GLY	C-O	6.61	1.34	1.23
8	H	9	LYS	C-O	6.61	1.35	1.23
7	G	36	TRP	CD2-CE2	6.59	1.49	1.41
6	S	71	TRP	CD2-CE2	6.58	1.49	1.41
8	H	8	ILE	N-CA	6.50	1.59	1.46
3	P	57	TRP	CD2-CE2	6.42	1.49	1.41
1	A	378	HIS	CG-CD2	6.36	1.46	1.35
1	N	340	TRP	CD2-CE2	6.34	1.49	1.41
1	A	61	HIS	CG-CD2	6.31	1.46	1.35
1	A	275	TRP	CD2-CE2	6.30	1.49	1.41
4	D	138	TRP	CD2-CE2	6.28	1.48	1.41
3	P	259	TRP	CD2-CE2	6.24	1.48	1.41
14	1	59	TRP	CD2-CE2	6.22	1.48	1.41
6	F	71	TRP	CD2-CE2	6.22	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	259	TRP	CD2-CE2	6.20	1.48	1.41
8	H	72	TRP	CD2-CE2	6.08	1.48	1.41
4	D	98	TRP	CD2-CE2	6.05	1.48	1.41
8	U	72	TRP	CD2-CE2	6.04	1.48	1.41
4	Q	145	TRP	CD2-CE2	5.98	1.48	1.41
3	P	99	TRP	CD2-CE2	5.97	1.48	1.41
8	U	55	TRP	CD2-CE2	5.88	1.48	1.41
3	P	58	TRP	CD2-CE2	5.87	1.48	1.41
6	S	73	TRP	CD2-CE2	5.86	1.48	1.41
3	C	57	TRP	CD2-CE2	5.84	1.48	1.41
7	G	62	TRP	CD2-CE2	5.81	1.48	1.41
7	T	36	TRP	CD2-CE2	5.78	1.48	1.41
1	A	450	TRP	CD2-CE2	5.78	1.48	1.41
1	A	6	TRP	CD2-CE2	5.77	1.48	1.41
1	N	81	TRP	CD2-CE2	5.75	1.48	1.41
11	K	29	TRP	CD2-CE2	5.72	1.48	1.41
8	U	68	TRP	CD2-CE2	5.66	1.48	1.41
1	N	473	TRP	CD2-CE2	5.65	1.48	1.41
4	Q	138	TRP	CD2-CE2	5.64	1.48	1.41
4	D	112	GLU	CD-OE1	5.63	1.31	1.25
2	B	222	TRP	CD2-CE2	5.61	1.48	1.41
4	Q	22	TYR	CG-CD1	5.60	1.46	1.39
8	U	30	TRP	CD2-CE2	5.59	1.48	1.41
1	N	126	TRP	CD2-CE2	5.58	1.48	1.41
11	X	53	TRP	CD2-CE2	5.57	1.48	1.41
4	Q	9	GLU	CD-OE2	5.56	1.31	1.25
4	D	48	TRP	CD2-CE2	5.55	1.48	1.41
2	O	104	TRP	CD2-CE2	5.55	1.48	1.41
5	R	15	TRP	CD2-CE2	5.51	1.48	1.41
1	A	493	GLU	CD-OE2	-5.47	1.19	1.25
2	O	65	TRP	CD2-CE2	5.46	1.48	1.41
10	W	52	TRP	CD2-CE2	5.37	1.47	1.41
1	N	494	TRP	CD2-CE2	5.33	1.47	1.41
2	B	198	GLU	CD-OE2	-5.31	1.19	1.25
6	F	94	HIS	CB-CG	5.30	1.59	1.50
2	O	163	TRP	CD2-CE2	5.29	1.47	1.41
8	H	30	TRP	CG-CD1	5.27	1.44	1.36
8	H	30	TRP	CD2-CE2	5.27	1.47	1.41
1	N	334	TRP	CD2-CE2	5.25	1.47	1.41
10	J	52	TRP	CD2-CE2	5.23	1.47	1.41
8	H	68	TRP	CD2-CE2	5.20	1.47	1.41
2	O	222	TRP	CD2-CE2	5.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	67	SER	CB-OG	5.17	1.49	1.42
6	S	82	CYS	CB-SG	-5.17	1.73	1.81
8	H	55	TRP	CD2-CE2	5.16	1.47	1.41
3	C	258	TRP	CD2-CE2	5.11	1.47	1.41
2	O	198	GLU	C-O	5.11	1.33	1.23
3	P	240	TRP	CD2-CE2	5.09	1.47	1.41
1	N	6	TRP	CD2-CE2	5.08	1.47	1.41
1	A	187	SER	CA-CB	5.08	1.60	1.52
4	Q	98	TRP	CD2-CE2	5.08	1.47	1.41
1	A	103	TRP	CD2-CE2	5.08	1.47	1.41
4	D	115	TRP	CG-CD1	5.04	1.43	1.36
13	Z	32	TRP	CD2-CE2	5.03	1.47	1.41
2	B	104	TRP	CD2-CE2	5.03	1.47	1.41
14	2	59	TRP	CD2-CE2	5.03	1.47	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-11.62	114.49	120.30
2	B	82	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	A	71	MET	CG-SD-CE	-11.09	82.46	100.20
1	A	486	ASP	CB-CG-OD1	10.23	127.51	118.30
5	E	90	ARG	NE-CZ-NH1	9.99	125.29	120.30
8	H	9	LYS	CA-CB-CG	-9.89	91.63	113.40
8	H	8	ILE	CG1-CB-CG2	9.71	132.77	111.40
4	D	20	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	486	ASP	CB-CG-OD2	-8.95	110.25	118.30
5	E	90	ARG	NE-CZ-NH2	-8.82	115.89	120.30
4	D	19	ARG	NE-CZ-NH2	8.12	124.36	120.30
9	I	21	ILE	CG1-CB-CG2	-7.64	94.60	111.40
8	U	27	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	B	82	ARG	NE-CZ-NH1	-7.26	116.67	120.30
8	H	9	LYS	O-C-N	7.16	134.15	122.70
2	O	82	ARG	NE-CZ-NH2	-7.04	116.78	120.30
7	G	17	ARG	NE-CZ-NH2	-6.89	116.86	120.30
6	F	96	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	N	71	MET	CG-SD-CE	-6.86	89.23	100.20
7	T	12	GLY	N-CA-C	6.74	129.95	113.10
7	T	5	LYS	CD-CE-NZ	6.61	126.91	111.70
4	D	51	LEU	CB-CG-CD2	6.49	122.04	111.00
13	Z	19	LEU	CA-CB-CG	6.40	130.02	115.30
6	S	60	CYS	O-C-N	6.27	132.73	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	73	ASP	CB-CG-OD1	6.05	123.75	118.30
8	H	9	LYS	CB-CG-CD	-6.04	95.91	111.60
7	T	33	LEU	CA-CB-CG	5.99	129.08	115.30
6	S	18	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	189	MET	CA-CB-CG	-5.92	103.23	113.30
5	E	14	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	49	GLY	N-CA-C	-5.89	98.39	113.10
6	S	65	ASP	CB-CG-OD2	-5.84	113.05	118.30
5	E	49	ASP	CB-CG-OD1	5.83	123.55	118.30
8	U	27	ARG	NE-CZ-NH1	5.78	123.19	120.30
7	T	17	ARG	CB-CG-CD	-5.77	96.61	111.60
5	E	14	ARG	NE-CZ-NH1	5.75	123.18	120.30
4	Q	51	LEU	CB-CG-CD1	5.68	120.66	111.00
2	B	167	SER	CB-CA-C	-5.66	99.34	110.10
1	A	212	ASP	CB-CG-OD2	5.66	123.39	118.30
4	D	51	LEU	CB-CG-CD1	5.63	120.58	111.00
13	M	34	LEU	CB-CG-CD1	5.61	120.53	111.00
9	I	31	PHE	N-CA-C	-5.60	95.88	111.00
1	A	208	MET	CG-SD-CE	5.58	109.13	100.20
7	G	17	ARG	CB-CG-CD	-5.58	97.09	111.60
4	D	26	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	N	96	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	F	3	GLY	N-CA-C	-5.53	99.27	113.10
9	V	29	LEU	CA-CB-CG	5.51	127.97	115.30
3	C	59	ARG	NE-CZ-NH2	-5.50	117.55	120.30
4	D	19	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	363	LEU	CB-CG-CD2	5.46	120.29	111.00
10	J	40	LEU	CB-CG-CD2	5.45	120.27	111.00
7	G	54	ARG	NE-CZ-NH2	-5.44	117.58	120.30
8	U	74	ASP	CB-CG-OD1	5.43	123.19	118.30
6	S	60	CYS	CA-C-N	-5.37	105.39	117.20
2	B	168	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	N	302	ARG	NE-CZ-NH1	-5.34	117.63	120.30
7	T	17	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	199	LEU	CB-CG-CD2	-5.25	102.07	111.00
4	D	19	ARG	CB-CA-C	-5.18	100.04	110.40
12	Y	20	ARG	NE-CZ-NH1	5.17	122.88	120.30
6	S	53	THR	CB-CA-C	-5.13	97.75	111.60
1	N	208	MET	CG-SD-CE	5.11	108.38	100.20
1	N	50	ASP	CB-CG-OD1	5.10	122.89	118.30
4	Q	20	ARG	NE-CZ-NH2	-5.07	117.77	120.30
13	Z	19	LEU	CB-CG-CD2	-5.04	102.43	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	8	ILE	Peptide
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
6	S	94	HIS	Peptide
6	S	95	GLN	Peptide
9	V	32	ALA	Peptide
9	V	33	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4084	0	4069	63	0
1	N	4065	0	4046	44	0
2	B	1836	0	1843	43	0
2	O	1824	0	1833	40	0
3	C	2149	0	2075	24	0
3	P	2143	0	2067	29	0
4	D	1195	0	1183	16	0
4	Q	1203	0	1196	30	0
5	E	852	0	845	8	0
5	R	852	0	845	5	0
6	F	748	0	728	25	0
6	S	748	0	729	25	0
7	G	675	0	643	20	0
7	T	675	0	644	26	0
8	H	662	0	623	36	0
8	U	662	0	623	7	0
9	I	601	0	613	39	0
9	V	601	0	613	19	0
10	J	460	0	459	7	0
10	W	460	0	459	12	0
11	K	384	0	366	5	0
11	X	384	0	366	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	380	0	380	12	0
12	Y	380	0	380	6	0
13	M	335	0	352	1	0
13	Z	335	0	352	4	0
14	1	826	0	849	27	0
14	2	826	0	848	40	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	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	129	0	88	9	0
18	N	129	0	88	10	0
19	A	2	0	0	0	0
19	N	2	0	0	1	0
20	A	102	0	152	9	0
20	C	102	0	152	14	0
20	N	51	0	76	1	0
20	P	102	0	152	10	0
21	B	63	0	110	6	0
21	D	63	0	110	12	0
21	L	63	0	110	20	0
21	N	63	0	110	2	0
21	Q	63	0	110	10	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	4	0	6	0	0
23	C	4	0	6	0	0
23	E	4	0	6	1	0
23	F	4	0	6	0	0
23	G	4	0	6	0	0
23	I	4	0	6	0	0
23	N	8	0	12	0	0
23	S	4	0	6	0	0
24	C	58	0	78	4	0
24	G	29	0	39	0	0
24	J	29	0	38	5	0
24	P	58	0	78	2	0
24	T	29	0	39	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	W	29	0	37	5	0
25	C	53	0	77	7	0
25	P	53	0	77	3	0
26	C	100	0	156	15	0
26	G	100	0	156	23	0
26	P	100	0	156	12	0
26	T	100	0	156	24	0
27	C	42	0	0	4	0
27	J	10	0	0	1	0
27	L	10	0	0	1	0
27	N	63	0	0	2	0
27	P	43	0	0	6	0
27	T	18	0	0	1	0
27	W	9	0	0	1	0
27	Y	10	0	0	1	0
28	E	52	0	80	19	0
28	V	52	0	80	21	0
29	F	1	0	0	0	0
29	S	1	0	0	2	0
30	M	33	0	42	1	0
30	Z	33	0	42	1	0
31	1	43	0	30	5	0
31	2	43	0	30	3	0
32	1	53	0	0	6	0
32	2	28	0	0	7	0
32	A	252	0	0	19	0
32	B	193	0	0	6	0
32	C	137	0	0	7	0
32	D	122	0	0	7	0
32	E	119	0	0	6	0
32	F	97	0	0	2	2
32	G	60	0	0	11	0
32	H	76	0	0	7	0
32	I	49	0	0	5	0
32	J	30	0	0	3	0
32	K	29	0	0	1	0
32	L	33	0	0	1	0
32	M	26	0	0	2	0
32	N	229	0	0	6	0
32	O	141	0	0	3	0
32	P	110	0	0	9	0
32	Q	99	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R	83	0	0	1	0
32	S	95	0	0	5	0
32	T	41	0	0	3	0
32	U	54	0	0	4	2
32	V	17	0	0	2	0
32	W	10	0	0	0	0
32	X	17	0	0	3	0
32	Y	21	0	0	0	0
32	Z	16	0	0	0	0
All	All	34765	0	32732	716	2

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 (716) 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)
14:1:17:CYS:SG	31:1:201:HEM:CAC	2.06	1.41
27:C:310:UNL:C4	27:C:310:UNL:C6	1.76	1.36
32:A:927:HOH:O	26:T:101:CDL:H412	1.17	1.28
5:E:79:LYS:HE3	32:E:387:HOH:O	1.31	1.24
27:W:102:UNL:C5	27:W:102:UNL:C4	2.17	1.23
1:A:486:ASP:OD2	4:D:19:ARG:HD2	1.32	1.21
19:N:607:PER:O2	19:N:607:PER:O1	1.54	1.21
9:I:29:LEU:O	9:I:32:ALA:N	1.71	1.20
32:P:475:HOH:O	10:W:58:LYS:HE2	1.38	1.20
24:J:101:CHD:H212	32:J:221:HOH:O	1.41	1.17
28:V:101:PSC:H343	28:V:101:PSC:H12	1.22	1.14
28:E:201:PSC:C01	28:E:201:PSC:H221	1.79	1.13
32:C:526:HOH:O	26:G:101:CDL:H551	0.98	1.12
9:I:29:LEU:O	9:I:32:ALA:CA	1.98	1.12
32:A:927:HOH:O	26:T:101:CDL:C40	1.97	1.12
28:E:201:PSC:H221	28:E:201:PSC:O03	1.37	1.10
26:P:306:CDL:OB3	32:P:401:HOH:O	1.65	1.10
14:1:17:CYS:SG	31:1:201:HEM:HAC	1.78	1.09
8:H:7:LYS:O	8:H:8:ILE:CG2	2.01	1.09
21:L:101:TGL:HC41	21:L:101:TGL:OC1	1.29	1.08
26:G:101:CDL:CB2	32:G:244:HOH:O	2.00	1.07
6:F:94:HIS:HB2	6:F:96:LEU:HB2	1.09	1.06
8:H:7:LYS:O	8:H:8:ILE:HB	1.47	1.06
27:P:310:UNL:C5	27:P:310:UNL:C4	2.33	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:310:UNL:C5	27:C:310:UNL:C6	2.33	1.06
2:B:220:GLU:OE2	32:B:401:HOH:O	1.73	1.05
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.36	1.05
9:I:26:MET:O	9:I:30:GLY:CA	2.05	1.05
8:H:7:LYS:O	8:H:8:ILE:CB	2.05	1.04
28:E:201:PSC:H343	28:E:201:PSC:H12	1.40	1.04
20:A:607:PGV:H22	32:A:701:HOH:O	1.57	1.04
27:L:102:UNL:C10	27:L:102:UNL:C4	2.35	1.04
3:C:133:ASN:ND2	32:C:402:HOH:O	1.89	1.04
28:V:101:PSC:H22	32:V:212:HOH:O	1.58	1.03
9:V:29:LEU:O	9:V:31:PHE:N	1.91	1.03
4:D:6:VAL:HG21	4:D:31:LYS:NZ	1.75	1.01
21:D:201:TGL:HA91	21:D:201:TGL:H231	1.40	1.00
9:I:26:MET:O	9:I:30:GLY:HA3	1.61	1.00
9:I:31:PHE:CZ	9:I:32:ALA:O	2.15	1.00
10:W:33:ARG:HG2	24:W:101:CHD:H152	1.42	0.99
8:H:9:LYS:N	8:H:9:LYS:HD3	1.49	0.98
6:F:85:CYS:SG	6:F:87:THR:HG23	2.02	0.98
26:C:306:CDL:O1	32:C:401:HOH:O	1.83	0.97
8:H:7:LYS:O	8:H:8:ILE:HG22	1.62	0.97
8:H:8:ILE:N	32:H:101:HOH:O	1.94	0.96
2:O:226:MET:CE	2:O:226:MET:HA	1.96	0.96
25:C:303:PEK:H161	25:C:303:PEK:H11	1.47	0.94
7:G:11:TPO:O	32:G:201:HOH:O	1.87	0.94
3:P:133:ASN:ND2	32:P:402:HOH:O	2.02	0.93
2:B:29:MET:HG3	9:I:31:PHE:HZ	1.33	0.92
26:G:101:CDL:HB21	32:G:244:HOH:O	1.62	0.91
32:A:927:HOH:O	26:T:101:CDL:C41	1.82	0.91
3:P:37:PHE:CE1	10:W:58:LYS:HG3	2.05	0.91
6:F:30:PRO:O	6:F:96:LEU:HD21	1.70	0.91
26:P:306:CDL:H1	32:P:403:HOH:O	1.70	0.91
9:I:29:LEU:O	9:I:32:ALA:CB	2.19	0.90
1:N:514:LYS:HE2	32:S:258:HOH:O	1.70	0.90
32:P:493:HOH:O	6:S:1:ALA:HB1	1.67	0.90
21:L:101:TGL:CC4	21:L:101:TGL:OC1	2.16	0.90
4:Q:21:ASP:HB2	32:Q:301:HOH:O	1.72	0.90
2:O:58:ALA:O	2:O:62:GLU:HG3	1.71	0.90
6:F:75:HIS:H	6:F:80:GLN:HE22	1.19	0.89
6:S:85:CYS:SG	6:S:87:THR:HG23	2.13	0.88
14:2:81:ILE:HD12	32:2:328:HOH:O	1.74	0.87
26:G:101:CDL:H241	26:G:101:CDL:H522	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:2:HIS:CD2	12:L:3:TYR:H	1.93	0.87
21:B:301:TGL:H302	21:B:301:TGL:H121	1.56	0.87
9:I:29:LEU:O	9:I:32:ALA:HB2	1.75	0.86
1:A:417[B]:MET:HE3	32:A:921:HOH:O	1.75	0.86
20:P:305:PGV:H062	32:U:103:HOH:O	1.76	0.86
12:L:20:ARG:HH21	21:L:101:TGL:HC52	1.39	0.86
3:P:37:PHE:CD1	10:W:58:LYS:HG3	2.11	0.85
27:Y:101:UNL:C4	27:Y:101:UNL:C5	2.54	0.85
6:F:30:PRO:O	6:F:96:LEU:CD2	2.24	0.85
1:A:282:PHE:HA	7:T:4:ALA:CB	2.07	0.84
26:G:101:CDL:HA21	26:G:101:CDL:H111	1.57	0.84
26:G:101:CDL:HB22	32:G:244:HOH:O	1.70	0.84
9:I:33:THR:HG22	9:I:37:PHE:HB3	1.57	0.84
28:E:201:PSC:O03	28:E:201:PSC:C22	2.23	0.84
6:F:94:HIS:CB	6:F:96:LEU:HB2	2.02	0.84
8:H:84:LYS:HA	8:H:84:LYS:HZ3	1.42	0.83
27:C:310:UNL:C5	27:C:310:UNL:C4	2.56	0.83
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.43	0.83
20:P:304:PGV:H151	20:P:304:PGV:H11	1.58	0.83
6:F:94:HIS:HB2	6:F:96:LEU:CB	2.02	0.83
2:B:16:ILE:HD13	32:B:549:HOH:O	1.79	0.82
9:I:30:GLY:O	9:I:31:PHE:C	2.16	0.82
9:I:26:MET:O	9:I:30:GLY:N	2.12	0.81
6:S:75:HIS:H	6:S:80:GLN:HE22	1.23	0.81
4:D:6:VAL:HG21	4:D:31:LYS:HZ1	1.41	0.81
3:P:205:GLY:HA3	25:P:303:PEK:H161	1.63	0.81
4:Q:31:LYS:HE3	32:Q:376:HOH:O	1.80	0.81
20:A:607:PGV:H211	32:M:216:HOH:O	1.80	0.80
8:U:46:LYS:HE3	32:U:143:HOH:O	1.80	0.80
14:2:20:VAL:HG12	14:2:102:THR:HG22	1.64	0.80
2:B:81:LEU:HD12	26:T:101:CDL:H351	1.64	0.80
6:S:64:GLU:O	6:S:65:ASP:HB2	1.81	0.79
32:N:737:HOH:O	21:Q:201:TGL:HB32	1.83	0.79
28:V:101:PSC:H291	28:V:101:PSC:H331	1.65	0.79
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.79
24:P:307:CHD:H231	32:P:504:HOH:O	1.83	0.79
20:A:608:PGV:H343	25:C:303:PEK:H383	1.65	0.78
21:L:101:TGL:C36	21:L:101:TGL:H312	2.13	0.78
14:2:3:VAL:HG13	14:2:97:TYR:HA	1.65	0.78
12:L:2:HIS:HD2	12:L:3:TYR:H	1.30	0.78
20:P:305:PGV:C06	32:U:103:HOH:O	2.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:17:CYS:SG	31:1:201:HEM:C3C	2.75	0.78
32:N:725:HOH:O	3:P:77:LYS:HE3	1.83	0.78
7:G:6:GLY:O	7:G:7:ASP:HB2	1.83	0.78
1:N:417:MET:HE3	32:N:928:HOH:O	1.83	0.78
27:J:102:UNL:C6	27:J:102:UNL:C10	2.62	0.77
12:L:24:MET:HG3	32:L:223:HOH:O	1.83	0.77
2:B:29:MET:HG3	9:I:31:PHE:CZ	2.17	0.77
4:Q:21:ASP:CB	32:Q:301:HOH:O	2.29	0.77
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.67	0.77
12:L:20:ARG:NH2	21:L:101:TGL:HC52	1.99	0.77
14:2:70:ASN:HB3	14:2:73:LYS:HB3	1.67	0.76
6:F:94:HIS:HD2	6:F:97:ALA:H	1.33	0.76
1:A:28:MET:CE	18:A:604[B]:HEA:H271	2.15	0.76
14:2:21:GLU:OE2	14:2:24:GLY:HA3	1.86	0.76
14:2:19:THR:HG23	14:2:27:LYS:HD2	1.67	0.76
4:Q:21:ASP:CG	32:Q:301:HOH:O	2.23	0.75
7:G:38:HIS:NE2	26:G:101:CDL:H122	2.01	0.75
9:I:31:PHE:CE1	9:I:32:ALA:O	2.38	0.75
9:V:10:ARG:HD3	28:V:101:PSC:H063	1.67	0.75
2:B:58:ALA:O	2:B:62:GLU:HG3	1.87	0.75
14:1:81:ILE:CG2	32:1:346:HOH:O	2.34	0.74
6:F:94:HIS:O	32:F:201:HOH:O	2.06	0.74
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.69	0.74
4:D:100:LYS:NZ	32:D:301:HOH:O	2.21	0.73
28:E:201:PSC:C34	28:E:201:PSC:H12	2.14	0.73
1:N:28:MET:HE1	18:N:605[B]:HEA:C27	2.18	0.73
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.69	0.73
2:O:56:MET:HB3	28:V:101:PSC:H211	1.70	0.73
9:I:2:THR:N	32:I:201:HOH:O	1.94	0.73
26:P:306:CDL:OB9	26:P:306:CDL:H521	1.87	0.73
2:O:226:MET:HA	2:O:226:MET:HE2	1.70	0.73
2:B:19:GLU:OE2	2:B:82:ARG:NH1	2.22	0.72
8:H:43:MET:CE	8:H:49:ASP:H	2.02	0.72
9:I:31:PHE:CD2	9:I:32:ALA:N	2.57	0.72
4:D:6:VAL:HG21	4:D:31:LYS:HZ2	1.51	0.72
28:E:201:PSC:H011	28:E:201:PSC:H221	1.71	0.72
14:2:71:PRO:HD2	14:2:83:ALA:O	1.89	0.72
1:A:28:MET:CE	18:A:604[B]:HEA:C27	2.68	0.72
2:O:226:MET:HA	2:O:226:MET:HE3	1.71	0.72
2:O:57:ASP:H	28:V:101:PSC:H202	1.55	0.71
8:H:84:LYS:HZ2	8:H:85:ILE:H	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:87:PHE:HB2	32:X:113:HOH:O	1.90	0.71
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.53	0.71
8:H:8:ILE:C	8:H:9:LYS:HD3	2.11	0.71
28:E:201:PSC:H343	28:E:201:PSC:C12	2.18	0.71
9:I:29:LEU:C	9:I:32:ALA:H	1.94	0.71
20:A:608:PGV:H183	25:C:303:PEK:H322	1.72	0.70
26:G:101:CDL:H271	27:N:601:UNL:C17	2.21	0.70
14:1:17:CYS:SG	31:1:201:HEM:CBC	2.76	0.70
28:V:101:PSC:H343	28:V:101:PSC:C12	2.13	0.70
2:B:66:THR:HG22	2:B:67:ILE:HD13	1.72	0.70
14:2:16:GLN:H	14:2:16:GLN:HE21	1.38	0.70
8:H:7:LYS:C	32:H:101:HOH:O	2.26	0.69
4:Q:19[B]:ARG:HD3	4:Q:21:ASP:OD1	1.92	0.69
3:P:37:PHE:HE1	10:W:58:LYS:HG3	1.57	0.69
14:2:32:LEU:HD22	14:2:35:LEU:HD22	1.74	0.69
4:Q:28:ALA:O	4:Q:31:LYS:HD2	1.93	0.69
9:I:31:PHE:O	9:I:34:PHE:N	2.18	0.69
9:V:31:PHE:C	9:V:31:PHE:CD1	2.66	0.69
21:D:201:TGL:H122	21:D:201:TGL:HB81	1.75	0.68
7:T:34:ASN:O	7:T:38:HIS:HB3	1.92	0.68
20:A:608:PGV:H343	25:C:303:PEK:C38	2.23	0.68
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.19	0.68
2:B:57:ASP:H	28:E:201:PSC:H211	1.58	0.68
1:A:239:GLY:CA	32:A:900:HOH:O	2.42	0.68
6:S:60:CYS:HG	29:S:101:ZN:ZN	1.05	0.68
12:L:14:SER:H	21:L:101:TGL:HC31	1.60	0.67
1:N:28:MET:HE1	18:N:605[B]:HEA:H271	1.75	0.67
2:O:116:LEU:HD11	2:O:226:MET:CG	2.24	0.67
1:A:304:TYR:HD1	26:T:101:CDL:HB32	1.59	0.67
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.76	0.67
26:T:101:CDL:H271	27:T:102:UNL:C17	2.24	0.67
6:F:64:GLU:O	6:F:65:ASP:HB2	1.95	0.67
28:V:101:PSC:H072	32:V:201:HOH:O	1.94	0.67
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.77	0.67
7:T:38:HIS:O	7:T:38:HIS:CD2	2.48	0.67
21:B:301:TGL:H342	21:B:301:TGL:H211	1.76	0.66
8:H:84:LYS:HA	8:H:84:LYS:NZ	2.09	0.66
1:N:28:MET:CE	18:N:605[B]:HEA:H271	2.25	0.66
26:C:306:CDL:OB9	26:C:306:CDL:H522	1.96	0.66
9:I:30:GLY:C	9:I:32:ALA:N	2.38	0.66
9:V:73:LYS:NZ	9:V:73:LYS:HB3	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:PRO:HG2	2:B:148:MET:HE2	1.77	0.66
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.77	0.66
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.94	0.66
26:T:101:CDL:H382	26:T:101:CDL:H152	1.78	0.66
14:1:86:LYS:HA	14:1:86:LYS:HE3	1.77	0.66
2:B:64:ILE:HG22	32:B:554:HOH:O	1.95	0.66
1:A:28:MET:HE2	18:A:604[B]:HEA:C27	2.24	0.66
1:N:145:LEU:HD11	27:P:310:UNL:C6	2.26	0.66
1:A:172:LYS:HZ1	7:T:9:GLY:HA3	1.60	0.65
32:A:927:HOH:O	26:T:101:CDL:H401	1.76	0.65
28:V:101:PSC:C28	28:V:101:PSC:H322	2.27	0.65
4:Q:4:SER:N	4:Q:31:LYS:H	1.95	0.65
7:G:45:PRO:O	7:G:46:ALA:CB	2.44	0.65
12:L:25:MET:HG2	21:L:101:TGL:HA62	1.78	0.65
14:1:19:THR:HG23	14:1:27:LYS:HD2	1.79	0.64
14:2:26:HIS:CD2	14:2:26:HIS:H	2.15	0.64
1:A:28:MET:HE2	18:A:604[B]:HEA:H273	1.79	0.64
6:F:94:HIS:O	6:F:95:GLN:HB3	1.94	0.64
7:T:7:ASP:O	7:T:8:HIS:HB2	1.97	0.64
28:V:101:PSC:H012	28:V:101:PSC:P	2.37	0.64
1:A:239:GLY:HA3	32:A:900:HOH:O	1.98	0.64
9:I:33:THR:HG22	9:I:37:PHE:CB	2.27	0.64
8:U:9:LYS:O	8:U:10:ASN:HB2	1.97	0.64
4:D:109:HIS:HD2	32:D:355:HOH:O	1.80	0.64
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.06	0.64
21:D:201:TGL:HA91	21:D:201:TGL:C23	2.17	0.63
9:I:73:LYS:N	9:I:73:LYS:HD3	2.12	0.63
3:P:80[B]:ARG:HH22	27:P:308:UNL:C1	2.10	0.63
31:2:201:HEM:CBC	32:2:317:HOH:O	2.46	0.63
3:C:220:PHE:HB2	26:C:306:CDL:H711	1.81	0.63
7:T:17:ARG:HD3	32:T:205:HOH:O	1.98	0.63
20:C:305:PGV:C06	8:H:22:ASN:HD22	2.12	0.63
5:R:44:GLU:OE1	32:R:201:HOH:O	2.15	0.63
1:N:28:MET:CE	18:N:605[B]:HEA:C27	2.77	0.63
21:N:608:TGL:H221	21:N:608:TGL:HA72	1.79	0.63
6:S:94:HIS:O	6:S:95:GLN:HB2	1.99	0.63
1:A:339:MET:HE2	32:D:392:HOH:O	1.99	0.63
2:B:57:ASP:H	28:E:201:PSC:C21	2.11	0.62
3:C:51[A]:MET:SD	26:C:306:CDL:H612	2.38	0.62
2:B:68:LEU:HD23	28:E:201:PSC:H171	1.80	0.62
14:2:30:PRO:HD3	14:2:46:PHE:CE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:101:TGL:HA92	21:L:101:TGL:C23	2.29	0.62
32:A:892:HOH:O	12:L:2:HIS:HE1	1.81	0.62
1:A:278[B]:MET:HE1	7:T:6:GLY:H	1.65	0.62
6:S:60:CYS:SG	29:S:101:ZN:ZN	1.88	0.62
14:1:7:LYS:HG3	14:1:97:TYR:CE1	2.35	0.62
14:2:16:GLN:H	14:2:16:GLN:NE2	1.96	0.62
4:Q:43:LYS:HE3	4:Q:55:GLU:OE1	1.98	0.62
4:Q:9:GLU:OE1	4:Q:9:GLU:HA	2.00	0.62
28:V:101:PSC:H281	28:V:101:PSC:H322	1.82	0.62
32:B:554:HOH:O	28:E:201:PSC:H151	2.00	0.62
26:G:101:CDL:C27	27:N:601:UNL:C17	2.76	0.62
9:I:30:GLY:O	9:I:32:ALA:N	2.32	0.62
8:H:84:LYS:NZ	8:H:85:ILE:H	1.97	0.61
2:O:57:ASP:N	28:V:101:PSC:H202	2.15	0.61
26:G:101:CDL:OB2	26:G:101:CDL:H142	1.99	0.61
2:O:198:GLU:OE2	32:O:401:HOH:O	2.16	0.61
2:O:116:LEU:CD1	2:O:226:MET:CG	2.79	0.61
14:2:22:LYS:HA	14:2:33:HIS:HB2	1.82	0.61
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.46	0.61
26:T:101:CDL:OA7	26:T:101:CDL:H322	1.99	0.61
31:2:201:HEM:HBC1	32:2:317:HOH:O	2.01	0.61
7:T:37:LEU:O	7:T:38:HIS:CB	2.49	0.61
1:A:310:MET:CE	2:B:77:ALA:HB2	2.31	0.61
10:W:33:ARG:HG2	24:W:101:CHD:C15	2.25	0.61
2:B:86:MET:O	2:B:89:GLU:HG2	2.00	0.61
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.83	0.61
7:G:38:HIS:NE2	26:G:101:CDL:H362	2.16	0.60
20:N:612:PGV:H61	3:P:54:MET:HG2	1.83	0.60
14:2:5:LYS:HD3	14:2:93:ASP:OD2	2.02	0.60
7:G:84:LYS:N	32:G:203:HOH:O	2.19	0.60
3:C:3:HIS:HA	32:C:410:HOH:O	2.01	0.60
10:J:7:GLU:HG3	32:J:220:HOH:O	2.01	0.60
1:N:486:ASP:OD2	4:Q:19[A]:ARG:NE	2.34	0.60
26:T:101:CDL:H311	26:T:101:CDL:CA5	2.31	0.60
26:P:306:CDL:H222	26:P:306:CDL:H262	1.84	0.60
7:G:7:ASP:O	7:G:8:HIS:HB2	2.02	0.60
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.83	0.59
20:P:304:PGV:C15	20:P:304:PGV:H11	2.27	0.59
26:G:101:CDL:H201	26:G:101:CDL:HB32	1.84	0.59
21:Q:201:TGL:HG2	21:Q:201:TGL:HB32	1.83	0.59
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:ARG:HD3	32:G:208:HOH:O	2.01	0.59
7:G:9:GLY:HA3	1:N:172:LYS:HZ1	1.68	0.59
8:H:9:LYS:HB3	32:H:102:HOH:O	2.03	0.59
3:C:224:LYS:HE3	26:C:306:CDL:HB32	1.85	0.59
26:G:101:CDL:H371	2:O:81:LEU:HD12	1.85	0.59
3:C:210:ILE:HG12	20:C:304:PGV:H132	1.85	0.58
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.33	0.58
1:A:282:PHE:HZ	26:T:101:CDL:H752	1.68	0.58
21:L:101:TGL:HA92	21:L:101:TGL:H231	1.85	0.58
1:A:278[B]:MET:CE	7:T:5:LYS:HB3	2.33	0.58
32:P:493:HOH:O	6:S:1:ALA:CB	2.35	0.58
6:F:96:LEU:C	6:F:98:HIS:H	2.07	0.58
26:T:101:CDL:OB4	26:T:101:CDL:H1	2.03	0.58
7:G:5:LYS:HA	1:N:278[B]:MET:CE	2.34	0.58
20:C:305:PGV:H061	8:H:22:ASN:ND2	2.18	0.57
9:I:31:PHE:HE1	9:I:35:TYR:CB	2.17	0.57
1:A:112:LEU:HD23	1:A:112:LEU:C	2.24	0.57
21:D:201:TGL:OB1	21:D:201:TGL:HG32	2.04	0.57
2:B:56:MET:HA	28:E:201:PSC:H212	1.87	0.57
9:I:28:SER:O	9:I:31:PHE:HD2	1.88	0.57
1:A:304:TYR:CD1	26:T:101:CDL:HB32	2.40	0.57
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.86	0.57
1:A:278[B]:MET:SD	7:T:5:LYS:HB3	2.45	0.57
25:C:303:PEK:H161	25:C:303:PEK:C11	2.28	0.57
20:C:304:PGV:H12	26:C:306:CDL:H622	1.86	0.57
11:X:24:PHE:O	11:X:28:VAL:HG12	2.05	0.57
6:F:85:CYS:SG	6:F:87:THR:CG2	2.87	0.56
32:A:858:HOH:O	6:F:96:LEU:CD1	2.53	0.56
21:Q:201:TGL:HC21	21:Q:201:TGL:HG11	1.88	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.04	0.56
4:Q:27:VAL:HG21	4:Q:31:LYS:HE2	1.87	0.56
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.87	0.56
1:A:28:MET:HE1	18:A:604[B]:HEA:H271	1.86	0.56
8:H:43:MET:HE2	8:H:49:ASP:H	1.70	0.56
8:H:9:LYS:CD	8:H:9:LYS:N	2.41	0.56
1:A:514:LYS:HE2	32:F:237:HOH:O	2.06	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
24:C:307:CHD:O7	24:C:307:CHD:H41	2.06	0.55
14:1:48:TYR:HB2	14:1:53:LYS:HG3	1.87	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.89	0.55
1:A:406:ASN:HD21	20:A:607:PGV:H31	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:201:TGL:CC2	21:Q:201:TGL:HG11	2.36	0.55
1:A:514:LYS:HA	6:F:38:ALA:CB	2.35	0.55
2:B:84:LEU:HA	2:B:87:MET:HE2	1.87	0.55
26:G:101:CDL:H111	26:G:101:CDL:CA2	2.32	0.55
4:D:121:LYS:HE2	11:K:52:GLU:OE2	2.07	0.55
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.39	0.55
6:S:64:GLU:O	6:S:65:ASP:CB	2.48	0.55
4:Q:109:HIS:HD2	32:Q:371:HOH:O	1.89	0.55
21:D:201:TGL:CA3	32:D:392:HOH:O	2.54	0.55
6:F:94:HIS:CD2	6:F:97:ALA:H	2.19	0.55
9:I:33:THR:HA	9:I:36:LYS:HB3	1.89	0.55
24:P:301:CHD:H212	24:P:301:CHD:H12	1.88	0.55
21:D:201:TGL:HA31	32:D:392:HOH:O	2.06	0.54
28:E:201:PSC:H072	32:I:221:HOH:O	2.07	0.54
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.07	0.54
26:G:101:CDL:O1	32:G:202:HOH:O	2.18	0.54
6:S:60:CYS:SG	6:S:85:CYS:SG	3.05	0.54
14:1:19:THR:CG2	14:1:27:LYS:HD2	2.37	0.54
1:A:365:ILE:HD11	32:A:899:HOH:O	2.06	0.54
9:I:30:GLY:C	9:I:32:ALA:H	2.09	0.54
6:S:53:THR:CG2	32:S:292:HOH:O	2.55	0.54
32:A:858:HOH:O	6:F:96:LEU:HD11	2.07	0.54
6:F:94:HIS:CG	6:F:95:GLN:N	2.75	0.54
9:V:17:LEU:CD2	28:V:101:PSC:H271	2.38	0.54
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.43	0.54
8:U:9:LYS:O	8:U:10:ASN:CB	2.55	0.54
32:A:911:HOH:O	26:T:101:CDL:H131	2.07	0.54
2:B:57:ASP:H	28:E:201:PSC:C20	2.21	0.54
9:V:31:PHE:CD1	9:V:31:PHE:O	2.60	0.54
11:X:54:ARG:NH2	11:X:54:ARG:CG	2.64	0.54
4:Q:9:GLU:HB3	32:S:275:HOH:O	2.07	0.53
1:A:177:SER:H	1:A:180:GLN:HE21	1.56	0.53
1:A:312[A]:ILE:HD12	32:A:763:HOH:O	2.07	0.53
1:N:379:TYR:O	1:N:383[A]:MET:HB2	2.08	0.53
2:O:59:GLN:O	2:O:60:GLU:HG3	2.09	0.53
14:1:49:THR:HG23	14:1:79:LYS:HD3	1.90	0.53
23:E:202:EDO:H22	32:E:391:HOH:O	2.08	0.53
8:H:49:ASP:O	8:H:50:VAL:HB	2.09	0.53
9:V:17:LEU:HD21	28:V:101:PSC:H271	1.90	0.53
21:Q:201:TGL:H352	9:V:16:ARG:HE	1.73	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:28:ALA:O	4:Q:31:LYS:CD	2.56	0.53
32:N:737:HOH:O	21:Q:201:TGL:HG2	2.08	0.53
28:V:101:PSC:H291	28:V:101:PSC:C33	2.32	0.53
2:B:57:ASP:N	28:E:201:PSC:H211	2.24	0.52
8:H:7:LYS:CA	8:H:7:LYS:HE3	2.39	0.52
2:B:33:LEU:HD11	9:I:29:LEU:HD13	1.91	0.52
26:T:101:CDL:H132	26:T:101:CDL:H342	1.91	0.52
1:A:513:LEU:O	1:A:514:LYS:CB	2.55	0.52
1:N:365:ILE:HD11	32:N:863:HOH:O	2.08	0.52
6:S:85:CYS:SG	6:S:87:THR:CG2	2.94	0.52
8:U:9:LYS:O	8:U:10:ASN:ND2	2.40	0.52
14:1:16:GLN:CB	32:1:338:HOH:O	2.58	0.52
8:H:43:MET:HE3	8:H:49:ASP:H	1.75	0.52
9:I:31:PHE:HE1	9:I:35:TYR:H	1.57	0.52
21:L:101:TGL:CA9	21:L:101:TGL:H231	2.39	0.52
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.92	0.52
7:T:31:CYS:SG	26:T:101:CDL:H551	2.49	0.52
11:X:54:ARG:HH21	11:X:54:ARG:CB	2.23	0.52
7:G:31:CYS:SG	26:G:101:CDL:H512	2.50	0.52
8:H:8:ILE:C	8:H:9:LYS:O	2.46	0.52
14:1:52:ASN:C	14:1:52:ASN:HD22	2.14	0.52
2:O:13:THR:OG1	2:O:167:SER:HB2	2.09	0.52
7:T:7:ASP:CG	7:T:8:HIS:N	2.63	0.52
5:E:78:HIS:HD2	32:E:364:HOH:O	1.91	0.51
21:L:101:TGL:C36	21:L:101:TGL:C31	2.88	0.51
14:2:62:GLU:HG2	14:2:63:THR:HG23	1.92	0.51
3:C:161[B]:GLN:HG2	24:C:307:CHD:O7	2.10	0.51
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.92	0.51
3:P:5:THR:HG21	6:S:96:LEU:HD13	1.92	0.51
26:C:306:CDL:H262	26:C:306:CDL:H381	1.91	0.51
3:C:156:ARG:HE	24:C:307:CHD:C24	2.23	0.51
27:P:310:UNL:C4	27:P:310:UNL:C6	2.89	0.51
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.41	0.51
8:U:7:LYS:HE3	8:U:10:ASN:HD21	1.74	0.51
14:2:36:PHE:CE2	14:2:61:GLU:HG3	2.46	0.51
10:J:2:GLU:HG2	32:J:209:HOH:O	2.11	0.51
1:N:24:ALA:HA	18:N:605[A]:HEA:H22	1.93	0.51
26:P:306:CDL:H201	26:P:306:CDL:H162	1.93	0.51
9:I:29:LEU:O	9:I:32:ALA:HA	2.05	0.51
6:S:82:CYS:C	6:S:84:SER:N	2.63	0.51
1:A:343:GLY:HA2	21:D:201:TGL:H201	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:ASN:N	32:H:102:HOH:O	1.98	0.51
32:A:950:HOH:O	14:1:81:ILE:HG21	2.10	0.51
14:2:30:PRO:HD3	14:2:46:PHE:CZ	2.46	0.51
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.93	0.50
9:I:1:SAC:H2A1	9:I:1:SAC:CB	2.40	0.50
8:H:7:LYS:HA	8:H:7:LYS:HE3	1.93	0.50
26:G:101:CDL:H372	2:O:78:LEU:HD12	1.94	0.50
4:D:107:ILE:HD11	4:D:111:PHE:CB	2.42	0.50
24:J:101:CHD:H21	24:J:101:CHD:H61	1.94	0.50
4:D:118:LYS:HB3	11:K:53:TRP:HB3	1.94	0.50
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.45	0.50
20:C:305:PGV:H061	8:H:22:ASN:HD22	1.76	0.50
1:N:309:THR:HG22	18:N:606:HEA:HMB2	1.92	0.50
26:T:101:CDL:H791	26:T:101:CDL:H832	1.93	0.50
26:C:306:CDL:HB21	10:J:8:LYS:HD2	1.92	0.50
14:2:3:VAL:O	14:2:97:TYR:HB2	2.11	0.50
14:2:42:GLN:O	14:2:44:PRO:HD3	2.11	0.50
14:2:9:ILE:O	14:2:13:LYS:HG2	2.11	0.50
1:N:514:LYS:HA	6:S:38:ALA:CB	2.41	0.50
2:O:137:GLU:OE1	4:Q:122:ARG:NH1	2.37	0.50
20:C:305:PGV:H11	3:P:258:TRP:HH2	1.76	0.50
3:P:59:ARG:HG3	26:P:306:CDL:HA22	1.92	0.50
9:I:33:THR:O	9:I:34:PHE:C	2.49	0.50
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.94	0.50
2:O:56:MET:CB	28:V:101:PSC:H211	2.41	0.50
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.11	0.50
14:1:72:LYS:HD2	32:1:334:HOH:O	2.12	0.50
1:A:49:GLY:HA3	32:A:908:HOH:O	2.10	0.50
14:2:3:VAL:HG11	14:2:100:LYS:HD2	1.94	0.49
20:C:304:PGV:H172	26:C:306:CDL:H631	1.93	0.49
21:L:101:TGL:H362	21:L:101:TGL:C31	2.42	0.49
6:F:46:PRO:O	6:F:48:LEU:HD22	2.12	0.49
2:O:58:ALA:O	2:O:62:GLU:CG	2.53	0.49
26:C:306:CDL:OB9	26:C:306:CDL:HB4	2.11	0.49
8:H:46:LYS:HA	8:H:46:LYS:HE2	1.94	0.49
2:B:70:ALA:HB1	26:T:101:CDL:H441	1.95	0.49
2:O:116:LEU:CD1	2:O:226:MET:HG3	2.42	0.49
10:W:36:MET:HB3	24:W:101:CHD:C18	2.42	0.49
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.48	0.49
6:F:52:ILE:HA	6:F:94:HIS:HB3	1.94	0.49
14:2:13:LYS:HE3	32:2:311:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:SER:H	4:D:37:GLN:NE2	2.11	0.49
14:1:16:GLN:HB3	32:1:338:HOH:O	2.12	0.49
1:A:333:LYS:HE2	32:M:212:HOH:O	2.11	0.49
8:H:9:LYS:N	32:H:101:HOH:O	2.18	0.48
9:V:33:THR:O	9:V:36:LYS:N	2.46	0.48
14:1:47:THR:HB	32:1:332:HOH:O	2.12	0.48
1:A:24:ALA:HB2	18:A:604[B]:HEA:H253	1.95	0.48
28:E:201:PSC:H21	28:E:201:PSC:H222	1.95	0.48
9:I:31:PHE:CE2	9:I:32:ALA:O	2.64	0.48
14:2:72:LYS:NZ	14:2:83:ALA:HA	2.29	0.48
21:B:301:TGL:H301	21:B:301:TGL:HA72	1.96	0.48
2:B:86:MET:HB3	32:B:536:HOH:O	2.14	0.48
26:G:101:CDL:H172	26:G:101:CDL:H402	1.95	0.48
1:N:240:HIS:C	1:N:240:HIS:CD2	2.86	0.48
10:W:36:MET:HG2	24:W:101:CHD:H183	1.94	0.48
7:T:31:CYS:SG	26:T:101:CDL:H532	2.54	0.48
4:D:63:LYS:HG2	4:D:64:PHE:CE2	2.49	0.48
9:I:33:THR:O	9:I:36:LYS:N	2.47	0.48
1:N:485:VAL:HG22	13:Z:1:ILE:HG13	1.95	0.48
14:2:32:LEU:O	14:2:102:THR:HB	2.13	0.47
1:A:309:THR:HG22	18:A:605:HEA:HMB2	1.96	0.47
7:G:11:TPO:HG22	32:G:210:HOH:O	2.13	0.47
3:P:246:ASP:HB2	32:P:485:HOH:O	2.13	0.47
12:Y:47:LYS:HD2	12:Y:47:LYS:OXT	2.14	0.47
9:I:61:GLU:OE1	9:I:64:ARG:NE	2.40	0.47
21:L:101:TGL:H363	21:L:101:TGL:H312	1.92	0.47
3:P:107:ALA:HB2	20:P:305:PGV:H031	1.96	0.47
2:B:129[A]:LYS:NZ	2:B:132:GLU:OE1	2.43	0.47
8:H:9:LYS:HG3	8:H:11:TYR:H	1.80	0.47
6:S:53:THR:HG22	32:S:292:HOH:O	2.14	0.47
7:G:37:LEU:HD23	26:G:101:CDL:H381	1.96	0.47
8:H:7:LYS:C	8:H:8:ILE:HG22	2.34	0.47
3:P:37:PHE:CE2	27:P:310:UNL:C1	2.98	0.47
28:V:101:PSC:O02	28:V:101:PSC:H011	2.15	0.47
7:G:10:GLY:N	32:G:205:HOH:O	2.47	0.47
9:I:33:THR:HA	9:I:36:LYS:HE3	1.95	0.47
1:N:437:PRO:HG2	1:N:440:TYR:CZ	2.49	0.47
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.47
4:Q:78:TRP:N	21:Q:201:TGL:HB22	2.30	0.47
7:T:3:ALA:O	32:T:201:HOH:O	2.20	0.47
21:Q:201:TGL:H362	9:V:20:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:306:CDL:HB21	10:J:8:LYS:CD	2.45	0.47
14:1:3:VAL:HG13	14:1:97:TYR:HA	1.97	0.47
14:2:16:GLN:N	14:2:16:GLN:NE2	2.63	0.47
14:2:49:THR:O	14:2:53:LYS:HB2	2.14	0.47
20:P:304:PGV:C11	20:P:304:PGV:C15	2.92	0.47
7:T:44:ARG:HD2	7:T:82:TYR:CE1	2.50	0.47
1:N:468:MET:HE3	18:N:605[B]:HEA:H22	1.96	0.46
4:Q:19[B]:ARG:CD	4:Q:21:ASP:OD1	2.61	0.46
8:H:52:VAL:HG11	8:U:48:GLY:HA3	1.97	0.46
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.98	0.46
14:1:3:VAL:HG21	14:1:100:LYS:HE2	1.97	0.46
21:D:201:TGL:HA32	32:D:392:HOH:O	2.16	0.46
8:H:43:MET:HE3	8:H:49:ASP:N	2.31	0.46
20:P:304:PGV:C11	20:P:304:PGV:H151	2.37	0.46
2:O:33:LEU:HD12	9:V:28:SER:HB3	1.96	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.50	0.46
3:C:76:GLN:NE2	3:C:80[A]:ARG:HH21	2.13	0.46
3:C:133:ASN:HB3	3:C:173:PHE:CE2	2.50	0.46
26:G:101:CDL:H212	1:N:311:ILE:CD1	2.44	0.46
3:C:131:LEU:HD11	26:G:101:CDL:H552	1.96	0.46
14:2:11:VAL:HA	14:2:15:ALA:HB2	1.96	0.46
20:C:305:PGV:H321	7:T:1:ALA:HB2	1.96	0.46
3:P:16:TRP:N	3:P:17:PRO:CD	2.78	0.46
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.79	0.46
6:S:51:SER:O	6:S:94:HIS:N	2.49	0.46
21:D:201:TGL:CG3	21:D:201:TGL:OB1	2.64	0.46
28:E:201:PSC:H011	28:E:201:PSC:C22	2.44	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.46
26:C:306:CDL:O1	26:C:306:CDL:OA3	2.34	0.46
1:N:28:MET:CE	18:N:605[B]:HEA:H273	2.46	0.46
32:A:911:HOH:O	26:T:101:CDL:H151	2.15	0.46
1:A:310:MET:HB3	2:B:73:LEU:HD22	1.97	0.46
12:L:46:LYS:O	12:L:47:LYS:HB2	2.15	0.46
2:B:13:THR:HG21	2:B:192:TYR:CZ	2.51	0.45
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.87	0.45
2:B:145:PRO:HG2	2:B:148:MET:CE	2.43	0.45
21:B:301:TGL:H101	21:B:301:TGL:HA62	1.98	0.45
20:P:305:PGV:H041	32:U:103:HOH:O	2.15	0.45
5:E:90:ARG:HD3	32:E:370:HOH:O	2.16	0.45
9:I:31:PHE:HE1	9:I:35:TYR:HB3	1.81	0.45
12:L:20:ARG:HH22	21:L:101:TGL:HC72	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:44:PRO:HG3	32:X:115:HOH:O	2.15	0.45
1:A:399:LEU:O	1:A:499:PRO:HA	2.16	0.45
1:A:217:THR:HG22	3:C:188:ILE:HG12	1.99	0.45
5:E:46:LYS:HG2	32:E:333:HOH:O	2.16	0.45
21:L:101:TGL:H362	21:L:101:TGL:H312	1.93	0.45
21:D:201:TGL:H362	9:I:20:HIS:CE1	2.51	0.45
1:N:368:HIS:CD2	1:N:369:ASP:HB2	2.51	0.45
1:N:390:MET:HE1	1:N:468:MET:SD	2.57	0.45
28:V:101:PSC:C34	28:V:101:PSC:H12	2.16	0.45
1:A:378:HIS:CG	1:A:425:PHE:CE1	3.05	0.45
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.98	0.45
20:A:607:PGV:C2	32:A:701:HOH:O	2.35	0.45
2:B:129[A]:LYS:NZ	32:B:407:HOH:O	2.49	0.45
24:C:301:CHD:O7	20:C:305:PGV:H42	2.17	0.45
6:F:53:THR:OG1	6:F:54:ASN:N	2.43	0.45
8:H:43:MET:CE	8:H:49:ASP:N	2.77	0.45
1:N:250:GLY:O	1:N:254:ILE:HG12	2.17	0.45
2:O:116:LEU:HD11	2:O:226:MET:HG3	1.98	0.45
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.51	0.45
1:A:311:ILE:CD1	26:T:101:CDL:H201	2.47	0.45
1:A:310:MET:HE3	2:B:77:ALA:HB2	1.98	0.45
9:V:33:THR:HA	9:V:37:PHE:HD2	1.82	0.45
5:E:6:GLU:O	28:E:201:PSC:H081	2.17	0.45
7:G:45:PRO:O	7:G:46:ALA:HB3	2.17	0.45
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.99	0.45
14:1:40:THR:HG22	14:1:59:TRP:CE2	2.52	0.45
6:S:44:GLU:CD	6:S:44:GLU:H	2.19	0.45
7:T:37:LEU:O	7:T:38:HIS:HB2	2.16	0.44
14:1:16:GLN:HB2	32:1:338:HOH:O	2.17	0.44
20:C:305:PGV:H032	32:C:502:HOH:O	2.17	0.44
14:1:25:LYS:HZ3	14:1:26:HIS:H	1.64	0.44
14:2:11:VAL:O	14:2:15:ALA:HB3	2.18	0.44
1:N:321:PHE:CE2	28:V:101:PSC:H162	2.53	0.44
28:E:201:PSC:H041	32:I:221:HOH:O	2.18	0.44
6:S:53:THR:HG23	32:S:292:HOH:O	2.17	0.44
2:B:58:ALA:O	2:B:62:GLU:CG	2.61	0.44
21:L:101:TGL:HC81	21:L:101:TGL:HC22	2.00	0.44
2:O:144:LEU:HD22	2:O:150:ILE:HD13	1.99	0.44
1:A:278[B]:MET:HE1	7:T:5:LYS:HB3	2.00	0.44
2:O:129:LYS:HE2	32:O:516:HOH:O	2.18	0.44
26:P:306:CDL:H471	26:P:306:CDL:H441	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.18	0.44
21:Q:201:TGL:H231	21:Q:201:TGL:HA91	1.99	0.44
5:R:12:ASP:OD2	5:R:44:GLU:HG3	2.18	0.44
1:A:281:GLY:O	7:T:4:ALA:HB1	2.18	0.44
2:O:4:PRO:HG2	32:X:115:HOH:O	2.17	0.44
2:O:146:MET:HA	2:O:213:LEU:HD12	2.00	0.43
3:P:62:ILE:CD1	26:P:306:CDL:H522	2.48	0.43
1:A:367:LEU:HD21	1:A:433:LEU:HD23	2.01	0.43
20:A:608:PGV:H311	25:C:303:PEK:H382	2.00	0.43
3:C:54:MET:HE1	20:C:304:PGV:H141	2.01	0.43
8:H:37:HIS:HD2	32:H:127:HOH:O	2.00	0.43
1:N:309:THR:CG2	18:N:606:HEA:HMB2	2.49	0.43
3:P:37:PHE:HE1	10:W:58:LYS:CG	2.27	0.43
20:C:305:PGV:C06	8:H:22:ASN:ND2	2.76	0.43
26:C:306:CDL:C19	26:C:306:CDL:H602	2.49	0.43
5:E:41:LEU:HA	32:I:228:HOH:O	2.17	0.43
10:J:33:ARG:HG2	24:J:101:CHD:H151	1.99	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.18	0.43
6:S:82:CYS:C	6:S:84:SER:H	2.21	0.43
21:N:608:TGL:CA7	21:N:608:TGL:H221	2.47	0.43
26:T:101:CDL:H241	26:T:101:CDL:H542	2.00	0.43
14:2:35:LEU:O	14:2:37:GLY:N	2.52	0.43
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.75	0.43
3:C:210:ILE:HD13	20:C:304:PGV:H302	1.99	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.99	0.43
5:E:79:LYS:HD2	32:E:412:HOH:O	2.19	0.43
10:J:40:LEU:HD12	24:J:101:CHD:H183	2.01	0.43
20:P:304:PGV:H312	20:P:304:PGV:H282	1.86	0.43
9:V:18:ARG:NH2	28:V:101:PSC:C7	2.82	0.43
4:Q:114:GLU:HG3	11:X:51:LYS:HE3	2.01	0.43
1:N:136[A]:LEU:HD11	32:2:328:HOH:O	2.18	0.43
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.99	0.43
2:O:150:ILE:HD12	2:O:184:LEU:HD22	2.01	0.43
14:1:100:LYS:HE3	14:1:100:LYS:HB3	1.73	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.43
21:L:101:TGL:H232	21:L:101:TGL:H261	1.67	0.43
9:V:29:LEU:O	9:V:31:PHE:CA	2.65	0.43
25:C:303:PEK:H041	7:G:70:PHE:HB2	2.01	0.43
4:D:34:SER:H	4:D:37:GLN:HE21	1.67	0.43
1:N:302:ARG:HD2	1:N:302:ARG:HH11	1.70	0.43
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:303:PEK:H31	25:P:303:PEK:H71	2.00	0.43
9:I:2:THR:CA	32:I:201:HOH:O	2.59	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42
14:2:26:HIS:ND1	14:2:46:PHE:HB2	2.33	0.42
14:2:58:THR:HG22	14:2:59:TRP:N	2.34	0.42
2:B:7:LEU:HD11	21:B:301:TGL:H152	2.01	0.42
2:O:92:ASN:HD22	2:O:92:ASN:N	2.18	0.42
4:Q:78:TRP:CE2	4:Q:79:LYS:HG3	2.54	0.42
3:C:151:LEU:HB2	3:C:159:MET:HG3	2.00	0.42
26:G:101:CDL:HA22	32:G:244:HOH:O	2.19	0.42
2:B:68:LEU:HB3	2:B:69:PRO:HD3	2.02	0.42
2:B:74:ILE:HG12	26:T:101:CDL:H402	2.02	0.42
6:S:96:LEU:O	6:S:97:ALA:HB3	2.19	0.42
26:T:101:CDL:H152	26:T:101:CDL:H362	2.00	0.42
14:1:17:CYS:CB	31:1:201:HEM:C3C	3.02	0.42
14:2:38:ARG:NH2	14:2:38:ARG:HB2	2.35	0.42
26:P:306:CDL:OB6	26:P:306:CDL:HB22	2.20	0.42
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.01	0.42
4:Q:19[A]:ARG:HG2	32:Q:385:HOH:O	2.19	0.42
4:Q:81:VAL:HG11	21:Q:201:TGL:HB62	2.02	0.42
6:S:52:ILE:CG2	6:S:96:LEU:HB2	2.50	0.42
10:W:24:GLY:N	10:W:28:ASP:OD2	2.50	0.42
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.42
6:F:94:HIS:CG	6:F:95:GLN:H	2.38	0.42
6:F:94:HIS:HD2	6:F:97:ALA:N	2.11	0.42
9:I:27:VAL:O	9:I:31:PHE:N	2.49	0.42
2:O:57:ASP:O	2:O:60:GLU:OE2	2.38	0.42
8:U:9:LYS:HG3	8:U:11:TYR:H	1.84	0.42
9:V:25:PHE:O	9:V:29:LEU:HB2	2.20	0.42
1:N:48:LEU:O	13:Z:41:LYS:HE2	2.20	0.42
14:2:16:GLN:NE2	32:2:303:HOH:O	2.51	0.42
14:2:49:THR:CG2	14:2:79:LYS:HG2	2.50	0.42
4:D:107:ILE:HD11	4:D:111:PHE:HB2	2.01	0.42
26:P:306:CDL:H612	26:P:306:CDL:H642	1.65	0.42
6:S:54:ASN:HD22	6:S:54:ASN:H	1.66	0.42
3:P:37:PHE:HD1	10:W:58:LYS:HG3	1.71	0.42
1:A:309:THR:CG2	18:A:605:HEA:HMB2	2.50	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.42
1:N:112:LEU:HD23	1:N:112:LEU:C	2.40	0.42
3:P:257:TYR:O	3:P:261:SER:HB3	2.20	0.42
25:P:303:PEK:H221	7:T:69:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:306:CDL:CB5	26:P:306:CDL:HA21	2.49	0.42
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.50	0.42
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.18	0.42
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.79	0.42
30:M:101:DMU:H30	30:M:101:DMU:O1	2.19	0.42
1:N:242:GLU:O	1:N:246:LEU:HG	2.20	0.42
3:P:76:GLN:HE21	3:P:233:PHE:HB2	1.84	0.42
9:V:22:VAL:O	9:V:26:MET:HG2	2.20	0.42
14:1:86:LYS:CA	14:1:86:LYS:HE3	2.45	0.42
5:E:7:THR:OG1	5:E:10:GLU:HG3	2.20	0.42
11:K:50:PRO:HD2	32:K:105:HOH:O	2.19	0.42
1:A:472:ILE:HG21	21:L:101:TGL:HA91	2.02	0.42
14:2:97:TYR:CE1	14:2:101:ALA:HB2	2.55	0.41
2:B:148:MET:HB3	2:B:148:MET:HE3	1.63	0.41
2:B:91:ASN:OD1	2:B:183:THR:HG21	2.20	0.41
3:C:122:HIS:CE1	32:C:498:HOH:O	2.73	0.41
1:A:3:ILE:HG12	1:A:7:LEU:HD22	2.02	0.41
20:C:305:PGV:H161	32:T:241:HOH:O	2.21	0.41
2:O:129:LYS:HE3	2:O:129:LYS:HB3	1.61	0.41
3:P:105:SER:HA	3:P:116:TRP:CE3	2.56	0.41
3:P:51[B]:MET:HE1	20:P:304:PGV:H172	2.02	0.41
3:P:146:TRP:HB2	7:T:16:TRP:HB3	2.02	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.87	0.41
11:K:32:MET:O	11:K:32:MET:HG2	2.19	0.41
12:L:2:HIS:HD2	12:L:3:TYR:N	2.08	0.41
2:O:49:LYS:HE3	32:O:437:HOH:O	2.20	0.41
7:T:3:ALA:O	7:T:4:ALA:CB	2.68	0.41
14:2:59:TRP:CE3	14:2:59:TRP:HA	2.56	0.41
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.84	0.41
3:C:257:TYR:O	3:C:261:SER:HB3	2.21	0.41
7:G:31:CYS:SG	26:G:101:CDL:H532	2.61	0.41
26:P:306:CDL:CA2	32:P:403:HOH:O	2.67	0.41
8:H:7:LYS:N	32:H:101:HOH:O	2.53	0.41
2:O:78:LEU:HA	2:O:78:LEU:HD12	1.84	0.41
4:Q:107:ILE:HB	4:Q:108:PRO:CD	2.51	0.41
10:W:36:MET:HB3	24:W:101:CHD:H183	2.02	0.41
1:A:48:LEU:HB2	32:A:721:HOH:O	2.20	0.41
2:B:200:CYS:SG	2:B:204:HIS:HA	2.61	0.41
9:I:29:LEU:O	9:I:30:GLY:C	2.59	0.41
10:J:36:MET:HG2	24:J:101:CHD:H162	2.02	0.41
1:N:383[A]:MET:O	1:N:387:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.56	0.41
26:C:306:CDL:H602	26:C:306:CDL:H201	2.02	0.41
1:N:136[B]:LEU:HD11	32:N:925:HOH:O	2.21	0.41
21:L:101:TGL:H122	21:L:101:TGL:H291	1.71	0.41
1:N:236:TRP:CH2	18:N:606:HEA:HBD1	2.56	0.41
24:T:103:CHD:H12	24:T:103:CHD:H212	2.02	0.41
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.41
3:C:246:ASP:HB2	32:C:477:HOH:O	2.20	0.41
30:Z:101:DMU:H15	30:Z:101:DMU:H9	1.98	0.41
14:2:16:GLN:HG3	32:2:316:HOH:O	2.21	0.41
2:O:116:LEU:HD13	2:O:226:MET:CG	2.51	0.41
1:A:127:THR:HB	1:A:129:TYR:CE1	2.56	0.41
2:B:36:SER:HB3	21:B:301:TGL:C13	2.51	0.41
14:1:69:GLU:HG3	14:1:91:ARG:CZ	2.50	0.40
14:2:104:GLU:HA	14:2:104:GLU:OE1	2.21	0.40
1:A:335:SER:HB2	1:A:336:PRO:HD2	2.03	0.40
1:A:236:TRP:CH2	18:A:605:HEA:HBD1	2.56	0.40
3:C:59:ARG:HG3	26:C:306:CDL:H512	2.03	0.40
1:A:415:ALA:HB1	21:D:201:TGL:H121	2.03	0.40
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.03	0.40
2:O:68:LEU:CD2	28:V:101:PSC:H172	2.50	0.40
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.40
14:1:68:LEU:HD23	14:1:68:LEU:HA	1.89	0.40
14:2:80:MET:HB2	31:2:201:HEM:C4D	2.57	0.40
14:2:3:VAL:CG1	14:2:97:TYR:HA	2.45	0.40
3:C:29:SER:HB2	27:C:310:UNL:C4	2.51	0.40
7:G:10:GLY:HA3	32:G:205:HOH:O	2.21	0.40
12:L:25:MET:HG2	21:L:101:TGL:CA6	2.48	0.40
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.83	0.40
3:P:80[B]:ARG:NH2	27:P:308:UNL:C1	2.81	0.40
4:Q:31:LYS:HG3	32:Q:399:HOH:O	2.21	0.40
20:A:607:PGV:H231	13:M:12:PRO:HG3	2.03	0.40
4:D:112:GLU:HB3	32:D:363:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:266:HOH:O	32:U:148:HOH:O[1_455]	2.11	0.09
32:F:276:HOH:O	32:U:141:HOH:O[1_455]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	520/514 (101%)	504 (97%)	16 (3%)	0	100	100
2	B	227/227 (100%)	217 (96%)	9 (4%)	1 (0%)	39	33
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	39	33
3	C	263/259 (102%)	259 (98%)	4 (2%)	0	100	100
3	P	262/259 (101%)	256 (98%)	5 (2%)	1 (0%)	39	33
4	D	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
4	Q	143/144 (99%)	136 (95%)	5 (4%)	2 (1%)	14	6
5	E	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	9	3
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	1
7	G	81/84 (96%)	65 (80%)	10 (12%)	6 (7%)	1	0
7	T	81/84 (96%)	64 (79%)	10 (12%)	7 (9%)	1	0
8	H	77/79 (98%)	70 (91%)	4 (5%)	3 (4%)	4	1
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	15	7
9	I	71/73 (97%)	67 (94%)	1 (1%)	3 (4%)	3	1
9	V	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	6	2
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	55 (98%)	0	1 (2%)	11	4
11	K	47/49 (96%)	47 (100%)	0	0	100	100
11	X	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
12	L	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	38 (93%)	3 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
14	1	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	10	4
14	2	103/105 (98%)	81 (79%)	15 (15%)	7 (7%)	1	0
All	All	3744/3768 (99%)	3557 (95%)	145 (4%)	42 (1%)	17	9

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	96	LEU
7	G	3	ALA
7	G	7	ASP
7	G	8	HIS
7	G	46	ALA
8	H	8	ILE
8	H	9	LYS
8	H	50	VAL
9	I	2	THR
9	I	32	ALA
3	P	38	ASN
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	38	HIS
8	U	10	ASN
9	V	30	GLY
10	W	56	PRO
14	2	25	LYS
14	2	36	PHE
14	2	39	LYS
2	B	60	GLU
7	G	5	LYS
2	O	60	GLU
6	S	94	HIS
7	T	3	ALA
14	1	24	GLY
7	G	38	HIS
6	S	95	GLN
7	T	37	LEU
14	2	56	GLY

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Mol	Chain	Res	Type
4	Q	5	VAL
7	T	6	GLY
9	V	29	LEU
4	Q	6	VAL
14	1	37	GLY
14	2	1	GLY
9	I	30	GLY
14	2	23	GLY
14	2	41	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	437/426 (103%)	429 (98%)	8 (2%)	66	69
1	N	433/426 (102%)	425 (98%)	8 (2%)	66	69
2	B	212/210 (101%)	204 (96%)	8 (4%)	40	36
2	O	210/210 (100%)	196 (93%)	14 (7%)	20	14
3	C	230/224 (103%)	225 (98%)	5 (2%)	60	62
3	P	229/224 (102%)	225 (98%)	4 (2%)	68	71
4	D	128/128 (100%)	123 (96%)	5 (4%)	39	35
4	Q	129/128 (101%)	123 (95%)	6 (5%)	32	27
5	E	92/92 (100%)	90 (98%)	2 (2%)	60	62
5	R	92/92 (100%)	90 (98%)	2 (2%)	60	62
6	F	81/81 (100%)	77 (95%)	4 (5%)	31	25
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	11
7	G	67/67 (100%)	60 (90%)	7 (10%)	9	4
7	T	67/67 (100%)	60 (90%)	7 (10%)	9	4
8	H	71/71 (100%)	63 (89%)	8 (11%)	7	4
8	U	71/71 (100%)	69 (97%)	2 (3%)	51	50
9	I	57/57 (100%)	50 (88%)	7 (12%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	51 (90%)	6 (10%)	8	4
10	J	49/49 (100%)	48 (98%)	1 (2%)	63	65
10	W	49/49 (100%)	47 (96%)	2 (4%)	37	32
11	K	39/39 (100%)	37 (95%)	2 (5%)	29	23
11	X	39/39 (100%)	38 (97%)	1 (3%)	54	54
12	L	39/39 (100%)	36 (92%)	3 (8%)	16	10
12	Y	39/39 (100%)	36 (92%)	3 (8%)	16	10
13	M	37/37 (100%)	34 (92%)	3 (8%)	15	9
13	Z	37/37 (100%)	35 (95%)	2 (5%)	27	21
14	1	86/86 (100%)	78 (91%)	8 (9%)	11	6
14	2	86/86 (100%)	75 (87%)	11 (13%)	5	3
All	All	3244/3212 (101%)	3099 (96%)	145 (4%)	34	29

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	338	MET
1	A	363	LEU
1	A	369	ASP
1	A	514	LYS
2	B	16	ILE
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	171	LYS
3	C	40	MET
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	7	LYS

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Mol	Chain	Res	Type
4	D	8	SER
4	D	51	LEU
4	D	58	GLU
4	D	107	ILE
5	E	5	HIS
5	E	90	ARG
6	F	54	ASN
6	F	80	GLN
6	F	87	THR
6	F	95	GLN
7	G	5	LYS
7	G	18	PHE
7	G	33	LEU
7	G	37	LEU
7	G	42	ARG
7	G	54	ARG
7	G	83	GLU
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	50	VAL
8	H	60	TYR
8	H	61	LYS
8	H	84	LYS
9	I	18	ARG
9	I	21	ILE
9	I	29	LEU
9	I	31	PHE
9	I	33	THR
9	I	37	PHE
9	I	41	GLU
10	J	50	LEU
11	K	7	PRO
11	K	54	ARG
12	L	2	HIS
12	L	5	GLU
12	L	47	LYS
13	M	34	LEU
13	M	38	ASP
13	M	40	TYR
1	N	35	LEU

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Mol	Chain	Res	Type
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	363	LEU
1	N	369	ASP
2	O	59	GLN
2	O	60	GLU
2	O	65	TRP
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	113	TYR
2	O	115	ASP
2	O	158	ASP
2	O	167	SER
2	O	171	LYS
2	O	217	LYS
2	O	226	MET
3	P	110	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	6	VAL
4	Q	7	LYS
4	Q	21	ASP
4	Q	31	LYS
4	Q	51	LEU
5	R	6	GLU
5	R	80	GLU
6	S	44	GLU
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
6	S	87	THR
7	T	18	PHE
7	T	33	LEU
7	T	35	SER

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Mol	Chain	Res	Type
7	T	36	TRP
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	27	ARG
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	21	ILE
9	V	31	PHE
9	V	36	LYS
9	V	73	LYS
10	W	2	GLU
10	W	50	LEU
11	X	54	ARG
12	Y	2	HIS
12	Y	5	GLU
12	Y	20	ARG
13	Z	34	LEU
13	Z	43	SER
14	1	14	CYS
14	1	20	VAL
14	1	25	LYS
14	1	38	ARG
14	1	52	ASN
14	1	69	GLU
14	1	86	LYS
14	1	103	ASN
14	2	14	CYS
14	2	16	GLN
14	2	17	CYS
14	2	19	THR
14	2	20	VAL
14	2	26	HIS
14	2	38	ARG
14	2	39	LYS
14	2	40	THR
14	2	47	THR
14	2	72	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
6	F	94	HIS
6	F	95	GLN
6	F	98	HIS
7	G	8	HIS
8	H	22	ASN
9	I	20	HIS
10	J	29	ASN
12	L	2	HIS
1	N	4	ASN
1	N	80	ASN
1	N	98	ASN
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	92	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN

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Mol	Chain	Res	Type
6	S	54	ASN
6	S	80	GLN
7	T	38	HIS
8	U	10	ASN
8	U	12	GLN
8	U	37	HIS
9	V	20	HIS
10	W	29	ASN
14	1	103	ASN
14	2	16	GLN
14	2	26	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	1.47	1 (12%)	5,9,11	2.73	4 (80%)
2	FME	B	1	2	8,9,10	2.54	3 (37%)	5,9,11	4.86	2 (40%)
7	TPO	G	11	7	7,10,11	1.58	1 (14%)	10,14,16	1.62	2 (20%)
9	SAC	I	1	9	7,8,9	2.19	2 (28%)	7,9,11	2.08	2 (28%)
1	FME	N	1	1	8,9,10	0.80	0	5,9,11	3.22	3 (60%)
2	FME	O	1	2	8,9,10	0.77	0	5,9,11	1.13	1 (20%)
7	TPO	T	11	7	7,10,11	1.97	1 (14%)	10,14,16	1.62	4 (40%)
9	SAC	V	1	9	7,8,9	2.46	2 (28%)	7,9,11	1.52	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	1/8/11/13	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	-	0/6/9/11	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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.62	1.10	1.22
2	B	1	FME	CB-CA	2.51	1.58	1.53
7	G	11	TPO	P-O1P	3.11	1.60	1.50
9	I	1	SAC	CA-N	3.28	1.50	1.46
7	T	11	TPO	P-O1P	3.57	1.62	1.50
1	A	1	FME	CA-N	3.74	1.51	1.46
9	V	1	SAC	CA-N	4.23	1.52	1.46
9	I	1	SAC	OAC-C1A	4.56	1.33	1.23
9	V	1	SAC	OAC-C1A	4.71	1.34	1.23
2	B	1	FME	CA-N	5.47	1.54	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O-C-CA	-2.40	119.13	125.69
1	A	1	FME	CG-CB-CA	-2.40	105.87	113.07
1	N	1	FME	CG-CB-CA	-2.28	106.21	113.07
1	A	1	FME	O-C-CA	-2.26	119.51	125.69
2	O	1	FME	O-C-CA	-2.08	120.01	125.69
7	T	11	TPO	O2P-P-OG1	2.02	112.65	106.62
7	T	11	TPO	OG1-P-O1P	2.04	112.33	107.48
7	T	11	TPO	P-OG1-CB	2.19	131.00	121.42
7	G	11	TPO	OG1-P-O1P	2.21	112.76	107.48
9	V	1	SAC	C2A-C1A-N	2.24	120.40	116.10
7	T	11	TPO	C-CA-N	2.40	115.25	109.95
9	I	1	SAC	CA-N-C1A	3.03	131.72	121.32
9	I	1	SAC	C2A-C1A-N	3.04	121.92	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CE-SD-CG	3.06	111.00	100.36
7	G	11	TPO	C-CA-N	3.10	116.80	109.95
1	N	1	FME	CE-SD-CG	3.90	113.91	100.36
1	A	1	FME	O1-CN-N	4.10	131.07	124.80
1	N	1	FME	O1-CN-N	5.33	132.96	124.80
2	B	1	FME	O1-CN-N	10.36	140.65	124.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	OG1-CB-CA-N
1	N	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	2	0
9	I	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 15 are unknown and 10 are monoatomic - leaving 51 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
31	HEM	1	201	14	24,50,50	0.66	0	16,82,82	1.94	5 (31%)
31	HEM	2	201	14	24,50,50	0.80	1 (4%)	16,82,82	1.44	2 (12%)
18	HEA	A	604[A]	-	40,67,67	1.18	3 (7%)	36,103,103	2.34	12 (33%)
18	HEA	A	604[B]	-	40,67,67	1.17	2 (5%)	36,103,103	2.22	11 (30%)
18	HEA	A	605	1,19	40,67,67	1.43	7 (17%)	36,103,103	2.13	9 (25%)
19	PER	A	606	18,15	0,1,1	0.00	-	0,0,0	0.00	-
20	PGV	A	607	-	50,50,50	1.09	2 (4%)	51,56,56	1.09	5 (9%)
20	PGV	A	608	-	50,50,50	1.05	5 (10%)	51,56,56	1.27	6 (11%)
21	TGL	B	301	-	62,62,62	1.43	8 (12%)	65,65,65	1.95	10 (15%)
22	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
23	EDO	B	303	-	3,3,3	0.75	0	2,2,2	0.46	0
24	CHD	C	301	-	29,32,32	1.29	4 (13%)	48,51,51	1.82	12 (25%)
25	PEK	C	303	-	51,52,52	0.95	2 (3%)	52,57,57	1.29	5 (9%)
20	PGV	C	304	-	50,50,50	0.79	2 (4%)	51,56,56	1.31	6 (11%)
20	PGV	C	305	-	50,50,50	1.38	3 (6%)	51,56,56	1.50	6 (11%)
26	CDL	C	306	-	99,99,99	1.35	12 (12%)	101,111,111	1.44	10 (9%)
24	CHD	C	307	-	29,32,32	0.87	0	48,51,51	3.57	25 (52%)
23	EDO	C	311	-	3,3,3	0.59	0	2,2,2	0.36	0
21	TGL	D	201	-	62,62,62	1.37	6 (9%)	65,65,65	1.53	8 (12%)
28	PSC	E	201	-	51,51,51	1.29	3 (5%)	55,59,59	1.56	9 (16%)
23	EDO	E	202	-	3,3,3	0.49	0	2,2,2	0.80	0
23	EDO	F	102	-	3,3,3	0.43	0	2,2,2	0.62	0
26	CDL	G	101	-	99,99,99	1.41	12 (12%)	101,111,111	1.39	13 (12%)
24	CHD	G	102	-	29,32,32	1.12	2 (6%)	48,51,51	2.06	13 (27%)
23	EDO	G	103	-	3,3,3	0.80	0	2,2,2	0.74	0
23	EDO	I	101	-	3,3,3	0.61	0	2,2,2	0.34	0
24	CHD	J	101	-	29,32,32	0.83	0	48,51,51	2.20	15 (31%)
21	TGL	L	101	-	62,62,62	1.53	7 (11%)	65,65,65	1.62	13 (20%)
30	DMU	M	101	-	34,34,34	0.73	0	45,45,45	1.77	10 (22%)
18	HEA	N	605[A]	-	40,67,67	1.10	4 (10%)	36,103,103	2.34	14 (38%)
18	HEA	N	605[B]	-	40,67,67	1.09	4 (10%)	36,103,103	2.33	15 (41%)
18	HEA	N	606	1,19	40,67,67	1.40	8 (20%)	36,103,103	1.71	7 (19%)
19	PER	N	607	18,15	0,1,1	0.00	-	0,0,0	0.00	-
21	TGL	N	608	-	62,62,62	1.45	7 (11%)	65,65,65	2.14	14 (21%)
20	PGV	N	612	-	50,50,50	0.84	1 (2%)	51,56,56	1.20	4 (7%)
23	EDO	N	613	-	3,3,3	0.56	0	2,2,2	0.36	0
23	EDO	N	614	-	3,3,3	0.40	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
24	CHD	P	301	-	29,32,32	1.05	2 (6%)	48,51,51	1.87	13 (27%)
25	PEK	P	303	-	51,52,52	0.97	3 (5%)	52,57,57	1.00	3 (5%)
20	PGV	P	304	-	50,50,50	0.81	2 (4%)	51,56,56	1.17	6 (11%)
20	PGV	P	305	-	50,50,50	1.26	2 (4%)	51,56,56	1.42	5 (9%)
26	CDL	P	306	-	99,99,99	1.38	12 (12%)	101,111,111	1.25	11 (10%)
24	CHD	P	307	-	29,32,32	0.57	0	48,51,51	2.43	18 (37%)
21	TGL	Q	201	-	62,62,62	1.38	6 (9%)	65,65,65	1.29	8 (12%)
23	EDO	S	102	-	3,3,3	0.61	0	2,2,2	0.88	0
26	CDL	T	101	-	99,99,99	1.40	12 (12%)	101,111,111	1.51	12 (11%)
24	CHD	T	103	-	29,32,32	1.06	2 (6%)	48,51,51	2.02	16 (33%)
28	PSC	V	101	-	51,51,51	1.19	3 (5%)	55,59,59	1.33	5 (9%)
24	CHD	W	101	-	29,32,32	0.85	1 (3%)	48,51,51	3.28	22 (45%)
30	DMU	Z	101	-	34,34,34	0.73	1 (2%)	45,45,45	1.08	5 (11%)

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
31	HEM	1	201	14	-	0/6/54/54	0/0/8/8
31	HEM	2	201	14	-	0/6/54/54	0/0/8/8
18	HEA	A	604[A]	-	-	0/24/76/76	0/0/8/8
18	HEA	A	604[B]	-	-	0/24/76/76	0/0/8/8
18	HEA	A	605	1,19	2/2/7/16	0/24/76/76	0/0/8/8
19	PER	A	606	18,15	-	0/0/0/0	0/0/0/0
20	PGV	A	607	-	-	0/55/55/55	0/0/0/0
20	PGV	A	608	-	-	0/55/55/55	0/0/0/0
21	TGL	B	301	-	-	0/65/65/65	0/0/0/0
22	CUA	B	302	2	-	0/0/0/0	0/0/0/0
23	EDO	B	303	-	-	0/1/1/1	0/0/0/0
24	CHD	C	301	-	-	0/7/74/74	0/4/4/4
25	PEK	C	303	-	-	0/56/56/56	0/0/0/0
20	PGV	C	304	-	-	0/55/55/55	0/0/0/0
20	PGV	C	305	-	-	0/55/55/55	0/0/0/0
26	CDL	C	306	-	-	0/110/110/110	0/0/0/0
24	CHD	C	307	-	-	0/7/74/74	0/4/4/4
23	EDO	C	311	-	-	0/1/1/1	0/0/0/0
21	TGL	D	201	-	-	0/65/65/65	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	PSC	E	201	-	-	0/55/55/55	0/0/0/0
23	EDO	E	202	-	-	0/1/1/1	0/0/0/0
23	EDO	F	102	-	-	0/1/1/1	0/0/0/0
26	CDL	G	101	-	-	0/110/110/110	0/0/0/0
24	CHD	G	102	-	-	0/7/74/74	0/4/4/4
23	EDO	G	103	-	-	0/1/1/1	0/0/0/0
23	EDO	I	101	-	-	0/1/1/1	0/0/0/0
24	CHD	J	101	-	-	0/7/74/74	0/4/4/4
21	TGL	L	101	-	-	0/65/65/65	0/0/0/0
30	DMU	M	101	-	-	0/19/59/59	0/2/2/2
18	HEA	N	605[A]	-	-	0/24/76/76	0/0/8/8
18	HEA	N	605[B]	-	-	0/24/76/76	0/0/8/8
18	HEA	N	606	1,19	2/2/7/16	0/24/76/76	0/0/8/8
19	PER	N	607	18,15	-	0/0/0/0	0/0/0/0
21	TGL	N	608	-	-	0/65/65/65	0/0/0/0
20	PGV	N	612	-	-	0/55/55/55	0/0/0/0
23	EDO	N	613	-	-	0/1/1/1	0/0/0/0
23	EDO	N	614	-	-	0/1/1/1	0/0/0/0
22	CUA	O	301	2	-	0/0/0/0	0/0/0/0
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
25	PEK	P	303	-	-	0/56/56/56	0/0/0/0
20	PGV	P	304	-	-	0/55/55/55	0/0/0/0
20	PGV	P	305	-	-	0/55/55/55	0/0/0/0
26	CDL	P	306	-	-	0/110/110/110	0/0/0/0
24	CHD	P	307	-	-	0/7/74/74	0/4/4/4
21	TGL	Q	201	-	-	1/65/65/65	0/0/0/0
23	EDO	S	102	-	-	0/1/1/1	0/0/0/0
26	CDL	T	101	-	-	0/110/110/110	0/0/0/0
24	CHD	T	103	-	-	0/7/74/74	0/4/4/4
28	PSC	V	101	-	-	0/55/55/55	0/0/0/0
24	CHD	W	101	-	-	0/7/74/74	0/4/4/4
30	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	605	HEA	C4A-NA	-4.15	1.31	1.36
21	B	301	TGL	OC1-CC1	-3.93	1.11	1.22
26	P	306	CDL	C59-C58	-3.37	1.32	1.51
21	L	101	TGL	C20-CA9	-3.23	1.33	1.51
26	C	306	CDL	C59-C58	-3.16	1.33	1.51
26	P	306	CDL	C82-C81	-3.10	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	CDL	C59-C58	-3.09	1.33	1.51
21	N	608	TGL	C20-CA9	-3.05	1.34	1.51
21	L	101	TGL	C10-CB9	-3.05	1.34	1.51
26	C	306	CDL	C79-C78	-3.04	1.34	1.51
26	C	306	CDL	C62-C61	-3.03	1.34	1.51
26	C	306	CDL	C19-C18	-3.02	1.34	1.51
21	Q	201	TGL	C15-CC9	-3.00	1.34	1.51
26	G	101	CDL	C42-C41	-2.99	1.34	1.51
26	P	306	CDL	C79-C78	-2.98	1.34	1.51
26	T	101	CDL	C19-C18	-2.97	1.34	1.51
26	G	101	CDL	C22-C21	-2.97	1.34	1.51
26	G	101	CDL	C62-C61	-2.96	1.34	1.51
21	D	201	TGL	C10-CB9	-2.94	1.34	1.51
26	C	306	CDL	C82-C81	-2.93	1.34	1.51
26	C	306	CDL	C22-C21	-2.93	1.34	1.51
26	P	306	CDL	C19-C18	-2.93	1.34	1.51
21	D	201	TGL	C15-CC9	-2.92	1.34	1.51
26	T	101	CDL	C62-C61	-2.91	1.34	1.51
26	P	306	CDL	C62-C61	-2.89	1.35	1.51
21	N	608	TGL	C15-CC9	-2.88	1.35	1.51
26	P	306	CDL	C39-C38	-2.88	1.35	1.51
26	C	306	CDL	C42-C41	-2.88	1.35	1.51
26	P	306	CDL	C22-C21	-2.88	1.35	1.51
26	P	306	CDL	C42-C41	-2.87	1.35	1.51
26	T	101	CDL	C39-C38	-2.87	1.35	1.51
21	B	301	TGL	C15-CC9	-2.87	1.35	1.51
21	Q	201	TGL	C10-CB9	-2.86	1.35	1.51
26	G	101	CDL	C19-C18	-2.86	1.35	1.51
26	G	101	CDL	C39-C38	-2.86	1.35	1.51
21	B	301	TGL	C20-CA9	-2.85	1.35	1.51
26	T	101	CDL	C82-C81	-2.84	1.35	1.51
26	G	101	CDL	C82-C81	-2.82	1.35	1.51
24	G	102	CHD	C13-C14	-2.78	1.50	1.55
26	G	101	CDL	C79-C78	-2.77	1.35	1.51
26	G	101	CDL	C59-C58	-2.76	1.35	1.51
18	A	605	HEA	C1A-NA	-2.76	1.33	1.36
26	T	101	CDL	C22-C21	-2.74	1.35	1.51
21	N	608	TGL	C10-CB9	-2.73	1.35	1.51
18	A	605	HEA	C3A-C2A	-2.73	1.36	1.40
26	T	101	CDL	C42-C41	-2.72	1.36	1.51
21	D	201	TGL	C20-CA9	-2.71	1.36	1.51
18	N	606	HEA	C1D-ND	-2.66	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	CDL	C79-C78	-2.66	1.36	1.51
21	L	101	TGL	C15-CC9	-2.65	1.36	1.51
26	C	306	CDL	C39-C38	-2.58	1.36	1.51
18	N	605[A]	HEA	C4A-NA	-2.52	1.33	1.36
18	N	605[B]	HEA	C4A-NA	-2.52	1.33	1.36
21	Q	201	TGL	C20-CA9	-2.45	1.37	1.51
21	B	301	TGL	C10-CB9	-2.45	1.37	1.51
21	N	608	TGL	OC1-CC1	-2.43	1.15	1.22
25	P	303	PEK	O03-C01	-2.35	1.40	1.45
18	A	605	HEA	CAA-C2A	-2.35	1.49	1.52
31	2	201	HEM	C3B-C2B	-2.23	1.37	1.40
18	N	606	HEA	C4A-NA	-2.20	1.33	1.36
21	B	301	TGL	OG1-CG1	-2.13	1.40	1.45
18	N	606	HEA	C3C-C2C	-2.11	1.37	1.40
20	A	608	PGV	O01-C02	-2.05	1.41	1.46
20	A	608	PGV	C01-C02	2.00	1.56	1.50
21	L	101	TGL	CG3-CG2	2.06	1.56	1.50
18	N	605[A]	HEA	C1C-CHC	2.07	1.45	1.40
18	N	605[B]	HEA	C1C-CHC	2.07	1.45	1.40
18	N	606	HEA	C4C-CHD	2.10	1.45	1.40
20	C	304	PGV	O01-C1	2.14	1.40	1.34
24	W	101	CHD	C20-C17	2.15	1.58	1.54
18	N	605[A]	HEA	C1B-CHB	2.15	1.45	1.40
18	N	605[B]	HEA	C1B-CHB	2.15	1.45	1.40
24	C	301	CHD	C18-C13	2.15	1.57	1.54
18	N	606	HEA	C18-C19	2.16	1.38	1.32
18	A	604[A]	HEA	C22-C23	2.16	1.38	1.32
18	A	604[B]	HEA	C3C-CAC	2.18	1.52	1.47
18	A	604[A]	HEA	C3C-CAC	2.18	1.52	1.47
18	A	605	HEA	C1C-CHC	2.26	1.46	1.40
18	A	605	HEA	C18-C19	2.33	1.38	1.32
30	Z	101	DMU	O16-C6	2.41	1.44	1.40
24	C	301	CHD	C16-C17	2.42	1.59	1.54
20	A	608	PGV	O03-C01	2.42	1.50	1.45
18	A	605	HEA	CMC-C2C	2.44	1.56	1.51
24	T	103	CHD	C11-C9	2.45	1.57	1.53
24	P	301	CHD	C8-C7	2.52	1.57	1.53
24	C	301	CHD	C11-C9	2.53	1.57	1.53
18	N	605[A]	HEA	O11-C11	2.55	1.48	1.42
18	N	605[B]	HEA	O11-C11	2.55	1.48	1.42
20	C	305	PGV	C01-C02	2.57	1.58	1.50
18	A	604[B]	HEA	CAA-C2A	2.58	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	604[A]	HEA	CAA-C2A	2.58	1.55	1.52
24	P	301	CHD	C18-C13	2.61	1.58	1.54
20	A	608	PGV	O01-C1	2.66	1.42	1.34
24	C	301	CHD	C8-C7	2.67	1.58	1.53
20	P	304	PGV	O03-C19	2.79	1.41	1.33
18	N	606	HEA	O11-C11	2.87	1.49	1.42
24	T	103	CHD	C4-C3	2.94	1.57	1.51
25	C	303	PEK	O03-C21	2.94	1.42	1.33
18	N	606	HEA	C1C-CHC	3.03	1.48	1.40
20	P	304	PGV	O01-C1	3.04	1.43	1.34
20	C	304	PGV	O03-C19	3.04	1.42	1.33
24	G	102	CHD	C4-C3	3.24	1.58	1.51
25	P	303	PEK	O03-C21	3.28	1.43	1.33
18	N	606	HEA	CAA-C2A	3.56	1.56	1.52
26	C	306	CDL	OB6-CB5	3.61	1.44	1.34
28	V	101	PSC	C13-C12	3.64	1.53	1.31
28	E	201	PSC	C13-C12	3.67	1.53	1.31
28	V	101	PSC	O03-C19	3.73	1.44	1.33
20	A	608	PGV	O03-C19	3.88	1.44	1.33
20	A	607	PGV	O01-C1	4.06	1.46	1.34
21	B	301	TGL	OG2-CB1	4.12	1.46	1.34
25	C	303	PEK	O01-C1	4.15	1.46	1.34
25	P	303	PEK	O01-C1	4.22	1.46	1.34
26	G	101	CDL	OA6-CA5	4.40	1.47	1.34
20	N	612	PGV	O03-C19	4.47	1.46	1.33
26	P	306	CDL	OB6-CB5	4.48	1.47	1.34
26	T	101	CDL	OB8-CB7	4.58	1.46	1.33
28	E	201	PSC	O03-C19	4.61	1.47	1.33
21	D	201	TGL	OG3-CC1	4.61	1.47	1.33
21	L	101	TGL	OG1-CA1	4.68	1.47	1.33
26	G	101	CDL	OA8-CA7	4.69	1.47	1.33
21	Q	201	TGL	OG1-CA1	4.79	1.47	1.33
26	P	306	CDL	OA6-CA5	4.79	1.48	1.34
21	D	201	TGL	OG2-CB1	4.81	1.48	1.34
26	P	306	CDL	OB8-CB7	4.84	1.47	1.33
21	B	301	TGL	OG1-CA1	4.85	1.47	1.33
26	T	101	CDL	OA6-CA5	4.85	1.48	1.34
26	C	306	CDL	OA8-CA7	4.86	1.47	1.33
21	Q	201	TGL	OG2-CB1	4.91	1.48	1.34
21	Q	201	TGL	OG3-CC1	4.93	1.48	1.33
20	P	305	PGV	O01-C1	4.94	1.48	1.34
26	G	101	CDL	OB8-CB7	4.95	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	608	TGL	OG3-CC1	4.95	1.48	1.33
20	A	607	PGV	O03-C19	4.96	1.48	1.33
26	T	101	CDL	OA8-CA7	4.99	1.48	1.33
26	C	306	CDL	OA6-CA5	4.99	1.49	1.34
26	P	306	CDL	OA8-CA7	5.02	1.48	1.33
26	T	101	CDL	OB6-CB5	5.05	1.49	1.34
21	B	301	TGL	OG3-CC1	5.06	1.48	1.33
20	C	305	PGV	O03-C19	5.10	1.48	1.33
21	D	201	TGL	OG1-CA1	5.13	1.48	1.33
21	N	608	TGL	OG2-CB1	5.17	1.49	1.34
21	N	608	TGL	OG1-CA1	5.19	1.48	1.33
20	P	305	PGV	O03-C19	5.20	1.48	1.33
26	G	101	CDL	OB6-CB5	5.23	1.49	1.34
26	C	306	CDL	OB8-CB7	5.27	1.49	1.33
28	V	101	PSC	O01-C1	5.36	1.50	1.34
28	E	201	PSC	O01-C1	5.39	1.50	1.34
20	C	305	PGV	O01-C1	5.62	1.50	1.34
21	L	101	TGL	OG3-CC1	5.67	1.50	1.33
21	L	101	TGL	OG2-CB1	6.69	1.54	1.34

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	307	CHD	C6-C5-C4	-7.94	102.55	111.07
18	N	605[A]	HEA	C13-C12-C11	-7.39	106.05	114.74
18	N	605[B]	HEA	C13-C12-C11	-7.39	106.05	114.74
18	A	604[B]	HEA	C13-C12-C11	-6.92	106.60	114.74
18	A	604[A]	HEA	C13-C12-C11	-6.92	106.60	114.74
18	A	605	HEA	C13-C12-C11	-6.41	107.20	114.74
18	A	605	HEA	C3C-CAC-CBC	-6.10	114.14	126.40
24	C	307	CHD	C19-C10-C1	-6.08	97.94	108.23
24	C	307	CHD	C11-C9-C8	-6.07	102.02	110.77
24	G	102	CHD	C6-C5-C4	-5.86	104.78	111.07
24	C	307	CHD	C6-C7-C8	-5.68	105.45	111.46
24	P	307	CHD	C9-C11-C12	-5.67	107.27	114.38
24	T	103	CHD	C18-C13-C12	-5.66	103.42	109.09
26	C	306	CDL	CB4-OB6-CB5	-5.66	103.92	117.91
24	W	101	CHD	C17-C13-C14	-5.40	94.62	100.08
24	W	101	CHD	C6-C5-C4	-5.08	105.61	111.07
18	N	605[A]	HEA	C20-C21-C22	-5.06	98.32	111.61
24	W	101	CHD	C14-C8-C9	-5.02	102.55	109.63
18	N	606	HEA	CAD-CBD-CGD	-4.86	103.33	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	604[B]	HEA	CAA-CBA-CGA	-4.79	103.47	112.78
18	A	604[A]	HEA	CAA-CBA-CGA	-4.79	103.47	112.78
31	1	201	HEM	CBD-CAD-C3D	-4.64	104.33	112.47
24	C	301	CHD	C21-C20-C22	-4.53	102.96	110.33
30	M	101	DMU	C18-O16-C6	-4.37	106.37	114.00
24	W	101	CHD	C18-C13-C12	-4.34	104.75	109.09
18	N	605[A]	HEA	C1A-C2A-C3A	-4.28	102.78	107.07
18	N	605[B]	HEA	C1A-C2A-C3A	-4.28	102.78	107.07
21	N	608	TGL	OG3-CC1-OC1	-4.25	112.36	123.51
24	P	307	CHD	C14-C8-C9	-4.22	103.69	109.63
18	A	605	HEA	CAD-CBD-CGD	-4.10	104.80	112.78
30	M	101	DMU	O2-C8-C9	-4.02	98.63	109.23
24	C	307	CHD	C21-C20-C22	-4.00	103.83	110.33
18	A	604[B]	HEA	C13-C14-C15	-3.95	119.04	127.75
18	A	604[A]	HEA	C13-C14-C15	-3.95	119.04	127.75
25	C	303	PEK	O03-C01-C02	-3.90	98.17	108.70
24	P	301	CHD	C9-C11-C12	-3.89	109.50	114.38
18	A	604[B]	HEA	C26-C15-C16	-3.85	109.51	115.37
18	A	604[A]	HEA	C26-C15-C16	-3.85	109.51	115.37
24	G	102	CHD	O12-C12-C13	-3.82	104.74	111.12
21	N	608	TGL	OG1-CA1-OA1	-3.81	113.52	123.51
24	W	101	CHD	C1-C10-C9	-3.80	105.39	111.43
24	C	307	CHD	C14-C8-C9	-3.80	104.28	109.63
24	J	101	CHD	C17-C13-C14	-3.78	96.25	100.08
24	T	103	CHD	C13-C17-C20	-3.77	114.84	119.44
20	N	612	PGV	O03-C19-O04	-3.75	113.69	123.51
21	N	608	TGL	CG3-CG2-CG1	-3.75	103.36	112.08
28	V	101	PSC	C21-C20-C19	-3.68	99.21	113.57
24	P	307	CHD	C23-C22-C20	-3.61	110.33	114.79
24	G	102	CHD	C18-C13-C12	-3.58	105.51	109.09
31	1	201	HEM	C3B-CAB-CBB	-3.52	119.31	126.40
18	A	604[A]	HEA	C20-C19-C18	-3.50	114.45	120.98
25	C	303	PEK	O03-C21-O04	-3.48	114.39	123.51
20	A	608	PGV	O03-C19-O04	-3.46	114.44	123.51
24	P	301	CHD	C13-C14-C8	-3.42	110.23	114.73
30	M	101	DMU	O3-C5-C10	-3.42	102.43	110.01
24	C	307	CHD	C23-C22-C20	-3.40	110.58	114.79
24	P	307	CHD	C1-C10-C9	-3.36	106.09	111.43
20	C	304	PGV	O03-C19-O04	-3.36	114.71	123.51
31	2	201	HEM	C3B-CAB-CBB	-3.32	119.72	126.40
18	N	606	HEA	C20-C19-C18	-3.29	114.84	120.98
18	A	605	HEA	CBA-CAA-C2A	-3.28	106.72	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	605	HEA	CMC-C2C-C1C	-3.25	122.78	128.31
24	J	101	CHD	C9-C11-C12	-3.22	110.34	114.38
20	A	608	PGV	O01-C1-O02	-3.18	115.01	123.67
20	C	304	PGV	O01-C1-O02	-3.12	115.17	123.67
24	C	301	CHD	C17-C13-C14	-3.11	96.94	100.08
24	C	301	CHD	C5-C4-C3	-3.09	108.30	112.88
24	J	101	CHD	C23-C22-C20	-3.09	110.97	114.79
24	G	102	CHD	C13-C17-C20	-3.09	115.67	119.44
24	P	301	CHD	C17-C13-C14	-3.08	96.96	100.08
18	N	605[A]	HEA	CAD-CBD-CGD	-3.08	106.79	112.78
18	N	605[B]	HEA	CAD-CBD-CGD	-3.08	106.79	112.78
24	P	307	CHD	O7-C7-C6	-2.98	102.74	110.02
21	L	101	TGL	OB1-CB1-CB2	-2.93	112.56	123.76
18	N	605[A]	HEA	C16-C15-C14	-2.92	115.55	120.98
18	N	605[B]	HEA	C16-C15-C14	-2.92	115.55	120.98
24	T	103	CHD	O3-C3-C2	-2.91	103.00	110.04
18	N	605[A]	HEA	CAA-CBA-CGA	-2.89	107.15	112.78
18	N	605[B]	HEA	CAA-CBA-CGA	-2.89	107.15	112.78
24	C	301	CHD	C23-C22-C20	-2.85	111.27	114.79
21	B	301	TGL	OB1-CB1-CB2	-2.82	112.96	123.76
30	M	101	DMU	C10-C5-C7	-2.82	104.39	109.98
31	I	201	HEM	C3B-C4B-NB	-2.76	105.64	109.21
26	T	101	CDL	CB6-CB4-CB3	-2.76	105.64	112.08
28	V	101	PSC	C28-C27-C26	-2.76	100.20	114.54
21	N	608	TGL	OB1-CB1-CB2	-2.72	113.35	123.76
24	T	103	CHD	C6-C5-C4	-2.71	108.16	111.07
28	E	201	PSC	C28-C27-C26	-2.71	100.47	114.54
24	T	103	CHD	C23-C22-C20	-2.69	111.47	114.79
31	2	201	HEM	C3C-CAC-CBC	-2.68	121.01	126.40
18	A	604[B]	HEA	C17-C18-C19	-2.68	121.84	127.75
26	C	306	CDL	C52-C51-CB5	-2.67	103.14	113.57
24	J	101	CHD	C13-C14-C8	-2.66	111.23	114.73
28	E	201	PSC	O01-C1-O02	-2.66	116.45	123.67
18	A	604[B]	HEA	C20-C19-C18	-2.65	116.03	120.98
24	W	101	CHD	O7-C7-C6	-2.64	103.59	110.02
24	G	102	CHD	C1-C10-C9	-2.60	107.30	111.43
20	C	304	PGV	C27-C26-C25	-2.57	101.17	114.54
26	P	306	CDL	OB8-CB6-CB4	-2.57	101.76	108.70
18	A	605	HEA	C1A-C2A-C3A	-2.55	104.52	107.07
21	D	201	TGL	OG2-CB1-OB1	-2.55	116.74	123.67
24	C	307	CHD	C9-C11-C12	-2.55	111.19	114.38
28	E	201	PSC	C11-C12-C13	-2.52	109.19	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E	201	PSC	C31-C30-C29	-2.50	101.54	114.54
24	T	103	CHD	O12-C12-C11	-2.50	103.91	109.09
21	Q	201	TGL	OG3-CC1-OC1	-2.48	117.01	123.51
20	P	305	PGV	O03-C19-O04	-2.47	117.02	123.51
24	T	103	CHD	C5-C4-C3	-2.47	109.22	112.88
21	Q	201	TGL	OG1-CA1-OA1	-2.47	117.04	123.51
24	C	301	CHD	C16-C15-C14	-2.46	100.18	105.11
24	C	307	CHD	O12-C12-C13	-2.44	107.05	111.12
26	G	101	CDL	OA6-CA5-OA7	-2.43	117.05	123.67
24	P	301	CHD	C22-C23-C24	-2.40	103.26	113.05
20	P	304	PGV	O03-C19-O04	-2.40	117.23	123.51
18	N	605[A]	HEA	CBD-CAD-C3D	-2.39	108.28	112.49
18	N	605[B]	HEA	CBD-CAD-C3D	-2.39	108.28	112.49
30	M	101	DMU	O4-C7-C8	-2.39	104.97	110.36
24	W	101	CHD	C9-C11-C12	-2.38	111.39	114.38
24	G	102	CHD	O7-C7-C6	-2.36	104.26	110.02
24	G	102	CHD	C19-C10-C1	-2.34	104.26	108.23
24	P	307	CHD	C19-C10-C5	-2.34	106.14	110.28
24	W	101	CHD	C14-C13-C12	-2.33	105.26	107.37
20	A	607	PGV	C5-C4-C3	-2.31	102.53	114.54
20	C	304	PGV	C03-C02-C01	-2.31	106.70	112.08
24	P	301	CHD	C13-C17-C20	-2.30	116.63	119.44
26	G	101	CDL	OB8-CB7-OB9	-2.30	117.49	123.51
18	A	605	HEA	CAA-CBA-CGA	-2.30	108.31	112.78
26	P	306	CDL	C56-C55-C54	-2.30	102.62	114.54
30	M	101	DMU	O1-C9-C8	-2.29	105.30	109.67
24	P	301	CHD	C14-C13-C12	-2.28	105.31	107.37
18	A	604[B]	HEA	C1A-C2A-C3A	-2.28	104.79	107.07
18	A	604[A]	HEA	C1A-C2A-C3A	-2.28	104.79	107.07
26	P	306	CDL	OB8-CB7-OB9	-2.27	117.55	123.51
28	V	101	PSC	C25-C24-C23	-2.27	102.75	114.54
20	A	607	PGV	C8-C9-C10	-2.26	104.58	113.79
26	P	306	CDL	C54-C53-C52	-2.25	102.86	114.54
28	E	201	PSC	C03-C02-C01	-2.24	106.86	112.08
26	T	101	CDL	OB8-CB7-OB9	-2.23	117.67	123.51
21	L	101	TGL	CA5-CA4-CA3	-2.22	103.00	114.54
24	P	307	CHD	C5-C4-C3	-2.22	109.59	112.88
20	P	305	PGV	O04-C19-C20	-2.22	115.27	123.76
21	L	101	TGL	CC4-CC3-CC2	-2.20	105.14	113.30
21	B	301	TGL	OG3-CC1-OC1	-2.18	117.80	123.51
26	T	101	CDL	OB7-CB5-C51	-2.17	115.44	123.76
18	N	606	HEA	CAA-CBA-CGA	-2.17	108.55	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	103	CHD	C1-C10-C9	-2.16	108.00	111.43
20	P	304	PGV	C22-C21-C20	-2.14	105.39	113.30
28	V	101	PSC	C29-C28-C27	-2.13	103.47	114.54
24	C	301	CHD	C13-C14-C8	-2.11	111.96	114.73
18	N	605[A]	HEA	C13-C14-C15	-2.11	123.11	127.75
18	N	605[B]	HEA	C13-C14-C15	-2.11	123.11	127.75
24	P	307	CHD	C21-C20-C22	-2.10	106.91	110.33
21	L	101	TGL	OC1-CC1-CC2	-2.10	115.73	123.76
20	N	612	PGV	O01-C1-O02	-2.10	117.97	123.67
24	P	307	CHD	O3-C3-C4	-2.09	105.63	109.86
21	B	301	TGL	OG1-CA1-OA1	-2.09	118.04	123.51
31	I	201	HEM	C3C-C4C-NC	-2.08	107.02	110.94
20	P	304	PGV	O01-C1-O02	-2.06	118.06	123.67
24	W	101	CHD	C19-C10-C5	-2.06	106.63	110.28
30	Z	101	DMU	O55-C2-C1	-2.06	105.72	110.36
24	T	103	CHD	C13-C14-C8	-2.05	112.03	114.73
18	N	605[A]	HEA	CMB-C2B-C1B	-2.05	124.83	128.31
18	N	605[B]	HEA	CMB-C2B-C1B	-2.05	124.83	128.31
26	G	101	CDL	CB6-CB4-CB3	-2.01	107.39	112.08
24	G	102	CHD	C15-C14-C13	2.01	105.52	103.59
21	B	301	TGL	C10-CB9-CB8	2.01	124.98	114.54
24	P	301	CHD	C17-C13-C12	2.01	119.44	117.68
18	A	604[B]	HEA	C26-C15-C14	2.03	127.52	123.58
18	A	604[A]	HEA	C26-C15-C14	2.03	127.52	123.58
21	N	608	TGL	C10-CB9-CB8	2.03	125.10	114.54
21	D	201	TGL	CG1-OG1-CA1	2.04	123.08	117.00
26	G	101	CDL	C82-C81-C80	2.04	125.15	114.54
24	C	307	CHD	C5-C4-C3	2.05	115.92	112.88
26	T	101	CDL	C83-C82-C81	2.06	125.23	114.54
26	P	306	CDL	C82-C81-C80	2.06	125.24	114.54
26	C	306	CDL	C40-C39-C38	2.07	125.28	114.54
24	C	307	CHD	C2-C1-C10	2.08	116.53	112.81
18	N	605[B]	HEA	C25-C23-C24	2.08	119.66	114.61
18	A	605	HEA	C3C-C4C-NC	2.08	111.90	109.21
18	N	606	HEA	C3C-C4C-NC	2.09	111.91	109.21
26	C	306	CDL	C39-C38-C37	2.09	125.40	114.54
26	C	306	CDL	C83-C82-C81	2.10	125.44	114.54
20	N	612	PGV	O01-C1-C2	2.11	115.98	111.53
30	M	101	DMU	O16-C6-C1	2.11	110.60	108.00
24	G	102	CHD	C18-C13-C14	2.12	114.55	111.20
21	Q	201	TGL	C21-C20-CA9	2.13	125.60	114.54
30	Z	101	DMU	C7-C8-C9	2.14	114.05	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	201	TGL	C21-C20-CA9	2.14	125.66	114.54
26	P	306	CDL	CB6-OB8-CB7	2.14	123.38	117.00
25	C	303	PEK	O13-P-O14	2.16	123.79	112.56
24	P	301	CHD	C23-C22-C20	2.18	117.48	114.79
24	C	307	CHD	C16-C17-C20	2.18	115.60	112.12
26	G	101	CDL	C60-C59-C58	2.18	125.86	114.54
28	E	201	PSC	C02-O01-C1	2.19	123.32	117.91
26	T	101	CDL	OA6-CA4-CA6	2.20	116.08	108.36
18	A	604[B]	HEA	CMC-C2C-C3C	2.20	129.40	125.09
18	A	604[A]	HEA	CMC-C2C-C3C	2.20	129.40	125.09
24	G	102	CHD	C2-C1-C10	2.20	116.76	112.81
24	P	301	CHD	C18-C13-C14	2.24	114.73	111.20
21	L	101	TGL	OG3-CG3-CG2	2.25	114.79	108.70
20	C	305	PGV	O01-C02-C01	2.27	116.34	108.36
30	Z	101	DMU	O5-C4-C57	2.27	112.26	106.38
24	J	101	CHD	C11-C12-C13	2.28	113.52	111.22
20	P	304	PGV	O14-P-O13	2.29	124.45	112.56
20	A	608	PGV	O14-P-O13	2.29	124.45	112.56
20	P	304	PGV	C02-O01-C1	2.29	123.57	117.91
18	N	605[A]	HEA	C21-C20-C19	2.29	120.19	112.61
21	Q	201	TGL	C11-C10-CB9	2.29	126.44	114.54
24	G	102	CHD	C1-C10-C5	2.29	110.29	107.76
24	T	103	CHD	C6-C7-C8	2.29	113.89	111.46
26	T	101	CDL	C82-C81-C80	2.31	126.56	114.54
24	W	101	CHD	C18-C13-C17	2.32	114.86	111.20
21	D	201	TGL	OG3-CG3-CG2	2.33	115.00	108.70
24	C	301	CHD	C16-C17-C13	2.35	105.86	103.59
30	Z	101	DMU	C1-C2-C3	2.36	114.84	109.63
30	M	101	DMU	O4-C7-C5	2.36	115.69	110.36
20	A	608	PGV	O03-C01-C02	2.37	115.11	108.70
25	P	303	PEK	C01-O03-C21	2.40	124.14	117.00
24	C	301	CHD	C1-C10-C5	2.41	110.42	107.76
24	W	101	CHD	C9-C10-C5	2.41	112.11	108.68
30	Z	101	DMU	O1-C9-C11	2.42	112.64	106.38
24	W	101	CHD	C2-C1-C10	2.44	117.18	112.81
20	C	305	PGV	O03-C01-C02	2.44	115.29	108.70
24	T	103	CHD	C9-C10-C5	2.45	112.17	108.68
24	P	307	CHD	C15-C14-C13	2.46	105.96	103.59
31	1	201	HEM	CMC-C2C-C3C	2.47	129.91	125.09
28	E	201	PSC	O01-C02-C03	2.47	117.03	108.36
26	G	101	CDL	C83-C82-C81	2.47	127.36	114.54
20	A	607	PGV	O01-C1-C2	2.48	116.74	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	608	TGL	OG1-CG1-CG2	2.48	115.39	108.70
18	A	604[B]	HEA	C3C-C4C-NC	2.48	112.42	109.21
18	A	604[A]	HEA	C3C-C4C-NC	2.48	112.42	109.21
18	N	605[A]	HEA	CBA-CAA-C2A	2.48	116.82	112.47
18	N	605[B]	HEA	CBA-CAA-C2A	2.48	116.82	112.47
21	L	101	TGL	C11-C10-CB9	2.48	127.43	114.54
24	P	307	CHD	C4-C3-C2	2.49	113.72	110.53
21	L	101	TGL	OG2-CG2-CG3	2.50	117.16	108.36
24	C	301	CHD	C18-C13-C12	2.51	111.60	109.09
24	J	101	CHD	C15-C14-C8	2.52	122.07	118.34
26	G	101	CDL	CB4-OB6-CB5	2.53	124.17	117.91
20	P	305	PGV	O03-C01-C02	2.58	115.66	108.70
24	C	307	CHD	O7-C7-C8	2.62	115.25	109.28
24	G	102	CHD	C1-C2-C3	2.63	113.91	110.41
26	G	101	CDL	OA8-CA7-C31	2.64	119.96	111.85
18	A	604[A]	HEA	C16-C17-C18	2.65	118.57	111.61
26	G	101	CDL	CA6-OA8-CA7	2.67	124.95	117.00
24	C	301	CHD	C11-C12-C13	2.69	113.94	111.22
20	C	304	PGV	O03-C19-C20	2.70	120.15	111.85
26	C	306	CDL	OA8-CA7-C31	2.70	120.17	111.85
18	N	605[A]	HEA	CMB-C2B-C3B	2.70	130.67	125.14
18	N	605[B]	HEA	CMB-C2B-C3B	2.70	130.67	125.14
28	E	201	PSC	O03-C19-C20	2.73	120.24	111.85
18	N	605[B]	HEA	C17-C18-C19	2.73	133.76	127.75
18	N	606	HEA	C16-C15-C14	2.75	126.11	120.98
24	W	101	CHD	C11-C12-C13	2.76	114.01	111.22
18	N	606	HEA	C16-C17-C18	2.77	118.88	111.61
18	N	605[A]	HEA	C26-C15-C16	2.77	119.59	115.37
18	N	605[B]	HEA	C26-C15-C16	2.77	119.59	115.37
24	T	103	CHD	C14-C13-C12	2.82	109.92	107.37
24	C	307	CHD	C16-C17-C13	2.83	106.31	103.59
26	C	306	CDL	OB6-CB5-C51	2.83	117.48	111.53
26	G	101	CDL	OB8-CB7-C71	2.83	120.56	111.85
26	P	306	CDL	OA8-CA7-C31	2.84	120.60	111.85
21	L	101	TGL	OG1-CA1-CA2	2.85	120.63	111.85
20	A	607	PGV	O03-C19-C20	2.88	120.72	111.85
24	C	307	CHD	C18-C13-C12	2.91	112.00	109.09
26	P	306	CDL	CA6-OA8-CA7	2.93	125.72	117.00
26	T	101	CDL	OB8-CB6-CB4	2.98	116.75	108.70
21	L	101	TGL	OG1-CG1-CG2	2.99	116.76	108.70
26	P	306	CDL	OB6-CB5-C51	2.99	117.82	111.53
24	J	101	CHD	C1-C2-C3	3.01	114.41	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	304	PGV	O01-C1-C2	3.03	117.90	111.53
25	P	303	PEK	C2-C3-C4	3.03	119.21	113.65
25	C	303	PEK	O01-C1-C2	3.03	117.92	111.53
25	P	303	PEK	O01-C1-C2	3.04	117.94	111.53
24	P	301	CHD	C11-C12-C13	3.05	114.30	111.22
24	T	103	CHD	C4-C3-C2	3.08	114.47	110.53
24	C	301	CHD	C11-C9-C8	3.09	115.22	110.77
24	P	301	CHD	C6-C7-C8	3.09	114.74	111.46
20	A	608	PGV	O03-C19-C20	3.11	121.41	111.85
24	J	101	CHD	C10-C9-C8	3.12	115.23	111.86
26	T	101	CDL	OA8-CA6-CA4	3.16	117.22	108.70
21	Q	201	TGL	OG1-CG1-CG2	3.17	117.25	108.70
20	C	305	PGV	C02-O01-C1	3.17	125.75	117.91
24	T	103	CHD	C9-C8-C7	3.19	115.75	111.89
21	Q	201	TGL	OG2-CB1-CB2	3.24	118.34	111.53
24	J	101	CHD	C4-C3-C2	3.24	114.67	110.53
21	D	201	TGL	OG1-CA1-CA2	3.25	121.86	111.85
24	T	103	CHD	C1-C10-C5	3.25	111.35	107.76
18	N	605[B]	HEA	C27-C19-C20	3.26	120.34	115.37
21	N	608	TGL	OG2-CG2-CG1	3.27	119.86	108.36
18	N	605[A]	HEA	C3C-C4C-NC	3.27	113.44	109.21
18	N	605[B]	HEA	C3C-C4C-NC	3.27	113.44	109.21
24	W	101	CHD	C6-C5-C10	3.29	116.19	112.66
24	C	307	CHD	C14-C8-C7	3.29	116.48	111.77
21	L	101	TGL	CG2-OG2-CB1	3.30	126.07	117.91
26	P	306	CDL	OA6-CA5-C11	3.33	118.54	111.53
21	D	201	TGL	OG3-CC1-CC2	3.33	122.11	111.85
24	W	101	CHD	C4-C5-C10	3.34	116.24	112.66
20	P	304	PGV	O01-C1-C2	3.34	118.56	111.53
24	P	307	CHD	O7-C7-C8	3.34	116.89	109.28
21	D	201	TGL	OG1-CG1-CG2	3.35	117.75	108.70
21	B	301	TGL	OG3-CC1-CC2	3.36	122.20	111.85
24	T	103	CHD	C15-C14-C13	3.39	106.85	103.59
24	C	307	CHD	C9-C10-C5	3.39	113.50	108.68
18	A	604[A]	HEA	C21-C20-C19	3.40	123.87	112.61
20	A	607	PGV	C01-O03-C19	3.41	127.17	117.00
24	J	101	CHD	C14-C8-C7	3.43	116.67	111.77
21	N	608	TGL	OG3-CG3-CG2	3.43	117.95	108.70
24	W	101	CHD	C10-C9-C8	3.44	115.58	111.86
18	N	606	HEA	C27-C19-C20	3.48	120.68	115.37
24	P	307	CHD	C15-C14-C8	3.48	123.50	118.34
18	A	605	HEA	CMC-C2C-C3C	3.60	132.12	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	201	TGL	OG3-CC1-CC2	3.62	123.00	111.85
24	C	307	CHD	C1-C2-C3	3.63	115.24	110.41
20	A	608	PGV	O01-C1-C2	3.63	119.19	111.53
21	Q	201	TGL	OG1-CA1-CA2	3.64	123.04	111.85
24	C	307	CHD	C21-C20-C17	3.66	118.63	112.99
26	T	101	CDL	OA8-CA7-C31	3.67	123.14	111.85
24	J	101	CHD	C1-C10-C5	3.71	111.84	107.76
24	P	307	CHD	C14-C8-C7	3.71	117.08	111.77
21	N	608	TGL	OG2-CG2-CG3	3.73	121.47	108.36
21	L	101	TGL	CG3-OG3-CC1	3.74	128.15	117.00
24	J	101	CHD	C15-C14-C13	3.75	107.20	103.59
24	J	101	CHD	C16-C17-C20	3.84	118.26	112.12
26	P	306	CDL	OB8-CB7-C71	3.85	123.70	111.85
30	M	101	DMU	O1-C9-C11	3.87	116.42	106.38
21	B	301	TGL	OG1-CA1-CA2	3.88	123.80	111.85
26	T	101	CDL	CA4-OA6-CA5	3.94	127.65	117.91
20	C	305	PGV	O03-C19-C20	3.94	123.98	111.85
26	C	306	CDL	OB8-CB7-C71	3.95	124.01	111.85
26	C	306	CDL	CA6-OA8-CA7	3.95	128.77	117.00
24	C	307	CHD	C15-C14-C13	3.99	107.43	103.59
30	M	101	DMU	O3-C5-C7	4.01	119.40	110.36
24	P	307	CHD	C4-C5-C10	4.02	116.97	112.66
21	L	101	TGL	OG3-CC1-CC2	4.02	124.22	111.85
26	G	101	CDL	CB6-OB8-CB7	4.02	128.98	117.00
24	W	101	CHD	C6-C7-C8	4.03	115.73	111.46
18	A	604[B]	HEA	C27-C19-C20	4.09	121.60	115.37
26	G	101	CDL	OA6-CA5-C11	4.12	120.22	111.53
25	C	303	PEK	C01-O03-C21	4.15	129.37	117.00
24	P	301	CHD	C1-C10-C5	4.16	112.34	107.76
24	P	307	CHD	C16-C17-C13	4.16	107.59	103.59
18	A	604[A]	HEA	C27-C19-C20	4.37	122.03	115.37
20	C	305	PGV	C01-O03-C19	4.50	130.41	117.00
20	N	612	PGV	O03-C19-C20	4.62	126.07	111.85
24	P	301	CHD	C15-C14-C13	4.73	108.15	103.59
26	C	306	CDL	OA6-CA5-C11	4.84	121.72	111.53
24	W	101	CHD	C14-C8-C7	4.91	118.80	111.77
24	C	307	CHD	C11-C9-C10	5.14	119.11	113.77
24	J	101	CHD	C22-C20-C17	5.14	121.07	110.24
20	P	305	PGV	O03-C19-C20	5.15	127.70	111.85
28	V	101	PSC	O01-C1-C2	5.17	122.42	111.53
20	C	305	PGV	O01-C1-C2	5.20	122.49	111.53
21	N	608	TGL	OG2-CB1-CB2	5.21	122.50	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	608	TGL	OG1-CA1-CA2	5.31	128.20	111.85
26	T	101	CDL	OA6-CA5-C11	5.35	122.80	111.53
21	B	301	TGL	OG2-CB1-CB2	5.39	122.89	111.53
21	N	608	TGL	CG3-OG3-CC1	5.42	133.13	117.00
24	J	101	CHD	C13-C17-C20	5.49	126.13	119.44
24	P	307	CHD	C10-C9-C8	5.53	117.84	111.86
20	P	305	PGV	O01-C1-C2	5.57	123.26	111.53
26	G	101	CDL	OB6-CB5-C51	5.59	123.30	111.53
21	B	301	TGL	OG2-CG2-CG1	5.66	128.27	108.36
24	P	307	CHD	C9-C10-C5	5.70	116.79	108.68
24	C	301	CHD	C15-C14-C13	5.75	109.13	103.59
24	W	101	CHD	C15-C14-C8	5.88	127.05	118.34
24	C	307	CHD	C11-C12-C13	5.89	117.16	111.22
21	L	101	TGL	OG2-CB1-CB2	5.91	123.98	111.53
21	N	608	TGL	OG3-CC1-CC2	6.00	130.33	111.85
24	C	307	CHD	C15-C14-C8	6.05	127.30	118.34
26	T	101	CDL	OB6-CB5-C51	6.09	124.36	111.53
21	N	608	TGL	CG2-OG2-CB1	6.52	134.03	117.91
28	E	201	PSC	O01-C1-C2	6.56	125.35	111.53
21	D	201	TGL	OG2-CB1-CB2	6.66	125.56	111.53
21	B	301	TGL	CG2-OG2-CB1	6.66	134.38	117.91
24	G	102	CHD	C6-C7-C8	6.86	118.73	111.46
24	C	307	CHD	C4-C5-C10	7.15	120.33	112.66
21	B	301	TGL	CG3-OG3-CC1	7.21	138.47	117.00
24	W	101	CHD	C13-C17-C20	7.38	128.43	119.44
24	W	101	CHD	C1-C10-C5	7.81	116.36	107.76
24	W	101	CHD	C17-C13-C12	10.22	126.64	117.68
24	C	307	CHD	C10-C9-C8	10.26	122.96	111.86

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	606	HEA	ND
18	N	606	HEA	NB
18	A	605	HEA	ND
18	A	605	HEA	NB

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	CG2-OG2-CB1-CB2

There are no ring outliers.

38 monomers are involved in 249 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	1	201	HEM	5	0
31	2	201	HEM	3	0
18	A	604[B]	HEA	6	0
18	A	605	HEA	3	0
20	A	607	PGV	5	0
20	A	608	PGV	4	0
21	B	301	TGL	6	0
24	C	301	CHD	1	0
25	C	303	PEK	7	0
20	C	304	PGV	5	0
20	C	305	PGV	9	0
26	C	306	CDL	15	0
24	C	307	CHD	3	0
21	D	201	TGL	12	0
28	E	201	PSC	19	0
23	E	202	EDO	1	0
26	G	101	CDL	23	0
24	J	101	CHD	5	0
21	L	101	TGL	20	0
30	M	101	DMU	1	0
18	N	605[A]	HEA	1	0
18	N	605[B]	HEA	6	0
18	N	606	HEA	3	0
19	N	607	PER	1	0
21	N	608	TGL	2	0
20	N	612	PGV	1	0
24	P	301	CHD	1	0
25	P	303	PEK	3	0
20	P	304	PGV	6	0
20	P	305	PGV	4	0
26	P	306	CDL	12	0
24	P	307	CHD	1	0
21	Q	201	TGL	10	0
26	T	101	CDL	24	0
24	T	103	CHD	1	0
28	V	101	PSC	21	0
24	W	101	CHD	5	0
30	Z	101	DMU	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.21	20 (3%) 43 45	22, 30, 39, 74	0
1	N	513/514 (99%)	0.22	26 (5%) 32 33	27, 36, 48, 71	0
2	B	226/227 (99%)	-0.34	2 (0%) 85 86	26, 35, 59, 109	0
2	O	226/227 (99%)	-0.15	2 (0%) 85 86	34, 49, 78, 98	0
3	C	259/259 (100%)	-0.54	2 (0%) 87 88	26, 35, 48, 83	0
3	P	259/259 (100%)	-0.55	4 (1%) 76 77	28, 38, 52, 87	0
4	D	144/144 (100%)	-0.54	6 (4%) 40 41	30, 38, 63, 144	0
4	Q	144/144 (100%)	0.16	13 (9%) 12 12	32, 50, 81, 139	0
5	E	105/105 (100%)	-0.41	2 (1%) 70 70	30, 38, 62, 134	0
5	R	105/105 (100%)	-0.61	1 (0%) 84 84	33, 41, 62, 123	0
6	F	98/98 (100%)	-0.05	8 (8%) 14 15	30, 40, 95, 141	0
6	S	98/98 (100%)	0.25	8 (8%) 14 15	32, 45, 106, 141	0
7	G	83/84 (98%)	0.56	15 (18%) 2 2	34, 44, 116, 138	0
7	T	83/84 (98%)	0.80	17 (20%) 1 1	31, 47, 111, 136	0
8	H	79/79 (100%)	-0.11	7 (8%) 12 13	33, 43, 90, 106	0
8	U	79/79 (100%)	-0.17	2 (2%) 61 61	38, 49, 69, 137	0
9	I	72/73 (98%)	-0.15	3 (4%) 40 41	33, 46, 66, 79	0
9	V	72/73 (98%)	0.99	11 (15%) 3 3	36, 63, 85, 111	0
10	J	58/58 (100%)	0.36	7 (12%) 6 6	36, 46, 75, 135	0
10	W	58/58 (100%)	0.72	8 (13%) 4 4	39, 53, 84, 144	0
11	K	49/49 (100%)	-0.15	3 (6%) 25 26	35, 42, 58, 70	0
11	X	49/49 (100%)	0.61	4 (8%) 14 15	47, 58, 77, 78	0
12	L	46/46 (100%)	-0.53	1 (2%) 65 66	30, 38, 59, 104	0
12	Y	46/46 (100%)	-0.51	1 (2%) 65 66	36, 46, 69, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	-0.21	2 (4%) 35 37	32, 40, 79, 127	0
13	Z	43/43 (100%)	-0.05	3 (6%) 19 21	36, 50, 81, 108	0
14	1	104/105 (99%)	2.81	65 (62%) 0 1	45, 90, 118, 125	0
14	2	104/105 (99%)	4.61	79 (75%) 0 1	67, 115, 139, 147	0
All	All	3758/3768 (99%)	0.17	322 (8%) 13 14	22, 40, 98, 147	0

All (322) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	13.6
4	Q	7	LYS	13.4
6	S	1	ALA	13.2
10	W	57	HIS	12.5
14	2	57	ILE	12.1
14	2	35	LEU	11.9
6	S	98	HIS	11.7
14	2	58	THR	11.3
6	F	1	ALA	10.7
10	J	58	LYS	10.5
14	2	36	PHE	10.4
10	J	57	HIS	10.3
6	S	97	ALA	10.3
14	2	32	LEU	10.2
6	S	96	LEU	10.1
14	2	95	ILE	9.8
4	Q	6	VAL	9.5
14	2	59	TRP	9.3
6	F	98	HIS	9.2
14	2	40	THR	9.0
9	V	30	GLY	8.8
14	2	43	ALA	8.6
14	2	22	LYS	8.5
7	T	10	GLY	8.5
6	F	97	ALA	8.3
14	2	64	LEU	8.3
14	2	46	PHE	8.2
5	E	5	HIS	8.2
14	2	33	HIS	7.9
14	2	38	ARG	7.9
14	2	74	TYR	7.8
7	G	3	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
14	2	103	ASN	7.5
14	1	37	GLY	7.5
14	2	76	PRO	7.5
4	D	5	VAL	7.5
14	2	104	GLU	7.4
8	U	8	ILE	7.3
14	2	45	GLY	7.2
14	2	39	LYS	7.2
6	S	94	HIS	7.1
14	2	75	ILE	7.0
14	1	43	ALA	7.0
14	2	1	GLY	7.0
14	1	102	THR	7.0
14	1	34	GLY	6.9
14	2	42	GLN	6.6
14	2	77	GLY	6.6
13	M	43	SER	6.5
14	2	21	GLU	6.5
14	1	101	ALA	6.5
14	2	67	TYR	6.4
7	T	40	GLY	6.4
6	S	2	SER	6.4
7	G	40	GLY	6.4
8	U	7	LYS	6.3
10	W	58	LYS	6.2
14	2	102	THR	6.2
14	1	58	THR	6.2
14	1	42	GLN	6.1
7	T	42	ARG	6.1
14	2	98	LEU	6.1
14	1	36	PHE	6.1
14	1	95	ILE	6.1
7	G	10	GLY	6.1
14	2	101	ALA	6.0
14	2	19	THR	6.0
14	2	37	GLY	6.0
14	1	57	ILE	6.0
14	1	53	LYS	5.9
14	2	23	GLY	5.8
14	2	61	GLU	5.8
14	2	55	LYS	5.8
14	2	3	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
14	1	47	THR	5.7
14	2	97	TYR	5.7
14	2	20	VAL	5.7
5	R	5	HIS	5.7
14	2	96	ALA	5.6
9	V	33	THR	5.6
4	Q	4	SER	5.6
4	D	4	SER	5.6
14	1	74	TYR	5.5
7	G	36	TRP	5.5
4	D	7	LYS	5.4
14	2	34	GLY	5.4
7	G	39	SER	5.4
14	2	44	PRO	5.3
14	2	99	LYS	5.3
14	2	63	THR	5.3
14	1	24	GLY	5.3
14	2	24	GLY	5.2
14	1	41	GLY	5.2
14	2	18	HIS	5.2
14	2	56	GLY	5.2
14	2	68	LEU	5.2
9	V	2	THR	5.1
7	G	2	SER	5.1
14	1	98	LEU	5.1
6	F	2	SER	5.1
14	2	28	THR	5.1
14	2	60	LYS	5.1
14	2	78	THR	5.1
14	1	99	LYS	5.0
14	1	46	PHE	4.9
4	Q	8	SER	4.9
14	1	35	LEU	4.9
14	1	40	THR	4.9
8	H	48	GLY	4.8
14	1	3	VAL	4.8
14	1	33	HIS	4.8
14	2	25	LYS	4.8
14	2	54	ASN	4.7
7	T	36	TRP	4.7
14	1	32	LEU	4.7
14	1	59	TRP	4.7

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Mol	Chain	Res	Type	RSRZ
6	F	96	LEU	4.6
4	Q	147	LYS	4.6
7	T	84	LYS	4.6
8	H	45	ALA	4.6
14	1	44	PRO	4.6
7	G	9	GLY	4.6
14	2	48	TYR	4.6
7	T	37	LEU	4.5
14	2	71	PRO	4.5
7	G	5	LYS	4.5
14	2	62	GLU	4.5
7	G	41	HIS	4.5
14	2	65	MET	4.5
14	2	26	HIS	4.5
14	1	39	LYS	4.4
10	W	55	PHE	4.4
14	1	54	ASN	4.4
7	T	41	HIS	4.4
14	1	96	ALA	4.4
10	W	1	PHE	4.3
14	1	50	ASP	4.3
7	T	2	SER	4.3
2	O	227	LEU	4.3
14	1	68	LEU	4.2
14	1	62	GLU	4.2
4	D	6	VAL	4.2
14	2	41	GLY	4.2
9	V	32	ALA	4.1
14	1	48	TYR	4.1
10	J	1	PHE	4.1
12	Y	47	LYS	4.1
14	1	51	ALA	4.1
7	T	39	SER	4.1
14	2	47	THR	4.1
9	I	37	PHE	4.1
9	I	30	GLY	4.1
2	B	59	GLN	4.0
14	1	25	LYS	4.0
14	1	38	ARG	4.0
10	W	48	TYR	4.0
14	1	104	GLU	4.0
14	1	1	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
14	2	4	GLU	3.9
8	H	49	ASP	3.9
14	1	49	THR	3.8
10	J	56	PRO	3.8
6	F	95	GLN	3.8
14	2	94	LEU	3.8
14	2	30	PRO	3.7
14	2	100	LYS	3.7
9	V	37	PHE	3.7
14	2	49	THR	3.7
14	2	15	ALA	3.7
6	S	93	PRO	3.7
14	2	72	LYS	3.7
4	Q	102	TYR	3.7
7	G	42	ARG	3.7
9	V	34	PHE	3.7
4	Q	101	HIS	3.6
7	T	38	HIS	3.6
2	O	113	TYR	3.6
14	1	23	GLY	3.6
14	1	56	GLY	3.6
14	2	29	GLY	3.6
3	P	3	HIS	3.5
14	1	64	LEU	3.5
11	K	7	PRO	3.5
14	2	52	ASN	3.4
14	2	66	GLU	3.4
14	1	103	ASN	3.4
1	A	113[A]	LEU	3.4
14	1	100	LYS	3.4
14	2	2	ASP	3.3
7	T	9	GLY	3.3
14	2	31	ASN	3.3
13	Z	42	LYS	3.3
1	N	199	LEU	3.3
7	G	84	LYS	3.2
8	H	8	ILE	3.2
14	1	63	THR	3.2
14	1	60	LYS	3.2
7	G	4	ALA	3.1
14	2	53	LYS	3.1
6	S	95	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
13	Z	35	TYR	3.1
6	F	94	HIS	3.1
1	A	73	ILE	3.1
10	W	56	PRO	3.0
14	1	55	LYS	3.0
7	T	3	ALA	3.0
14	1	61	GLU	3.0
1	N	374	VAL	3.0
12	L	47	LYS	3.0
7	T	8	HIS	2.9
7	T	43	GLU	2.9
4	Q	140	TYR	2.9
8	H	47	GLY	2.9
14	1	52	ASN	2.9
9	I	33	THR	2.8
14	1	97	TYR	2.8
13	Z	43	SER	2.8
14	1	45	GLY	2.8
5	E	109	VAL	2.8
10	W	52	TRP	2.8
14	2	73	LYS	2.8
14	1	22	LYS	2.8
14	1	26	HIS	2.8
2	B	58	ALA	2.7
11	X	6	ALA	2.7
14	2	10	PHE	2.7
7	G	38	HIS	2.7
14	2	88	LYS	2.7
14	1	66	GLU	2.7
9	V	53	ASN	2.7
14	1	65	MET	2.7
1	N	373	VAL	2.6
14	1	2	ASP	2.6
7	G	37	LEU	2.6
8	H	46	LYS	2.6
7	T	4	ALA	2.6
10	J	2	GLU	2.6
14	2	79	LYS	2.6
4	Q	87	PHE	2.6
8	H	43	MET	2.5
14	1	4	GLU	2.5
1	N	377	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
4	Q	138	TRP	2.5
7	G	1	ALA	2.5
10	W	4	ARG	2.5
1	N	63	PHE	2.5
11	X	27	ALA	2.4
14	1	89	THR	2.4
1	N	246	LEU	2.4
1	A	386	VAL	2.4
1	A	82	LEU	2.4
1	N	66	ILE	2.4
14	1	67	TYR	2.4
3	C	37	PHE	2.4
1	A	70	VAL	2.4
14	2	92	GLU	2.4
9	V	42	LYS	2.4
1	N	126	TRP	2.4
14	1	93	ASP	2.4
9	V	65	LYS	2.3
1	N	127	THR	2.3
1	N	238	PHE	2.3
3	P	41	THR	2.3
6	F	3	GLY	2.3
1	A	199	LEU	2.3
3	P	38	ASN	2.3
14	1	6	GLY	2.3
1	N	202	LEU	2.2
13	M	42	LYS	2.2
11	X	23	THR	2.2
14	2	50	ASP	2.2
1	A	247	ILE	2.2
1	N	245	ILE	2.2
3	P	40	MET	2.2
1	N	247	ILE	2.2
9	V	36	LYS	2.2
1	A	245	ILE	2.2
1	A	196	LEU	2.2
1	A	78	PHE	2.2
1	N	128	VAL	2.2
1	N	372	TYR	2.2
9	V	31	PHE	2.2
14	1	20	VAL	2.2
14	2	91	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
14	2	69	GLU	2.2
1	A	150	LEU	2.2
1	A	197	LEU	2.2
1	A	389	ILE	2.1
1	A	74	MET	2.1
14	1	88	LYS	2.1
1	A	195	LEU	2.1
1	N	150	LEU	2.1
10	J	55	PHE	2.1
4	Q	141	ASP	2.1
1	A	188	VAL	2.1
1	A	190	ILE	2.1
3	C	261	SER	2.1
4	Q	46	ALA	2.1
1	N	206	ILE	2.1
1	N	113[A]	LEU	2.1
1	N	248	LEU	2.1
11	K	6	ALA	2.1
1	N	251	PHE	2.1
7	T	5	LYS	2.1
10	J	48	TYR	2.1
1	A	72	PRO	2.0
7	T	33	LEU	2.0
1	A	388	ALA	2.0
11	X	34	THR	2.0
14	1	92	GLU	2.0
1	N	190	ILE	2.0
14	1	94	LEU	2.0
1	N	370	THR	2.0
1	N	243	VAL	2.0
1	N	244	TYR	2.0
4	D	8	SER	2.0
14	1	79	LYS	2.0
1	N	191	THR	2.0
1	N	389	ILE	2.0
11	K	23	THR	2.0
1	A	193	VAL	2.0
4	D	147	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	FME	N	1	10/11	0.96	0.17	-	43,61,73,95	0
7	TPO	T	11	11/12	0.45	0.34	-	85,109,117,125	0
7	TPO	G	11	11/12	0.50	0.33	-	81,97,160,160	0
1	FME	A	1	10/11	0.95	0.13	-	40,52,71,88	0
9	SAC	I	1	9/10	0.75	0.39	-	98,106,110,119	0
2	FME	O	1	10/11	0.98	0.14	-	49,56,65,78	0
9	SAC	V	1	9/10	0.31	0.91	-	131,137,150,153	0
2	FME	B	1	10/11	0.98	0.10	-	30,35,39,51	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	UNL	Y	101	10/-	0.78	0.39	8.44	69,76,86,94	0
24	CHD	J	101	29/29	0.84	0.33	7.80	61,75,106,109	0
27	UNL	J	102	10/-	0.73	0.29	7.36	61,65,77,92	0
26	CDL	P	306	100/100	0.79	0.27	6.77	49,97,149,159	0
24	CHD	W	101	29/29	0.70	0.43	6.71	73,114,126,130	0
27	UNL	L	102	10/-	0.80	0.27	6.68	61,75,82,86	0
20	PGV	A	607	51/51	0.77	0.30	6.28	44,84,151,159	0
27	UNL	P	310	7/-	0.84	0.27	6.24	53,60,76,88	0
26	CDL	C	306	100/100	0.83	0.23	5.11	51,86,124,152	0
27	UNL	C	310	7/-	0.79	0.34	5.11	41,64,76,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	TGL	Q	201	63/63	0.74	0.21	4.63	52,82,104,109	0
16	MG	A	602	1/1	0.95	0.21	3.83	36,36,36,36	0
27	UNL	C	308	18/-	0.85	0.20	3.81	55,66,77,81	0
27	UNL	N	609	16/-	0.77	0.32	3.80	54,59,79,85	0
20	PGV	C	305	51/51	0.74	0.25	3.41	55,80,122,138	0
21	TGL	D	201	63/63	0.76	0.22	3.36	47,70,101,105	0
26	CDL	T	101	100/100	0.73	0.25	3.21	61,95,153,161	0
27	UNL	P	308	20/-	0.86	0.20	3.03	58,64,72,73	0
21	TGL	B	301	63/63	0.90	0.18	2.54	33,68,103,114	0
30	DMU	Z	101	33/33	0.77	0.30	2.54	55,76,107,113	0
21	TGL	L	101	63/63	0.78	0.26	2.48	45,70,98,107	0
26	CDL	G	101	100/100	0.66	0.30	2.47	58,103,158,163	0
27	UNL	N	610	18/-	0.85	0.19	2.43	51,59,69,70	0
23	EDO	N	613	4/4	0.98	0.16	2.42	38,38,39,41	0
16	MG	N	603	1/1	0.96	0.25	2.38	42,42,42,42	0
21	TGL	N	608	63/63	0.83	0.19	2.28	51,73,104,115	0
27	UNL	N	601	17/-	0.76	0.18	2.23	52,60,83,85	0
20	PGV	P	305	51/51	0.73	0.23	2.21	54,86,135,150	0
24	CHD	P	307	29/29	0.89	0.29	2.08	71,80,88,95	0
27	UNL	P	309	16/-	0.68	0.17	1.99	70,79,89,95	0
23	EDO	F	102	4/4	0.97	0.14	1.93	45,47,49,49	0
27	UNL	W	102	9/-	0.78	0.24	1.79	59,62,79,82	0
23	EDO	N	614	4/4	0.94	0.16	1.78	56,59,63,85	0
20	PGV	P	304	51/51	0.95	0.13	1.78	30,46,73,76	0
29	ZN	F	101	1/1	1.00	0.10	1.71	36,36,36,36	0
27	UNL	C	309	17/-	0.77	0.16	1.68	60,71,87,90	0
24	CHD	C	307	29/29	0.82	0.26	1.47	73,85,93,99	0
28	PSC	V	101	52/52	0.82	0.23	1.44	49,77,145,166	0
30	DMU	M	101	33/33	0.92	0.14	1.41	40,46,62,65	0
28	PSC	E	201	52/52	0.76	0.26	1.29	50,79,162,163	0
27	UNL	N	611	12/-	0.84	0.15	1.24	48,56,68,69	0
20	PGV	C	304	51/51	0.96	0.12	1.23	31,38,95,103	0
23	EDO	B	303	4/4	0.98	0.13	1.19	30,31,33,36	0
25	PEK	C	303	53/53	0.93	0.16	1.04	34,48,88,97	0
20	PGV	N	612	51/51	0.97	0.15	0.99	33,43,70,80	0
23	EDO	I	101	4/4	0.83	0.14	0.79	55,59,63,72	0
20	PGV	A	608	51/51	0.97	0.15	0.70	29,41,68,74	0
27	UNL	T	102	18/-	0.76	0.18	0.54	47,66,85,92	0
24	CHD	P	301	29/29	0.91	0.12	0.31	40,45,52,55	0
18	HEA	N	606	60/60	0.99	0.19	0.29	27,33,41,47	0
18	HEA	N	605[A]	60/60	0.98	0.18	0.28	32,38,47,50	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	PEK	P	303	53/53	0.95	0.13	0.28	39,53,94,101	0
18	HEA	N	605[B]	60/60	0.98	0.18	0.28	32,38,44,47	9
23	EDO	S	102	4/4	0.97	0.08	0.26	44,45,46,53	0
18	HEA	A	605	60/60	0.99	0.14	0.07	22,26,33,39	0
23	EDO	G	103	4/4	0.97	0.09	-0.36	37,39,49,51	0
24	CHD	G	102	29/29	0.96	0.08	-0.37	35,38,43,52	0
24	CHD	T	103	29/29	0.96	0.08	-0.42	30,36,42,53	0
18	HEA	A	604[B]	60/60	0.99	0.15	-0.56	23,28,35,40	9
31	HEM	1	201	43/43	0.95	0.19	-0.65	57,81,94,99	0
31	HEM	2	201	43/43	0.94	0.27	-0.70	79,101,135,149	0
17	NA	N	604	1/1	0.97	0.09	-0.74	45,45,45,45	0
23	EDO	C	311	4/4	0.97	0.08	-0.74	48,51,51,52	0
18	HEA	A	604[A]	60/60	0.99	0.15	-0.82	23,28,38,40	9
24	CHD	C	301	29/29	0.96	0.08	-1.16	34,40,48,53	0
22	CUA	B	302	2/2	1.00	0.11	-1.63	27,27,27,29	0
22	CUA	O	301	2/2	0.99	0.09	-2.24	42,42,42,43	0
17	NA	A	603	1/1	1.00	0.05	-2.65	31,31,31,31	0
29	ZN	S	101	1/1	0.99	0.05	-2.66	37,37,37,37	0
19	PER	A	606	2/2	0.99	0.10	-3.27	40,40,40,54	0
19	PER	N	607	2/2	0.98	0.10	-4.93	36,36,36,48	0
23	EDO	E	202	4/4	0.85	0.33	-	57,61,68,79	0
17	NA	C	302	1/1	0.58	0.58	-	59,59,59,59	0
15	CU	N	602	1/1	1.00	0.14	-	35,35,35,35	0
15	CU	A	601	1/1	1.00	0.13	-	29,29,29,29	0
17	NA	P	302	1/1	0.55	0.51	-	57,57,57,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.