



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:21 PM GMT

PDB ID : 3WG7  
Title : A 1.9 angstrom radiation damage free X-ray structure of large (420KDa) protein by femtosecond crystallography  
Authors : Hirata, K.; Shinzawa-Itoh, K.; Yano, N.; Takemura, S.; Kato, K.; Hatanaka, M.; Muramoto, K.; Kawahara, T.; Tsukihara, T.; Yamashita, E.; Tono, K.; Ueno, G.; Hikima, T.; Murakami, H.; Inubushi, Y.; Yabashi, M.; Ishikawa, T.; Yamamoto, M.; Ogura, T.; Sugimoto, H.; Shen, J.R.; Yoshikawa, S.; Ago, H.  
Deposited on : 2013-07-29  
Resolution : 1.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

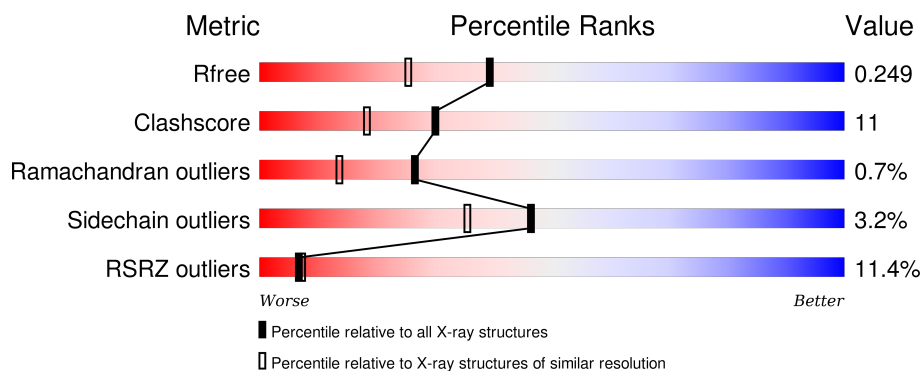
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



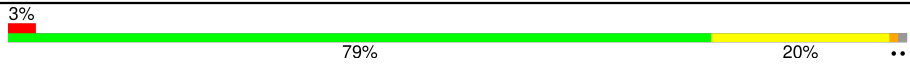
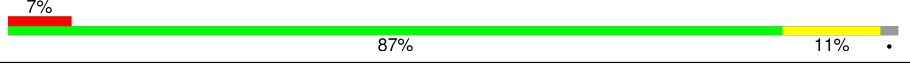
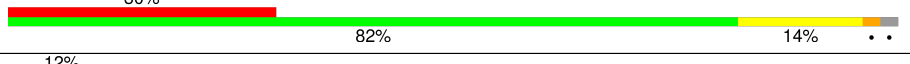


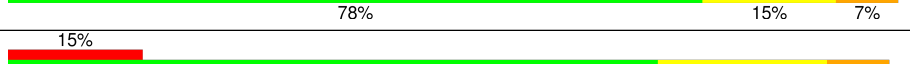
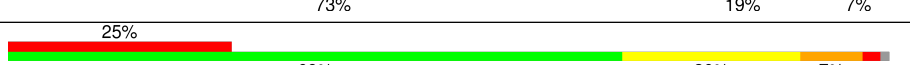
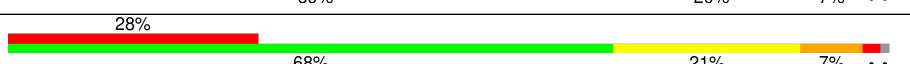
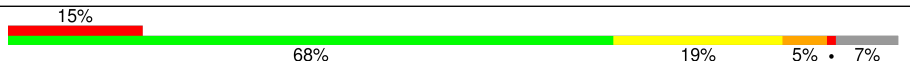
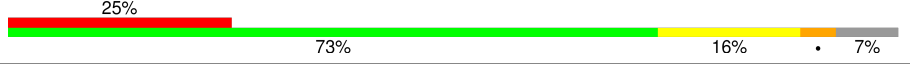

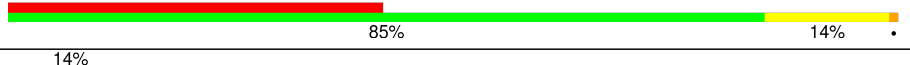
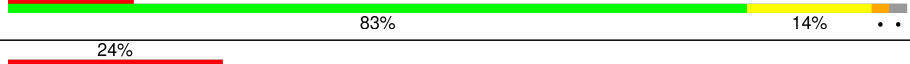

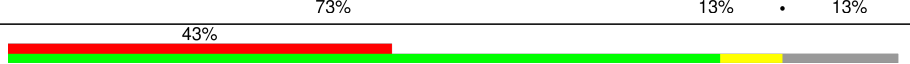





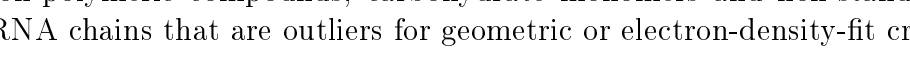
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>84%</div> <div>16%</div> <div>.</div> </div>
1	N	514	<div> <div>2%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
2	B	227	<div> <div>6%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
2	O	227	<div> <div>10%</div> <div>74%</div> <div>25%</div> <div>.</div> </div>
3	C	261	<div> <div>3%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
14	HEA	N	602	X	-	-	-
16	MG	N	604	-	-	-	X
18	PER	A	606[A]	-	-	-	X
18	PER	A	606[B]	-	-	-	X
19	PGV	A	607	-	-	-	X
19	PGV	A	608	-	-	-	X
19	PGV	C	303	-	-	-	X
19	PGV	C	308	-	-	-	X
19	PGV	N	607	-	-	-	X
19	PGV	N	608	-	-	-	X
19	PGV	P	301	-	-	-	X
19	PGV	P	304	-	-	-	X
2	FME	O	1	-	-	X	-
20	TGL	B	301	-	-	-	X
20	TGL	D	201	-	-	-	X
20	TGL	L	101	-	-	-	X
20	TGL	N	609	-	-	-	X
20	TGL	Q	201	-	-	-	X
20	TGL	Y	101	-	-	-	X
22	CHD	C	305	-	-	-	X
22	CHD	J	101	-	-	-	X
22	CHD	W	101	-	-	-	X
23	PSC	N	610	-	-	X	-
24	PEK	C	302	-	-	-	X
25	CDL	C	304	-	-	X	X
25	CDL	G	101	-	-	X	-
25	CDL	P	305	-	-	-	X
25	CDL	T	102	-	-	X	X
27	DMU	M	101	X	-	-	-
27	DMU	Z	101	X	-	-	-

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 33302 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	6	0
			4074	2725	629	684	36			
1	N	514	Total	C	N	O	S	0	6	0
			4074	2725	629	684	36			

- 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	1	0
			1832	1189	282	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	3	0
			2134	1427	339	353	15			
3	P	259	Total	C	N	O	S	0	3	0
			2134	1427	339	353	15			

- 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	0	0
			1195	777	196	218	4			

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

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

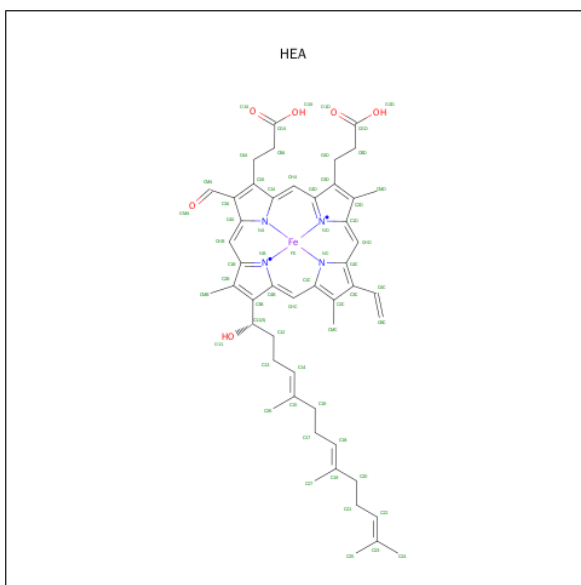
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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 HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

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

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

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

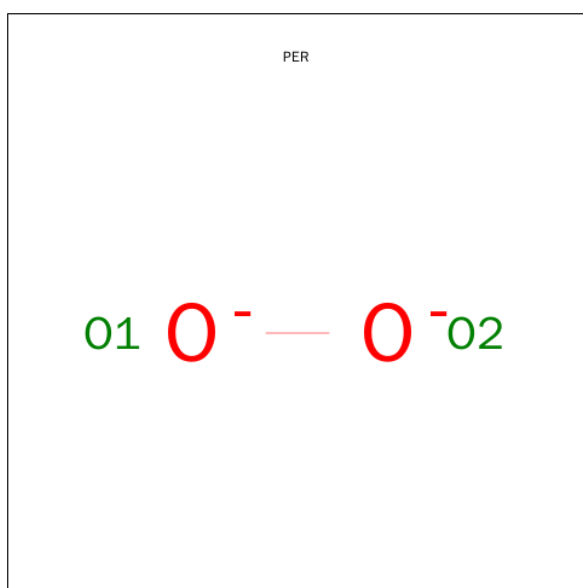
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

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



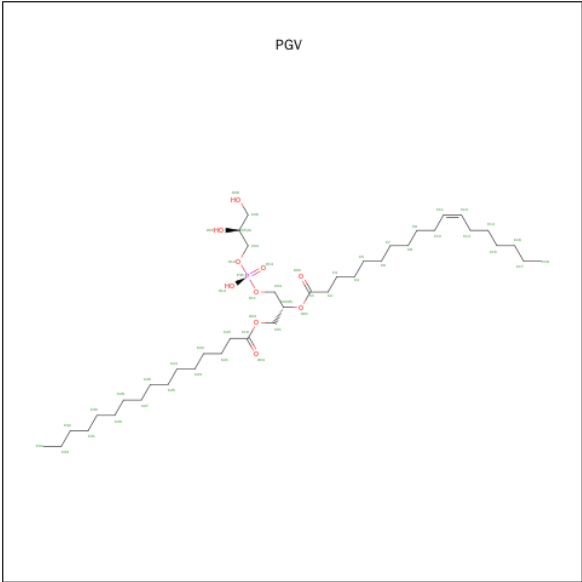
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	1	Total Na 1 1	0	0
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



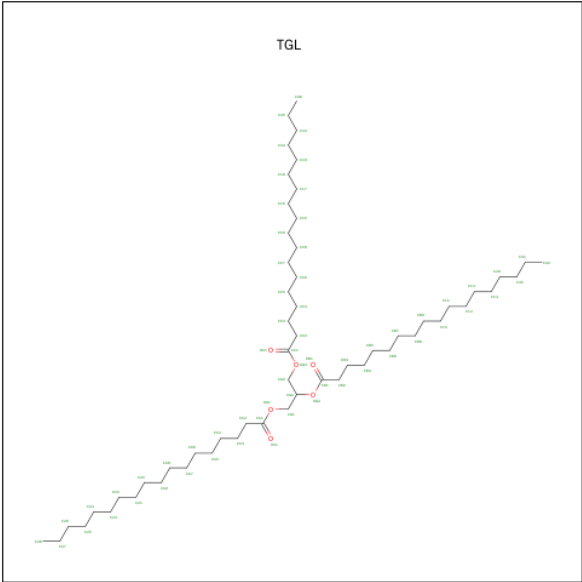
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 4 4	0	1
18	N	1	Total O 4 4	0	1

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



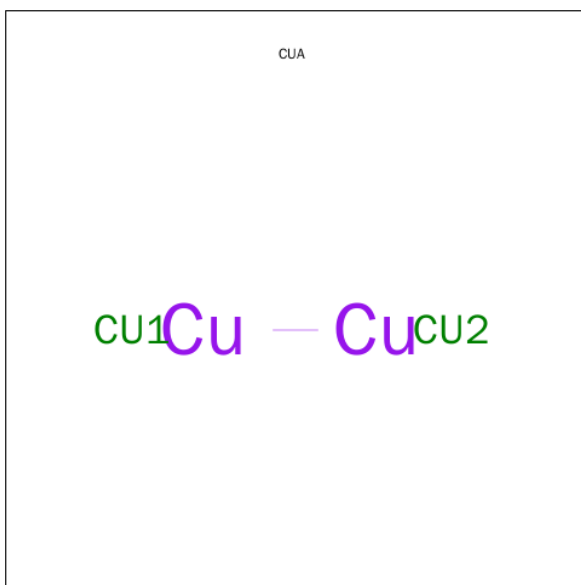
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



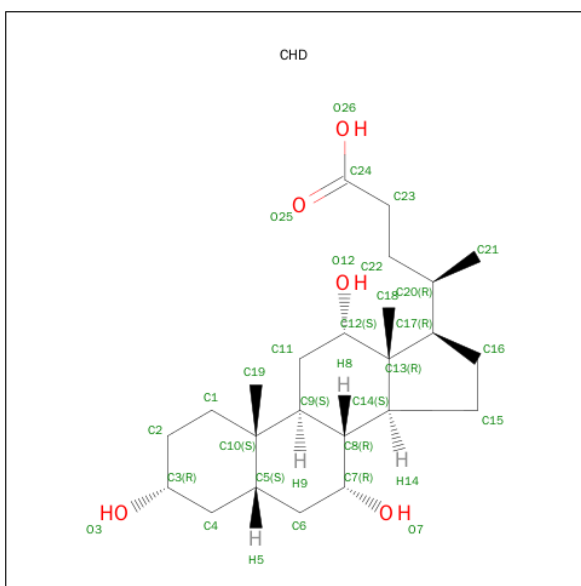
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



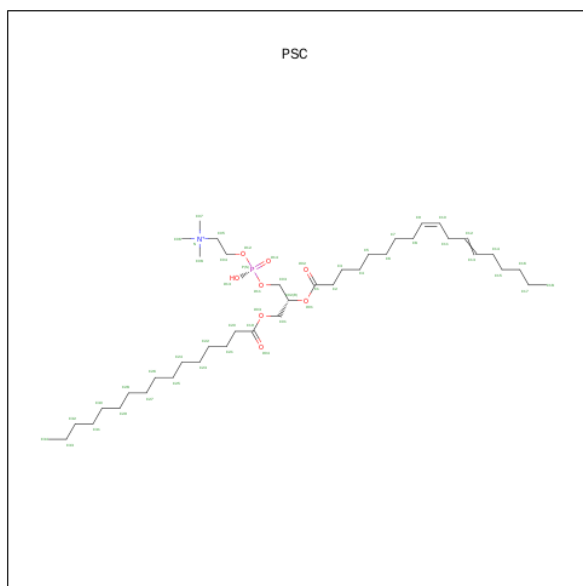
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	C	O	0
			29	24	5	0
22	C	1	Total	C	O	0
			29	24	5	0

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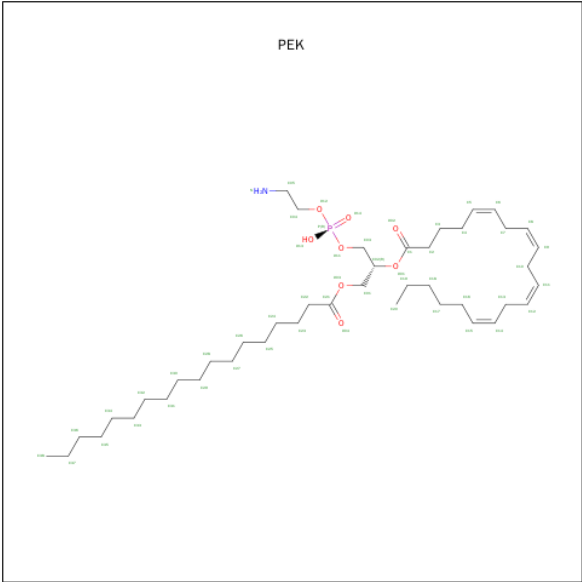
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



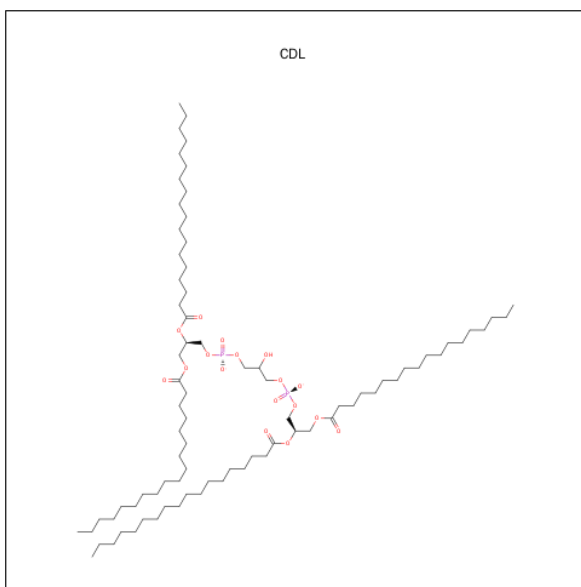
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	N	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).

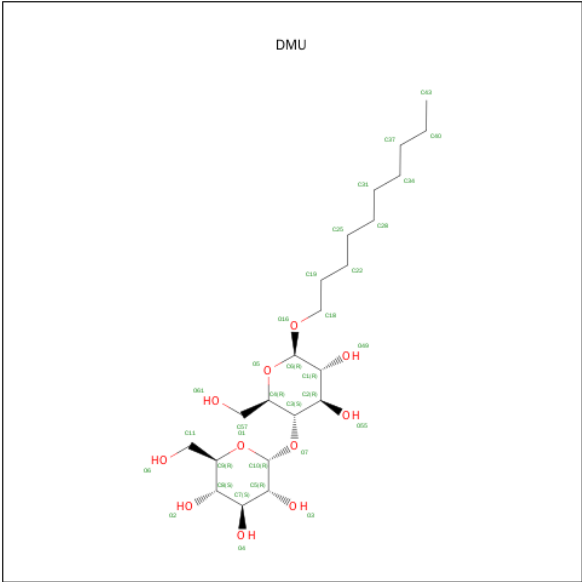


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	265	Total	O	0	0
			265	265		
28	B	194	Total	O	0	0
			194	194		
28	C	141	Total	O	0	0
			141	141		
28	D	160	Total	O	0	0
			160	160		
28	E	125	Total	O	0	0
			125	125		
28	F	112	Total	O	0	0
			112	112		
28	G	70	Total	O	0	0
			70	70		
28	H	70	Total	O	0	0
			70	70		
28	I	52	Total	O	0	0
			52	52		
28	J	31	Total	O	0	0
			31	31		

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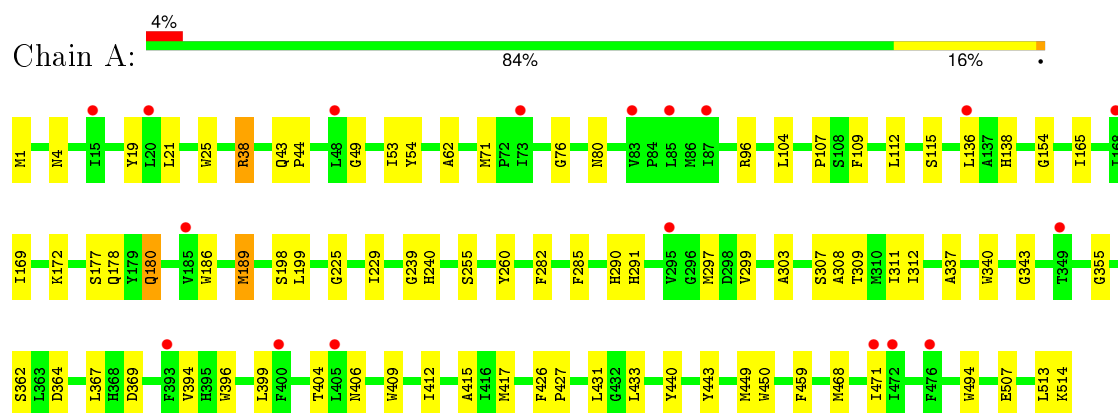
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	40	Total 40	O 40	0	0
28	L	31	Total 31	O 31	0	0
28	M	31	Total 31	O 31	0	0
28	N	259	Total 259	O 259	0	0
28	O	157	Total 157	O 157	0	0
28	P	143	Total 143	O 143	0	0
28	Q	90	Total 90	O 90	0	0
28	R	103	Total 103	O 103	0	0
28	S	122	Total 122	O 122	0	0
28	T	56	Total 56	O 56	0	0
28	U	51	Total 51	O 51	0	0
28	V	42	Total 42	O 42	0	0
28	W	38	Total 38	O 38	0	0
28	X	34	Total 34	O 34	0	0
28	Y	37	Total 37	O 37	0	0
28	Z	24	Total 24	O 24	0	0

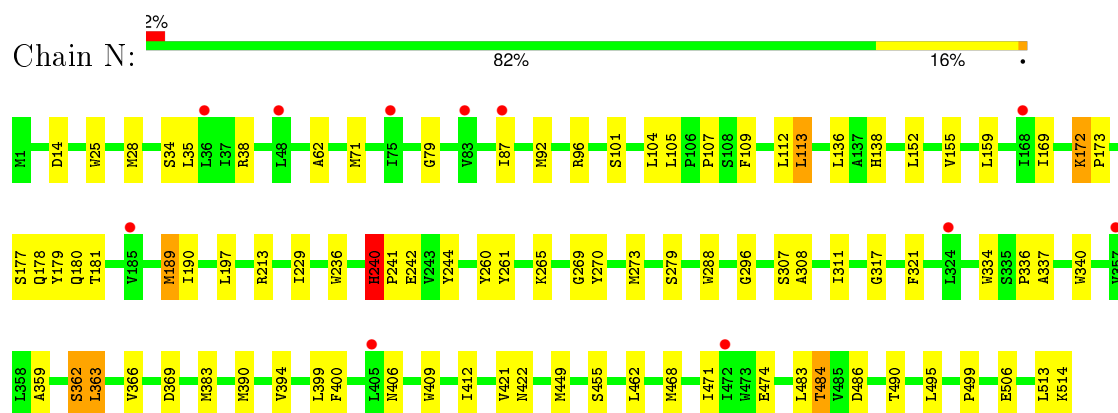
### 3 Residue-property plots [i](#)

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.

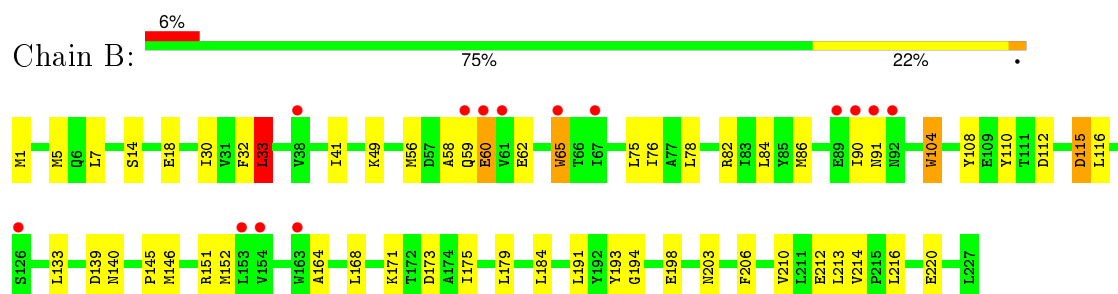
#### • Molecule 1: Cytochrome c oxidase subunit 1



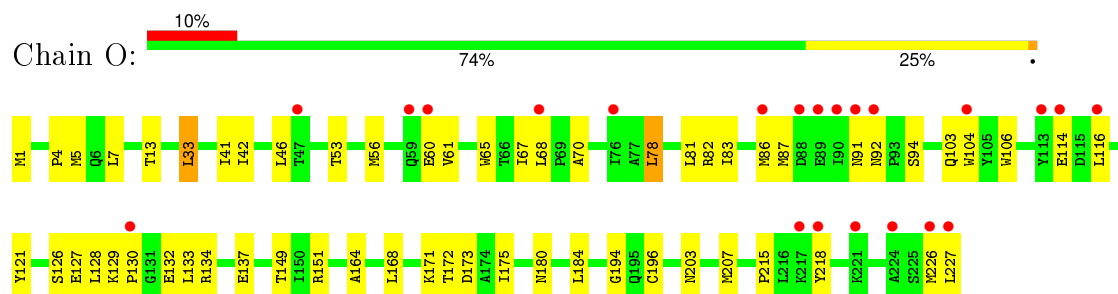
#### • Molecule 1: Cytochrome c oxidase subunit 1



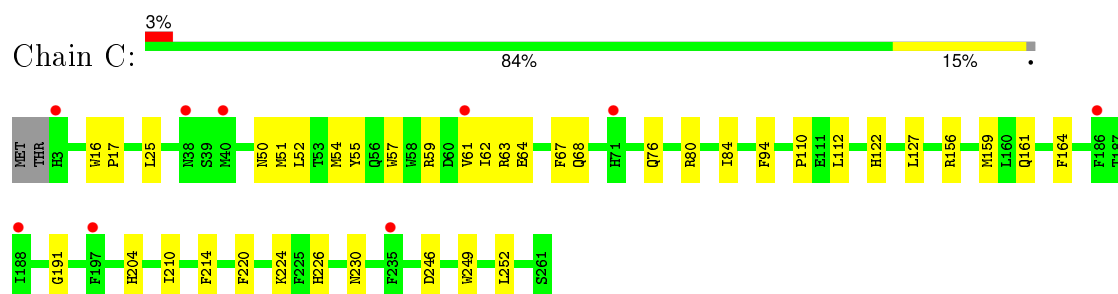
#### • Molecule 2: Cytochrome c oxidase subunit 2



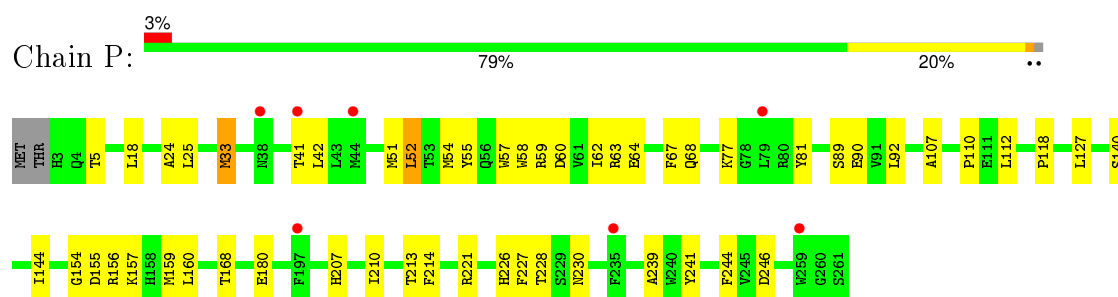
- Molecule 2: Cytochrome c oxidase subunit 2



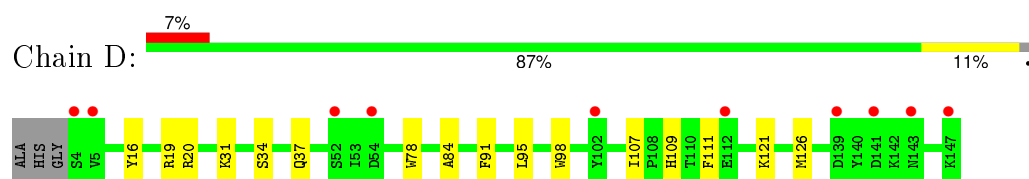
- Molecule 3: Cytochrome c oxidase subunit 3



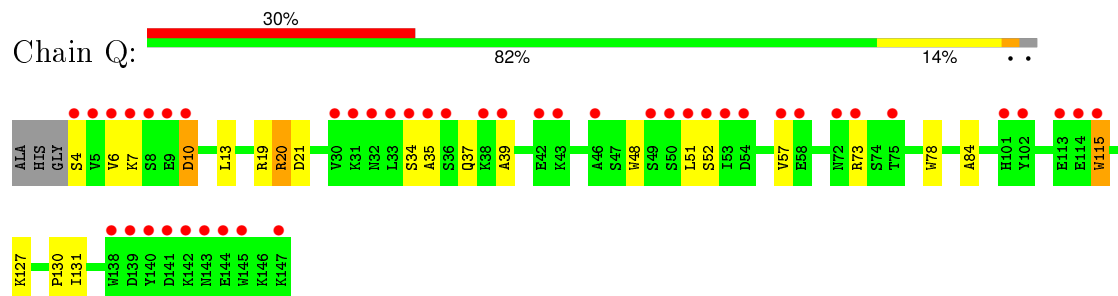
- Molecule 3: Cytochrome c oxidase subunit 3



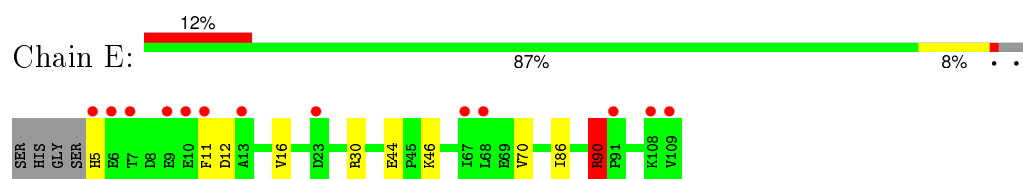
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



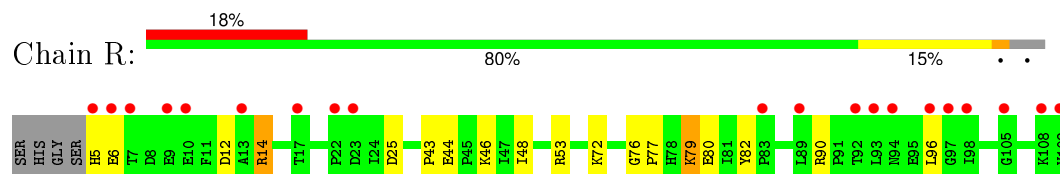
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



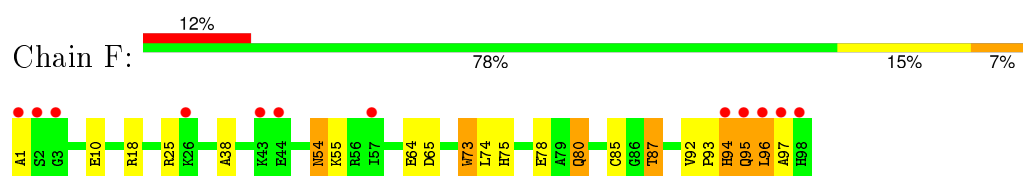
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



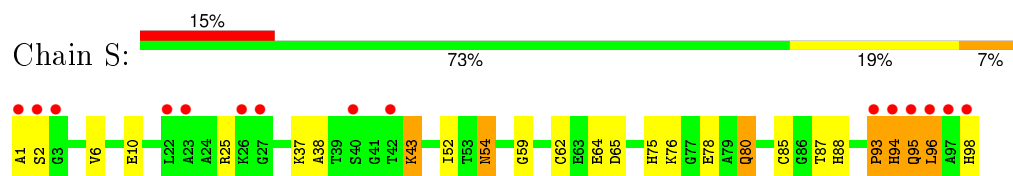
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



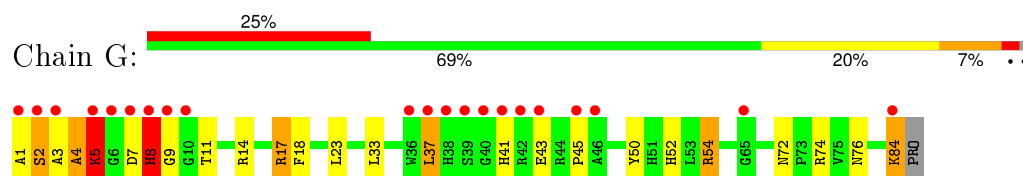
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



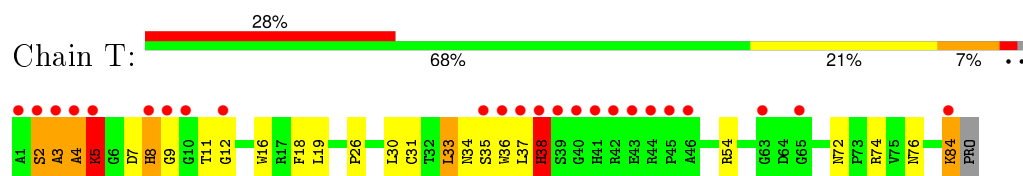
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



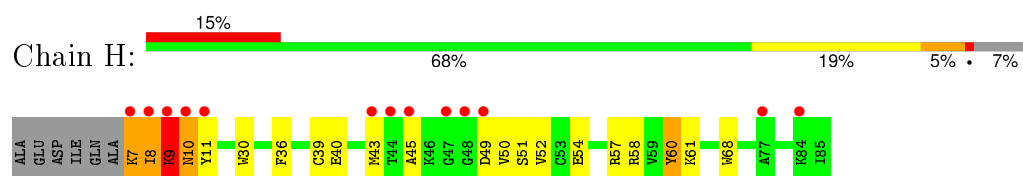
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



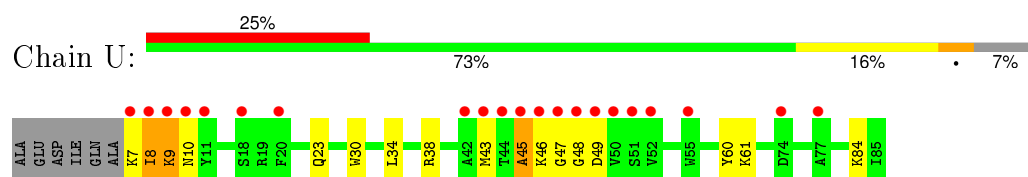
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



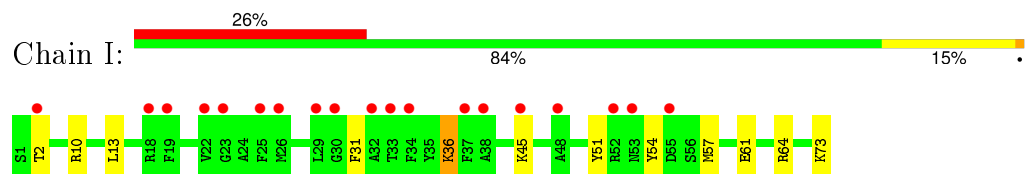
- Molecule 8: Cytochrome c oxidase subunit 6B1



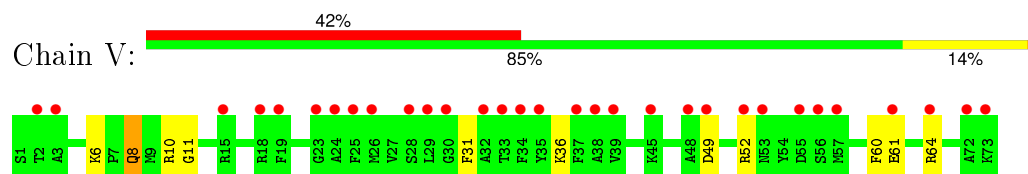
- Molecule 8: Cytochrome c oxidase subunit 6B1



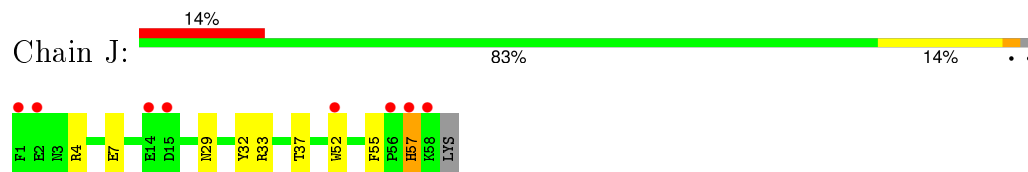
- Molecule 9: Cytochrome c oxidase subunit 6C



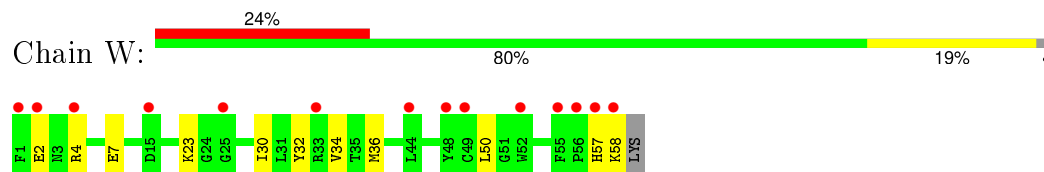
- Molecule 9: Cytochrome c oxidase subunit 6C



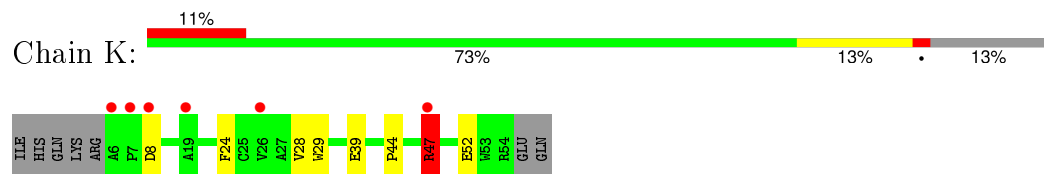
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



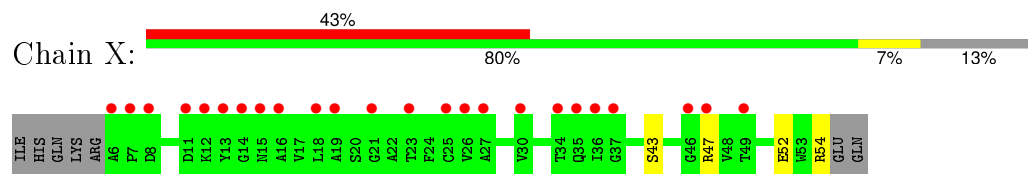
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



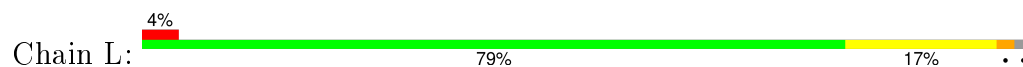
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



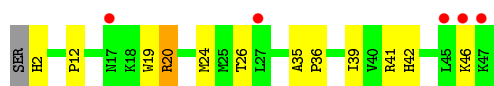
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



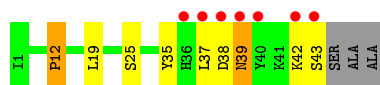
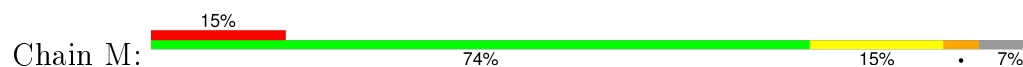
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



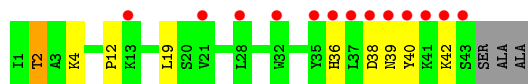
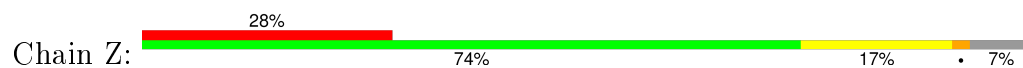
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.60Å 204.51Å 178.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 27.31 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.0 (40.00-1.90) 95.3 (27.31-1.89)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.195 , 0.230 0.220 , 0.249	Depositor DCC
$R_{free}$ test set	25150 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 77.8	EDS
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 500579 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.46	22/4203 (0.5%)	1.15	11/5742 (0.2%)
1	N	1.40	17/4203 (0.4%)	1.14	17/5742 (0.3%)
2	B	1.24	4/1868 (0.2%)	1.13	8/2545 (0.3%)
2	O	1.11	2/1860 (0.1%)	1.06	3/2534 (0.1%)
3	C	1.32	3/2221 (0.1%)	0.98	2/3035 (0.1%)
3	P	1.29	7/2221 (0.3%)	1.02	4/3035 (0.1%)
4	D	1.20	2/1229 (0.2%)	1.05	4/1658 (0.2%)
4	Q	0.99	1/1229 (0.1%)	0.90	1/1658 (0.1%)
5	E	1.18	1/871 (0.1%)	1.02	2/1182 (0.2%)
5	R	1.00	0/871	1.07	7/1182 (0.6%)
6	F	1.08	1/765 (0.1%)	1.07	2/1038 (0.2%)
6	S	1.18	1/765 (0.1%)	1.05	0/1038
7	G	1.16	0/690	1.04	5/937 (0.5%)
7	T	1.12	1/690 (0.1%)	1.01	3/937 (0.3%)
8	H	1.14	2/682 (0.3%)	0.95	1/921 (0.1%)
8	U	0.97	0/682	0.95	0/921
9	I	0.94	0/605	1.01	3/802 (0.4%)
9	V	0.87	0/605	0.93	0/802
10	J	0.96	0/471	1.01	1/636 (0.2%)
10	W	0.97	0/471	1.00	0/636
11	K	1.11	1/398 (0.3%)	1.04	1/546 (0.2%)
11	X	0.96	0/398	0.84	0/546
12	L	1.20	0/393	1.20	2/526 (0.4%)
12	Y	1.13	0/393	0.95	1/526 (0.2%)
13	M	1.21	1/345 (0.3%)	1.01	1/470 (0.2%)
13	Z	1.09	0/345	0.90	0/470
All	All	1.24	66/29474 (0.2%)	1.06	79/40065 (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	N	0	1
6	F	0	1
6	S	0	1
8	H	0	1
10	J	0	1
10	W	0	1
All	All	0	6

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	36	TRP	CB-CG	8.63	1.65	1.50
1	N	242	GLU	CD-OE1	8.41	1.34	1.25
1	A	154	GLY	N-CA	7.80	1.57	1.46
1	N	236	TRP	CE3-CZ3	7.54	1.51	1.38
1	N	260	TYR	CG-CD2	7.26	1.48	1.39
3	P	227	PHE	CG-CD1	7.24	1.49	1.38
1	N	260	TYR	CE1-CZ	7.22	1.48	1.38
1	N	79	GLY	N-CA	7.13	1.56	1.46
1	N	340	TRP	CB-CG	6.90	1.62	1.50
1	A	260	TYR	CG-CD2	6.88	1.48	1.39
1	N	179	TYR	CE1-CZ	6.82	1.47	1.38
1	A	355	GLY	N-CA	6.67	1.56	1.46
1	A	260	TYR	CE1-CZ	6.66	1.47	1.38
1	A	198	SER	CA-CB	6.60	1.62	1.52
1	N	244	TYR	CG-CD1	6.50	1.47	1.39
1	A	404	THR	C-O	6.26	1.35	1.23
1	A	54	TYR	CE1-CZ	6.12	1.46	1.38
1	A	186	TRP	CE3-CZ3	6.11	1.48	1.38
1	N	474	GLU	CD-OE2	6.11	1.32	1.25
6	S	59	GLY	C-O	6.09	1.33	1.23
1	N	270	TYR	CG-CD1	6.05	1.47	1.39
1	N	337	ALA	N-CA	5.99	1.58	1.46
13	M	35	TYR	CB-CG	5.93	1.60	1.51
1	N	288	TRP	N-CA	5.93	1.58	1.46
2	O	106	TRP	CG-CD1	5.89	1.45	1.36
2	B	18	GLU	CD-OE2	5.86	1.32	1.25
1	A	38	ARG	CZ-NH1	5.85	1.40	1.33
3	P	90	GLU	CD-OE1	5.81	1.32	1.25
3	C	16	TRP	CB-CG	5.75	1.60	1.50
1	N	359	ALA	N-CA	5.75	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	89	SER	CB-OG	5.74	1.49	1.42
1	A	440	TYR	CE1-CZ	5.73	1.46	1.38
3	C	249	TRP	CG-CD1	5.73	1.44	1.36
4	D	16	TYR	CG-CD1	5.70	1.46	1.39
2	O	121	TYR	CE1-CZ	5.70	1.46	1.38
5	E	30	ARG	CZ-NH2	5.69	1.40	1.33
3	P	58	TRP	CZ3-CH2	5.69	1.49	1.40
4	Q	115	TRP	CB-CG	5.67	1.60	1.50
1	A	340	TRP	CB-CG	5.63	1.60	1.50
1	N	362	SER	CB-OG	-5.62	1.34	1.42
2	B	108	TYR	CE1-CZ	5.58	1.45	1.38
11	K	29	TRP	CB-CG	5.57	1.60	1.50
8	H	68	TRP	CG-CD1	5.53	1.44	1.36
1	A	362	SER	CB-OG	-5.52	1.35	1.42
1	A	239	GLY	N-CA	5.49	1.54	1.46
6	F	73	TRP	CG-CD1	5.49	1.44	1.36
1	A	396	TRP	CD1-NE1	5.48	1.47	1.38
1	A	440	TYR	CG-CD2	5.48	1.46	1.39
2	B	198	GLU	C-O	5.45	1.33	1.23
1	A	115	SER	CB-OG	-5.39	1.35	1.42
1	N	506	GLU	CD-OE2	-5.38	1.19	1.25
1	A	19	TYR	CD1-CE1	5.29	1.47	1.39
3	P	228	THR	CB-CG2	5.25	1.69	1.52
2	B	104	TRP	CE3-CZ3	5.25	1.47	1.38
1	A	396	TRP	CE3-CZ3	5.24	1.47	1.38
1	A	255	SER	CA-CB	5.22	1.60	1.52
8	H	68	TRP	CZ3-CH2	5.20	1.48	1.40
3	C	57	TRP	CB-CG	5.17	1.59	1.50
1	A	49	GLY	C-O	5.15	1.31	1.23
1	A	443	TYR	C-O	5.12	1.33	1.23
3	P	226	HIS	N-CA	5.10	1.56	1.46
4	D	91	PHE	CG-CD1	5.08	1.46	1.38
1	A	25	TRP	CG-CD1	5.04	1.43	1.36
1	N	261	TYR	CD1-CE1	5.01	1.46	1.39
3	P	140	SER	CB-OG	5.01	1.48	1.42
1	N	455	SER	CB-OG	5.01	1.48	1.42

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ARG	NE-CZ-NH2	-13.88	113.36	120.30
5	R	90	ARG	NE-CZ-NH2	-10.73	114.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	47	ARG	NE-CZ-NH1	10.01	125.31	120.30
12	L	20	ARG	NE-CZ-NH2	-9.56	115.52	120.30
4	D	20	ARG	NE-CZ-NH2	9.53	125.06	120.30
2	O	151	ARG	NE-CZ-NH1	9.28	124.94	120.30
6	F	18	ARG	NE-CZ-NH2	-9.02	115.79	120.30
5	E	90	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	N	71	MET	CG-SD-CE	-8.28	86.95	100.20
1	N	38	ARG	NE-CZ-NH1	8.25	124.42	120.30
5	R	14	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	71	MET	CG-SD-CE	-7.92	87.53	100.20
1	N	92	MET	CG-SD-CE	7.84	112.75	100.20
2	O	151	ARG	NE-CZ-NH2	-7.67	116.46	120.30
5	R	90	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	96	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	N	38	ARG	NE-CZ-NH2	-7.28	116.66	120.30
6	F	18	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	A	38	ARG	NE-CZ-NH1	7.17	123.89	120.30
2	B	179	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	152	MET	CG-SD-CE	7.00	111.40	100.20
4	D	20	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	N	363	LEU	CB-CG-CD2	6.74	122.47	111.00
5	E	90	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	N	96	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	B	173	ASP	CB-CG-OD1	6.48	124.14	118.30
1	N	486	ASP	CB-CG-OD1	6.40	124.06	118.30
9	I	64	ARG	NE-CZ-NH1	6.37	123.49	120.30
8	H	58	ARG	NE-CZ-NH2	-6.37	117.11	120.30
4	D	19	ARG	NE-CZ-NH2	6.25	123.42	120.30
4	Q	51	LEU	CA-CB-CG	6.00	129.10	115.30
1	A	240	HIS	N-CA-CB	6.00	121.40	110.60
12	L	20	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	N	96	ARG	NE-CZ-NH2	-5.98	117.31	120.30
9	I	64	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	199	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	N	213	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	N	113	LEU	CB-CG-CD1	5.81	120.88	111.00
1	A	364	ASP	CB-CG-OD2	-5.80	113.08	118.30
7	T	19	LEU	CB-CG-CD1	-5.78	101.17	111.00
12	Y	19	TRP	CA-CB-CG	-5.78	102.72	113.70
5	R	25	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	104	LEU	CB-CG-CD1	-5.74	101.23	111.00
7	G	14	ARG	NE-CZ-NH1	-5.74	117.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	5	LYS	CB-CA-C	5.72	121.84	110.40
1	N	172	LYS	CD-CE-NZ	-5.70	98.59	111.70
1	N	240	HIS	N-CA-CB	5.69	120.85	110.60
3	C	80	ARG	CG-CD-NE	-5.68	99.86	111.80
7	T	5	LYS	CB-CA-C	5.64	121.68	110.40
5	R	53	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	38	ARG	CG-CD-NE	5.59	123.55	111.80
1	A	189	MET	CG-SD-CE	-5.55	91.31	100.20
1	N	366	VAL	CG1-CB-CG2	-5.55	102.02	110.90
13	M	37	LEU	CB-CG-CD1	-5.55	101.57	111.00
2	B	139	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	65	TRP	CB-CA-C	5.49	121.38	110.40
1	N	14	ASP	CB-CG-OD2	5.44	123.20	118.30
3	P	92	LEU	CB-CG-CD1	-5.42	101.79	111.00
10	J	4	ARG	NE-CZ-NH1	5.41	123.01	120.30
3	P	180	GLU	OE1-CD-OE2	5.39	129.77	123.30
2	B	112	ASP	CB-CG-OD1	5.38	123.14	118.30
3	C	61	VAL	CG1-CB-CG2	-5.36	102.33	110.90
7	G	17	ARG	NE-CZ-NH1	-5.32	117.64	120.30
3	P	18	LEU	CB-CG-CD1	5.31	120.02	111.00
2	B	33	LEU	CA-CB-CG	5.29	127.46	115.30
2	B	151	ARG	NE-CZ-NH1	5.28	122.94	120.30
9	I	13	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	N	189	MET	CB-CG-SD	-5.20	96.80	112.40
2	O	173	ASP	CB-CG-OD1	5.18	122.97	118.30
3	P	52	LEU	CB-CG-CD2	-5.16	102.22	111.00
5	R	12	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	21	LEU	CB-CG-CD2	-5.16	102.24	111.00
5	R	25	ASP	CB-CG-OD2	-5.13	113.68	118.30
4	D	95	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	N	213	ARG	NE-CZ-NH2	-5.13	117.74	120.30
7	T	74	ARG	NE-CZ-NH2	-5.07	117.77	120.30
7	G	54	ARG	NE-CZ-NH1	5.07	122.83	120.30
7	G	8	HIS	N-CA-C	5.04	124.59	111.00
1	N	101	SER	CA-CB-OG	-5.02	97.64	111.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
8	H	9	LYS	Peptide

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Mol	Chain	Res	Type	Group
10	J	57	HIS	Peptide
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
10	W	57	HIS	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	4074	0	4058	53	0
1	N	4074	0	4058	73	0
2	B	1832	0	1836	36	0
2	O	1824	0	1833	51	2
3	C	2134	0	2051	39	0
3	P	2134	0	2051	46	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	30	0
5	E	852	0	845	7	0
5	R	852	0	845	10	2
6	F	748	0	728	16	1
6	S	748	0	728	36	7
7	G	675	0	643	29	0
7	T	675	0	643	34	0
8	H	662	0	623	19	0
8	U	662	0	623	11	0
9	I	601	0	613	8	2
9	V	601	0	613	8	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	7	0
11	X	384	0	366	4	0
12	L	380	0	380	14	0
12	Y	380	0	380	16	0
13	M	335	0	352	10	0
13	Z	335	0	352	9	0
14	A	120	0	108	10	0
14	N	120	0	108	6	0
15	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	1	0
18	N	4	0	0	1	0
19	A	102	0	152	10	0
19	C	102	0	152	5	0
19	N	102	0	152	16	0
19	P	102	0	152	10	0
20	B	63	0	110	3	0
20	D	63	0	110	13	0
20	L	63	0	110	12	0
20	N	63	0	110	4	0
20	Q	63	0	110	11	0
20	Y	63	0	110	16	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	1	0
22	C	58	0	78	4	0
22	G	29	0	39	0	0
22	J	29	0	39	5	0
22	P	58	0	78	5	0
22	W	29	0	38	5	0
23	B	52	0	80	13	0
23	N	52	0	80	21	0
24	C	106	0	154	23	0
24	G	53	0	77	6	0
24	P	106	0	154	22	0
24	T	53	0	77	12	0
25	C	100	0	156	23	0
25	G	100	0	156	37	0
25	P	100	0	156	17	0
25	T	100	0	156	29	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	42	1	0
27	Z	33	0	42	0	0
28	A	265	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	B	194	0	0	10	2
28	C	141	0	0	8	0
28	D	160	0	0	1	1
28	E	125	0	0	3	0
28	F	112	0	0	2	1
28	G	70	0	0	6	0
28	H	70	0	0	5	0
28	I	52	0	0	1	0
28	J	31	0	0	2	0
28	K	40	0	0	3	1
28	L	31	0	0	1	0
28	M	31	0	0	1	2
28	N	259	0	0	11	0
28	O	157	0	0	11	6
28	P	143	0	0	8	0
28	Q	90	0	0	5	0
28	R	103	0	0	3	0
28	S	122	0	0	7	1
28	T	56	0	0	2	0
28	U	51	0	0	2	0
28	V	42	0	0	5	0
28	W	38	0	0	2	0
28	X	34	0	0	3	0
28	Y	37	0	0	4	0
28	Z	24	0	0	1	0
All	All	33302	0	31396	691	14

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 (691) 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)
6:S:76:LYS:CE	6:S:93:PRO:HG2	1.47	1.41
6:S:43:LYS:CD	6:S:43:LYS:H	1.28	1.39
6:S:43:LYS:N	6:S:43:LYS:HD3	1.33	1.29
6:S:76:LYS:HD3	28:S:271:HOH:O	1.36	1.25
18:A:606[A]:PER:O2	18:A:606[A]:PER:O1	1.55	1.22
18:N:606[A]:PER:O1	18:N:606[A]:PER:O2	1.55	1.19
20:L:101:TGL:HC41	20:L:101:TGL:OC1	1.41	1.18
7:G:5:LYS:HB2	24:G:102:PEK:H362	1.21	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:76:LYS:HE3	6:S:93:PRO:CG	1.80	1.11
1:N:513:LEU:O	1:N:514:LYS:HB2	1.49	1.07
19:P:304:PGV:H172	25:P:305:CDL:H651	1.35	1.07
20:Q:201:TGL:H231	20:Q:201:TGL:HA91	1.29	1.06
23:N:610:PSC:H342	2:O:41:ILE:HD13	1.36	1.04
7:T:5:LYS:HB2	24:T:101:PEK:H351	1.39	1.03
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.04	1.02
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.38	1.01
12:L:20:ARG:HH22	20:L:101:TGL:HC32	1.22	1.01
3:C:67:PHE:HE1	25:C:304:CDL:H1	1.25	1.01
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.46	0.97
6:S:95:GLN:HB2	28:S:240:HOH:O	1.64	0.97
1:N:321:PHE:CD2	23:N:610:PSC:H341	2.00	0.96
10:W:23:LYS:HE3	28:W:221:HOH:O	1.64	0.95
11:X:47:ARG:HD3	28:X:116:HOH:O	1.67	0.95
7:G:5:LYS:HG3	24:G:102:PEK:H383	1.48	0.94
7:G:72:ASN:H	7:G:76:ASN:HD22	1.16	0.93
19:A:608:PGV:O14	19:A:608:PGV:H02	1.67	0.93
6:F:85:CYS:SG	6:F:87:THR:HG23	2.08	0.93
23:N:610:PSC:H22	28:V:101:HOH:O	1.68	0.92
3:C:224:LYS:CD	25:C:304:CDL:HB31	1.98	0.92
3:P:33[A]:MET:HE1	3:P:42:LEU:H	1.34	0.91
24:C:307:PEK:H383	25:G:101:CDL:C27	2.01	0.90
14:N:601:HEA:HMC1	14:N:601:HEA:HBC1	1.54	0.89
17:C:301:NA:NA	28:C:404:HOH:O	1.45	0.89
7:G:5:LYS:HB2	24:G:102:PEK:C36	2.01	0.89
7:T:5:LYS:CB	24:T:101:PEK:H351	2.02	0.89
3:C:67:PHE:CE1	25:C:304:CDL:H1	2.08	0.88
6:S:76:LYS:CE	6:S:93:PRO:CG	2.42	0.88
3:P:67:PHE:HE1	25:P:305:CDL:H1	1.36	0.88
2:O:1:FME:HE1	2:O:133:LEU:HD13	1.55	0.87
19:N:608:PGV:H343	24:P:303:PEK:H382	1.56	0.87
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.57	0.86
25:G:101:CDL:H202	25:G:101:CDL:H522	1.58	0.86
19:P:301:PGV:H11	22:P:307:CHD:H152	1.58	0.86
6:S:98:HIS:HB3	28:S:268:HOH:O	1.76	0.85
12:L:20:ARG:NH2	20:L:101:TGL:HC32	1.91	0.85
25:T:102:CDL:H202	25:T:102:CDL:H511	1.57	0.85
8:U:7:LYS:O	8:U:8:ILE:HG22	1.77	0.84
4:D:78:TRP:HB3	20:D:201:TGL:HB22	1.56	0.84
1:A:513:LEU:O	1:A:514:LYS:HB2	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:101:TGL:CC4	20:L:101:TGL:OC1	2.23	0.83
25:G:101:CDL:H352	2:O:78:LEU:HD12	1.59	0.83
6:S:85:CYS:SG	6:S:87:THR:HG23	2.19	0.83
7:T:72:ASN:H	7:T:76:ASN:HD22	1.23	0.83
3:C:224:LYS:HD2	25:C:304:CDL:HB31	1.59	0.82
6:S:75:HIS:H	6:S:80:GLN:HE22	1.23	0.82
2:O:1:FME:CE	2:O:133:LEU:HD13	2.10	0.81
3:P:63:ARG:HE	25:P:305:CDL:HA22	1.46	0.81
8:H:40:GLU:OE2	28:H:130:HOH:O	1.98	0.80
25:C:304:CDL:OB9	25:C:304:CDL:H522	1.81	0.80
19:A:608:PGV:H311	13:M:19:LEU:HD23	1.64	0.80
12:L:2:HIS:CG	12:L:3:TYR:H	1.99	0.80
7:G:84:LYS:HD2	7:G:84:LYS:H	1.47	0.79
28:A:955:HOH:O	2:B:206:PHE:HE1	1.63	0.79
2:O:1:FME:HE3	2:O:133:LEU:CD2	2.12	0.79
24:C:302:PEK:HN2	7:G:76:ASN:HD21	1.27	0.79
28:C:528:HOH:O	25:G:101:CDL:H673	1.81	0.79
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.63	0.79
3:P:33[A]:MET:HG2	28:P:455:HOH:O	1.83	0.78
1:N:321:PHE:HD2	23:N:610:PSC:H341	1.48	0.78
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.16	0.78
24:P:303:PEK:H203	24:P:303:PEK:H15	1.65	0.78
6:S:43:LYS:CD	6:S:43:LYS:N	2.08	0.77
25:P:305:CDL:HB21	25:P:305:CDL:OB6	1.82	0.77
24:C:307:PEK:H361	25:G:101:CDL:H273	1.66	0.77
7:G:11:TPO:HA	7:G:11:TPO:O2P	1.81	0.77
7:T:5:LYS:HG3	24:T:101:PEK:H371	1.67	0.77
5:E:90:ARG:HD2	28:E:279:HOH:O	1.83	0.77
6:S:52:ILE:O	6:S:94:HIS:CE1	2.37	0.77
28:N:953:HOH:O	24:P:303:PEK:H372	1.83	0.77
24:C:307:PEK:C38	25:G:101:CDL:C27	2.62	0.77
23:B:304:PSC:C12	23:B:304:PSC:H342	2.14	0.75
25:T:102:CDL:CA5	25:T:102:CDL:H311	2.17	0.75
28:P:530:HOH:O	6:S:1:ALA:HB2	1.87	0.75
25:P:305:CDL:H532	25:P:305:CDL:OB9	1.87	0.74
2:O:1:FME:HE3	2:O:133:LEU:CD1	2.18	0.74
1:A:311[A]:ILE:HD13	25:T:102:CDL:H221	1.69	0.74
7:G:84:LYS:N	7:G:84:LYS:HD2	2.02	0.74
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.86	0.73
3:C:161:GLN:HE22	24:C:307:PEK:H21	1.52	0.73
8:H:30:TRP:HB2	28:H:158:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:26:THR:HG23	13:M:25:SER:CB	2.19	0.73
19:N:607:PGV:H302	13:Z:19:LEU:CD2	2.19	0.73
4:Q:6:VAL:HG13	4:Q:10:ASP:OD2	1.89	0.72
12:Y:12:PRO:HB2	20:Y:101:TGL:HG11	1.68	0.72
2:O:1:FME:CE	2:O:133:LEU:CD1	2.67	0.72
4:Q:6:VAL:CG1	4:Q:10:ASP:OD2	2.37	0.72
25:G:101:CDL:HA21	25:G:101:CDL:H111	1.71	0.72
28:O:536:HOH:O	4:Q:21:ASP:HB2	1.89	0.72
24:C:307:PEK:C38	25:G:101:CDL:H272	2.20	0.72
25:P:305:CDL:H251	25:P:305:CDL:H391	1.72	0.72
5:R:80:GLU:CD	5:R:80:GLU:H	1.93	0.72
3:C:161:GLN:NE2	24:C:307:PEK:H21	2.05	0.72
25:G:101:CDL:H751	25:G:101:CDL:H561	1.70	0.72
3:P:107:ALA:HB2	19:P:301:PGV:H031	1.72	0.72
19:N:607:PGV:H202	19:N:607:PGV:H31	1.72	0.72
12:Y:20:ARG:HH21	20:Y:101:TGL:HC32	1.55	0.71
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.20	0.71
4:Q:78:TRP:CA	20:Q:201:TGL:HB22	2.21	0.71
24:P:303:PEK:HN2	7:T:76:ASN:HD21	1.34	0.71
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.26	0.71
2:B:56:MET:HG2	23:B:304:PSC:H221	1.73	0.70
1:A:311[B]:ILE:HD11	24:P:308:PEK:H342	1.72	0.70
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.73	0.70
12:L:14:SER:H	20:L:101:TGL:HC31	1.55	0.70
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.72	0.70
20:Q:201:TGL:OB1	20:Q:201:TGL:HG32	1.92	0.70
7:T:30:LEU:HD21	25:T:102:CDL:H471	1.74	0.69
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	1.91	0.69
4:D:78:TRP:N	20:D:201:TGL:HB21	2.06	0.69
24:C:307:PEK:H382	25:G:101:CDL:H272	1.74	0.69
1:N:321:PHE:CD2	23:N:610:PSC:C34	2.75	0.69
7:T:3:ALA:O	7:T:4:ALA:CB	2.40	0.69
3:C:63:ARG:HE	25:C:304:CDL:HA22	1.56	0.69
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.57	0.69
3:P:63:ARG:HE	25:P:305:CDL:CA2	2.06	0.69
3:C:63:ARG:HE	25:C:304:CDL:CA2	2.06	0.68
1:N:113:LEU:HD12	20:Y:101:TGL:H141	1.75	0.68
4:D:78:TRP:CB	20:D:201:TGL:HB22	2.23	0.68
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.93	0.68
7:G:2:SER:OG	24:G:102:PEK:H301	1.93	0.68
25:G:101:CDL:H182	25:G:101:CDL:CB5	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PHE:CE2	20:B:301:TGL:HA52	2.29	0.68
3:P:67:PHE:CE1	25:P:305:CDL:H1	2.25	0.67
1:N:321:PHE:CE2	23:N:610:PSC:H341	2.30	0.67
24:P:308:PEK:H382	25:T:102:CDL:H271	1.76	0.67
6:S:64:GLU:O	6:S:65:ASP:HB2	1.94	0.67
23:B:304:PSC:H342	23:B:304:PSC:H12	1.77	0.67
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.77	0.67
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.77	0.66
4:D:34:SER:H	4:D:37:GLN:HE21	1.43	0.66
11:K:39:GLU:HB3	28:K:137:HOH:O	1.95	0.66
1:N:406:ASN:HD21	19:N:607:PGV:H22	1.60	0.66
8:H:9:LYS:O	8:H:10:ASN:HB2	1.94	0.66
2:B:115[B]:ASP:OD1	28:B:501:HOH:O	2.13	0.66
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.31	0.66
19:A:608:PGV:H152	19:A:608:PGV:H322	1.77	0.66
7:G:1:ALA:HB2	19:P:301:PGV:H321	1.76	0.66
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.42	0.66
20:Q:201:TGL:HA91	20:Q:201:TGL:C23	2.15	0.66
8:H:7:LYS:O	8:H:8:ILE:HB	1.96	0.66
2:O:218:TYR:HB3	28:O:513:HOH:O	1.94	0.66
7:T:31:CYS:SG	25:T:102:CDL:H551	2.36	0.66
1:A:417:MET:CE	14:A:601:HEA:H263	2.25	0.66
4:Q:78:TRP:CB	20:Q:201:TGL:HB22	2.27	0.65
1:A:417:MET:HE3	14:A:601:HEA:H263	1.77	0.65
1:N:159:LEU:HD21	28:P:499:HOH:O	1.96	0.65
1:A:406:ASN:HD21	19:A:608:PGV:H22	1.62	0.65
25:C:304:CDL:OB6	25:C:304:CDL:HB21	1.98	0.64
4:Q:20:ARG:HG2	28:Q:317:HOH:O	1.96	0.64
6:S:52:ILE:O	6:S:94:HIS:ND1	2.31	0.64
1:N:273:MET:HE2	28:N:921:HOH:O	1.97	0.63
4:Q:78:TRP:HB3	20:Q:201:TGL:HB22	1.79	0.63
3:C:224:LYS:HD3	25:C:304:CDL:HB31	1.80	0.63
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.80	0.63
23:N:610:PSC:H342	2:O:41:ILE:CD1	2.23	0.62
3:P:5:THR:HG22	6:S:96:LEU:CD1	2.29	0.62
23:N:610:PSC:C32	23:N:610:PSC:H12	2.29	0.62
4:D:109:HIS:HD2	28:D:306:HOH:O	1.83	0.62
2:O:227:LEU:HD21	28:O:546:HOH:O	2.00	0.61
25:G:101:CDL:H462	2:O:70:ALA:HB1	1.82	0.61
12:L:26:THR:HG23	13:M:25:SER:HB3	1.81	0.61
10:J:7:GLU:HG3	28:J:209:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ASP:OD1	5:E:44:GLU:HG3	1.98	0.61
1:N:136[B]:LEU:HD21	28:N:892:HOH:O	2.00	0.61
7:T:3:ALA:O	7:T:4:ALA:HB3	1.99	0.61
2:B:140:ASN:HB3	28:B:502:HOH:O	2.00	0.61
12:Y:12:PRO:CB	20:Y:101:TGL:HG11	2.31	0.61
2:B:7:LEU:HD12	20:B:301:TGL:HC52	1.83	0.61
1:N:136[B]:LEU:CD2	28:N:893:HOH:O	2.48	0.61
4:Q:78:TRP:HA	20:Q:201:TGL:HB22	1.83	0.60
12:Y:24:MET:SD	20:Y:101:TGL:H152	2.41	0.60
7:T:2:SER:OG	24:T:101:PEK:H292	2.00	0.60
1:A:311[A]:ILE:HG13	25:T:102:CDL:H432	1.83	0.60
10:J:33:ARG:HG2	22:J:101:CHD:H152	1.82	0.60
3:P:59:ARG:HA	25:P:305:CDL:H512	1.82	0.60
13:M:42:LYS:HB3	28:M:2326:HOH:O	2.01	0.60
7:T:31:CYS:SG	25:T:102:CDL:C55	2.90	0.60
3:P:246:ASP:HB2	28:P:473:HOH:O	2.02	0.60
6:S:43:LYS:H	6:S:43:LYS:HD3	0.48	0.60
4:D:121:LYS:HD3	11:K:52:GLU:HA	1.83	0.60
3:C:246:ASP:HB2	28:C:459:HOH:O	2.02	0.59
1:N:177:SER:H	1:N:180:GLN:HE21	1.50	0.59
5:R:72:LYS:HB2	5:R:82:TYR:CD2	2.37	0.59
9:I:45:LYS:HG3	28:I:144:HOH:O	2.02	0.59
1:N:484:THR:HG22	13:Z:2:THR:HG23	1.84	0.59
20:D:201:TGL:H202	20:D:201:TGL:H242	1.84	0.59
5:R:80:GLU:HG3	28:R:279:HOH:O	2.02	0.59
3:P:60:ASP:O	3:P:64:GLU:HG3	2.03	0.59
2:O:83:ILE:O	2:O:87:MET:HG3	2.02	0.59
6:F:92:VAL:O	6:F:92:VAL:HG23	2.02	0.59
7:T:31:CYS:SG	25:T:102:CDL:H532	2.42	0.59
5:R:79:LYS:HD2	5:R:79:LYS:N	2.16	0.59
6:S:43:LYS:HD2	6:S:88:HIS:CE1	2.38	0.59
3:C:161:GLN:HE22	24:C:307:PEK:C2	2.15	0.59
23:B:304:PSC:H22	23:B:304:PSC:H231	1.83	0.59
12:Y:12:PRO:CG	20:Y:101:TGL:HG11	2.32	0.58
7:G:3:ALA:O	7:G:4:ALA:CB	2.51	0.58
3:C:210:ILE:HG12	19:C:303:PGV:H132	1.84	0.58
12:Y:20:ARG:NH2	20:Y:101:TGL:HC32	2.18	0.58
1:N:449:MET:SD	2:O:5:MET:HG2	2.43	0.58
4:Q:73:ARG:HG2	4:Q:73:ARG:HH11	1.67	0.58
6:F:75:HIS:H	6:F:80:GLN:HE22	1.51	0.58
20:L:101:TGL:HC61	20:L:101:TGL:HC22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:N:610:PSC:H21	23:N:610:PSC:H222	1.84	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.02	0.58
4:Q:127:LYS:HD2	28:V:109:HOH:O	2.04	0.58
1:A:136[B]:LEU:HD11	28:A:927:HOH:O	2.04	0.58
6:S:94:HIS:CD2	6:S:95:GLN:H	2.21	0.58
2:O:127:GLU:HG2	28:O:543:HOH:O	2.04	0.58
10:J:37:THR:OG1	22:J:101:CHD:H5	2.04	0.57
25:G:101:CDL:H242	25:G:101:CDL:H542	1.86	0.57
25:G:101:CDL:H171	1:N:307:SER:HB3	1.85	0.57
19:N:607:PGV:H322	13:Z:19:LEU:HD23	1.86	0.57
3:P:33[A]:MET:HE1	3:P:42:LEU:N	2.13	0.57
3:C:161:GLN:NE2	24:C:307:PEK:C2	2.67	0.57
1:N:422:ASN:OD1	20:N:609:TGL:H262	2.03	0.57
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.87	0.57
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.85	0.57
7:G:72:ASN:H	7:G:76:ASN:ND2	1.96	0.57
24:P:308:PEK:H311	7:T:26:PRO:HB3	1.86	0.57
28:N:945:HOH:O	2:O:56:MET:SD	2.58	0.57
7:T:5:LYS:CG	24:T:101:PEK:H371	2.34	0.57
1:A:177:SER:H	1:A:180:GLN:HE21	1.53	0.57
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.87	0.57
6:F:95:GLN:C	6:F:97:ALA:H	2.06	0.57
2:O:1:FME:HE3	2:O:133:LEU:HD22	1.86	0.57
1:N:400:PHE:O	20:Y:101:TGL:H281	2.04	0.57
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.05	0.57
22:C:305:CHD:C23	22:C:305:CHD:H162	2.35	0.57
12:L:13:PHE:HB3	20:L:101:TGL:HG12	1.85	0.57
3:C:50:ASN:HD22	3:C:51[A]:MET:HE2	1.69	0.56
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	2.04	0.56
6:F:95:GLN:HB3	28:F:280:HOH:O	2.03	0.56
7:G:45:PRO:HD2	28:G:203:HOH:O	2.06	0.56
7:T:84:LYS:H	7:T:84:LYS:HZ3	1.52	0.56
25:G:101:CDL:H561	25:G:101:CDL:H771	1.87	0.56
12:L:26:THR:HG22	28:L:226:HOH:O	2.05	0.56
25:G:101:CDL:C56	25:G:101:CDL:H771	2.35	0.56
6:S:78:GLU:HB2	28:S:317:HOH:O	2.05	0.56
23:B:304:PSC:H241	23:B:304:PSC:H42	1.86	0.56
2:B:32:PHE:HE2	20:B:301:TGL:HA52	1.67	0.56
1:N:169[B]:ILE:HD11	1:N:189:MET:CE	2.36	0.56
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.71	0.56
8:H:43:MET:HE3	8:H:49:ASP:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:307:PEK:H361	25:G:101:CDL:C27	2.34	0.56
24:C:307:PEK:H041	7:G:17:ARG:HH22	1.71	0.56
25:G:101:CDL:C35	2:O:78:LEU:HD12	2.35	0.56
12:L:26:THR:HG23	13:M:25:SER:HB2	1.88	0.56
24:P:308:PEK:H383	25:T:102:CDL:H273	1.88	0.56
1:N:113:LEU:HD12	20:Y:101:TGL:C14	2.36	0.56
20:L:101:TGL:CC1	20:L:101:TGL:HC61	2.36	0.56
4:Q:6:VAL:HG12	4:Q:7:LYS:N	2.20	0.56
24:G:102:PEK:H241	28:G:266:HOH:O	2.06	0.56
1:A:297:MET:HG2	28:C:531:HOH:O	2.05	0.56
3:P:210:ILE:HD13	19:P:304:PGV:H301	1.87	0.55
7:T:72:ASN:N	7:T:76:ASN:HD22	1.99	0.55
20:Y:101:TGL:OG3	20:Y:101:TGL:OA1	2.24	0.55
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.36	0.55
1:N:409:TRP:HB3	1:N:471:ILE:HG12	1.88	0.55
1:N:483:LEU:HD21	13:Z:4:LYS:HE3	1.87	0.55
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.88	0.55
20:N:609:TGL:HC31	28:V:102:HOH:O	2.07	0.55
6:S:43:LYS:HE3	28:S:282:HOH:O	2.06	0.55
8:U:48:GLY:HA2	28:U:133:HOH:O	2.06	0.55
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.88	0.55
12:Y:12:PRO:HG2	20:Y:101:TGL:HG11	1.89	0.54
3:P:168:THR:HG22	24:P:308:PEK:H14	1.88	0.54
2:B:33:LEU:HD13	9:I:31:PHE:HD1	1.70	0.54
6:F:64:GLU:O	6:F:65:ASP:HB2	2.07	0.54
3:C:94:PHE:HD2	28:C:509:HOH:O	1.90	0.54
11:X:52:GLU:HG2	28:X:120:HOH:O	2.06	0.54
1:N:308:ALA:O	1:N:311[B]:ILE:HG22	2.08	0.54
8:H:50:VAL:HG23	28:H:156:HOH:O	2.07	0.54
1:N:321:PHE:HD2	23:N:610:PSC:C34	2.15	0.54
4:Q:10:ASP:HB3	4:Q:13:LEU:HD12	1.88	0.54
1:N:513:LEU:O	1:N:514:LYS:CB	2.31	0.54
1:A:513:LEU:O	1:A:514:LYS:CB	2.46	0.54
7:T:5:LYS:HD2	24:T:101:PEK:H371	1.89	0.54
28:P:529:HOH:O	25:T:102:CDL:H673	2.06	0.54
2:O:91:ASN:HD22	2:O:149:THR:HG21	1.73	0.54
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.37	0.54
25:G:101:CDL:H171	1:N:307:SER:CB	2.38	0.53
12:Y:12:PRO:HB2	20:Y:101:TGL:CG1	2.37	0.53
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.90	0.53
2:O:53:THR:HG21	28:Q:344:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:102:CDL:H781	25:T:102:CDL:H571	1.91	0.53
28:B:452:HOH:O	20:D:201:TGL:HC61	2.08	0.53
1:N:113:LEU:HD12	20:Y:101:TGL:C13	2.38	0.53
4:Q:19:ARG:CD	4:Q:21:ASP:OD1	2.57	0.53
3:P:77:LYS:NZ	3:P:81:TYR:OH	2.40	0.53
25:T:102:CDL:H172	28:T:222:HOH:O	2.07	0.53
7:G:84:LYS:HG2	28:G:253:HOH:O	2.08	0.53
1:A:309:THR:O	1:A:312[B]:ILE:HG22	2.08	0.53
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.91	0.53
1:A:311[B]:ILE:CD1	24:P:308:PEK:H342	2.39	0.53
8:H:43:MET:CE	8:H:49:ASP:H	2.22	0.53
8:U:45:ALA:O	8:U:47:GLY:N	2.42	0.53
25:G:101:CDL:H542	25:G:101:CDL:C24	2.38	0.53
2:B:49:LYS:HD3	20:D:201:TGL:HC72	1.91	0.53
3:C:191:GLY:HA3	28:G:204:HOH:O	2.09	0.53
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.44	0.53
23:N:610:PSC:H12	23:N:610:PSC:H321	1.90	0.53
7:T:5:LYS:HG3	24:T:101:PEK:C37	2.37	0.53
4:Q:6:VAL:HG12	4:Q:10:ASP:OD2	2.07	0.53
1:A:165:ILE:HG22	1:A:169[B]:ILE:HD12	1.91	0.53
28:O:479:HOH:O	20:Q:201:TGL:HC72	2.09	0.53
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.23	0.53
1:N:152:LEU:HD22	3:P:24:ALA:HB1	1.91	0.53
3:C:156:ARG:HE	22:C:305:CHD:C24	2.22	0.53
1:A:112:LEU:HG	28:A:749:HOH:O	2.10	0.52
10:J:55:PHE:HB2	28:J:230:HOH:O	2.09	0.52
12:L:2:HIS:CG	12:L:3:TYR:N	2.70	0.52
1:N:321:PHE:CZ	23:N:610:PSC:H162	2.45	0.52
8:H:8:ILE:HG23	8:H:8:ILE:O	2.09	0.52
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.92	0.52
2:B:1:FME:HE3	2:B:133:LEU:HD22	1.92	0.52
28:B:582:HOH:O	24:P:308:PEK:H301	2.08	0.52
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.92	0.52
2:O:116:LEU:HD13	2:O:226:MET:HG3	1.91	0.52
10:W:2:GLU:HA	28:W:218:HOH:O	2.09	0.52
20:L:101:TGL:CC2	20:L:101:TGL:HC61	2.39	0.52
23:N:610:PSC:H322	23:N:610:PSC:H12	1.92	0.52
2:O:1:FME:HE3	2:O:133:LEU:HD21	1.90	0.52
3:C:84:ILE:HD11	24:T:101:PEK:H031	1.92	0.52
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.91	0.52
3:C:59:ARG:HG3	25:C:304:CDL:H512	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:301:PGV:H21	28:P:512:HOH:O	2.09	0.52
3:P:168:THR:CG2	24:P:308:PEK:H14	2.40	0.52
23:B:304:PSC:C13	23:B:304:PSC:H342	2.39	0.52
1:N:390:MET:O	1:N:394[A]:VAL:HG22	2.10	0.52
25:T:102:CDL:HA21	25:T:102:CDL:H122	1.93	0.51
9:V:8:GLN:HG3	28:V:116:HOH:O	2.08	0.51
1:N:62:ALA:HB1	14:N:601:HEA:HMD3	1.92	0.51
20:N:609:TGL:H191	28:N:933:HOH:O	2.09	0.51
1:A:177:SER:H	1:A:180:GLN:NE2	2.08	0.51
6:S:76:LYS:CD	28:S:271:HOH:O	2.19	0.51
1:A:297:MET:HB2	28:A:924:HOH:O	2.11	0.51
7:G:8:HIS:O	7:G:9:GLY:C	2.47	0.51
1:A:76:GLY:O	1:A:80:ASN:HB2	2.11	0.51
19:P:301:PGV:H42	22:P:307:CHD:H151	1.93	0.51
19:A:608:PGV:P	19:A:608:PGV:H061	2.50	0.51
3:P:77:LYS:NZ	28:P:482:HOH:O	2.36	0.51
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	1.93	0.51
1:N:112:LEU:HD23	1:N:113:LEU:HD23	1.93	0.51
5:E:16:VAL:HG21	5:E:46:LYS:HG3	1.92	0.51
23:B:304:PSC:H042	28:E:217:HOH:O	2.10	0.50
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.46	0.50
23:N:610:PSC:H21	23:N:610:PSC:C22	2.40	0.50
24:C:307:PEK:C04	7:G:17:ARG:HH22	2.25	0.50
1:A:308:ALA:HA	25:T:102:CDL:H212	1.94	0.50
1:N:406:ASN:HD21	19:N:607:PGV:C2	2.25	0.50
1:N:136[B]:LEU:HD22	28:N:893:HOH:O	2.09	0.50
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.94	0.50
3:P:51[A]:MET:SD	25:P:305:CDL:H621	2.51	0.50
28:O:458:HOH:O	8:U:61:LYS:HE3	2.10	0.50
1:A:299:VAL:HG23	2:B:84:LEU:HG	1.94	0.50
7:T:2:SER:OG	24:T:101:PEK:C29	2.59	0.50
3:C:55:TYR:CE1	25:C:304:CDL:H521	2.47	0.50
6:F:87:THR:HG21	28:F:222:HOH:O	2.12	0.50
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
23:N:610:PSC:H072	9:V:10:ARG:HH21	1.77	0.50
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.47	0.50
19:C:303:PGV:H12	25:C:304:CDL:H651	1.93	0.50
1:A:343:GLY:HA2	20:D:201:TGL:H211	1.92	0.50
7:G:9:GLY:HA3	28:N:812:HOH:O	2.12	0.50
3:P:210:ILE:HG21	19:P:304:PGV:H282	1.93	0.50
23:B:304:PSC:H212	23:B:304:PSC:O01	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:LYS:HG3	8:H:11:TYR:H	1.77	0.50
19:A:608:PGV:H251	13:M:12:PRO:HG3	1.93	0.49
3:P:107:ALA:HB2	19:P:301:PGV:C03	2.41	0.49
2:B:82:ARG:HG2	2:B:86:MET:HE3	1.94	0.49
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.65	0.49
25:C:304:CDL:CB5	25:C:304:CDL:HB22	2.42	0.49
3:C:127:LEU:HD13	25:G:101:CDL:OB3	2.11	0.49
24:P:303:PEK:C20	24:P:303:PEK:H15	2.36	0.49
6:F:55:LYS:HG3	6:F:73:TRP:CZ3	2.48	0.49
1:N:155:VAL:HG21	19:N:608:PGV:H142	1.95	0.49
5:E:86:ILE:O	5:E:90:ARG:HG2	2.12	0.49
3:C:164:PHE:CD1	22:C:305:CHD:H192	2.48	0.49
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	1.94	0.49
19:N:608:PGV:H21	3:P:57:TRP:CZ2	2.47	0.49
19:N:608:PGV:H61	3:P:54:MET:HG2	1.94	0.49
1:A:415:ALA:HB1	20:D:201:TGL:H132	1.94	0.49
4:Q:7:LYS:HA	28:Q:373:HOH:O	2.13	0.49
25:P:305:CDL:H431	10:W:34:VAL:HG11	1.93	0.49
7:T:2:SER:O	7:T:3:ALA:HB3	2.11	0.49
4:D:34:SER:H	4:D:37:GLN:NE2	2.10	0.49
1:A:1:FME:HE3	1:A:4:ASN:HD22	1.76	0.49
2:B:58:ALA:O	2:B:62:GLU:HG3	2.12	0.49
25:G:101:CDL:HA21	25:G:101:CDL:C11	2.39	0.49
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.93	0.49
13:Z:40:TYR:O	13:Z:42:LYS:N	2.45	0.49
2:O:13:THR:HB	2:O:168:LEU:HD23	1.95	0.49
3:C:224:LYS:HD3	25:C:304:CDL:CB3	2.42	0.49
24:C:307:PEK:H292	28:O:486:HOH:O	2.13	0.49
1:N:317:GLY:O	1:N:321:PHE:CD1	2.66	0.49
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.49
19:N:608:PGV:C34	24:P:303:PEK:H382	2.35	0.48
28:R:294:HOH:O	9:V:11:GLY:HA2	2.12	0.48
1:A:459:PHE:HE2	28:A:949:HOH:O	1.96	0.48
7:G:2:SER:HB2	1:N:197:LEU:HD21	1.95	0.48
3:P:62:ILE:HD12	25:P:305:CDL:H511	1.94	0.48
25:G:101:CDL:H522	25:G:101:CDL:C20	2.37	0.48
1:N:28:MET:HE2	14:N:601:HEA:H271	1.95	0.48
2:B:30:ILE:HD13	28:B:571:HOH:O	2.13	0.48
1:A:1:FME:CE	1:A:4:ASN:HD22	2.27	0.48
7:G:2:SER:HB2	1:N:197:LEU:HD11	1.96	0.48
25:T:102:CDL:H571	25:T:102:CDL:C78	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ALA:HB1	25:T:102:CDL:H132	1.95	0.48
24:P:303:PEK:H161	24:P:303:PEK:H11	1.96	0.48
4:D:78:TRP:CA	20:D:201:TGL:CB2	2.92	0.48
1:A:409:TRP:HB3	1:A:471:ILE:HG12	1.95	0.48
9:I:57:MET:O	9:I:61:GLU:HG2	2.13	0.48
11:K:44:PRO:CA	11:K:47:ARG:HH21	2.27	0.48
2:B:41:ILE:HD13	23:B:304:PSC:H341	1.96	0.48
2:B:56:MET:CG	23:B:304:PSC:H221	2.43	0.47
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.12	0.47
23:N:610:PSC:C13	23:N:610:PSC:H343	2.44	0.47
7:G:37:LEU:HD21	25:G:101:CDL:H361	1.96	0.47
2:O:1:FME:CE	2:O:133:LEU:HD22	2.43	0.47
2:O:1:FME:HE3	2:O:133:LEU:HD11	1.95	0.47
3:C:204:HIS:HB2	3:C:252:LEU:HD11	1.97	0.47
12:Y:46:LYS:HG2	28:Y:229:HOH:O	2.15	0.47
12:L:20:ARG:HH22	20:L:101:TGL:HC52	1.79	0.47
12:Y:41:ARG:HG3	13:Z:40:TYR:CE1	2.50	0.47
10:W:36:MET:HB3	22:W:101:CHD:H181	1.97	0.47
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.13	0.47
1:N:87:ILE:O	1:N:173:PRO:HD3	2.14	0.47
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.45	0.47
3:C:226:HIS:CE1	25:C:304:CDL:HB32	2.50	0.47
8:U:7:LYS:HB2	28:U:139:HOH:O	2.14	0.47
24:P:308:PEK:C38	25:T:102:CDL:C27	2.93	0.47
8:H:9:LYS:O	8:H:10:ASN:CB	2.62	0.47
1:N:169[B]:ILE:HD11	1:N:189:MET:HE3	1.96	0.47
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.96	0.47
23:N:610:PSC:H241	23:N:610:PSC:H42	1.97	0.47
24:P:308:PEK:H332	24:P:308:PEK:H362	1.78	0.47
22:J:101:CHD:H3	22:J:101:CHD:H192	1.96	0.47
8:U:43:MET:HE3	8:U:49:ASP:N	2.29	0.47
6:S:76:LYS:CE	28:S:271:HOH:O	2.57	0.47
7:T:2:SER:O	24:T:101:PEK:H322	2.15	0.47
1:A:311[A]:ILE:HD13	25:T:102:CDL:C22	2.41	0.47
19:N:607:PGV:H302	13:Z:19:LEU:HD22	1.96	0.47
2:O:42:ILE:HG21	20:Q:201:TGL:H232	1.96	0.47
3:C:52:LEU:HD23	25:C:304:CDL:H362	1.97	0.47
25:T:102:CDL:H712	25:T:102:CDL:H521	1.97	0.47
3:P:127:LEU:HD22	25:T:102:CDL:HB62	1.96	0.47
12:L:24:MET:SD	20:L:101:TGL:HC82	2.55	0.46
25:G:101:CDL:H541	25:G:101:CDL:H732	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:MET:HG2	23:B:304:PSC:H201	1.95	0.46
28:C:536:HOH:O	24:T:101:PEK:H262	2.14	0.46
7:G:23:LEU:HD12	25:G:101:CDL:H271	1.97	0.46
2:O:4:PRO:HB2	11:X:43:SER:HA	1.96	0.46
9:I:36:LYS:HE3	9:I:36:LYS:HB2	1.64	0.46
7:T:7:ASP:O	7:T:9:GLY:N	2.49	0.46
24:C:302:PEK:H72	24:C:302:PEK:H102	1.73	0.46
4:D:78:TRP:N	20:D:201:TGL:CB2	2.77	0.46
19:N:607:PGV:H52	19:N:607:PGV:H21	1.64	0.46
24:C:302:PEK:C12	24:C:302:PEK:H161	2.45	0.46
25:G:101:CDL:H152	1:N:307:SER:OG	2.15	0.46
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	1.96	0.46
4:D:78:TRP:CA	20:D:201:TGL:HB22	2.45	0.46
2:B:14:SER:HB3	2:B:168:LEU:CD2	2.46	0.46
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.50	0.46
24:C:307:PEK:H383	25:G:101:CDL:H271	1.89	0.46
19:N:608:PGV:H343	24:P:303:PEK:C38	2.36	0.46
1:A:468:MET:HG3	28:A:937:HOH:O	2.15	0.46
2:O:67:ILE:CD1	28:O:486:HOH:O	2.62	0.46
25:T:102:CDL:OA7	25:T:102:CDL:H342	2.16	0.46
19:A:607:PGV:H343	24:C:302:PEK:H382	1.97	0.46
10:W:32:TYR:OH	22:W:101:CHD:H213	2.15	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
3:C:54:MET:HE1	19:C:303:PGV:H142	1.98	0.46
5:R:76:GLY:O	5:R:79:LYS:HE3	2.16	0.46
8:H:54:GLU:HA	8:H:54:GLU:OE1	2.16	0.46
7:T:2:SER:O	7:T:3:ALA:CB	2.64	0.45
6:F:95:GLN:O	6:F:97:ALA:N	2.40	0.45
3:C:62:ILE:HD12	25:C:304:CDL:H511	1.99	0.45
2:O:129:LYS:O	2:O:132:GLU:HG3	2.17	0.45
2:B:30:ILE:CD1	28:B:571:HOH:O	2.63	0.45
11:K:44:PRO:HA	11:K:47:ARG:HH21	1.80	0.45
22:W:101:CHD:H222	22:W:101:CHD:O12	2.15	0.45
13:M:39:ASN:N	13:M:39:ASN:OD1	2.49	0.45
25:P:305:CDL:H561	25:P:305:CDL:H531	1.50	0.45
2:O:128:LEU:HD22	2:O:132:GLU:HB2	1.97	0.45
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.52	0.45
2:O:114:GLU:HG3	28:O:505:HOH:O	2.15	0.45
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.99	0.45
19:A:608:PGV:H311	13:M:19:LEU:CD2	2.41	0.45
1:N:25:TRP:CH2	20:Y:101:TGL:H292	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:201:TGL:HG31	20:Q:201:TGL:HC21	1.77	0.45
5:R:77:PRO:O	5:R:79:LYS:HD2	2.16	0.45
7:T:11:TPO:CG2	7:T:11:TPO:O	2.65	0.45
4:D:98:TRP:CE2	27:M:101:DMU:H11	2.52	0.45
1:A:311[B]:ILE:HG12	1:A:311[B]:ILE:O	2.15	0.45
1:A:307:SER:HB2	25:T:102:CDL:H192	1.99	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.45
20:Y:101:TGL:H172	28:Y:235:HOH:O	2.17	0.45
13:M:39:ASN:O	13:M:43:SER:HB2	2.16	0.45
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.97	0.45
3:P:154:GLY:HA2	6:S:6:VAL:HB	1.97	0.45
23:B:304:PSC:H073	5:E:11:PHE:CG	2.52	0.45
7:G:43:GLU:HA	28:G:269:HOH:O	2.16	0.45
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.97	0.45
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.04	0.45
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.17	0.45
5:E:90:ARG:HG3	28:E:239:HOH:O	2.16	0.45
3:C:50:ASN:HD22	3:C:51[A]:MET:CE	2.30	0.45
11:K:8:ASP:HB2	28:K:111:HOH:O	2.16	0.45
1:N:468:MET:HG3	28:N:923:HOH:O	2.17	0.45
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.52	0.45
11:K:24:PHE:CE1	11:K:28:VAL:HG21	2.52	0.45
7:G:2:SER:CB	1:N:197:LEU:HD11	2.47	0.44
1:N:321:PHE:HD2	23:N:610:PSC:C33	2.30	0.44
28:B:452:HOH:O	20:D:201:TGL:CC6	2.64	0.44
4:Q:73:ARG:NH1	4:Q:73:ARG:HG2	2.32	0.44
8:H:43:MET:HE3	8:H:49:ASP:H	1.80	0.44
22:W:101:CHD:H232	22:W:101:CHD:H211	1.60	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.44
3:C:220:PHE:HB2	25:C:304:CDL:H712	1.99	0.44
2:O:116:LEU:CD2	2:O:226:MET:HG2	2.48	0.44
4:Q:19:ARG:CG	4:Q:21:ASP:OD1	2.65	0.44
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.81	0.44
6:F:64:GLU:O	6:F:65:ASP:CB	2.62	0.44
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.00	0.44
24:P:308:PEK:C38	25:T:102:CDL:H271	2.46	0.44
22:W:101:CHD:H111	22:W:101:CHD:H12A	1.85	0.44
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.53	0.44
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.83	0.44
3:P:52:LEU:HD23	25:P:305:CDL:H362	2.00	0.44
19:N:607:PGV:H251	13:Z:12:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:FME:HE2	28:B:418:HOH:O	2.18	0.44
2:B:76:ILE:HG13	28:B:571:HOH:O	2.18	0.44
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.49	0.44
14:A:601:HEA:H122	14:A:601:HEA:HHC	2.00	0.44
28:N:951:HOH:O	6:S:37:LYS:HE2	2.18	0.44
1:N:321:PHE:HB3	23:N:610:PSC:H331	2.00	0.44
24:C:307:PEK:H372	1:N:279:SER:OG	2.18	0.44
22:C:306:CHD:H212	22:C:306:CHD:H12	1.99	0.44
3:C:55:TYR:CD1	25:C:304:CDL:H181	2.53	0.43
14:A:601:HEA:H271	14:A:601:HEA:H212	1.44	0.43
12:Y:42:HIS:O	12:Y:46:LYS:HG3	2.18	0.43
8:U:34:LEU:O	8:U:38:ARG:HG3	2.19	0.43
3:C:122:HIS:HD2	28:C:467:HOH:O	2.00	0.43
23:N:610:PSC:H21	23:N:610:PSC:C21	2.48	0.43
25:G:101:CDL:H352	2:O:78:LEU:CD1	2.38	0.43
24:P:308:PEK:H382	25:T:102:CDL:C27	2.47	0.43
19:N:607:PGV:H211	28:Z:222:HOH:O	2.18	0.43
20:Y:101:TGL:H202	20:Y:101:TGL:H231	1.67	0.43
7:T:12:GLY:CA	28:T:207:HOH:O	2.65	0.43
1:N:105:LEU:HD23	1:N:105:LEU:HA	1.86	0.43
10:J:29:ASN:HD22	10:J:29:ASN:H	1.66	0.43
8:H:7:LYS:HA	28:H:145:HOH:O	2.18	0.43
5:R:44:GLU:OE1	9:V:6:LYS:NZ	2.40	0.43
2:B:146:MET:HA	2:B:213:LEU:HD12	2.01	0.43
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.99	0.43
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.01	0.43
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.00	0.43
3:P:144:ILE:CD1	3:P:239:ALA:HA	2.48	0.43
1:N:399:LEU:O	1:N:499:PRO:HA	2.18	0.43
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.54	0.43
10:J:37:THR:OG1	22:J:101:CHD:H191	2.18	0.43
1:N:240:HIS:O	1:N:241:PRO:C	2.56	0.43
13:Z:36:HIS:HD2	13:Z:39:ASN:HD22	1.67	0.43
6:F:54:ASN:HD22	6:F:54:ASN:H	1.65	0.43
6:S:54:ASN:C	6:S:54:ASN:HD22	2.22	0.43
12:L:20:ARG:HH22	20:L:101:TGL:CC3	2.11	0.43
24:C:302:PEK:H171	24:C:302:PEK:H203	1.81	0.43
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.44	0.43
1:A:449:MET:SD	2:B:5:MET:HG2	2.59	0.43
22:B:303:CHD:H212	22:B:303:CHD:H12	2.00	0.43
19:A:607:PGV:H183	24:C:302:PEK:H322	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:P:308:PEK:H6	24:P:308:PEK:H221	2.01	0.43
3:P:62:ILE:CD1	3:P:221:ARG:HD2	2.49	0.43
14:A:602:HEA:HAD2	14:A:602:HEA:HH A	1.76	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.18	0.43
4:Q:52:SER:HB2	28:Q:340:HOH:O	2.18	0.43
4:D:78:TRP:CA	20:D:201:TGL:HB21	2.49	0.42
1:A:309:THR:HG22	14:A:602:HEA:HMB2	2.00	0.42
7:G:3:ALA:HA	28:G:261:HOH:O	2.19	0.42
25:C:304:CDL:H182	25:C:304:CDL:H352	2.00	0.42
24:C:307:PEK:H383	25:G:101:CDL:H273	1.93	0.42
19:P:301:PGV:H202	19:P:301:PGV:H231	1.74	0.42
25:T:102:CDL:H181	25:T:102:CDL:CB5	2.50	0.42
12:Y:39:ILE:O	12:Y:42:HIS:HB3	2.19	0.42
3:P:213:THR:HG23	25:P:305:CDL:H771	2.01	0.42
25:C:304:CDL:CB2	25:C:304:CDL:CB5	2.98	0.42
25:C:304:CDL:OB6	25:C:304:CDL:CB2	2.67	0.42
25:G:101:CDL:C52	25:G:101:CDL:H202	2.39	0.42
2:O:103:GLN:HB3	2:O:104:TRP:CE2	2.55	0.42
25:P:305:CDL:H192	25:P:305:CDL:H222	1.80	0.42
20:Q:201:TGL:HB51	20:Q:201:TGL:HA32	2.00	0.42
12:Y:46:LYS:CD	28:Y:229:HOH:O	2.67	0.42
1:A:367:LEU:HD21	1:A:433:LEU:HD23	2.02	0.42
19:C:308:PGV:H51	19:C:308:PGV:H21	1.88	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.20	0.42
25:G:101:CDL:H591	25:G:101:CDL:C77	2.49	0.42
8:U:43:MET:HE3	8:U:49:ASP:H	1.85	0.42
23:N:610:PSC:H042	23:N:610:PSC:H062	1.85	0.42
1:A:282:PHE:HA	7:T:4:ALA:CB	2.49	0.42
1:N:169[B]:ILE:CD1	1:N:189:MET:HE1	2.50	0.42
2:B:216:LEU:O	2:B:220:GLU:HG3	2.20	0.42
28:A:955:HOH:O	2:B:206:PHE:CE1	2.51	0.42
2:O:168:LEU:HD13	2:O:184:LEU:HG	2.01	0.42
1:N:269:GLY:HA2	28:O:500:HOH:O	2.19	0.42
3:P:155:ASP:OD2	6:S:2:SER:HA	2.20	0.42
6:S:43:LYS:N	6:S:43:LYS:HD2	2.24	0.42
3:P:33[A]:MET:CE	3:P:41:THR:HB	2.50	0.42
3:P:5:THR:HG22	6:S:96:LEU:HD11	1.99	0.42
11:K:52:GLU:HG3	28:K:131:HOH:O	2.18	0.42
28:B:580:HOH:O	4:D:126:MET:SD	2.62	0.42
10:W:58:LYS:HD3	10:W:58:LYS:HA	1.70	0.42
25:G:101:CDL:H132	2:O:81:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:104:LEU:C	1:N:107:PRO:HD2	2.40	0.42
9:I:51:TYR:HA	9:I:54:TYR:HB2	2.02	0.42
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.50	0.42
3:P:157:LYS:HD3	28:P:520:HOH:O	2.20	0.42
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.54	0.42
25:G:101:CDL:H591	25:G:101:CDL:H771	2.02	0.41
2:B:191:LEU:HD23	2:B:212:GLU:HA	2.01	0.41
19:A:608:PGV:C31	13:M:19:LEU:HD23	2.42	0.41
22:P:307:CHD:H12	22:P:307:CHD:H212	2.01	0.41
7:T:38:HIS:HE1	25:T:102:CDL:H121	1.83	0.41
19:N:607:PGV:H131	19:N:607:PGV:H301	2.02	0.41
20:N:609:TGL:H152	2:O:7:LEU:HD11	2.01	0.41
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.55	0.41
8:H:52:VAL:HG12	28:H:166:HOH:O	2.19	0.41
7:G:5:LYS:CG	24:G:102:PEK:H383	2.35	0.41
3:C:210:ILE:HG21	19:C:303:PGV:H281	2.01	0.41
3:C:63:ARG:HE	25:C:304:CDL:HA21	1.83	0.41
24:C:307:PEK:C36	25:G:101:CDL:H273	2.45	0.41
5:E:12:ASP:HB3	5:E:46:LYS:HE2	2.03	0.41
4:Q:57:VAL:HG21	28:R:258:HOH:O	2.20	0.41
9:V:49:ASP:HB3	28:V:132:HOH:O	2.20	0.41
1:A:426:PHE:HB3	1:A:427:PRO:HD3	2.03	0.41
3:C:76:GLN:NE2	28:C:435:HOH:O	2.46	0.41
24:P:303:PEK:H161	24:P:303:PEK:C11	2.49	0.41
7:T:30:LEU:CD2	25:T:102:CDL:H471	2.44	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.55	0.41
7:T:33:LEU:O	7:T:34:ASN:C	2.59	0.41
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.50	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.93	0.41
12:Y:20:ARG:HD3	28:Y:211:HOH:O	2.20	0.41
7:T:11:TPO:HG22	7:T:11:TPO:O	2.20	0.41
6:F:55:LYS:HA	6:F:74:LEU:O	2.20	0.41
2:B:60:GLU:HG3	2:B:60:GLU:H	1.56	0.41
2:B:90:ILE:H	2:B:90:ILE:HG13	1.73	0.41
4:Q:39:ALA:HB1	28:Q:354:HOH:O	2.21	0.41
25:G:101:CDL:H602	25:G:101:CDL:H631	1.87	0.41
1:N:169[B]:ILE:HD11	1:N:189:MET:HE1	2.02	0.41
8:U:9:LYS:HB3	8:U:10:ASN:H	1.66	0.41
3:P:33[A]:MET:CE	3:P:42:LEU:H	2.18	0.41
1:N:136[B]:LEU:HD11	28:N:935:HOH:O	2.20	0.41
3:P:144:ILE:HD13	3:P:239:ALA:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLU:CD	28:A:945:HOH:O	2.59	0.41
2:B:145:PRO:HA	2:B:214:VAL:O	2.20	0.41
25:G:101:CDL:H541	25:G:101:CDL:H712	2.03	0.41
14:N:601:HEA:HHC	14:N:601:HEA:H122	2.03	0.41
6:F:92:VAL:O	6:F:92:VAL:CG2	2.66	0.41
1:A:412:ILE:HG12	4:D:84:ALA:HB3	2.03	0.41
7:T:5:LYS:CD	24:T:101:PEK:H371	2.49	0.40
2:O:67:ILE:HD13	28:O:486:HOH:O	2.20	0.40
25:T:102:CDL:H712	25:T:102:CDL:C52	2.51	0.40
3:P:64:GLU:HA	3:P:68:GLN:HE21	1.86	0.40
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.03	0.40
3:P:156:ARG:HE	22:P:306:CHD:C23	2.33	0.40
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.03	0.40
2:B:168:LEU:HA	2:B:168:LEU:HD23	1.94	0.40
1:N:189:MET:HG3	1:N:190:ILE:N	2.29	0.40
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.56	0.40
3:P:160:LEU:HD13	22:P:306:CHD:H181	2.03	0.40
9:I:73:LYS:HA	9:I:73:LYS:HD2	1.60	0.40
23:B:304:PSC:C07	9:I:10:ARG:HH21	2.34	0.40
1:A:417:MET:HE1	14:A:601:HEA:H263	2.03	0.40
10:J:52:TRP:O	10:J:57:HIS:HE1	2.02	0.40
3:P:55:TYR:CE1	25:P:305:CDL:H171	2.57	0.40
7:T:72:ASN:H	7:T:76:ASN:ND2	2.03	0.40
10:J:32:TYR:OH	22:J:101:CHD:H213	2.22	0.40
8:H:39:CYS:O	8:H:43:MET:HG2	2.21	0.40
11:X:54:ARG:NH2	28:X:130:HOH:O	2.53	0.40
1:N:412:ILE:HD13	4:Q:84:ALA:HB3	2.04	0.40

All (14) 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)
28:F:294:HOH:O	28:K:114:HOH:O[2_585]	1.63	0.57
9:I:2:THR:CG2	5:R:80:GLU:OE1[3_647]	1.83	0.37
28:B:586:HOH:O	28:M:2318:HOH:O[2_584]	1.90	0.30
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	1.93	0.27
6:S:95:GLN:N	28:O:535:HOH:O[2_685]	1.95	0.25
6:F:94:HIS:CE1	28:D:393:HOH:O[2_585]	1.98	0.22
6:S:94:HIS:CD2	28:O:535:HOH:O[2_685]	2.00	0.20
9:I:2:THR:CB	5:R:80:GLU:OE1[3_647]	2.06	0.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:CA	28:O:547:HOH:O[2_685]	2.07	0.13
28:B:592:HOH:O	28:M:2318:HOH:O[2_584]	2.09	0.11
6:S:95:GLN:CA	28:O:535:HOH:O[2_685]	2.10	0.10
28:O:533:HOH:O	28:S:307:HOH:O[2_684]	2.10	0.10
2:O:126:SER:O	6:S:94:HIS:CG[2_684]	2.12	0.08
6:S:95:GLN:N	28:O:547:HOH:O[2_685]	2.18	0.02

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/514 (101%)	500 (96%)	18 (4%)	0	100	100
1	N	518/514 (101%)	501 (97%)	17 (3%)	0	100	100
2	B	226/227 (100%)	213 (94%)	13 (6%)	0	100	100
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	39	27
3	C	260/261 (100%)	254 (98%)	6 (2%)	0	100	100
3	P	260/261 (100%)	255 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	136 (96%)	5 (4%)	1 (1%)	26	14
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100
6	F	96/98 (98%)	91 (95%)	2 (2%)	3 (3%)	5	1
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	1
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	2	0
7	T	81/85 (95%)	68 (84%)	8 (10%)	5 (6%)	2	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	4	0
8	U	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3523/3614 (98%)	3376 (96%)	123 (4%)	24 (1%)	26	14

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	5	LYS
7	T	8	HIS
8	U	8	ILE
8	U	46	LYS
6	F	95	GLN
7	G	37	LEU
7	T	38	HIS
7	G	7	ASP
2	O	92	ASN
7	T	4	ALA
8	U	45	ALA
4	Q	35	ALA
6	S	96	LEU
7	G	5	LYS
8	H	10	ASN
8	H	45	ALA

### 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	432/426 (101%)	426 (99%)	6 (1%)	74	71
1	N	432/426 (101%)	424 (98%)	8 (2%)	65	59
2	B	211/210 (100%)	199 (94%)	12 (6%)	25	13
2	O	210/210 (100%)	202 (96%)	8 (4%)	40	28
3	C	227/226 (100%)	223 (98%)	4 (2%)	66	61
3	P	227/226 (100%)	221 (97%)	6 (3%)	54	45
4	D	128/129 (99%)	127 (99%)	1 (1%)	86	86
4	Q	128/129 (99%)	125 (98%)	3 (2%)	58	51
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	34
5	R	92/95 (97%)	89 (97%)	3 (3%)	45	34
6	F	81/81 (100%)	76 (94%)	5 (6%)	23	11
6	S	81/81 (100%)	78 (96%)	3 (4%)	41	29
7	G	67/68 (98%)	62 (92%)	5 (8%)	17	7
7	T	67/68 (98%)	58 (87%)	9 (13%)	5	1
8	H	71/75 (95%)	66 (93%)	5 (7%)	19	8
8	U	71/75 (95%)	68 (96%)	3 (4%)	36	24
9	I	57/57 (100%)	56 (98%)	1 (2%)	66	61
9	V	57/57 (100%)	54 (95%)	3 (5%)	28	16
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	57
11	K	39/46 (85%)	38 (97%)	1 (3%)	54	45
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	45
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16	6
13	M	37/38 (97%)	34 (92%)	3 (8%)	15	5
13	Z	37/38 (97%)	35 (95%)	2 (5%)	27	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3059/3082 (99%)	2960 (97%)	99 (3%)	46 35

All (99) 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	189	MET
1	A	369	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	116	LEU
2	B	171	LYS
3	C	17	PRO
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	31	LYS
5	E	5	HIS
5	E	70	VAL
5	E	90	ARG
6	F	54	ASN
6	F	78	GLU
6	F	80	GLN
6	F	87	THR
6	F	96	LEU
7	G	2	SER
7	G	18	PHE
7	G	33	LEU
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS

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Mol	Chain	Res	Type
8	H	9	LYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
11	K	47	ARG
12	L	47	LYS
13	M	12	PRO
13	M	38	ASP
13	M	39	ASN
1	N	34	SER
1	N	109	PHE
1	N	138	HIS
1	N	362	SER
1	N	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	495	LEU
2	O	33	LEU
2	O	60	GLU
2	O	61	VAL
2	O	65	TRP
2	O	68	LEU
2	O	78	LEU
2	O	94	SER
2	O	171	LYS
3	P	33[A]	MET
3	P	33[B]	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
3	P	244	PHE
4	Q	4	SER
4	Q	10	ASP
4	Q	20	ARG
5	R	5	HIS
5	R	46	LYS
5	R	79	LYS
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
7	T	2	SER

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Mol	Chain	Res	Type
7	T	8	HIS
7	T	18	PHE
7	T	33	LEU
7	T	35	SER
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	9	LYS
8	U	60	TYR
8	U	84	LYS
9	V	8	GLN
9	V	36	LYS
9	V	52	ARG
10	W	50	LEU
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
13	Z	2	THR
13	Z	38	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
2	B	59	GLN
2	B	91	ASN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
3	C	161	GLN
4	D	37	GLN
4	D	109	HIS
4	D	143	ASN
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	76	ASN
8	H	37	HIS

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Mol	Chain	Res	Type
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN
8	U	37	HIS
10	W	29	ASN
13	Z	36	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	A	1	1	8,9,10	0.49	0	6,9,11	1.57	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FME	B	1	2	8,9,10	1.59	1 (12%)	6,9,11	9.21	3 (50%)
7	TPO	G	11	7	8,10,11	1.39	1 (12%)	7,14,16	1.79	1 (14%)
9	SAC	I	1	9	7,8,9	2.26	2 (28%)	7,9,11	1.10	1 (14%)
1	FME	N	1	1	8,9,10	0.87	0	6,9,11	1.48	1 (16%)
2	FME	O	1	2	8,9,10	0.87	0	6,9,11	2.62	3 (50%)
7	TPO	T	11	7	8,10,11	1.60	1 (12%)	7,14,16	1.83	1 (14%)
9	SAC	V	1	9	7,8,9	2.21	2 (28%)	7,9,11	1.71	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	0/6/9/11	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	-	0/6/9/11	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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.42	1.12	1.22
7	G	11	TPO	P-O1P	2.46	1.59	1.51
9	I	1	SAC	CA-N	2.88	1.50	1.46
7	T	11	TPO	P-O1P	3.08	1.61	1.51
9	V	1	SAC	CA-N	3.27	1.51	1.46
9	V	1	SAC	OAC-C1A	4.71	1.34	1.23
9	I	1	SAC	OAC-C1A	4.98	1.34	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.41	91.43	122.82
2	O	1	FME	O1-CN-N	-5.03	117.51	124.76
2	B	1	FME	O-C-CA	-3.13	117.18	125.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CG-CB-CA	-2.86	104.68	113.06
1	N	1	FME	O-C-CA	-2.29	119.39	125.44
9	I	1	SAC	CB-CA-N	-2.16	105.87	110.60
9	V	1	SAC	CB-CA-N	-2.11	105.99	110.60
9	V	1	SAC	O-C-CA	-2.10	119.89	125.44
2	O	1	FME	O-C-CA	-2.02	120.11	125.44
9	V	1	SAC	C2A-C1A-N	2.03	120.00	116.11
7	G	11	TPO	CG2-CB-CA	2.86	119.00	113.17
1	A	1	FME	CE-SD-CG	2.95	110.43	100.37
7	T	11	TPO	CG2-CB-CA	3.10	119.47	113.17
2	B	1	FME	O1-CN-N	8.86	137.52	124.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
2	B	1	FME	2	0
7	G	11	TPO	1	0
2	O	1	FME	9	0
7	T	11	TPO	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 10 are monoatomic - leaving 46 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	HEA	A	601	1	40,67,67	1.45	5 (12%)	41,103,103	2.42	14 (34%)
14	HEA	A	602	1,18	40,67,67	1.89	13 (32%)	41,103,103	2.33	13 (31%)
18	PER	A	606[A]	15,14	0,1,1	0.00	-	0,0,0	0.00	-
18	PER	A	606[B]	15	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	A	607	-	50,50,50	1.12	4 (8%)	51,56,56	1.29	5 (9%)
19	PGV	A	608	-	50,50,50	1.17	2 (4%)	51,56,56	1.50	6 (11%)
20	TGL	B	301	-	62,62,62	1.27	6 (9%)	65,65,65	1.75	11 (16%)
21	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	B	303	-	29,32,32	1.41	4 (13%)	48,51,51	1.85	11 (22%)
23	PSC	B	304	-	51,51,51	1.18	3 (5%)	55,59,59	1.18	3 (5%)
24	PEK	C	302	-	51,52,52	0.98	2 (3%)	52,57,57	1.14	6 (11%)
19	PGV	C	303	-	50,50,50	0.92	2 (4%)	51,56,56	1.40	8 (15%)
25	CDL	C	304	-	99,99,99	1.38	13 (13%)	101,111,111	1.51	12 (11%)
22	CHD	C	305	-	29,32,32	0.66	0	48,51,51	2.28	16 (33%)
22	CHD	C	306	-	29,32,32	1.15	3 (10%)	48,51,51	1.79	12 (25%)
24	PEK	C	307	-	51,52,52	1.07	2 (3%)	52,57,57	1.27	5 (9%)
19	PGV	C	308	-	50,50,50	1.15	3 (6%)	51,56,56	1.26	3 (5%)
20	TGL	D	201	-	62,62,62	1.51	7 (11%)	65,65,65	1.63	14 (21%)
25	CDL	G	101	-	99,99,99	1.32	12 (12%)	101,111,111	1.32	9 (8%)
24	PEK	G	102	-	51,52,52	1.10	2 (3%)	52,57,57	1.32	5 (9%)
22	CHD	G	103	-	29,32,32	1.50	5 (17%)	48,51,51	2.38	18 (37%)
22	CHD	J	101	-	29,32,32	0.65	0	48,51,51	2.66	24 (50%)
20	TGL	L	101	-	62,62,62	1.36	6 (9%)	65,65,65	1.47	9 (13%)
27	DMU	M	101	-	34,34,34	0.66	0	45,45,45	2.42	13 (28%)
14	HEA	N	601	1	40,67,67	1.14	5 (12%)	41,103,103	2.05	13 (31%)
14	HEA	N	602	1,18	40,67,67	1.41	4 (10%)	41,103,103	1.81	11 (26%)
18	PER	N	606[A]	15,14	0,1,1	0.00	-	0,0,0	0.00	-
18	PER	N	606[B]	15	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	N	607	-	50,50,50	0.99	2 (4%)	51,56,56	1.33	8 (15%)
19	PGV	N	608	-	50,50,50	1.02	2 (4%)	51,56,56	1.52	5 (9%)
20	TGL	N	609	-	62,62,62	1.30	6 (9%)	65,65,65	1.67	9 (13%)
23	PSC	N	610	-	51,51,51	1.21	3 (5%)	55,59,59	1.29	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	P	301	-	50,50,50	1.02	2 (4%)	51,56,56	1.21	5 (9%)
24	PEK	P	303	-	51,52,52	1.06	3 (5%)	52,57,57	1.46	6 (11%)
19	PGV	P	304	-	50,50,50	0.95	2 (4%)	51,56,56	1.06	3 (5%)
25	CDL	P	305	-	99,99,99	1.35	14 (14%)	101,111,111	1.40	10 (9%)
22	CHD	P	306	-	29,32,32	0.84	1 (3%)	48,51,51	2.45	18 (37%)
22	CHD	P	307	-	29,32,32	1.29	2 (6%)	48,51,51	1.39	4 (8%)
24	PEK	P	308	-	51,52,52	1.12	2 (3%)	52,57,57	1.11	4 (7%)
20	TGL	Q	201	-	62,62,62	1.51	7 (11%)	65,65,65	1.32	11 (16%)
24	PEK	T	101	-	51,52,52	1.03	2 (3%)	52,57,57	1.28	4 (7%)
25	CDL	T	102	-	99,99,99	1.31	12 (12%)	101,111,111	1.35	12 (11%)
22	CHD	W	101	-	29,32,32	0.77	0	48,51,51	3.12	17 (35%)
20	TGL	Y	101	-	62,62,62	1.34	6 (9%)	65,65,65	1.56	11 (16%)
27	DMU	Z	101	-	34,34,34	0.74	1 (2%)	45,45,45	1.84	11 (24%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	G	101	-	-	0/110/110/110	0/0/0/0
24	PEK	G	102	-	-	0/56/56/56	0/0/0/0
22	CHD	G	103	-	-	0/7/74/74	0/4/4/4
22	CHD	J	101	-	-	0/7/74/74	0/4/4/4
20	TGL	L	101	-	-	0/65/65/65	0/0/0/0
27	DMU	M	101	-	2/2/10/10	0/19/59/59	0/2/2/2
14	HEA	N	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1,18	2/2/7/16	0/24/76/76	0/0/8/8
18	PER	N	606[A]	15,14	-	0/0/0/0	0/0/0/0
18	PER	N	606[B]	15	-	0/0/0/0	0/0/0/0
19	PGV	N	607	-	-	0/55/55/55	0/0/0/0
19	PGV	N	608	-	-	0/55/55/55	0/0/0/0
20	TGL	N	609	-	-	0/65/65/65	0/0/0/0
23	PSC	N	610	-	-	0/55/55/55	0/0/0/0
21	CUA	O	301	2	-	0/0/0/0	0/0/0/0
19	PGV	P	301	-	-	0/55/55/55	0/0/0/0
24	PEK	P	303	-	-	0/56/56/56	0/0/0/0
19	PGV	P	304	-	-	0/55/55/55	0/0/0/0
25	CDL	P	305	-	-	0/110/110/110	0/0/0/0
22	CHD	P	306	-	-	0/7/74/74	0/4/4/4
22	CHD	P	307	-	-	0/7/74/74	0/4/4/4
24	PEK	P	308	-	-	0/56/56/56	0/0/0/0
20	TGL	Q	201	-	-	0/65/65/65	0/0/0/0
24	PEK	T	101	-	-	0/56/56/56	0/0/0/0
25	CDL	T	102	-	-	1/110/110/110	0/0/0/0
22	CHD	W	101	-	-	0/7/74/74	0/4/4/4
20	TGL	Y	101	-	-	0/65/65/65	0/0/0/0
27	DMU	Z	101	-	2/2/10/10	0/19/59/59	0/2/2/2

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C1A-NA	-4.28	1.30	1.36
14	N	602	HEA	C1A-NA	-3.91	1.31	1.36
25	T	102	CDL	C42-C41	-3.66	1.30	1.51
22	G	103	CHD	C10-C5	-3.53	1.49	1.55
25	C	304	CDL	C59-C58	-3.37	1.32	1.51
20	Y	101	TGL	C20-CA9	-3.36	1.32	1.51
25	C	304	CDL	C79-C78	-3.34	1.32	1.51
14	A	602	HEA	C3C-C2C	-3.33	1.35	1.40
20	N	609	TGL	C10-CB9	-3.24	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	305	CDL	C59-C58	-3.23	1.32	1.51
20	L	101	TGL	C20-CA9	-3.20	1.33	1.51
20	D	201	TGL	C10-CB9	-3.19	1.33	1.51
25	P	305	CDL	C62-C61	-3.17	1.33	1.51
25	T	102	CDL	C39-C38	-3.14	1.33	1.51
20	Q	201	TGL	C10-CB9	-3.13	1.33	1.51
25	P	305	CDL	C79-C78	-3.13	1.33	1.51
25	G	101	CDL	C82-C81	-3.12	1.33	1.51
20	N	609	TGL	C20-CA9	-3.11	1.33	1.51
25	G	101	CDL	C59-C58	-3.06	1.33	1.51
25	T	102	CDL	C59-C58	-3.06	1.33	1.51
25	T	102	CDL	C22-C21	-3.05	1.33	1.51
25	C	304	CDL	C82-C81	-3.05	1.33	1.51
25	G	101	CDL	C79-C78	-3.05	1.33	1.51
25	P	305	CDL	C39-C38	-3.05	1.33	1.51
25	T	102	CDL	C82-C81	-3.05	1.33	1.51
25	C	304	CDL	C19-C18	-3.03	1.34	1.51
20	L	101	TGL	C10-CB9	-3.02	1.34	1.51
25	C	304	CDL	C22-C21	-3.01	1.34	1.51
25	C	304	CDL	C39-C38	-3.01	1.34	1.51
25	C	304	CDL	C62-C61	-2.99	1.34	1.51
25	C	304	CDL	C42-C41	-2.98	1.34	1.51
25	T	102	CDL	C19-C18	-2.98	1.34	1.51
25	G	101	CDL	C62-C61	-2.98	1.34	1.51
20	Y	101	TGL	C10-CB9	-2.96	1.34	1.51
20	B	301	TGL	C20-CA9	-2.96	1.34	1.51
25	P	305	CDL	C82-C81	-2.95	1.34	1.51
25	T	102	CDL	C79-C78	-2.93	1.34	1.51
20	B	301	TGL	C10-CB9	-2.93	1.34	1.51
25	P	305	CDL	C19-C18	-2.93	1.34	1.51
25	G	101	CDL	C42-C41	-2.93	1.34	1.51
25	P	305	CDL	C42-C41	-2.90	1.34	1.51
14	N	601	HEA	C4A-NA	-2.82	1.32	1.36
14	N	601	HEA	C1D-ND	-2.81	1.32	1.36
25	P	305	CDL	C22-C21	-2.81	1.35	1.51
20	Q	201	TGL	C15-CC9	-2.80	1.35	1.51
25	G	101	CDL	C39-C38	-2.80	1.35	1.51
20	Y	101	TGL	C15-CC9	-2.78	1.35	1.51
20	D	201	TGL	C15-CC9	-2.78	1.35	1.51
20	N	609	TGL	C15-CC9	-2.72	1.35	1.51
20	Q	201	TGL	C20-CA9	-2.72	1.35	1.51
25	T	102	CDL	C62-C61	-2.71	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	201	TGL	C20-CA9	-2.68	1.36	1.51
25	G	101	CDL	C19-C18	-2.67	1.36	1.51
20	L	101	TGL	C15-CC9	-2.62	1.36	1.51
20	B	301	TGL	C15-CC9	-2.58	1.36	1.51
25	G	101	CDL	C22-C21	-2.53	1.36	1.51
25	C	304	CDL	OB6-CB4	-2.34	1.40	1.46
19	A	607	PGV	P-O14	-2.34	1.45	1.54
14	A	602	HEA	CAA-C2A	-2.27	1.48	1.52
14	A	602	HEA	C1A-NA	-2.03	1.33	1.36
19	C	308	PGV	C01-C02	2.03	1.56	1.50
14	N	602	HEA	C16-C15	2.04	1.55	1.51
19	N	608	PGV	O06-C06	2.04	1.51	1.42
22	B	303	CHD	C13-C12	2.07	1.57	1.54
25	P	305	CDL	PB2-OB3	2.09	1.58	1.51
25	P	305	CDL	O1-C1	2.10	1.49	1.43
14	A	602	HEA	C20-C19	2.10	1.56	1.51
22	B	303	CHD	C11-C9	2.10	1.57	1.53
14	N	601	HEA	CMB-C2B	2.11	1.56	1.51
14	N	601	HEA	C1C-CHC	2.15	1.45	1.39
22	P	306	CHD	C8-C9	2.15	1.58	1.53
14	A	602	HEA	CMC-C2C	2.17	1.56	1.51
14	A	602	HEA	C4C-CHD	2.18	1.45	1.39
27	Z	101	DMU	O16-C6	2.18	1.44	1.40
14	N	602	HEA	C18-C19	2.19	1.37	1.33
14	A	602	HEA	C1C-CHC	2.20	1.45	1.39
19	A	607	PGV	C01-C02	2.25	1.57	1.50
14	A	601	HEA	O11-C11	2.26	1.48	1.42
22	C	306	CHD	C11-C9	2.28	1.57	1.53
14	N	601	HEA	O11-C11	2.31	1.48	1.42
22	G	103	CHD	C11-C9	2.36	1.57	1.53
22	C	306	CHD	C21-C20	2.39	1.59	1.53
14	A	602	HEA	C3A-C2A	2.42	1.43	1.40
19	A	607	PGV	O01-C1	2.44	1.41	1.34
22	G	103	CHD	C13-C12	2.45	1.58	1.54
22	P	307	CHD	C11-C12	2.49	1.57	1.53
22	B	303	CHD	C4-C5	2.73	1.58	1.53
22	G	103	CHD	C6-C5	2.80	1.58	1.53
14	A	601	HEA	C3A-CMA	2.83	1.53	1.46
22	G	103	CHD	C18-C13	2.86	1.59	1.54
22	C	306	CHD	C18-C13	2.89	1.59	1.54
19	P	304	PGV	O01-C1	2.92	1.43	1.34
19	C	303	PGV	O01-C1	2.97	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	303	PEK	O01-C1	2.98	1.43	1.34
20	B	301	TGL	OG2-CB1	3.06	1.43	1.34
14	A	601	HEA	C1C-CHC	3.17	1.48	1.39
25	C	304	CDL	OB6-CB5	3.19	1.43	1.34
14	A	601	HEA	CMB-C2B	3.36	1.58	1.51
14	A	602	HEA	CMB-C2B	3.45	1.58	1.51
22	B	303	CHD	C4-C3	3.45	1.58	1.51
22	P	307	CHD	C8-C7	3.46	1.59	1.53
24	P	303	PEK	C2-C1	3.51	1.61	1.50
25	P	305	CDL	OB6-CB5	3.54	1.44	1.34
19	C	303	PGV	O03-C19	3.58	1.44	1.33
14	A	602	HEA	C18-C19	3.59	1.40	1.33
14	N	602	HEA	CMD-C2D	3.62	1.59	1.51
14	A	602	HEA	CAD-C3D	3.70	1.58	1.52
24	C	302	PEK	O01-C1	3.76	1.45	1.34
20	Y	101	TGL	OG1-CA1	3.77	1.44	1.33
19	N	607	PGV	O01-C1	3.85	1.45	1.34
19	P	301	PGV	O01-C1	3.92	1.46	1.34
20	D	201	TGL	OG3-CC1	3.92	1.45	1.33
19	P	304	PGV	O03-C19	3.96	1.45	1.33
25	T	102	CDL	OB8-CB7	3.97	1.45	1.33
19	A	607	PGV	O03-C19	4.01	1.45	1.33
20	N	609	TGL	OG2-CB1	4.05	1.46	1.34
23	B	304	PSC	C13-C12	4.07	1.55	1.31
23	B	304	PSC	O03-C19	4.09	1.45	1.33
25	G	101	CDL	OA8-CA7	4.10	1.45	1.33
24	T	101	PEK	O01-C1	4.13	1.46	1.34
23	N	610	PSC	C13-C12	4.15	1.55	1.31
25	T	102	CDL	OB6-CB5	4.15	1.46	1.34
14	A	602	HEA	C1D-ND	4.17	1.42	1.36
24	P	303	PEK	O03-C21	4.19	1.45	1.33
25	G	101	CDL	OB6-CB5	4.21	1.46	1.34
25	P	305	CDL	OA6-CA5	4.21	1.46	1.34
20	Q	201	TGL	OG3-CC1	4.25	1.46	1.33
25	C	304	CDL	OB8-CB7	4.25	1.46	1.33
19	N	608	PGV	O03-C19	4.35	1.46	1.33
25	P	305	CDL	OB8-CB7	4.36	1.46	1.33
24	C	302	PEK	O03-C21	4.36	1.46	1.33
23	N	610	PSC	O03-C19	4.39	1.46	1.33
19	A	608	PGV	O01-C1	4.41	1.47	1.34
14	A	602	HEA	CMD-C2D	4.42	1.61	1.51
19	C	308	PGV	O03-C19	4.44	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	304	CDL	OA6-CA5	4.46	1.47	1.34
20	L	101	TGL	OG3-CC1	4.47	1.46	1.33
20	L	101	TGL	OG1-CA1	4.50	1.46	1.33
25	T	102	CDL	OA6-CA5	4.52	1.47	1.34
23	B	304	PSC	O01-C1	4.53	1.47	1.34
24	P	308	PEK	O03-C21	4.54	1.47	1.33
25	G	101	CDL	OA6-CA5	4.55	1.47	1.34
19	P	301	PGV	O03-C19	4.55	1.47	1.33
19	C	308	PGV	O01-C1	4.57	1.48	1.34
24	G	102	PEK	O01-C1	4.57	1.48	1.34
25	T	102	CDL	OA8-CA7	4.66	1.47	1.33
24	T	101	PEK	O03-C21	4.68	1.47	1.33
19	N	607	PGV	O03-C19	4.68	1.47	1.33
20	B	301	TGL	OG3-CC1	4.68	1.47	1.33
24	C	307	PEK	O01-C1	4.69	1.48	1.34
20	N	609	TGL	OG1-CA1	4.74	1.47	1.33
23	N	610	PSC	O01-C1	4.77	1.48	1.34
25	P	305	CDL	OA8-CA7	4.78	1.47	1.33
24	G	102	PEK	O03-C21	4.82	1.47	1.33
24	C	307	PEK	O03-C21	4.86	1.48	1.33
20	N	609	TGL	OG3-CC1	4.89	1.48	1.33
24	P	308	PEK	O01-C1	4.89	1.48	1.34
25	C	304	CDL	OA8-CA7	4.90	1.48	1.33
20	D	201	TGL	OG1-CA1	4.90	1.48	1.33
25	G	101	CDL	OB8-CB7	4.90	1.48	1.33
20	Y	101	TGL	OG3-CC1	5.00	1.48	1.33
20	Q	201	TGL	OG1-CA1	5.01	1.48	1.33
20	Q	201	TGL	OB1-CB1	5.03	1.37	1.22
20	D	201	TGL	OG2-CB1	5.07	1.49	1.34
20	Q	201	TGL	OG2-CB1	5.10	1.49	1.34
20	Y	101	TGL	OG2-CB1	5.13	1.49	1.34
20	B	301	TGL	OG1-CA1	5.15	1.48	1.33
19	A	608	PGV	O03-C19	5.27	1.49	1.33
20	D	201	TGL	OB1-CB1	5.39	1.38	1.22
20	L	101	TGL	OG2-CB1	5.64	1.51	1.34

All (383) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	305	CHD	C23-C22-C20	-9.90	103.09	114.75
14	A	602	HEA	CAD-C3D-C4D	-8.17	118.14	127.01
22	W	101	CHD	C18-C13-C12	-8.16	101.13	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	103	CHD	C1-C2-C3	-7.77	97.84	110.43
14	A	601	HEA	OMA-CMA-C3A	-7.47	110.01	125.11
22	W	101	CHD	C17-C13-C14	-7.19	92.79	100.05
27	M	101	DMU	O7-C10-C5	-6.77	91.64	108.10
22	P	306	CHD	C18-C13-C12	-6.06	103.18	109.09
14	A	601	HEA	CAA-C2A-C1A	-6.05	120.44	127.01
22	G	103	CHD	C4-C5-C10	-5.93	106.12	112.66
20	D	201	TGL	OG2-CB1-CB2	-5.89	98.72	111.53
14	N	602	HEA	OMA-CMA-C3A	-5.80	113.40	125.11
14	A	602	HEA	OMA-CMA-C3A	-5.29	114.42	125.11
22	J	101	CHD	C6-C5-C4	-5.20	105.24	111.05
19	N	608	PGV	O03-C19-O04	-5.18	110.13	123.49
14	A	602	HEA	C13-C12-C11	-5.11	107.72	114.51
25	P	305	CDL	CB4-OB6-CB5	-4.94	106.03	117.89
14	N	601	HEA	C3C-CAC-CBC	-4.62	116.88	126.32
19	C	303	PGV	O03-C19-O04	-4.54	111.76	123.49
14	A	601	HEA	CAA-CBA-CGA	-4.46	104.56	112.75
22	P	306	CHD	O7-C7-C6	-4.30	99.52	110.06
22	J	101	CHD	C14-C8-C9	-4.25	103.78	109.62
14	N	601	HEA	C1A-C2A-C3A	-4.23	102.84	107.07
19	A	608	PGV	C4-C3-C2	-4.20	97.87	113.29
25	C	304	CDL	CB4-OB6-CB5	-4.11	108.03	117.89
22	P	306	CHD	C19-C10-C9	-4.05	105.11	111.18
22	J	101	CHD	C23-C22-C20	-4.00	110.04	114.75
27	Z	101	DMU	O49-C1-C2	-3.98	101.38	110.34
24	P	303	PEK	O01-C1-O02	-3.97	113.02	123.67
27	M	101	DMU	O7-C10-O1	-3.97	100.64	110.68
22	B	303	CHD	C19-C10-C5	-3.88	103.40	110.25
19	N	608	PGV	C01-O03-C19	-3.86	106.05	116.85
22	B	303	CHD	C18-C13-C12	-3.83	105.36	109.09
27	Z	101	DMU	C18-O16-C6	-3.73	107.42	113.94
22	C	305	CHD	C18-C13-C12	-3.69	105.49	109.09
22	P	306	CHD	O3-C3-C4	-3.67	102.57	109.86
22	G	103	CHD	C13-C14-C8	-3.67	110.02	114.75
22	P	306	CHD	C19-C10-C1	-3.65	102.06	108.20
20	Q	201	TGL	OG2-CB1-CB2	-3.63	103.63	111.53
22	P	307	CHD	C23-C22-C20	-3.62	110.49	114.75
22	G	103	CHD	C19-C10-C1	-3.61	102.12	108.20
14	A	601	HEA	C26-C15-C16	-3.59	109.93	115.41
14	N	602	HEA	C3C-CAC-CBC	-3.58	119.00	126.32
22	C	305	CHD	C17-C13-C12	-3.57	114.52	117.68
22	C	306	CHD	C16-C17-C13	-3.51	100.11	103.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C19-C10-C9	-3.45	106.00	111.18
19	N	607	PGV	C4-C3-C2	-3.43	100.70	113.29
22	G	103	CHD	C17-C13-C12	-3.42	114.65	117.68
14	N	602	HEA	C13-C12-C11	-3.41	109.98	114.51
22	B	303	CHD	C13-C17-C20	-3.39	115.37	119.50
14	A	602	HEA	C16-C15-C14	-3.37	114.66	121.05
14	N	601	HEA	OMA-CMA-C3A	-3.32	118.41	125.11
14	N	601	HEA	CAA-C2A-C1A	-3.31	123.42	127.01
25	P	305	CDL	OB8-CB7-OB9	-3.28	115.03	123.49
22	P	307	CHD	C19-C10-C1	-3.26	102.72	108.20
19	A	607	PGV	O03-C19-O04	-3.22	115.18	123.49
22	C	306	CHD	C23-C22-C20	-3.21	110.97	114.75
22	G	103	CHD	C18-C13-C12	-3.20	105.97	109.09
14	N	601	HEA	CMB-C2B-C1B	-3.19	123.09	128.36
20	D	201	TGL	OG3-CG3-CG2	-3.18	100.14	108.69
20	B	301	TGL	CB3-CB2-CB1	-3.15	101.23	113.59
22	P	307	CHD	C4-C5-C10	-3.15	109.19	112.66
20	Y	101	TGL	OG1-CA1-OA1	-3.13	115.40	123.49
22	W	101	CHD	C6-C5-C4	-3.12	107.56	111.05
24	P	308	PEK	O03-C21-O04	-3.11	115.47	123.49
14	N	601	HEA	C13-C12-C11	-3.06	110.45	114.51
22	J	101	CHD	C19-C10-C1	-3.05	103.08	108.20
19	N	608	PGV	O01-C1-O02	-3.01	115.60	123.67
22	C	306	CHD	C6-C5-C4	-3.00	107.69	111.05
19	N	607	PGV	C3-C2-C1	-2.98	101.87	113.59
24	T	101	PEK	O01-C1-O02	-2.96	115.74	123.67
14	N	602	HEA	CAD-CBD-CGD	-2.93	107.38	112.75
25	C	304	CDL	C52-C51-CB5	-2.89	102.22	113.59
22	C	306	CHD	C1-C2-C3	-2.89	105.74	110.43
22	G	103	CHD	C5-C4-C3	-2.87	108.64	112.91
22	W	101	CHD	C23-C22-C20	-2.84	111.40	114.75
19	A	607	PGV	C23-C22-C21	-2.78	100.15	114.53
22	P	306	CHD	C21-C20-C22	-2.73	105.79	110.35
24	C	302	PEK	O03-C21-O04	-2.72	116.47	123.49
22	G	103	CHD	C16-C15-C14	-2.71	99.67	105.12
22	P	306	CHD	C14-C8-C9	-2.71	105.90	109.62
27	M	101	DMU	C22-C25-C28	-2.70	100.61	114.53
22	C	306	CHD	C5-C4-C3	-2.69	108.91	112.91
14	A	601	HEA	CMC-C2C-C1C	-2.69	123.92	128.36
22	P	307	CHD	C11-C9-C10	-2.67	111.02	113.79
22	J	101	CHD	C11-C9-C8	-2.67	106.94	110.73
14	N	601	HEA	C4B-C3B-C11	-2.65	124.13	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	101	DMU	O6-C11-C9	-2.64	102.60	111.33
27	M	101	DMU	O7-C3-C4	-2.64	102.39	109.32
19	A	608	PGV	O03-C19-O04	-2.64	116.69	123.49
24	C	302	PEK	C2-C3-C4	-2.55	108.22	113.30
19	C	303	PGV	O01-C02-C03	-2.54	99.40	108.36
25	G	101	CDL	OA6-CA5-OA7	-2.54	116.85	123.67
25	G	101	CDL	OA8-CA7-OA9	-2.53	116.95	123.49
25	T	102	CDL	OB8-CB7-OB9	-2.53	116.97	123.49
27	Z	101	DMU	O4-C7-C8	-2.52	104.66	110.34
25	P	305	CDL	C52-C51-CB5	-2.51	103.72	113.59
20	D	201	TGL	OG3-CC1-OC1	-2.48	117.08	123.49
25	C	304	CDL	OA6-CA5-OA7	-2.48	117.01	123.67
24	C	302	PEK	O01-C02-C01	-2.47	99.65	108.36
22	C	305	CHD	C19-C10-C1	-2.45	104.08	108.20
20	Y	101	TGL	OG3-CC1-OC1	-2.44	117.18	123.49
20	Y	101	TGL	CA4-CA3-CA2	-2.43	104.36	113.29
14	A	601	HEA	C4B-C3B-C11	-2.40	124.40	127.01
25	T	102	CDL	OA6-CA5-OA7	-2.40	117.23	123.67
22	C	305	CHD	C14-C8-C9	-2.39	106.34	109.62
19	P	301	PGV	O04-C19-C20	-2.38	114.18	123.72
22	B	303	CHD	C10-C9-C8	-2.38	109.27	111.88
27	Z	101	DMU	O4-C7-C5	-2.37	105.01	110.34
20	L	101	TGL	CC4-CC3-CC2	-2.35	104.65	113.29
25	P	305	CDL	C57-C56-C55	-2.35	102.41	114.53
14	N	602	HEA	O11-C11-C3B	-2.32	104.98	111.82
22	J	101	CHD	C18-C13-C12	-2.32	106.83	109.09
20	L	101	TGL	OG3-CC1-OC1	-2.32	117.52	123.49
22	J	101	CHD	C5-C6-C7	-2.31	111.86	114.44
14	A	602	HEA	C20-C21-C22	-2.30	105.66	111.69
19	C	303	PGV	O01-C1-O02	-2.29	117.53	123.67
25	G	101	CDL	OB6-CB5-OB7	-2.28	117.54	123.67
14	A	602	HEA	CAA-CBA-CGA	-2.28	108.57	112.75
20	Y	101	TGL	OG2-CB1-OB1	-2.28	117.56	123.67
23	N	610	PSC	O01-C1-O02	-2.26	117.61	123.67
19	N	607	PGV	C9-C8-C7	-2.24	102.95	114.53
22	W	101	CHD	C19-C10-C1	-2.23	104.46	108.20
22	C	306	CHD	C17-C13-C14	-2.22	97.81	100.05
25	C	304	CDL	C56-C55-C54	-2.22	103.07	114.53
22	C	306	CHD	C22-C20-C17	-2.21	105.59	110.24
19	P	301	PGV	O01-C1-O02	-2.21	117.74	123.67
23	N	610	PSC	C21-C20-C19	-2.20	104.94	113.59
14	A	602	HEA	CBA-CAA-C2A	-2.19	108.61	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C13-C14-C15	-2.18	123.02	127.76
14	N	601	HEA	C27-C19-C18	-2.15	119.27	123.50
22	G	103	CHD	C19-C10-C5	-2.14	106.48	110.25
19	N	607	PGV	C26-C25-C24	-2.11	103.63	114.53
22	B	303	CHD	C11-C12-C13	-2.10	109.06	111.20
20	B	301	TGL	OA1-CA1-CA2	-2.10	115.31	123.72
22	B	303	CHD	C19-C10-C1	-2.10	104.68	108.20
22	G	103	CHD	C6-C5-C10	-2.08	110.36	112.66
14	N	602	HEA	C12-C13-C14	-2.08	106.58	112.40
14	A	601	HEA	C27-C19-C18	-2.07	119.43	123.50
22	P	306	CHD	C22-C23-C24	-2.06	104.61	113.02
23	B	304	PSC	O03-C19-O04	-2.06	118.18	123.49
14	A	601	HEA	C21-C20-C19	-2.05	106.03	112.71
14	A	601	HEA	C20-C21-C22	-2.05	106.32	111.69
14	N	602	HEA	CAA-C2A-C1A	-2.05	124.78	127.01
20	L	101	TGL	C29-C14-C13	-2.04	103.98	114.53
22	C	306	CHD	C16-C15-C14	-2.04	101.03	105.12
25	T	102	CDL	C12-C11-CA5	-2.03	105.61	113.59
24	C	307	PEK	O03-C21-O04	-2.02	118.27	123.49
19	P	304	PGV	O01-C02-C01	-2.02	101.24	108.36
20	L	101	TGL	CA9-CA8-CA7	-2.02	104.12	114.53
24	P	303	PEK	O03-C21-O04	-2.01	118.30	123.49
25	P	305	CDL	OA6-CA5-OA7	-2.01	118.27	123.67
22	J	101	CHD	C17-C13-C14	-2.00	98.03	100.05
22	C	305	CHD	C4-C5-C10	2.00	114.86	112.66
20	B	301	TGL	C16-C15-CC9	2.01	124.89	114.53
20	D	201	TGL	C11-C10-CB9	2.01	124.90	114.53
27	Z	101	DMU	C8-C7-C5	2.01	114.55	110.79
14	A	601	HEA	C17-C16-C15	2.02	119.28	112.71
20	D	201	TGL	OG2-CG2-CG1	2.02	115.46	108.36
19	A	607	PGV	C02-O01-C1	2.02	122.73	117.89
22	G	103	CHD	C15-C14-C8	2.02	121.25	118.32
20	N	609	TGL	C15-CC9-CC8	2.02	124.97	114.53
24	C	302	PEK	C03-C02-C01	2.02	116.80	112.07
22	G	103	CHD	C6-C5-C4	2.04	113.32	111.05
19	C	303	PGV	O14-P-O13	2.05	123.62	112.53
22	W	101	CHD	C16-C17-C20	2.06	115.73	112.05
14	N	602	HEA	C3C-C4C-NC	2.06	111.87	109.21
20	L	101	TGL	OG2-CG2-CG1	2.08	115.67	108.36
25	T	102	CDL	C63-C62-C61	2.09	125.32	114.53
25	T	102	CDL	C59-C58-C57	2.09	125.33	114.53
24	P	303	PEK	C01-O03-C21	2.10	122.72	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	608	PGV	O01-C1-C2	2.11	116.10	111.53
27	Z	101	DMU	O5-C4-C57	2.11	111.68	106.36
25	T	102	CDL	C83-C82-C81	2.13	125.53	114.53
20	Q	201	TGL	CG1-OG1-CA1	2.14	122.82	116.85
25	C	304	CDL	C39-C38-C37	2.14	125.59	114.53
19	P	304	PGV	C01-O03-C19	2.15	122.85	116.85
25	T	102	CDL	CA4-OA6-CA5	2.15	123.04	117.89
20	Q	201	TGL	CG2-OG2-CB1	2.15	123.04	117.89
19	P	301	PGV	O03-C01-C02	2.15	114.47	108.69
22	J	101	CHD	C15-C14-C13	2.15	105.74	103.60
22	C	305	CHD	C6-C5-C10	2.15	115.03	112.66
24	P	308	PEK	O03-C01-C02	2.16	114.51	108.69
19	A	607	PGV	O01-C1-C2	2.17	116.23	111.53
20	L	101	TGL	CG2-OG2-CB1	2.17	123.09	117.89
24	C	302	PEK	C23-C22-C21	2.17	122.13	113.59
20	Q	201	TGL	C21-C20-CA9	2.18	125.81	114.53
24	G	102	PEK	O01-C02-C01	2.20	116.11	108.36
20	Q	201	TGL	C16-C15-CC9	2.21	125.92	114.53
22	C	305	CHD	C16-C17-C13	2.21	105.80	103.60
20	D	201	TGL	OG1-CA1-CA2	2.22	118.66	111.90
20	Q	201	TGL	C15-CC9-CC8	2.22	125.99	114.53
22	P	306	CHD	C2-C1-C10	2.22	116.81	112.84
20	Y	101	TGL	CG2-OG2-CB1	2.22	123.23	117.89
14	N	601	HEA	CBA-CAA-C2A	2.23	116.52	112.53
14	A	602	HEA	C27-C19-C20	2.23	118.82	115.41
22	J	101	CHD	C19-C10-C5	2.25	114.22	110.25
14	N	602	HEA	C21-C20-C19	2.26	120.06	112.71
22	C	305	CHD	C11-C9-C8	2.27	113.96	110.73
22	C	306	CHD	C14-C8-C9	2.29	112.77	109.62
22	C	305	CHD	O12-C12-C11	2.30	113.77	109.06
22	G	103	CHD	C1-C10-C9	2.31	115.17	111.45
19	N	607	PGV	O01-C02-C01	2.31	116.49	108.36
25	T	102	CDL	CA6-OA8-CA7	2.33	123.36	116.85
20	D	201	TGL	C16-C15-CC9	2.33	126.56	114.53
27	Z	101	DMU	O1-C10-C5	2.33	115.06	110.28
22	C	305	CHD	C18-C13-C17	2.34	114.91	111.22
20	Q	201	TGL	OG2-CG2-CG1	2.34	116.62	108.36
19	C	303	PGV	C01-O03-C19	2.36	123.45	116.85
25	G	101	CDL	OB8-CB6-CB4	2.36	115.05	108.69
22	G	103	CHD	C15-C16-C17	2.37	109.90	105.12
22	J	101	CHD	C22-C20-C17	2.38	115.25	110.24
25	P	305	CDL	OB2-PB2-OB3	2.39	118.90	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	303	PEK	O02-C1-C2	2.40	133.34	123.72
22	B	303	CHD	C4-C5-C10	2.41	115.31	112.66
20	Q	201	TGL	OG2-CB1-OB1	2.41	130.14	123.67
14	A	602	HEA	C26-C15-C14	2.42	128.26	123.50
22	C	305	CHD	C5-C6-C7	2.44	117.16	114.44
19	C	303	PGV	C02-O01-C1	2.46	123.78	117.89
20	B	301	TGL	C15-CC9-CC8	2.46	127.22	114.53
25	C	304	CDL	CA4-OA6-CA5	2.46	123.78	117.89
19	N	607	PGV	O03-C19-C20	2.47	119.42	111.90
14	N	601	HEA	C3C-C4C-NC	2.47	112.41	109.21
22	G	103	CHD	C14-C13-C12	2.48	109.61	107.39
14	A	602	HEA	C17-C18-C19	2.50	133.19	127.76
22	C	305	CHD	C21-C20-C17	2.55	117.20	112.96
22	J	101	CHD	C6-C7-C8	2.56	114.19	111.47
19	N	607	PGV	C02-O01-C1	2.57	124.05	117.89
24	C	302	PEK	O01-C1-C2	2.57	117.10	111.53
22	P	306	CHD	C1-C10-C9	2.57	115.59	111.45
20	N	609	TGL	OG3-CC1-CC2	2.58	119.75	111.90
25	T	102	CDL	OB8-CB7-C71	2.60	119.82	111.90
22	J	101	CHD	C16-C17-C13	2.60	106.19	103.60
22	W	101	CHD	C11-C9-C10	2.61	116.50	113.79
19	A	608	PGV	O01-C02-C03	2.61	117.56	108.36
22	J	101	CHD	O7-C7-C8	2.62	115.04	109.26
14	A	602	HEA	CMB-C2B-C1B	2.62	132.70	128.36
20	D	201	TGL	CG2-OG2-CB1	2.63	124.20	117.89
24	C	307	PEK	C01-O03-C21	2.66	124.28	116.85
22	W	101	CHD	O12-C12-C11	2.66	114.51	109.06
14	A	601	HEA	CMC-C2C-C3C	2.67	130.30	125.09
22	C	305	CHD	C14-C13-C12	2.67	109.78	107.39
25	G	101	CDL	C19-C18-C17	2.67	128.34	114.53
25	C	304	CDL	OA8-CA6-CA4	2.68	115.91	108.69
14	A	601	HEA	C16-C15-C14	2.69	126.16	121.05
20	Y	101	TGL	OG3-CG3-CG2	2.70	115.97	108.69
14	A	602	HEA	C21-C20-C19	2.71	121.53	112.71
19	P	304	PGV	O01-C1-C2	2.73	117.45	111.53
24	C	307	PEK	O03-C01-C02	2.73	116.04	108.69
22	J	101	CHD	C1-C2-C3	2.73	114.87	110.43
14	A	602	HEA	C4B-C3B-C11	2.73	129.98	127.01
20	D	201	TGL	C21-C20-CA9	2.74	128.71	114.53
23	B	304	PSC	O03-C19-C20	2.75	120.27	111.90
25	C	304	CDL	CA6-OA8-CA7	2.75	124.53	116.85
24	G	102	PEK	C01-O03-C21	2.75	124.54	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	101	DMU	C7-C8-C9	2.76	115.00	110.20
22	G	103	CHD	C14-C8-C9	2.78	113.45	109.62
14	N	601	HEA	C20-C21-C22	2.79	118.99	111.69
20	Y	101	TGL	OG1-CG1-CG2	2.79	116.20	108.69
14	N	602	HEA	C4B-C3B-C11	2.84	130.09	127.01
20	Q	201	TGL	OG3-CC1-CC2	2.85	120.59	111.90
22	B	303	CHD	C1-C10-C5	2.86	112.51	107.81
24	T	101	PEK	C01-O03-C21	2.88	124.90	116.85
14	N	601	HEA	CMB-C2B-C3B	2.90	131.07	125.14
22	J	101	CHD	C15-C14-C8	2.91	122.55	118.32
22	C	306	CHD	C11-C12-C13	2.93	114.18	111.20
20	D	201	TGL	OG1-CG1-CG2	2.94	116.62	108.69
20	D	201	TGL	CG1-OG1-CA1	2.96	125.11	116.85
22	W	101	CHD	C1-C10-C5	2.96	112.67	107.81
20	L	101	TGL	OG2-CB1-CB2	2.96	117.97	111.53
20	N	609	TGL	OG2-CG2-CG3	2.96	118.80	108.36
25	C	304	CDL	OA8-CA7-C31	2.99	121.03	111.90
14	N	601	HEA	C17-C18-C19	3.02	134.32	127.76
22	P	306	CHD	C6-C5-C10	3.02	115.99	112.66
22	C	305	CHD	C1-C10-C5	3.03	112.79	107.81
20	D	201	TGL	CB3-CB2-CB1	3.04	125.53	113.59
25	C	304	CDL	OB8-CB7-C71	3.04	121.17	111.90
20	Y	101	TGL	CG3-OG3-CC1	3.05	125.38	116.85
20	N	609	TGL	CG1-OG1-CA1	3.07	125.43	116.85
25	C	304	CDL	OB6-CB5-C51	3.08	118.23	111.53
25	P	305	CDL	OA8-CA7-C31	3.08	121.29	111.90
24	G	102	PEK	O03-C01-C02	3.09	117.02	108.69
22	P	306	CHD	C15-C14-C8	3.10	122.81	118.32
25	T	102	CDL	OA8-CA7-C31	3.11	121.36	111.90
20	D	201	TGL	CG3-OG3-CC1	3.12	125.58	116.85
24	T	101	PEK	O03-C21-C22	3.15	121.51	111.90
20	Y	101	TGL	OG1-CA1-CA2	3.15	121.51	111.90
25	G	101	CDL	OA8-CA7-C31	3.16	121.53	111.90
27	M	101	DMU	C10-O1-C9	3.18	119.92	113.75
22	C	306	CHD	C5-C6-C7	3.19	117.99	114.44
19	C	303	PGV	O03-C19-C20	3.19	121.61	111.90
27	Z	101	DMU	O2-C8-C9	3.24	117.83	109.24
22	P	306	CHD	C11-C9-C8	3.25	115.34	110.73
20	Q	201	TGL	OG1-CG1-CG2	3.28	117.53	108.69
22	B	303	CHD	C6-C5-C10	3.28	116.27	112.66
22	W	101	CHD	C22-C20-C17	3.33	117.25	110.24
20	Q	201	TGL	OG1-CA1-CA2	3.35	122.12	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	609	TGL	OG1-CA1-CA2	3.38	122.19	111.90
20	N	609	TGL	OG2-CG2-CG1	3.38	120.26	108.36
20	L	101	TGL	OG1-CA1-CA2	3.41	122.29	111.90
14	A	601	HEA	C20-C19-C18	3.43	127.55	121.05
27	M	101	DMU	C7-C8-C9	3.45	116.21	110.20
19	A	608	PGV	C02-O01-C1	3.45	126.17	117.89
20	B	301	TGL	OG3-CC1-CC2	3.46	122.45	111.90
27	M	101	DMU	O16-C6-C1	3.46	112.41	108.04
23	N	610	PSC	O03-C19-C20	3.47	122.47	111.90
20	Y	101	TGL	OG3-CC1-CC2	3.48	122.50	111.90
24	G	102	PEK	O03-C21-C22	3.50	122.57	111.90
19	N	607	PGV	O01-C1-C2	3.52	119.17	111.53
24	P	308	PEK	O03-C21-C22	3.56	122.75	111.90
25	P	305	CDL	OB6-CB5-C51	3.58	119.31	111.53
24	P	308	PEK	O01-C1-C2	3.59	119.33	111.53
22	P	306	CHD	C11-C12-C13	3.60	114.86	111.20
22	W	101	CHD	C6-C5-C10	3.62	116.64	112.66
22	P	306	CHD	C16-C17-C13	3.63	107.21	103.60
27	M	101	DMU	C10-C5-C7	3.68	117.22	109.97
25	G	101	CDL	CB6-OB8-CB7	3.69	127.17	116.85
19	A	607	PGV	O03-C19-C20	3.70	123.17	111.90
27	M	101	DMU	O3-C5-C7	3.71	118.70	110.34
22	W	101	CHD	C15-C14-C8	3.75	123.76	118.32
19	C	303	PGV	O01-C1-C2	3.75	119.68	111.53
22	B	303	CHD	C15-C14-C13	3.77	107.35	103.60
20	B	301	TGL	OG2-CG2-CG1	3.78	121.68	108.36
19	C	308	PGV	C01-O03-C19	3.81	127.52	116.85
19	P	301	PGV	O01-C1-C2	3.86	119.92	111.53
22	C	305	CHD	C6-C7-C8	3.88	115.58	111.47
24	P	303	PEK	O03-C21-C22	3.90	123.78	111.90
19	C	308	PGV	O03-C19-C20	3.91	123.80	111.90
22	W	101	CHD	C18-C13-C17	3.92	117.40	111.22
19	A	608	PGV	C01-O03-C19	3.93	127.85	116.85
20	B	301	TGL	OG2-CB1-CB2	4.02	120.25	111.53
19	N	608	PGV	O03-C19-C20	4.05	124.24	111.90
22	J	101	CHD	C11-C12-C13	4.11	115.38	111.20
27	M	101	DMU	C8-C7-C5	4.11	118.47	110.79
20	L	101	TGL	OG3-CC1-CC2	4.15	124.55	111.90
20	B	301	TGL	OG1-CA1-CA2	4.17	124.60	111.90
20	B	301	TGL	CG1-OG1-CA1	4.18	128.53	116.85
20	N	609	TGL	OG2-CB1-CB2	4.20	120.66	111.53
22	J	101	CHD	C14-C13-C12	4.21	111.16	107.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	101	CHD	C13-C17-C20	4.21	124.63	119.50
24	C	307	PEK	O03-C21-C22	4.24	124.83	111.90
22	G	103	CHD	C18-C13-C14	4.25	117.91	111.22
25	P	305	CDL	OB8-CB7-C71	4.26	124.87	111.90
19	A	608	PGV	O03-C19-C20	4.26	124.88	111.90
22	P	306	CHD	C4-C5-C10	4.28	117.37	112.66
22	W	101	CHD	C14-C8-C7	4.28	117.68	111.74
25	P	305	CDL	OA6-CA5-C11	4.30	120.88	111.53
24	C	307	PEK	O01-C1-C2	4.36	121.01	111.53
22	J	101	CHD	C14-C8-C7	4.37	117.80	111.74
22	W	101	CHD	C11-C12-C13	4.38	115.65	111.20
22	J	101	CHD	C4-C5-C10	4.39	117.49	112.66
22	G	103	CHD	C15-C14-C13	4.42	108.00	103.60
25	T	102	CDL	OB6-CB5-C51	4.42	121.14	111.53
22	P	306	CHD	C15-C14-C13	4.43	108.00	103.60
27	Z	101	DMU	O1-C9-C8	4.62	118.36	109.68
23	B	304	PSC	O01-C1-C2	4.65	121.64	111.53
19	C	308	PGV	O01-C1-C2	4.77	121.89	111.53
19	P	301	PGV	O03-C19-C20	4.92	126.88	111.90
20	D	201	TGL	OG2-CB1-OB1	4.96	136.97	123.67
23	N	610	PSC	O01-C1-C2	5.00	122.40	111.53
22	C	306	CHD	C18-C13-C12	5.04	114.01	109.09
20	B	301	TGL	CG2-OG2-CB1	5.06	130.04	117.89
20	N	609	TGL	CG3-OG3-CC1	5.09	131.09	116.85
24	G	102	PEK	O01-C1-C2	5.10	122.61	111.53
25	G	101	CDL	OA6-CA5-C11	5.10	122.62	111.53
27	M	101	DMU	O1-C10-C5	5.11	120.76	110.28
22	P	306	CHD	C6-C7-C8	5.22	117.01	111.47
27	Z	101	DMU	C10-O1-C9	5.23	123.89	113.75
14	A	601	HEA	C17-C18-C19	5.36	139.42	127.76
22	B	303	CHD	C4-C3-C2	5.52	117.56	110.52
22	J	101	CHD	C9-C8-C7	5.70	118.65	111.92
27	M	101	DMU	O1-C9-C8	5.70	120.38	109.68
20	B	301	TGL	CG3-OG3-CC1	5.72	132.85	116.85
24	P	303	PEK	C2-C3-C4	5.74	124.73	113.30
25	G	101	CDL	OB6-CB5-C51	5.91	124.38	111.53
25	C	304	CDL	OA6-CA5-C11	5.97	124.51	111.53
24	T	101	PEK	O01-C1-C2	6.00	124.56	111.53
22	J	101	CHD	C10-C9-C8	6.09	118.56	111.88
25	T	102	CDL	OA6-CA5-C11	6.20	125.01	111.53
20	Y	101	TGL	OG2-CB1-CB2	6.37	125.37	111.53
20	N	609	TGL	CG2-OG2-CB1	6.79	134.19	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	C13-C17-C20	8.56	129.93	119.50
22	W	101	CHD	C17-C13-C12	9.96	126.50	117.68

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	Z	101	DMU	C5
27	Z	101	DMU	C9
14	N	602	HEA	ND
14	N	602	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	601	HEA	NB
27	M	101	DMU	C5
27	M	101	DMU	C9
14	A	601	HEA	ND
14	A	601	HEA	NB
14	A	602	HEA	NB

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	T	102	CDL	CA4-OA6-CA5-C11

There are no ring outliers.

40 monomers are involved in 319 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	7	0
14	A	602	HEA	3	0
18	A	606[A]	PER	1	0
19	A	607	PGV	2	0
19	A	608	PGV	8	0
20	B	301	TGL	3	0
22	B	303	CHD	1	0
23	B	304	PSC	13	0
24	C	302	PEK	6	0
19	C	303	PGV	4	0
25	C	304	CDL	23	0
22	C	305	CHD	3	0
22	C	306	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	307	PEK	17	0
19	C	308	PGV	1	0
20	D	201	TGL	13	0
25	G	101	CDL	37	0
24	G	102	PEK	6	0
22	J	101	CHD	5	0
20	L	101	TGL	12	0
27	M	101	DMU	1	0
14	N	601	HEA	5	0
14	N	602	HEA	1	0
18	N	606[A]	PER	1	0
19	N	607	PGV	10	0
19	N	608	PGV	6	0
20	N	609	TGL	4	0
23	N	610	PSC	21	0
19	P	301	PGV	7	0
24	P	303	PEK	9	0
19	P	304	PGV	3	0
25	P	305	CDL	17	0
22	P	306	CHD	2	0
22	P	307	CHD	3	0
24	P	308	PEK	13	0
20	Q	201	TGL	11	0
24	T	101	PEK	12	0
25	T	102	CDL	29	0
22	W	101	CHD	5	0
20	Y	101	TGL	16	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	0.44	18 (3%) 48 51	12, 15, 22, 51	0
1	N	513/514 (99%)	0.14	11 (2%) 67 70	9, 14, 20, 51	0
2	B	226/227 (99%)	0.35	14 (6%) 24 27	9, 18, 39, 65	0
2	O	226/227 (99%)	0.57	22 (9%) 10 11	11, 17, 41, 62	0
3	C	259/261 (99%)	0.21	9 (3%) 48 51	11, 17, 26, 59	0
3	P	259/261 (99%)	0.17	7 (2%) 58 61	10, 16, 26, 46	0
4	D	144/147 (97%)	0.35	10 (6%) 20 22	12, 18, 35, 57	0
4	Q	144/147 (97%)	1.65	44 (30%) 1 0	13, 23, 48, 106	0
5	E	105/109 (96%)	0.63	13 (12%) 5 5	11, 17, 41, 88	0
5	R	105/109 (96%)	1.13	20 (19%) 2 2	13, 18, 36, 89	0
6	F	98/98 (100%)	1.02	12 (12%) 5 6	15, 23, 68, 118	0
6	S	98/98 (100%)	0.95	15 (15%) 3 3	13, 20, 61, 97	0
7	G	83/85 (97%)	1.28	21 (25%) 1 1	11, 20, 73, 90	0
7	T	83/85 (97%)	1.59	24 (28%) 1 0	10, 20, 77, 101	0
8	H	79/85 (92%)	1.04	13 (16%) 2 2	16, 24, 62, 76	0
8	U	79/85 (92%)	1.39	21 (26%) 1 1	14, 22, 63, 76	0
9	I	72/73 (98%)	1.22	19 (26%) 1 1	15, 26, 53, 63	0
9	V	72/73 (98%)	2.11	31 (43%) 0 0	13, 26, 47, 58	0
10	J	58/59 (98%)	0.81	8 (13%) 4 4	17, 25, 45, 86	0
10	W	58/59 (98%)	1.30	14 (24%) 1 1	13, 22, 51, 91	0
11	K	49/56 (87%)	1.01	6 (12%) 5 6	16, 22, 36, 42	0
11	X	49/56 (87%)	2.22	24 (48%) 0 0	16, 21, 37, 43	0
12	L	46/47 (97%)	0.38	2 (4%) 39 42	15, 19, 37, 64	0
12	Y	46/47 (97%)	0.72	5 (10%) 7 8	12, 19, 38, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.76	7 (16%) 2 3	14, 18, 44, 77	0
13	Z	43/46 (93%)	1.62	13 (30%) 1 0	12, 18, 48, 66	0
All	All	3550/3614 (98%)	0.67	403 (11%) 7 7	9, 17, 43, 118	0

All (403) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	16.6
6	S	97	ALA	15.4
6	F	97	ALA	15.2
4	Q	6	VAL	13.9
6	F	98	HIS	13.1
7	G	10	GLY	12.5
8	H	8	ILE	11.4
6	F	1	ALA	10.9
8	U	8	ILE	10.9
2	O	90	ILE	10.3
9	V	37	PHE	10.1
8	U	44	THR	9.5
5	R	5	HIS	9.4
7	T	40	GLY	9.3
6	S	1	ALA	9.1
7	T	8	HIS	9.0
8	H	44	THR	8.8
10	W	58	LYS	8.4
9	I	37	PHE	8.4
5	E	5	HIS	8.2
13	M	42	LYS	7.9
7	T	39	SER	7.9
7	T	36	TRP	7.9
11	X	6	ALA	7.8
6	S	96	LEU	7.8
8	H	45	ALA	7.7
4	Q	35	ALA	7.6
4	D	4	SER	7.6
6	F	96	LEU	7.6
8	H	10	ASN	7.5
10	W	57	HIS	7.5
2	B	90	ILE	7.4
8	U	10	ASN	7.4
9	V	2	THR	7.3

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Mol	Chain	Res	Type	RSRZ
7	T	84	LYS	7.0
7	G	40	GLY	6.9
6	S	95	GLN	6.8
4	Q	8	SER	6.8
12	Y	47	LYS	6.8
9	I	25	PHE	6.6
6	F	95	GLN	6.6
13	Z	39	ASN	6.6
6	S	94	HIS	6.5
6	F	94	HIS	6.5
6	S	98	HIS	6.5
5	E	109	VAL	6.5
10	J	58	LYS	6.5
4	Q	7	LYS	6.3
7	T	9	GLY	6.2
9	V	25	PHE	6.2
7	G	84	LYS	6.2
7	G	9	GLY	6.1
13	M	43	SER	5.9
7	T	41	HIS	5.8
10	W	1	PHE	5.7
2	O	227	LEU	5.7
9	V	34	PHE	5.7
4	Q	4	SER	5.6
11	K	7	PRO	5.6
9	V	33	THR	5.6
7	T	10	GLY	5.5
2	O	224	ALA	5.4
7	T	42	ARG	5.4
8	H	47	GLY	5.4
5	R	7	THR	5.4
9	V	3	ALA	5.4
10	W	56	PRO	5.4
9	V	30	GLY	5.3
4	D	5	VAL	5.3
7	T	2	SER	5.3
7	G	2	SER	5.3
2	B	60	GLU	5.3
12	Y	27	LEU	5.3
4	Q	36	SER	5.2
13	Z	43	SER	5.2
6	F	3	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
9	V	26	MET	5.2
7	G	8	HIS	5.1
11	K	6	ALA	5.0
7	G	42	ARG	5.0
6	S	2	SER	5.0
4	Q	147	LYS	5.0
13	Z	42	LYS	4.9
5	R	109	VAL	4.9
7	T	3	ALA	4.9
11	X	27	ALA	4.9
9	I	33	THR	4.9
12	L	2	HIS	4.9
10	W	52	TRP	4.9
4	Q	33	LEU	4.8
9	V	29	LEU	4.8
4	Q	32	ASN	4.8
7	T	43	GLU	4.8
8	U	11	TYR	4.8
7	G	39	SER	4.7
8	U	49	ASP	4.7
4	Q	53	ILE	4.7
9	I	29	LEU	4.6
7	G	37	LEU	4.6
9	I	30	GLY	4.6
7	T	38	HIS	4.5
2	O	91	ASN	4.5
5	E	7	THR	4.5
8	U	7	LYS	4.4
2	O	60	GLU	4.4
8	U	18	SER	4.4
2	O	113	TYR	4.4
13	Z	32	TRP	4.3
11	X	13	TYR	4.3
6	F	2	SER	4.3
5	R	6	GLU	4.3
7	T	46	ALA	4.3
11	X	34	THR	4.2
4	Q	34	SER	4.2
10	J	52	TRP	4.2
4	Q	140	TYR	4.2
7	G	38	HIS	4.2
4	Q	102	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
7	G	41	HIS	4.2
5	R	13	ALA	4.2
11	X	23	THR	4.1
8	U	48	GLY	4.1
7	G	43	GLU	4.1
2	O	217	LYS	4.1
10	W	48	TYR	4.1
9	I	26	MET	4.1
9	I	22	VAL	4.1
11	X	30	VAL	4.1
5	R	108	LYS	4.0
8	U	51	SER	4.0
4	Q	50	SER	4.0
11	X	7	PRO	4.0
9	V	19	PHE	4.0
6	S	3	GLY	4.0
9	I	18	ARG	4.0
4	Q	31	LYS	4.0
4	Q	39	ALA	4.0
13	Z	35	TYR	3.9
8	H	43	MET	3.9
6	S	93	PRO	3.9
12	L	47	LYS	3.9
4	Q	52	SER	3.9
5	R	10	GLU	3.9
4	Q	49	SER	3.8
3	P	235	PHE	3.8
8	U	45	ALA	3.8
13	M	39	ASN	3.7
2	O	221	LYS	3.7
4	Q	46	ALA	3.7
13	M	38	ASP	3.7
1	N	36	LEU	3.7
2	O	59	GLN	3.7
13	Z	38	ASP	3.7
4	Q	30	VAL	3.6
11	X	19	ALA	3.6
9	V	53	ASN	3.6
9	V	73	LYS	3.6
4	Q	54	ASP	3.6
8	U	52	VAL	3.6
5	R	23	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
2	O	116	LEU	3.5
8	H	9	LYS	3.5
7	G	3	ALA	3.5
4	Q	9	GLU	3.5
10	W	25	GLY	3.5
4	Q	42	GLU	3.5
9	V	57	MET	3.5
13	Z	41	LYS	3.4
4	Q	10	ASP	3.4
2	B	91	ASN	3.4
8	U	46	LYS	3.4
11	X	21	GLY	3.4
8	U	42	ALA	3.4
5	R	17	THR	3.4
7	G	7	ASP	3.4
11	X	14	GLY	3.4
5	E	6	GLU	3.4
10	J	56	PRO	3.3
4	D	147	LYS	3.3
4	Q	73	ARG	3.3
12	Y	45	LEU	3.3
11	X	37	GLY	3.3
4	Q	58	GLU	3.3
7	T	45	PRO	3.3
2	O	86	MET	3.2
10	W	2	GLU	3.2
10	J	14	GLU	3.2
13	Z	37	LEU	3.2
13	Z	40	TYR	3.2
2	O	89	GLU	3.2
10	J	57	HIS	3.2
9	I	23	GLY	3.2
4	Q	144	GLU	3.2
5	R	94	ASN	3.2
11	K	19	ALA	3.2
5	R	98	ILE	3.2
5	E	10	GLU	3.2
9	V	61	GLU	3.2
13	Z	13	LYS	3.1
9	I	19	PHE	3.1
6	F	44	GLU	3.1
4	Q	51	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	38	ASN	3.1
7	G	36	TRP	3.1
5	R	89	LEU	3.1
4	Q	38	LYS	3.1
11	X	26	VAL	3.1
11	X	47	ARG	3.0
10	J	1	PHE	3.0
11	K	8	ASP	3.0
8	U	9	LYS	3.0
9	V	52	ARG	3.0
5	R	9	GLU	3.0
8	U	47	GLY	3.0
13	M	40	TYR	3.0
9	V	49	ASP	3.0
9	V	23	GLY	3.0
4	Q	139	ASP	3.0
9	V	48	ALA	3.0
7	T	37	LEU	3.0
2	B	59	GLN	3.0
4	Q	43	LYS	3.0
3	C	235	PHE	2.9
4	D	143	ASN	2.9
2	B	67	ILE	2.9
11	X	25	CYS	2.9
8	H	7	LYS	2.9
1	A	83	VAL	2.9
3	C	186	PHE	2.9
9	V	28	SER	2.9
4	Q	115	TRP	2.9
5	E	9	GLU	2.9
4	Q	57	VAL	2.9
7	T	35	SER	2.9
11	K	47	ARG	2.9
8	U	50	VAL	2.9
4	D	102	TYR	2.9
1	A	405	LEU	2.9
1	A	471	ILE	2.9
7	T	5	LYS	2.9
9	V	15	ARG	2.9
5	E	11	PHE	2.8
1	N	83	VAL	2.8
3	P	38	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
4	Q	113	GLU	2.8
8	H	49	ASP	2.8
9	V	45	LYS	2.8
10	W	55	PHE	2.8
7	G	5	LYS	2.8
9	I	52	ARG	2.8
4	Q	143	ASN	2.8
11	X	12	LYS	2.8
8	H	48	GLY	2.8
2	O	218	TYR	2.8
9	V	18	ARG	2.7
2	O	226	MET	2.7
4	D	112	GLU	2.7
8	U	77	ALA	2.7
1	N	87	ILE	2.7
8	H	11	TYR	2.7
5	E	13	ALA	2.7
1	A	393	PHE	2.7
1	A	20	LEU	2.7
5	E	108	LYS	2.7
6	S	26	LYS	2.7
1	A	295	VAL	2.7
3	C	188	ILE	2.7
9	I	2	THR	2.6
1	A	87	ILE	2.6
13	M	36	HIS	2.6
1	A	472	ILE	2.6
2	O	68	LEU	2.6
9	I	32	ALA	2.6
11	K	26	VAL	2.6
2	O	76	ILE	2.6
7	G	6	GLY	2.6
11	X	8	ASP	2.6
1	A	476	PHE	2.6
7	G	65	GLY	2.6
11	X	46	GLY	2.6
5	E	23	ASP	2.6
11	X	11	ASP	2.6
12	Y	46	LYS	2.5
1	A	136[A]	LEU	2.5
7	G	46	ALA	2.5
7	T	4	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
9	V	24	ALA	2.5
9	V	32	ALA	2.5
13	Z	36	HIS	2.5
5	E	67	ILE	2.5
8	U	20	PHE	2.5
4	Q	114	GLU	2.5
11	X	16	ALA	2.5
9	V	56	SER	2.5
11	X	49	THR	2.5
1	N	168	ILE	2.5
13	M	37	LEU	2.5
9	I	34	PHE	2.4
6	F	26	LYS	2.4
1	A	168	ILE	2.4
2	O	92	ASN	2.4
3	P	79	LEU	2.4
8	U	43	MET	2.4
10	W	44	LEU	2.4
8	U	74	ASP	2.4
11	X	35	GLN	2.4
11	X	18	LEU	2.4
2	O	47	THR	2.4
4	Q	141	ASP	2.4
1	N	472	ILE	2.4
6	S	23	ALA	2.4
4	Q	138	TRP	2.3
5	R	92	THR	2.3
13	Z	21	VAL	2.3
8	U	55	TRP	2.3
2	B	92	ASN	2.3
5	E	68	LEU	2.3
7	G	45	PRO	2.3
7	G	1	ALA	2.3
5	E	91	PRO	2.3
2	O	88	ASP	2.3
3	P	41	THR	2.3
7	T	12	GLY	2.3
9	V	38	ALA	2.3
1	A	85	LEU	2.3
4	Q	72	ASN	2.3
9	I	38	ALA	2.3
10	J	2	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
10	W	4	ARG	2.2
10	W	33	ARG	2.2
13	Z	28	LEU	2.2
9	I	55	ASP	2.2
10	W	49	CYS	2.2
2	O	130	PRO	2.2
7	T	63	GLY	2.2
9	V	72	ALA	2.2
2	B	38	VAL	2.2
2	B	61	VAL	2.2
2	B	163	TRP	2.2
9	V	39	VAL	2.2
7	T	1	ALA	2.2
8	H	77	ALA	2.2
1	A	15	ILE	2.2
9	V	64	ARG	2.2
1	N	185	VAL	2.2
2	O	104	TRP	2.2
4	Q	75	THR	2.2
4	Q	145	TRP	2.2
1	N	75	ILE	2.2
6	F	57	ILE	2.2
9	I	45	LYS	2.2
4	Q	142	LYS	2.2
6	S	27	GLY	2.2
10	J	15	ASP	2.2
2	O	114	GLU	2.2
9	V	35	TYR	2.2
3	P	44[A]	MET	2.2
4	D	141	ASP	2.1
5	R	97	GLY	2.1
2	B	65	TRP	2.1
3	C	3	HIS	2.1
1	A	400	PHE	2.1
3	P	197	PHE	2.1
1	N	324	LEU	2.1
2	B	126	SER	2.1
3	C	197	PHE	2.1
6	S	42	THR	2.1
10	W	15	ASP	2.1
1	A	48	LEU	2.1
7	T	65	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	185	VAL	2.1
1	N	357	VAL	2.1
9	V	55	ASP	2.1
11	X	15	ASN	2.1
3	C	40	MET	2.1
3	P	259	TRP	2.1
11	X	36	ILE	2.1
5	R	96	LEU	2.1
4	D	139	ASP	2.1
9	I	53	ASN	2.1
1	A	349	THR	2.1
2	B	89	GLU	2.1
7	T	44	ARG	2.1
5	R	22	PRO	2.1
2	B	153	LEU	2.1
6	S	22	LEU	2.1
3	C	61	VAL	2.1
6	S	40	SER	2.1
4	Q	101	HIS	2.1
9	I	48	ALA	2.0
5	R	93	LEU	2.0
2	B	154	VAL	2.0
6	F	43	LYS	2.0
4	D	54	ASP	2.0
12	Y	17	ASN	2.0
4	D	52	SER	2.0
1	A	73	ILE	2.0
1	N	48	LEU	2.0
1	N	405	LEU	2.0
3	C	71	HIS	2.0
5	R	105	GLY	2.0
5	R	83	PRO	2.0
8	H	84	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	FME	A	1	10/11	0.94	0.18	-	25,33,52,71	0
9	SAC	I	1	9/10	0.66	0.50	-	43,49,64,67	0
9	SAC	V	1	9/10	0.34	0.70	-	63,69,72,74	0
7	TPO	G	11	11/12	0.60	0.43	-	65,74,106,115	0
2	FME	O	1	10/11	0.97	0.12	-	15,16,24,24	0
2	FME	B	1	10/11	0.96	0.15	-	15,16,24,33	0
1	FME	N	1	10/11	0.93	0.21	-	18,28,48,58	0
7	TPO	T	11	11/12	0.52	0.34	-	52,69,96,97	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
22	CHD	J	101	29/29	0.44	0.37	8.88	56,93,101,102	0
19	PGV	A	608	51/51	0.67	0.27	7.73	24,51,72,84	0
19	PGV	N	607	51/51	0.58	0.29	5.43	27,49,103,114	0
22	CHD	W	101	29/29	0.58	0.39	4.81	52,82,95,101	0
16	MG	N	604	1/1	0.90	0.14	4.51	17,17,17,17	0
18	PER	A	606[A]	2/2	0.99	0.17	4.41	10,10,10,12	0
25	CDL	P	305	100/100	0.70	0.27	4.11	28,60,102,116	0
19	PGV	C	308	51/51	0.68	0.26	4.10	34,64,99,101	0
18	PER	A	606[B]	2/2	0.99	0.17	3.96	11,11,11,11	2
20	TGL	L	101	63/63	0.53	0.30	3.92	28,44,70,80	0
20	TGL	Y	101	63/63	0.47	0.33	3.80	33,49,76,81	0
20	TGL	D	201	63/63	0.71	0.21	3.78	23,45,66,74	0
20	TGL	B	301	63/63	0.75	0.20	3.74	28,51,75,84	0
22	CHD	C	305	29/29	0.77	0.29	3.70	41,47,53,59	0
20	TGL	N	609	63/63	0.74	0.20	3.66	31,54,73,76	0
25	CDL	C	304	100/100	0.74	0.23	3.63	26,59,88,108	0
19	PGV	N	608	51/51	0.95	0.24	3.13	12,30,49,58	0
25	CDL	T	102	100/100	0.56	0.29	2.96	31,67,118,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
19	PGV	A	607	51/51	0.95	0.24	2.91	13,26,49,57	0
19	PGV	P	301	51/51	0.65	0.25	2.89	45,70,102,114	0
19	PGV	P	304	51/51	0.93	0.24	2.37	12,27,51,54	0
19	PGV	C	303	51/51	0.94	0.23	2.21	13,22,55,63	0
24	PEK	C	302	53/53	0.93	0.20	2.21	13,33,60,65	0
20	TGL	Q	201	63/63	0.60	0.26	2.19	30,47,66,71	0
24	PEK	P	303	53/53	0.91	0.18	1.90	13,29,70,77	0
27	DMU	Z	101	33/33	0.72	0.27	1.65	18,31,34,39	0
24	PEK	G	102	53/53	0.56	0.30	1.60	37,71,111,121	0
27	DMU	M	101	33/33	0.68	0.22	1.60	25,29,39,40	0
25	CDL	G	101	100/100	0.63	0.24	1.51	34,66,99,138	0
23	PSC	B	304	52/52	0.48	0.36	1.50	36,84,130,137	0
18	PER	N	606[A]	2/2	0.99	0.12	1.38	10,10,10,12	0
24	PEK	T	101	53/53	0.53	0.32	1.36	36,76,114,118	0
14	HEA	N	601	60/60	0.94	0.15	1.28	10,13,32,39	0
18	PER	N	606[B]	2/2	0.99	0.12	1.22	11,11,11,11	2
24	PEK	P	308	53/53	0.50	0.27	0.99	25,55,100,118	0
24	PEK	C	307	53/53	0.56	0.24	0.86	34,59,94,103	0
23	PSC	N	610	52/52	0.71	0.29	0.85	24,61,117,126	0
22	CHD	P	306	29/29	0.82	0.20	0.71	34,44,49,56	0
14	HEA	N	602	60/60	0.96	0.14	0.64	9,12,18,21	0
14	HEA	A	601	60/60	0.96	0.15	0.49	10,12,37,46	0
14	HEA	A	602	60/60	0.95	0.16	0.47	9,12,18,19	0
16	MG	A	604	1/1	0.97	0.10	-0.16	14,14,14,14	0
22	CHD	G	103	29/29	0.95	0.09	-0.51	8,10,12,16	0
22	CHD	B	303	29/29	0.95	0.09	-0.57	8,10,13,19	0
17	NA	A	605	1/1	0.98	0.09	-0.90	14,14,14,14	0
22	CHD	P	307	29/29	0.94	0.09	-0.97	12,19,23,26	0
22	CHD	C	306	29/29	0.94	0.09	-1.25	17,21,25,29	0
21	CUA	O	301	2/2	0.98	0.05	-2.15	14,14,14,15	0
17	NA	N	605	1/1	0.98	0.04	-2.47	12,12,12,12	0
21	CUA	B	302	2/2	0.99	0.04	-2.99	14,14,14,15	0
26	ZN	F	101	1/1	1.00	0.02	-3.16	19,19,19,19	0
26	ZN	S	101	1/1	0.99	0.04	-3.54	18,18,18,18	0
15	CU	N	603	1/1	1.00	0.07	-	14,14,14,14	0
17	NA	C	301	1/1	0.94	0.25	-	37,37,37,37	0
17	NA	P	302	1/1	0.92	0.11	-	29,29,29,29	0
15	CU	A	603	1/1	1.00	0.09	-	15,15,15,15	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.