



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:32 am GMT

PDB ID : 3ASN  
Title : Bovine heart cytochrome C oxidase in the fully oxidized state measured at 1.7470 angstrom wavelength  
Authors : Suga, M.; Yano, N.; Muramoto, K.; Shinzawa-Itoh, K.; Maeda, T.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2010-12-17  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

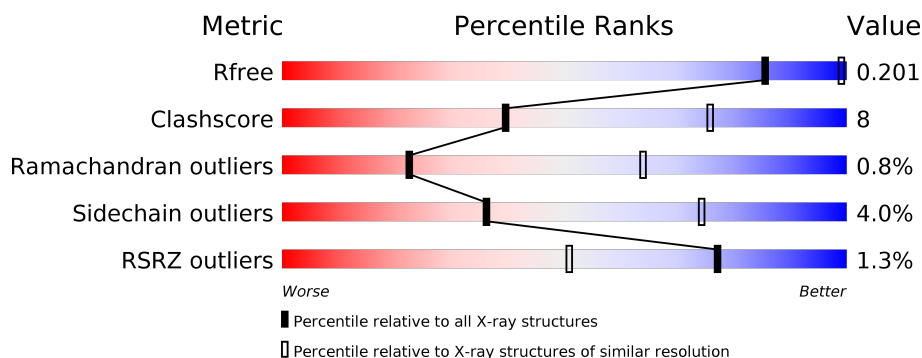
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



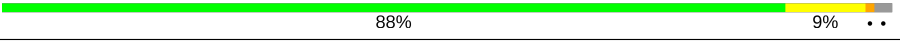


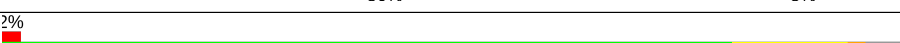
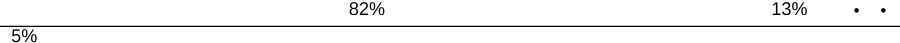




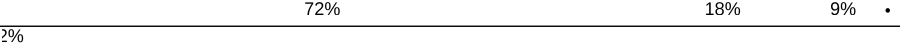




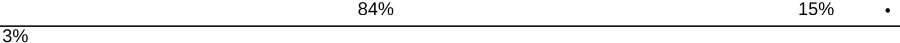
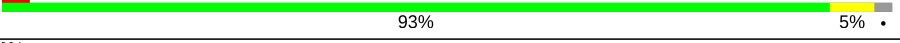




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>86%</div> <div>13%</div> <div>.</div> </div>
1	N	514	<div> <div>87%</div> <div>13%</div> </div>
2	B	227	<div> <div>81%</div> <div>19%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>..</div> </div>
3	C	261	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
3	P	261	<div> <div>85%</div> <div>14%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
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	515	X	-	-	-
14	HEA	A	516	X	-	-	-
14	HEA	N	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	516	X	-	-	-
18	TGL	A	521	-	-	-	X
18	TGL	D	523	-	-	-	X
18	TGL	L	522	-	-	-	X
18	TGL	N	1521	-	-	-	X
18	TGL	N	1522	-	-	-	X
18	TGL	N	1523	-	-	-	X
19	PGV	A	522	-	-	-	X
19	PGV	A	524	-	-	-	X
19	PGV	C	267	-	-	-	X
19	PGV	C	268	-	-	-	X
19	PGV	N	1266	-	-	-	X
19	PGV	N	1524	-	-	-	X
19	PGV	P	1267	-	-	-	X
19	PGV	P	1268	-	-	-	X
21	PSC	B	229	-	-	-	X
21	PSC	O	1229	-	-	-	X
22	CHD	J	60	-	-	-	X
22	CHD	P	1271	-	-	-	X
22	CHD	W	1059	-	-	-	X
24	PEK	C	264	-	-	-	X
24	PEK	G	1263	-	-	-	X
24	PEK	P	1265	-	-	-	X
24	PEK	T	263	-	-	-	X
25	CDL	C	270	-	-	-	X
25	CDL	G	269	-	-	-	X
25	CDL	P	1270	-	-	-	X
25	CDL	T	1269	-	-	X	X
27	DMU	M	526	X	-	-	-
27	DMU	Z	1526	X	-	-	X

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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.

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.

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.

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.

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			

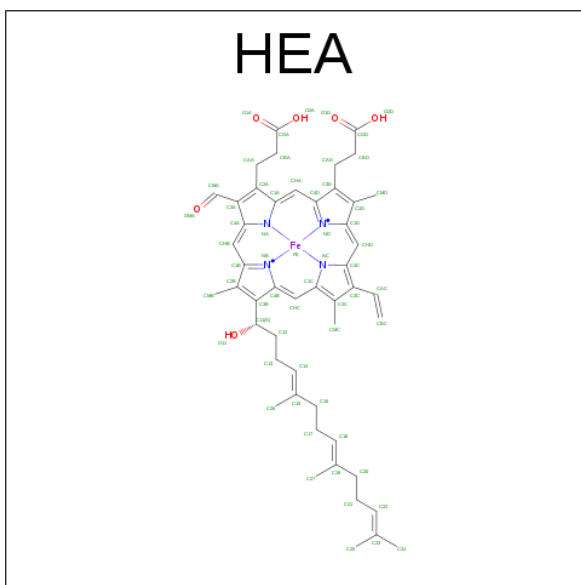
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

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	
			60	49	1	4	6	0
14	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
14	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

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

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

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

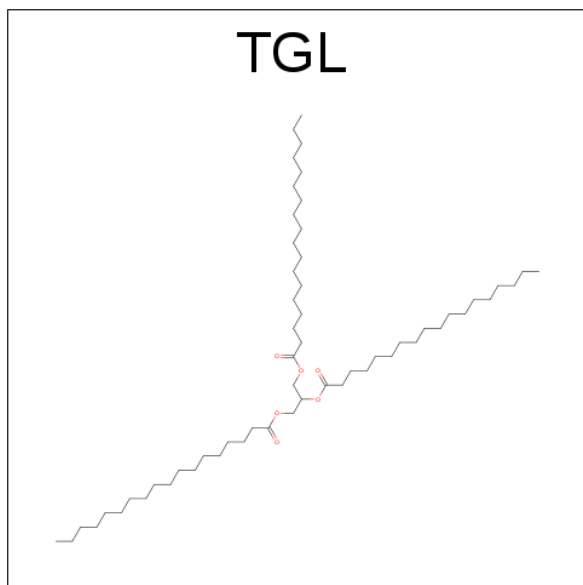
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg		
			1	1	0	0
16	N	1	Total	Mg		
			1	1	0	0

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



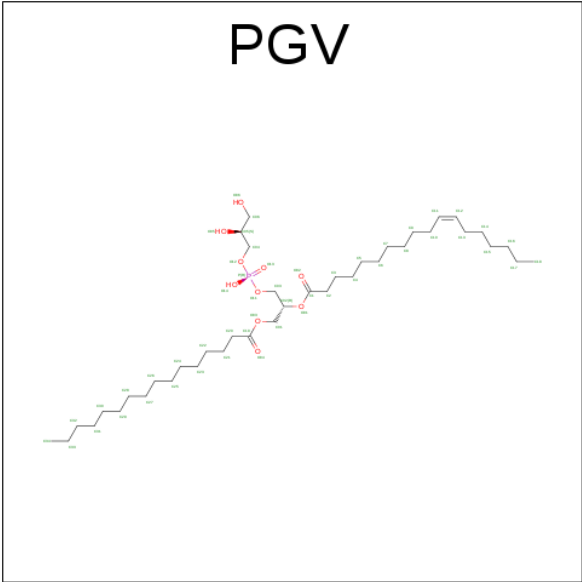
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula:  $C_{57}H_{110}O_6$ ).



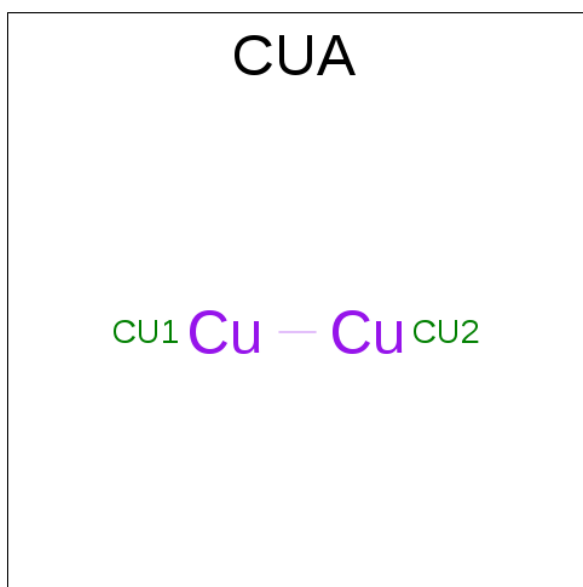
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		

- 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:  $C_{40}H_{77}O_{10}P$ ).



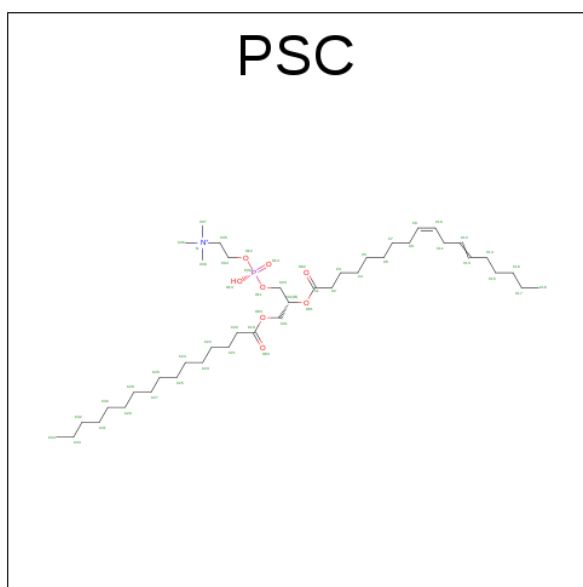
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



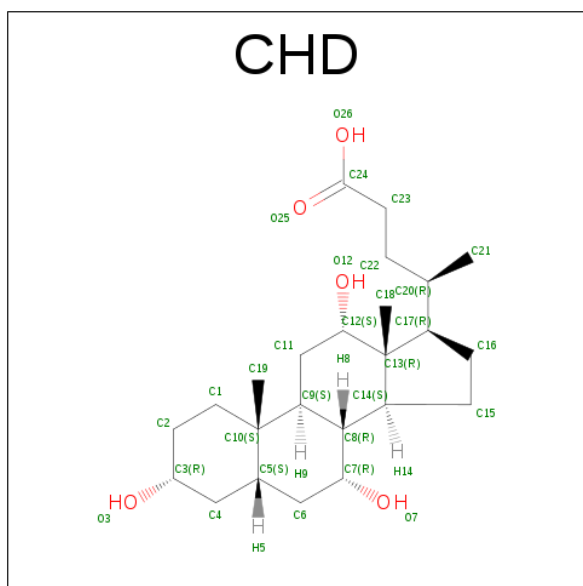
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

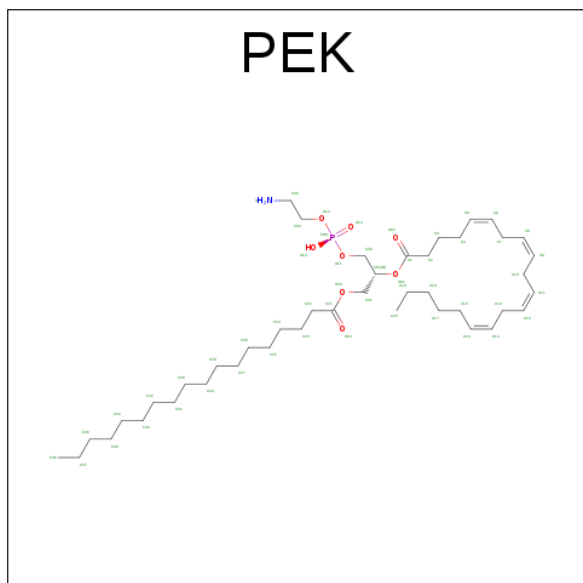


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0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

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

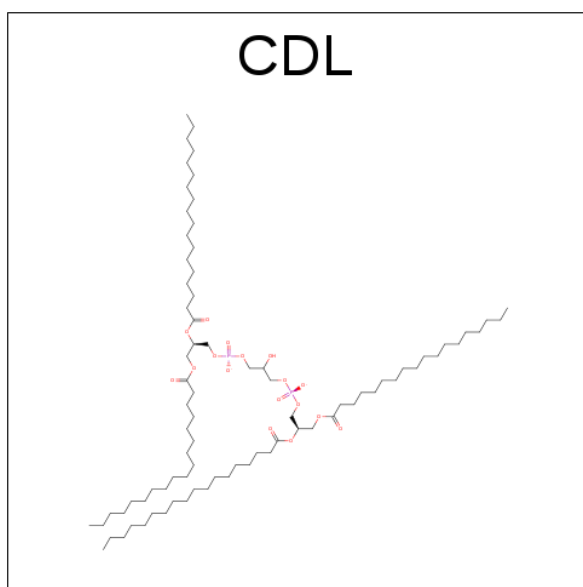
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	P	1	Total X 1 1	0	0
23	C	1	Total X 1 1	0	0

- 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>).

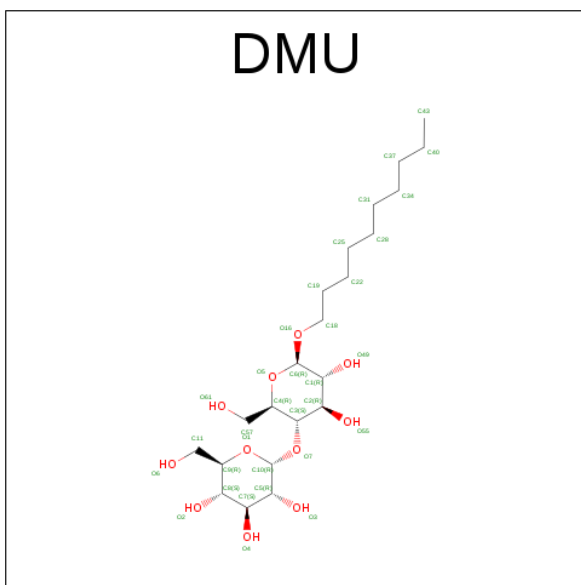


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- 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 33	C 22	O 11	0	0
27	Z	1	Total 33	C 22	O 11	0	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	212	Total O 212 212	0	0
28	B	127	Total O 127 127	0	0
28	C	110	Total O 110 110	0	0
28	D	104	Total O 104 104	0	0
28	E	66	Total O 66 66	0	0
28	F	81	Total O 81 81	0	0
28	G	52	Total O 52 52	0	0
28	H	47	Total O 47 47	0	0
28	I	32	Total O 32 32	0	0
28	J	18	Total O 18 18	0	0

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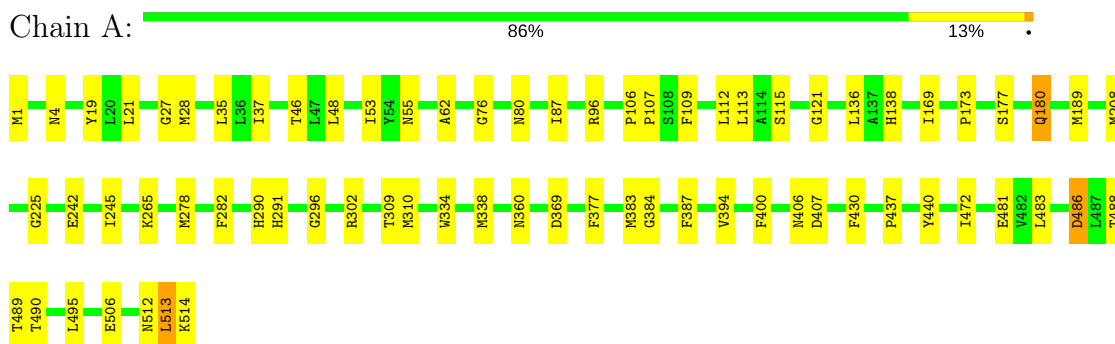
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	20	Total 20	O 20	0	0
28	L	27	Total 27	O 27	0	0
28	M	20	Total 20	O 20	0	0
28	N	210	Total 210	O 210	0	0
28	O	115	Total 115	O 115	0	0
28	P	109	Total 109	O 109	0	0
28	Q	60	Total 60	O 60	0	0
28	R	45	Total 45	O 45	0	0
28	S	79	Total 79	O 79	0	0
28	T	42	Total 42	O 42	0	0
28	U	47	Total 47	O 47	0	0
28	V	24	Total 24	O 24	0	0
28	W	17	Total 17	O 17	0	0
28	X	18	Total 18	O 18	0	0
28	Y	17	Total 17	O 17	0	0
28	Z	12	Total 12	O 12	0	0



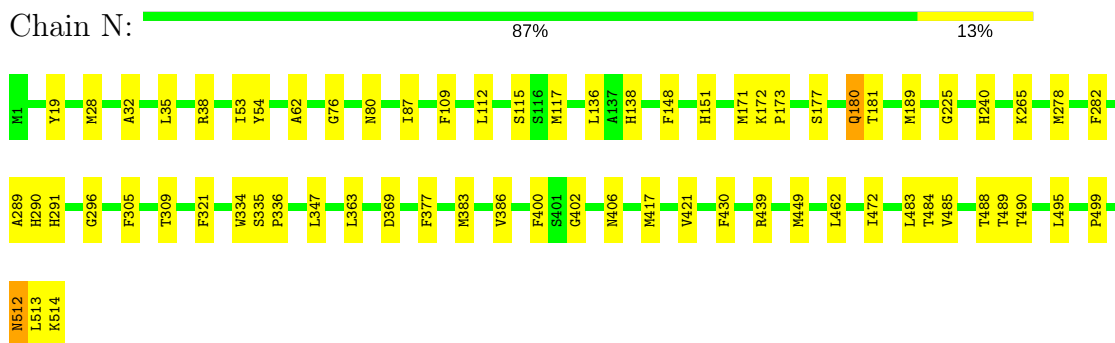
### 3 Residue-property plots [i](#)

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

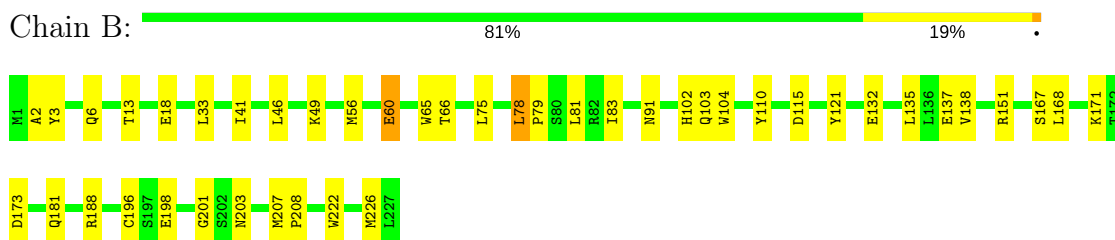
#### • Molecule 1: Cytochrome c oxidase subunit 1



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

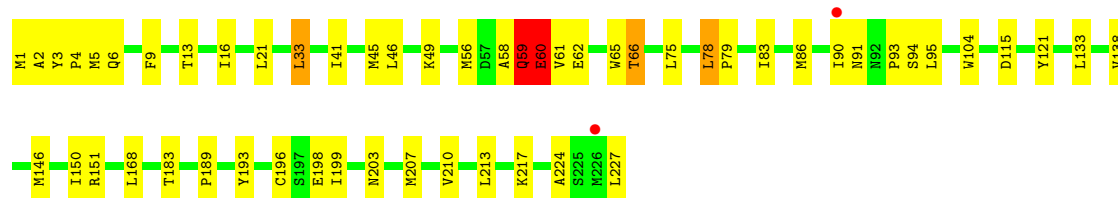


#### • Molecule 2: Cytochrome c oxidase subunit 2



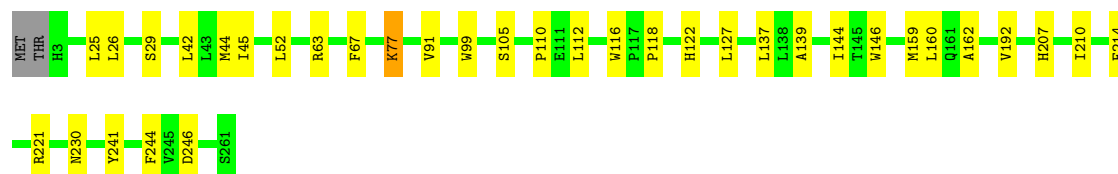
#### • Molecule 2: Cytochrome c oxidase subunit 2





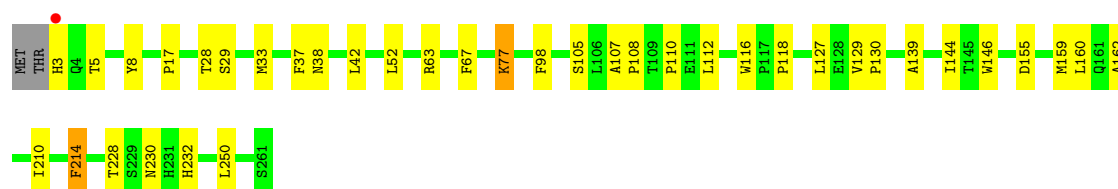
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 86% 13%



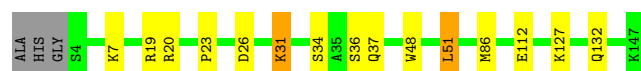
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 85% 14%



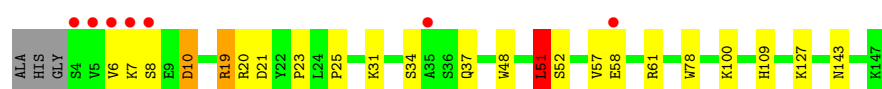
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 88% 9%



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 5% 82% 14%

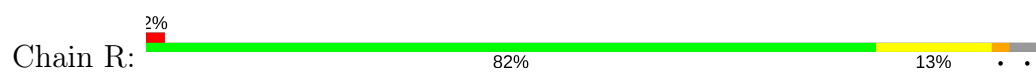


• Molecule 5: Cytochrome c oxidase subunit 5A

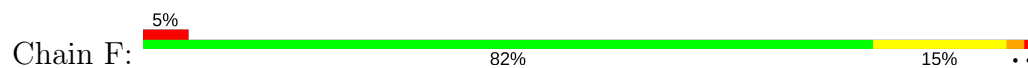
Chain E: 86% 8%



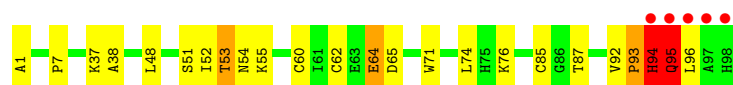
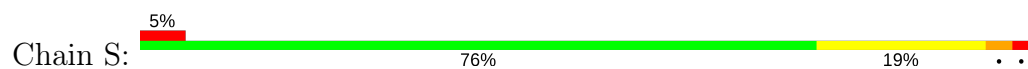
• Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 6: Cytochrome c oxidase subunit 5B



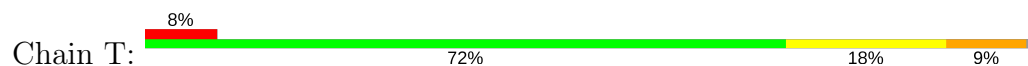
- Molecule 6: Cytochrome c oxidase subunit 5B



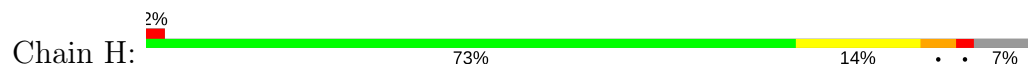
- Molecule 7: Cytochrome c oxidase subunit 6A2



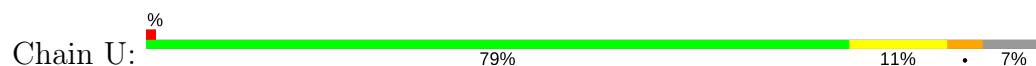
- Molecule 7: Cytochrome c oxidase subunit 6A2



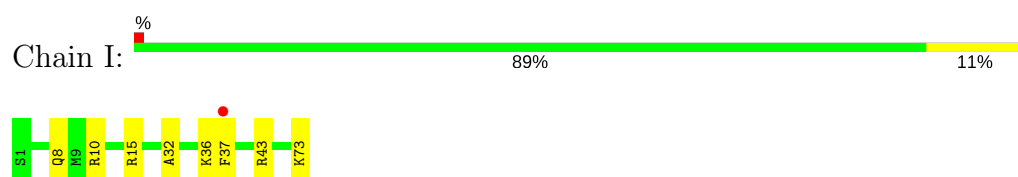
- Molecule 8: Cytochrome c oxidase subunit 6B1



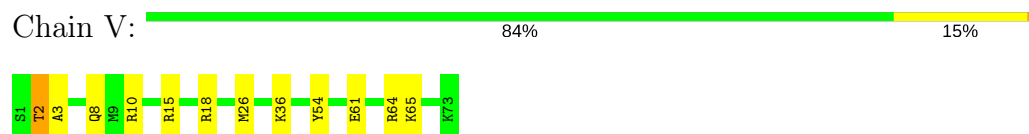
- Molecule 8: Cytochrome c oxidase subunit 6B1



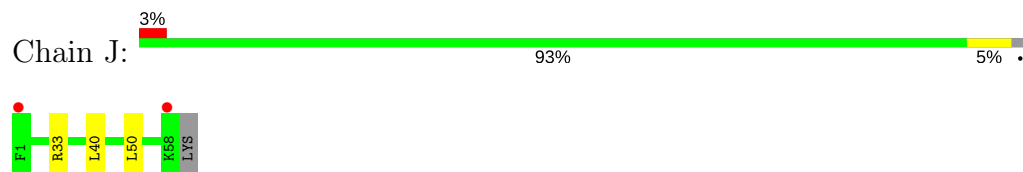
- Molecule 9: Cytochrome c oxidase subunit 6C



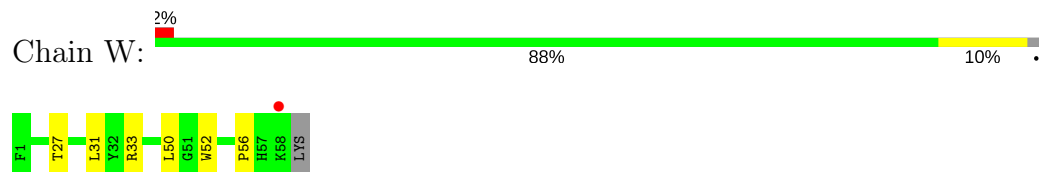
- Molecule 9: Cytochrome c oxidase subunit 6C



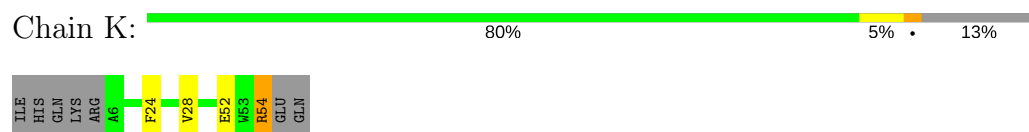
- Molecule 10: Cytochrome c oxidase subunit 7A1



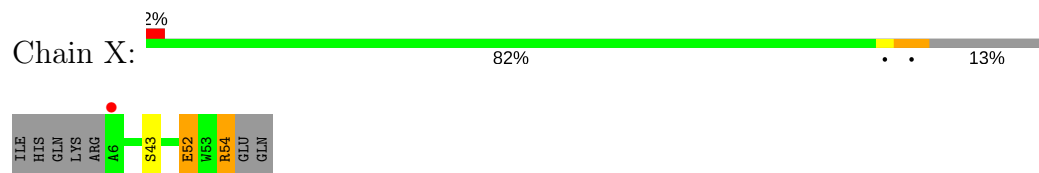
- Molecule 10: Cytochrome c oxidase subunit 7A1



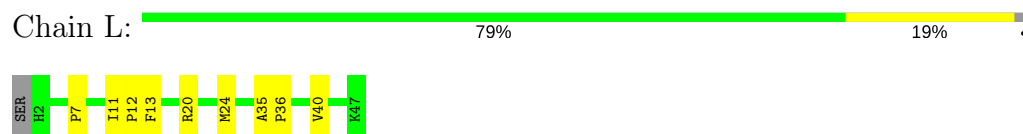
- Molecule 11: Cytochrome c oxidase subunit 7B



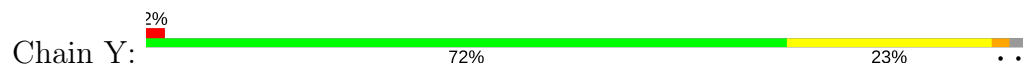
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 12: Cytochrome c oxidase subunit 7C

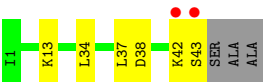
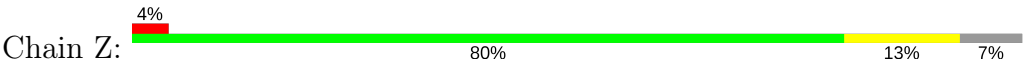




• Molecule 13: Cytochrome c oxidase subunit 8B



• Molecule 13: Cytochrome c oxidase subunit 8B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.83Å 204.10Å 177.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 135.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-3.00) 100.0 (135.76-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	27.93 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5	Depositor
R, $R_{free}$	0.150 , 0.187 0.166 , 0.201	Depositor DCC
$R_{free}$ test set	6633 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.96	0/4156	0.91	13/5678 (0.2%)
1	N	0.92	0/4156	0.84	3/5678 (0.1%)
2	B	0.98	2/1860 (0.1%)	0.94	2/2534 (0.1%)
2	O	0.98	3/1860 (0.2%)	0.94	0/2534
3	C	0.96	1/2197 (0.0%)	0.81	2/3005 (0.1%)
3	P	0.92	0/2197	0.82	1/3005 (0.0%)
4	D	1.01	1/1229 (0.1%)	0.94	3/1658 (0.2%)
4	Q	0.97	2/1229 (0.2%)	0.85	2/1658 (0.1%)
5	E	0.94	1/871 (0.1%)	0.94	2/1182 (0.2%)
5	R	0.86	1/871 (0.1%)	0.85	3/1182 (0.3%)
6	F	0.91	0/765	0.97	1/1038 (0.1%)
6	S	1.06	2/765 (0.3%)	1.07	3/1038 (0.3%)
7	G	1.07	2/690 (0.3%)	0.92	0/937
7	T	1.00	2/690 (0.3%)	0.91	0/937
8	H	0.94	0/682	0.88	1/921 (0.1%)
8	U	0.86	0/682	0.88	2/921 (0.2%)
9	I	1.07	0/605	0.87	0/802
9	V	1.07	0/605	0.88	0/802
10	J	1.01	0/471	0.86	0/636
10	W	0.92	0/471	0.88	0/636
11	K	0.96	0/398	0.89	1/546 (0.2%)
11	X	1.00	1/398 (0.3%)	0.77	0/546
12	L	0.87	0/393	0.83	0/526
12	Y	1.08	1/393 (0.3%)	0.81	0/526
13	M	0.94	0/345	0.93	1/470 (0.2%)
13	Z	0.81	0/345	0.86	0/470
All	All	0.96	19/29324 (0.1%)	0.89	40/39866 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	8.62	1.65	1.50
7	T	36	TRP	CB-CG	8.62	1.65	1.50
12	Y	16	GLU	CG-CD	8.15	1.64	1.51
2	O	198	GLU	C-O	6.50	1.35	1.23
2	B	198	GLU	C-O	6.47	1.35	1.23
6	S	54	ASN	CB-CG	-6.20	1.36	1.51
2	O	59	GLN	CG-CD	5.88	1.64	1.51
6	S	60	CYS	CB-SG	-5.71	1.72	1.81
4	Q	58	GLU	CG-CD	5.65	1.60	1.51
7	T	5	LYS	CB-CG	5.58	1.67	1.52
4	D	36	SER	CB-OG	-5.44	1.35	1.42
5	R	80	GLU	CG-CD	5.33	1.59	1.51
2	O	60	GLU	CB-CG	5.17	1.61	1.52
2	B	18	GLU	CD-OE1	5.13	1.31	1.25
5	E	9	GLU	CG-CD	5.12	1.59	1.51
7	G	5	LYS	CB-CG	5.11	1.66	1.52
4	Q	10	ASP	CB-CG	5.10	1.62	1.51
3	C	192	VAL	CB-CG2	-5.03	1.42	1.52
11	X	52	GLU	CB-CG	5.02	1.61	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	LEU	CB-CG-CD2	-10.95	92.39	111.00
1	A	136	LEU	CA-CB-CG	8.60	135.08	115.30
1	A	136	LEU	CB-CG-CD1	8.13	124.81	111.00
8	H	27	ARG	NE-CZ-NH1	7.85	124.23	120.30
4	D	20	ARG	NE-CZ-NH2	-7.71	116.44	120.30
5	E	90	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	407	ASP	CB-CG-OD1	-7.32	111.71	118.30
1	A	486	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	486	ASP	CB-CG-OD2	-6.97	112.03	118.30
11	K	54	ARG	NE-CZ-NH1	-6.87	116.86	120.30
5	R	25	ASP	CB-CG-OD1	6.78	124.40	118.30
3	C	44	MET	CG-SD-CE	6.76	111.01	100.20
1	A	96	ARG	NE-CZ-NH2	-6.54	117.03	120.30
6	S	54	ASN	CB-CA-C	-6.46	97.47	110.40
5	E	90	ARG	NE-CZ-NH1	6.46	123.53	120.30
4	D	26	ASP	CB-CG-OD1	6.42	124.08	118.30
2	B	188	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	B	173	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	208	MET	CG-SD-CE	5.89	109.62	100.20
1	A	35	LEU	CA-CB-CG	-5.79	101.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	LEU	CB-CG-CD2	5.79	120.84	111.00
13	M	37	LEU	CB-CG-CD1	-5.76	101.20	111.00
1	N	136	LEU	CB-CG-CD1	5.62	120.55	111.00
4	Q	10	ASP	CB-CG-OD1	5.61	123.35	118.30
6	S	94	HIS	N-CA-C	5.59	126.09	111.00
1	N	117	MET	CA-CB-CG	5.56	122.75	113.30
3	C	221	ARG	NE-CZ-NH1	-5.50	117.55	120.30
8	U	38	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	96	ARG	NE-CZ-NH1	5.39	122.99	120.30
4	D	20	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	A	512	ASN	CB-CA-C	-5.31	99.78	110.40
6	F	74	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	A	169	ILE	CG1-CB-CG2	-5.21	99.93	111.40
6	S	93	PRO	C-N-CA	5.19	134.66	121.70
3	P	155	ASP	CB-CG-OD1	5.17	122.95	118.30
4	Q	51	LEU	CA-CB-CG	5.16	127.17	115.30
5	R	14	ARG	NE-CZ-NH1	5.14	122.87	120.30
5	R	30	ARG	NE-CZ-NH2	-5.13	117.73	120.30
8	U	35	ASP	CB-CG-OD2	5.11	122.90	118.30
1	N	512	ASN	CB-CA-C	-5.01	100.38	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	53	0
1	N	4027	0	4001	61	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	34	0
3	C	2110	0	2027	28	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	852	0	845	8	0
6	F	748	0	728	13	0
6	S	748	0	728	27	0
7	G	675	0	644	31	0
7	T	675	0	644	33	0
8	H	662	0	623	11	0
8	U	662	0	623	5	0
9	I	601	0	613	7	0
9	V	601	0	613	10	0
10	J	460	0	459	2	0
10	W	460	0	459	6	0
11	K	384	0	366	2	0
11	X	384	0	366	6	0
12	L	380	0	380	12	0
12	Y	380	0	380	11	1
13	M	335	0	352	3	0
13	Z	335	0	352	1	0
14	A	120	0	108	10	0
14	N	120	0	108	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	63	0	110	6	0
18	D	63	0	110	5	0
18	L	63	0	110	14	0
18	N	189	0	330	22	0
19	A	102	0	152	13	0
19	C	102	0	152	10	0
19	N	102	0	152	9	0
19	P	102	0	152	7	0
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	52	0	80	11	0
21	O	52	0	80	17	0
22	B	29	0	39	2	0
22	C	58	0	78	2	0
22	G	29	0	39	0	0
22	J	29	0	38	2	0
22	P	58	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	29	0	38	3	0
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	106	0	154	8	0
24	G	53	0	77	10	0
24	P	106	0	154	13	0
24	T	53	0	77	12	0
25	C	100	0	156	19	0
25	G	100	0	156	20	0
25	P	100	0	156	9	0
25	T	100	0	156	24	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	39	0	0
27	Z	33	0	39	0	0
28	A	212	0	0	13	0
28	B	127	0	0	2	0
28	C	110	0	0	2	0
28	D	104	0	0	4	0
28	E	66	0	0	3	0
28	F	81	0	0	5	0
28	G	52	0	0	3	0
28	H	47	0	0	2	0
28	I	32	0	0	5	0
28	J	18	0	0	0	0
28	K	20	0	0	2	0
28	L	27	0	0	1	0
28	M	20	0	0	0	0
28	N	210	0	0	8	0
28	O	115	0	0	1	0
28	P	109	0	0	5	0
28	Q	60	0	0	4	0
28	R	45	0	0	0	0
28	S	79	0	0	4	0
28	T	42	0	0	4	0
28	U	47	0	0	0	0
28	V	24	0	0	5	1
28	W	17	0	0	1	0
28	X	18	0	0	1	0
28	Y	17	0	0	1	0
28	Z	12	0	0	0	0
All	All	32377	0	31226	521	1

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 8.

All (521) 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)
24:P:1265:PEK:H383	25:T:1269:CDL:C27	1.54	1.35
24:P:1265:PEK:C38	25:T:1269:CDL:H273	1.66	1.25
24:C:265:PEK:H383	25:G:269:CDL:H273	1.20	1.19
6:S:52:ILE:O	6:S:94:HIS:CE1	1.96	1.18
28:N:4772:HOH:O	24:P:1264:PEK:H381	1.44	1.14
6:S:52:ILE:O	6:S:94:HIS:NE2	1.80	1.14
7:T:84:LYS:H	7:T:84:LYS:HD2	1.02	1.13
1:A:1:FME:HG3	28:L:4907:HOH:O	1.50	1.11
24:C:265:PEK:H383	25:G:269:CDL:C27	1.83	1.07
21:O:1229:PSC:H142	21:O:1229:PSC:H343	1.07	1.06
25:G:269:CDL:H541	25:G:269:CDL:H231	1.37	1.06
21:O:1229:PSC:C34	21:O:1229:PSC:H142	1.86	1.06
18:D:523:TGL:H361	28:I:4610:HOH:O	1.54	1.04
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.39	1.03
2:O:224:ALA:O	2:O:227:LEU:HG	1.59	1.02
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.22	1.02
24:C:265:PEK:C38	25:G:269:CDL:H273	1.88	1.02
21:B:229:PSC:H142	21:B:229:PSC:H343	1.41	1.01
7:G:84:LYS:HD2	7:G:84:LYS:H	1.19	0.99
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.42	0.98
6:F:54:ASN:HB2	28:F:4662:HOH:O	1.61	0.96
21:O:1229:PSC:H343	21:O:1229:PSC:C14	1.94	0.96
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.49	0.93
6:S:53:THR:HA	6:S:94:HIS:CE1	2.03	0.93
1:N:513:LEU:O	1:N:514:LYS:HB2	1.64	0.92
7:T:84:LYS:H	7:T:84:LYS:CD	1.82	0.92
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.50	0.92
7:T:84:LYS:N	7:T:84:LYS:HD2	1.84	0.90
18:D:523:TGL:HC21	18:D:523:TGL:HG11	1.51	0.90
1:A:55:ASN:HB2	28:A:2299:HOH:O	1.70	0.90
19:P:1268:PGV:H062	28:P:4397:HOH:O	1.68	0.90
7:G:72:ASN:H	7:G:76:ASN:HD22	1.19	0.89
6:S:53:THR:HA	6:S:94:HIS:HE1	1.38	0.89
7:T:72:ASN:H	7:T:76:ASN:HD22	1.18	0.88
7:G:5:LYS:HB2	24:G:1263:PEK:H362	1.56	0.87
1:A:112:LEU:HG	28:A:2701:HOH:O	1.73	0.87
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.57	0.86
19:A:524:PGV:H311	13:M:19:LEU:HD23	1.57	0.86
3:P:3:HIS:HB3	28:P:4285:HOH:O	1.73	0.86
6:F:85:CYS:SG	6:F:87:THR:HG23	2.16	0.85
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.41	0.85
18:A:521:TGL:HC82	28:A:4504:HOH:O	1.76	0.84
1:A:278:MET:SD	7:T:5:LYS:HB3	2.17	0.84
1:N:112:LEU:HG	28:N:3701:HOH:O	1.77	0.84
6:S:64:GLU:O	6:S:65:ASP:HB2	1.77	0.82
25:T:1269:CDL:H541	25:T:1269:CDL:H231	1.62	0.82
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.20	0.82
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.45	0.82
25:G:269:CDL:C54	25:G:269:CDL:H231	2.11	0.80
25:G:269:CDL:H522	25:G:269:CDL:H202	1.63	0.80
24:P:1265:PEK:H383	25:T:1269:CDL:H273	0.82	0.80
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.64	0.79
1:N:513:LEU:O	1:N:514:LYS:CB	2.30	0.79
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.22	0.78
3:C:246:ASP:HB2	28:C:4249:HOH:O	1.82	0.78
7:G:5:LYS:HB3	1:N:278:MET:SD	2.23	0.78
19:A:524:PGV:H062	28:A:2126:HOH:O	1.83	0.78
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.66	0.77
7:T:3:ALA:HB1	24:T:263:PEK:H382	1.64	0.77
2:B:56:MET:HG2	21:B:229:PSC:H211	1.67	0.77
18:N:1523:TGL:HC21	18:N:1523:TGL:HG11	1.67	0.77
14:A:516:HEA:HMC1	14:A:516:HEA:HBC1	1.67	0.76
4:D:34:SER:H	4:D:37:GLN:HE21	1.34	0.76
6:S:52:ILE:C	6:S:94:HIS:CE1	2.59	0.76
6:S:85:CYS:SG	6:S:87:THR:HG23	2.25	0.76
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.68	0.75
18:N:1521:TGL:H201	18:N:1521:TGL:H241	1.69	0.75
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.34	0.74
1:A:506:GLU:HG3	28:A:4882:HOH:O	1.87	0.74
6:S:52:ILE:O	6:S:94:HIS:CD2	2.40	0.73
21:B:229:PSC:H072	9:I:10:ARG:HH21	1.54	0.73
7:G:5:LYS:HG3	24:G:1263:PEK:H383	1.70	0.72
7:G:84:LYS:H	7:G:84:LYS:CD	2.01	0.72
24:P:1265:PEK:H041	6:S:1:ALA:N	2.05	0.72
2:B:13:THR:HB	2:B:168:LEU:HD23	1.70	0.72
21:B:229:PSC:C07	9:I:10:ARG:HH21	2.02	0.71
7:G:2:SER:O	24:G:1263:PEK:H322	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:N:4478:HOH:O	4:Q:100:LYS:HE2	1.90	0.71
9:V:18:ARG:HD3	28:V:4483:HOH:O	1.90	0.71
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.27	0.70
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.73	0.70
24:P:1264:PEK:H161	24:P:1264:PEK:H101	1.74	0.70
10:W:33:ARG:HG2	22:W:1059:CHD:H151	1.74	0.69
7:G:3:ALA:HB1	24:G:1263:PEK:H382	1.73	0.69
2:B:41:ILE:HD13	21:B:229:PSC:H342	1.74	0.69
1:A:406:ASN:HD21	19:A:524:PGV:H22	1.57	0.69
9:I:73:LYS:HB3	28:I:4200:HOH:O	1.91	0.68
18:D:523:TGL:HB62	18:D:523:TGL:HA52	1.74	0.68
19:A:524:PGV:H82	19:A:524:PGV:H262	1.75	0.68
18:N:1521:TGL:C28	18:N:1521:TGL:H101	2.24	0.68
24:C:264:PEK:H101	24:C:264:PEK:H161	1.76	0.68
24:P:1265:PEK:H383	25:T:1269:CDL:H272	1.72	0.68
7:G:30:LEU:CD2	25:G:269:CDL:H462	2.24	0.67
6:F:95:GLN:OE1	6:F:95:GLN:HA	1.94	0.67
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.58	0.67
28:G:4789:HOH:O	19:P:1268:PGV:H341	1.94	0.67
1:A:513:LEU:O	1:A:514:LYS:HB2	1.94	0.67
28:B:2562:HOH:O	18:D:523:TGL:HC72	1.95	0.67
7:T:5:LYS:HD2	24:T:263:PEK:H371	1.76	0.67
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.77	0.67
7:G:72:ASN:H	7:G:76:ASN:ND2	1.92	0.66
7:T:72:ASN:H	7:T:76:ASN:ND2	1.90	0.66
7:G:30:LEU:HD21	25:G:269:CDL:H462	1.77	0.66
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.76	0.66
28:B:3446:HOH:O	7:T:17:ARG:HD2	1.96	0.66
6:S:95:GLN:HB2	28:S:4523:HOH:O	1.96	0.65
7:T:3:ALA:CB	24:T:263:PEK:H382	2.27	0.64
7:G:3:ALA:O	7:G:4:ALA:HB2	1.97	0.64
24:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.43	0.64
11:X:54:ARG:HG3	11:X:54:ARG:NH2	2.12	0.64
21:O:1229:PSC:O01	21:O:1229:PSC:H212	1.98	0.64
3:C:210:ILE:HG12	19:C:267:PGV:H132	1.79	0.63
12:L:11:ILE:CG2	18:L:522:TGL:H271	2.29	0.63
9:V:65:LYS:O	11:X:54:ARG:NH1	2.32	0.63
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.80	0.63
7:T:3:ALA:O	7:T:4:ALA:HB2	1.99	0.63
4:Q:31:LYS:HB3	28:Q:4834:HOH:O	1.97	0.62
25:T:1269:CDL:H172	25:T:1269:CDL:H511	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:HIS:HD2	28:P:4343:HOH:O	1.81	0.62
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.82	0.62
2:O:41:ILE:HD13	21:O:1229:PSC:H342	1.82	0.62
1:A:430:PHE:HE1	18:A:521:TGL:HB21	1.65	0.62
19:C:267:PGV:H182	25:C:270:CDL:C67	2.30	0.62
18:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.80	0.62
25:T:1269:CDL:H171	28:T:4708:HOH:O	2.00	0.62
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.11	0.62
10:W:33:ARG:HG2	22:W:1059:CHD:C15	2.30	0.62
1:A:302:ARG:NH1	28:A:4472:HOH:O	2.29	0.61
4:D:7:LYS:HE3	28:D:4308:HOH:O	2.01	0.61
7:T:2:SER:O	24:T:263:PEK:H322	2.00	0.61
6:S:96:LEU:HD12	28:S:4273:HOH:O	1.99	0.61
1:N:321:PHE:CD2	21:O:1229:PSC:H341	2.36	0.61
7:T:7:ASP:HB2	28:T:4216:HOH:O	2.01	0.61
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.66	0.60
19:C:268:PGV:H42	28:P:4823:HOH:O	2.01	0.60
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	2.01	0.60
12:L:20:ARG:HH22	18:L:522:TGL:HC62	1.67	0.59
6:F:64:GLU:O	6:F:65:ASP:HB2	2.02	0.59
3:P:52:LEU:HD21	25:P:1270:CDL:H412	1.83	0.59
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.84	0.59
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.37	0.59
1:A:46:THR:HG23	28:A:2466:HOH:O	2.03	0.59
3:C:52:LEU:HD21	25:C:270:CDL:H412	1.83	0.59
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.68	0.59
1:A:406:ASN:HD21	19:A:524:PGV:C2	2.16	0.59
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.02	0.59
6:F:19:GLU:HG2	28:F:4411:HOH:O	2.00	0.59
7:T:5:LYS:CB	24:T:263:PEK:H362	2.26	0.59
1:N:430:PHE:HE1	18:N:1521:TGL:HB21	1.68	0.58
4:Q:127:LYS:HD2	28:V:3618:HOH:O	2.03	0.58
18:D:523:TGL:H242	18:D:523:TGL:HA91	1.85	0.58
9:V:2:THR:HG22	9:V:3:ALA:H	1.69	0.58
25:G:269:CDL:C52	25:G:269:CDL:H202	2.33	0.58
1:N:400:PHE:HB3	18:N:1522:TGL:H282	1.86	0.58
2:O:41:ILE:CD1	21:O:1229:PSC:H342	2.33	0.58
18:N:1521:TGL:H281	18:N:1521:TGL:H101	1.85	0.58
9:I:32:ALA:O	9:I:36:LYS:HE3	2.04	0.57
18:N:1523:TGL:HB22	4:Q:78:TRP:HA	1.85	0.57
19:A:524:PGV:H02	19:A:524:PGV:O14	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:522:PGV:H183	24:C:264:PEK:H332	1.86	0.57
25:C:270:CDL:H642	25:C:270:CDL:H191	1.85	0.57
1:N:177:SER:H	1:N:180:GLN:NE2	2.02	0.57
21:B:229:PSC:H042	28:E:2664:HOH:O	2.05	0.57
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.85	0.57
1:N:28:MET:CE	14:N:515:HEA:C27	2.83	0.57
21:O:1229:PSC:H222	21:O:1229:PSC:H21	1.87	0.57
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.85	0.57
1:A:383:MET:O	1:A:387:PHE:HB2	2.04	0.56
1:N:112:LEU:HD12	28:N:4714:HOH:O	2.04	0.56
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.86	0.56
18:L:522:TGL:CC6	18:L:522:TGL:HC22	2.35	0.56
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.87	0.56
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.88	0.56
6:S:53:THR:CA	6:S:94:HIS:CE1	2.84	0.56
24:P:1265:PEK:C38	25:T:1269:CDL:C27	2.47	0.56
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.18	0.56
25:G:269:CDL:H1	25:G:269:CDL:OB4	2.06	0.55
25:T:1269:CDL:OB4	25:T:1269:CDL:H1	2.07	0.55
8:H:27:ARG:HD3	28:H:4760:HOH:O	2.07	0.55
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.22	0.55
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.88	0.55
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.95	0.54
1:N:400:PHE:HB3	18:N:1522:TGL:C28	2.37	0.54
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.90	0.54
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.07	0.54
21:O:1229:PSC:C07	9:V:10:ARG:HH21	2.21	0.54
7:T:3:ALA:O	7:T:4:ALA:CB	2.54	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.54
4:D:31:LYS:HE2	28:D:4278:HOH:O	2.07	0.54
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.47	0.54
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.73	0.54
1:A:514:LYS:HE2	28:F:2514:HOH:O	2.06	0.54
1:N:151:HIS:CD2	24:P:1264:PEK:H382	2.43	0.54
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.90	0.54
24:P:1265:PEK:H041	6:S:1:ALA:H1	1.72	0.54
6:S:87:THR:HG21	28:S:3514:HOH:O	2.07	0.54
8:H:7:LYS:O	8:H:8:ILE:HB	2.07	0.54
7:G:31:CYS:SG	25:G:269:CDL:H552	2.49	0.53
28:A:2527:HOH:O	12:L:7:PRO:HG3	2.07	0.53
1:A:87:ILE:O	1:A:173:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:488:THR:HB	1:N:495:LEU:HD13	1.90	0.53
6:F:87:THR:HG21	28:F:4250:HOH:O	2.08	0.53
18:N:1521:TGL:C10	18:N:1521:TGL:H281	2.38	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.49	0.53
21:B:229:PSC:C14	21:B:229:PSC:H343	2.27	0.52
2:O:59:GLN:O	2:O:59:GLN:CG	2.57	0.52
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.91	0.52
24:G:1263:PEK:H042	3:P:77:LYS:NZ	2.24	0.52
19:N:1524:PGV:H011	19:N:1524:PGV:H221	1.90	0.52
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.92	0.52
19:N:1524:PGV:H011	19:N:1524:PGV:H22	1.91	0.52
3:P:63:ARG:NE	25:P:1270:CDL:HA22	2.07	0.52
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.91	0.52
21:O:1229:PSC:H322	21:O:1229:PSC:H12	1.92	0.52
25:C:270:CDL:CB3	25:C:270:CDL:HB21	2.40	0.52
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.45	0.52
7:G:2:SER:OG	24:G:1263:PEK:H301	2.10	0.52
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.45	0.52
21:O:1229:PSC:H071	9:V:10:ARG:HE	1.75	0.52
7:G:37:LEU:CD2	25:G:269:CDL:H361	2.40	0.51
3:P:250:LEU:HD22	25:T:1269:CDL:H662	1.91	0.51
19:C:267:PGV:H12	19:C:267:PGV:H161	1.91	0.51
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.92	0.51
14:A:515:HEA:HMC1	14:A:515:HEA:CB3	2.31	0.51
14:N:516:HEA:HBC1	14:N:516:HEA:HMC1	1.92	0.51
7:G:3:ALA:O	7:G:4:ALA:CB	2.58	0.51
1:A:400:PHE:HB3	18:L:522:TGL:H282	1.93	0.51
28:N:4478:HOH:O	4:Q:100:LYS:CE	2.54	0.51
5:R:80:GLU:N	5:R:80:GLU:OE1	2.42	0.51
24:P:1265:PEK:H041	6:S:1:ALA:H2	1.76	0.51
1:A:1:FME:HCN	1:A:4:ASN:H	1.76	0.51
7:T:5:LYS:HD2	24:T:263:PEK:C37	2.39	0.51
7:G:17:ARG:HD2	28:G:2446:HOH:O	2.10	0.51
1:N:400:PHE:O	18:N:1522:TGL:H283	2.11	0.51
1:A:48:LEU:N	28:A:2466:HOH:O	2.44	0.51
19:A:524:PGV:H201	28:A:4726:HOH:O	2.11	0.50
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.92	0.50
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.94	0.50
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.93	0.50
19:N:1266:PGV:H182	3:P:28:THR:HG22	1.93	0.50
2:O:58:ALA:O	2:O:62:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.36	0.50
12:L:11:ILE:HG22	18:L:522:TGL:H271	1.92	0.50
25:G:269:CDL:H352	2:O:78:LEU:HD12	1.93	0.50
1:A:21:LEU:HD23	18:L:522:TGL:H211	1.94	0.50
1:A:76:GLY:O	1:A:80:ASN:HB2	2.12	0.49
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.93	0.49
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.00	0.49
9:V:15:ARG:HB2	28:V:4449:HOH:O	2.12	0.49
18:N:1521:TGL:HC22	28:Q:3606:HOH:O	2.12	0.49
21:B:229:PSC:H322	21:B:229:PSC:H12	1.94	0.49
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.11	0.49
2:B:135:LEU:O	2:B:208:PRO:HG3	2.12	0.49
10:J:33:ARG:HG2	22:J:60:CHD:H151	1.95	0.49
2:O:1:FME:CE	2:O:133:LEU:HD13	2.43	0.49
19:A:524:PGV:H011	19:A:524:PGV:H221	1.95	0.49
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.12	0.49
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.95	0.49
3:C:122:HIS:HD2	28:C:4770:HOH:O	1.95	0.49
24:C:265:PEK:C37	25:G:269:CDL:H273	2.42	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.95	0.49
8:H:27:ARG:NH1	28:H:2431:HOH:O	2.44	0.49
1:N:112:LEU:HD23	1:N:112:LEU:C	2.33	0.49
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.43	0.49
1:N:514:LYS:HE2	28:S:3514:HOH:O	2.13	0.48
25:C:270:CDL:OA5	25:C:270:CDL:HB22	2.11	0.48
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.28	0.48
6:F:76:LYS:HD2	6:F:93:PRO:HG2	1.94	0.48
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.48	0.48
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.49	0.48
2:O:1:FME:HE1	2:O:133:LEU:HD13	1.94	0.48
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.13	0.48
12:L:20:ARG:NH2	18:L:522:TGL:HC42	2.29	0.48
18:N:1522:TGL:H271	12:Y:11:ILE:CG2	2.44	0.48
2:O:56:MET:HA	21:O:1229:PSC:H202	1.96	0.47
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.47
19:N:1524:PGV:H132	19:N:1524:PGV:H301	1.96	0.47
1:A:488:THR:HB	1:A:495:LEU:HD13	1.95	0.47
1:A:27:GLY:HA3	14:A:515:HEA:H273	1.97	0.47
3:C:52:LEU:HD23	25:C:270:CDL:H382	1.96	0.47
21:B:229:PSC:H21	21:B:229:PSC:H222	1.97	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:334:TRP:CZ3	18:N:1523:TGL:HA51	2.50	0.47
2:O:59:GLN:HG3	2:O:59:GLN:O	2.14	0.47
2:O:62:GLU:O	2:O:66:THR:HB	2.14	0.47
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.51	0.47
12:Y:15:VAL:HG12	12:Y:21:LEU:HD22	1.95	0.47
5:E:105:GLY:O	5:E:108:LYS:HG2	2.14	0.47
1:N:489:THR:HA	6:S:71:TRP:O	2.15	0.47
25:C:270:CDL:H172	25:C:270:CDL:H741	1.97	0.47
3:C:26:LEU:HD13	3:C:45:ILE:HG22	1.97	0.47
1:N:417:MET:O	1:N:421:VAL:HG22	2.15	0.47
5:R:5:HIS:HB3	5:R:6:GLU:H	1.64	0.47
6:S:64:GLU:O	6:S:65:ASP:CB	2.51	0.47
1:A:486:ASP:OD2	4:D:19:ARG:HD3	2.15	0.46
5:R:82:TYR:N	5:R:83:PRO:HD2	2.29	0.46
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.46
3:P:214:PHE:CD1	19:P:1267:PGV:H62	2.51	0.46
1:A:377:PHE:HB2	14:A:516:HEA:HMD3	1.96	0.46
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.51	0.46
2:B:79:PRO:O	2:B:83:ILE:HG13	2.15	0.46
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.43	0.46
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.96	0.46
11:K:52:GLU:HG3	28:K:4808:HOH:O	2.15	0.46
2:O:79:PRO:O	2:O:83:ILE:HG13	2.15	0.46
2:B:78:LEU:CD1	25:T:1269:CDL:H352	2.42	0.46
3:C:77:LYS:NZ	24:T:263:PEK:H042	2.29	0.46
18:A:521:TGL:H281	18:A:521:TGL:C10	2.46	0.46
7:G:5:LYS:CG	24:G:1263:PEK:H383	2.44	0.46
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.40	0.46
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.16	0.46
6:S:94:HIS:HB3	6:S:95:GLN:H	1.02	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.64	0.46
4:Q:109:HIS:HD2	28:Q:3122:HOH:O	1.98	0.46
3:C:77:LYS:HZ1	24:T:263:PEK:H042	1.81	0.46
7:G:37:LEU:HD21	25:G:269:CDL:H361	1.97	0.46
5:E:25:ASP:OD1	5:E:28:GLU:HG3	2.16	0.46
18:N:1521:TGL:H252	18:N:1521:TGL:HA91	1.98	0.46
2:O:13:THR:HB	2:O:168:LEU:HD23	1.98	0.46
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.16	0.46
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.97	0.46
2:B:102:HIS:O	2:B:104:TRP:HA	2.16	0.46
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:CG	28:A:2701:HOH:O	2.45	0.45
12:L:20:ARG:HH22	18:L:522:TGL:HC42	1.81	0.45
4:D:86:MET:CE	28:K:4688:HOH:O	2.63	0.45
8:H:17:ASP:OD1	8:H:17:ASP:C	2.54	0.45
19:A:524:PGV:O02	19:A:524:PGV:O13	2.34	0.45
6:S:92:VAL:HG23	6:S:92:VAL:O	2.15	0.45
10:W:56:PRO:HD3	12:Y:46:LYS:HG2	1.98	0.45
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.51	0.45
1:N:309:THR:HG22	14:N:516:HEA:HMB2	1.97	0.45
3:P:108:PRO:HA	28:P:3226:HOH:O	2.16	0.45
19:N:1266:PGV:H183	24:P:1264:PEK:H332	1.98	0.45
2:B:222:TRP:O	2:B:226:MET:HB2	2.17	0.45
19:C:267:PGV:H182	25:C:270:CDL:H671	1.97	0.45
8:H:60:TYR:C	8:H:60:TYR:CD1	2.89	0.45
1:N:402:GLY:HA3	1:N:499:PRO:HD3	1.99	0.45
3:C:112:LEU:HD13	3:C:118:PRO:HG3	1.99	0.45
3:C:139:ALA:CB	7:G:24:ALA:HB1	2.46	0.45
7:G:84:LYS:HD2	7:G:84:LYS:N	2.05	0.45
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.98	0.45
22:B:1085:CHD:H212	22:B:1085:CHD:H12	1.98	0.45
18:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.98	0.45
7:T:12:GLY:HA3	28:T:3372:HOH:O	2.17	0.45
28:O:4335:HOH:O	8:U:61:LYS:HD2	2.17	0.45
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.45
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.98	0.45
6:F:25:ARG:HD2	28:F:4164:HOH:O	2.17	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.98	0.45
4:D:132:GLN:OE1	9:I:43:ARG:HD3	2.17	0.44
11:K:24:PHE:O	11:K:28:VAL:HG12	2.17	0.44
1:N:335:SER:HB2	1:N:336:PRO:HD2	1.98	0.44
19:A:524:PGV:H232	19:A:524:PGV:H42	1.98	0.44
7:G:5:LYS:HD2	24:G:1263:PEK:H371	1.99	0.44
19:N:1524:PGV:O13	19:N:1524:PGV:O02	2.35	0.44
21:O:1229:PSC:H251	21:O:1229:PSC:H221	1.73	0.44
1:A:430:PHE:CE1	18:A:521:TGL:HB21	2.48	0.44
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.62	0.44
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.52	0.44
24:G:1263:PEK:H182	3:P:98:PHE:CD2	2.53	0.44
1:A:483:LEU:HD21	13:M:4:LYS:HD3	2.00	0.44
1:N:472:ILE:HG21	18:N:1522:TGL:CA9	2.47	0.44
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:MET:HG2	7:T:5:LYS:HA	2.00	0.44
2:B:81:LEU:HD12	25:T:1269:CDL:H351	1.99	0.44
7:G:31:CYS:SG	25:G:269:CDL:H532	2.57	0.44
18:N:1523:TGL:C36	28:V:4391:HOH:O	2.66	0.44
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	2.00	0.44
3:C:105:SER:HA	3:C:116:TRP:CE3	2.53	0.44
7:G:2:SER:OG	24:G:1263:PEK:H291	2.18	0.44
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.52	0.44
2:O:95:LEU:HD23	2:O:150:ILE:HG12	2.00	0.44
1:A:310:MET:CE	1:A:360:ASN:HD21	2.30	0.44
25:C:270:CDL:H652	25:C:270:CDL:H611	1.98	0.44
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.18	0.44
3:P:228:THR:HA	6:S:7:PRO:O	2.18	0.44
6:S:55:LYS:HA	6:S:74:LEU:O	2.18	0.44
12:Y:2:HIS:N	28:Y:4664:HOH:O	2.50	0.44
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.53	0.44
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.98	0.44
2:O:146:MET:HA	2:O:213:LEU:HD12	2.00	0.44
25:C:270:CDL:H202	25:C:270:CDL:H171	1.81	0.43
25:C:270:CDL:HB32	25:C:270:CDL:HB21	2.00	0.43
7:G:30:LEU:HD23	25:G:269:CDL:C46	2.48	0.43
3:P:107:ALA:HB2	19:P:1268:PGV:H031	1.99	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.18	0.43
22:W:1059:CHD:H193	22:W:1059:CHD:H111	1.77	0.43
6:F:92:VAL:O	6:F:92:VAL:HG23	2.18	0.43
12:L:24:MET:SD	18:L:522:TGL:H161	2.58	0.43
1:A:37:ILE:HG21	14:A:515:HEA:CMA	2.47	0.43
21:B:229:PSC:H251	21:B:229:PSC:H221	1.67	0.43
4:D:112:GLU:HB2	28:D:4721:HOH:O	2.17	0.43
1:N:148:PHE:HB3	3:P:28:THR:HB	2.00	0.43
25:T:1269:CDL:C57	25:T:1269:CDL:H782	2.29	0.43
1:N:87:ILE:O	1:N:173:PRO:HD3	2.18	0.43
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.18	0.43
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.43
1:A:310:MET:HE1	1:A:360:ASN:HD21	1.84	0.43
11:X:52:GLU:HG2	28:X:4813:HOH:O	2.18	0.43
1:A:309:THR:HG22	14:A:516:HEA:HMB2	2.01	0.43
5:E:14:ARG:HD2	28:E:4284:HOH:O	2.18	0.43
18:N:1523:TGL:H361	28:V:4391:HOH:O	2.17	0.43
2:O:121:TYR:O	2:O:138:VAL:HA	2.18	0.43
1:A:37:ILE:HG21	14:A:515:HEA:HMA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:TYR:CG	1:N:76:GLY:HA3	2.53	0.43
1:N:54:TYR:HB2	28:N:4621:HOH:O	2.19	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.43
21:O:1229:PSC:C02	21:O:1229:PSC:H212	2.49	0.43
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.19	0.43
1:A:489:THR:HA	6:F:71:TRP:O	2.19	0.43
2:B:121:TYR:O	2:B:138:VAL:HA	2.19	0.43
4:D:34:SER:H	4:D:37:GLN:NE2	2.07	0.43
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.54	0.43
1:N:400:PHE:C	18:N:1522:TGL:H283	2.39	0.43
2:O:93:PRO:HG3	2:O:151:ARG:HB2	2.00	0.43
25:T:1269:CDL:H182	25:T:1269:CDL:H152	1.85	0.43
25:C:270:CDL:H532	25:C:270:CDL:H561	1.81	0.42
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.19	0.42
1:N:347:LEU:HD13	1:N:383:MET:SD	2.59	0.42
1:N:76:GLY:O	1:N:80:ASN:HB2	2.18	0.42
22:C:271:CHD:H12A	22:C:271:CHD:H112	1.87	0.42
24:C:265:PEK:C38	25:G:269:CDL:C27	2.66	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
7:T:11:TPO:O	7:T:11:TPO:CG2	2.66	0.42
1:A:437:PRO:HG2	1:A:440:TYR:CZ	2.54	0.42
18:L:522:TGL:HA81	18:L:522:TGL:H211	1.55	0.42
1:N:386:VAL:HG11	14:N:515:HEA:H261	2.01	0.42
1:N:495:LEU:HA	1:N:495:LEU:HD12	1.92	0.42
12:L:12:PRO:HB2	18:L:522:TGL:HG2	2.01	0.42
21:O:1229:PSC:H081	5:R:8:ASP:OD1	2.18	0.42
7:T:38:HIS:NE2	25:T:1269:CDL:H111	2.35	0.42
7:G:25:LEU:HA	7:G:25:LEU:HD23	1.90	0.42
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.19	0.42
1:A:28:MET:CE	14:A:515:HEA:H271	2.49	0.42
3:C:91:VAL:HG22	24:T:263:PEK:H14	2.00	0.42
4:D:23:PRO:HG3	5:E:70:VAL:HG21	2.01	0.42
25:T:1269:CDL:H522	25:T:1269:CDL:H202	2.01	0.42
19:A:524:PGV:H061	19:A:524:PGV:P	2.59	0.42
8:H:37:HIS:NE2	8:H:76:ARG:NH2	2.67	0.42
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
28:G:4541:HOH:O	19:P:1268:PGV:H301	2.18	0.42
25:T:1269:CDL:HA62	25:T:1269:CDL:H322	2.00	0.42
1:A:514:LYS:NZ	28:A:2645:HOH:O	2.41	0.42
18:A:521:TGL:H281	18:A:521:TGL:H102	2.02	0.42
19:C:268:PGV:H341	28:T:4364:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.55	0.42
1:N:377:PHE:HB2	14:N:516:HEA:HMD3	2.01	0.42
21:O:1229:PSC:C07	9:V:10:ARG:HE	2.33	0.42
22:P:1525:CHD:H152	19:P:1268:PGV:H11	2.02	0.42
1:N:472:ILE:HG21	18:N:1522:TGL:HA91	2.02	0.42
25:C:270:CDL:C19	25:C:270:CDL:H642	2.49	0.42
4:D:127:LYS:HD2	28:I:2618:HOH:O	2.20	0.42
6:F:55:LYS:HA	6:F:74:LEU:O	2.19	0.42
25:G:269:CDL:H511	25:G:269:CDL:H172	2.02	0.42
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.59	0.42
7:T:84:LYS:N	7:T:84:LYS:CD	2.62	0.42
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.82	0.42
3:C:210:ILE:HD13	19:C:267:PGV:H301	2.01	0.41
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.71	0.41
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.33	0.41
22:B:1085:CHD:H212	22:B:1085:CHD:H183	2.01	0.41
25:P:1270:CDL:H242	25:P:1270:CDL:H661	2.01	0.41
4:Q:7:LYS:HA	28:Q:4706:HOH:O	2.19	0.41
10:W:27:THR:HB	28:W:4729:HOH:O	2.20	0.41
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.84	0.41
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	2.02	0.41
2:B:49:LYS:HE2	28:E:4606:HOH:O	2.19	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.02	0.41
3:C:207:HIS:CE1	19:C:267:PGV:H343	2.56	0.41
28:N:3199:HOH:O	3:P:17:PRO:HG2	2.20	0.41
7:T:2:SER:OG	24:T:263:PEK:H301	2.21	0.41
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.50	0.41
5:R:52:LEU:O	5:R:55:CYS:HB2	2.20	0.41
21:B:229:PSC:H031	21:B:229:PSC:O02	2.20	0.41
4:D:112:GLU:CB	28:D:4721:HOH:O	2.68	0.41
18:N:1523:TGL:HA32	18:N:1523:TGL:HB42	2.02	0.41
2:O:33:LEU:HD12	2:O:33:LEU:HA	1.93	0.41
3:P:37:PHE:CD1	10:W:52:TRP:HZ3	2.38	0.41
19:A:524:PGV:H152	19:A:524:PGV:H321	2.03	0.41
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.02	0.41
3:P:129:VAL:N	3:P:130:PRO:CD	2.82	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.55	0.41
2:O:41:ILE:O	2:O:45:MET:HG2	2.21	0.41
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.50	0.41
1:A:177:SER:H	1:A:180:GLN:HE21	1.69	0.41
18:A:521:TGL:HC22	28:I:2606:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:TYR:O	3:C:244:PHE:HB3	2.20	0.41
2:B:103:GLN:HA	2:B:104:TRP:HA	1.90	0.41
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.34	0.41
3:C:137:LEU:HD23	3:C:137:LEU:HA	1.85	0.41
12:L:20:ARG:HH12	18:L:522:TGL:HC62	1.86	0.41
3:P:139:ALA:CB	7:T:24:ALA:HB1	2.51	0.41
9:I:73:LYS:CB	28:I:4200:HOH:O	2.61	0.41
1:N:240:HIS:C	1:N:240:HIS:CD2	2.94	0.41
1:N:62:ALA:HB1	14:N:515:HEA:HMD3	2.03	0.41
19:C:267:PGV:H182	25:C:270:CDL:H673	2.01	0.41
10:J:40:LEU:HD12	22:J:60:CHD:H183	2.03	0.41
2:O:193:TYR:CD1	2:O:210:VAL:HG22	2.56	0.41
8:U:9:LYS:HB3	8:U:10:ASN:H	1.61	0.41
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.92	0.41
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.03	0.40
28:A:2690:HOH:O	2:B:201:GLY:HA2	2.21	0.40
1:N:172:LYS:HD2	1:N:181:THR:HG22	2.02	0.40
2:O:16:ILE:HD11	2:O:86:MET:HG2	2.04	0.40
3:P:105:SER:HA	3:P:116:TRP:CE3	2.55	0.40
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.57	0.40
6:F:53:THR:HB	6:F:54:ASN:H	1.74	0.40
2:O:3:TYR:CZ	2:O:6:GLN:HG3	2.56	0.40
2:O:4:PRO:HB2	11:X:43:SER:HA	2.03	0.40
6:S:51:SER:O	6:S:94:HIS:HA	2.20	0.40
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.56	0.40
8:H:9:LYS:HD3	8:H:9:LYS:HA	1.91	0.40
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.31	0.40
8:H:39:CYS:O	8:H:43:MET:HG2	2.22	0.40
2:O:90:ILE:HG12	8:U:16:PHE:CE2	2.56	0.40
21:O:1229:PSC:H071	9:V:10:ARG:HH21	1.87	0.40
8:H:75:ARG:HG2	8:H:80:THR:OG1	2.21	0.40
1:N:335:SER:HB2	28:N:3257:HOH:O	2.20	0.40
7:T:37:LEU:HD23	25:T:1269:CDL:H361	2.03	0.40

All (1) 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)
12:Y:2:HIS:N	28:V:4556:HOH:O[2_685]	2.13	0.07



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	494 (96%)	17 (3%)	1 (0%)	51	86
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	38	78
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	38	78
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	250 (97%)	5 (2%)	2 (1%)	22	64
4	D	142/147 (97%)	136 (96%)	6 (4%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
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%)	87 (91%)	8 (8%)	1 (1%)	18	59
6	S	96/98 (98%)	88 (92%)	6 (6%)	2 (2%)	8	38
7	G	81/85 (95%)	65 (80%)	8 (10%)	8 (10%)	1	3
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	2	10
8	H	77/85 (91%)	69 (90%)	5 (6%)	3 (4%)	3	20
8	U	77/85 (91%)	71 (92%)	4 (5%)	2 (3%)	6	31
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	13	49
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	47 (100%)	0	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3504/3614 (97%)	3351 (96%)	126 (4%)	27 (1%)	22	64

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
8	H	8	ILE
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
1	A	384	GLY
2	B	60	GLU
7	G	6	GLY
7	T	3	ALA
8	U	8	ILE
7	T	6	GLY
7	G	3	ALA
8	H	45	ALA
8	H	46	LYS
2	O	60	GLU
3	P	38	ASN
3	P	232	HIS
7	G	37	LEU
8	U	10	ASN
7	G	40	GLY
9	V	36	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	418 (98%)	8 (2%)	62	88
1	N	426/426 (100%)	415 (97%)	11 (3%)	51	83
2	B	210/210 (100%)	199 (95%)	11 (5%)	27	65
2	O	210/210 (100%)	197 (94%)	13 (6%)	21	58
3	C	224/226 (99%)	218 (97%)	6 (3%)	50	82
3	P	224/226 (99%)	217 (97%)	7 (3%)	45	80
4	D	128/129 (99%)	126 (98%)	2 (2%)	68	90
4	Q	128/129 (99%)	123 (96%)	5 (4%)	37	75
5	E	92/95 (97%)	90 (98%)	2 (2%)	57	86
5	R	92/95 (97%)	90 (98%)	2 (2%)	57	86
6	F	81/81 (100%)	77 (95%)	4 (5%)	29	68
6	S	81/81 (100%)	76 (94%)	5 (6%)	21	58
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	25
7	T	67/68 (98%)	61 (91%)	6 (9%)	11	40
8	H	71/75 (95%)	65 (92%)	6 (8%)	12	43
8	U	71/75 (95%)	66 (93%)	5 (7%)	18	53
9	I	57/57 (100%)	54 (95%)	3 (5%)	26	65
9	V	57/57 (100%)	54 (95%)	3 (5%)	26	65
10	J	49/50 (98%)	48 (98%)	1 (2%)	60	87
10	W	49/50 (98%)	48 (98%)	1 (2%)	60	87
11	K	39/46 (85%)	38 (97%)	1 (3%)	51	83
11	X	39/46 (85%)	38 (97%)	1 (3%)	51	83
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	38 (97%)	1 (3%)	51	83
13	M	37/38 (97%)	31 (84%)	6 (16%)	3	14
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	19
All	All	3040/3082 (99%)	2917 (96%)	123 (4%)	36	74

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	189	MET
1	A	338	MET
1	A	369	ASP
1	A	394	VAL
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
3	C	77	LYS
3	C	127	LEU
3	C	144	ILE
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	31	LYS
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	84	SER
6	F	87	THR
6	F	95	GLN
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	35	SER
7	G	36	TRP
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	27	ARG

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Mol	Chain	Res	Type
8	H	51	SER
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	189	MET
1	N	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	485	VAL
1	N	512	ASN
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	65	TRP
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	183	THR
2	O	217	LYS
3	P	33	MET
3	P	77	LYS
3	P	127	LEU
3	P	144	ILE
3	P	159	MET

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Mol	Chain	Res	Type
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	19	ARG
4	Q	51	LEU
4	Q	52	SER
4	Q	143	ASN
5	R	5	HIS
5	R	79	LYS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	64	GLU
6	S	95	GLN
7	T	17	ARG
7	T	18	PHE
7	T	38	HIS
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
8	U	70	SER
9	V	2	THR
9	V	8	GLN
9	V	26	MET
10	W	50	LEU
11	X	54	ARG
12	Y	20	ARG
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN

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Mol	Chain	Res	Type
1	A	512	ASN
2	B	22	HIS
2	B	52	HIS
2	B	181	GLN
3	C	68	GLN
3	C	122	HIS
4	D	29	HIS
4	D	37	GLN
4	D	109	HIS
4	D	143	ASN
5	E	94	ASN
7	G	8	HIS
7	G	71	HIS
7	G	76	ASN
9	I	8	GLN
10	J	29	ASN
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	181	GLN
3	P	3	HIS
3	P	68	GLN
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
7	T	76	ASN
10	W	57	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	A	1	1	9,9,10	0.90	0	7,9,11	4.71	4 (57%)
2	FME	B	1	2	9,9,10	1.06	0	7,9,11	5.80	3 (42%)
7	TPO	G	11	7	9,10,11	3.15	5 (55%)	10,14,16	1.43	2 (20%)
9	SAC	I	1	9	8,8,9	2.52	3 (37%)	6,9,11	1.81	2 (33%)
1	FME	N	1	1	9,9,10	0.97	1 (11%)	7,9,11	5.69	4 (57%)
2	FME	O	1	2	9,9,10	0.73	0	7,9,11	4.98	2 (28%)
7	TPO	T	11	7	9,10,11	2.61	4 (44%)	10,14,16	1.59	2 (20%)
9	SAC	V	1	9	8,8,9	2.98	3 (37%)	6,9,11	3.75	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	1/6/9/11	0/0/0/0
2	FME	O	1	2	-	1/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O2P	2.09	1.63	1.54
7	T	11	TPO	P-O2P	2.09	1.63	1.54
7	G	11	TPO	CB-CA	2.18	1.57	1.53
1	N	1	FME	CA-C	2.27	1.53	1.50
9	I	1	SAC	CA-C	2.67	1.53	1.50
7	G	11	TPO	P-O1P	3.04	1.61	1.50
7	T	11	TPO	P-O1P	3.23	1.61	1.50
9	I	1	SAC	CA-N	3.64	1.51	1.46
7	T	11	TPO	P-OG1	3.81	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	4.30	1.33	1.23
7	T	11	TPO	CA-C	4.62	1.56	1.50
9	V	1	SAC	CA-N	4.69	1.53	1.46
9	I	1	SAC	OAC-C1A	5.09	1.35	1.23
9	V	1	SAC	CA-C	5.31	1.57	1.50
7	G	11	TPO	P-OG1	5.46	1.69	1.59
7	G	11	TPO	CA-C	5.67	1.57	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CA-N-CN	-14.36	100.73	122.82
2	B	1	FME	CA-N-CN	-14.25	100.91	122.82
2	O	1	FME	CA-N-CN	-12.59	103.45	122.82
1	A	1	FME	CA-N-CN	-11.19	105.61	122.82
9	V	1	SAC	CB-CA-N	-8.46	90.89	110.60
2	B	1	FME	CG-CB-CA	-4.30	100.52	112.97
1	A	1	FME	CG-CB-CA	-3.35	103.26	112.97
9	I	1	SAC	C2A-C1A-N	-2.81	111.03	116.11
2	O	1	FME	CG-CB-CA	-2.52	105.69	112.97
7	T	11	TPO	O-C-CA	-2.49	119.34	125.15
7	G	11	TPO	O-C-CA	-2.34	119.70	125.15
2	B	1	FME	CB-CA-C	-2.33	107.81	111.65
9	V	1	SAC	O-C-CA	-2.31	119.75	125.15
1	N	1	FME	O-C-CA	-2.07	120.31	125.15
1	A	1	FME	CB-CA-C	2.08	115.08	111.65
9	I	1	SAC	OG-CB-CA	2.11	116.38	111.02
1	N	1	FME	CE-SD-CG	2.33	108.72	100.35
7	G	11	TPO	O2P-P-OG1	2.82	118.81	106.00
7	T	11	TPO	CG2-CB-CA	2.90	118.59	113.22
1	N	1	FME	CB-CA-C	2.90	116.42	111.65
1	A	1	FME	CE-SD-CG	3.57	113.16	100.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 8 are monoatomic and 2 are unknown - leaving 42 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	515	1	44,67,67	1.16	4 (9%)	37,103,103	2.84	17 (45%)
14	HEA	A	516	1	44,67,67	1.18	4 (9%)	37,103,103	1.83	7 (18%)
18	TGL	A	521	-	62,62,62	1.26	6 (9%)	65,65,65	1.88	15 (23%)
19	PGV	A	522	-	50,50,50	0.85	2 (4%)	51,56,56	1.21	2 (3%)
19	PGV	A	524	-	50,50,50	1.27	2 (4%)	51,56,56	1.30	8 (15%)
22	CHD	B	1085	-	29,32,32	0.76	0	47,51,51	1.88	15 (31%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	PSC	B	229	-	51,51,51	1.20	3 (5%)	56,59,59	1.15	2 (3%)
24	PEK	C	264	-	52,52,52	0.97	4 (7%)	54,57,57	1.48	8 (14%)
24	PEK	C	265	-	52,52,52	1.27	3 (5%)	54,57,57	1.29	6 (11%)
19	PGV	C	267	-	50,50,50	0.83	3 (6%)	51,56,56	1.12	4 (7%)
19	PGV	C	268	-	50,50,50	1.25	2 (4%)	51,56,56	1.41	6 (11%)
25	CDL	C	270	-	99,99,99	1.36	13 (13%)	101,111,111	1.41	15 (14%)
22	CHD	C	271	-	29,32,32	0.59	0	47,51,51	2.28	19 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CHD	C	525	-	29,32,32	0.78	0	47,51,51	1.24	5 (10%)
18	TGL	D	523	-	62,62,62	1.37	6 (9%)	65,65,65	1.68	9 (13%)
24	PEK	G	1263	-	52,52,52	1.32	4 (7%)	54,57,57	1.38	6 (11%)
22	CHD	G	229	-	29,32,32	0.54	0	47,51,51	1.25	2 (4%)
25	CDL	G	269	-	99,99,99	1.41	12 (12%)	101,111,111	1.39	12 (11%)
22	CHD	J	60	-	29,32,32	0.94	0	47,51,51	3.06	23 (48%)
18	TGL	L	522	-	62,62,62	1.38	7 (11%)	65,65,65	1.66	12 (18%)
27	DMU	M	526	-	34,34,34	0.96	2 (5%)	45,45,45	2.74	16 (35%)
19	PGV	N	1266	-	50,50,50	0.84	2 (4%)	51,56,56	1.44	6 (11%)
18	TGL	N	1521	-	62,62,62	1.27	6 (9%)	65,65,65	1.67	10 (15%)
18	TGL	N	1522	-	62,62,62	1.59	7 (11%)	65,65,65	1.66	14 (21%)
18	TGL	N	1523	-	62,62,62	1.38	6 (9%)	65,65,65	1.54	12 (18%)
19	PGV	N	1524	-	50,50,50	0.99	2 (4%)	51,56,56	1.27	8 (15%)
14	HEA	N	515	1	44,67,67	1.56	7 (15%)	37,103,103	3.36	17 (45%)
14	HEA	N	516	1	44,67,67	1.13	3 (6%)	37,103,103	1.55	11 (29%)
21	PSC	O	1229	-	51,51,51	1.18	3 (5%)	56,59,59	1.15	4 (7%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
24	PEK	P	1264	-	52,52,52	0.99	4 (7%)	54,57,57	1.43	10 (18%)
24	PEK	P	1265	-	52,52,52	1.33	5 (9%)	54,57,57	1.35	5 (9%)
19	PGV	P	1267	-	50,50,50	0.91	3 (6%)	51,56,56	1.10	4 (7%)
19	PGV	P	1268	-	50,50,50	1.22	2 (4%)	51,56,56	1.57	6 (11%)
25	CDL	P	1270	-	99,99,99	1.39	12 (12%)	101,111,111	1.48	17 (16%)
22	CHD	P	1271	-	29,32,32	0.60	0	47,51,51	2.25	18 (38%)
22	CHD	P	1525	-	29,32,32	0.68	0	47,51,51	1.59	9 (19%)
25	CDL	T	1269	-	99,99,99	1.36	12 (12%)	101,111,111	1.33	11 (10%)
24	PEK	T	263	-	52,52,52	1.31	4 (7%)	54,57,57	1.27	6 (11%)
22	CHD	W	1059	-	29,32,32	0.92	1 (3%)	47,51,51	3.37	22 (46%)
27	DMU	Z	1526	-	34,34,34	0.90	2 (5%)	45,45,45	2.69	17 (37%)

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	515	1	3/3/7/16	0/24/76/76	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
18	TGL	A	521	-	-	0/65/65/65	0/0/0/0
19	PGV	A	522	-	-	0/55/55/55	0/0/0/0
19	PGV	A	524	-	-	1/55/55/55	0/0/0/0
22	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	PSC	B	229	-	-	0/55/55/55	0/0/0/0
24	PEK	C	264	-	-	0/56/56/56	0/0/0/0
24	PEK	C	265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	268	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	0/110/110/110	0/0/0/0
22	CHD	C	271	-	-	0/7/74/74	0/4/4/4
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
18	TGL	D	523	-	-	0/65/65/65	0/0/0/0
24	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
22	CHD	G	229	-	-	0/7/74/74	0/4/4/4
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
22	CHD	J	60	-	-	0/7/74/74	0/4/4/4
18	TGL	L	522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	526	-	4/4/10/10	0/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
18	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
19	PGV	N	1524	-	-	1/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
21	PSC	O	1229	-	-	0/55/55/55	0/0/0/0
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
24	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
24	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
19	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
22	CHD	P	1271	-	-	0/7/74/74	0/4/4/4
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
24	PEK	T	263	-	-	0/56/56/56	0/0/0/0
22	CHD	W	1059	-	-	0/7/74/74	0/4/4/4
27	DMU	Z	1526	-	4/4/10/10	0/19/59/59	0/2/2/2

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	515	HEA	C4A-NA	-4.77	1.31	1.36
14	N	515	HEA	C1A-NA	-3.96	1.32	1.36
14	N	515	HEA	C1D-ND	-3.90	1.32	1.36
25	P	1270	CDL	C59-C58	-3.70	1.30	1.51
25	C	270	CDL	C59-C58	-3.58	1.31	1.51
18	L	522	TGL	C10-CB9	-3.55	1.31	1.51
18	L	522	TGL	C20-CA9	-3.48	1.31	1.51
25	P	1270	CDL	C79-C78	-3.43	1.32	1.51
18	N	1521	TGL	C10-CB9	-3.41	1.32	1.51
18	N	1522	TGL	C20-CA9	-3.38	1.32	1.51
14	A	515	HEA	C4A-NA	-3.37	1.32	1.36
25	T	1269	CDL	C59-C58	-3.31	1.32	1.51
25	P	1270	CDL	C62-C61	-3.29	1.32	1.51
18	A	521	TGL	C10-CB9	-3.29	1.32	1.51
25	T	1269	CDL	C42-C41	-3.23	1.33	1.51
25	C	270	CDL	C62-C61	-3.23	1.33	1.51
25	G	269	CDL	C59-C58	-3.23	1.33	1.51
18	N	1522	TGL	C10-CB9	-3.22	1.33	1.51
25	T	1269	CDL	C62-C61	-3.22	1.33	1.51
25	G	269	CDL	C42-C41	-3.15	1.33	1.51
14	N	515	HEA	C3A-C2A	-3.12	1.36	1.40
25	P	1270	CDL	C19-C18	-3.09	1.34	1.51
25	C	270	CDL	C19-C18	-3.09	1.34	1.51
25	C	270	CDL	C79-C78	-3.06	1.34	1.51
14	N	516	HEA	C4B-NB	-3.06	1.33	1.36
18	D	523	TGL	C20-CA9	-3.03	1.34	1.51
27	M	526	DMU	C3-C4	-3.03	1.44	1.52
25	P	1270	CDL	C82-C81	-3.03	1.34	1.51
27	Z	1526	DMU	C3-C4	-3.02	1.44	1.52
18	N	1523	TGL	C20-CA9	-3.01	1.34	1.51
25	C	270	CDL	C82-C81	-3.01	1.34	1.51
25	T	1269	CDL	C79-C78	-2.97	1.34	1.51
18	N	1523	TGL	C10-CB9	-2.96	1.34	1.51
14	A	515	HEA	C1D-ND	-2.96	1.33	1.36
18	A	521	TGL	C20-CA9	-2.94	1.34	1.51
25	C	270	CDL	C22-C21	-2.93	1.34	1.51
25	G	269	CDL	C62-C61	-2.93	1.34	1.51
18	D	523	TGL	C10-CB9	-2.92	1.35	1.51
25	G	269	CDL	C39-C38	-2.90	1.35	1.51
25	P	1270	CDL	C22-C21	-2.89	1.35	1.51
25	G	269	CDL	C22-C21	-2.89	1.35	1.51
18	D	523	TGL	C15-CC9	-2.88	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	264	PEK	O01-C02	-2.88	1.39	1.46
25	T	1269	CDL	C39-C38	-2.87	1.35	1.51
14	N	516	HEA	C4A-NA	-2.86	1.33	1.36
25	G	269	CDL	C19-C18	-2.85	1.35	1.51
24	P	1264	PEK	O03-C01	-2.85	1.38	1.45
18	N	1523	TGL	C15-CC9	-2.84	1.35	1.51
25	T	1269	CDL	C19-C18	-2.83	1.35	1.51
14	A	516	HEA	C4A-NA	-2.82	1.33	1.36
25	T	1269	CDL	C22-C21	-2.80	1.35	1.51
25	G	269	CDL	C82-C81	-2.79	1.35	1.51
25	T	1269	CDL	C82-C81	-2.78	1.35	1.51
25	G	269	CDL	C79-C78	-2.76	1.35	1.51
18	N	1521	TGL	C20-CA9	-2.73	1.36	1.51
14	A	516	HEA	C4B-NB	-2.67	1.33	1.36
18	N	1522	TGL	C15-CC9	-2.65	1.36	1.51
25	P	1270	CDL	C39-C38	-2.59	1.36	1.51
14	N	515	HEA	C4B-NB	-2.58	1.33	1.36
18	N	1521	TGL	C15-CC9	-2.57	1.36	1.51
24	C	264	PEK	O03-C01	-2.54	1.39	1.45
25	C	270	CDL	C42-C41	-2.54	1.37	1.51
25	C	270	CDL	C39-C38	-2.53	1.37	1.51
18	A	521	TGL	C15-CC9	-2.50	1.37	1.51
18	L	522	TGL	C15-CC9	-2.50	1.37	1.51
25	P	1270	CDL	C42-C41	-2.45	1.37	1.51
19	P	1267	PGV	O01-C02	-2.36	1.40	1.46
24	P	1264	PEK	O01-C02	-2.35	1.40	1.46
14	A	515	HEA	C4B-NB	-2.33	1.34	1.36
25	C	270	CDL	OB6-CB4	-2.18	1.40	1.46
14	A	516	HEA	C1A-NA	-2.14	1.34	1.36
19	C	267	PGV	O01-C02	-2.14	1.41	1.46
14	N	515	HEA	C1B-NB	-2.09	1.31	1.36
14	N	515	HEA	C4D-ND	-2.07	1.31	1.36
14	A	516	HEA	C14-C15	2.01	1.38	1.33
24	C	265	PEK	P-O11	2.03	1.67	1.59
14	A	515	HEA	C1B-CHB	2.06	1.45	1.40
22	W	1059	CHD	C13-C17	2.06	1.59	1.55
24	G	1263	PEK	C01-C02	2.07	1.56	1.50
24	G	1263	PEK	C03-C02	2.17	1.56	1.50
14	N	516	HEA	C1B-CHB	2.19	1.46	1.40
24	P	1265	PEK	C03-C02	2.21	1.57	1.50
24	P	1265	PEK	P-O12	2.22	1.68	1.59
18	L	522	TGL	CG1-CG2	2.24	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	1522	TGL	CG1-CG2	2.33	1.57	1.50
24	T	263	PEK	C03-C02	2.34	1.57	1.50
24	T	263	PEK	P-O11	2.36	1.69	1.59
27	Z	1526	DMU	O16-C6	2.54	1.44	1.40
19	P	1267	PGV	O01-C1	2.63	1.41	1.34
24	P	1265	PEK	P-O11	2.71	1.70	1.59
18	L	522	TGL	OG3-CC1	2.88	1.41	1.33
19	C	267	PGV	O01-C1	2.96	1.42	1.34
27	M	526	DMU	O16-C6	3.06	1.45	1.40
19	N	1266	PGV	O01-C1	3.13	1.43	1.34
24	C	264	PEK	O03-C21	3.15	1.42	1.33
19	N	1524	PGV	O01-C1	3.29	1.43	1.34
25	C	270	CDL	OB6-CB5	3.34	1.44	1.34
18	A	521	TGL	OG3-CC1	3.34	1.43	1.33
19	C	267	PGV	O03-C19	3.35	1.43	1.33
24	C	264	PEK	O01-C1	3.42	1.44	1.34
19	A	522	PGV	O01-C1	3.45	1.44	1.34
19	A	522	PGV	O03-C19	3.48	1.43	1.33
24	P	1264	PEK	O01-C1	3.60	1.44	1.34
24	P	1264	PEK	O03-C21	3.60	1.43	1.33
25	P	1270	CDL	OB8-CB7	3.78	1.44	1.33
19	N	1266	PGV	O03-C19	3.90	1.44	1.33
21	B	229	PSC	C13-C12	3.97	1.54	1.31
25	P	1270	CDL	OB6-CB5	4.00	1.45	1.34
21	O	1229	PSC	O03-C19	4.00	1.45	1.33
19	P	1267	PGV	O03-C19	4.04	1.45	1.33
21	O	1229	PSC	C13-C12	4.09	1.54	1.31
25	T	1269	CDL	OA8-CA7	4.13	1.45	1.33
19	A	524	PGV	O01-C1	4.22	1.46	1.34
18	N	1521	TGL	OG3-CC1	4.32	1.46	1.33
18	N	1521	TGL	OG2-CB1	4.42	1.47	1.34
25	C	270	CDL	OA6-CA5	4.42	1.47	1.34
21	O	1229	PSC	O01-C1	4.42	1.47	1.34
25	T	1269	CDL	OB6-CB5	4.43	1.47	1.34
18	N	1522	TGL	OG3-CC1	4.47	1.46	1.33
25	C	270	CDL	OB8-CB7	4.47	1.46	1.33
21	B	229	PSC	O01-C1	4.50	1.47	1.34
18	A	521	TGL	OG2-CB1	4.52	1.47	1.34
25	G	269	CDL	OA8-CA7	4.54	1.46	1.33
21	B	229	PSC	O03-C19	4.56	1.46	1.33
25	T	1269	CDL	OB8-CB7	4.59	1.46	1.33
19	P	1268	PGV	O03-C19	4.61	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1524	PGV	O03-C19	4.62	1.46	1.33
25	T	1269	CDL	OA6-CA5	4.63	1.47	1.34
18	N	1521	TGL	OG1-CA1	4.69	1.47	1.33
25	G	269	CDL	OB8-CB7	4.69	1.47	1.33
18	D	523	TGL	OG1-CA1	4.70	1.47	1.33
18	N	1523	TGL	OG1-CA1	4.76	1.47	1.33
25	G	269	CDL	OB6-CB5	4.82	1.48	1.34
19	C	268	PGV	O03-C19	4.82	1.47	1.33
18	N	1523	TGL	OG3-CC1	4.82	1.47	1.33
24	T	263	PEK	O01-C1	4.85	1.48	1.34
18	D	523	TGL	OG3-CC1	4.88	1.47	1.33
24	G	1263	PEK	O01-C1	4.95	1.48	1.34
25	P	1270	CDL	OA6-CA5	4.98	1.48	1.34
25	C	270	CDL	OA8-CA7	4.99	1.48	1.33
24	C	265	PEK	O01-C1	5.04	1.48	1.34
24	P	1265	PEK	O03-C21	5.07	1.48	1.33
18	L	522	TGL	OG1-CA1	5.09	1.48	1.33
25	P	1270	CDL	OA8-CA7	5.14	1.48	1.33
18	A	521	TGL	OG1-CA1	5.18	1.48	1.33
18	D	523	TGL	OG2-CB1	5.20	1.49	1.34
25	G	269	CDL	OA6-CA5	5.40	1.50	1.34
24	P	1265	PEK	O01-C1	5.62	1.50	1.34
18	N	1523	TGL	OG2-CB1	5.62	1.50	1.34
24	C	265	PEK	O03-C21	5.68	1.50	1.33
19	C	268	PGV	O01-C1	5.72	1.50	1.34
18	L	522	TGL	OG2-CB1	5.79	1.51	1.34
19	P	1268	PGV	O01-C1	5.81	1.51	1.34
24	G	1263	PEK	O03-C21	5.98	1.51	1.33
18	N	1522	TGL	OG2-CB1	6.05	1.51	1.34
24	T	263	PEK	O03-C21	6.10	1.51	1.33
19	A	524	PGV	O03-C19	6.13	1.51	1.33
18	N	1522	TGL	OG1-CA1	6.72	1.53	1.33

All (416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	C17-C18-C19	-8.80	105.58	127.68
14	N	515	HEA	C17-C18-C19	-8.53	106.25	127.68
14	N	515	HEA	C4B-C3B-C2B	-7.84	101.39	106.87
22	W	1059	CHD	C18-C13-C12	-7.34	101.61	109.08
22	W	1059	CHD	C17-C13-C14	-6.80	93.16	100.08
22	J	60	CHD	C17-C13-C14	-5.98	94.00	100.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	522	TGL	OG3-CC1-OC1	-5.67	109.47	123.55
14	A	516	HEA	CAD-CBD-CGD	-5.60	103.09	112.66
14	N	515	HEA	C12-C13-C14	-5.01	99.17	112.33
22	C	271	CHD	C19-C10-C1	-4.91	100.18	108.24
18	D	523	TGL	CG3-CG2-CG1	-4.70	101.26	111.86
22	P	1271	CHD	C19-C10-C1	-4.70	100.53	108.24
19	N	1266	PGV	O03-C19-O04	-4.63	112.05	123.55
22	C	271	CHD	C18-C13-C12	-4.63	104.37	109.08
14	N	515	HEA	C26-C15-C16	-4.59	107.31	115.29
18	N	1523	TGL	CG3-CG2-CG1	-4.52	101.65	111.86
22	J	60	CHD	C6-C5-C4	-4.13	106.43	111.13
19	A	522	PGV	O03-C19-O04	-4.07	113.44	123.55
18	A	521	TGL	CG3-CG2-CG1	-4.06	102.69	111.86
18	A	521	TGL	CA3-CA2-CA1	-4.03	98.86	113.58
24	C	264	PEK	O01-C1-O02	-4.00	113.69	123.68
14	A	515	HEA	C12-C13-C14	-3.98	101.87	112.33
22	P	1271	CHD	C18-C13-C12	-3.94	105.07	109.08
14	A	516	HEA	CAA-CBA-CGA	-3.93	105.95	112.66
22	G	229	CHD	O12-C12-C13	-3.88	104.64	111.12
24	P	1264	PEK	O01-C1-O02	-3.87	114.02	123.68
14	N	515	HEA	OMA-CMA-C3A	-3.74	116.47	125.08
14	N	515	HEA	C27-C19-C18	-3.74	113.72	123.69
14	A	515	HEA	C4B-C3B-C2B	-3.57	104.37	106.87
22	B	1085	CHD	C14-C13-C12	-3.55	104.02	107.39
24	C	264	PEK	O03-C01-C02	-3.53	99.79	108.66
24	P	1264	PEK	O03-C01-C02	-3.48	99.90	108.66
25	P	1270	CDL	OB8-CB7-OB9	-3.48	114.91	123.55
19	A	524	PGV	C4-C3-C2	-3.45	100.59	113.24
22	W	1059	CHD	C1-C10-C9	-3.43	105.92	111.39
18	A	521	TGL	OG3-CC1-OC1	-3.42	115.05	123.55
24	P	1265	PEK	O03-C21-O04	-3.40	115.10	123.55
22	C	525	CHD	C6-C5-C10	-3.34	109.01	112.66
22	J	60	CHD	C19-C10-C5	-3.34	104.55	110.30
25	T	1269	CDL	OA6-CA5-OA7	-3.32	115.39	123.68
14	A	516	HEA	OMA-CMA-C3A	-3.29	117.52	125.08
22	W	1059	CHD	C6-C5-C4	-3.25	107.44	111.13
22	J	60	CHD	C19-C10-C1	-3.24	102.92	108.24
22	W	1059	CHD	C19-C10-C5	-3.22	104.74	110.30
19	N	1524	PGV	O01-C1-O02	-3.18	115.74	123.68
22	G	229	CHD	C14-C13-C12	-3.16	104.38	107.39
22	J	60	CHD	C18-C13-C12	-3.15	105.88	109.08
22	P	1525	CHD	C6-C5-C4	-3.14	107.56	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C19-C10-C5	-3.13	104.91	110.30
19	C	267	PGV	O03-C19-O04	-3.12	115.80	123.55
25	C	270	CDL	OB8-CB6-CB4	-3.11	100.83	108.66
14	A	515	HEA	C21-C20-C19	-3.09	102.47	112.93
14	N	515	HEA	C21-C20-C19	-3.09	102.47	112.93
25	C	270	CDL	C52-C51-CB5	-3.09	102.30	113.58
19	P	1268	PGV	C03-C02-C01	-3.01	105.06	111.86
14	A	516	HEA	C13-C12-C11	-3.01	109.90	114.46
14	A	516	HEA	C1B-C2B-C3B	-2.98	104.92	107.00
14	N	516	HEA	OMA-CMA-C3A	-2.96	118.28	125.08
14	A	515	HEA	C25-C23-C22	-2.95	113.75	122.65
22	J	60	CHD	C1-C10-C9	-2.93	106.71	111.39
22	P	1271	CHD	C5-C4-C3	-2.90	108.61	112.87
24	C	264	PEK	C03-C02-C01	-2.88	105.35	111.86
22	P	1525	CHD	O12-C12-C13	-2.85	106.36	111.12
19	C	268	PGV	C03-C02-C01	-2.84	105.46	111.86
18	A	521	TGL	CB3-CB2-CB1	-2.83	103.23	113.58
18	D	523	TGL	CC3-CC2-CC1	-2.82	103.29	113.58
18	N	1521	TGL	CG1-OG1-CA1	-2.80	108.72	117.13
22	C	271	CHD	C23-C22-C20	-2.79	110.96	114.72
19	N	1524	PGV	O03-C19-O04	-2.76	116.69	123.55
19	N	1266	PGV	C01-O03-C19	-2.76	108.84	117.13
24	C	265	PEK	O03-C21-O04	-2.76	116.71	123.55
14	A	515	HEA	C26-C15-C16	-2.73	110.55	115.29
22	P	1525	CHD	C21-C20-C22	-2.71	106.08	110.35
14	N	515	HEA	C25-C23-C22	-2.71	114.47	122.65
18	D	523	TGL	OG1-CA1-OA1	-2.71	116.83	123.55
18	N	1523	TGL	CC3-CC2-CC1	-2.68	103.81	113.58
19	P	1268	PGV	O03-C19-O04	-2.68	116.90	123.55
18	L	522	TGL	CB6-CB5-CB4	-2.68	100.66	114.45
24	P	1264	PEK	C28-C27-C26	-2.68	100.67	114.45
18	N	1522	TGL	OG3-CC1-OC1	-2.67	116.91	123.55
14	A	515	HEA	O11-C11-C3B	-2.67	104.15	111.83
14	N	515	HEA	CMB-C2B-C1B	-2.66	124.38	128.46
14	N	516	HEA	CAD-CBD-CGD	-2.64	108.16	112.66
22	C	525	CHD	O12-C12-C13	-2.63	106.74	111.12
25	P	1270	CDL	OA8-CA7-OA9	-2.61	117.06	123.55
25	C	270	CDL	C53-C52-C51	-2.61	103.68	113.24
14	N	516	HEA	CAA-CBA-CGA	-2.59	108.23	112.66
22	C	271	CHD	C5-C4-C3	-2.59	109.07	112.87
22	B	1085	CHD	C6-C5-C4	-2.59	108.19	111.13
22	P	1525	CHD	C18-C13-C12	-2.59	106.44	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	269	CDL	OA6-CA5-OA7	-2.59	117.23	123.68
19	C	268	PGV	O03-C19-O04	-2.58	117.14	123.55
14	A	515	HEA	C27-C19-C18	-2.57	116.83	123.69
19	P	1267	PGV	C8-C9-C10	-2.57	103.88	113.74
25	G	269	CDL	OB8-CB7-OB9	-2.56	117.20	123.55
18	N	1522	TGL	C25-C24-C23	-2.56	101.28	114.45
24	P	1264	PEK	C30-C29-C28	-2.55	101.30	114.45
18	A	521	TGL	CB7-CB6-CB5	-2.53	101.43	114.45
18	N	1522	TGL	C23-C22-C21	-2.52	101.46	114.45
27	Z	1526	DMU	C10-O1-C9	-2.51	109.00	113.72
22	J	60	CHD	C21-C20-C17	-2.49	109.05	112.95
25	C	270	CDL	CA6-CA4-CA3	-2.47	106.29	111.86
25	T	1269	CDL	OA8-CA7-OA9	-2.44	117.49	123.55
18	L	522	TGL	CB4-CB3-CB2	-2.43	104.32	113.24
24	C	264	PEK	C24-C23-C22	-2.42	104.36	113.24
19	N	1524	PGV	C8-C9-C10	-2.42	104.46	113.74
24	P	1264	PEK	C03-C02-C01	-2.41	106.43	111.86
24	C	264	PEK	O01-C02-C01	-2.39	99.75	108.44
19	P	1268	PGV	O02-C1-C2	-2.38	114.27	123.68
19	N	1266	PGV	C15-C14-C13	-2.37	104.65	113.74
25	C	270	CDL	OB8-CB7-OB9	-2.37	117.68	123.55
18	N	1521	TGL	CA3-CA2-CA1	-2.36	104.97	113.58
21	O	1229	PSC	C32-C31-C30	-2.35	102.33	114.45
14	N	516	HEA	O11-C11-C3B	-2.33	105.13	111.83
22	B	1085	CHD	C18-C13-C17	-2.30	107.60	111.23
25	P	1270	CDL	C52-C51-CB5	-2.29	105.24	113.58
18	N	1522	TGL	OA1-CA1-CA2	-2.25	114.80	123.68
22	W	1059	CHD	C19-C10-C1	-2.24	104.56	108.24
19	C	268	PGV	O02-C1-C2	-2.24	114.85	123.68
18	A	521	TGL	OB1-CB1-CB2	-2.23	114.87	123.68
22	B	1085	CHD	O12-C12-C13	-2.21	107.43	111.12
19	C	267	PGV	C8-C9-C10	-2.21	105.25	113.74
22	P	1271	CHD	C14-C8-C9	-2.20	106.65	109.64
22	B	1085	CHD	O3-C3-C2	-2.19	104.78	110.10
25	P	1270	CDL	CB6-CB4-CB3	-2.19	106.91	111.86
25	C	270	CDL	C57-C56-C55	-2.19	103.16	114.45
24	P	1264	PEK	C24-C23-C22	-2.19	105.21	113.24
18	L	522	TGL	C22-C21-C20	-2.18	103.21	114.45
24	G	1263	PEK	O03-C21-O04	-2.18	118.14	123.55
22	B	1085	CHD	C13-C17-C20	-2.18	116.85	119.49
19	N	1524	PGV	C4-C3-C2	-2.17	105.29	113.24
18	L	522	TGL	CB9-CB8-CB7	-2.14	103.43	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	516	HEA	C13-C12-C11	-2.14	111.22	114.46
27	Z	1526	DMU	O2-C8-C7	-2.13	105.73	110.36
19	A	524	PGV	O03-C19-O04	-2.12	118.28	123.55
24	T	263	PEK	O04-C21-C22	-2.11	115.33	123.68
18	N	1523	TGL	OG1-CA1-OA1	-2.09	118.36	123.55
18	N	1522	TGL	OB1-CB1-CB2	-2.08	115.48	123.68
19	P	1267	PGV	C9-C8-C7	-2.07	103.81	114.45
19	P	1267	PGV	O03-C19-O04	-2.06	118.44	123.55
18	N	1522	TGL	C26-C25-C24	-2.05	103.87	114.45
19	A	524	PGV	C03-C02-C01	-2.04	107.24	111.86
18	N	1523	TGL	OG2-CB1-OB1	-2.04	118.58	123.68
14	N	516	HEA	C26-C15-C14	-2.04	118.26	123.69
25	P	1270	CDL	CB4-OB6-CB5	-2.02	113.11	117.88
14	N	516	HEA	C1B-C2B-C3B	-2.02	105.59	107.00
24	P	1264	PEK	C34-C33-C32	-2.01	104.10	114.45
19	A	524	PGV	C3-C2-C1	-2.00	106.26	113.58
14	A	515	HEA	C3C-C4C-NC	2.01	111.81	109.21
25	C	270	CDL	CA6-OA8-CA7	2.01	123.19	117.13
25	P	1270	CDL	C82-C81-C80	2.02	124.86	114.45
27	Z	1526	DMU	O16-C6-C1	2.03	111.54	108.23
22	C	525	CHD	C15-C14-C13	2.03	105.59	103.57
22	C	525	CHD	C5-C6-C7	2.04	116.70	114.44
22	W	1059	CHD	C16-C17-C20	2.06	115.44	112.14
25	C	270	CDL	C43-C42-C41	2.07	125.12	114.45
24	C	264	PEK	C2-C3-C4	2.07	116.99	113.29
14	A	515	HEA	CMD-C2D-C3D	2.07	128.85	124.94
24	C	264	PEK	C01-O03-C21	2.08	123.38	117.13
18	N	1523	TGL	C11-C10-CB9	2.08	125.15	114.45
19	C	267	PGV	O01-C1-C2	2.08	115.87	111.55
25	T	1269	CDL	C19-C18-C17	2.08	125.18	114.45
22	C	271	CHD	C9-C8-C7	2.09	114.38	111.92
18	N	1523	TGL	C21-C20-CA9	2.09	125.23	114.45
25	T	1269	CDL	C83-C82-C81	2.11	125.31	114.45
25	T	1269	CDL	C82-C81-C80	2.12	125.36	114.45
25	G	269	CDL	OB8-CB7-C71	2.12	118.07	111.90
22	P	1271	CHD	C13-C14-C8	2.12	117.51	114.77
18	N	1521	TGL	C16-C15-CC9	2.13	125.45	114.45
27	Z	1526	DMU	C10-C5-C7	2.15	113.97	109.98
27	M	526	DMU	C57-C4-C3	2.15	119.10	113.24
14	A	516	HEA	CMC-C2C-C3C	2.15	128.88	124.89
22	C	271	CHD	C14-C8-C7	2.15	114.72	111.80
25	G	269	CDL	C82-C81-C80	2.17	125.65	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C14-C8-C7	2.18	114.76	111.80
22	P	1525	CHD	C11-C9-C8	2.19	114.00	110.82
25	G	269	CDL	C83-C82-C81	2.20	125.78	114.45
18	A	521	TGL	C15-CC9-CC8	2.20	125.80	114.45
25	P	1270	CDL	C43-C42-C41	2.20	125.81	114.45
14	N	515	HEA	CMD-C2D-C3D	2.21	129.10	124.94
22	C	271	CHD	C16-C17-C13	2.21	105.77	103.57
27	M	526	DMU	O16-C6-C1	2.22	111.86	108.23
24	P	1264	PEK	O13-P-O14	2.23	123.81	112.28
22	C	271	CHD	C9-C10-C5	2.23	111.85	108.63
18	L	522	TGL	CC3-CC2-CC1	2.24	121.76	113.58
18	L	522	TGL	OG2-CB1-CB2	2.25	116.22	111.55
19	N	1524	PGV	O01-C02-C03	2.26	116.67	108.44
21	O	1229	PSC	C02-O01-C1	2.27	123.23	117.88
25	T	1269	CDL	CA6-OA8-CA7	2.27	123.97	117.13
25	P	1270	CDL	C40-C39-C38	2.28	126.21	114.45
14	N	516	HEA	C26-C15-C16	2.30	119.28	115.29
14	A	515	HEA	CBA-CAA-C2A	2.30	116.86	112.47
25	C	270	CDL	C40-C39-C38	2.30	126.32	114.45
25	P	1270	CDL	CA6-OA8-CA7	2.30	124.06	117.13
22	P	1271	CHD	C9-C10-C5	2.31	111.97	108.63
25	P	1270	CDL	OA4-PA1-OA3	2.32	124.31	112.28
22	B	1085	CHD	C1-C10-C5	2.32	111.39	107.79
19	C	268	PGV	O03-C01-C02	2.33	114.52	108.66
22	B	1085	CHD	C18-C13-C14	2.34	114.92	111.23
14	N	515	HEA	C1B-C2B-C3B	2.35	108.63	107.00
19	A	524	PGV	O03-C01-C02	2.36	114.59	108.66
18	L	522	TGL	C15-CC9-CC8	2.37	126.64	114.45
19	N	1524	PGV	C01-O03-C19	2.37	124.25	117.13
18	N	1523	TGL	OG1-CG1-CG2	2.37	114.61	108.66
19	C	267	PGV	O03-C19-C20	2.37	118.80	111.90
19	P	1268	PGV	O01-C02-C03	2.38	117.07	108.44
25	C	270	CDL	C42-C41-C40	2.38	126.70	114.45
25	P	1270	CDL	OA8-CA6-CA4	2.39	114.65	108.66
18	A	521	TGL	OG3-CC1-CC2	2.42	118.95	111.90
24	P	1264	PEK	O01-C1-C2	2.44	116.61	111.55
27	M	526	DMU	C10-C5-C7	2.47	114.57	109.98
18	N	1521	TGL	C21-C20-CA9	2.48	127.21	114.45
22	P	1271	CHD	C14-C8-C7	2.49	115.17	111.80
19	A	524	PGV	C01-O03-C19	2.50	124.65	117.13
25	T	1269	CDL	OB8-CB6-CB4	2.52	115.00	108.66
25	P	1270	CDL	C39-C38-C37	2.55	127.57	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	1526	DMU	C7-C8-C9	2.56	114.72	110.22
25	G	269	CDL	CA6-OA8-CA7	2.57	124.85	117.13
22	P	1525	CHD	C15-C14-C13	2.59	106.14	103.57
22	J	60	CHD	C18-C13-C17	2.61	115.35	111.23
24	C	264	PEK	O01-C1-C2	2.61	116.97	111.55
22	J	60	CHD	C16-C17-C20	2.61	116.32	112.14
18	D	523	TGL	CB3-CB2-CB1	2.63	123.20	113.58
21	O	1229	PSC	O03-C19-C20	2.64	119.58	111.90
25	P	1270	CDL	C42-C41-C40	2.64	128.07	114.45
18	N	1523	TGL	OG2-CG2-CG3	2.64	118.05	108.44
22	P	1525	CHD	C11-C9-C10	2.65	116.55	113.74
25	P	1270	CDL	OB6-CB5-C51	2.65	117.06	111.55
25	G	269	CDL	CB6-OB8-CB7	2.65	125.12	117.13
14	N	516	HEA	C20-C21-C22	2.66	121.08	111.97
22	W	1059	CHD	C5-C6-C7	2.66	117.38	114.44
24	C	265	PEK	O03-C01-C02	2.67	115.38	108.66
14	A	515	HEA	C20-C19-C18	2.69	126.61	121.10
22	J	60	CHD	O7-C7-C8	2.70	115.35	109.33
27	M	526	DMU	O55-C2-C1	2.70	116.23	110.36
14	N	516	HEA	C12-C11-C3B	2.72	119.28	112.65
25	C	270	CDL	C39-C38-C37	2.73	128.51	114.45
22	W	1059	CHD	C4-C5-C10	2.74	115.65	112.66
22	J	60	CHD	C5-C6-C7	2.74	117.47	114.44
24	P	1265	PEK	O03-C01-C02	2.74	115.55	108.66
18	N	1522	TGL	CC3-CC2-CC1	2.76	123.64	113.58
22	P	1271	CHD	O7-C7-C8	2.77	115.50	109.33
22	C	271	CHD	C14-C13-C12	2.77	110.01	107.39
24	P	1265	PEK	C01-O03-C21	2.77	125.47	117.13
22	W	1059	CHD	C4-C3-C2	2.78	114.00	110.55
22	J	60	CHD	C14-C8-C7	2.80	115.60	111.80
27	M	526	DMU	C11-C9-C8	2.80	119.56	113.00
22	C	271	CHD	C15-C14-C13	2.81	106.37	103.57
14	N	516	HEA	C17-C18-C19	2.81	134.74	127.68
25	T	1269	CDL	CB6-OB8-CB7	2.81	125.59	117.13
22	P	1271	CHD	C6-C5-C10	2.81	115.73	112.66
24	G	1263	PEK	C01-O03-C21	2.83	125.65	117.13
19	N	1266	PGV	O01-C1-C2	2.85	117.47	111.55
27	M	526	DMU	C6-C1-C2	2.86	115.28	109.98
27	Z	1526	DMU	C6-C1-C2	2.86	115.30	109.98
18	L	522	TGL	OG1-CG1-CG2	2.87	115.86	108.66
25	G	269	CDL	C80-C79-C78	2.87	129.25	114.45
22	J	60	CHD	C17-C13-C12	2.88	120.32	117.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C6-C7-C8	2.89	114.57	111.50
22	C	271	CHD	C5-C6-C7	2.89	117.64	114.44
19	A	524	PGV	O01-C02-C01	2.90	118.97	108.44
24	P	1264	PEK	C01-O03-C21	2.94	125.97	117.13
19	N	1266	PGV	O03-C01-C02	2.95	116.06	108.66
25	G	269	CDL	OA8-CA7-C31	2.95	120.49	111.90
24	C	265	PEK	C24-C23-C22	2.97	124.11	113.24
22	P	1271	CHD	C16-C17-C13	2.97	106.53	103.57
18	A	521	TGL	OG1-CA1-CA2	3.00	120.61	111.90
27	M	526	DMU	C7-C8-C9	3.00	115.50	110.22
22	P	1525	CHD	O12-C12-C11	3.00	115.27	109.11
21	B	229	PSC	O03-C19-C20	3.01	120.67	111.90
22	W	1059	CHD	C10-C9-C8	3.01	115.12	111.87
24	T	263	PEK	C01-O03-C21	3.03	126.24	117.13
19	P	1267	PGV	O14-P-O13	3.05	128.04	112.28
22	B	1085	CHD	C9-C10-C5	3.06	113.04	108.63
18	A	521	TGL	OG2-CG2-CG1	3.07	119.58	108.44
18	A	521	TGL	CG3-OG3-CC1	3.08	126.38	117.13
22	B	1085	CHD	C22-C20-C17	3.08	116.73	110.26
14	N	515	HEA	C13-C12-C11	3.10	119.16	114.46
18	A	521	TGL	OG2-CG2-CG3	3.10	119.70	108.44
25	C	270	CDL	OA8-CA6-CA4	3.10	116.45	108.66
24	C	265	PEK	C01-O03-C21	3.11	126.48	117.13
22	P	1271	CHD	C15-C14-C8	3.12	122.73	118.32
27	Z	1526	DMU	O7-C3-C4	3.12	117.03	109.34
14	A	516	HEA	C27-C19-C20	3.14	120.75	115.29
18	N	1522	TGL	OG1-CG1-CG2	3.18	116.64	108.66
14	A	515	HEA	C13-C12-C11	3.21	119.32	114.46
22	C	271	CHD	C6-C5-C10	3.23	116.19	112.66
22	C	271	CHD	C15-C14-C8	3.23	122.89	118.32
24	T	263	PEK	O03-C01-C02	3.23	116.78	108.66
18	N	1522	TGL	OG3-CC1-CC2	3.24	121.34	111.90
27	Z	1526	DMU	O1-C10-C5	3.25	116.56	110.30
24	T	263	PEK	C02-O01-C1	3.25	125.57	117.88
18	N	1522	TGL	OG2-CB1-CB2	3.27	118.35	111.55
18	N	1523	TGL	CG3-OG3-CC1	3.28	127.00	117.13
25	G	269	CDL	C79-C78-C77	3.28	131.36	114.45
22	W	1059	CHD	C5-C4-C3	3.28	117.69	112.87
22	P	1525	CHD	C14-C13-C12	3.28	110.50	107.39
22	W	1059	CHD	C22-C20-C17	3.28	117.16	110.26
27	Z	1526	DMU	C11-C9-C8	3.29	120.69	113.00
22	C	271	CHD	C6-C7-C8	3.29	115.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1085	CHD	C1-C2-C3	3.30	114.62	110.42
25	C	270	CDL	OA8-CA7-C31	3.32	121.55	111.90
18	D	523	TGL	OG1-CA1-CA2	3.35	121.64	111.90
14	A	515	HEA	C25-C23-C24	3.37	122.48	114.60
18	N	1522	TGL	CG1-OG1-CA1	3.38	127.30	117.13
22	C	525	CHD	O12-C12-C11	3.39	116.07	109.11
25	C	270	CDL	OB8-CB7-C71	3.41	121.82	111.90
19	N	1524	PGV	O03-C19-C20	3.41	121.82	111.90
18	N	1521	TGL	OG1-CG1-CG2	3.48	117.41	108.66
18	N	1522	TGL	CG3-OG3-CC1	3.48	127.61	117.13
21	O	1229	PSC	O01-C1-C2	3.49	118.80	111.55
19	A	524	PGV	O03-C19-C20	3.50	122.07	111.90
18	N	1523	TGL	OG1-CA1-CA2	3.51	122.11	111.90
18	N	1521	TGL	OG1-CA1-CA2	3.53	122.18	111.90
22	P	1271	CHD	C18-C13-C14	3.54	116.82	111.23
22	J	60	CHD	C4-C5-C10	3.54	116.53	112.66
18	L	522	TGL	CG2-OG2-CB1	3.56	126.28	117.88
25	P	1270	CDL	OA8-CA7-C31	3.56	122.27	111.90
22	W	1059	CHD	C1-C10-C5	3.58	113.34	107.79
25	T	1269	CDL	OA8-CA7-C31	3.60	122.38	111.90
18	N	1522	TGL	OG1-CA1-CA2	3.61	122.41	111.90
22	C	271	CHD	C2-C1-C10	3.63	119.13	112.80
22	P	1271	CHD	C1-C10-C5	3.68	113.49	107.79
18	N	1523	TGL	OG3-CC1-CC2	3.71	122.69	111.90
27	M	526	DMU	O5-C4-C3	3.72	117.37	109.75
18	L	522	TGL	OG1-CA1-CA2	3.74	122.79	111.90
22	C	271	CHD	C1-C10-C5	3.77	113.64	107.79
22	J	60	CHD	C14-C13-C12	3.77	110.97	107.39
25	P	1270	CDL	OB8-CB7-C71	3.78	122.89	111.90
19	N	1524	PGV	O01-C1-C2	3.79	119.42	111.55
24	C	265	PEK	O01-C1-C2	3.80	119.45	111.55
22	J	60	CHD	C22-C20-C17	3.81	118.26	110.26
24	T	263	PEK	O01-C1-C2	3.82	119.49	111.55
24	G	1263	PEK	C02-O01-C1	3.84	126.95	117.88
22	C	271	CHD	O7-C7-C8	3.84	117.91	109.33
24	G	1263	PEK	O03-C01-C02	3.86	118.37	108.66
18	A	521	TGL	OG1-CG1-CG2	3.86	118.37	108.66
22	P	1271	CHD	C15-C14-C13	3.89	107.44	103.57
14	A	515	HEA	C12-C11-C3B	3.90	122.18	112.65
22	J	60	CHD	C4-C3-C2	3.91	115.40	110.55
18	D	523	TGL	CG3-OG3-CC1	3.99	129.13	117.13
18	D	523	TGL	OG2-CB1-CB2	4.06	119.97	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	CBA-CAA-C2A	4.06	120.22	112.47
21	B	229	PSC	O01-C1-C2	4.09	120.04	111.55
18	N	1521	TGL	OG2-CG2-CG3	4.09	123.31	108.44
24	T	263	PEK	O03-C21-C22	4.09	123.81	111.90
18	L	522	TGL	OG3-CC1-CC2	4.12	123.89	111.90
22	P	1271	CHD	C10-C9-C8	4.14	116.33	111.87
14	N	515	HEA	C16-C15-C14	4.16	129.63	121.10
18	D	523	TGL	OG3-CC1-CC2	4.18	124.07	111.90
18	N	1521	TGL	OG2-CB1-CB2	4.19	120.25	111.55
22	C	271	CHD	C10-C9-C8	4.23	116.43	111.87
27	M	526	DMU	C8-C7-C5	4.24	118.32	110.84
24	P	1265	PEK	O03-C21-C22	4.31	124.43	111.90
18	N	1521	TGL	CG3-OG3-CC1	4.31	130.10	117.13
14	N	515	HEA	C20-C19-C18	4.32	129.94	121.10
14	A	515	HEA	C16-C15-C14	4.33	129.96	121.10
22	J	60	CHD	C5-C4-C3	4.35	119.25	112.87
18	A	521	TGL	OG2-CB1-CB2	4.37	120.63	111.55
19	C	268	PGV	O03-C19-C20	4.38	124.64	111.90
19	A	522	PGV	O03-C19-C20	4.45	124.84	111.90
14	N	515	HEA	C12-C11-C3B	4.47	123.56	112.65
22	B	1085	CHD	C6-C7-C8	4.48	116.26	111.50
22	P	1271	CHD	C2-C1-C10	4.48	120.61	112.80
27	Z	1526	DMU	C2-C3-C4	4.50	120.43	110.88
27	M	526	DMU	O1-C9-C8	4.51	117.97	109.66
24	G	1263	PEK	O01-C1-C2	4.51	120.93	111.55
27	Z	1526	DMU	C8-C7-C5	4.54	118.84	110.84
24	C	265	PEK	O03-C21-C22	4.57	125.20	111.90
22	W	1059	CHD	C17-C13-C12	4.57	121.88	117.67
24	G	1263	PEK	O03-C21-C22	4.60	125.28	111.90
22	W	1059	CHD	C18-C13-C17	4.65	118.57	111.23
25	G	269	CDL	OA6-CA5-C11	4.77	121.46	111.55
22	B	1085	CHD	C4-C3-C2	4.79	116.50	110.55
22	W	1059	CHD	C9-C11-C12	4.81	120.66	114.32
22	J	60	CHD	C1-C10-C5	4.81	115.25	107.79
19	P	1268	PGV	O03-C19-C20	4.82	125.93	111.90
27	Z	1526	DMU	O1-C9-C11	4.83	117.98	106.41
25	T	1269	CDL	OB6-CB5-C51	4.85	121.62	111.55
27	M	526	DMU	O5-C6-C1	4.89	119.73	110.30
22	C	271	CHD	C1-C2-C3	4.92	116.69	110.42
27	Z	1526	DMU	O1-C9-C8	5.01	118.89	109.66
22	J	60	CHD	C9-C10-C5	5.05	115.92	108.63
18	N	1523	TGL	OG2-CB1-CB2	5.07	122.09	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	1522	TGL	CG2-OG2-CB1	5.09	129.90	117.88
27	Z	1526	DMU	O5-C4-C3	5.09	120.17	109.75
25	T	1269	CDL	OA6-CA5-C11	5.10	122.14	111.55
25	G	269	CDL	OB6-CB5-C51	5.13	122.20	111.55
24	P	1265	PEK	O01-C1-C2	5.13	122.20	111.55
18	D	523	TGL	OG1-CG1-CG2	5.18	121.68	108.66
25	C	270	CDL	OA6-CA5-C11	5.23	122.42	111.55
22	P	1271	CHD	C1-C2-C3	5.33	117.21	110.42
19	N	1266	PGV	O03-C19-C20	5.36	127.49	111.90
27	M	526	DMU	O1-C10-C5	5.38	120.67	110.30
27	Z	1526	DMU	O5-C4-C57	5.38	119.30	106.41
18	N	1521	TGL	CG2-OG2-CB1	5.47	130.80	117.88
19	C	268	PGV	O01-C1-C2	5.51	123.00	111.55
25	P	1270	CDL	OA6-CA5-C11	5.61	123.20	111.55
22	W	1059	CHD	C9-C10-C5	5.83	117.05	108.63
22	J	60	CHD	C10-C9-C8	5.86	118.19	111.87
27	M	526	DMU	C2-C3-C4	5.92	123.44	110.88
22	W	1059	CHD	C14-C13-C12	5.94	113.03	107.39
22	W	1059	CHD	C6-C5-C10	5.97	119.18	112.66
27	M	526	DMU	O1-C9-C11	6.00	120.78	106.41
27	M	526	DMU	O5-C4-C57	6.13	121.09	106.41
27	Z	1526	DMU	O5-C6-C1	6.28	122.42	110.30
27	Z	1526	DMU	O7-C3-C2	6.37	122.51	107.19
27	M	526	DMU	O7-C3-C2	6.45	122.72	107.19
22	J	60	CHD	C13-C17-C20	7.01	127.99	119.49
18	A	521	TGL	CG2-OG2-CB1	7.09	134.63	117.88
22	W	1059	CHD	C11-C12-C13	7.16	118.64	111.22
22	J	60	CHD	C6-C5-C10	7.19	120.52	112.66
19	P	1268	PGV	O01-C1-C2	7.20	126.50	111.55
14	A	515	HEA	C17-C16-C15	7.39	137.93	112.93
14	N	515	HEA	C17-C16-C15	8.12	140.40	112.93
22	W	1059	CHD	C13-C17-C20	8.31	129.57	119.49

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB

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Mol	Chain	Res	Type	Atom
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
27	M	526	DMU	C2
27	M	526	DMU	C3
27	M	526	DMU	C9
27	M	526	DMU	C5
27	Z	1526	DMU	C2
27	Z	1526	DMU	C3
27	Z	1526	DMU	C5
27	Z	1526	DMU	C4

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C02-O01-C1-C2
19	N	1524	PGV	C02-O01-C1-C2

There are no ring outliers.

36 monomers are involved in 242 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	7	0
14	A	516	HEA	3	0
18	A	521	TGL	6	0
19	A	522	PGV	1	0
19	A	524	PGV	12	0
22	B	1085	CHD	2	0
21	B	229	PSC	11	0
24	C	264	PEK	3	0
24	C	265	PEK	5	0
19	C	267	PGV	7	0
19	C	268	PGV	3	0
25	C	270	CDL	19	0
22	C	271	CHD	2	0
18	D	523	TGL	5	0
24	G	1263	PEK	10	0
25	G	269	CDL	20	0
22	J	60	CHD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	522	TGL	14	0
19	N	1266	PGV	2	0
18	N	1521	TGL	7	0
18	N	1522	TGL	9	0
18	N	1523	TGL	6	0
19	N	1524	PGV	7	0
14	N	515	HEA	5	0
14	N	516	HEA	3	0
21	O	1229	PSC	17	0
24	P	1264	PEK	5	0
24	P	1265	PEK	8	0
19	P	1267	PGV	2	0
19	P	1268	PGV	5	0
25	P	1270	CDL	9	0
22	P	1271	CHD	1	0
22	P	1525	CHD	1	0
25	T	1269	CDL	24	0
24	T	263	PEK	12	0
22	W	1059	CHD	3	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%)	-0.33	0 100 100	13, 17, 24, 50	0
1	N	513/514 (99%)	-0.35	0 100 100	13, 19, 26, 49	0
2	B	226/227 (99%)	-0.27	0 100 100	12, 21, 49, 70	0
2	O	226/227 (99%)	-0.15	2 (0%) 84 61	16, 24, 50, 68	0
3	C	259/261 (99%)	-0.45	0 100 100	13, 18, 30, 48	0
3	P	259/261 (99%)	-0.43	1 (0%) 92 77	14, 20, 33, 52	0
4	D	144/147 (97%)	-0.38	0 100 100	14, 20, 41, 64	0
4	Q	144/147 (97%)	0.14	7 (4%) 30 12	19, 31, 56, 99	0
5	E	105/109 (96%)	-0.49	1 (0%) 82 58	13, 20, 48, 85	0
5	R	105/109 (96%)	-0.36	2 (1%) 67 37	17, 24, 56, 88	0
6	F	98/98 (100%)	-0.06	5 (5%) 29 12	15, 24, 72, 108	0
6	S	98/98 (100%)	0.03	5 (5%) 29 12	14, 23, 74, 106	0
7	G	83/85 (97%)	0.07	4 (4%) 31 12	13, 24, 92, 96	0
7	T	83/85 (97%)	0.20	7 (8%) 12 4	16, 26, 92, 97	0
8	H	79/85 (92%)	-0.07	2 (2%) 58 29	16, 27, 76, 99	0
8	U	79/85 (92%)	-0.05	1 (1%) 77 51	19, 29, 76, 100	0
9	I	72/73 (98%)	-0.17	1 (1%) 75 49	16, 29, 54, 62	0
9	V	72/73 (98%)	-0.02	0 100 100	16, 35, 55, 79	0
10	J	58/59 (98%)	-0.15	2 (3%) 46 20	19, 28, 55, 89	0
10	W	58/59 (98%)	-0.15	1 (1%) 70 42	18, 27, 61, 95	0
11	K	49/56 (87%)	-0.34	0 100 100	19, 26, 37, 49	0
11	X	49/56 (87%)	-0.09	1 (2%) 65 36	24, 32, 47, 61	0
12	L	46/47 (97%)	-0.30	0 100 100	17, 23, 46, 70	0
12	Y	46/47 (97%)	-0.24	1 (2%) 62 33	18, 24, 51, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.14	0 100 100	15, 21, 66, 91	0
13	Z	43/46 (93%)	-0.16	2 (4%) 32 13	22, 26, 75, 94	0
All	All	3550/3614 (98%)	-0.25	45 (1%) 77 51	12, 21, 52, 108	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	12.6
4	Q	4	SER	12.2
6	S	97	ALA	9.2
4	Q	6	VAL	7.5
4	Q	8	SER	6.7
6	F	98	HIS	5.9
7	T	3	ALA	5.8
7	T	1	ALA	5.6
6	F	97	ALA	5.2
7	T	2	SER	5.2
7	T	8	HIS	5.1
6	S	98	HIS	5.0
5	R	5	HIS	4.1
10	J	58	LYS	3.7
8	U	7	LYS	3.7
3	P	3	HIS	3.6
7	G	2	SER	3.4
6	S	94	HIS	3.4
7	G	4	ALA	3.4
6	F	96	LEU	3.4
7	G	8	HIS	3.3
11	X	6	ALA	3.3
7	G	3	ALA	3.2
4	Q	7	LYS	3.2
5	E	5	HIS	3.1
2	O	226	MET	3.0
10	W	58	LYS	3.0
13	Z	42	LYS	3.0
8	H	46	LYS	2.9
6	F	95	GLN	2.9
13	Z	43	SER	2.8
6	S	96	LEU	2.8
7	T	4	ALA	2.6
5	R	109	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
10	J	1	PHE	2.6
6	F	1	ALA	2.5
9	I	37	PHE	2.5
6	S	95	GLN	2.4
7	T	7	ASP	2.4
7	T	5	LYS	2.4
12	Y	47	LYS	2.4
4	Q	35	ALA	2.3
4	Q	58	GLU	2.2
8	H	47	GLY	2.2
2	O	90	ILE	2.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
2	FME	O	1	10/11	0.97	0.26	-	23,24,32,39	0
7	TPO	T	11	11/12	0.72	0.41	-	64,70,88,88	0
2	FME	B	1	10/11	0.97	0.22	-	20,21,29,35	0
9	SAC	I	1	9/10	0.59	0.44	-	71,74,76,78	0
1	FME	N	1	10/11	0.95	0.31	-	35,35,51,53	0
9	SAC	V	1	9/10	0.73	0.52	-	84,85,86,86	0
1	FME	A	1	10/11	0.96	0.29	-	34,36,49,58	0
7	TPO	G	11	11/12	0.60	0.35	-	61,67,86,87	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(Å <sup>2</sup> )	Q<0.9
25	CDL	P	1270	100/100	0.83	0.48	9.94	39,83,105,108	0
22	CHD	J	60	29/29	0.71	0.52	7.30	98,105,109,109	0
19	PGV	A	524	51/51	0.85	0.40	7.23	29,64,91,94	0
22	CHD	W	1059	29/29	0.65	0.47	6.85	91,103,105,105	0
18	TGL	L	522	63/63	0.86	0.36	6.63	32,55,78,82	0
18	TGL	A	521	63/63	0.88	0.35	6.63	40,64,86,90	0
25	CDL	G	269	100/100	0.77	0.56	6.48	56,82,107,111	0
25	CDL	C	270	100/100	0.86	0.52	6.46	38,80,104,106	0
19	PGV	N	1524	51/51	0.80	0.40	5.84	36,64,98,101	0
19	PGV	P	1268	51/51	0.76	0.46	5.58	74,86,100,101	0
18	TGL	N	1522	63/63	0.83	0.39	5.25	41,65,81,83	0
25	CDL	T	1269	100/100	0.76	0.50	5.17	51,83,107,108	0
18	TGL	D	523	63/63	0.83	0.33	4.47	44,64,89,90	0
18	TGL	N	1521	63/63	0.85	0.40	4.45	40,68,88,92	0
18	TGL	N	1523	63/63	0.75	0.40	4.16	45,70,89,91	0
19	PGV	N	1266	51/51	0.98	0.29	3.42	20,34,52,53	0
21	PSC	B	229	52/52	0.78	0.47	3.11	44,89,112,114	0
22	CHD	P	1271	29/29	0.85	0.37	3.09	78,87,88,88	0
21	PSC	O	1229	52/52	0.79	0.45	2.51	34,82,109,112	0
24	PEK	P	1265	53/53	0.74	0.45	2.29	34,86,99,100	0
19	PGV	A	522	51/51	0.98	0.27	2.29	14,25,49,51	0
19	PGV	P	1267	51/51	0.98	0.27	2.25	17,25,63,65	0
27	DMU	Z	1526	33/33	0.94	0.27	2.09	29,41,54,57	0
24	PEK	C	264	53/53	0.96	0.25	2.07	14,34,69,70	0
19	PGV	C	267	51/51	0.98	0.25	2.06	15,23,61,65	0
24	PEK	P	1264	53/53	0.96	0.24	1.89	14,35,68,70	0
14	HEA	N	515	60/60	0.96	0.25	1.77	22,41,66,70	0
24	PEK	C	265	53/53	0.74	0.39	1.44	36,87,96,98	0
19	PGV	C	268	51/51	0.80	0.45	1.33	57,84,99,100	0
24	PEK	T	263	53/53	0.70	0.52	1.20	38,90,112,114	0
22	CHD	C	271	29/29	0.86	0.38	1.13	76,85,87,88	0
24	PEK	G	1263	53/53	0.78	0.41	0.98	42,92,110,110	0
14	HEA	A	516	60/60	0.98	0.22	0.61	10,15,23,26	0
14	HEA	A	515	60/60	0.98	0.21	0.38	6,18,35,40	0
14	HEA	N	516	60/60	0.98	0.21	0.19	5,17,25,27	0
22	CHD	C	525	29/29	0.97	0.21	0.01	18,26,28,28	0
22	CHD	P	1525	29/29	0.96	0.20	-0.10	19,26,29,33	0
27	DMU	M	526	33/33	0.96	0.19	-0.41	26,34,43,43	0
22	CHD	B	1085	29/29	0.97	0.17	-0.62	7,13,15,22	0
22	CHD	G	229	29/29	0.98	0.17	-0.72	6,12,14,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
26	ZN	F	99	1/1	1.00	0.12	-2.01	22,22,22,22	0
17	NA	N	519	1/1	0.97	0.10	-2.06	21,21,21,21	0
26	ZN	S	99	1/1	0.99	0.11	-2.22	22,22,22,22	0
20	CUA	B	228	2/2	0.99	0.10	-2.28	17,17,17,18	0
17	NA	A	519	1/1	0.97	0.13	-2.75	18,18,18,18	0
20	CUA	O	228	2/2	0.99	0.10	-3.70	20,20,20,22	0
16	MG	N	518	1/1	0.95	0.12	-6.13	18,18,18,18	0
16	MG	A	518	1/1	0.99	0.10	-6.70	15,15,15,15	0
15	CU	N	517	1/1	0.98	0.16	-	24,24,24,24	0
15	CU	A	517	1/1	0.97	0.17	-	22,22,22,22	0
23	UNX	P	262	1/1	0.56	0.26	-	42,42,42,42	0
23	UNX	C	262	1/1	0.81	0.30	-	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.