



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 AM GMT

PDB ID : 2Y69  
Title : Bovine heart cytochrome c oxidase re-refined with molecular oxygen  
Authors : Kaila, V.R.I.; Oksanen, E.; Goldman, A.; Verkhovsky, M.I.; Sundholm, D.; Wikstrom, M.  
Deposited on : 2011-01-20  
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

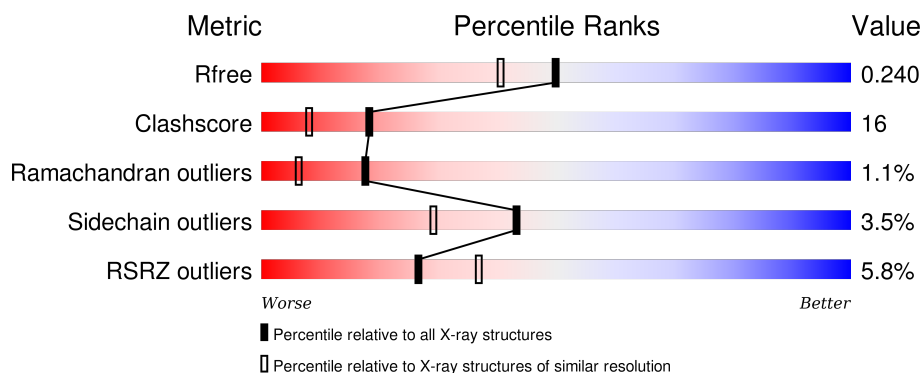
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

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



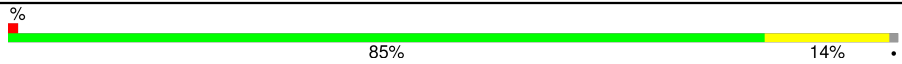


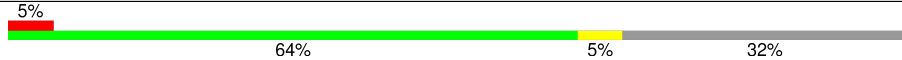
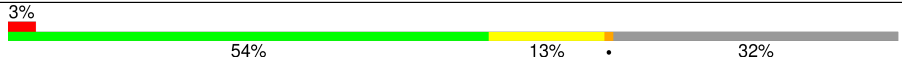
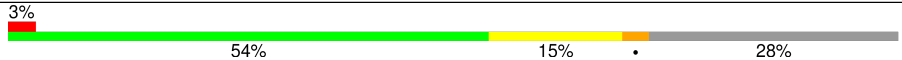
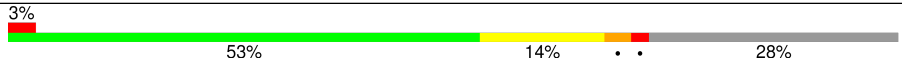
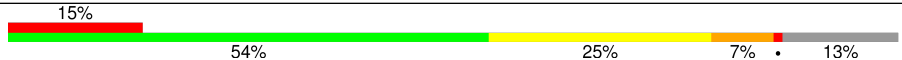
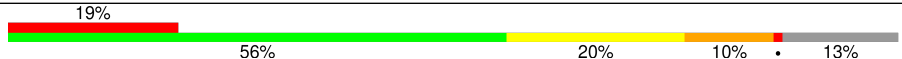
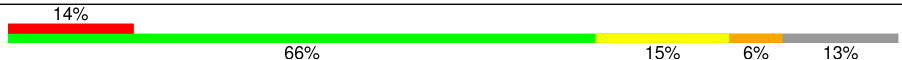



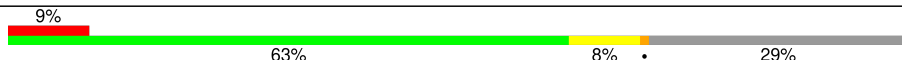
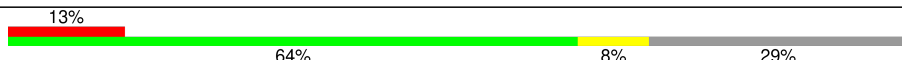

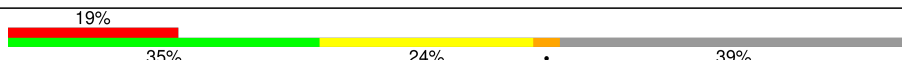
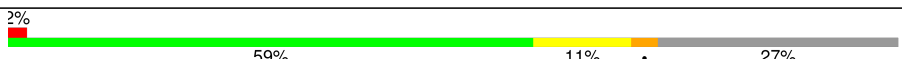

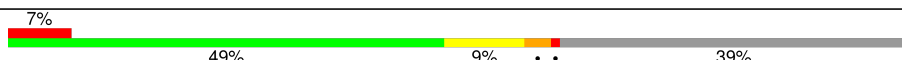
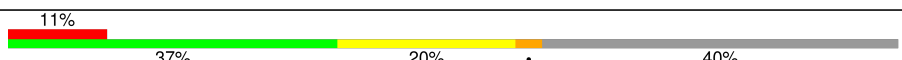
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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>3%</div> <div>86% 13%</div> </div>
1	N	514	<div> <div>3%</div> <div>82% 18%</div> </div>
2	B	227	<div> <div>2%</div> <div>79% 18% .</div> </div>
2	O	227	<div> <div>3%</div> <div>74% 22% .</div> </div>
3	C	261	<div> <div>90% 8% ..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	169	
4	Q	169	
5	E	152	
5	R	152	
6	F	129	
6	S	129	
7	G	97	
7	T	97	
8	H	86	
8	U	86	
9	I	74	
9	V	74	
10	J	80	
10	W	80	
11	K	80	
11	X	80	
12	L	63	
12	Y	63	
13	M	70	
13	Z	70	

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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	515	X	-	-	-
14	HEA	N	516	X	-	-	-
16	OXY	A	1515	-	-	-	X
23	DMU	M	1044	X	-	-	-
23	DMU	Z	1043	X	-	-	-

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 30116 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	513	Total	C	N	O	S	0	0	0
			4017	2685	622	676	34			
1	N	513	Total	C	N	O	S	0	0	0
			4017	2685	622	676	34			

- 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
			1822	1184	281	339	18			
2	O	226	Total	C	N	O	S	0	0	0
			1814	1179	280	338	17			

- 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	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

- Molecule 6 is a protein called CYTOCHROME C OXIDASE SUBUNIT 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

- Molecule 7 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 6A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			671	428	128	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

- Molecule 8 is a protein called CYTOCHROME C OXIDASE SUBUNIT VIB ISOFORM 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE VIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

- Molecule 10 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

- Molecule 11 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE 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			

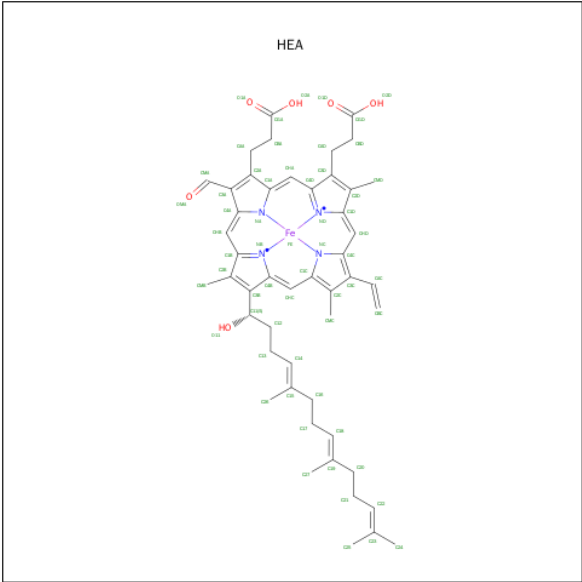
- Molecule 12 is a protein called CYTOCHROME C OXIDASE SUBUNIT 7C.

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 POLYPEPTIDE 8H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	42	Total	C	N	O	0	0	0
			329	220	52	57			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



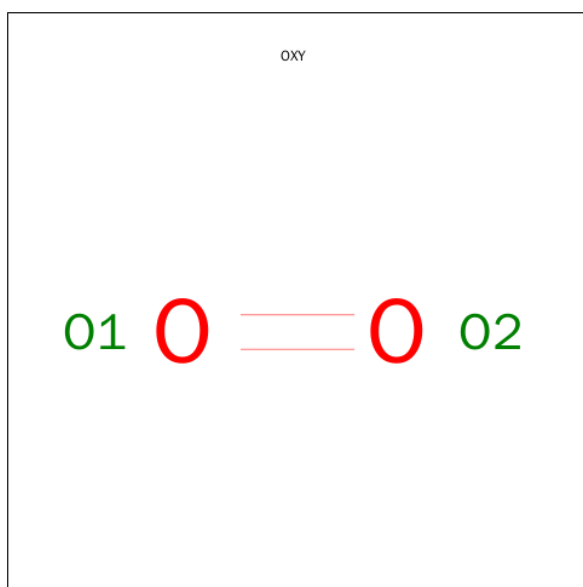
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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

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

- Molecule 16 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



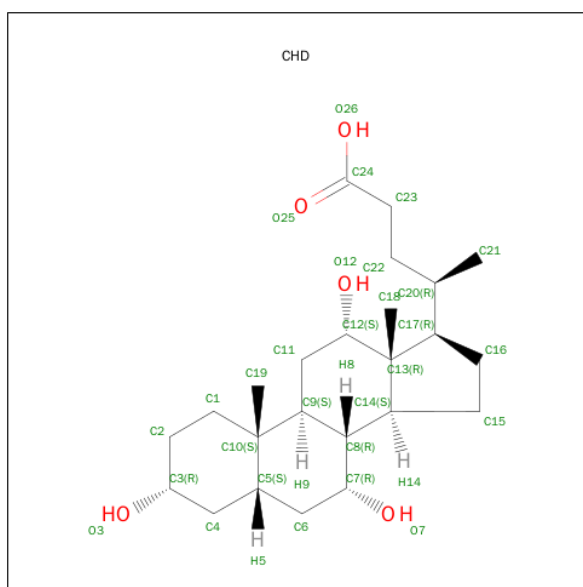


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O 2 2	0	0
16	N	1	Total O 2 2	0	0

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

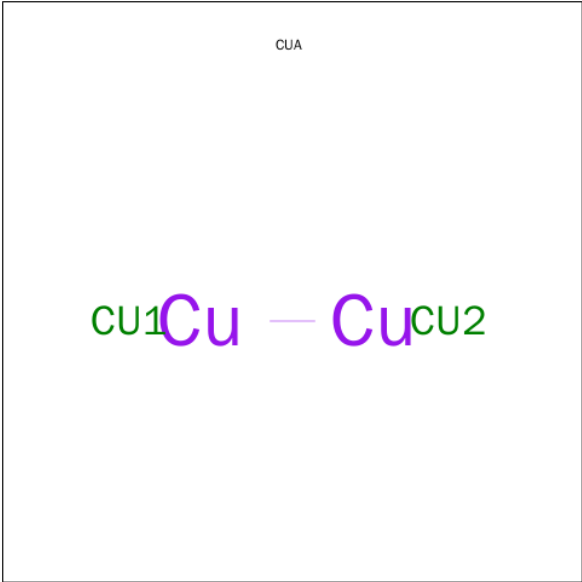
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Mg 1 1	0	0
17	N	1	Total Mg 1 1	0	0

- Molecule 18 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



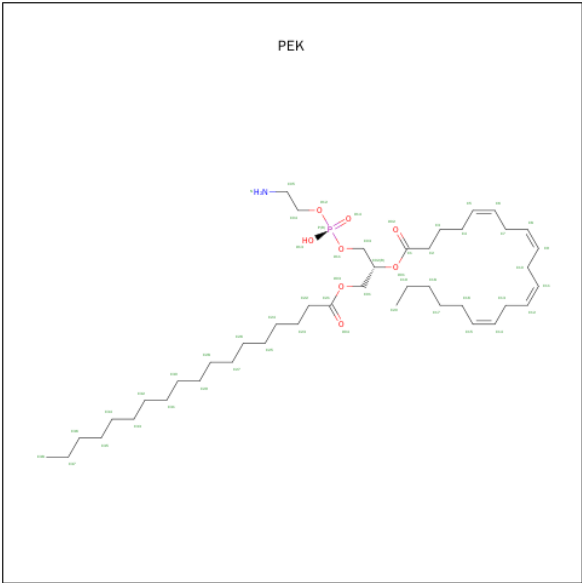
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			29	24	5		
18	C	1	Total	C	O	0	0
			29	24	5		
18	G	1	Total	C	O	0	0
			29	24	5		
18	N	1	Total	C	O	0	0
			29	24	5		
18	P	1	Total	C	O	0	0
			29	24	5		
18	T	1	Total	C	O	0	0
			29	24	5		

- Molecule 19 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 20 is (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).



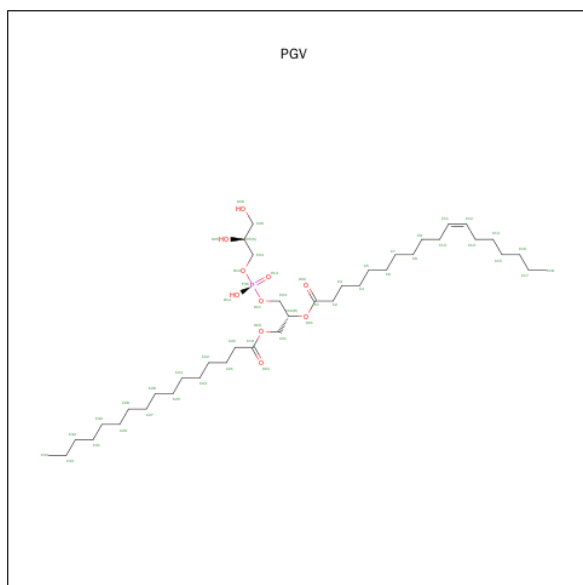
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

- Molecule 21 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).

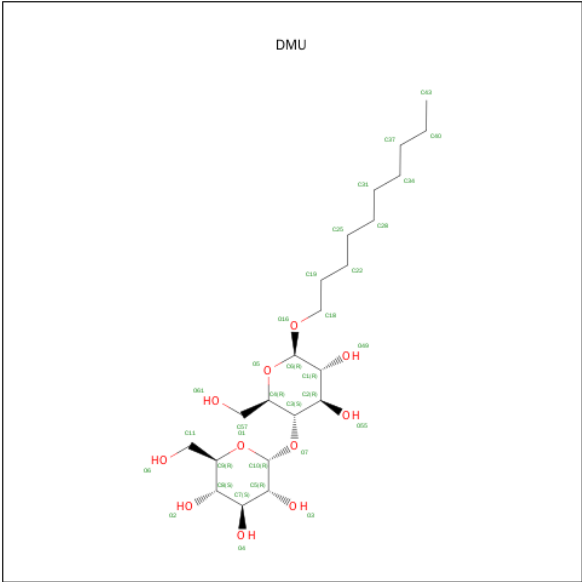


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	C	1	Total	C	O	P	0	0
			51	40	10	1		
21	C	1	Total	C	O	P	0	0
			51	40	10	1		
21	P	1	Total	C	O	P	0	0
			51	40	10	1		
21	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 23 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
23	M	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	114	Total	O	0	0
			114	114		
24	B	102	Total	O	0	0
			102	102		
24	C	85	Total	O	0	0
			85	85		
24	D	43	Total	O	0	0
			43	43		
24	F	45	Total	O	0	0
			45	45		
24	G	41	Total	O	0	0
			41	41		
24	H	49	Total	O	0	0
			49	49		
24	I	20	Total	O	0	0
			20	20		
24	J	26	Total	O	0	0
			26	26		
24	K	10	Total	O	0	0
			10	10		

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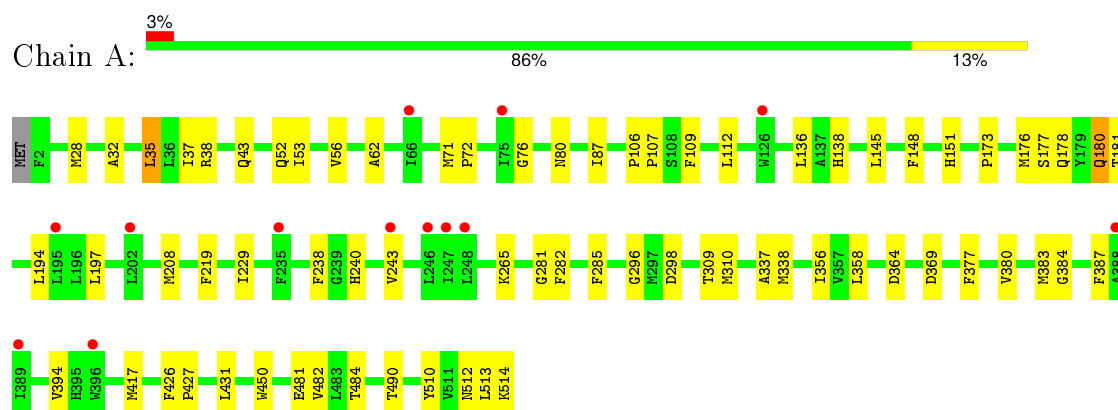
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	L	11	Total 11	O 11	0	0
24	M	10	Total 10	O 10	0	0
24	N	118	Total 118	O 118	0	0
24	O	88	Total 88	O 88	0	0
24	P	17	Total 17	O 17	0	0
24	Q	54	Total 54	O 54	0	0
24	R	56	Total 56	O 56	0	0
24	S	46	Total 46	O 46	0	0
24	T	30	Total 30	O 30	0	0
24	U	32	Total 32	O 32	0	0
24	V	23	Total 23	O 23	0	0
24	X	12	Total 12	O 12	0	0
24	Y	6	Total 6	O 6	0	0
24	Z	10	Total 10	O 10	0	0

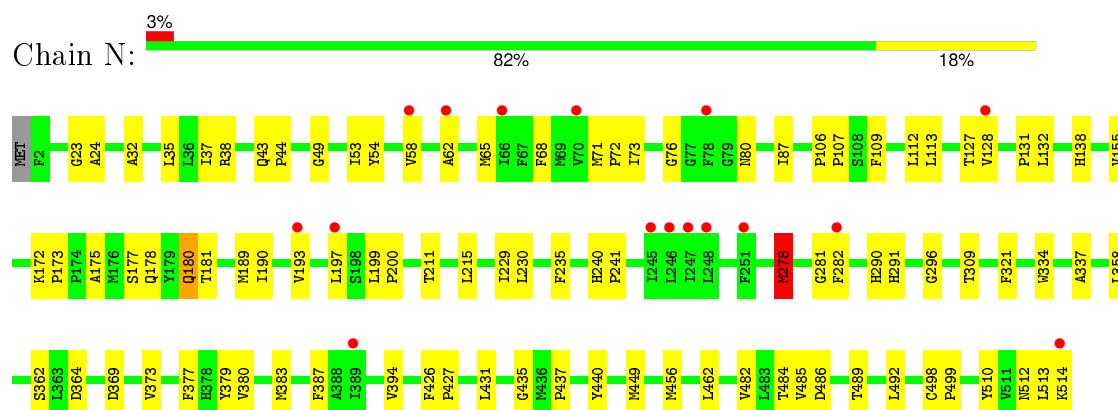
### 3 Residue-property plots [i](#)

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

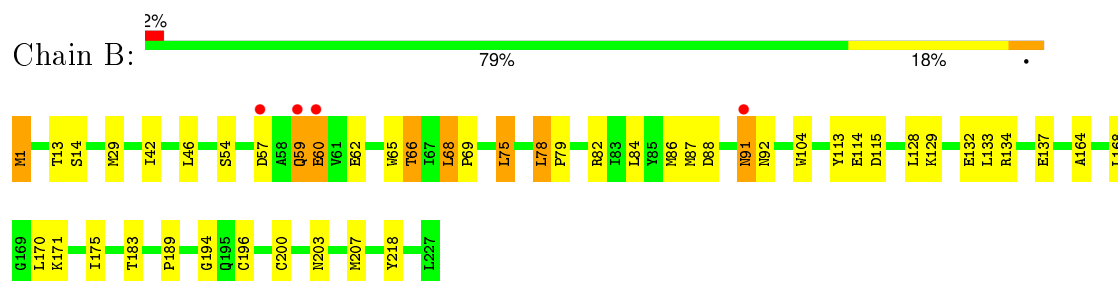
#### • Molecule 1: CYTOCHROME C OXIDASE SUBUNIT 1



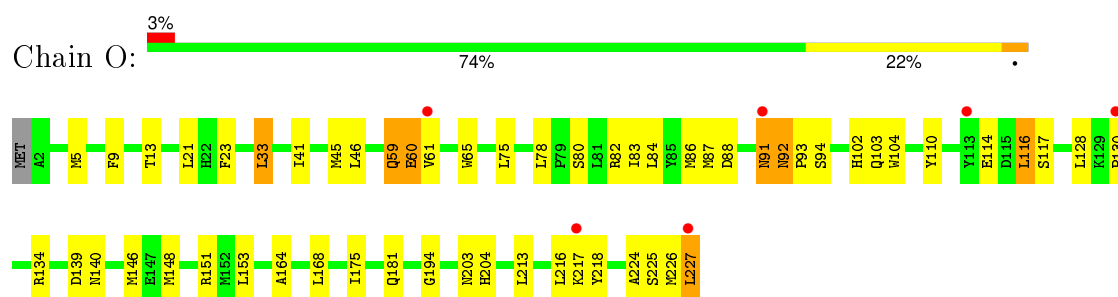
#### • Molecule 1: CYTOCHROME C OXIDASE SUBUNIT 1



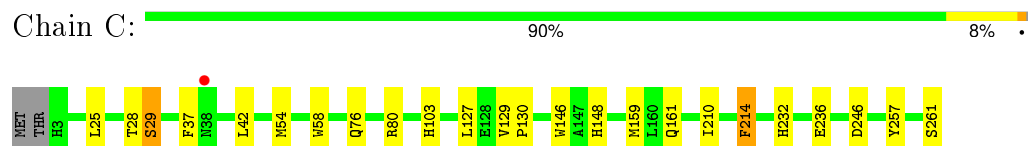
#### • Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2



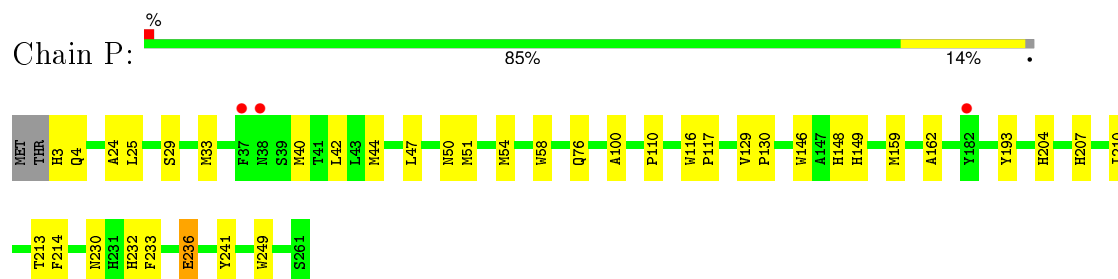
#### • Molecule 2: CYTOCHROME C OXIDASE SUBUNIT 2



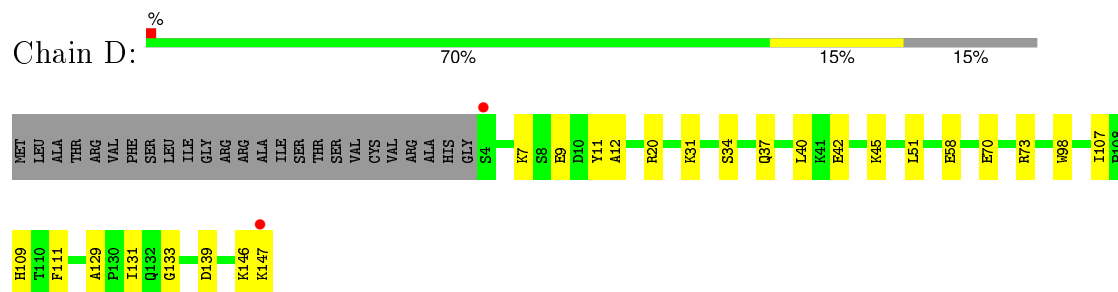
• Molecule 3: CYTOCHROME C OXIDASE SUBUNIT 3



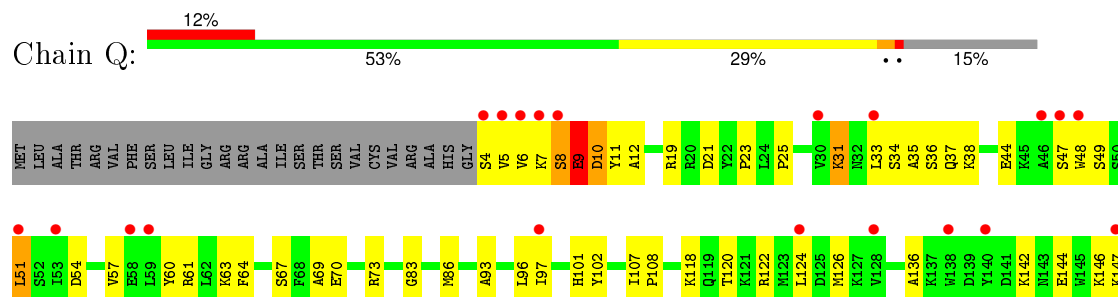
• Molecule 3: CYTOCHROME C OXIDASE SUBUNIT 3



• Molecule 4: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1



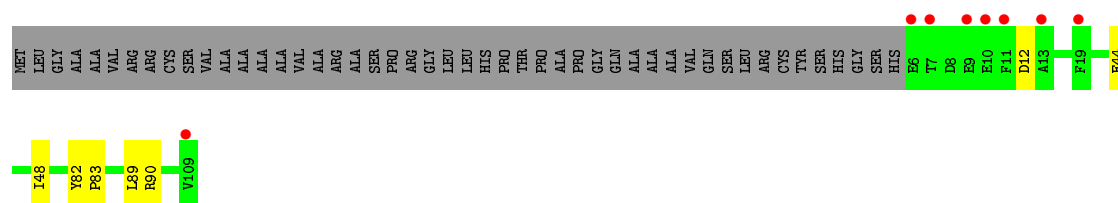
• Molecule 4: CYTOCHROME C OXIDASE SUBUNIT 4 ISOFORM 1



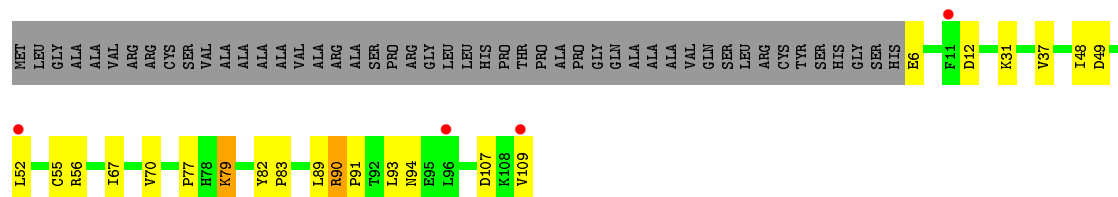
• Molecule 5: CYTOCHROME C OXIDASE SUBUNIT 5A



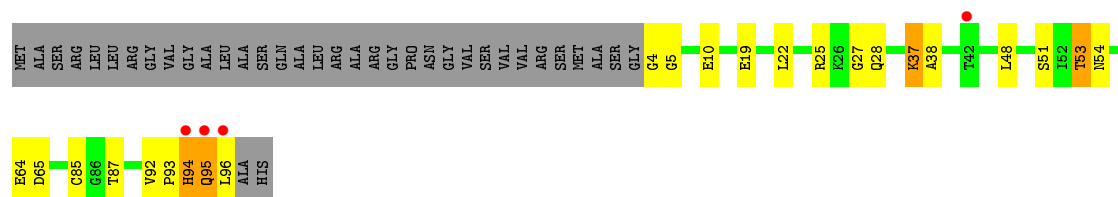




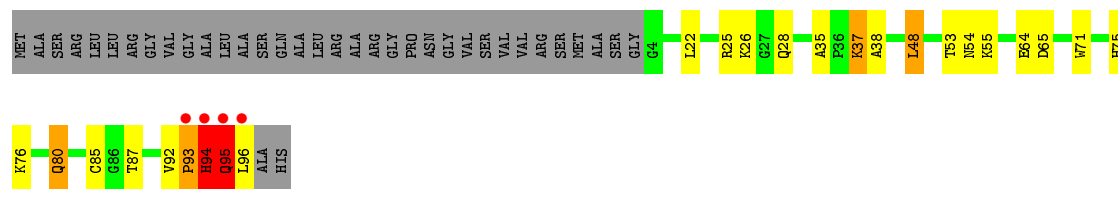
• Molecule 5: CYTOCHROME C OXIDASE SUBUNIT 5A



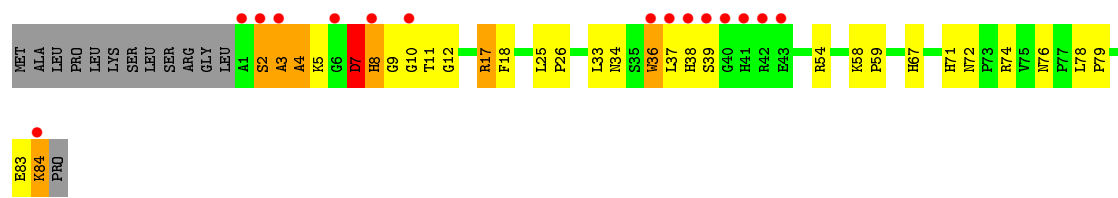
• Molecule 6: CYTOCHROME C OXIDASE SUBUNIT 5B



• Molecule 6: CYTOCHROME C OXIDASE SUBUNIT 5B

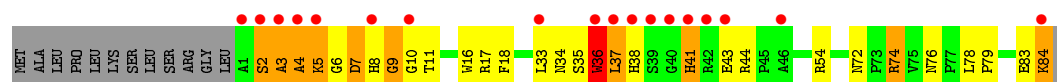


• Molecule 7: CYTOCHROME C OXIDASE POLYPEPTIDE 6A2

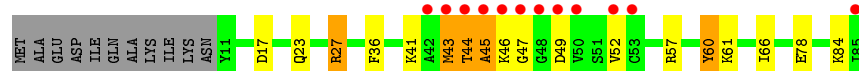


• Molecule 7: CYTOCHROME C OXIDASE POLYPEPTIDE 6A2

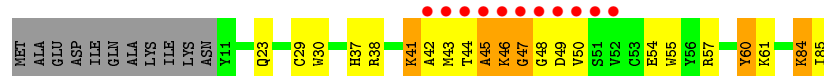




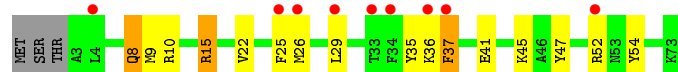
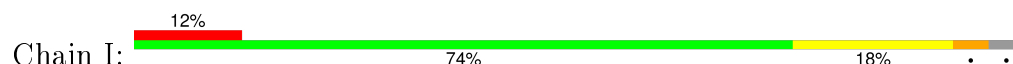
• Molecule 8: CYTOCHROME C OXIDASE SUBUNIT VIB ISOFORM 1



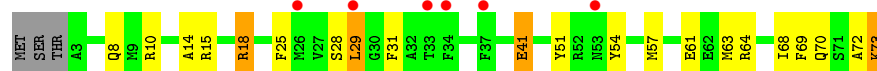
• Molecule 8: CYTOCHROME C OXIDASE SUBUNIT VIB ISOFORM 1



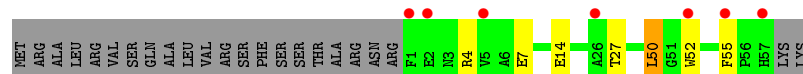
• Molecule 9: CYTOCHROME C OXIDASE POLYPEPTIDE VIC



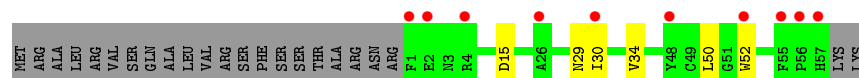
• Molecule 9: CYTOCHROME C OXIDASE POLYPEPTIDE VIC



• Molecule 10: CYTOCHROME C OXIDASE POLYPEPTIDE 7A1



• Molecule 10: CYTOCHROME C OXIDASE POLYPEPTIDE 7A1

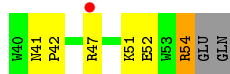
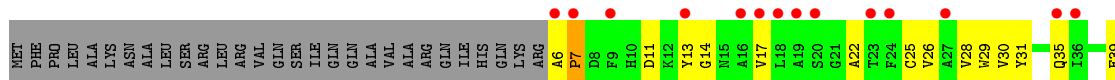
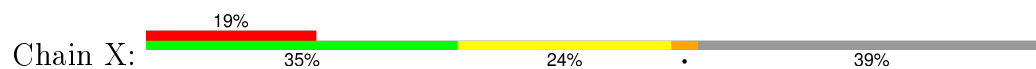


• Molecule 11: CYTOCHROME C OXIDASE POLYPEPTIDE 7B

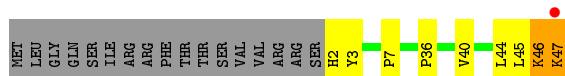




• Molecule 11: CYTOCHROME C OXIDASE POLYPEPTIDE 7B



• Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 7C



• Molecule 12: CYTOCHROME C OXIDASE SUBUNIT 7C



• Molecule 13: CYTOCHROME C OXIDASE POLYPEPTIDE 8H



• Molecule 13: CYTOCHROME C OXIDASE POLYPEPTIDE 8H



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.70Å 206.99Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.15 – 1.95 64.10 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.15-1.95) 96.4 (64.10-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.211 , 0.245 0.210 , 0.240	Depositor DCC
$R_{free}$ test set	16433 reflections (3.61%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 67.5	EDS
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 471933 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	30116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CHD, OXY, TPO, ZN, PGV, DMU, CUA, PEK, CU, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.75	0/4156	0.72	1/5678 (0.0%)
1	N	0.60	0/4156	0.65	1/5678 (0.0%)
2	B	0.67	1/1868 (0.1%)	0.74	0/2544
2	O	0.50	0/1860	0.65	0/2534
3	C	0.59	0/2197	0.61	0/3005
3	P	0.65	3/2197 (0.1%)	0.63	1/3005 (0.0%)
4	D	0.61	0/1229	0.67	2/1658 (0.1%)
4	Q	0.39	0/1229	0.53	0/1658
5	E	0.56	0/860	0.62	0/1167
5	R	0.45	0/860	0.58	0/1167
6	F	0.58	0/733	0.71	0/996
6	S	0.53	0/733	0.66	0/996
7	G	0.48	0/686	0.60	0/933
7	T	0.46	0/690	0.63	0/937
8	H	0.52	0/648	0.57	0/877
8	U	0.44	0/648	0.57	0/877
9	I	0.53	0/598	0.57	0/792
9	V	0.43	0/598	0.50	0/792
10	J	0.44	0/462	0.54	0/625
10	W	0.42	0/462	0.56	0/625
11	K	0.55	0/398	0.59	0/546
11	X	0.37	0/398	0.50	0/546
12	L	0.60	0/393	0.59	0/526
12	Y	0.44	0/393	0.51	0/526
13	M	0.54	0/345	0.60	0/470
13	Z	0.40	0/339	0.52	0/462
All	All	0.58	4/29136 (0.0%)	0.64	5/39620 (0.0%)

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

of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	S	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	236	GLU	CB-CG	9.64	1.70	1.52
3	P	236	GLU	CD-OE2	6.80	1.33	1.25
2	B	200	CYS	CB-SG	5.69	1.92	1.82
3	P	236	GLU	CG-CD	5.24	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	CA-CB-CG	-6.75	99.77	115.30
3	P	236	GLU	CB-CA-C	5.79	121.97	110.40
4	D	20	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	N	278	MET	CG-SD-CE	-5.61	91.23	100.20
4	D	20	ARG	NE-CZ-NH2	-5.47	117.57	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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	4017	0	3990	78	0
1	N	4017	0	3990	91	0
2	B	1822	0	1834	51	0
2	O	1814	0	1822	48	0
3	C	2110	0	2027	19	0
3	P	2110	0	2027	36	0
4	D	1195	0	1183	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1195	0	1183	109	0
5	E	842	0	838	4	0
5	R	842	0	838	29	0
6	F	717	0	700	33	0
6	S	717	0	700	44	0
7	G	671	0	633	54	0
7	T	675	0	644	46	0
8	H	628	0	578	20	0
8	U	628	0	580	32	0
9	I	585	0	597	36	0
9	V	585	0	597	57	0
10	J	451	0	446	11	0
10	W	451	0	446	7	1
11	K	384	0	366	4	0
11	X	384	0	366	35	1
12	L	380	0	380	15	0
12	Y	380	0	380	33	0
13	M	335	0	351	19	0
13	Z	329	0	347	32	0
14	A	120	0	108	22	0
14	N	120	0	108	23	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	2	0	0	0	0
16	N	2	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	29	0	39	1	0
18	C	29	0	39	2	0
18	G	29	0	39	1	0
18	N	29	0	39	2	0
18	P	29	0	39	1	0
18	T	29	0	39	1	0
19	B	2	0	0	0	0
19	O	2	0	0	0	0
20	C	53	0	77	10	0
20	P	53	0	77	13	0
21	C	102	0	152	6	0
21	P	102	0	152	11	0
22	F	1	0	0	0	0
22	S	1	0	0	0	0
23	M	33	0	40	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Z	33	0	40	8	0
24	A	114	0	0	11	0
24	B	102	0	0	12	0
24	C	85	0	0	2	0
24	D	43	0	0	4	0
24	F	45	0	0	15	0
24	G	41	0	0	7	0
24	H	49	0	0	11	0
24	I	20	0	0	3	0
24	J	26	0	0	5	0
24	K	10	0	0	0	0
24	L	11	0	0	1	0
24	M	10	0	0	1	0
24	N	118	0	0	1	0
24	O	88	0	0	3	0
24	P	17	0	0	0	0
24	Q	54	0	0	28	0
24	R	56	0	0	16	0
24	S	46	0	0	6	0
24	T	30	0	0	1	0
24	U	32	0	0	4	0
24	V	23	0	0	8	0
24	X	12	0	0	3	0
24	Y	6	0	0	5	0
24	Z	10	0	0	4	0
All	All	30116	0	28831	900	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 16.

All (900) 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)
9:V:18:ARG:CB	9:V:18:ARG:HH11	1.09	1.59
13:M:42:LYS:CE	13:M:42:LYS:O	1.66	1.40
9:V:18:ARG:NH1	9:V:18:ARG:HB3	1.07	1.38
7:G:37:LEU:HD23	7:G:38:HIS:CE1	1.59	1.38
4:Q:4:SER:HB2	24:Q:2001:HOH:O	1.18	1.36
9:I:45:LYS:HE2	24:I:2006:HOH:O	1.26	1.32
12:Y:47:LYS:HD3	24:Y:2006:HOH:O	1.27	1.31
4:Q:48:TRP:HA	4:Q:51:LEU:CD2	1.62	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:73:LYS:CE	9:V:73:LYS:CA	2.01	1.29
9:V:73:LYS:CE	9:V:73:LYS:HA	1.16	1.27
11:X:47:ARG:NH1	11:X:47:ARG:HB3	1.48	1.25
2:B:1:MET:CE	2:B:133:LEU:HD13	1.65	1.25
7:G:9:GLY:HA3	24:G:2003:HOH:O	1.10	1.23
8:H:27:ARG:CD	24:H:2014:HOH:O	1.86	1.23
6:F:95:GLN:CG	24:F:2045:HOH:O	1.87	1.23
2:O:218:TYR:HD2	24:V:2022:HOH:O	1.22	1.21
4:Q:49:SER:HB2	24:Q:2026:HOH:O	1.38	1.21
5:R:79:LYS:CE	24:R:2050:HOH:O	1.87	1.21
4:Q:63:LYS:HD3	24:Q:2033:HOH:O	1.04	1.20
13:M:42:LYS:HE3	13:M:42:LYS:O	1.15	1.20
2:O:217:LYS:HG3	24:O:2087:HOH:O	1.39	1.20
6:F:95:GLN:HG3	24:F:2045:HOH:O	1.39	1.20
7:G:37:LEU:CD2	7:G:38:HIS:CE1	2.24	1.19
8:H:27:ARG:HD3	24:H:2014:HOH:O	1.38	1.18
20:P:1262:PEK:H71	20:P:1262:PEK:H32	1.19	1.16
10:J:55:PHE:HB3	24:J:2024:HOH:O	1.44	1.15
2:B:129:LYS:HE3	24:B:2059:HOH:O	1.00	1.15
11:X:54:ARG:HH11	11:X:54:ARG:CG	1.59	1.15
2:O:116:LEU:HD12	2:O:117:SER:N	1.63	1.14
7:G:9:GLY:CA	24:G:2003:HOH:O	1.71	1.13
6:S:94:HIS:O	6:S:95:GLN:HG2	1.47	1.13
9:I:15:ARG:HH11	9:I:15:ARG:CG	1.60	1.13
6:S:95:GLN:CA	6:S:95:GLN:HE21	1.61	1.13
6:S:53:THR:HG22	6:S:54:ASN:H	1.03	1.11
11:X:47:ARG:HH11	11:X:47:ARG:HB3	0.98	1.11
6:F:94:HIS:O	6:F:95:GLN:HG2	1.51	1.11
9:V:68:ILE:HD12	9:V:69:PHE:N	1.65	1.11
2:B:1:MET:HE1	2:B:133:LEU:CD1	1.82	1.10
11:X:54:ARG:HH11	11:X:54:ARG:HG3	1.03	1.09
6:S:95:GLN:NE2	6:S:95:GLN:HA	1.55	1.09
4:Q:48:TRP:HA	4:Q:51:LEU:HD21	1.08	1.08
1:A:298:ASP:HB2	24:A:2069:HOH:O	0.92	1.08
13:Z:39:ASN:OD1	24:Z:2008:HOH:O	1.68	1.08
4:Q:34:SER:O	4:Q:38:LYS:HG3	1.52	1.08
12:Y:26:THR:HG23	13:Z:25:SER:CB	1.83	1.08
13:M:38:ASP:OD1	13:M:42:LYS:HG3	1.53	1.08
1:A:136:LEU:HB2	24:A:2032:HOH:O	1.53	1.08
7:G:11:TPO:HA	7:G:11:TPO:O3P	1.35	1.07
12:Y:46:LYS:HA	24:Y:2004:HOH:O	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:73:LYS:HA	9:V:73:LYS:HE2	1.14	1.06
9:I:15:ARG:HH11	9:I:15:ARG:HG3	1.17	1.06
9:V:68:ILE:HD11	9:V:69:PHE:CE2	1.91	1.06
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.53	1.06
4:Q:86:MET:CE	11:X:22:ALA:HA	1.86	1.06
5:R:79:LYS:CD	24:R:2050:HOH:O	2.02	1.06
12:Y:47:LYS:CD	24:Y:2006:HOH:O	1.91	1.05
7:T:37:LEU:HD23	7:T:38:HIS:ND1	1.70	1.05
20:C:1262:PEK:H71	20:C:1262:PEK:H32	1.35	1.05
7:G:10:GLY:O	7:G:11:TPO:HB	1.57	1.05
4:Q:48:TRP:CA	4:Q:51:LEU:CD2	2.35	1.04
2:B:1:MET:CE	2:B:133:LEU:CD1	2.33	1.04
20:P:1262:PEK:H102	20:P:1262:PEK:H161	1.38	1.04
9:V:73:LYS:HE2	9:V:73:LYS:CA	1.62	1.03
6:F:19:GLU:OE1	24:F:2028:HOH:O	1.75	1.03
6:S:85:CYS:SG	6:S:87:THR:HG23	1.98	1.03
5:R:79:LYS:HA	5:R:79:LYS:HE3	1.38	1.02
13:Z:28:LEU:HD23	23:Z:1043:DMU:H7	1.41	1.02
9:V:68:ILE:HD11	9:V:69:PHE:CD2	1.95	1.02
6:F:95:GLN:OE1	6:F:95:GLN:HA	1.58	1.01
4:Q:63:LYS:HA	24:Q:2033:HOH:O	1.61	1.01
3:P:148:HIS:NE2	3:P:236:GLU:OE2	1.92	1.00
9:V:18:ARG:CG	9:V:18:ARG:HH11	1.72	1.00
14:N:515:HEA:C27	14:N:515:HEA:C16	2.38	1.00
14:N:515:HEA:H273	14:N:515:HEA:H162	1.43	1.00
9:V:41:GLU:OE1	9:V:41:GLU:HA	1.56	0.99
4:Q:86:MET:HE2	11:X:22:ALA:HA	1.03	0.99
12:Y:24:MET:HE2	12:Y:24:MET:HA	1.45	0.99
3:P:33:MET:HE3	10:W:52:TRP:HZ3	1.24	0.99
6:S:22:LEU:HD23	6:S:25:ARG:NH1	1.78	0.98
9:V:73:LYS:HB2	24:V:2023:HOH:O	1.61	0.97
3:P:232:HIS:NE2	3:P:236:GLU:OE2	1.97	0.97
9:V:68:ILE:CD1	9:V:69:PHE:CG	2.46	0.97
13:M:38:ASP:OD1	13:M:42:LYS:HG2	1.61	0.97
11:X:54:ARG:NH1	11:X:54:ARG:HG3	1.74	0.97
4:Q:5:VAL:HG11	13:Z:4:LYS:HE2	1.42	0.97
4:Q:49:SER:CB	24:Q:2026:HOH:O	1.98	0.97
7:G:72:ASN:H	7:G:76:ASN:HD22	1.12	0.97
13:M:42:LYS:C	13:M:42:LYS:HE3	1.85	0.96
2:B:1:MET:HE1	2:B:133:LEU:HD13	1.40	0.96
9:V:68:ILE:CD1	9:V:69:PHE:CD1	2.49	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:22:LEU:HD23	6:S:25:ARG:HH12	1.26	0.96
9:I:15:ARG:HH11	9:I:15:ARG:CB	1.78	0.95
6:S:26:LYS:HB3	6:S:28:GLN:NE2	1.81	0.95
9:I:8:GLN:HE21	9:I:9:MET:N	1.62	0.95
7:G:11:TPO:O1P	7:G:12:GLY:N	1.99	0.95
14:N:515:HEA:H272	14:N:515:HEA:H161	1.47	0.94
13:M:42:LYS:HE2	13:M:42:LYS:O	1.65	0.94
7:T:7:ASP:CG	7:T:8:HIS:H	1.65	0.94
12:L:47:LYS:OXT	12:L:47:LYS:HD2	1.68	0.94
1:A:296:GLY:HA2	8:H:23:GLN:OE1	1.66	0.94
4:Q:63:LYS:CB	24:Q:2033:HOH:O	2.14	0.94
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.07	0.94
8:U:84:LYS:C	8:U:84:LYS:HD2	1.87	0.94
4:Q:48:TRP:O	4:Q:51:LEU:HD23	1.67	0.93
9:I:15:ARG:NH1	9:I:15:ARG:CB	2.31	0.93
5:R:79:LYS:HD2	24:R:2050:HOH:O	1.62	0.93
9:V:18:ARG:CB	9:V:18:ARG:NH1	1.86	0.93
9:V:18:ARG:HB3	9:V:18:ARG:CZ	1.99	0.92
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.49	0.92
7:T:72:ASN:H	7:T:76:ASN:HD22	1.17	0.92
11:X:47:ARG:NH1	11:X:47:ARG:CB	2.32	0.92
4:Q:9:GLU:N	4:Q:9:GLU:OE1	2.02	0.92
6:S:53:THR:HG22	6:S:54:ASN:N	1.85	0.91
13:Z:35:TYR:OH	23:Z:1043:DMU:H41	1.69	0.91
6:F:94:HIS:O	6:F:95:GLN:CG	2.19	0.91
1:A:37:ILE:HG21	14:A:515:HEA:HMA	1.49	0.91
7:G:37:LEU:CD2	7:G:38:HIS:HE1	1.80	0.90
4:Q:49:SER:N	24:Q:2026:HOH:O	2.01	0.90
4:Q:7:LYS:HB2	24:Q:2002:HOH:O	1.70	0.90
7:T:37:LEU:HD23	7:T:38:HIS:CE1	2.05	0.90
6:F:28:GLN:HA	24:F:2032:HOH:O	1.71	0.90
9:V:68:ILE:HD11	9:V:69:PHE:CZ	2.06	0.90
4:Q:8:SER:CB	4:Q:9:GLU:OE1	2.21	0.89
23:Z:1043:DMU:H29	23:Z:1043:DMU:H35	1.51	0.89
7:G:11:TPO:O3P	7:G:11:TPO:CA	2.18	0.89
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.73	0.89
12:Y:26:THR:CG2	13:Z:25:SER:HB3	2.03	0.88
6:S:94:HIS:O	6:S:95:GLN:CG	2.22	0.88
7:G:4:ALA:HB1	1:N:281:GLY:C	1.92	0.88
9:V:41:GLU:OE1	9:V:41:GLU:CA	2.21	0.88
12:Y:24:MET:CE	12:Y:24:MET:HA	2.00	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:CG2	14:A:515:HEA:HMA	2.03	0.87
2:B:59:GLN:O	2:B:59:GLN:HG3	1.73	0.87
1:A:282:PHE:HA	7:T:4:ALA:CB	2.04	0.87
9:V:73:LYS:HA	9:V:73:LYS:HE3	0.87	0.87
12:Y:24:MET:HE3	12:Y:24:MET:N	1.89	0.86
9:I:15:ARG:NH1	9:I:15:ARG:CG	2.32	0.86
6:F:28:GLN:CG	24:F:2032:HOH:O	2.23	0.86
12:Y:26:THR:CG2	13:Z:25:SER:CB	2.53	0.86
12:Y:24:MET:CE	12:Y:24:MET:CA	2.54	0.85
7:T:7:ASP:CG	7:T:8:HIS:N	2.27	0.85
4:Q:86:MET:HE2	11:X:22:ALA:CA	1.99	0.85
14:N:515:HEA:C27	14:N:515:HEA:H162	2.03	0.85
1:N:215:LEU:HD11	20:P:1262:PEK:C27	2.06	0.85
11:X:7:PRO:HB3	11:X:11:ASP:CB	2.06	0.85
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.10	0.85
9:V:73:LYS:HE3	9:V:73:LYS:CA	1.81	0.85
1:N:37:ILE:HG21	14:N:515:HEA:HMA	1.58	0.84
8:U:45:ALA:O	8:U:47:GLY:N	2.10	0.84
6:S:95:GLN:HE21	6:S:95:GLN:HA	0.72	0.84
7:G:4:ALA:CB	1:N:282:PHE:N	2.40	0.84
2:B:1:MET:HE3	2:B:133:LEU:HD13	1.59	0.84
14:N:515:HEA:H272	14:N:515:HEA:C16	2.05	0.83
7:G:7:ASP:O	7:G:9:GLY:N	2.12	0.83
4:Q:8:SER:HB3	4:Q:9:GLU:OE1	1.77	0.83
13:Z:35:TYR:CZ	23:Z:1043:DMU:H41	2.14	0.83
1:A:136:LEU:CB	24:A:2032:HOH:O	2.19	0.83
9:I:8:GLN:NE2	9:I:9:MET:H	1.75	0.83
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.78	0.83
3:P:33:MET:CE	10:W:52:TRP:HZ3	1.90	0.82
6:F:95:GLN:O	6:F:96:LEU:HB3	1.77	0.82
11:X:7:PRO:HB3	11:X:11:ASP:HB3	1.62	0.82
12:Y:24:MET:CE	12:Y:24:MET:N	2.43	0.82
4:D:42:GLU:OE1	4:D:45:LYS:HE3	1.78	0.82
5:R:79:LYS:HE2	24:R:2050:HOH:O	1.59	0.82
4:Q:48:TRP:O	4:Q:51:LEU:CD2	2.26	0.81
9:I:15:ARG:NH1	9:I:15:ARG:HG3	1.93	0.81
7:G:4:ALA:HB1	1:N:282:PHE:N	1.95	0.81
9:V:68:ILE:HD13	9:V:69:PHE:CD1	2.15	0.81
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	1.95	0.81
3:P:33:MET:HE3	10:W:52:TRP:CZ3	2.15	0.81
6:S:26:LYS:CB	6:S:28:GLN:NE2	2.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:1264:PGV:C16	21:P:1264:PGV:H12	2.09	0.81
2:B:13:THR:HB	2:B:168:LEU:HD23	1.62	0.81
1:N:215:LEU:HD11	20:P:1262:PEK:H272	1.61	0.81
9:V:68:ILE:CD1	9:V:69:PHE:CD2	2.63	0.81
8:H:49:ASP:O	8:H:52:VAL:HG13	1.80	0.81
20:P:1262:PEK:C3	20:P:1262:PEK:H71	2.05	0.81
9:I:8:GLN:HE21	9:I:8:GLN:CA	1.93	0.80
1:A:281:GLY:C	7:T:4:ALA:HB1	2.01	0.80
6:F:28:GLN:CA	24:F:2032:HOH:O	2.25	0.80
7:G:4:ALA:HB2	1:N:282:PHE:HA	1.62	0.80
9:V:14:ALA:O	9:V:18:ARG:HG3	1.81	0.79
2:O:91:ASN:HD22	2:O:92:ASN:N	1.80	0.79
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.65	0.79
2:B:1:MET:HE1	2:B:133:LEU:HD11	1.65	0.79
7:G:2:SER:O	7:G:3:ALA:CB	2.30	0.79
20:P:1262:PEK:H102	20:P:1262:PEK:C16	2.13	0.79
8:U:48:GLY:HA2	24:U:2016:HOH:O	1.82	0.79
3:P:232:HIS:CD2	3:P:236:GLU:HG3	2.17	0.79
6:F:85:CYS:SG	6:F:87:THR:HG23	2.23	0.79
7:G:37:LEU:HD21	7:G:38:HIS:HE1	1.47	0.78
8:H:61:LYS:NZ	24:H:2031:HOH:O	1.93	0.78
4:Q:34:SER:N	4:Q:37:GLN:HE21	1.82	0.78
1:N:49:GLY:HA2	24:N:2007:HOH:O	1.84	0.78
8:H:27:ARG:NE	24:H:2014:HOH:O	2.02	0.78
4:Q:47:SER:OG	24:Q:2026:HOH:O	2.01	0.78
21:P:1264:PGV:H161	21:P:1264:PGV:C12	2.13	0.78
11:X:47:ARG:CB	11:X:47:ARG:HH11	1.90	0.77
3:P:232:HIS:HD2	3:P:236:GLU:HG3	1.47	0.77
11:X:6:ALA:N	24:X:2001:HOH:O	2.15	0.77
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.66	0.77
9:V:68:ILE:HD11	9:V:69:PHE:CG	2.16	0.77
1:A:510:TYR:CZ	1:A:512:ASN:ND2	2.53	0.77
11:X:54:ARG:C	11:X:54:ARG:HD3	2.05	0.77
20:P:1262:PEK:C7	20:P:1262:PEK:H32	2.06	0.77
2:B:91:ASN:HD22	2:B:92:ASN:N	1.83	0.77
11:X:54:ARG:NH1	11:X:54:ARG:CG	2.31	0.76
13:Z:38:ASP:OD2	24:Z:2006:HOH:O	2.04	0.76
4:Q:48:TRP:C	4:Q:51:LEU:CD2	2.54	0.76
9:I:45:LYS:CE	24:I:2006:HOH:O	2.02	0.76
2:B:88:ASP:HB3	24:B:2024:HOH:O	1.86	0.76
4:Q:48:TRP:CA	4:Q:51:LEU:HD21	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:116:LEU:HD12	2:O:116:LEU:C	2.06	0.76
9:I:8:GLN:NE2	9:I:9:MET:N	2.31	0.76
6:S:64:GLU:CG	24:S:2028:HOH:O	2.34	0.76
6:S:64:GLU:OE2	24:S:2028:HOH:O	2.03	0.76
6:F:51:SER:O	6:F:94:HIS:N	2.19	0.75
6:S:94:HIS:CD2	6:S:95:GLN:H	2.03	0.75
9:V:18:ARG:CA	9:V:18:ARG:HH11	1.96	0.75
1:A:510:TYR:CE1	1:A:512:ASN:ND2	2.54	0.74
1:N:37:ILE:CG2	14:N:515:HEA:HMA	2.16	0.74
9:I:8:GLN:HE21	9:I:9:MET:H	1.30	0.74
6:F:27:GLY:O	24:F:2032:HOH:O	2.05	0.74
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.35	0.74
6:F:95:GLN:OE1	6:F:95:GLN:CA	2.34	0.74
13:M:13:LYS:C	13:M:13:LYS:HD2	2.08	0.74
9:V:15:ARG:HD3	24:V:2009:HOH:O	1.86	0.74
4:D:146:LYS:HA	24:D:2030:HOH:O	1.87	0.74
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.69	0.74
9:V:73:LYS:N	24:V:2023:HOH:O	2.13	0.74
12:Y:24:MET:HE2	12:Y:24:MET:CA	2.15	0.74
7:G:4:ALA:CB	1:N:282:PHE:CA	2.65	0.74
20:C:1262:PEK:HN2	7:G:76:ASN:HD21	1.35	0.74
7:T:41:HIS:HB3	7:T:74:ARG:NH2	2.02	0.74
4:D:34:SER:H	4:D:37:GLN:HE21	1.36	0.74
8:U:84:LYS:C	8:U:84:LYS:CD	2.56	0.73
2:O:116:LEU:HD22	2:O:226:MET:HG2	1.71	0.73
9:V:68:ILE:CD1	9:V:69:PHE:CE1	2.72	0.73
9:V:68:ILE:HD12	9:V:69:PHE:CG	2.22	0.73
7:G:5:LYS:O	1:N:193:VAL:HG21	1.89	0.73
12:L:47:LYS:HE2	12:L:47:LYS:C	2.09	0.73
9:I:8:GLN:C	9:I:8:GLN:HE21	1.91	0.72
12:L:47:LYS:OXT	12:L:47:LYS:CD	2.37	0.72
2:B:1:MET:HE3	2:B:133:LEU:CD1	2.15	0.72
9:V:68:ILE:HD11	9:V:69:PHE:CE1	2.23	0.72
7:T:4:ALA:O	7:T:5:LYS:O	2.07	0.72
6:S:22:LEU:CD2	6:S:25:ARG:HH12	2.00	0.72
6:S:53:THR:CG2	6:S:54:ASN:H	1.82	0.72
6:S:22:LEU:CD2	6:S:25:ARG:NH1	2.51	0.72
12:Y:15:VAL:HG12	12:Y:21:LEU:HD22	1.70	0.72
7:G:4:ALA:CB	1:N:282:PHE:HA	2.20	0.72
4:Q:6:VAL:CG1	4:Q:10:ASP:OD1	2.38	0.72
3:P:232:HIS:CD2	3:P:236:GLU:CG	2.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.53	0.71
1:A:514:LYS:OXT	6:F:37:LYS:NZ	2.23	0.71
2:B:57:ASP:OD1	2:B:59:GLN:HB3	1.90	0.71
1:N:215:LEU:HD11	20:P:1262:PEK:C26	2.20	0.71
4:Q:35:ALA:HB3	24:Q:2019:HOH:O	1.88	0.71
4:Q:35:ALA:N	24:Q:2019:HOH:O	2.23	0.71
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.21	0.71
6:S:26:LYS:HB3	6:S:28:GLN:HE21	1.50	0.71
1:N:155:VAL:HG21	21:P:1263:PGV:H142	1.72	0.71
5:R:6:GLU:N	24:R:2002:HOH:O	2.23	0.70
2:B:91:ASN:HB2	24:B:2027:HOH:O	1.91	0.70
7:G:37:LEU:HD21	7:G:38:HIS:CE1	2.19	0.70
3:P:33:MET:CE	10:W:52:TRP:CZ3	2.74	0.70
13:Z:10:THR:HA	13:Z:14:GLU:OE1	1.92	0.70
1:A:484:THR:HB	13:M:2:THR:OG1	1.90	0.70
13:Z:39:ASN:HA	24:Z:2007:HOH:O	1.91	0.70
7:G:72:ASN:H	7:G:76:ASN:ND2	1.89	0.70
3:P:148:HIS:HE2	3:P:236:GLU:CD	1.95	0.70
12:L:46:LYS:O	12:L:47:LYS:HB2	1.90	0.69
4:Q:54:ASP:O	24:Q:2030:HOH:O	2.10	0.69
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	1.71	0.69
4:Q:63:LYS:CA	24:Q:2033:HOH:O	2.17	0.69
8:U:84:LYS:HD2	8:U:85:ILE:N	2.08	0.69
10:J:50:LEU:HD22	10:J:50:LEU:O	1.92	0.69
1:A:37:ILE:HG21	14:A:515:HEA:CMA	2.22	0.69
6:S:64:GLU:CD	24:S:2028:HOH:O	2.30	0.69
4:Q:48:TRP:CA	4:Q:51:LEU:HD23	2.22	0.69
9:V:68:ILE:HD11	9:V:69:PHE:CD1	2.27	0.69
3:P:232:HIS:HD2	3:P:236:GLU:CG	2.04	0.69
10:J:27:THR:N	24:J:2017:HOH:O	2.23	0.69
13:M:42:LYS:O	13:M:42:LYS:CD	2.40	0.69
1:N:215:LEU:HD11	20:P:1262:PEK:H262	1.75	0.69
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.23	0.69
4:D:109:HIS:HD2	24:D:2015:HOH:O	1.76	0.68
6:F:92:VAL:O	6:F:92:VAL:HG23	1.92	0.68
2:O:116:LEU:HD12	2:O:117:SER:H	1.53	0.68
9:V:73:LYS:CB	24:V:2023:HOH:O	2.28	0.68
6:F:95:GLN:HG2	24:F:2045:HOH:O	1.65	0.68
2:B:114:GLU:HG2	24:B:2043:HOH:O	1.93	0.68
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.29	0.68
5:R:12:ASP:OD2	24:R:2011:HOH:O	2.12	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:63:LYS:HG2	4:Q:64:PHE:CE2	2.28	0.68
6:F:64:GLU:O	6:F:65:ASP:HB2	1.94	0.68
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.75	0.68
20:P:1262:PEK:HN2	7:T:76:ASN:HD21	1.38	0.67
3:P:148:HIS:NE2	3:P:236:GLU:CD	2.46	0.67
2:O:88:ASP:OD2	24:O:2034:HOH:O	2.11	0.67
7:T:37:LEU:CD2	7:T:38:HIS:CE1	2.78	0.67
3:C:210:ILE:HD13	21:C:1264:PGV:C30	2.24	0.67
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	1.95	0.67
1:A:136:LEU:HD13	24:A:2032:HOH:O	1.93	0.67
5:R:77:PRO:O	24:R:2047:HOH:O	2.11	0.67
9:I:15:ARG:NH1	9:I:15:ARG:HB3	2.08	0.67
4:Q:8:SER:HB2	4:Q:9:GLU:OE1	1.91	0.67
13:Z:35:TYR:CZ	23:Z:1043:DMU:C11	2.78	0.66
2:B:218:TYR:OH	24:B:2096:HOH:O	2.12	0.66
11:X:26:VAL:O	11:X:30:VAL:HG23	1.94	0.66
6:S:64:GLU:O	6:S:65:ASP:HB2	1.94	0.66
3:P:40:MET:O	3:P:44:MET:HG2	1.95	0.66
6:S:37:LYS:N	6:S:37:LYS:HD2	2.10	0.66
4:Q:6:VAL:HG11	4:Q:10:ASP:OD1	1.96	0.66
7:T:84:LYS:N	7:T:84:LYS:HD2	2.11	0.66
1:A:282:PHE:CA	7:T:4:ALA:CB	2.73	0.66
11:K:42:PRO:HG2	11:K:47:ARG:NH1	2.10	0.66
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.79	0.65
4:Q:31:LYS:CB	4:Q:31:LYS:NZ	2.59	0.65
4:Q:48:TRP:C	4:Q:51:LEU:HD23	2.17	0.65
4:Q:8:SER:O	4:Q:10:ASP:N	2.28	0.65
8:U:45:ALA:O	8:U:46:LYS:C	2.35	0.65
8:U:49:ASP:OD1	8:U:50:VAL:N	2.30	0.65
4:Q:102:TYR:CD1	13:Z:35:TYR:HE1	2.14	0.65
4:Q:48:TRP:CB	24:Q:2025:HOH:O	2.44	0.65
13:M:42:LYS:CG	13:M:42:LYS:O	2.44	0.65
7:T:72:ASN:H	7:T:76:ASN:ND2	1.92	0.65
1:A:151:HIS:CD2	20:C:1262:PEK:H382	2.32	0.65
7:G:2:SER:O	7:G:3:ALA:HB2	1.98	0.65
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.78	0.65
13:M:38:ASP:OD1	13:M:42:LYS:CB	2.44	0.64
1:A:28:MET:CE	14:A:515:HEA:H271	2.25	0.64
9:V:15:ARG:CD	24:V:2009:HOH:O	2.45	0.64
12:L:47:LYS:OXT	12:L:47:LYS:CE	2.45	0.64
6:S:64:GLU:HG3	24:S:2028:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:1264:PGV:H161	21:P:1264:PGV:H12	1.74	0.64
2:O:13:THR:HB	2:O:168:LEU:HD23	1.80	0.64
6:S:75:HIS:H	6:S:80:GLN:HE22	1.45	0.64
3:P:210:ILE:HD13	21:P:1264:PGV:H301	1.78	0.64
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.80	0.64
4:Q:107:ILE:CD1	11:X:39:GLU:HB2	2.28	0.64
8:U:84:LYS:CE	8:U:84:LYS:O	2.46	0.64
11:X:7:PRO:HB3	11:X:11:ASP:HB2	1.78	0.64
8:U:50:VAL:N	24:U:2017:HOH:O	2.31	0.64
9:V:64:ARG:HG3	9:V:72:ALA:O	1.97	0.64
7:T:7:ASP:OD1	7:T:8:HIS:N	2.31	0.64
1:N:435:GLY:O	1:N:437:PRO:HD3	1.97	0.64
1:A:178:GLN:HE21	7:T:9:GLY:HA3	1.61	0.63
2:O:103:GLN:HB3	2:O:104:TRP:CE2	2.33	0.63
8:U:54:GLU:OE1	8:U:54:GLU:HA	1.97	0.63
5:E:12:ASP:OD2	5:E:44:GLU:HG3	1.99	0.63
12:L:2:HIS:HA	24:L:2001:HOH:O	1.99	0.63
5:R:94:ASN:HB2	24:R:2054:HOH:O	1.97	0.63
9:I:8:GLN:NE2	9:I:8:GLN:CA	2.61	0.63
6:F:94:HIS:O	6:F:95:GLN:CB	2.46	0.63
9:V:68:ILE:C	9:V:68:ILE:HD12	2.19	0.63
2:O:139:ASP:OD1	2:O:140:ASN:N	2.31	0.63
10:J:55:PHE:CB	24:J:2024:HOH:O	2.08	0.62
1:A:417:MET:CE	14:A:515:HEA:H263	2.29	0.62
1:N:112:LEU:HD23	1:N:113:LEU:HD23	1.80	0.62
1:N:486:ASP:OD2	4:Q:19:ARG:NH2	2.22	0.62
2:B:13:THR:HB	2:B:168:LEU:CD2	2.30	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.39	0.62
12:Y:26:THR:CG2	13:Z:25:SER:HB2	2.28	0.62
7:T:2:SER:O	7:T:3:ALA:HB3	1.98	0.62
20:C:1262:PEK:C7	20:C:1262:PEK:H32	2.20	0.62
7:G:34:ASN:O	7:G:37:LEU:HB3	1.99	0.61
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.82	0.61
11:X:41:ASN:ND2	24:X:2011:HOH:O	2.19	0.61
11:X:52:GLU:OE2	24:X:2012:HOH:O	2.16	0.61
4:Q:48:TRP:HB2	24:Q:2025:HOH:O	1.98	0.61
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.65	0.61
13:Z:28:LEU:CD2	23:Z:1043:DMU:H7	2.26	0.61
6:S:95:GLN:CA	6:S:95:GLN:NE2	2.34	0.61
7:T:11:TPO:O2P	7:T:16:TRP:NE1	2.33	0.61
3:P:24:ALA:HB2	21:P:1263:PGV:H12	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:LYS:CG	24:H:2048:HOH:O	2.49	0.61
12:L:47:LYS:CE	12:L:47:LYS:C	2.68	0.61
14:N:515:HEA:H122	14:N:515:HEA:HHC	1.82	0.61
2:B:91:ASN:C	2:B:91:ASN:HD22	2.04	0.61
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.82	0.61
12:L:47:LYS:C	12:L:47:LYS:CD	2.69	0.60
12:L:47:LYS:HD2	12:L:47:LYS:C	2.21	0.60
9:I:22:VAL:O	9:I:26:MET:HG2	2.01	0.60
4:Q:49:SER:CA	24:Q:2026:HOH:O	2.28	0.60
8:U:38:ARG:NH2	8:U:84:LYS:HE2	2.16	0.60
4:Q:34:SER:O	4:Q:38:LYS:CG	2.41	0.60
6:S:94:HIS:C	24:S:2046:HOH:O	2.40	0.60
11:X:47:ARG:CZ	11:X:47:ARG:CB	2.79	0.60
9:V:68:ILE:HD12	9:V:69:PHE:H	1.60	0.60
4:D:34:SER:H	4:D:37:GLN:NE2	1.99	0.60
8:U:44:THR:O	8:U:45:ALA:O	2.18	0.60
2:O:84:LEU:HA	2:O:87:MET:HE2	1.84	0.60
2:B:114:GLU:HB3	24:B:2044:HOH:O	2.02	0.60
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.29	0.60
9:V:68:ILE:CD1	9:V:69:PHE:N	2.54	0.60
11:X:54:ARG:CD	11:X:54:ARG:C	2.67	0.60
9:V:18:ARG:CG	9:V:18:ARG:NH1	2.43	0.59
6:F:95:GLN:O	6:F:96:LEU:CB	2.47	0.59
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.78	0.59
2:B:84:LEU:HA	2:B:87:MET:HE2	1.85	0.59
3:C:37:PHE:CD1	10:J:52:TRP:HZ3	2.20	0.59
4:Q:147:LYS:N	24:Q:2053:HOH:O	2.34	0.59
7:T:83:GLU:HA	7:T:84:LYS:NZ	2.18	0.59
7:T:44:ARG:NH1	24:T:2006:HOH:O	2.04	0.59
7:G:83:GLU:O	7:G:84:LYS:C	2.41	0.59
5:R:90:ARG:NH2	24:R:2053:HOH:O	2.29	0.59
3:C:210:ILE:HD13	21:C:1264:PGV:H302	1.84	0.59
11:X:7:PRO:HA	11:X:11:ASP:OD2	2.03	0.58
3:C:210:ILE:HD13	21:C:1264:PGV:H301	1.84	0.58
8:H:27:ARG:NH1	24:H:2015:HOH:O	2.36	0.58
6:F:27:GLY:C	24:F:2032:HOH:O	2.40	0.58
6:F:28:GLN:HG2	24:F:2032:HOH:O	1.93	0.58
8:H:41:LYS:NZ	24:H:2023:HOH:O	2.36	0.58
6:S:94:HIS:O	6:S:95:GLN:CB	2.51	0.58
23:Z:1043:DMU:H29	23:Z:1043:DMU:C9	2.27	0.58
4:Q:70:GLU:O	4:Q:73:ARG:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:44:LEU:HD22	13:Z:41:LYS:HG2	1.85	0.58
5:R:31:LYS:HE2	24:R:2030:HOH:O	2.04	0.58
4:Q:7:LYS:CB	24:Q:2002:HOH:O	2.41	0.57
4:Q:122:ARG:HG2	4:Q:126:MET:HE1	1.85	0.57
9:V:18:ARG:NH1	9:V:18:ARG:CA	2.63	0.57
6:F:10:GLU:HG3	24:F:2004:HOH:O	2.04	0.57
4:D:7:LYS:HD2	4:D:9:GLU:OE2	2.05	0.57
6:F:28:GLN:HG3	24:F:2032:HOH:O	1.99	0.57
6:S:92:VAL:HG23	6:S:92:VAL:O	2.04	0.57
1:A:112:LEU:HG	24:A:2037:HOH:O	2.03	0.57
2:B:91:ASN:O	24:B:2027:HOH:O	2.17	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.40	0.57
4:Q:122:ARG:HG2	4:Q:126:MET:CE	2.34	0.57
9:I:45:LYS:NZ	24:I:2006:HOH:O	2.30	0.56
4:Q:51:LEU:HD22	4:Q:51:LEU:H	1.71	0.56
9:V:68:ILE:HD13	9:V:69:PHE:CE1	2.37	0.56
2:B:62:GLU:O	2:B:66:THR:HB	2.05	0.56
1:A:513:LEU:O	1:A:514:LYS:HB2	2.04	0.56
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.88	0.56
5:R:79:LYS:HA	5:R:79:LYS:CE	2.24	0.56
11:X:54:ARG:HH11	11:X:54:ARG:HG2	1.60	0.56
10:J:50:LEU:CD2	10:J:50:LEU:O	2.53	0.56
3:P:47:LEU:O	3:P:51:MET:HG2	2.06	0.56
7:G:9:GLY:HA2	24:G:2003:HOH:O	1.68	0.56
1:N:383:MET:O	1:N:387:PHE:HB2	2.04	0.56
2:O:116:LEU:CD2	2:O:226:MET:HG2	2.35	0.56
8:U:38:ARG:HH21	8:U:84:LYS:HE2	1.70	0.56
14:A:515:HEA:C27	14:A:515:HEA:C16	2.84	0.56
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.71	0.56
4:Q:9:GLU:HB3	24:Q:2003:HOH:O	2.04	0.56
14:N:516:HEA:HBC1	14:N:516:HEA:HMC1	1.88	0.56
1:A:43:GLN:CD	4:D:107:ILE:HG22	2.27	0.55
9:I:8:GLN:NE2	9:I:10:ARG:H	2.03	0.55
7:T:84:LYS:N	7:T:84:LYS:CD	2.69	0.55
3:P:149:HIS:CE1	7:T:11:TPO:HG22	2.40	0.55
1:A:37:ILE:HG22	14:A:515:HEA:HMA	1.87	0.55
1:A:383:MET:O	1:A:387:PHE:HB2	2.06	0.55
4:Q:142:LYS:HE3	4:Q:144:GLU:OE2	2.05	0.55
10:J:14:GLU:CG	24:J:2012:HOH:O	2.54	0.55
4:Q:48:TRP:N	24:Q:2025:HOH:O	1.87	0.55
6:S:26:LYS:HB2	6:S:28:GLN:NE2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:LEU:HD22	10:J:50:LEU:C	2.26	0.55
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.89	0.55
1:A:87:ILE:O	1:A:173:PRO:HD3	2.07	0.55
2:B:59:GLN:O	2:B:59:GLN:CG	2.50	0.54
1:A:177:SER:H	1:A:180:GLN:NE2	2.05	0.54
20:C:1262:PEK:C3	20:C:1262:PEK:H71	2.22	0.54
8:U:49:ASP:C	8:U:49:ASP:OD1	2.46	0.54
2:O:139:ASP:O	9:V:70:GLN:NE2	2.39	0.54
13:Z:39:ASN:CG	24:Z:2008:HOH:O	2.27	0.54
4:Q:63:LYS:CD	24:Q:2033:HOH:O	1.83	0.54
2:B:164:ALA:O	2:B:194:GLY:HA3	2.07	0.54
9:V:51:TYR:HA	9:V:54:TYR:HB2	1.90	0.54
9:I:15:ARG:CZ	9:I:15:ARG:HB3	2.37	0.54
1:A:197:LEU:HD11	7:T:2:SER:HB3	1.88	0.54
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.89	0.54
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.89	0.54
4:Q:34:SER:N	4:Q:37:GLN:NE2	2.38	0.54
4:Q:4:SER:CB	24:Q:2001:HOH:O	2.03	0.54
4:Q:48:TRP:C	4:Q:51:LEU:HD22	2.27	0.54
1:N:37:ILE:HG21	14:N:515:HEA:CMA	2.36	0.54
7:T:8:HIS:O	7:T:9:GLY:C	2.44	0.54
7:G:17:ARG:HD2	24:G:2007:HOH:O	2.08	0.53
1:N:358:LEU:HB3	14:N:516:HEA:HMA	1.89	0.53
1:A:309:THR:HG22	14:A:516:HEA:HMB2	1.90	0.53
7:T:72:ASN:N	7:T:76:ASN:HD22	1.97	0.53
7:G:4:ALA:CB	1:N:281:GLY:C	2.70	0.53
1:N:486:ASP:CG	4:Q:19:ARG:HH21	2.10	0.53
2:O:103:GLN:HB3	2:O:104:TRP:CD2	2.43	0.53
1:A:112:LEU:HD12	24:A:2038:HOH:O	2.07	0.53
10:J:50:LEU:CD2	10:J:50:LEU:C	2.77	0.53
20:C:1262:PEK:C11	20:C:1262:PEK:H162	2.39	0.53
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.90	0.53
9:V:8:GLN:NE2	24:V:2003:HOH:O	2.41	0.53
6:F:93:PRO:HB2	6:F:94:HIS:ND1	2.22	0.53
8:H:84:LYS:HG3	24:H:2048:HOH:O	2.08	0.53
1:N:87:ILE:O	1:N:173:PRO:HD3	2.09	0.53
2:O:164:ALA:O	2:O:194:GLY:HA3	2.08	0.53
6:F:94:HIS:C	6:F:95:GLN:CG	2.77	0.53
1:A:282:PHE:N	7:T:4:ALA:HB1	2.24	0.53
8:H:43:MET:O	8:H:44:THR:C	2.47	0.53
2:B:13:THR:OG1	24:B:2007:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:8:GLN:HA	9:I:8:GLN:NE2	2.22	0.52
8:H:84:LYS:HG2	24:H:2048:HOH:O	2.08	0.52
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.91	0.52
12:Y:45:LEU:HD21	13:Z:40:TYR:CD1	2.44	0.52
4:Q:33:LEU:O	4:Q:38:LYS:HE2	2.09	0.52
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.91	0.52
11:X:42:PRO:HG2	11:X:47:ARG:HH21	1.74	0.52
20:C:1262:PEK:H102	20:C:1262:PEK:H162	1.91	0.52
12:Y:24:MET:HE2	12:Y:24:MET:N	2.22	0.52
4:D:11:TYR:C	4:D:11:TYR:CD1	2.82	0.52
4:D:31:LYS:HE3	24:D:2004:HOH:O	2.09	0.52
1:N:68:PHE:O	1:N:72:PRO:HG2	2.09	0.52
6:S:53:THR:CG2	6:S:54:ASN:N	2.55	0.52
2:B:91:ASN:O	2:B:92:ASN:HB2	2.09	0.52
1:A:358:LEU:HB3	14:A:516:HEA:HMA	1.91	0.52
4:D:98:TRP:CE3	23:M:1044:DMU:H12	2.45	0.52
2:B:82:ARG:HG2	2:B:86:MET:HE3	1.92	0.52
6:S:48:LEU:HG	6:S:92:VAL:HG11	1.91	0.52
1:N:76:GLY:O	1:N:80:ASN:HB2	2.09	0.52
4:Q:35:ALA:CB	24:Q:2019:HOH:O	2.55	0.52
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	1.92	0.52
7:T:11:TPO:O	7:T:11:TPO:HG23	2.08	0.52
4:Q:11:TYR:CD1	4:Q:11:TYR:C	2.83	0.52
8:H:60:TYR:C	8:H:60:TYR:CD1	2.82	0.52
4:Q:31:LYS:HB2	4:Q:31:LYS:NZ	2.26	0.51
1:N:362:SER:HA	2:O:87:MET:HE1	1.91	0.51
12:Y:47:LYS:HD2	24:Y:2006:HOH:O	1.83	0.51
9:V:25:PHE:CE1	9:V:29:LEU:HD22	2.45	0.51
1:N:211:THR:HG22	1:N:215:LEU:HD12	1.92	0.51
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.37	0.51
3:C:232:HIS:NE2	3:C:236:GLU:OE2	2.42	0.51
7:G:36:TRP:HA	7:G:36:TRP:CE3	2.45	0.51
13:M:42:LYS:O	13:M:42:LYS:HG3	2.10	0.51
2:B:1:MET:CE	2:B:133:LEU:HD11	2.26	0.51
9:V:68:ILE:C	9:V:68:ILE:CD1	2.77	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.51
4:Q:5:VAL:CG1	13:Z:4:LYS:HE2	2.29	0.51
1:N:309:THR:HG22	14:N:516:HEA:HMB2	1.93	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.46	0.51
4:Q:35:ALA:CA	24:Q:2019:HOH:O	2.58	0.51
4:D:98:TRP:CD2	23:M:1044:DMU:H12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.92	0.51
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.92	0.51
1:A:112:LEU:CG	24:A:2037:HOH:O	2.58	0.51
1:A:177:SER:H	1:A:180:GLN:HE21	1.57	0.51
5:R:67:ILE:O	5:R:70:VAL:HG12	2.11	0.51
1:N:215:LEU:CD1	20:P:1262:PEK:H262	2.39	0.50
1:A:282:PHE:N	7:T:4:ALA:CB	2.74	0.50
7:G:2:SER:O	7:G:3:ALA:HB3	2.08	0.50
1:N:112:LEU:CD2	1:N:113:LEU:HD23	2.41	0.50
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	1.92	0.50
2:O:114:GLU:CD	2:O:227:LEU:HD21	2.32	0.50
9:I:36:LYS:O	9:I:41:GLU:HG2	2.11	0.50
5:R:79:LYS:CA	5:R:79:LYS:HE3	2.25	0.50
6:F:92:VAL:O	6:F:92:VAL:CG2	2.59	0.50
1:A:136:LEU:CD1	24:A:2032:HOH:O	2.54	0.50
4:Q:7:LYS:O	4:Q:8:SER:C	2.50	0.50
1:A:417:MET:HE1	14:A:515:HEA:H263	1.93	0.50
3:P:213:THR:HB	21:P:1264:PGV:H11	1.94	0.50
4:Q:19:ARG:CD	4:Q:21:ASP:OD1	2.60	0.50
4:Q:107:ILE:CD1	11:X:39:GLU:CB	2.90	0.50
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.42	0.50
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.77	0.50
1:A:52:GLN:O	1:A:56:VAL:HG23	2.12	0.50
4:Q:48:TRP:O	4:Q:51:LEU:HD22	2.10	0.50
4:Q:7:LYS:N	24:Q:2002:HOH:O	2.40	0.50
11:K:42:PRO:CG	11:K:47:ARG:NH1	2.75	0.50
9:V:25:PHE:O	9:V:28:SER:HB2	2.11	0.50
4:D:131:ILE:HD13	9:I:47:TYR:CE2	2.46	0.50
5:R:79:LYS:NZ	24:R:2050:HOH:O	2.27	0.49
7:G:36:TRP:HE3	7:G:36:TRP:HA	1.77	0.49
7:T:35:SER:O	7:T:37:LEU:N	2.41	0.49
7:T:4:ALA:C	7:T:5:LYS:O	2.49	0.49
8:H:43:MET:O	8:H:45:ALA:N	2.45	0.49
2:B:129:LYS:CE	24:B:2059:HOH:O	1.89	0.49
7:T:36:TRP:HE3	7:T:36:TRP:N	2.11	0.49
8:U:84:LYS:HE2	8:U:84:LYS:O	2.11	0.49
5:R:49:ASP:OD2	24:R:2039:HOH:O	2.18	0.49
6:S:94:HIS:HD2	6:S:95:GLN:H	1.58	0.49
7:T:2:SER:O	7:T:3:ALA:CB	2.58	0.49
5:R:89:LEU:O	5:R:93:LEU:HG	2.13	0.49
1:A:208:MET:HG2	1:A:219:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.95	0.49
4:Q:6:VAL:HB	4:Q:10:ASP:OD1	2.13	0.49
7:T:3:ALA:O	7:T:4:ALA:HB2	2.13	0.49
1:A:310:MET:HE2	1:A:356:ILE:HG23	1.94	0.49
13:M:38:ASP:OD1	13:M:42:LYS:HB3	2.13	0.48
5:R:48:ILE:O	5:R:52:LEU:HG	2.13	0.48
10:W:30:ILE:O	10:W:34:VAL:HG23	2.13	0.48
5:R:90:ARG:NE	24:R:2053:HOH:O	2.24	0.48
4:Q:69:ALA:O	5:R:109:VAL:HG12	2.13	0.48
12:Y:20:ARG:NH2	12:Y:24:MET:HG2	2.29	0.48
3:P:76:GLN:HE21	3:P:233:PHE:HB2	1.78	0.48
4:Q:19:ARG:CG	4:Q:21:ASP:OD1	2.61	0.48
7:G:36:TRP:CA	7:G:36:TRP:CE3	2.96	0.48
7:G:39:SER:O	24:G:2014:HOH:O	2.20	0.48
8:H:78:GLU:HG2	8:H:78:GLU:O	2.12	0.48
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.77	0.48
4:D:11:TYR:CD1	4:D:12:ALA:N	2.81	0.48
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.48
1:N:65:MET:HB3	14:N:515:HEA:CAC	2.44	0.48
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.95	0.48
1:N:449:MET:SD	2:O:5:MET:CG	3.02	0.48
1:A:380:VAL:HG21	14:A:516:HEA:C3C	2.44	0.48
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.48	0.48
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.95	0.48
4:Q:51:LEU:HD22	4:Q:51:LEU:N	2.29	0.48
6:S:53:THR:HG22	6:S:54:ASN:HB2	1.96	0.48
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.51	0.48
12:Y:41:ARG:HD2	13:Z:40:TYR:OH	2.14	0.48
1:N:240:HIS:O	1:N:241:PRO:C	2.52	0.48
9:V:63:MET:HB3	9:V:68:ILE:CG1	2.44	0.47
14:A:515:HEA:H272	14:A:515:HEA:C16	2.44	0.47
2:B:14:SER:HB3	2:B:168:LEU:HD22	1.96	0.47
3:P:204:HIS:CE1	3:P:249:TRP:HB2	2.49	0.47
12:Y:39:ILE:O	12:Y:42:HIS:HB3	2.14	0.47
13:M:34:LEU:HA	13:M:37:LEU:HG	1.95	0.47
3:P:210:ILE:HG23	21:P:1264:PGV:H91	1.96	0.47
24:R:2006:HOH:O	9:V:10:ARG:HD3	2.14	0.47
2:B:29:MET:HG3	9:I:35:TYR:CD1	2.50	0.47
2:B:78:LEU:CB	2:B:79:PRO:CD	2.92	0.47
14:A:515:HEA:H272	14:A:515:HEA:H161	1.95	0.47
7:G:4:ALA:HB3	1:N:282:PHE:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:43:MET:HE3	8:U:49:ASP:N	2.29	0.47
2:O:148:MET:CE	2:O:216:LEU:HD22	2.45	0.47
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.96	0.47
4:Q:36:SER:N	24:Q:2019:HOH:O	2.46	0.47
8:U:38:ARG:NE	8:U:84:LYS:HE3	2.28	0.47
9:I:15:ARG:HH11	9:I:15:ARG:HB2	1.71	0.47
12:Y:46:LYS:CA	24:Y:2004:HOH:O	2.33	0.47
4:Q:9:GLU:CB	24:Q:2003:HOH:O	2.60	0.47
9:V:57:MET:O	9:V:61:GLU:HG2	2.14	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.49	0.47
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.47
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.15	0.47
2:B:68:LEU:CB	2:B:69:PRO:HD3	2.45	0.47
7:G:10:GLY:O	7:G:11:TPO:CB	2.42	0.47
1:N:321:PHE:CD2	2:O:65:TRP:HB2	2.49	0.47
10:J:4:ARG:HD2	10:J:7:GLU:OE2	2.15	0.47
4:Q:9:GLU:H	4:Q:9:GLU:CD	2.18	0.47
1:A:309:THR:CG2	14:A:516:HEA:HMB2	2.45	0.47
6:F:53:THR:HB	6:F:54:ASN:H	1.60	0.47
1:N:112:LEU:HD23	1:N:112:LEU:C	2.35	0.46
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.15	0.46
11:X:42:PRO:HG2	11:X:47:ARG:NH2	2.30	0.46
8:U:43:MET:CE	8:U:49:ASP:O	2.64	0.46
2:O:130:PRO:HB3	4:Q:118:LYS:HD3	1.96	0.46
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.96	0.46
4:Q:86:MET:CE	11:X:22:ALA:CA	2.74	0.46
14:A:515:HEA:H122	14:A:515:HEA:HHC	1.98	0.46
11:K:16:ALA:O	11:K:20:SER:OG	2.33	0.46
3:P:33:MET:HE1	10:W:52:TRP:CZ3	2.51	0.46
7:G:5:LYS:HA	1:N:190:ILE:HG12	1.97	0.46
7:T:11:TPO:O2P	7:T:16:TRP:CD1	2.68	0.46
1:N:309:THR:CG2	14:N:516:HEA:HMB2	2.45	0.46
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.96	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.46
8:U:60:TYR:OH	24:U:2018:HOH:O	2.19	0.46
8:U:43:MET:HE1	8:U:48:GLY:HA3	1.98	0.46
6:F:22:LEU:O	6:F:25:ARG:HB3	2.15	0.46
18:P:1265:CHD:H12	18:P:1265:CHD:H212	1.97	0.46
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.96	0.46
1:N:23:GLY:HA3	1:N:73:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:VAL:HG22	13:M:1:ILE:HD11	1.98	0.46
21:C:1263:PGV:H42	21:C:1263:PGV:H71	1.75	0.46
8:U:43:MET:HE2	8:U:49:ASP:O	2.15	0.46
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.97	0.46
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.50	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.96	0.46
13:M:13:LYS:O	13:M:13:LYS:HD2	2.16	0.46
1:A:364:ASP:OD1	14:A:516:HEA:O2A	2.33	0.46
4:Q:60:TYR:OH	4:Q:67:SER:HA	2.16	0.46
13:Z:37:LEU:HA	13:Z:37:LEU:HD23	1.78	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.46
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.98	0.46
6:F:5:GLY:N	24:F:2006:HOH:O	2.48	0.46
4:Q:44:GLU:O	5:R:56:ARG:NH2	2.39	0.46
6:S:95:GLN:O	6:S:96:LEU:HB3	2.15	0.46
1:N:58:VAL:CG2	14:N:515:HEA:HBA1	2.46	0.46
8:U:44:THR:C	8:U:45:ALA:O	2.54	0.46
12:L:2:HIS:ND1	12:L:3:TYR:N	2.53	0.46
9:I:35:TYR:C	9:I:37:PHE:H	2.19	0.46
8:U:37:HIS:HD2	24:U:2014:HOH:O	1.99	0.45
2:O:59:GLN:NE2	24:O:2024:HOH:O	2.49	0.45
4:Q:63:LYS:HB2	24:Q:2033:HOH:O	2.02	0.45
7:G:4:ALA:HB3	1:N:282:PHE:CA	2.45	0.45
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.16	0.45
3:C:76:GLN:O	3:C:80:ARG:HG3	2.17	0.45
11:X:13:TYR:O	11:X:14:GLY:C	2.53	0.45
1:A:240:HIS:O	1:A:243:VAL:HG22	2.16	0.45
7:T:84:LYS:H	7:T:84:LYS:HD2	1.81	0.45
1:A:148:PHE:HB3	3:C:28:THR:HB	1.98	0.45
9:V:41:GLU:OE1	9:V:41:GLU:N	2.50	0.45
4:D:139:ASP:HB2	24:D:2030:HOH:O	2.15	0.45
3:P:58:TRP:CG	21:P:1264:PGV:H41	2.52	0.45
2:B:113:TYR:HB2	24:B:2043:HOH:O	2.17	0.45
21:C:1264:PGV:H183	21:C:1264:PGV:H151	1.71	0.45
1:A:180:GLN:HB2	1:A:180:GLN:HE21	1.64	0.45
7:G:79:PRO:HD2	24:G:2030:HOH:O	2.17	0.45
4:Q:63:LYS:HG2	4:Q:64:PHE:CZ	2.51	0.45
7:T:8:HIS:O	7:T:10:GLY:N	2.50	0.45
4:Q:10:ASP:C	4:Q:12:ALA:N	2.71	0.45
7:G:37:LEU:CD2	7:G:38:HIS:ND1	2.74	0.45
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:120:THR:O	4:Q:124:LEU:HG	2.17	0.45
20:C:1262:PEK:H102	20:C:1262:PEK:C16	2.47	0.44
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.35	0.44
1:A:28:MET:HE1	14:A:515:HEA:H271	1.98	0.44
2:O:33:LEU:HD13	9:V:31:PHE:CD2	2.53	0.44
1:N:24:ALA:HA	14:N:515:HEA:H22	2.00	0.44
3:C:148:HIS:NE2	3:C:236:GLU:OE2	2.39	0.44
9:I:25:PHE:O	9:I:29:LEU:HD13	2.17	0.44
4:D:147:LYS:HB2	4:D:147:LYS:HE3	1.63	0.44
2:O:224:ALA:C	2:O:226:MET:H	2.21	0.44
14:A:515:HEA:HBC1	14:A:515:HEA:HMC1	1.99	0.44
1:A:450:TRP:CE3	1:A:450:TRP:HA	2.52	0.44
7:G:37:LEU:HG	7:G:38:HIS:ND1	2.32	0.44
9:I:36:LYS:HE3	9:I:36:LYS:HB2	1.57	0.44
6:F:4:GLY:HA2	24:F:2006:HOH:O	2.17	0.44
3:C:76:GLN:NE2	24:C:2039:HOH:O	2.46	0.44
4:Q:136:ALA:O	4:Q:146:LYS:HE3	2.17	0.44
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.97	0.44
10:W:29:ASN:H	10:W:29:ASN:HD22	1.63	0.44
18:A:1517:CHD:O26	3:C:103:HIS:ND1	2.51	0.44
1:N:175:ALA:HB2	6:S:35:ALA:HB1	2.00	0.44
3:C:246:ASP:HB2	24:C:2056:HOH:O	2.16	0.44
4:Q:93:ALA:O	4:Q:97:ILE:HG13	2.18	0.44
4:Q:107:ILE:HD12	11:X:39:GLU:HG2	1.99	0.44
20:C:1262:PEK:C10	20:C:1262:PEK:H162	2.47	0.44
4:Q:31:LYS:CB	4:Q:31:LYS:HZ3	2.31	0.44
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.00	0.44
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.53	0.44
9:I:15:ARG:NH1	9:I:15:ARG:HB2	2.23	0.44
4:Q:9:GLU:HB3	4:Q:12:ALA:HB3	1.99	0.44
6:F:4:GLY:CA	24:F:2006:HOH:O	2.65	0.44
1:N:492:LEU:HD22	6:S:71:TRP:CE2	2.53	0.44
7:G:7:ASP:O	7:G:8:HIS:C	2.54	0.44
2:O:218:TYR:CD2	24:V:2022:HOH:O	2.15	0.44
4:Q:6:VAL:CB	4:Q:10:ASP:OD1	2.66	0.44
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.69	0.44
1:N:373:VAL:HG22	14:N:516:HEA:HBA1	1.99	0.44
11:K:24:PHE:O	11:K:28:VAL:HG12	2.17	0.44
6:S:95:GLN:O	6:S:96:LEU:CB	2.66	0.43
4:Q:35:ALA:HA	4:Q:38:LYS:HD2	2.00	0.43
6:S:26:LYS:HB3	6:S:28:GLN:HE22	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:P:1263:PGV:H42	21:P:1263:PGV:H71	1.85	0.43
4:Q:31:LYS:HE2	4:Q:31:LYS:HB3	1.85	0.43
2:O:60:GLU:OE1	2:O:61:VAL:N	2.47	0.43
2:O:146:MET:HA	2:O:213:LEU:HD12	2.00	0.43
1:N:199:LEU:N	1:N:200:PRO:CD	2.81	0.43
1:A:197:LEU:HD11	7:T:2:SER:CB	2.48	0.43
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.54	0.43
2:O:91:ASN:ND2	2:O:92:ASN:N	2.60	0.43
7:G:2:SER:HB3	1:N:197:LEU:HD11	2.00	0.43
13:M:13:LYS:HE2	24:M:2004:HOH:O	2.18	0.43
7:T:41:HIS:HB3	7:T:74:ARG:CZ	2.48	0.43
4:Q:69:ALA:HB2	5:R:107:ASP:O	2.17	0.43
1:N:364:ASP:OD1	14:N:516:HEA:O2A	2.36	0.43
7:G:7:ASP:HA	1:N:178:GLN:HG2	2.01	0.43
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.99	0.43
4:Q:31:LYS:HB3	4:Q:31:LYS:NZ	2.31	0.43
3:P:50:ASN:ND2	3:P:54:MET:CE	2.81	0.43
1:N:177:SER:H	1:N:180:GLN:NE2	2.16	0.43
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.53	0.43
2:B:128:LEU:HD11	2:B:134:ARG:HA	2.00	0.43
1:N:131:PRO:O	1:N:132:LEU:C	2.57	0.43
13:Z:35:TYR:OH	23:Z:1043:DMU:C11	2.53	0.43
1:N:190:ILE:CD1	1:N:278:MET:HG2	2.49	0.43
1:N:190:ILE:HD13	1:N:278:MET:HG2	2.01	0.43
7:G:8:HIS:CD2	24:G:2002:HOH:O	2.71	0.43
1:N:53:ILE:HG23	1:N:54:TYR:N	2.34	0.43
7:G:7:ASP:OD1	7:G:7:ASP:C	2.56	0.43
6:S:53:THR:HG21	24:S:2024:HOH:O	2.19	0.43
2:O:91:ASN:C	2:O:91:ASN:HD22	2.22	0.43
1:A:377:PHE:HB2	14:A:516:HEA:HMD3	2.01	0.43
5:R:52:LEU:O	5:R:55:CYS:HB2	2.18	0.43
8:U:46:LYS:HA	8:U:46:LYS:HD3	1.79	0.42
3:P:29:SER:HB3	3:P:42:LEU:HD13	2.01	0.42
1:A:310:MET:CE	1:A:356:ILE:HG23	2.49	0.42
1:N:489:THR:HA	6:S:71:TRP:O	2.19	0.42
1:N:37:ILE:HG22	14:N:515:HEA:HMA	2.01	0.42
8:U:50:VAL:CG1	8:U:50:VAL:O	2.67	0.42
2:O:103:GLN:HA	2:O:104:TRP:HA	1.84	0.42
8:H:66:ILE:HG23	24:H:2034:HOH:O	2.18	0.42
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.00	0.42
7:G:67:HIS:HD2	7:G:71:HIS:CD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:1517:CHD:H12	18:N:1517:CHD:H212	2.02	0.42
3:P:3:HIS:CG	3:P:4:GLN:N	2.87	0.42
11:X:25:CYS:O	11:X:28:VAL:HG12	2.19	0.42
1:A:112:LEU:HD12	24:A:2037:HOH:O	2.18	0.42
2:B:170:LEU:HD23	24:B:2073:HOH:O	2.19	0.42
18:G:1085:CHD:H212	18:G:1085:CHD:H12	2.01	0.42
7:T:11:TPO:O	7:T:11:TPO:CG2	2.63	0.42
1:N:175:ALA:HB1	1:N:513:LEU:HD23	2.02	0.42
4:D:129:ALA:HB1	4:D:133:GLY:HA3	1.99	0.42
1:A:76:GLY:O	1:A:80:ASN:HB2	2.20	0.42
2:O:224:ALA:O	2:O:226:MET:N	2.53	0.42
12:L:44:LEU:C	12:L:46:LYS:H	2.23	0.42
24:A:2094:HOH:O	13:M:4:LYS:HG3	2.19	0.42
2:B:29:MET:HB2	9:I:35:TYR:CE1	2.55	0.42
5:E:82:TYR:N	5:E:83:PRO:CD	2.82	0.42
4:Q:102:TYR:CD1	13:Z:35:TYR:CE1	3.01	0.42
3:C:214:PHE:CD1	21:C:1264:PGV:H62	2.54	0.42
1:A:106:PRO:N	1:A:107:PRO:CD	2.82	0.42
11:X:28:VAL:HG13	11:X:29:TRP:N	2.34	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.42
3:P:129:VAL:N	3:P:130:PRO:CD	2.81	0.42
9:V:68:ILE:CD1	9:V:69:PHE:CZ	2.90	0.42
4:Q:9:GLU:N	4:Q:9:GLU:CD	2.72	0.42
4:Q:9:GLU:HG2	6:S:55:LYS:NZ	2.35	0.42
14:A:515:HEA:H261	14:A:515:HEA:H172	1.49	0.42
18:N:1517:CHD:H212	18:N:1517:CHD:H183	2.01	0.42
11:X:31:TYR:CD1	11:X:35:GLN:CG	3.03	0.42
3:C:29:SER:HB2	3:C:42:LEU:HD13	2.01	0.42
2:B:75:LEU:HA	2:B:75:LEU:HD12	1.84	0.42
8:H:17:ASP:OD1	8:H:17:ASP:C	2.58	0.42
2:B:91:ASN:OD1	2:B:183:THR:HG21	2.18	0.42
1:N:53:ILE:O	1:N:54:TYR:C	2.57	0.42
1:N:230:LEU:HD21	3:P:100:ALA:HA	2.02	0.42
1:A:176:MET:SD	1:A:181:THR:HG22	2.60	0.42
1:A:28:MET:HE2	14:A:515:HEA:H271	1.99	0.42
2:B:82:ARG:HG2	2:B:86:MET:CE	2.49	0.42
2:B:29:MET:HG3	9:I:35:TYR:CG	2.54	0.42
5:E:48:ILE:HG21	5:E:89:LEU:HD11	2.02	0.42
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.92	0.42
1:N:107:PRO:HB3	3:P:25:LEU:HB2	2.02	0.41
5:R:37:VAL:HG11	5:R:70:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:26:THR:HG21	13:Z:25:SER:HB3	1.96	0.41
8:U:84:LYS:CD	8:U:84:LYS:O	2.68	0.41
7:G:4:ALA:HB3	1:N:282:PHE:N	2.33	0.41
9:I:52:ARG:HB2	9:I:52:ARG:CZ	2.50	0.41
1:N:172:LYS:HD3	1:N:181:THR:HG21	2.01	0.41
4:Q:101:HIS:CD2	4:Q:102:TYR:CZ	3.08	0.41
12:Y:20:ARG:HH22	12:Y:24:MET:HG3	1.81	0.41
8:U:43:MET:CE	8:U:49:ASP:N	2.83	0.41
10:J:14:GLU:HG3	24:J:2012:HOH:O	2.17	0.41
20:P:1262:PEK:C10	20:P:1262:PEK:H161	2.27	0.41
20:P:1262:PEK:H262	20:P:1262:PEK:H231	1.37	0.41
14:N:515:HEA:H261	14:N:515:HEA:H172	1.75	0.41
9:I:8:GLN:HE22	9:I:10:ARG:H	1.67	0.41
13:Z:41:LYS:HB2	13:Z:42:LYS:H	1.53	0.41
9:V:73:LYS:C	9:V:73:LYS:HE2	2.34	0.41
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.18	0.41
4:Q:101:HIS:HD2	4:Q:102:TYR:CZ	2.39	0.41
4:D:70:GLU:O	4:D:73:ARG:NH1	2.54	0.41
2:B:60:GLU:CD	2:B:60:GLU:N	2.74	0.41
3:C:54:MET:HB3	3:C:58:TRP:CZ3	2.55	0.41
2:B:113:TYR:CB	24:B:2043:HOH:O	2.68	0.41
8:U:41:LYS:HG3	8:U:42:ALA:N	2.33	0.41
1:A:282:PHE:HA	7:T:4:ALA:HB2	1.94	0.41
1:A:281:GLY:O	7:T:4:ALA:HB1	2.21	0.41
2:B:66:THR:HG21	18:T:1085:CHD:H3	2.03	0.41
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.74	0.41
24:A:2079:HOH:O	12:L:7:PRO:HG3	2.20	0.41
2:O:9:PHE:HB2	2:O:21:LEU:HD21	2.03	0.41
14:N:515:HEA:HAA2	14:N:515:HEA:HHA	1.94	0.41
7:G:36:TRP:N	7:G:36:TRP:CE3	2.88	0.41
7:T:34:ASN:O	7:T:37:LEU:HB3	2.21	0.41
20:C:1262:PEK:C12	20:C:1262:PEK:H162	2.51	0.41
8:H:44:THR:O	8:H:45:ALA:O	2.38	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
1:N:440:TYR:HE1	2:O:204:HIS:CE1	2.39	0.41
6:S:26:LYS:CB	6:S:28:GLN:HE22	2.29	0.41
3:P:24:ALA:HB2	21:P:1263:PGV:C12	2.48	0.41
1:A:383:MET:O	1:A:387:PHE:CB	2.69	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.98	0.41
1:N:431:LEU:HA	1:N:431:LEU:HD23	1.92	0.41
8:H:41:LYS:HD3	24:H:2023:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:31:LYS:CE	24:R:2030:HOH:O	2.64	0.40
5:R:49:ASP:HB3	24:R:2039:HOH:O	2.20	0.40
2:O:153:LEU:HD23	2:O:181:GLN:HB2	2.03	0.40
18:C:1265:CHD:H12	18:C:1265:CHD:H212	2.03	0.40
2:O:102:HIS:O	2:O:104:TRP:HA	2.21	0.40
1:N:426:PHE:N	1:N:427:PRO:CD	2.84	0.40
2:O:93:PRO:HG3	2:O:151:ARG:HB2	2.02	0.40
1:A:426:PHE:HB3	1:A:427:PRO:HD3	2.03	0.40
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	2.02	0.40
4:Q:73:ARG:HB3	5:R:109:VAL:HG11	2.02	0.40
13:Z:42:LYS:HE3	13:Z:42:LYS:HA	1.62	0.40
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.56	0.40
9:V:29:LEU:HA	9:V:29:LEU:HD12	1.79	0.40
9:I:29:LEU:N	9:I:29:LEU:HD12	2.37	0.40
9:I:29:LEU:N	9:I:29:LEU:CD1	2.84	0.40
18:C:1265:CHD:H211	18:C:1265:CHD:H231	1.91	0.40
7:G:58:LYS:HA	7:G:59:PRO:HD3	1.90	0.40
3:P:193:TYR:C	3:P:193:TYR:CD1	2.95	0.40
8:U:54:GLU:O	8:U:55:TRP:C	2.59	0.40
2:O:151:ARG:HH11	2:O:151:ARG:HD2	1.79	0.40
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.56	0.40
7:G:25:LEU:N	7:G:26:PRO:CD	2.84	0.40
12:L:45:LEU:HA	12:L:45:LEU:HD23	1.87	0.40
7:T:33:LEU:HD13	7:T:33:LEU:C	2.41	0.40
9:V:63:MET:O	9:V:68:ILE:HG13	2.21	0.40
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.51	0.40
2:O:83:ILE:O	2:O:87:MET:HG3	2.22	0.40
1:N:379:TYR:O	1:N:383:MET:HB2	2.21	0.40
3:C:232:HIS:CD2	3:C:236:GLU:OE2	2.75	0.40
3:C:257:TYR:O	3:C:261:SER:HB3	2.21	0.40
2:B:42:ILE:HG22	2:B:46:LEU:HD12	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)
10:W:15:ASP:OD2	11:X:52:GLU:OE1[2_685]	2.16	0.04

## 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	511/514 (99%)	497 (97%)	13 (2%)	1 (0%)	52	43
1	N	511/514 (99%)	496 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	39	27
2	O	224/227 (99%)	209 (93%)	13 (6%)	2 (1%)	21	9
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/169 (84%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/169 (84%)	126 (89%)	13 (9%)	3 (2%)	9	2
5	E	102/152 (67%)	101 (99%)	1 (1%)	0	100	100
5	R	102/152 (67%)	101 (99%)	1 (1%)	0	100	100
6	F	91/129 (70%)	87 (96%)	2 (2%)	2 (2%)	8	2
6	S	91/129 (70%)	87 (96%)	2 (2%)	2 (2%)	8	2
7	G	81/97 (84%)	69 (85%)	7 (9%)	5 (6%)	2	0
7	T	81/97 (84%)	65 (80%)	6 (7%)	10 (12%)	0	0
8	H	73/86 (85%)	68 (93%)	0	5 (7%)	1	0
8	U	73/86 (85%)	66 (90%)	4 (6%)	3 (4%)	3	0
9	I	69/74 (93%)	66 (96%)	3 (4%)	0	100	100
9	V	69/74 (93%)	64 (93%)	5 (7%)	0	100	100
10	J	55/80 (69%)	55 (100%)	0	0	100	100
10	W	55/80 (69%)	55 (100%)	0	0	100	100
11	K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
11	X	47/80 (59%)	42 (89%)	4 (8%)	1 (2%)	9	2
12	L	44/63 (70%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
13	M	41/70 (59%)	39 (95%)	1 (2%)	1 (2%)	7	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	40/70 (57%)	35 (88%)	4 (10%)	1 (2%)	7	1
All	All	3474/4004 (87%)	3314 (95%)	123 (4%)	37 (1%)	17	6

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	GLN
6	F	95	GLN
7	G	3	ALA
7	G	8	HIS
8	H	43	MET
8	H	45	ALA
8	H	46	LYS
13	M	42	LYS
4	Q	8	SER
4	Q	9	GLU
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	5	LYS
7	T	7	ASP
7	T	43	GLU
8	U	45	ALA
8	U	46	LYS
13	Z	41	LYS
7	G	7	ASP
8	H	47	GLY
7	G	2	SER
7	G	4	ALA
8	H	44	THR
7	T	41	HIS
7	T	36	TRP
7	T	37	LEU
6	F	94	HIS
2	O	59	GLN
4	Q	108	PRO
7	T	9	GLY
2	O	92	ASN
7	T	6	GLY
8	U	47	GLY
1	A	384	GLY

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Mol	Chain	Res	Type
11	X	7	PRO

### 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	426/427 (100%)	418 (98%)	8 (2%)	65	58
1	N	426/427 (100%)	417 (98%)	9 (2%)	61	53
2	B	211/211 (100%)	200 (95%)	11 (5%)	29	13
2	O	210/211 (100%)	200 (95%)	10 (5%)	31	15
3	C	224/226 (99%)	219 (98%)	5 (2%)	60	51
3	P	224/226 (99%)	221 (99%)	3 (1%)	76	72
4	D	128/148 (86%)	127 (99%)	1 (1%)	86	85
4	Q	128/148 (86%)	124 (97%)	4 (3%)	47	34
5	E	91/123 (74%)	90 (99%)	1 (1%)	80	77
5	R	91/123 (74%)	89 (98%)	2 (2%)	60	51
6	F	79/103 (77%)	76 (96%)	3 (4%)	40	25
6	S	79/103 (77%)	74 (94%)	5 (6%)	22	8
7	G	66/78 (85%)	58 (88%)	8 (12%)	6	1
7	T	67/78 (86%)	60 (90%)	7 (10%)	9	2
8	H	67/76 (88%)	65 (97%)	2 (3%)	48	36
8	U	67/76 (88%)	62 (92%)	5 (8%)	17	5
9	I	56/59 (95%)	53 (95%)	3 (5%)	27	12
9	V	56/59 (95%)	52 (93%)	4 (7%)	18	6
10	J	48/68 (71%)	47 (98%)	1 (2%)	61	53
10	W	48/68 (71%)	47 (98%)	1 (2%)	61	53
11	K	39/66 (59%)	37 (95%)	2 (5%)	29	13
11	X	39/66 (59%)	37 (95%)	2 (5%)	29	13
12	L	39/55 (71%)	37 (95%)	2 (5%)	29	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Y	39/55 (71%)	37 (95%)	2 (5%)	29	13
13	M	37/57 (65%)	33 (89%)	4 (11%)	8	2
13	Z	36/57 (63%)	34 (94%)	2 (6%)	26	11
All	All	3021/3394 (89%)	2914 (96%)	107 (4%)	43	29

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
2	B	1	MET
2	B	54	SER
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	29	SER
3	C	127	LEU
3	C	159	MET
3	C	161	GLN
3	C	214	PHE
4	D	51	LEU
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU
6	F	53	THR
7	G	7	ASP
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU

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Mol	Chain	Res	Type
7	G	36	TRP
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	27	ARG
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	50	LEU
11	K	47	ARG
11	K	54	ARG
12	L	46	LYS
12	L	47	LYS
13	M	4	LYS
13	M	34	LEU
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	128	VAL
1	N	138	HIS
1	N	180	GLN
1	N	189	MET
1	N	278	MET
1	N	369	ASP
1	N	485	VAL
2	O	33	LEU
2	O	60	GLU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	116	LEU
2	O	225	SER
2	O	227	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	9	GLU
4	Q	10	ASP

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Mol	Chain	Res	Type
4	Q	31	LYS
4	Q	51	LEU
5	R	79	LYS
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	2	SER
7	T	17	ARG
7	T	18	PHE
7	T	36	TRP
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	29	CYS
8	U	41	LYS
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	18	ARG
9	V	29	LEU
9	V	41	GLU
9	V	73	LYS
10	W	50	LEU
11	X	51	LYS
11	X	54	ARG
12	Y	20	ARG
12	Y	24	MET
13	Z	34	LEU
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	22	HIS
2	B	91	ASN

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Mol	Chain	Res	Type
2	B	181	GLN
3	C	68	GLN
3	C	161	GLN
4	D	37	GLN
4	D	143	ASN
5	E	94	ASN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
9	I	8	GLN
9	I	53	ASN
10	J	29	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
3	P	149	HIS
3	P	161	GLN
3	P	207	HIS
3	P	230	ASN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	28	GLN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
9	V	20	HIS
10	W	29	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 ⓘ

2 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	$\# Z  > 2$
7	TPO	G	11	7	8,10,11	0.62	0	7,14,16	1.48	0
7	TPO	T	11	7	8,10,11	0.62	0	7,14,16	1.39	0

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
7	TPO	G	11	7	-	1/8/11/13	0/0/0/0
7	TPO	T	11	7	-	1/8/11/13	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	11	TPO	P-OG1-CB-CA
7	T	11	TPO	P-OG1-CB-CA

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	5	0
7	T	11	TPO	5	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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$
16	OXY	A	1515	15,14	1,1,1	0.82	0	0,0,0	0.00	-
18	CHD	A	1517	-	29,32,32	0.75	1 (3%)	48,51,51	1.21	6 (12%)
14	HEA	A	515	1	40,67,67	1.14	4 (10%)	41,103,103	2.81	17 (41%)
14	HEA	A	516	1,16	40,67,67	1.12	6 (15%)	41,103,103	2.38	10 (24%)
19	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
20	PEK	C	1262	-	51,52,52	0.82	2 (3%)	52,57,57	1.02	3 (5%)
21	PGV	C	1263	-	50,50,50	0.87	2 (4%)	51,56,56	1.08	3 (5%)
21	PGV	C	1264	-	50,50,50	0.88	2 (4%)	51,56,56	0.96	4 (7%)
18	CHD	C	1265	-	29,32,32	0.71	0	48,51,51	1.24	6 (12%)
18	CHD	G	1085	-	29,32,32	0.70	0	48,51,51	1.24	5 (10%)
23	DMU	M	1044	-	34,34,34	1.34	1 (2%)	45,45,45	2.13	11 (24%)
16	OXY	N	1515	15,14	1,1,1	0.72	0	0,0,0	0.00	-
18	CHD	N	1517	-	29,32,32	0.69	1 (3%)	48,51,51	1.05	4 (8%)
14	HEA	N	515	1	40,67,67	1.13	4 (10%)	41,103,103	2.62	18 (43%)
14	HEA	N	516	1,16	40,67,67	1.00	3 (7%)	41,103,103	2.67	16 (39%)
19	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
20	PEK	P	1262	-	51,52,52	0.85	2 (3%)	52,57,57	1.07	4 (7%)
21	PGV	P	1263	-	50,50,50	0.87	2 (4%)	51,56,56	1.23	4 (7%)
21	PGV	P	1264	-	50,50,50	0.85	3 (6%)	51,56,56	0.98	4 (7%)
18	CHD	P	1265	-	29,32,32	0.69	0	48,51,51	1.37	11 (22%)
18	CHD	T	1085	-	29,32,32	0.61	0	48,51,51	1.41	6 (12%)
23	DMU	Z	1043	-	34,34,34	1.34	1 (2%)	45,45,45	1.90	7 (15%)

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
16	OXY	A	1515	15,14	-	0/0/0/0	0/0/0/0
18	CHD	A	1517	-	-	0/7/74/74	0/4/4/4
14	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1,16	3/3/7/16	0/24/76/76	0/0/8/8
19	CUA	B	228	2	-	0/0/0/0	0/0/0/0
20	PEK	C	1262	-	-	0/56/56/56	0/0/0/0
21	PGV	C	1263	-	-	0/55/55/55	0/0/0/0
21	PGV	C	1264	-	-	0/55/55/55	0/0/0/0
18	CHD	C	1265	-	-	0/7/74/74	0/4/4/4
18	CHD	G	1085	-	-	0/7/74/74	0/4/4/4
23	DMU	M	1044	-	4/4/10/10	0/19/59/59	0/2/2/2
16	OXY	N	1515	15,14	-	0/0/0/0	0/0/0/0
18	CHD	N	1517	-	-	0/7/74/74	0/4/4/4
14	HEA	N	515	1	3/3/7/16	1/24/76/76	0/0/8/8
14	HEA	N	516	1,16	3/3/7/16	0/24/76/76	0/0/8/8
19	CUA	O	228	2	-	0/0/0/0	0/0/0/0
20	PEK	P	1262	-	-	0/56/56/56	0/0/0/0
21	PGV	P	1263	-	-	0/55/55/55	0/0/0/0
21	PGV	P	1264	-	-	0/55/55/55	0/0/0/0
18	CHD	P	1265	-	-	0/7/74/74	0/4/4/4
18	CHD	T	1085	-	-	0/7/74/74	0/4/4/4
23	DMU	Z	1043	-	4/4/10/10	0/19/59/59	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	1044	DMU	C3-C4	-7.43	1.32	1.52
23	Z	1043	DMU	C3-C4	-7.40	1.32	1.52
18	A	1517	CHD	C10-C5	-2.41	1.51	1.55
21	P	1264	PGV	O01-C02	-2.07	1.41	1.46
18	N	1517	CHD	C13-C14	-2.06	1.51	1.55
14	A	516	HEA	C1D-ND	2.09	1.39	1.36
14	N	515	HEA	C1A-NA	2.16	1.39	1.36
14	A	516	HEA	C18-C19	2.18	1.37	1.33
14	N	516	HEA	C3D-C2D	2.30	1.44	1.37
14	N	515	HEA	C3D-C2D	2.30	1.44	1.37
14	A	516	HEA	C4B-NB	2.35	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	C3D-C2D	2.53	1.45	1.37
14	A	515	HEA	C3D-C2D	2.54	1.45	1.37
14	A	515	HEA	C3A-C2A	2.58	1.43	1.40
14	A	516	HEA	C3C-C2C	2.58	1.43	1.40
14	N	515	HEA	C3C-C2C	2.64	1.43	1.40
14	N	516	HEA	C3A-C2A	2.67	1.43	1.40
14	N	516	HEA	C3C-C2C	3.15	1.44	1.40
14	A	516	HEA	C3A-C2A	3.20	1.44	1.40
20	P	1262	PEK	O01-C1	3.26	1.44	1.34
14	A	515	HEA	C4B-NB	3.30	1.41	1.36
21	P	1264	PGV	O01-C1	3.31	1.44	1.34
21	C	1263	PGV	O01-C1	3.36	1.44	1.34
20	C	1262	PEK	O03-C21	3.49	1.43	1.33
14	A	515	HEA	C3C-C2C	3.54	1.45	1.40
20	C	1262	PEK	O01-C1	3.54	1.44	1.34
20	P	1262	PEK	O03-C21	3.56	1.44	1.33
21	P	1264	PGV	O03-C19	3.56	1.44	1.33
21	C	1264	PGV	O01-C1	3.58	1.45	1.34
21	C	1264	PGV	O03-C19	3.59	1.44	1.33
21	P	1263	PGV	O01-C1	3.77	1.45	1.34
21	P	1263	PGV	O03-C19	3.80	1.44	1.33
21	C	1263	PGV	O03-C19	4.06	1.45	1.33
14	N	515	HEA	C3A-C2A	4.46	1.46	1.40

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	515	HEA	C1A-C2A-C3A	-7.59	99.48	107.07
14	A	516	HEA	C1A-C2A-C3A	-7.49	99.57	107.07
14	A	515	HEA	C1A-C2A-C3A	-6.91	100.15	107.07
14	N	516	HEA	C1A-C2A-C3A	-6.48	100.59	107.07
14	A	515	HEA	CAA-CBA-CGA	-5.92	101.89	112.75
14	N	516	HEA	CAA-CBA-CGA	-5.75	102.21	112.75
14	A	515	HEA	OMA-CMA-C3A	-5.74	113.50	125.11
14	A	516	HEA	CAA-CBA-CGA	-5.72	102.27	112.75
14	N	516	HEA	CMC-C2C-C1C	-5.66	119.01	128.36
14	A	516	HEA	C13-C12-C11	-5.57	107.11	114.51
14	N	515	HEA	OMA-CMA-C3A	-5.11	114.79	125.11
23	M	1044	DMU	O16-C6-C1	-4.66	102.15	108.04
14	N	515	HEA	CMB-C2B-C1B	-4.46	120.99	128.36
14	N	516	HEA	CAD-CBD-CGD	-4.37	104.75	112.75
14	A	516	HEA	CMC-C2C-C1C	-4.15	121.50	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	1085	CHD	C18-C13-C12	-3.98	105.21	109.09
14	A	515	HEA	CMC-C2C-C1C	-3.88	121.94	128.36
14	N	515	HEA	CAA-CBA-CGA	-3.74	105.89	112.75
21	P	1263	PGV	C03-C02-C01	-3.53	103.81	112.07
14	N	516	HEA	OMA-CMA-C3A	-3.34	118.36	125.11
18	C	1265	CHD	C5-C4-C3	-3.32	107.97	112.91
14	A	515	HEA	C20-C21-C22	-3.22	103.26	111.69
14	N	516	HEA	CMB-C2B-C1B	-3.20	123.08	128.36
18	P	1265	CHD	C6-C5-C4	-3.12	107.57	111.05
21	C	1263	PGV	O03-C19-O04	-2.98	115.79	123.49
14	N	515	HEA	CBD-CAD-C3D	-2.96	107.22	112.53
14	N	516	HEA	C13-C12-C11	-2.95	110.59	114.51
20	C	1262	PEK	O03-C01-C02	-2.94	100.79	108.69
18	C	1265	CHD	C23-C22-C20	-2.92	111.31	114.75
14	N	515	HEA	C13-C14-C15	-2.91	121.44	127.76
18	G	1085	CHD	C10-C9-C8	-2.87	108.74	111.88
14	A	516	HEA	OMA-CMA-C3A	-2.86	119.33	125.11
18	A	1517	CHD	C11-C9-C10	-2.85	110.83	113.79
21	P	1263	PGV	O03-C19-O04	-2.84	116.15	123.49
18	A	1517	CHD	C5-C4-C3	-2.84	108.69	112.91
18	A	1517	CHD	C1-C2-C3	-2.84	105.83	110.43
23	Z	1043	DMU	C10-O7-C3	-2.83	110.61	118.01
18	N	1517	CHD	C5-C4-C3	-2.82	108.71	112.91
14	N	516	HEA	C3C-CAC-CBC	-2.81	120.56	126.32
18	P	1265	CHD	O12-C12-C13	-2.74	106.67	111.11
18	P	1265	CHD	C17-C13-C12	-2.68	115.30	117.68
20	P	1262	PEK	O01-C1-O02	-2.68	116.49	123.67
21	P	1264	PGV	O03-C19-O04	-2.66	116.62	123.49
14	N	515	HEA	C27-C19-C18	-2.64	118.32	123.50
14	N	515	HEA	C17-C18-C19	-2.64	122.03	127.76
18	A	1517	CHD	C6-C5-C10	-2.63	109.75	112.66
18	A	1517	CHD	C4-C5-C10	-2.61	109.78	112.66
14	N	516	HEA	C13-C14-C15	-2.56	122.19	127.76
14	A	515	HEA	C13-C12-C11	-2.55	111.12	114.51
14	A	515	HEA	CBD-CAD-C3D	-2.52	108.02	112.53
20	P	1262	PEK	O03-C01-C02	-2.51	101.93	108.69
18	G	1085	CHD	O12-C12-C13	-2.47	107.11	111.11
14	N	515	HEA	C26-C15-C14	-2.46	118.68	123.50
18	C	1265	CHD	C19-C10-C5	-2.44	105.94	110.25
14	A	515	HEA	C26-C15-C14	-2.44	118.72	123.50
14	N	515	HEA	C13-C12-C11	-2.42	111.30	114.51
14	N	515	HEA	CAD-CBD-CGD	-2.41	108.33	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	1085	CHD	C6-C5-C4	-2.41	108.36	111.05
18	G	1085	CHD	C6-C5-C4	-2.38	108.39	111.05
18	G	1085	CHD	C13-C17-C20	-2.35	116.64	119.50
18	P	1265	CHD	C14-C8-C9	-2.34	106.41	109.62
14	N	515	HEA	CMC-C2C-C1C	-2.33	124.50	128.36
18	T	1085	CHD	C19-C10-C5	-2.32	106.15	110.25
18	P	1265	CHD	C5-C4-C3	-2.26	109.55	112.91
18	G	1085	CHD	C11-C9-C10	-2.24	111.47	113.79
21	C	1264	PGV	O03-C19-O04	-2.24	117.72	123.49
18	P	1265	CHD	C13-C17-C20	-2.22	116.80	119.50
14	A	515	HEA	C17-C16-C15	-2.16	105.69	112.71
18	P	1265	CHD	C23-C22-C20	-2.15	112.22	114.75
23	M	1044	DMU	O7-C10-C5	-2.11	102.98	108.10
18	P	1265	CHD	C13-C14-C8	-2.10	112.05	114.75
18	C	1265	CHD	C10-C9-C8	-2.08	109.60	111.88
21	P	1264	PGV	O01-C1-O02	-2.08	118.10	123.67
18	N	1517	CHD	C1-C10-C9	-2.08	108.10	111.45
18	T	1085	CHD	C5-C4-C3	-2.07	109.84	112.91
18	C	1265	CHD	O12-C12-C13	-2.06	107.77	111.11
14	A	515	HEA	C13-C14-C15	-2.05	123.31	127.76
18	P	1265	CHD	C14-C8-C7	-2.04	108.92	111.74
23	M	1044	DMU	C6-C1-C2	2.01	113.94	109.97
14	A	515	HEA	C12-C11-C3B	2.03	116.78	112.59
18	N	1517	CHD	C15-C14-C13	2.08	105.66	103.60
23	M	1044	DMU	C8-C7-C5	2.12	114.75	110.79
18	A	1517	CHD	C13-C17-C20	2.17	122.14	119.50
21	C	1264	PGV	O14-P-O13	2.19	124.37	112.53
23	Z	1043	DMU	C6-C1-C2	2.26	114.42	109.97
14	A	516	HEA	CMD-C2D-C3D	2.27	129.99	125.24
18	N	1517	CHD	C1-C10-C5	2.32	111.61	107.81
18	P	1265	CHD	C16-C17-C13	2.37	105.96	103.60
18	C	1265	CHD	C9-C10-C5	2.38	112.19	108.67
20	C	1262	PEK	O01-C1-C2	2.39	116.71	111.53
18	P	1265	CHD	C15-C14-C13	2.41	105.99	103.60
14	A	515	HEA	CMD-C2D-C3D	2.43	130.33	125.24
21	C	1264	PGV	O01-C1-C2	2.48	116.92	111.53
14	A	516	HEA	CAA-C2A-C1A	2.48	129.71	127.01
14	N	515	HEA	C12-C11-C3B	2.56	117.90	112.59
21	P	1264	PGV	O03-C19-C20	2.66	120.00	111.90
14	A	516	HEA	CAD-C3D-C4D	2.71	129.95	127.01
14	N	516	HEA	C26-C15-C16	2.73	119.58	115.41
18	T	1085	CHD	C6-C7-C8	2.73	114.37	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	516	HEA	C27-C19-C20	2.75	119.61	115.41
14	A	516	HEA	C27-C19-C20	2.82	119.72	115.41
23	M	1044	DMU	O1-C9-C11	2.88	113.65	106.36
14	N	516	HEA	CAD-C3D-C4D	2.95	130.21	127.01
21	C	1264	PGV	O03-C19-C20	2.96	120.92	111.90
20	C	1262	PEK	C01-O03-C21	2.97	125.16	116.85
14	A	515	HEA	C16-C17-C18	2.98	119.49	111.69
21	P	1264	PGV	O01-C1-C2	2.99	118.03	111.53
23	M	1044	DMU	C10-C5-C7	3.05	115.98	109.97
21	C	1263	PGV	O01-C1-C2	3.10	118.26	111.53
14	A	515	HEA	C27-C19-C20	3.11	120.16	115.41
20	P	1262	PEK	O01-C1-C2	3.15	118.37	111.53
14	N	516	HEA	CAA-C2A-C1A	3.17	130.45	127.01
14	N	516	HEA	CMB-C2B-C3B	3.28	131.84	125.14
14	N	515	HEA	C27-C19-C20	3.36	120.54	115.41
14	N	516	HEA	CMD-C2D-C3D	3.40	132.35	125.24
21	P	1263	PGV	O01-C1-C2	3.42	118.97	111.53
20	P	1262	PEK	C01-O03-C21	3.50	126.62	116.85
23	M	1044	DMU	O7-C3-C4	3.51	118.53	109.32
14	N	515	HEA	CMC-C2C-C3C	3.67	132.26	125.09
23	Z	1043	DMU	O7-C3-C4	3.67	118.96	109.32
21	C	1263	PGV	O03-C19-C20	3.71	123.19	111.90
18	T	1085	CHD	C17-C13-C12	3.73	120.98	117.68
14	N	515	HEA	CMB-C2B-C3B	3.74	132.80	125.14
21	P	1263	PGV	O03-C19-C20	3.75	123.32	111.90
14	N	515	HEA	CBA-CAA-C2A	3.81	119.35	112.53
14	N	515	HEA	CMD-C2D-C3D	4.24	134.11	125.24
23	Z	1043	DMU	O5-C4-C3	4.28	118.78	109.75
23	M	1044	DMU	C2-C3-C4	4.46	120.92	110.84
14	A	516	HEA	CMC-C2C-C3C	4.51	133.91	125.09
23	M	1044	DMU	O5-C4-C3	4.51	119.28	109.75
14	A	515	HEA	CMC-C2C-C3C	4.63	134.15	125.09
23	Z	1043	DMU	C2-C3-C4	4.70	121.46	110.84
23	Z	1043	DMU	O7-C3-C2	4.80	119.57	107.17
23	M	1044	DMU	O7-C3-C2	5.18	120.54	107.17
14	A	515	HEA	CBA-CAA-C2A	5.67	122.68	112.53
14	N	516	HEA	CMC-C2C-C3C	5.90	136.64	125.09
23	M	1044	DMU	O5-C4-C57	6.27	122.19	106.36
14	A	515	HEA	CAA-C2A-C1A	6.32	133.87	127.01
23	Z	1043	DMU	O5-C4-C57	6.60	123.03	106.36

All (20) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
23	M	1044	DMU	C2
23	M	1044	DMU	C3
23	M	1044	DMU	C5
23	M	1044	DMU	C4
23	Z	1043	DMU	C2
23	Z	1043	DMU	C3
23	Z	1043	DMU	C5
23	Z	1043	DMU	C4
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
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

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	N	515	HEA	C19-C18-C17-C16

There are no ring outliers.

18 monomers are involved in 103 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1517	CHD	1	0
14	A	515	HEA	16	0
14	A	516	HEA	6	0
20	C	1262	PEK	10	0
21	C	1263	PGV	1	0
21	C	1264	PGV	5	0
18	C	1265	CHD	2	0
18	G	1085	CHD	1	0
23	M	1044	DMU	2	0
18	N	1517	CHD	2	0
14	N	515	HEA	17	0
14	N	516	HEA	6	0
20	P	1262	PEK	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	P	1263	PGV	4	0
21	P	1264	PGV	7	0
18	P	1265	CHD	1	0
18	T	1085	CHD	1	0
23	Z	1043	DMU	8	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%)	0.46	13 (2%) 61 71	24, 29, 36, 56	0
1	N	513/514 (99%)	0.39	16 (3%) 52 62	27, 37, 50, 106	0
2	B	227/227 (100%)	0.11	4 (1%) 71 80	24, 35, 54, 67	0
2	O	226/227 (99%)	0.13	6 (2%) 58 68	32, 46, 82, 136	0
3	C	259/261 (99%)	-0.06	1 (0%) 93 95	27, 35, 50, 114	0
3	P	259/261 (99%)	-0.05	3 (1%) 81 87	29, 37, 55, 122	0
4	D	144/169 (85%)	-0.15	2 (1%) 78 85	30, 38, 64, 99	0
4	Q	144/169 (85%)	0.88	20 (13%) 4 6	40, 59, 91, 210	0
5	E	104/152 (68%)	0.28	8 (7%) 16 25	31, 39, 67, 110	0
5	R	104/152 (68%)	0.60	4 (3%) 44 56	36, 49, 79, 109	0
6	F	93/129 (72%)	0.42	4 (4%) 39 50	29, 40, 83, 243	0
6	S	93/129 (72%)	0.33	4 (4%) 39 50	32, 43, 89, 168	0
7	G	83/97 (85%)	0.95	15 (18%) 2 2	30, 42, 138, 172	0
7	T	83/97 (85%)	1.05	18 (21%) 1 1	30, 47, 146, 256	0
8	H	75/86 (87%)	0.73	12 (16%) 3 4	31, 44, 88, 166	0
8	U	75/86 (87%)	0.78	11 (14%) 3 5	38, 51, 99, 141	0
9	I	71/74 (95%)	0.89	9 (12%) 5 8	31, 47, 90, 126	0
9	V	71/74 (95%)	1.02	6 (8%) 13 21	37, 59, 90, 106	0
10	J	57/80 (71%)	0.55	7 (12%) 5 9	34, 44, 81, 95	0
10	W	57/80 (71%)	0.68	10 (17%) 2 3	38, 50, 100, 127	0
11	K	49/80 (61%)	0.06	0 100 100	33, 43, 70, 118	0
11	X	49/80 (61%)	1.36	15 (30%) 1 0	49, 58, 84, 125	0
12	L	46/63 (73%)	-0.07	1 (2%) 65 74	27, 37, 58, 137	0
12	Y	46/63 (73%)	0.15	2 (4%) 39 50	37, 50, 89, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/70 (61%)	0.71	5 (11%) 6 10	28, 37, 122, 212	0
13	Z	42/70 (60%)	0.79	8 (19%) 2 2	44, 54, 120, 171	0
All	All	3526/4004 (88%)	0.38	204 (5%) 26 37	24, 39, 81, 256	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	13.2
13	M	43	SER	12.6
6	F	95	GLN	11.1
6	F	96	LEU	11.0
4	Q	4	SER	9.9
13	Z	42	LYS	9.8
7	T	10	GLY	8.3
6	S	96	LEU	8.0
8	U	46	LYS	7.9
7	G	42	ARG	7.7
9	I	37	PHE	7.4
7	G	1	ALA	7.2
13	M	42	LYS	7.0
4	Q	5	VAL	6.9
7	G	41	HIS	6.1
7	T	42	ARG	6.0
13	Z	40	TYR	6.0
8	H	44	THR	5.9
13	M	41	LYS	5.8
7	T	36	TRP	5.7
8	U	48	GLY	5.6
7	G	84	LYS	5.5
9	V	37	PHE	5.5
5	E	109	VAL	5.4
5	R	109	VAL	5.4
8	U	45	ALA	5.3
4	Q	7	LYS	5.2
7	G	3	ALA	5.2
11	X	13	TYR	5.1
8	H	48	GLY	5.0
10	W	52	TRP	5.0
13	M	40	TYR	5.0
8	H	45	ALA	5.0
7	T	41	HIS	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	Q	53	ILE	4.8
7	G	40	GLY	4.8
9	I	26	MET	4.5
8	H	43	MET	4.5
7	T	3	ALA	4.4
11	X	7	PRO	4.4
3	P	38	ASN	4.4
4	Q	147	LYS	4.4
2	O	113	TYR	4.3
7	G	2	SER	4.3
6	F	94	HIS	4.3
6	S	94	HIS	4.2
8	H	46	LYS	4.2
8	H	47	GLY	4.2
8	U	49	ASP	4.2
12	Y	47	LYS	4.1
11	X	6	ALA	4.1
13	Z	39	ASN	4.1
7	T	40	GLY	4.1
9	I	25	PHE	4.1
7	T	39	SER	4.1
8	U	44	THR	4.0
7	T	1	ALA	3.9
11	X	19	ALA	3.9
5	R	96	LEU	3.8
7	G	10	GLY	3.7
7	T	84	LYS	3.7
8	U	50	VAL	3.7
9	V	26	MET	3.7
9	I	36	LYS	3.6
8	H	50	VAL	3.6
8	H	52	VAL	3.6
10	W	1	PHE	3.6
7	T	2	SER	3.6
11	X	23	THR	3.6
7	T	43	GLU	3.5
9	I	29	LEU	3.5
8	U	42	ALA	3.5
1	N	70	VAL	3.5
10	J	1	PHE	3.5
9	I	33	THR	3.5
11	X	27	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
4	Q	58	GLU	3.4
7	G	8	HIS	3.4
5	E	7	THR	3.4
8	U	47	GLY	3.4
9	V	34	PHE	3.4
4	Q	48	TRP	3.3
7	G	36	TRP	3.3
2	B	91	ASN	3.3
7	G	43	GLU	3.3
8	H	42	ALA	3.3
8	U	43	MET	3.3
12	L	47	LYS	3.3
7	G	37	LEU	3.2
4	Q	51	LEU	3.2
9	I	34	PHE	3.2
2	B	59	GLN	3.2
13	Z	13	LYS	3.2
13	Z	32	TRP	3.2
10	W	57	HIS	3.2
13	Z	35	TYR	3.1
6	S	93	PRO	3.1
9	V	53	ASN	3.1
11	X	36	ILE	3.0
7	G	39	SER	3.0
1	A	126	TRP	3.0
4	Q	140	TYR	3.0
13	Z	41	LYS	3.0
7	T	8	HIS	3.0
2	O	91	ASN	2.9
9	V	33	THR	2.9
4	Q	138	TRP	2.9
2	O	61	VAL	2.9
8	U	52	VAL	2.9
13	Z	37	LEU	2.9
8	H	49	ASP	2.9
11	X	16	ALA	2.9
7	T	5	LYS	2.9
4	Q	30	VAL	2.8
1	A	246	LEU	2.8
1	N	246	LEU	2.8
1	A	66	ILE	2.8
1	N	66	ILE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	W	55	PHE	2.8
2	B	60	GLU	2.8
4	Q	128	VAL	2.7
4	Q	46	ALA	2.7
8	U	51	SER	2.7
4	D	147	LYS	2.7
1	A	202	LEU	2.7
12	Y	45	LEU	2.7
2	O	130	PRO	2.7
5	E	9	GLU	2.6
1	A	389	ILE	2.6
5	E	6	GLU	2.6
3	P	37	PHE	2.6
1	A	195	LEU	2.6
10	W	56	PRO	2.6
5	E	11	PHE	2.6
6	S	95	GLN	2.6
2	O	227	LEU	2.6
11	X	24	PHE	2.6
10	J	5	VAL	2.6
4	Q	97	ILE	2.5
7	T	38	HIS	2.5
11	X	18	LEU	2.5
10	J	52	TRP	2.5
1	N	58	VAL	2.5
1	A	75	ILE	2.5
7	T	37	LEU	2.5
1	A	235	PHE	2.4
4	Q	33	LEU	2.4
10	W	26	ALA	2.4
1	A	247	ILE	2.4
10	W	30	ILE	2.4
4	D	4	SER	2.4
11	X	17	VAL	2.3
10	J	57	HIS	2.3
1	N	62	ALA	2.3
4	Q	8	SER	2.3
3	P	182	TYR	2.3
6	F	42	THR	2.3
1	A	248	LEU	2.3
5	R	52	LEU	2.3
11	X	35	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
9	I	52	ARG	2.3
5	R	11	PHE	2.3
9	I	4	LEU	2.2
8	H	53	CYS	2.2
1	N	247	ILE	2.2
1	N	248	LEU	2.2
1	N	128	VAL	2.2
5	E	19	PHE	2.2
1	N	389	ILE	2.2
10	W	4	ARG	2.2
7	T	33	LEU	2.2
1	N	282	PHE	2.2
10	J	55	PHE	2.2
4	Q	59	LEU	2.2
8	H	85	ILE	2.1
11	X	47	ARG	2.1
3	C	38	ASN	2.1
10	J	26	ALA	2.1
1	N	78	PHE	2.1
9	V	29	LEU	2.1
10	W	2	GLU	2.1
10	W	48	TYR	2.1
5	E	13	ALA	2.1
1	N	193	VAL	2.1
7	G	38	HIS	2.1
1	A	388	ALA	2.1
1	N	197	LEU	2.1
4	Q	124	LEU	2.1
1	A	243	VAL	2.1
4	Q	47	SER	2.1
5	E	10	GLU	2.1
2	B	57	ASP	2.1
1	N	245	ILE	2.0
1	N	251	PHE	2.0
11	X	9	PHE	2.0
7	T	4	ALA	2.0
7	T	46	ALA	2.0
1	A	396	TRP	2.0
7	G	6	GLY	2.0
1	N	514	LYS	2.0
13	M	39	ASN	2.0
2	O	217	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
11	X	20	SER	2.0
10	J	2	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
7	TPO	G	11	11/12	0.58	0.34	-	73,140,486,493	0
7	TPO	T	11	11/12	0.68	0.39	-	65,143,410,489	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
16	OXY	A	1515	2/2	0.90	0.20	2.21	32,32,32,41	0
21	PGV	P	1264	51/51	0.95	0.14	1.95	28,43,86,192	0
23	DMU	Z	1043	33/33	0.84	0.20	1.58	42,72,127,190	0
23	DMU	M	1044	33/33	0.91	0.14	1.48	35,51,76,92	0
19	CUA	O	228	2/2	0.96	0.13	1.02	39,39,39,40	0
19	CUA	B	228	2/2	0.99	0.14	0.96	28,28,28,30	0
20	PEK	P	1262	53/53	0.94	0.14	0.92	35,52,149,483	0
20	PEK	C	1262	53/53	0.95	0.14	0.92	30,48,94,136	0
21	PGV	C	1263	51/51	0.97	0.14	0.91	26,46,86,132	0
14	HEA	N	516	60/60	0.97	0.17	0.70	21,31,40,48	0
18	CHD	A	1517	29/29	0.96	0.13	0.69	25,32,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
14	HEA	N	515	60/60	0.97	0.17	0.69	25,38,64,319	0
21	PGV	P	1263	51/51	0.97	0.12	0.46	30,48,80,146	0
18	CHD	C	1265	29/29	0.96	0.15	0.42	37,51,65,68	0
18	CHD	N	1517	29/29	0.97	0.13	0.37	27,37,42,44	0
21	PGV	C	1264	51/51	0.96	0.10	0.28	24,37,97,273	0
22	ZN	F	1097	1/1	1.00	0.10	0.25	35,35,35,35	0
14	HEA	A	515	60/60	0.98	0.16	0.13	19,26,49,53	0
14	HEA	A	516	60/60	0.98	0.13	-0.25	21,26,34,35	0
18	CHD	P	1265	29/29	0.94	0.15	-0.27	38,57,66,74	0
22	ZN	S	1097	1/1	0.99	0.09	-0.37	39,39,39,39	0
18	CHD	G	1085	29/29	0.98	0.09	-0.42	27,35,48,63	0
18	CHD	T	1085	29/29	0.97	0.08	-0.88	26,31,46,51	0
17	MG	N	1516	1/1	0.94	0.09	-1.01	35,35,35,35	0
17	MG	A	1516	1/1	0.99	0.08	-2.55	26,26,26,26	0
16	OXY	N	1515	2/2	0.95	0.09	-3.71	31,31,31,33	0
15	CU	N	517	1/1	0.99	0.16	-	32,32,32,32	0
15	CU	A	517	1/1	0.99	0.15	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.