



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:25 AM GMT

PDB ID : 3AG1  
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 280 K  
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2010-03-19  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

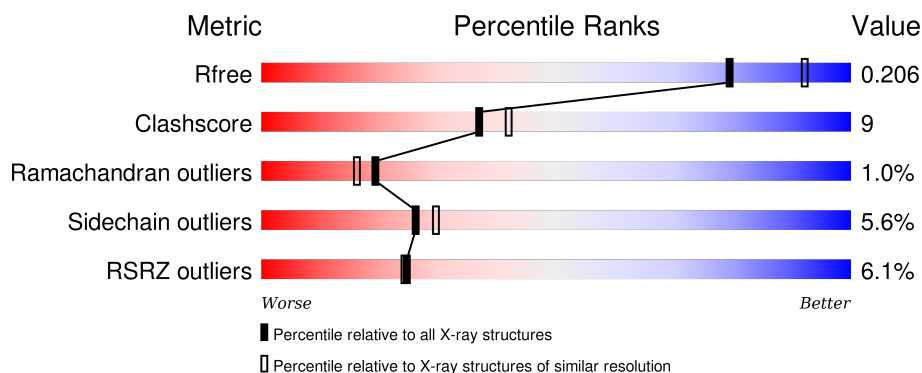
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



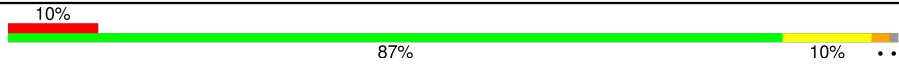
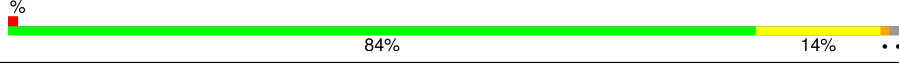
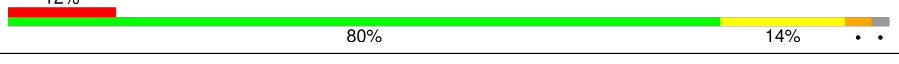


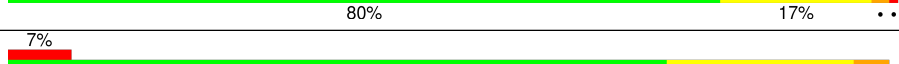
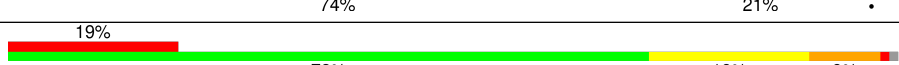
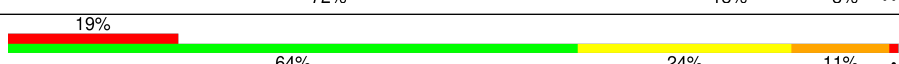
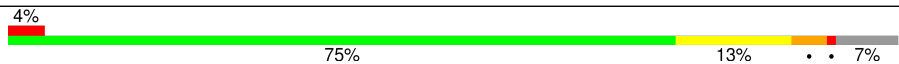
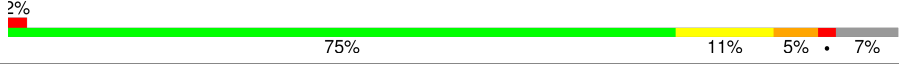

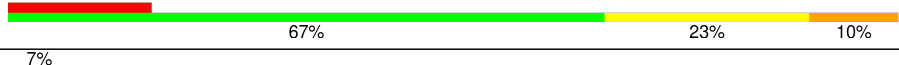
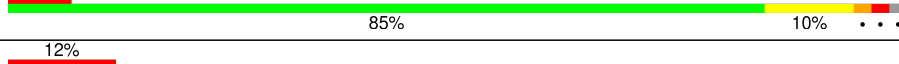

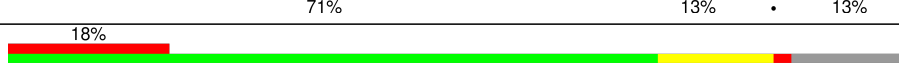





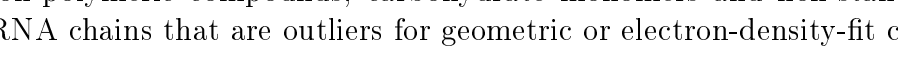
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>85%</div> <div>13%</div> <div>•</div> </div>
1	N	514	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>•</div> </div>
2	B	227	<div> <div>68%</div> <div>27%</div> <div>• •</div> </div>
2	O	227	<div> <div>4%</div> <div>75%</div> <div>19%</div> <div>5%</div> </div>
3	C	261	<div> <div>8%</div> <div>87%</div> <div>10%</div> <div>• •</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	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	-	-	-
17	MG	A	518	-	-	-	X
18	NA	N	519	-	-	-	X
19	TGL	A	523	-	-	-	X
19	TGL	B	521	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1521	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	N	1523	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	C	268	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	PSC	B	229	-	-	-	X
22	PSC	R	1229	-	-	-	X
23	CHD	B	1085	X	-	-	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	P	1525	-	-	-	X
23	CHD	W	1059	X	-	-	X
25	CDL	C	270	-	-	X	X
25	CDL	G	269	-	-	X	X
25	CDL	P	1270	-	-	-	X
25	CDL	T	1269	-	-	X	X
26	DMU	C	272	X	-	-	X
26	DMU	M	526	X	-	-	-
26	DMU	T	1272	X	-	-	X
26	DMU	Z	1526	X	-	-	-
27	ZN	F	99	-	-	-	X
28	PEK	G	1263	-	-	-	X
28	PEK	T	263	-	-	-	X

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 32105 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

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

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

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

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

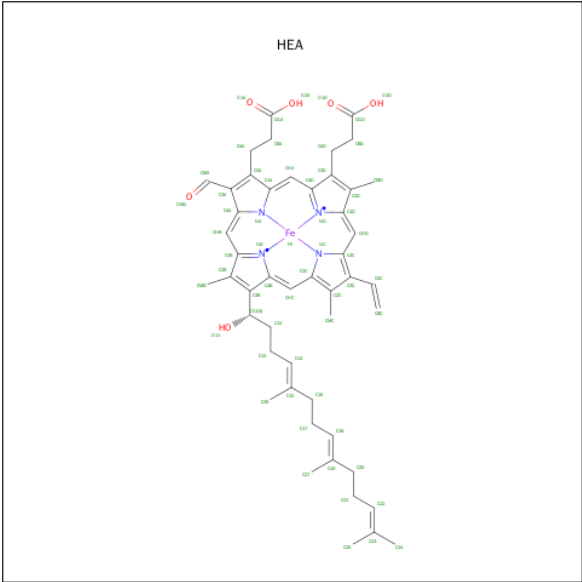
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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

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

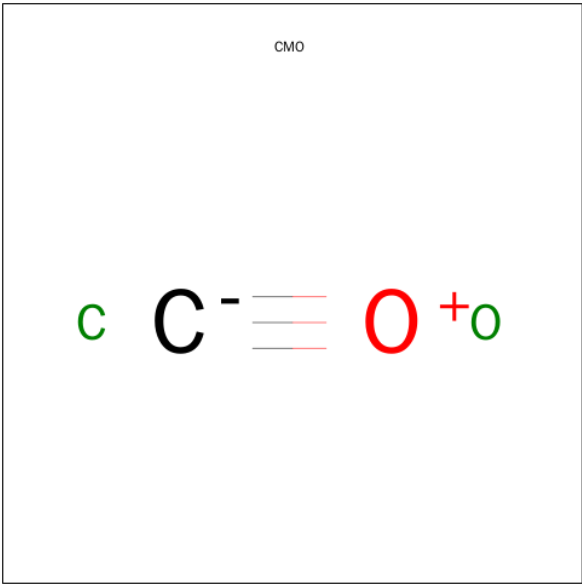
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	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 CARBON MONOXIDE (three-letter code: CMO) (formula: CO).





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

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

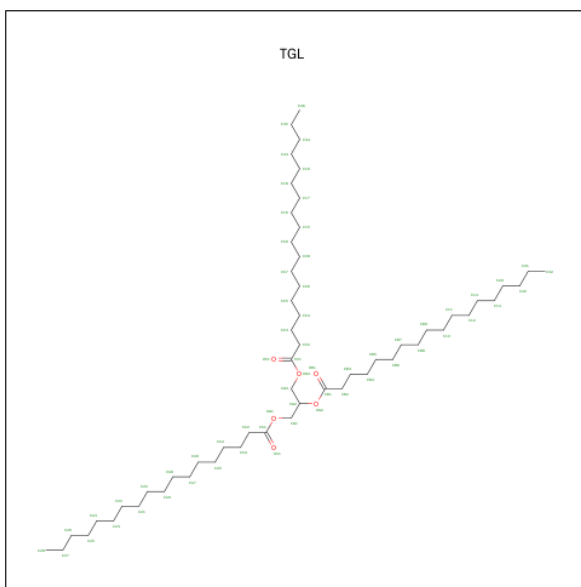
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

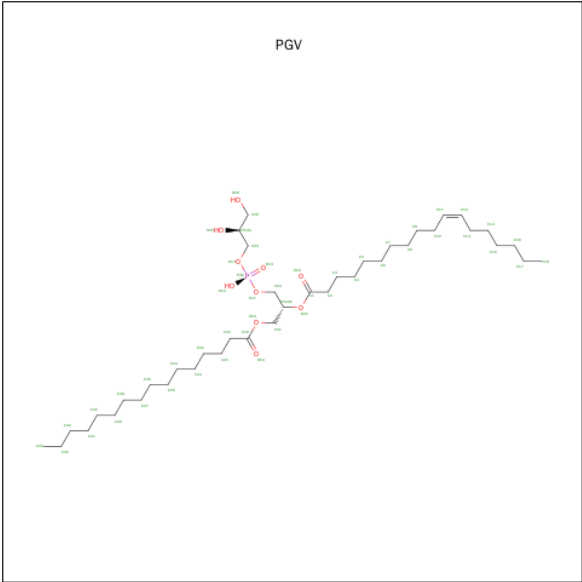
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



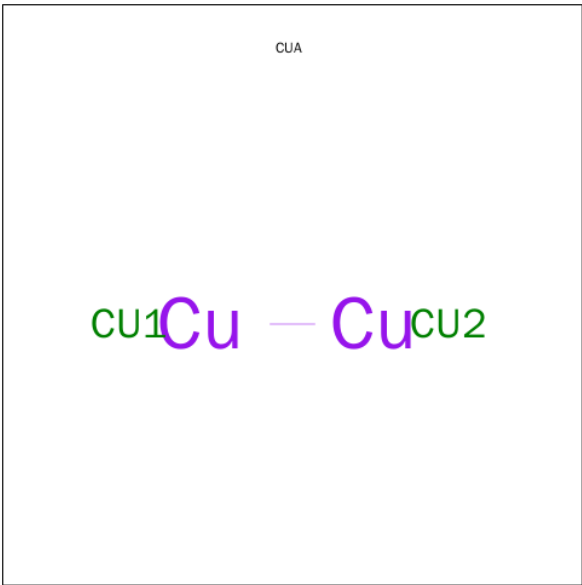
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



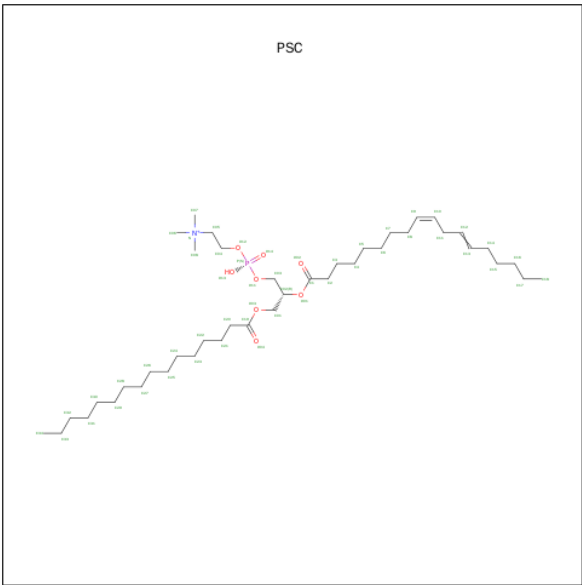
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

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



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

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



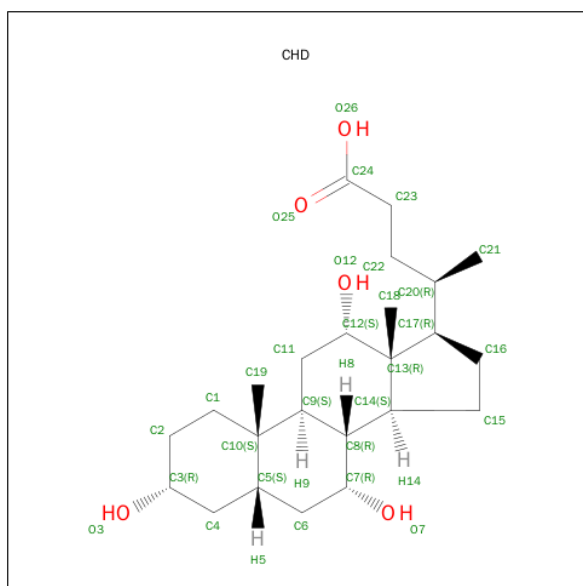
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).

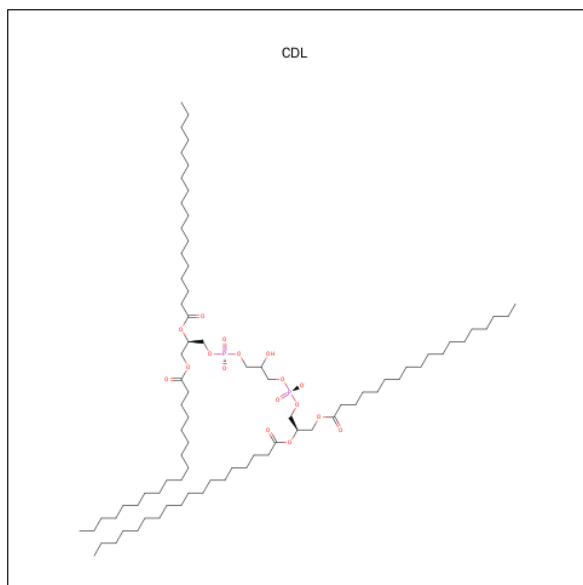


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total 29	C 24	O 5	0	0
23	C	1	Total 29	C 24	O 5	0	0
23	C	1	Total 29	C 24	O 5	0	0
23	J	1	Total 29	C 24	O 5	0	0
23	O	1	Total 29	C 24	O 5	0	0
23	P	1	Total 29	C 24	O 5	0	0
23	P	1	Total 29	C 24	O 5	0	0
23	W	1	Total 29	C 24	O 5	0	0

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

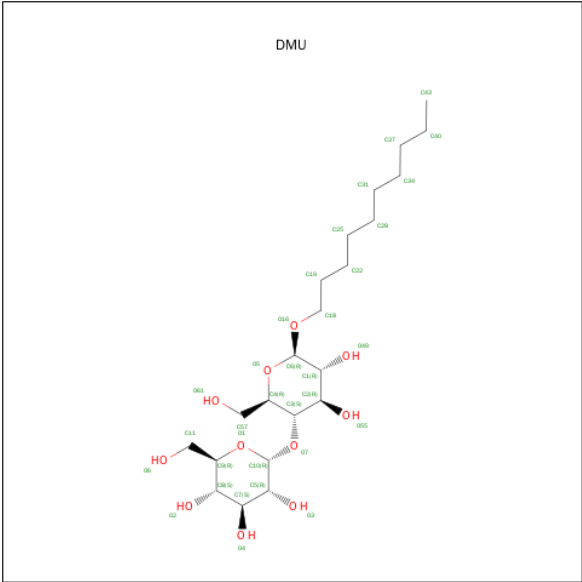
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 26 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula:  $C_{22}H_{42}O_{11}$ ).

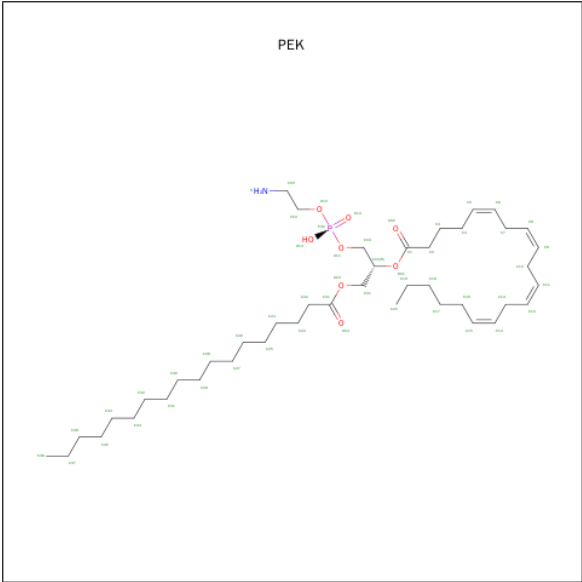


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	M	1	Total	C	O	0	0
			33	22	11		
26	T	1	Total	C	O	0	0
			33	22	11		
26	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 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
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	S	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	205	Total	O	0	0
			205	205		
29	B	121	Total	O	0	0
			121	121		
29	C	80	Total	O	0	0
			80	80		
29	D	75	Total	O	0	0
			75	75		
29	E	39	Total	O	0	0
			39	39		
29	F	70	Total	O	0	0
			70	70		

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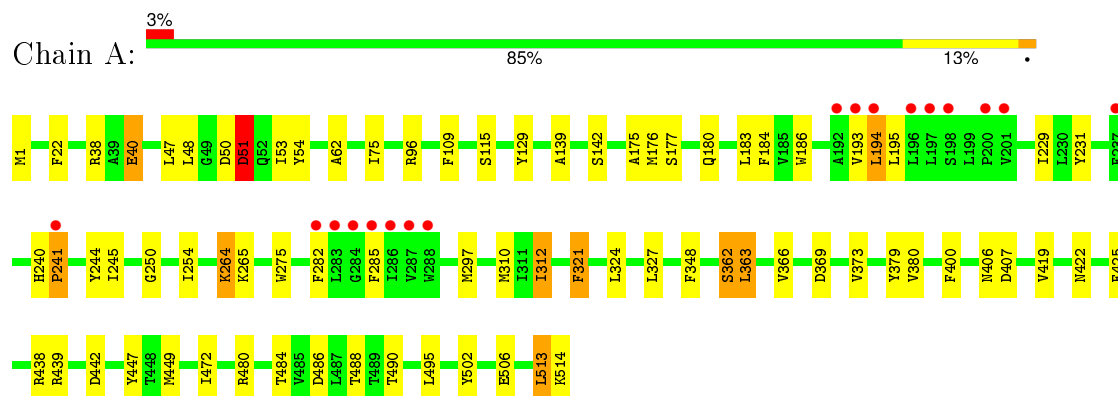
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	G	42	Total 42	O 42	0	0
29	H	33	Total 33	O 33	0	0
29	I	24	Total 24	O 24	0	0
29	J	9	Total 9	O 9	0	0
29	K	17	Total 17	O 17	0	0
29	L	20	Total 20	O 20	0	0
29	M	15	Total 15	O 15	0	0
29	N	184	Total 184	O 184	0	0
29	O	97	Total 97	O 97	0	0
29	P	81	Total 81	O 81	0	0
29	Q	47	Total 47	O 47	0	0
29	R	27	Total 27	O 27	0	0
29	S	52	Total 52	O 52	0	0
29	T	37	Total 37	O 37	0	0
29	U	28	Total 28	O 28	0	0
29	V	17	Total 17	O 17	0	0
29	W	12	Total 12	O 12	0	0
29	X	12	Total 12	O 12	0	0
29	Y	16	Total 16	O 16	0	0
29	Z	9	Total 9	O 9	0	0

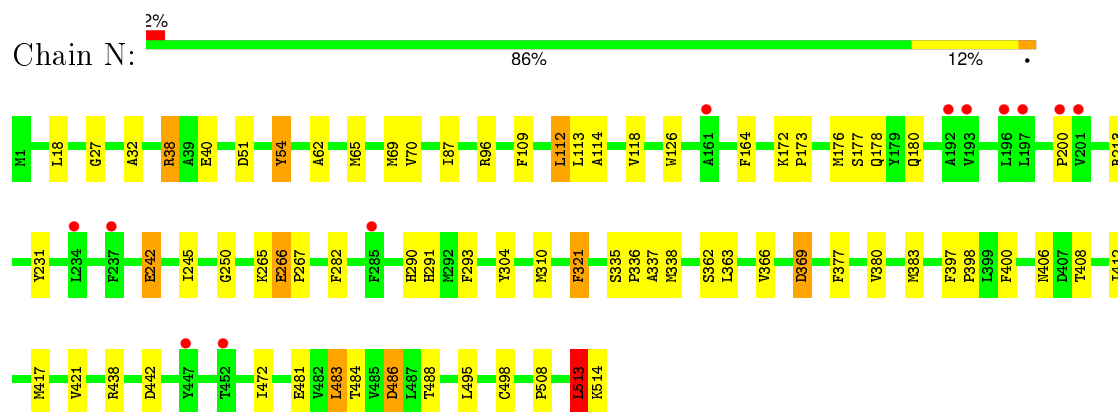
### 3 Residue-property plots [i](#)

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.

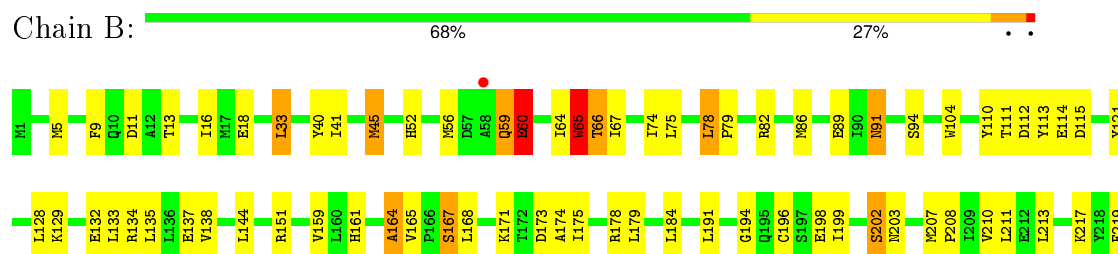
#### • Molecule 1: Cytochrome c oxidase subunit 1



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

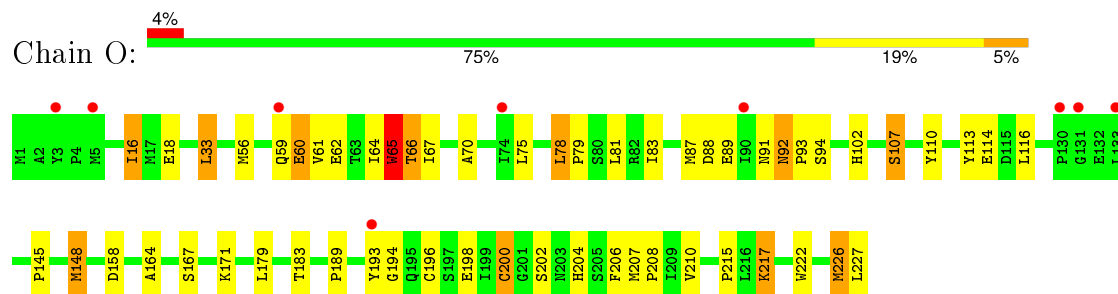


#### • Molecule 2: Cytochrome c oxidase subunit 2

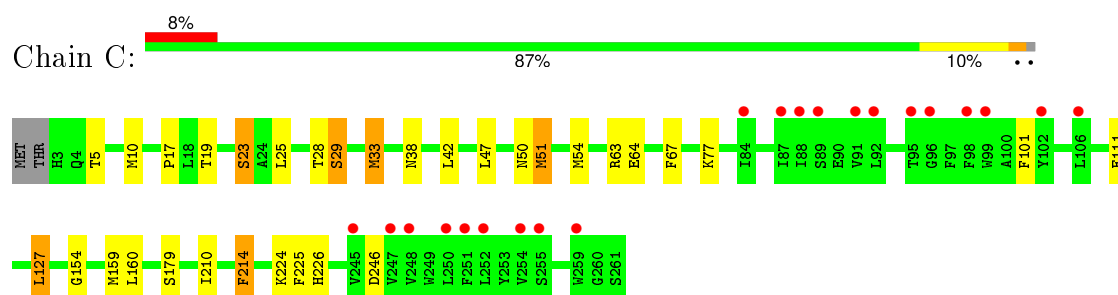




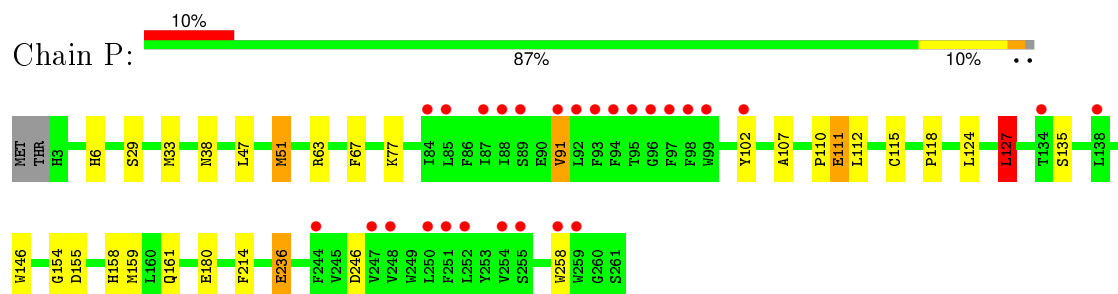
• Molecule 2: Cytochrome c oxidase subunit 2



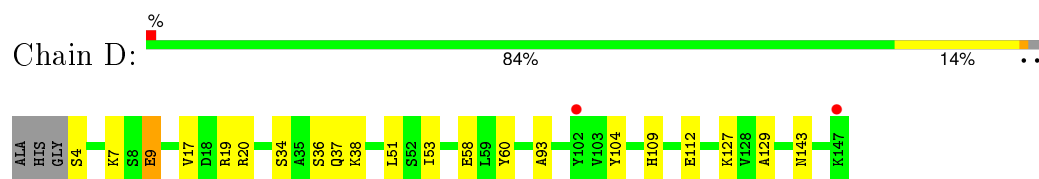
• Molecule 3: Cytochrome c oxidase subunit 3



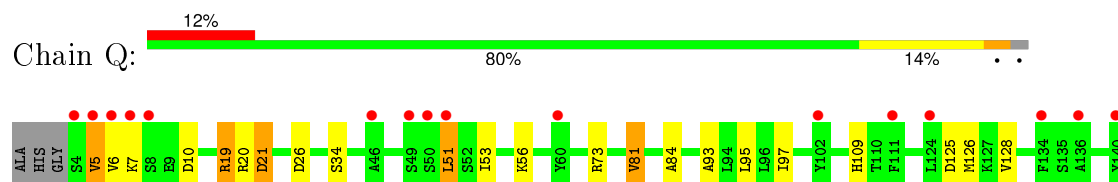
• Molecule 3: Cytochrome c oxidase subunit 3

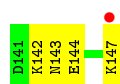


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



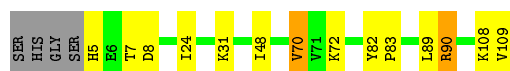
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1





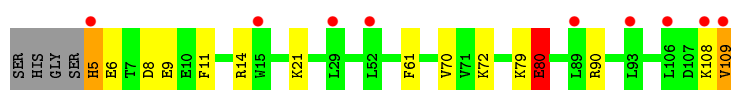
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 83% 11% ..



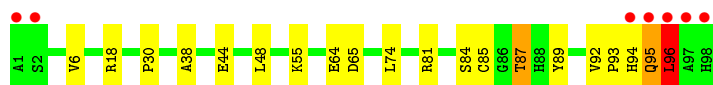
- Molecule 5: Cytochrome c oxidase subunit 5A

Chain R: 8% 83% 11% ..



- Molecule 6: Cytochrome c oxidase subunit 5B

Chain F: 7% 80% 17% ..



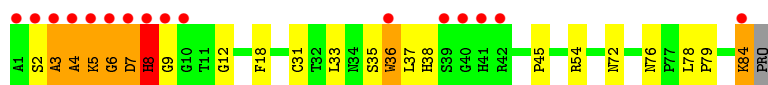
- Molecule 6: Cytochrome c oxidase subunit 5B

Chain S: 7% 74% 21% .



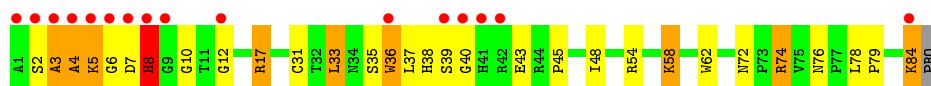
- Molecule 7: Cytochrome c oxidase subunit 6A2

Chain G: 19% 72% 18% 8% ..



- Molecule 7: Cytochrome c oxidase subunit 6A2

Chain T: 19% 64% 24% 11% ..

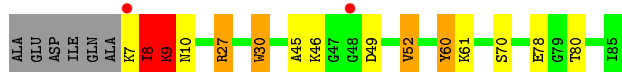
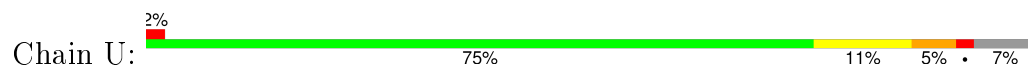


- Molecule 8: Cytochrome c oxidase subunit 6B1

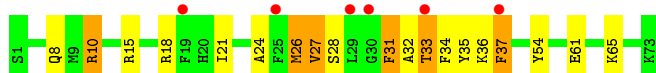
Chain H: 4% 75% 13% . . 7%



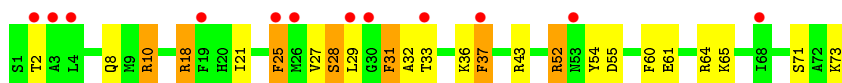
- Molecule 8: Cytochrome c oxidase subunit 6B1



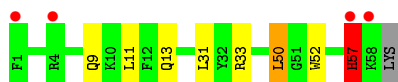
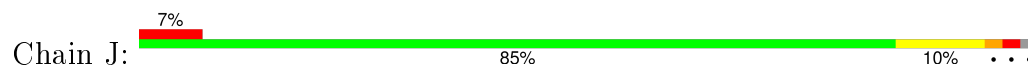
- Molecule 9: Cytochrome c oxidase subunit 6C



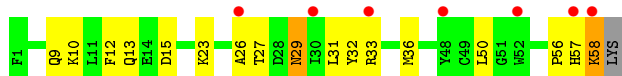
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1

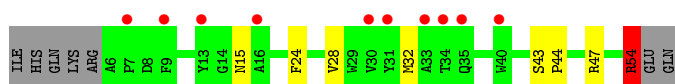


- Molecule 11: Cytochrome c oxidase subunit 7B

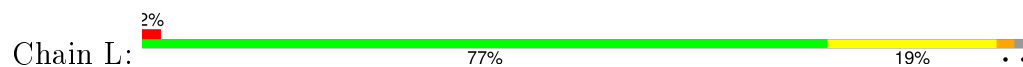


- Molecule 11: Cytochrome c oxidase subunit 7B

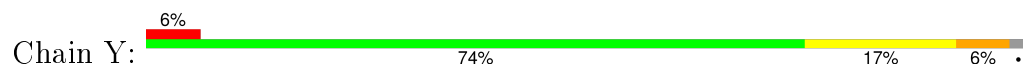




- Molecule 12: Cytochrome c oxidase subunit 7C



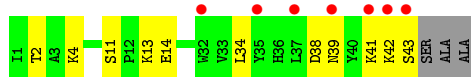
- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	189.49Å 210.89Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 94.75 – 2.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.20) 99.2 (94.75-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, $R_{free}$	0.162 , 0.192 0.178 , 0.206	Depositor DCC
$R_{free}$ test set	17411 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 61.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 352235 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	32105	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: CMO, ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, TGL, PGV, TPO, UNX, CUA, NA, FME, CU, DMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.52	24/4156 (0.6%)	1.14	17/5678 (0.3%)
1	N	1.30	13/4156 (0.3%)	1.00	9/5678 (0.2%)
2	B	1.52	17/1860 (0.9%)	1.22	15/2534 (0.6%)
2	O	1.19	5/1860 (0.3%)	1.02	3/2534 (0.1%)
3	C	1.44	6/2197 (0.3%)	1.00	2/3005 (0.1%)
3	P	1.26	7/2197 (0.3%)	0.96	4/3005 (0.1%)
4	D	1.42	8/1229 (0.7%)	1.12	1/1658 (0.1%)
4	Q	1.10	2/1229 (0.2%)	0.98	6/1658 (0.4%)
5	E	1.26	2/871 (0.2%)	1.07	3/1182 (0.3%)
5	R	1.03	2/871 (0.2%)	0.93	1/1182 (0.1%)
6	F	1.47	3/765 (0.4%)	1.25	4/1038 (0.4%)
6	S	1.25	2/765 (0.3%)	1.09	3/1038 (0.3%)
7	G	1.38	2/690 (0.3%)	1.12	3/937 (0.3%)
7	T	1.43	4/690 (0.6%)	1.09	4/937 (0.4%)
8	H	1.29	1/682 (0.1%)	1.01	1/921 (0.1%)
8	U	1.09	1/682 (0.1%)	0.94	0/921
9	I	1.45	3/605 (0.5%)	1.13	3/802 (0.4%)
9	V	1.31	2/605 (0.3%)	1.10	4/802 (0.5%)
10	J	1.35	0/471	1.12	2/636 (0.3%)
10	W	1.10	1/471 (0.2%)	0.98	0/636
11	K	1.34	3/398 (0.8%)	1.16	2/546 (0.4%)
11	X	0.97	0/398	0.93	1/546 (0.2%)
12	L	1.49	1/393 (0.3%)	1.07	1/526 (0.2%)
12	Y	1.10	0/393	0.98	1/526 (0.2%)
13	M	1.20	0/345	1.15	2/470 (0.4%)
13	Z	0.98	0/345	0.97	0/470
All	All	1.33	109/29324 (0.4%)	1.06	92/39866 (0.2%)

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



detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
10	J	0	1
10	W	0	1
All	All	0	4

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	36	TRP	CB-CG	12.12	1.72	1.50
7	G	36	TRP	CB-CG	10.31	1.68	1.50
7	T	58	LYS	CE-NZ	9.32	1.72	1.49
2	O	198	GLU	C-O	8.13	1.38	1.23
2	B	198	GLU	C-O	7.69	1.38	1.23
2	B	198	GLU	CG-CD	7.52	1.63	1.51
1	A	321	PHE	CE1-CZ	7.36	1.51	1.37
2	B	164	ALA	CA-CB	7.18	1.67	1.52
1	A	40	GLU	CG-CD	6.91	1.62	1.51
3	P	29	SER	CB-OG	-6.80	1.33	1.42
1	A	139	ALA	CA-CB	6.79	1.66	1.52
1	N	126	TRP	CZ3-CH2	6.73	1.50	1.40
9	V	37	PHE	CB-CG	6.71	1.62	1.51
7	T	17	ARG	CG-CD	-6.66	1.35	1.51
1	N	54	TYR	CD1-CE1	6.62	1.49	1.39
2	B	18	GLU	CD-OE2	6.60	1.32	1.25
1	A	129	TYR	CD1-CE1	-6.57	1.29	1.39
2	B	18	GLU	CD-OE1	6.50	1.32	1.25
4	D	17	VAL	CB-CG1	-6.46	1.39	1.52
6	F	89	TYR	CE2-CZ	6.40	1.46	1.38
7	G	5	LYS	CB-CG	6.39	1.69	1.52
8	U	30	TRP	CB-CG	6.33	1.61	1.50
1	N	231	TYR	CD2-CE2	6.33	1.48	1.39
1	A	348	PHE	CE1-CZ	6.31	1.49	1.37
2	B	121	TYR	CD1-CE1	6.26	1.48	1.39
5	R	9	GLU	CG-CD	6.25	1.61	1.51
11	K	39	GLU	CB-CG	6.25	1.64	1.52
3	C	214	PHE	CG-CD2	6.19	1.48	1.38
1	A	22	PHE	CD1-CE1	6.18	1.51	1.39
3	P	91	VAL	CB-CG1	6.16	1.65	1.52
1	A	231	TYR	CD1-CE1	6.16	1.48	1.39
3	C	29	SER	CB-OG	-6.14	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	214	PHE	CD1-CE1	6.13	1.51	1.39
10	W	26	ALA	CA-CB	6.10	1.65	1.52
1	A	480	ARG	CZ-NH2	6.08	1.41	1.33
2	B	115	ASP	CB-CG	6.06	1.64	1.51
1	A	373	VAL	CB-CG1	5.90	1.65	1.52
4	D	104	TYR	CD1-CE1	5.83	1.48	1.39
2	O	18	GLU	CD-OE1	5.79	1.32	1.25
1	A	175	ALA	CA-CB	5.76	1.64	1.52
3	P	258	TRP	CB-CG	-5.71	1.40	1.50
1	A	447	TYR	CD1-CE1	5.71	1.48	1.39
5	E	70	VAL	CB-CG1	-5.70	1.40	1.52
8	H	8	ILE	CA-CB	5.69	1.68	1.54
1	A	186	TRP	CE2-CZ2	5.67	1.49	1.39
1	A	275	TRP	CZ3-CH2	5.66	1.49	1.40
1	A	362	SER	CB-OG	-5.64	1.34	1.42
2	B	9	PHE	CE2-CZ	5.63	1.48	1.37
1	N	321	PHE	CE1-CZ	5.59	1.48	1.37
1	A	425	PHE	CE2-CZ	5.55	1.47	1.37
1	A	400	PHE	CB-CG	5.53	1.60	1.51
1	N	250	GLY	N-CA	5.52	1.54	1.46
5	R	80	GLU	CG-CD	5.50	1.60	1.51
1	N	242	GLU	CG-CD	5.49	1.60	1.51
1	A	506	GLU	CG-CD	5.46	1.60	1.51
1	A	193	VAL	CB-CG1	5.45	1.64	1.52
4	Q	5	VAL	CA-CB	5.44	1.66	1.54
2	B	167	SER	CB-OG	-5.43	1.35	1.42
2	B	138	VAL	CB-CG1	5.43	1.64	1.52
9	I	37	PHE	CB-CG	5.41	1.60	1.51
3	C	64	GLU	CB-CG	5.39	1.62	1.52
7	T	5	LYS	CB-CG	5.38	1.67	1.52
11	K	47	ARG	CG-CD	5.38	1.65	1.51
3	P	115	CYS	CB-SG	5.37	1.91	1.82
1	A	419	VAL	CB-CG2	5.37	1.64	1.52
6	S	19	GLU	CD-OE1	5.36	1.31	1.25
4	D	9	GLU	CG-CD	5.36	1.59	1.51
4	D	129	ALA	CA-CB	5.35	1.63	1.52
2	B	59	GLN	CG-CD	5.32	1.63	1.51
11	K	29	TRP	CB-CG	5.32	1.59	1.50
4	D	112	GLU	CD-OE1	5.32	1.31	1.25
1	A	184	PHE	CD1-CE1	5.31	1.49	1.39
2	O	65	TRP	CB-CG	-5.31	1.40	1.50
2	O	200	CYS	CB-SG	5.31	1.91	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	111	GLU	CD-OE1	5.28	1.31	1.25
1	N	293	PHE	CD1-CE1	5.25	1.49	1.39
1	A	366	VAL	CB-CG1	-5.25	1.41	1.52
9	I	36	LYS	CD-CE	5.23	1.64	1.51
1	A	379	TYR	CG-CD1	5.22	1.46	1.39
4	Q	81	VAL	CB-CG1	5.21	1.63	1.52
2	B	159	VAL	CB-CG2	5.21	1.63	1.52
1	A	310	MET	CG-SD	-5.19	1.67	1.81
2	B	199	ILE	C-O	5.19	1.33	1.23
1	A	438	ARG	CB-CG	-5.18	1.38	1.52
3	C	101	PHE	CE2-CZ	5.18	1.47	1.37
1	N	397	PHE	CE1-CZ	5.18	1.47	1.37
2	O	208	PRO	C-O	5.17	1.33	1.23
6	S	20	VAL	CB-CG2	5.15	1.63	1.52
6	F	89	TYR	CD1-CE1	5.15	1.47	1.39
1	N	164	PHE	CD1-CE1	5.15	1.49	1.39
3	P	161	GLN	CB-CG	-5.15	1.38	1.52
1	N	266	GLU	CD-OE2	5.14	1.31	1.25
12	L	38	PHE	CE1-CZ	5.13	1.47	1.37
4	D	104	TYR	CD2-CE2	5.13	1.47	1.39
6	F	44	GLU	CG-CD	5.12	1.59	1.51
2	B	65	TRP	CB-CG	-5.12	1.41	1.50
1	N	366	VAL	CB-CG1	-5.11	1.42	1.52
9	V	37	PHE	CD2-CE2	5.10	1.49	1.39
4	D	60	TYR	CD1-CE1	-5.09	1.31	1.39
9	I	54	TYR	CD2-CE2	5.09	1.47	1.39
2	B	219	PHE	CE1-CZ	5.08	1.47	1.37
2	B	210	VAL	CB-CG1	5.08	1.63	1.52
3	C	10	MET	CB-CG	5.07	1.67	1.51
2	B	202	SER	CB-OG	-5.05	1.35	1.42
4	D	58	GLU	CB-CG	-5.03	1.42	1.52
1	N	337	ALA	CA-CB	5.02	1.62	1.52
3	P	236	GLU	CB-CG	-5.02	1.42	1.52
5	E	70	VAL	CB-CG2	5.01	1.63	1.52
1	N	70	VAL	CB-CG1	5.01	1.63	1.52

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	32	MET	CG-SD-CE	8.85	114.36	100.20
6	F	18	ARG	NE-CZ-NH2	-8.74	115.93	120.30
4	D	20	ARG	NE-CZ-NH2	-8.70	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	MET	CG-SD-CE	-8.47	86.66	100.20
2	B	112	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	96	ARG	NE-CZ-NH2	-8.10	116.25	120.30
6	F	81	ARG	NE-CZ-NH2	-8.03	116.28	120.30
4	Q	20	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	297	MET	CG-SD-CE	7.71	112.53	100.20
1	A	438	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	N	310	MET	CG-SD-CE	-7.52	88.17	100.20
2	B	45	MET	CG-SD-CE	7.46	112.13	100.20
1	N	310	MET	CA-CB-CG	-7.37	100.77	113.30
12	Y	41	ARG	NE-CZ-NH1	7.16	123.88	120.30
13	M	34	LEU	CB-CG-CD1	7.12	123.10	111.00
9	I	10	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	N	213	ARG	NE-CZ-NH2	-6.95	116.83	120.30
4	Q	125	ASP	CB-CG-OD1	-6.93	112.07	118.30
7	T	8	HIS	N-CA-C	6.92	129.69	111.00
1	A	363	LEU	CB-CG-CD2	6.91	122.74	111.00
7	T	7	ASP	N-CA-C	6.80	129.35	111.00
2	B	167	SER	CB-CA-C	-6.71	97.36	110.10
4	Q	20	ARG	NE-CZ-NH1	6.64	123.62	120.30
7	T	6	GLY	N-CA-C	6.56	129.51	113.10
9	I	10	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	362	SER	N-CA-CB	-6.41	100.89	110.50
3	P	127	LEU	CA-CB-CG	6.32	129.84	115.30
6	S	18	ARG	NE-CZ-NH2	-6.29	117.16	120.30
5	E	90	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	A	96	ARG	NE-CZ-NH1	6.24	123.42	120.30
13	M	7	LYS	CD-CE-NZ	-6.20	97.44	111.70
1	A	442	ASP	CB-CG-OD2	6.20	123.88	118.30
2	B	11	ASP	CB-CG-OD2	6.19	123.87	118.30
2	B	178	ARG	NE-CZ-NH1	6.17	123.38	120.30
8	H	35	ASP	CB-CG-OD2	-6.15	112.76	118.30
11	X	54	ARG	NE-CZ-NH2	6.14	123.37	120.30
7	G	7	ASP	N-CA-C	6.04	127.31	111.00
1	N	366	VAL	CG1-CB-CG2	-5.99	101.31	110.90
1	A	373	VAL	CA-CB-CG2	-5.98	101.93	110.90
1	N	483	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	A	312	ILE	CG1-CB-CG2	-5.94	98.33	111.40
1	A	380	VAL	CG1-CB-CG2	-5.90	101.46	110.90
2	B	151	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	407	ASP	CB-CG-OD2	5.83	123.54	118.30
4	Q	51	LEU	CA-CB-CG	5.75	128.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	GLU	OE1-CD-OE2	5.73	130.18	123.30
9	V	55	ASP	CB-CG-OD1	5.72	123.45	118.30
5	R	72	LYS	CD-CE-NZ	-5.62	98.77	111.70
2	B	129	LYS	CD-CE-NZ	-5.60	98.83	111.70
1	A	244	TYR	CA-CB-CG	-5.57	102.81	113.40
2	B	173	ASP	CB-CG-OD1	5.53	123.28	118.30
2	B	33	LEU	CB-CG-CD2	-5.53	101.61	111.00
1	N	96	ARG	NE-CZ-NH2	-5.51	117.55	120.30
3	P	51	MET	CA-CB-CG	5.48	122.61	113.30
1	A	264	LYS	CD-CE-NZ	5.47	124.28	111.70
3	P	246	ASP	N-CA-CB	-5.47	100.75	110.60
9	V	43	ARG	NE-CZ-NH2	5.44	123.02	120.30
10	J	11	LEU	CB-CG-CD1	-5.44	101.75	111.00
5	E	70	VAL	CG1-CB-CG2	-5.43	102.21	110.90
1	N	442	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	439	ARG	NE-CZ-NH1	5.39	122.99	120.30
6	F	92	VAL	CG1-CB-CG2	-5.38	102.29	110.90
2	B	151	ARG	NE-CZ-NH2	-5.35	117.62	120.30
6	S	18	ARG	NE-CZ-NH1	5.35	122.98	120.30
2	O	92	ASN	CB-CA-C	5.34	121.08	110.40
10	J	57	HIS	CB-CA-C	5.34	121.07	110.40
7	T	5	LYS	CD-CE-NZ	5.32	123.93	111.70
2	B	112	ASP	CB-CG-OD1	5.31	123.08	118.30
1	N	176	MET	CG-SD-CE	-5.31	91.71	100.20
9	V	10	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	O	158	ASP	CB-CG-OD1	5.25	123.03	118.30
2	O	179	LEU	CA-CB-CG	5.25	127.37	115.30
2	B	65	TRP	N-CA-C	5.24	125.15	111.00
12	L	24	MET	CA-CB-CG	5.23	122.19	113.30
2	B	184	LEU	CB-CG-CD1	-5.23	102.12	111.00
3	P	102	TYR	CB-CG-CD2	-5.21	117.87	121.00
5	E	72	LYS	CD-CE-NZ	-5.19	99.76	111.70
2	B	133	LEU	CB-CG-CD1	-5.15	102.25	111.00
9	I	36	LYS	CD-CE-NZ	5.15	123.54	111.70
1	A	194	LEU	CB-CG-CD2	5.14	119.74	111.00
4	Q	26	ASP	CB-CG-OD1	5.12	122.91	118.30
11	K	47	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	51	ASP	CB-CG-OD1	-5.11	113.70	118.30
7	G	6	GLY	N-CA-C	5.11	125.88	113.10
3	C	25	LEU	CB-CG-CD2	-5.11	102.32	111.00
7	G	8	HIS	N-CA-C	5.10	124.77	111.00
3	C	51	MET	CA-CB-CG	5.09	121.95	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	513	LEU	CB-CG-CD1	-5.07	102.39	111.00
9	V	10	ARG	NE-CZ-NH2	-5.05	117.78	120.30
4	Q	21	ASP	CB-CG-OD1	5.04	122.84	118.30
6	F	18	ARG	NE-CZ-NH1	5.02	122.81	120.30
6	S	96	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
10	J	57	HIS	Peptide
6	S	93	PRO	Peptide
10	W	57	HIS	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	38	0
1	N	4027	0	4001	48	0
2	B	1824	0	1833	34	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	22	0
3	P	2110	0	2027	22	0
4	D	1195	0	1183	9	0
4	Q	1195	0	1183	15	0
5	E	852	0	845	11	0
5	R	852	0	845	9	0
6	F	748	0	728	10	0
6	S	748	0	728	14	0
7	G	675	0	643	26	0
7	T	675	0	644	41	0
8	H	662	0	623	8	0
8	U	662	0	623	12	0
9	I	601	0	613	22	0
9	V	601	0	613	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	460	0	459	5	0
10	W	460	0	459	12	0
11	K	384	0	366	3	0
11	X	384	0	366	6	0
12	L	380	0	380	14	0
12	Y	380	0	380	9	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0
14	A	120	0	108	4	0
14	N	120	0	108	7	0
15	A	2	0	0	0	0
15	N	2	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	3	0
19	B	63	0	109	9	0
19	L	63	0	110	19	0
19	N	189	0	330	21	0
20	A	102	0	152	13	0
20	C	102	0	152	7	0
20	N	102	0	152	9	0
20	P	102	0	152	7	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	17	0
22	R	52	0	80	16	0
23	B	29	0	37	3	0
23	C	58	0	71	3	0
23	J	29	0	36	2	0
23	O	29	0	37	1	0
23	P	58	0	72	4	0
23	W	29	0	36	3	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	100	0	156	22	0
25	G	100	0	156	24	0
25	P	100	0	156	16	0
25	T	100	0	156	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	C	33	0	38	2	0
26	M	33	0	38	0	0
26	T	33	0	39	6	0
26	Z	33	0	39	1	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	22	0
28	S	53	0	77	6	0
28	T	106	0	154	19	0
29	A	205	0	0	3	0
29	B	121	0	0	3	0
29	C	80	0	0	2	0
29	D	75	0	0	1	0
29	E	39	0	0	1	0
29	F	70	0	0	2	0
29	G	42	0	0	5	0
29	H	33	0	0	5	0
29	I	24	0	0	1	0
29	J	9	0	0	0	0
29	K	17	0	0	0	0
29	L	20	0	0	2	0
29	M	15	0	0	0	0
29	N	184	0	0	6	0
29	O	97	0	0	2	0
29	P	81	0	0	7	0
29	Q	47	0	0	2	0
29	R	27	0	0	0	0
29	S	52	0	0	1	0
29	T	37	0	0	8	0
29	U	28	0	0	4	0
29	V	17	0	0	4	0
29	W	12	0	0	2	0
29	X	12	0	0	1	0
29	Y	16	0	0	0	0
29	Z	9	0	0	0	0
All	All	32105	0	31279	581	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (581) 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)
1:A:75:ILE:CG1	1:A:75:ILE:CD1	1.76	1.62
28:G:265:PEK:C6	28:G:265:PEK:C7	1.81	1.53
7:T:58:LYS:NZ	7:T:58:LYS:CE	1.72	1.47
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.40	1.36
7:T:45:PRO:CD	29:T:3099:HOH:O	1.75	1.35
7:T:5:LYS:CD	28:T:263:PEK:H382	1.73	1.19
7:T:5:LYS:HD2	28:T:263:PEK:C38	1.74	1.17
28:G:265:PEK:H383	25:G:269:CDL:C27	1.74	1.17
7:T:84:LYS:N	7:T:84:LYS:HD2	1.60	1.16
19:A:523:TGL:HG12	19:A:523:TGL:HC21	1.29	1.12
7:G:45:PRO:HD2	29:G:2099:HOH:O	1.49	1.11
7:T:5:LYS:HD2	28:T:263:PEK:H382	1.28	1.08
7:T:84:LYS:H	7:T:84:LYS:CD	1.67	1.07
7:T:45:PRO:HD2	29:T:3099:HOH:O	1.34	1.06
25:G:269:CDL:HA21	25:G:269:CDL:H112	1.32	1.05
29:P:4533:HOH:O	28:S:1265:PEK:H71	1.56	1.05
20:P:1267:PGV:H182	25:P:1270:CDL:H662	1.08	1.04
28:G:265:PEK:C38	25:G:269:CDL:H273	1.86	1.04
28:G:265:PEK:H383	25:G:269:CDL:H273	1.06	1.04
20:C:267:PGV:C12	20:C:267:PGV:H161	1.89	1.03
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.23	1.00
20:C:267:PGV:H12	20:C:267:PGV:H161	1.42	1.00
8:H:9:LYS:O	8:H:10:ASN:HB2	1.57	0.99
20:P:1267:PGV:C18	25:P:1270:CDL:H662	1.92	0.99
20:P:1267:PGV:H182	25:P:1270:CDL:C66	1.93	0.98
1:A:321:PHE:CD2	22:B:229:PSC:H341	1.99	0.98
3:C:111:GLU:HG3	29:H:4073:HOH:O	1.62	0.97
22:B:229:PSC:H072	9:I:10:ARG:HH21	1.29	0.96
28:T:1264:PEK:H71	28:T:1264:PEK:H32	1.46	0.96
1:N:112:LEU:HD12	29:N:3701:HOH:O	1.64	0.95
8:U:8:ILE:HG21	29:U:4330:HOH:O	1.66	0.95
6:S:85:CYS:SG	6:S:87:THR:HG23	2.07	0.94
26:C:272:DMU:O1	26:C:272:DMU:H29	1.68	0.94
22:B:229:PSC:C07	9:I:10:ARG:HH21	1.80	0.93
5:R:8:ASP:OD1	22:R:1229:PSC:H081	1.69	0.93
25:G:269:CDL:H522	25:G:269:CDL:H231	1.51	0.92
7:T:45:PRO:HD3	29:T:3099:HOH:O	1.47	0.92
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.13	0.92
6:F:85:CYS:SG	6:F:87:THR:HG23	2.09	0.91
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.35	0.91
7:G:5:LYS:HD2	28:G:1263:PEK:H383	1.50	0.91
1:N:321:PHE:CD2	22:R:1229:PSC:H341	2.05	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:1269:CDL:H541	25:T:1269:CDL:H231	1.51	0.90
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.53	0.90
19:B:521:TGL:H281	19:B:521:TGL:H102	1.52	0.89
7:T:5:LYS:CD	28:T:263:PEK:C38	2.41	0.89
22:R:1229:PSC:C07	9:V:10:ARG:HH21	1.85	0.89
7:T:62:TRP:HB3	26:T:1272:DMU:H30	1.52	0.89
7:T:84:LYS:H	7:T:84:LYS:HD2	0.77	0.88
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.34	0.88
12:L:20:ARG:HH21	19:L:522:TGL:HC32	1.36	0.86
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.39	0.86
25:G:269:CDL:H873	29:G:4364:HOH:O	1.75	0.86
7:T:31:CYS:SG	25:T:1269:CDL:H532	2.17	0.85
8:H:9:LYS:O	8:H:10:ASN:CB	2.25	0.85
7:G:72:ASN:H	7:G:76:ASN:HD22	1.22	0.85
7:T:62:TRP:CB	26:T:1272:DMU:H30	2.07	0.83
19:N:1521:TGL:C28	19:N:1521:TGL:H102	2.08	0.83
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.43	0.83
9:V:36:LYS:HG3	29:V:4356:HOH:O	1.77	0.82
28:G:265:PEK:C5	28:G:265:PEK:C7	2.58	0.82
2:B:33:LEU:HD11	9:I:28:SER:HB3	1.59	0.82
20:C:267:PGV:H12	20:C:267:PGV:C16	2.07	0.82
25:T:1269:CDL:H511	25:T:1269:CDL:H181	1.61	0.81
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.64	0.81
7:G:45:PRO:CD	29:G:2099:HOH:O	2.16	0.80
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.46	0.80
7:T:72:ASN:H	7:T:76:ASN:HD22	1.26	0.80
7:T:76:ASN:HD21	28:T:1264:PEK:HN2	1.26	0.79
25:P:1270:CDL:HB21	25:P:1270:CDL:HB32	1.65	0.79
9:V:31:PHE:C	9:V:31:PHE:CD1	2.55	0.79
4:D:34:SER:H	4:D:37:GLN:HE21	1.31	0.78
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.49	0.78
19:N:1521:TGL:H222	19:N:1521:TGL:HA81	1.65	0.78
19:A:523:TGL:CC2	19:A:523:TGL:HG12	2.13	0.77
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.67	0.77
25:P:1270:CDL:H652	25:P:1270:CDL:H611	1.67	0.77
19:B:521:TGL:C28	19:B:521:TGL:H102	2.14	0.77
25:C:270:CDL:H231	25:C:270:CDL:H642	1.68	0.76
25:G:269:CDL:C11	25:G:269:CDL:HA21	2.14	0.76
7:T:62:TRP:HB3	26:T:1272:DMU:C57	2.15	0.75
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.01	0.75
28:S:1265:PEK:H383	25:T:1269:CDL:C27	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:522:TGL:HC51	19:L:522:TGL:OC1	1.86	0.74
22:R:1229:PSC:H072	9:V:10:ARG:HH21	1.51	0.74
22:B:229:PSC:O01	22:B:229:PSC:H212	1.87	0.74
19:N:1521:TGL:H281	19:N:1521:TGL:H102	1.69	0.73
8:H:27:ARG:NH1	29:H:2431:HOH:O	2.22	0.73
1:N:177:SER:H	1:N:180:GLN:HE21	1.36	0.73
2:O:226:MET:HE1	29:O:4398:HOH:O	1.89	0.73
28:G:265:PEK:C38	25:G:269:CDL:C27	2.57	0.72
28:G:265:PEK:C6	28:G:265:PEK:C8	2.67	0.72
1:A:50:ASP:HB3	1:A:53:ILE:HD12	1.71	0.72
20:A:524:PGV:C01	20:A:524:PGV:H221	2.19	0.72
9:I:31:PHE:CD1	9:I:31:PHE:C	2.63	0.72
22:R:1229:PSC:H071	9:V:10:ARG:HH21	1.55	0.72
14:N:516:HEA:HBC1	14:N:516:HEA:HMC1	1.71	0.71
3:P:111:GLU:OE1	29:P:3467:HOH:O	2.08	0.71
5:R:80:GLU:CD	5:R:80:GLU:H	1.93	0.71
7:G:31:CYS:SG	25:G:269:CDL:H532	2.30	0.71
7:G:5:LYS:CD	28:G:1263:PEK:H383	2.21	0.71
7:G:76:ASN:HD21	28:G:264:PEK:HN2	1.37	0.71
25:G:269:CDL:H562	25:G:269:CDL:H792	1.72	0.71
7:G:84:LYS:HD2	7:G:84:LYS:H	1.54	0.71
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.72	0.70
13:M:39:ASN:O	13:M:43:SER:HB2	1.91	0.70
19:A:523:TGL:H281	29:B:4178:HOH:O	1.91	0.70
25:T:1269:CDL:C51	25:T:1269:CDL:H181	2.22	0.69
25:G:269:CDL:C23	25:G:269:CDL:H522	2.21	0.69
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.58	0.69
6:F:64:GLU:O	6:F:65:ASP:HB2	1.92	0.69
3:P:107:ALA:HB2	20:P:1268:PGV:H031	1.73	0.69
3:C:67:PHE:CE1	25:C:270:CDL:H1	2.25	0.68
1:N:484:THR:HB	13:Z:2:THR:OG1	1.93	0.68
25:C:270:CDL:HB21	25:C:270:CDL:HB32	1.74	0.68
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.06	0.68
1:N:514:LYS:HA	6:S:38:ALA:CB	2.23	0.68
3:C:246:ASP:HB2	29:C:4122:HOH:O	1.94	0.68
1:A:484:THR:HB	13:M:2:THR:OG1	1.94	0.68
22:R:1229:PSC:H071	9:V:10:ARG:NH2	2.09	0.67
19:B:521:TGL:HC72	29:B:4575:HOH:O	1.94	0.67
1:N:177:SER:H	1:N:180:GLN:NE2	1.92	0.67
25:P:1270:CDL:HA4	25:P:1270:CDL:H122	1.75	0.67
25:G:269:CDL:C52	25:G:269:CDL:H231	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:26:MET:O	9:I:27:VAL:C	2.33	0.67
20:C:267:PGV:H182	25:C:270:CDL:H671	1.76	0.67
7:T:5:LYS:CG	28:T:263:PEK:H382	2.24	0.67
22:B:229:PSC:C07	9:I:10:ARG:NH2	2.56	0.67
5:E:109:VAL:OXT	5:E:109:VAL:HG23	1.93	0.66
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.76	0.66
28:S:1265:PEK:H383	25:T:1269:CDL:H272	1.77	0.66
25:T:1269:CDL:CB5	25:T:1269:CDL:H181	2.26	0.66
3:P:33:MET:HG2	29:P:4161:HOH:O	1.95	0.66
14:A:516:HEA:HBC1	14:A:516:HEA:HMC1	1.77	0.66
25:G:269:CDL:C56	25:G:269:CDL:H792	2.26	0.66
8:H:12:GLN:HG3	29:H:4563:HOH:O	1.95	0.66
20:A:524:PGV:H062	29:A:2126:HOH:O	1.95	0.65
1:A:75:ILE:CD1	1:A:75:ILE:CB	2.71	0.65
25:P:1270:CDL:HB21	25:P:1270:CDL:CB3	2.26	0.65
22:B:229:PSC:H142	22:B:229:PSC:H342	1.78	0.65
1:A:486:ASP:OD1	4:D:19:ARG:HD2	1.96	0.65
22:B:229:PSC:H142	22:B:229:PSC:C34	2.26	0.65
10:W:33:ARG:HG2	23:W:1059:CHD:C15	2.27	0.65
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.33	0.64
4:Q:19:ARG:HB3	4:Q:19:ARG:HH21	1.61	0.64
20:N:1524:PGV:H221	20:N:1524:PGV:C01	2.28	0.64
23:P:1271:CHD:H162	23:P:1271:CHD:H232	1.78	0.64
2:O:89:GLU:O	2:O:91:ASN:ND2	2.31	0.64
25:C:270:CDL:PA1	25:C:270:CDL:HB22	2.38	0.64
19:N:1521:TGL:H101	19:N:1521:TGL:HA71	1.79	0.64
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.09	0.64
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.80	0.63
1:N:488:THR:HB	1:N:495:LEU:HD13	1.81	0.63
2:B:33:LEU:HD11	9:I:28:SER:CB	2.26	0.63
10:W:33:ARG:HG2	23:W:1059:CHD:H152	1.81	0.63
7:G:5:LYS:HG3	28:G:1263:PEK:H382	1.81	0.63
23:P:1271:CHD:C16	23:P:1271:CHD:H232	2.29	0.63
7:G:8:HIS:ND1	28:G:1263:PEK:H332	2.13	0.63
2:B:59:GLN:O	2:B:60:GLU:HG3	1.99	0.63
7:G:72:ASN:H	7:G:76:ASN:ND2	1.97	0.62
8:H:57:ARG:HD2	29:H:4481:HOH:O	1.99	0.62
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.15	0.62
1:N:513:LEU:O	1:N:514:LYS:HB2	1.99	0.62
7:T:12:GLY:HA3	29:T:3372:HOH:O	1.99	0.62
20:A:524:PGV:C06	29:A:2126:HOH:O	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:61:VAL:HA	2:O:64:ILE:HD12	1.80	0.62
22:R:1229:PSC:C07	9:V:10:ARG:NH2	2.60	0.61
28:G:264:PEK:H71	28:G:264:PEK:H32	1.81	0.61
4:D:34:SER:H	4:D:37:GLN:NE2	1.98	0.61
7:T:36:TRP:HB3	29:T:4417:HOH:O	2.00	0.61
12:L:20:ARG:HH21	19:L:522:TGL:CC3	2.08	0.61
1:A:502:TYR:CD1	12:L:2:HIS:HE1	2.19	0.60
20:A:524:PGV:H011	20:A:524:PGV:H221	1.83	0.60
7:G:84:LYS:H	7:G:84:LYS:CD	2.13	0.60
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.01	0.60
9:V:18:ARG:CG	9:V:18:ARG:HH11	2.11	0.60
20:N:1524:PGV:H011	20:N:1524:PGV:H221	1.83	0.60
22:B:229:PSC:H081	5:E:8:ASP:OD1	2.01	0.59
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.31	0.59
7:T:3:ALA:O	7:T:4:ALA:HB2	2.03	0.59
9:I:31:PHE:CD1	9:I:32:ALA:N	2.71	0.59
28:S:1265:PEK:C38	25:T:1269:CDL:H273	2.32	0.59
7:G:3:ALA:O	7:G:4:ALA:HB2	2.02	0.59
3:P:127:LEU:HG	25:T:1269:CDL:OB3	2.03	0.58
25:T:1269:CDL:H111	25:T:1269:CDL:CA2	2.31	0.58
4:Q:109:HIS:CD2	29:Q:3122:HOH:O	2.47	0.58
19:N:1521:TGL:H281	19:N:1521:TGL:HB92	1.86	0.58
1:A:406:ASN:HD21	20:A:524:PGV:H21	1.69	0.58
5:E:31:LYS:HE3	29:F:4383:HOH:O	2.04	0.58
1:A:177:SER:H	1:A:180:GLN:NE2	2.02	0.58
19:N:1521:TGL:H283	19:N:1521:TGL:H102	1.86	0.58
7:G:4:ALA:CB	1:N:282:PHE:HA	2.34	0.57
8:U:49:ASP:O	8:U:52:VAL:HG22	2.04	0.57
1:A:47:LEU:O	13:M:41:LYS:HE3	2.04	0.57
5:R:8:ASP:HA	22:R:1229:PSC:H071	1.86	0.57
6:F:85:CYS:SG	6:F:87:THR:CG2	2.89	0.57
7:G:5:LYS:HG3	28:G:1263:PEK:C38	2.33	0.57
25:P:1270:CDL:H661	25:P:1270:CDL:H252	1.87	0.57
2:B:56:MET:HA	22:B:229:PSC:H202	1.85	0.57
7:T:5:LYS:HD3	28:T:263:PEK:H382	1.79	0.57
20:A:524:PGV:H222	13:M:15:GLN:HE22	1.70	0.56
26:C:272:DMU:H29	26:C:272:DMU:C10	2.35	0.56
9:I:31:PHE:O	9:I:34:PHE:N	2.32	0.56
4:Q:95:LEU:HD22	26:Z:1526:DMU:H13	1.86	0.56
3:C:19:THR:O	3:C:23:SER:HB3	2.06	0.56
25:P:1270:CDL:H431	29:W:4138:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:270:CDL:HB32	25:C:270:CDL:CB2	2.35	0.56
20:A:524:PGV:H221	20:A:524:PGV:H012	1.86	0.56
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.06	0.56
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.87	0.56
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	2.05	0.56
25:C:270:CDL:H672	25:C:270:CDL:H261	1.88	0.56
10:J:52:TRP:O	10:J:57:HIS:HE1	1.87	0.56
25:C:270:CDL:HB21	25:C:270:CDL:CB3	2.36	0.56
2:B:66:THR:HG22	2:B:67:ILE:N	2.20	0.56
23:B:1085:CHD:H212	23:B:1085:CHD:H12	1.87	0.56
1:A:513:LEU:O	1:A:514:LYS:HB2	2.06	0.56
4:Q:19:ARG:NH2	4:Q:21:ASP:OD1	2.39	0.55
28:G:264:PEK:H101	28:G:264:PEK:H161	1.88	0.55
25:T:1269:CDL:H522	25:T:1269:CDL:H202	1.87	0.55
25:C:270:CDL:H661	25:C:270:CDL:H242	1.88	0.55
10:J:50:LEU:HD22	10:J:50:LEU:O	2.06	0.55
25:T:1269:CDL:OA7	25:T:1269:CDL:H311	2.05	0.55
19:N:1523:TGL:HG11	19:N:1523:TGL:CC2	2.37	0.55
1:N:508:PRO:HG3	3:P:6:HIS:HB3	1.89	0.55
25:G:269:CDL:H371	2:O:81:LEU:HD12	1.88	0.55
7:T:62:TRP:HB2	26:T:1272:DMU:H30	1.89	0.55
13:Z:39:ASN:O	13:Z:43:SER:HB2	2.07	0.55
22:R:1229:PSC:H231	22:R:1229:PSC:H42	1.89	0.55
7:G:2:SER:OG	28:G:1263:PEK:H301	2.07	0.55
3:P:33:MET:CG	29:P:4161:HOH:O	2.53	0.55
19:B:521:TGL:H252	19:B:521:TGL:HA91	1.88	0.55
7:G:3:ALA:O	7:G:4:ALA:CB	2.55	0.54
5:R:6:GLU:OE1	5:R:14:ARG:NH2	2.39	0.54
3:C:226:HIS:CE1	25:C:270:CDL:HB31	2.42	0.54
3:C:54:MET:HE3	25:C:270:CDL:H601	1.89	0.54
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.90	0.54
3:P:124:LEU:HD13	3:P:180:GLU:OE1	2.07	0.54
8:U:8:ILE:HG12	29:U:4330:HOH:O	2.08	0.54
19:L:522:TGL:H362	29:L:4269:HOH:O	2.08	0.54
7:T:5:LYS:HD3	28:T:263:PEK:C38	2.35	0.54
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.40	0.54
1:N:408:THR:O	1:N:412:ILE:HD12	2.08	0.54
11:X:24:PHE:O	11:X:28:VAL:HG12	2.08	0.53
4:Q:73:ARG:HB3	5:R:109:VAL:HG11	1.91	0.53
10:J:9:GLN:O	10:J:13:GLN:HG3	2.09	0.53
20:C:267:PGV:H182	25:C:270:CDL:C67	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:521:TGL:H252	19:B:521:TGL:C20	2.39	0.53
3:C:226:HIS:HE1	25:C:270:CDL:HB31	1.74	0.53
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.91	0.53
10:W:29:ASN:HD22	10:W:29:ASN:H	1.54	0.53
12:L:25:MET:HG2	19:L:522:TGL:HA62	1.90	0.53
2:B:13:THR:OG1	2:B:167:SER:HB3	2.09	0.53
6:F:64:GLU:O	6:F:65:ASP:CB	2.57	0.53
25:C:270:CDL:OA5	25:C:270:CDL:HB22	2.08	0.52
1:N:112:LEU:CD1	29:N:3701:HOH:O	2.39	0.52
2:B:33:LEU:CD1	9:I:28:SER:HB3	2.36	0.52
19:N:1523:TGL:HB52	4:Q:81:VAL:HG11	1.92	0.52
25:T:1269:CDL:H172	29:T:4505:HOH:O	2.09	0.52
3:C:210:ILE:HG23	20:C:267:PGV:H102	1.90	0.52
6:S:64:GLU:O	6:S:65:ASP:HB2	2.09	0.52
25:G:269:CDL:C53	25:G:269:CDL:H231	2.39	0.52
1:N:38:ARG:HD2	14:N:515:HEA:OMA	2.09	0.52
29:P:4415:HOH:O	26:T:1272:DMU:H24	2.10	0.52
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.93	0.52
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.51	0.51
2:O:62:GLU:HB2	29:O:4150:HOH:O	2.10	0.51
9:V:31:PHE:CD1	9:V:32:ALA:N	2.78	0.51
10:W:29:ASN:ND2	10:W:29:ASN:H	2.09	0.51
4:Q:56:LYS:HG2	5:R:61:PHE:CZ	2.46	0.51
3:C:224:LYS:O	3:C:225:PHE:HB2	2.11	0.51
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.40	0.51
2:O:33:LEU:CD1	9:V:28:SER:HB3	2.40	0.51
2:O:116:LEU:HD11	2:O:226:MET:CG	2.40	0.51
25:G:269:CDL:H542	25:G:269:CDL:H251	1.92	0.51
7:G:5:LYS:HB2	28:G:1263:PEK:H361	1.91	0.51
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.92	0.51
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.91	0.51
2:B:89:GLU:O	2:B:91:ASN:OD1	2.29	0.51
3:C:51:MET:HB2	25:C:270:CDL:H392	1.94	0.50
19:B:521:TGL:C10	19:B:521:TGL:C28	2.87	0.50
7:T:3:ALA:O	7:T:4:ALA:CB	2.59	0.50
2:O:78:LEU:CB	2:O:79:PRO:CD	2.89	0.50
2:O:226:MET:HA	2:O:226:MET:CE	2.41	0.50
25:G:269:CDL:H761	1:N:282:PHE:HZ	1.77	0.50
2:O:56:MET:HG2	22:R:1229:PSC:H211	1.94	0.50
20:A:524:PGV:H132	20:A:524:PGV:H302	1.93	0.50
12:L:20:ARG:HH22	19:L:522:TGL:CC3	2.04	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:HB3	19:B:521:TGL:H242	1.94	0.50
20:A:524:PGV:H151	20:A:524:PGV:H322	1.94	0.50
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.08	0.49
8:U:7:LYS:C	8:U:9:LYS:H	2.16	0.49
6:S:34:LEU:HD22	29:S:4590:HOH:O	2.12	0.49
19:N:1523:TGL:H352	29:V:4468:HOH:O	2.12	0.49
2:O:66:THR:HG22	2:O:67:ILE:N	2.27	0.49
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.94	0.49
11:X:15:ASN:HB2	29:X:3609:HOH:O	2.11	0.49
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.95	0.49
11:K:24:PHE:O	11:K:28:VAL:HG12	2.12	0.49
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.78	0.49
20:A:521:PGV:H182	3:C:28:THR:HG22	1.94	0.49
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.48	0.49
2:O:78:LEU:HB3	2:O:79:PRO:HD3	1.95	0.49
2:O:62:GLU:O	2:O:66:THR:HB	2.13	0.48
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.94	0.48
12:L:20:ARG:NH2	19:L:522:TGL:HC62	2.08	0.48
10:W:9:GLN:O	10:W:13:GLN:HG3	2.12	0.48
19:N:1521:TGL:C10	19:N:1521:TGL:C28	2.88	0.48
4:D:93:ALA:HB3	11:K:28:VAL:HG22	1.95	0.48
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.95	0.48
19:L:522:TGL:H351	29:L:4252:HOH:O	2.13	0.48
19:N:1521:TGL:C10	19:N:1521:TGL:H281	2.39	0.48
4:D:34:SER:N	4:D:37:GLN:HE21	2.07	0.48
9:V:27:VAL:HG11	29:V:4562:HOH:O	2.13	0.48
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.25	0.48
9:V:36:LYS:CG	29:V:4356:HOH:O	2.49	0.48
4:Q:19:ARG:NH2	4:Q:21:ASP:CG	2.66	0.48
19:N:1523:TGL:H242	19:N:1523:TGL:HA91	1.95	0.48
2:O:59:GLN:HG3	2:O:59:GLN:O	2.13	0.48
8:U:60:TYR:CD1	8:U:60:TYR:C	2.87	0.48
2:O:102:HIS:HE2	2:O:107:SER:HG	1.61	0.48
6:F:55:LYS:HA	6:F:74:LEU:O	2.13	0.48
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.11	0.48
20:P:1267:PGV:H182	25:P:1270:CDL:C67	2.43	0.48
1:N:400:PHE:HB3	19:N:1522:TGL:H282	1.94	0.48
3:P:236:GLU:HG2	29:P:4386:HOH:O	2.12	0.48
6:S:92:VAL:HG23	6:S:92:VAL:O	2.14	0.48
7:T:2:SER:O	28:T:263:PEK:H331	2.14	0.48
7:T:5:LYS:CD	28:T:263:PEK:H383	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:87:ILE:O	1:N:173:PRO:HD3	2.14	0.48
29:W:4565:HOH:O	12:Y:47:LYS:HG3	2.13	0.48
25:T:1269:CDL:H561	25:T:1269:CDL:H762	1.96	0.48
22:B:229:PSC:H072	9:I:10:ARG:NH2	2.13	0.48
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.96	0.48
1:N:417:MET:CE	29:N:3166:HOH:O	2.62	0.48
3:P:154:GLY:HA2	6:S:6:VAL:HB	1.95	0.47
23:P:1525:CHD:H112	23:P:1525:CHD:H12A	1.72	0.47
20:N:1524:PGV:H012	20:N:1524:PGV:H221	1.95	0.47
1:A:177:SER:H	1:A:180:GLN:HE21	1.62	0.47
13:M:42:LYS:HA	13:M:42:LYS:CE	2.43	0.47
23:B:1085:CHD:H212	23:B:1085:CHD:C12	2.44	0.47
1:N:417:MET:HE1	29:N:3166:HOH:O	2.13	0.47
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.30	0.47
8:U:27:ARG:NH1	29:U:3431:HOH:O	2.46	0.47
2:B:94:SER:HB2	29:B:4446:HOH:O	2.15	0.47
2:B:217:LYS:HD2	2:B:217:LYS:HA	1.60	0.47
7:T:5:LYS:HD2	28:T:263:PEK:H383	1.83	0.46
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.80	0.46
20:N:1524:PGV:H152	20:N:1524:PGV:H322	1.96	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.46
1:N:472:ILE:HG21	19:N:1522:TGL:HA91	1.97	0.46
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.96	0.46
1:A:51:ASP:HB3	2:B:202:SER:O	2.15	0.46
3:C:33:MET:CG	29:C:4096:HOH:O	2.63	0.46
9:V:28:SER:O	9:V:32:ALA:N	2.41	0.46
13:M:39:ASN:O	13:M:43:SER:CB	2.61	0.46
4:Q:19:ARG:HB3	4:Q:19:ARG:NH2	2.29	0.46
2:O:78:LEU:CB	2:O:79:PRO:HD3	2.44	0.46
6:S:53:THR:HB	6:S:54:ASN:H	1.36	0.46
19:L:522:TGL:C24	19:L:522:TGL:H201	2.46	0.46
28:S:1265:PEK:H381	25:T:1269:CDL:H273	1.97	0.46
3:P:146:TRP:CE2	7:T:17:ARG:HG3	2.50	0.46
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.80	0.46
20:P:1268:PGV:H21	20:P:1268:PGV:H51	1.36	0.46
2:O:217:LYS:HA	2:O:217:LYS:HE2	1.95	0.46
2:O:33:LEU:HD11	9:V:28:SER:HB3	1.98	0.46
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.97	0.46
2:O:67:ILE:O	2:O:70:ALA:HB3	2.16	0.46
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.98	0.46
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:229:PSC:H142	22:B:229:PSC:H343	1.98	0.46
8:H:12:GLN:CG	29:H:4563:HOH:O	2.59	0.46
2:B:40:TYR:CE2	9:I:24:ALA:HB2	2.51	0.46
8:U:78:GLU:O	8:U:78:GLU:HG2	2.16	0.46
25:C:270:CDL:H411	25:C:270:CDL:H382	1.83	0.46
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.51	0.46
3:C:5:THR:HG22	6:F:96:LEU:HD22	1.97	0.46
10:W:56:PRO:HD3	12:Y:46:LYS:HG2	1.98	0.46
25:G:269:CDL:H552	25:G:269:CDL:H582	1.60	0.46
2:B:52:HIS:CE1	22:B:229:PSC:H211	2.51	0.46
23:B:1085:CHD:H112	23:B:1085:CHD:H12A	1.69	0.46
12:L:46:LYS:O	12:L:47:LYS:CB	2.64	0.46
28:G:1263:PEK:H282	28:G:1263:PEK:H312	1.85	0.46
2:B:165:VAL:HG11	2:B:168:LEU:HD12	1.98	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.45
7:G:9:GLY:HA3	29:N:4361:HOH:O	2.16	0.45
1:N:398:PRO:O	1:N:498:CYS:HB3	2.16	0.45
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.51	0.45
7:T:8:HIS:CE1	28:T:263:PEK:H341	2.50	0.45
9:V:18:ARG:CG	9:V:18:ARG:NH1	2.77	0.45
28:T:1264:PEK:C7	28:T:1264:PEK:H32	2.31	0.45
2:O:200:CYS:SG	2:O:204:HIS:HA	2.57	0.45
5:R:8:ASP:HA	22:R:1229:PSC:C07	2.47	0.45
19:N:1521:TGL:H222	19:N:1521:TGL:CA8	2.42	0.45
1:A:50:ASP:CB	1:A:53:ILE:HD12	2.44	0.45
12:Y:9:LYS:HA	12:Y:9:LYS:HD3	1.61	0.45
3:C:47:LEU:O	3:C:51:MET:HG2	2.16	0.45
8:U:7:LYS:O	8:U:8:ILE:HG22	2.16	0.45
22:R:1229:PSC:H251	22:R:1229:PSC:H221	1.39	0.45
1:A:514:LYS:HA	6:F:38:ALA:CB	2.47	0.45
12:Y:16:GLU:OE1	12:Y:16:GLU:HA	2.17	0.45
7:T:10:GLY:CA	29:T:4407:HOH:O	2.64	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.97	0.45
5:E:48:ILE:HG21	5:E:89:LEU:HD11	1.99	0.45
25:G:269:CDL:C87	29:G:4364:HOH:O	2.50	0.45
1:N:514:LYS:HA	6:S:38:ALA:HB2	1.98	0.45
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.05	0.45
2:O:83:ILE:O	2:O:87:MET:HG3	2.17	0.45
28:T:263:PEK:H231	28:T:263:PEK:H052	1.99	0.45
3:C:127:LEU:HG	25:G:269:CDL:OB3	2.16	0.45
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:127:LYS:HD2	29:I:2618:HOH:O	2.18	0.44
25:G:269:CDL:HB32	1:N:304:TYR:HD1	1.82	0.44
5:E:31:LYS:CE	29:F:4383:HOH:O	2.63	0.44
7:T:33:LEU:O	7:T:37:LEU:HB2	2.17	0.44
8:H:58:ARG:HD2	8:H:58:ARG:HA	1.85	0.44
25:T:1269:CDL:H541	25:T:1269:CDL:C23	2.34	0.44
19:B:521:TGL:C10	19:B:521:TGL:H281	2.36	0.44
20:A:524:PGV:H22	20:A:524:PGV:H011	1.99	0.44
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.00	0.44
3:C:154:GLY:HA2	6:F:6:VAL:HB	1.99	0.44
8:H:60:TYR:CD1	8:H:60:TYR:C	2.90	0.44
10:W:12:PHE:O	10:W:23:LYS:HE2	2.17	0.44
1:N:369:ASP:HA	1:N:438:ARG:HD3	2.00	0.44
11:X:43:SER:HA	11:X:44:PRO:HD3	1.84	0.44
22:B:229:PSC:H232	22:B:229:PSC:H201	1.33	0.44
7:G:5:LYS:CG	28:G:1263:PEK:H383	2.48	0.44
1:A:50:ASP:OD1	29:A:2067:HOH:O	2.21	0.44
2:O:66:THR:CG2	2:O:67:ILE:N	2.80	0.44
7:G:12:GLY:HA3	29:G:2372:HOH:O	2.18	0.44
1:A:513:LEU:O	1:A:514:LYS:CB	2.66	0.44
6:F:30:PRO:O	6:F:96:LEU:HD21	2.18	0.44
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.99	0.44
23:J:60:CHD:H12A	23:J:60:CHD:H112	1.41	0.44
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.99	0.44
5:E:24:ILE:HG23	5:E:24:ILE:O	2.17	0.44
1:A:321:PHE:CE2	22:B:229:PSC:H341	2.48	0.44
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.53	0.44
6:S:14:THR:HG1	10:W:13:GLN:HE22	1.64	0.43
3:P:155:ASP:OD2	3:P:158:HIS:ND1	2.38	0.43
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.53	0.43
2:B:111:THR:HA	2:B:114:GLU:O	2.19	0.43
28:G:265:PEK:H383	25:G:269:CDL:H272	1.84	0.43
1:N:321:PHE:HB3	2:O:65:TRP:CE3	2.53	0.43
20:N:1524:PGV:C01	20:N:1524:PGV:C22	2.96	0.43
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.99	0.43
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.99	0.43
1:N:114:ALA:O	1:N:118:VAL:HG13	2.18	0.43
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.52	0.43
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.52	0.43
19:N:1521:TGL:H281	19:N:1521:TGL:CB9	2.48	0.43
9:V:31:PHE:HD1	9:V:32:ALA:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:LEU:HD22	19:N:1522:TGL:HB32	2.01	0.43
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.01	0.43
20:N:1524:PGV:H242	20:N:1524:PGV:H41	1.99	0.43
2:B:78:LEU:CB	2:B:79:PRO:CD	2.97	0.43
2:O:33:LEU:HD13	2:O:33:LEU:HA	1.32	0.43
1:A:250:GLY:O	1:A:254:ILE:HG12	2.19	0.43
28:S:1265:PEK:C38	25:T:1269:CDL:C27	2.88	0.43
2:O:33:LEU:CD1	9:V:28:SER:CB	2.96	0.43
9:I:31:PHE:O	9:I:32:ALA:C	2.56	0.43
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.60	0.43
23:W:1059:CHD:H12A	23:W:1059:CHD:H112	1.40	0.43
1:N:200:PRO:HB3	20:N:1266:PGV:H341	2.01	0.43
22:B:229:PSC:H071	9:I:10:ARG:NH2	2.31	0.43
7:T:74:ARG:HB2	29:T:3608:HOH:O	2.19	0.43
12:Y:22:LEU:O	12:Y:26:THR:HB	2.19	0.43
7:T:2:SER:O	28:T:263:PEK:H322	2.19	0.43
22:R:1229:PSC:O01	22:R:1229:PSC:H212	2.19	0.43
2:B:13:THR:HG22	2:B:13:THR:O	2.18	0.43
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.68	0.43
2:O:114:GLU:HB3	2:O:227:LEU:HD21	2.01	0.43
14:N:515:HEA:HHC	14:N:515:HEA:H11	1.79	0.42
2:O:114:GLU:HG3	2:O:227:LEU:HD11	2.00	0.42
1:N:377:PHE:HA	1:N:380:VAL:HG22	2.01	0.42
2:O:33:LEU:HD11	9:V:28:SER:CB	2.49	0.42
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.85	0.42
3:P:47:LEU:O	3:P:51:MET:HG2	2.19	0.42
22:R:1229:PSC:H212	22:R:1229:PSC:C02	2.49	0.42
1:N:486:ASP:HB2	29:N:3142:HOH:O	2.18	0.42
20:C:267:PGV:H182	25:C:270:CDL:C66	2.49	0.42
28:T:1264:PEK:H71	28:T:1264:PEK:C3	2.34	0.42
6:S:16:LEU:HA	6:S:16:LEU:HD12	1.83	0.42
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.54	0.42
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.60	0.42
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.67	0.42
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.62	0.42
1:A:472:ILE:HG21	19:L:522:TGL:HA92	2.02	0.42
9:I:26:MET:O	9:I:27:VAL:O	2.36	0.42
1:A:48:LEU:C	1:A:50:ASP:H	2.21	0.42
6:S:37:LYS:HA	6:S:37:LYS:HD3	1.83	0.42
10:W:32:TYR:CE1	10:W:36:MET:HE3	2.54	0.42
2:O:222:TRP:HB2	9:V:71:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:14:SER:H	19:L:522:TGL:HC31	1.85	0.42
3:P:135:SER:HB3	25:T:1269:CDL:H572	2.02	0.42
9:I:31:PHE:O	9:I:34:PHE:HB3	2.20	0.42
1:N:412:ILE:HG12	4:Q:84:ALA:HB3	2.01	0.42
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.50	0.42
19:L:522:TGL:H231	19:L:522:TGL:H202	1.72	0.42
28:T:263:PEK:O04	28:T:263:PEK:H242	2.19	0.42
9:I:31:PHE:HD1	9:I:32:ALA:N	2.15	0.42
1:A:115:SER:HB2	1:A:142:SER:O	2.19	0.42
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.01	0.42
20:P:1267:PGV:H331	29:P:4415:HOH:O	2.19	0.42
14:N:515:HEA:HHD	14:N:515:HEA:HAC	1.91	0.42
10:J:31:LEU:HA	10:J:31:LEU:HD12	1.75	0.42
1:N:27:GLY:HA2	1:N:69:MET:HG3	2.02	0.42
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.85	0.41
9:V:25:PHE:CZ	9:V:29:LEU:HD22	2.54	0.41
9:I:61:GLU:HG3	9:I:65:LYS:HE3	2.02	0.41
6:S:81:ARG:HA	6:S:87:THR:O	2.19	0.41
19:N:1522:TGL:HC62	19:N:1522:TGL:HC32	1.90	0.41
3:C:160:LEU:HD13	23:C:271:CHD:H181	2.02	0.41
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.84	0.41
4:Q:144:GLU:OE1	4:Q:147:LYS:HE3	2.19	0.41
5:E:82:TYR:N	5:E:83:PRO:CD	2.83	0.41
1:N:266:GLU:HB2	1:N:267:PRO:HD2	2.02	0.41
1:A:488:THR:HB	1:A:495:LEU:HD13	2.02	0.41
10:W:58:LYS:HA	10:W:58:LYS:HD3	1.81	0.41
3:P:67:PHE:HA	10:W:9:GLN:HG2	2.02	0.41
10:J:33:ARG:HG2	23:J:60:CHD:H151	2.01	0.41
19:L:522:TGL:C24	19:L:522:TGL:C20	2.95	0.41
28:G:1263:PEK:H161	3:P:91:VAL:HG13	2.03	0.41
19:B:521:TGL:H201	19:B:521:TGL:C24	2.50	0.41
28:G:264:PEK:C10	28:G:264:PEK:H161	2.49	0.41
20:N:1524:PGV:H011	20:N:1524:PGV:C22	2.49	0.41
5:R:5:HIS:HB3	5:R:6:GLU:H	1.41	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.02	0.41
12:L:29:PHE:CZ	19:L:522:TGL:HA82	2.56	0.41
8:U:8:ILE:CG2	29:U:4330:HOH:O	2.44	0.41
2:O:196:CYS:CB	2:O:207:MET:HG3	2.50	0.41
7:T:58:LYS:NZ	7:T:58:LYS:CD	2.72	0.41
25:C:270:CDL:HA4	25:C:270:CDL:H122	2.02	0.41
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:335:SER:HB2	1:N:336:PRO:HD2	2.02	0.41
1:A:324:LEU:O	1:A:327:LEU:HB2	2.21	0.41
25:G:269:CDL:OA7	25:G:269:CDL:H342	2.21	0.41
25:C:270:CDL:H812	25:C:270:CDL:H852	2.03	0.41
9:I:27:VAL:HG12	9:I:28:SER:N	2.36	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.20	0.41
1:A:1:FME:HA	1:A:1:FME:CE	2.49	0.41
7:T:62:TRP:HB3	26:T:1272:DMU:H29	2.01	0.41
22:B:229:PSC:C02	22:B:229:PSC:H212	2.50	0.41
22:B:229:PSC:H071	5:E:8:ASP:HA	2.02	0.41
5:R:11:PHE:HB3	22:R:1229:PSC:H073	2.02	0.41
2:B:33:LEU:HD11	9:I:28:SER:CA	2.51	0.41
20:A:524:PGV:H242	13:M:15:GLN:NE2	2.35	0.41
2:B:41:ILE:O	2:B:45:MET:HG2	2.21	0.41
4:D:9:GLU:H	4:D:9:GLU:CD	2.24	0.41
2:B:144:LEU:HB2	2:B:213:LEU:HD13	2.03	0.41
25:T:1269:CDL:H821	25:T:1269:CDL:H791	1.70	0.40
14:A:515:HEA:H11	14:A:515:HEA:HHC	1.83	0.40
8:U:78:GLU:HG2	8:U:80:THR:HG23	2.04	0.40
5:E:90:ARG:NH2	29:E:4208:HOH:O	2.54	0.40
2:O:193:TYR:CD1	2:O:210:VAL:HG22	2.56	0.40
23:C:525:CHD:H12A	23:C:525:CHD:H112	1.52	0.40
2:B:191:LEU:HA	2:B:211:LEU:O	2.21	0.40
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.55	0.40
22:R:1229:PSC:H042	22:R:1229:PSC:H063	1.84	0.40
20:A:524:PGV:H202	20:A:524:PGV:H231	1.95	0.40
14:N:516:HEA:HAD2	14:N:516:HEA:HHA	1.83	0.40
23:P:1271:CHD:C16	23:P:1271:CHD:C23	2.96	0.40
5:E:108:LYS:HG2	5:E:108:LYS:O	2.20	0.40
1:A:183:LEU:HA	1:A:183:LEU:HD23	1.98	0.40
9:I:21:ILE:HA	9:I:21:ILE:HD13	1.96	0.40
8:U:9:LYS:O	8:U:10:ASN:CB	2.68	0.40
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.40
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.03	0.40
4:Q:93:ALA:O	4:Q:97:ILE:HG13	2.20	0.40
2:O:189:PRO:HD2	9:V:54:TYR:OH	2.21	0.40
11:K:31:TYR:CD2	11:K:35:GLN:HG3	2.56	0.40
2:B:135:LEU:O	2:B:208:PRO:HG3	2.22	0.40
2:B:74:ILE:HD11	25:T:1269:CDL:H461	2.04	0.40
19:N:1523:TGL:HC51	19:N:1523:TGL:HC22	1.88	0.40
1:A:449:MET:SD	2:B:5:MET:HG2	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:109:HIS:HD2	29:D:2122:HOH:O	2.03	0.40
7:T:8:HIS:ND1	28:T:263:PEK:H321	2.37	0.40
25:T:1269:CDL:OA7	25:T:1269:CDL:H342	2.22	0.40
4:D:34:SER:O	4:D:38:LYS:HG3	2.21	0.40
19:N:1522:TGL:HA51	12:Y:25:MET:HG2	2.02	0.40
9:V:52:ARG:CZ	9:V:52:ARG:HB2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
1	N	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
2	B	225/227 (99%)	213 (95%)	11 (5%)	1 (0%)	39	42
2	O	225/227 (99%)	212 (94%)	12 (5%)	1 (0%)	39	42
3	C	257/261 (98%)	253 (98%)	3 (1%)	1 (0%)	39	42
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	39	42
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	132 (93%)	9 (6%)	1 (1%)	26	25
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	5	2
6	S	96/98 (98%)	91 (95%)	3 (3%)	2 (2%)	9	5
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2	0
7	T	81/85 (95%)	65 (80%)	11 (14%)	5 (6%)	2	0
8	H	77/85 (91%)	66 (86%)	5 (6%)	6 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	1
9	I	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	6	3
9	V	71/73 (97%)	64 (90%)	4 (6%)	3 (4%)	3	1
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	7	4
All	All	3504/3614 (97%)	3339 (95%)	129 (4%)	36 (1%)	19	16

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	3	ALA
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	8	ILE
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	8	HIS
8	U	8	ILE
8	U	45	ALA
2	B	60	GLU
3	C	38	ASN
8	H	47	GLY
9	I	27	VAL
9	I	33	THR
2	O	60	GLU
3	P	38	ASN
7	T	3	ALA
7	T	40	GLY
6	F	95	GLN

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Mol	Chain	Res	Type
8	H	10	ASN
8	H	45	ALA
7	T	39	SER
8	U	46	LYS
6	F	96	LEU
8	H	9	LYS
8	U	9	LYS
9	V	28	SER
9	V	33	THR
9	V	37	PHE
4	Q	142	LYS
6	S	95	GLN
13	Z	41	LYS
7	G	6	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	416 (98%)	10 (2%)	58	71
1	N	426/426 (100%)	414 (97%)	12 (3%)	51	63
2	B	210/210 (100%)	199 (95%)	11 (5%)	29	33
2	O	210/210 (100%)	191 (91%)	19 (9%)	12	11
3	C	224/226 (99%)	216 (96%)	8 (4%)	42	52
3	P	224/226 (99%)	220 (98%)	4 (2%)	66	79
4	D	128/129 (99%)	122 (95%)	6 (5%)	32	39
4	Q	128/129 (99%)	121 (94%)	7 (6%)	27	30
5	E	92/95 (97%)	89 (97%)	3 (3%)	45	56
5	R	92/95 (97%)	84 (91%)	8 (9%)	13	12
6	F	81/81 (100%)	76 (94%)	5 (6%)	23	25
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	17
7	G	67/68 (98%)	60 (90%)	7 (10%)	9	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	59 (88%)	8 (12%)	6	5
8	H	71/75 (95%)	66 (93%)	5 (7%)	19	19
8	U	71/75 (95%)	64 (90%)	7 (10%)	10	9
9	I	57/57 (100%)	50 (88%)	7 (12%)	6	5
9	V	57/57 (100%)	48 (84%)	9 (16%)	3	2
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	76
10	W	49/50 (98%)	43 (88%)	6 (12%)	6	5
11	K	39/46 (85%)	36 (92%)	3 (8%)	16	16
11	X	39/46 (85%)	36 (92%)	3 (8%)	16	16
12	L	39/40 (98%)	37 (95%)	2 (5%)	29	34
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16	16
13	M	37/38 (97%)	32 (86%)	5 (14%)	5	3
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8	7
All	All	3040/3082 (99%)	2871 (94%)	169 (6%)	26	29

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	51	ASP
1	A	109	PHE
1	A	241	PRO
1	A	264	LYS
1	A	312	ILE
1	A	362	SER
1	A	363	LEU
1	A	369	ASP
1	A	513	LEU
2	B	60	GLU
2	B	64	ILE
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	113	TYR

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Mol	Chain	Res	Type
2	B	171	LYS
2	B	179	LEU
3	C	17	PRO
3	C	23	SER
3	C	33	MET
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	214	PHE
4	D	4	SER
4	D	7	LYS
4	D	36	SER
4	D	51	LEU
4	D	53	ILE
4	D	143	ASN
5	E	5	HIS
5	E	7	THR
5	E	70	VAL
6	F	48	LEU
6	F	84	SER
6	F	87	THR
6	F	95	GLN
6	F	96	LEU
7	G	8	HIS
7	G	18	PHE
7	G	33	LEU
7	G	35	SER
7	G	36	TRP
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	8	GLN
9	I	15	ARG
9	I	18	ARG
9	I	26	MET
9	I	31	PHE
9	I	33	THR

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Mol	Chain	Res	Type
9	I	37	PHE
10	J	50	LEU
11	K	32	MET
11	K	47	ARG
11	K	54	ARG
12	L	26	THR
12	L	46	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	65	MET
1	N	109	PHE
1	N	112	LEU
1	N	265	LYS
1	N	338	MET
1	N	362	SER
1	N	363	LEU
1	N	369	ASP
1	N	483	LEU
1	N	486	ASP
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	88	ASP
2	O	94	SER
2	O	107	SER
2	O	110	TYR
2	O	113	TYR
2	O	148	MET
2	O	167	SER
2	O	171	LYS
2	O	183	THR
2	O	202	SER
2	O	217	LYS

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Mol	Chain	Res	Type
2	O	226	MET
3	P	77	LYS
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
4	Q	5	VAL
4	Q	6	VAL
4	Q	19	ARG
4	Q	34	SER
4	Q	51	LEU
4	Q	53	ILE
4	Q	143	ASN
5	R	5	HIS
5	R	21	LYS
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
5	R	90	ARG
5	R	108	LYS
5	R	109	VAL
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	78	GLU
6	S	87	THR
7	T	33	LEU
7	T	35	SER
7	T	38	HIS
7	T	43	GLU
7	T	48	ILE
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	27	ARG
8	U	52	VAL
8	U	60	TYR
8	U	61	LYS
8	U	70	SER
9	V	2	THR

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Mol	Chain	Res	Type
9	V	8	GLN
9	V	18	ARG
9	V	21	ILE
9	V	25	PHE
9	V	31	PHE
9	V	52	ARG
9	V	65	LYS
9	V	73	LYS
10	W	10	LYS
10	W	15	ASP
10	W	27	THR
10	W	29	ASN
10	W	50	LEU
10	W	58	LYS
11	X	32	MET
11	X	47	ARG
11	X	54	ARG
12	Y	16	GLU
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	52	HIS
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	149	HIS
4	D	37	GLN
5	E	94	ASN
7	G	76	ASN
10	J	57	HIS

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Mol	Chain	Res	Type
12	L	2	HIS
13	M	15	GLN
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	161	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
7	T	76	ASN
8	U	22	ASN
9	V	8	GLN
10	W	29	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	A	1	1	8,9,10	0.76	0	6,9,11	5.94	5 (83%)
2	FME	B	1	2	8,9,10	1.32	1 (12%)	6,9,11	7.17	3 (50%)
7	TPO	G	11	7	8,10,11	2.23	4 (50%)	7,14,16	2.37	2 (28%)
9	SAC	I	1	9	7,8,9	3.70	2 (28%)	7,9,11	3.57	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	FME	N	1	1	8,9,10	0.90	0	6,9,11	5.05	3 (50%)
2	FME	O	1	2	8,9,10	0.84	0	6,9,11	4.49	3 (50%)
7	TPO	T	11	7	8,10,11	2.26	5 (62%)	7,14,16	2.31	2 (28%)
9	SAC	V	1	9	7,8,9	3.70	3 (42%)	7,9,11	2.78	4 (57%)

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

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-3.19	1.12	1.22
7	T	11	TPO	P-O2P	2.08	1.62	1.54
7	G	11	TPO	P-O3P	2.14	1.62	1.54
7	T	11	TPO	CG2-CB	2.32	1.57	1.51
7	G	11	TPO	P-O2P	2.32	1.63	1.54
7	T	11	TPO	P-OG1	2.42	1.67	1.60
7	G	11	TPO	CG2-CB	2.47	1.57	1.51
9	V	1	SAC	CB-CA	2.48	1.58	1.52
7	T	11	TPO	P-O3P	2.62	1.64	1.54
7	T	11	TPO	P-O1P	3.38	1.62	1.51
7	G	11	TPO	P-O1P	3.59	1.63	1.51
9	V	1	SAC	OAC-C1A	5.37	1.35	1.23
9	I	1	SAC	OAC-C1A	6.31	1.37	1.23
9	I	1	SAC	CA-N	6.85	1.56	1.46
9	V	1	SAC	CA-N	7.45	1.57	1.46

All (25) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.81	96.98	122.82
1	A	1	FME	CA-N-CN	-12.33	103.86	122.82
1	N	1	FME	CA-N-CN	-10.28	107.00	122.82
2	O	1	FME	CA-N-CN	-9.32	108.49	122.82
9	I	1	SAC	CB-CA-N	-7.68	93.78	110.60
2	O	1	FME	O1-CN-N	-4.57	118.17	124.76
2	B	1	FME	O1-CN-N	-3.75	119.36	124.76
7	T	11	TPO	O-C-CA	-3.06	117.37	125.44
2	B	1	FME	O-C-CA	-2.82	118.00	125.44
1	A	1	FME	CG-CB-CA	-2.80	104.84	113.06
9	V	1	SAC	OAC-C1A-C2A	-2.75	117.01	122.06
2	O	1	FME	O-C-CA	-2.51	118.80	125.44
7	G	11	TPO	O-C-CA	-2.48	118.88	125.44
1	A	1	FME	O-C-CA	-2.20	119.62	125.44
9	I	1	SAC	OAC-C1A-N	2.07	126.08	121.86
9	V	1	SAC	OG-CB-CA	2.35	116.38	111.04
9	V	1	SAC	C2A-C1A-N	3.72	123.22	116.11
1	A	1	FME	O1-CN-N	3.87	130.32	124.76
1	N	1	FME	O1-CN-N	4.08	130.63	124.76
9	I	1	SAC	CA-N-C1A	4.28	135.88	121.37
7	T	11	TPO	CG2-CB-CA	4.71	122.75	113.17
9	V	1	SAC	CA-N-C1A	4.86	137.86	121.37
1	N	1	FME	CE-SD-CG	4.94	117.22	100.37
7	G	11	TPO	CG2-CB-CA	5.40	124.15	113.17
1	A	1	FME	CE-SD-CG	5.63	119.60	100.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	HEA	A	515	1	40,67,67	1.52	8 (20%)	41,103,103	2.82	13 (31%)
14	HEA	A	516	1	40,67,67	1.36	6 (15%)	41,103,103	2.37	13 (31%)
15	CMO	A	520	-	0,1,1	0.00	-	0,0,0	0.00	-
20	PGV	A	521	-	50,50,50	0.81	2 (4%)	51,56,56	1.75	8 (15%)
19	TGL	A	523	-	62,62,62	1.38	6 (9%)	65,65,65	1.73	11 (16%)
20	PGV	A	524	-	50,50,50	1.30	4 (8%)	51,56,56	1.46	7 (13%)
23	CHD	B	1085	-	29,32,32	1.54	4 (13%)	48,51,51	5.60	36 (75%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	229	-	51,51,51	1.37	3 (5%)	55,59,59	1.34	7 (12%)
19	TGL	B	521	-	62,62,62	1.45	8 (12%)	65,65,65	2.64	16 (24%)
20	PGV	C	267	-	50,50,50	0.88	2 (4%)	51,56,56	1.23	7 (13%)
20	PGV	C	268	-	50,50,50	1.41	2 (4%)	51,56,56	1.76	9 (17%)
25	CDL	C	270	-	99,99,99	1.40	14 (14%)	101,111,111	1.46	15 (14%)
23	CHD	C	271	-	29,32,32	0.83	1 (3%)	48,51,51	5.01	33 (68%)
26	DMU	C	272	-	34,34,34	1.30	5 (14%)	45,45,45	3.46	21 (46%)
23	CHD	C	525	-	29,32,32	1.34	3 (10%)	48,51,51	5.10	37 (77%)
28	PEK	G	1263	-	51,52,52	1.39	5 (9%)	52,57,57	1.58	8 (15%)
28	PEK	G	264	-	51,52,52	1.03	5 (9%)	52,57,57	1.64	11 (21%)
28	PEK	G	265	-	51,52,52	1.70	7 (13%)	52,57,57	1.63	9 (17%)
25	CDL	G	269	-	99,99,99	1.41	13 (13%)	101,111,111	1.46	17 (16%)
23	CHD	J	60	-	29,32,32	0.88	0	48,51,51	5.36	36 (75%)
19	TGL	L	522	-	62,62,62	1.66	10 (16%)	65,65,65	2.01	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	DMU	M	526	-	34,34,34	1.24	2 (5%)	45,45,45	3.50	22 (48%)
20	PGV	N	1266	-	50,50,50	0.83	2 (4%)	51,56,56	1.41	6 (11%)
19	TGL	N	1521	-	62,62,62	1.39	9 (14%)	65,65,65	2.29	14 (21%)
19	TGL	N	1522	-	62,62,62	1.60	7 (11%)	65,65,65	1.81	17 (26%)
19	TGL	N	1523	-	62,62,62	1.40	7 (11%)	65,65,65	1.46	10 (15%)
20	PGV	N	1524	-	50,50,50	1.22	2 (4%)	51,56,56	1.27	7 (13%)
14	HEA	N	515	1	40,67,67	1.28	5 (12%)	41,103,103	2.63	15 (36%)
14	HEA	N	516	1,15	40,67,67	1.49	6 (15%)	41,103,103	2.39	14 (34%)
15	CMO	N	520	14	0,1,1	0.00	-	0,0,0	0.00	-
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.45	4 (13%)	48,51,51	5.50	35 (72%)
20	PGV	P	1267	-	50,50,50	0.99	2 (4%)	51,56,56	1.03	4 (7%)
20	PGV	P	1268	-	50,50,50	1.37	2 (4%)	51,56,56	1.64	9 (17%)
25	CDL	P	1270	-	99,99,99	1.42	13 (13%)	101,111,111	1.44	12 (11%)
23	CHD	P	1271	-	29,32,32	0.78	1 (3%)	48,51,51	5.24	34 (70%)
23	CHD	P	1525	-	29,32,32	1.03	2 (6%)	48,51,51	5.41	36 (75%)
22	PSC	R	1229	-	51,51,51	1.33	3 (5%)	55,59,59	1.28	4 (7%)
28	PEK	S	1265	-	51,52,52	1.26	2 (3%)	52,57,57	1.39	6 (11%)
28	PEK	T	1264	-	51,52,52	0.91	4 (7%)	52,57,57	1.49	10 (19%)
25	CDL	T	1269	-	99,99,99	1.47	13 (13%)	101,111,111	1.53	13 (12%)
26	DMU	T	1272	-	34,34,34	1.33	3 (8%)	45,45,45	3.22	23 (51%)
28	PEK	T	263	-	51,52,52	1.40	4 (7%)	52,57,57	1.29	6 (11%)
23	CHD	W	1059	-	29,32,32	0.58	0	48,51,51	5.10	35 (72%)
26	DMU	Z	1526	-	34,34,34	0.98	3 (8%)	45,45,45	3.21	21 (46%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
15	CMO	A	520	-	-	0/0/0/0	0/0/0/0
20	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	TGL	A	523	-	-	0/65/65/65	0/0/0/0
20	PGV	A	524	-	-	2/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	B	1085	-	1/1/12/12	0/7/74/74	0/4/4/4
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	229	-	-	0/55/55/55	0/0/0/0
19	TGL	B	521	-	-	0/65/65/65	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
25	CDL	C	270	-	-	1/110/110/110	0/0/0/0
23	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
26	DMU	C	272	-	5/5/10/10	0/19/59/59	0/2/2/2
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
28	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
28	PEK	G	264	-	-	0/56/56/56	0/0/0/0
28	PEK	G	265	-	-	0/56/56/56	0/0/0/0
25	CDL	G	269	-	-	0/110/110/110	0/0/0/0
23	CHD	J	60	-	1/1/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
26	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1521	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	1/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	CMO	N	520	14	-	0/0/0/0	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	1/1/12/12	0/7/74/74	0/4/4/4
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
25	CDL	P	1270	-	-	1/110/110/110	0/0/0/0
23	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
22	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
28	PEK	S	1265	-	-	0/56/56/56	0/0/0/0
28	PEK	T	1264	-	-	0/56/56/56	0/0/0/0
25	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
26	DMU	T	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
28	PEK	T	263	-	-	0/56/56/56	0/0/0/0
23	CHD	W	1059	-	2/2/12/12	0/7/74/74	0/4/4/4
26	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	521	TGL	OC1-CC1	-4.65	1.08	1.22
26	M	526	DMU	C3-C4	-3.83	1.42	1.52
23	O	229	CHD	C13-C14	-3.63	1.49	1.55
14	N	516	HEA	C3A-C2A	-3.54	1.35	1.40
25	T	1269	CDL	C59-C58	-3.53	1.31	1.51
14	A	516	HEA	C4A-NA	-3.47	1.32	1.36
14	A	516	HEA	C3A-C2A	-3.37	1.35	1.40
25	P	1270	CDL	C59-C58	-3.37	1.32	1.51
19	B	521	TGL	C10-CB9	-3.32	1.32	1.51
19	L	522	TGL	C20-CA9	-3.24	1.32	1.51
14	N	516	HEA	C4A-NA	-3.23	1.32	1.36
25	C	270	CDL	C59-C58	-3.22	1.32	1.51
25	G	269	CDL	C59-C58	-3.21	1.33	1.51
19	N	1521	TGL	C10-CB9	-3.19	1.33	1.51
25	T	1269	CDL	C62-C61	-3.18	1.33	1.51
25	G	269	CDL	C62-C61	-3.12	1.33	1.51
25	T	1269	CDL	C42-C41	-3.08	1.33	1.51
19	N	1522	TGL	C20-CA9	-3.08	1.33	1.51
19	N	1522	TGL	C10-CB9	-3.06	1.33	1.51
19	N	1523	TGL	C10-CB9	-3.06	1.33	1.51
28	G	264	PEK	O03-C01	-3.02	1.38	1.45
25	P	1270	CDL	C62-C61	-3.00	1.34	1.51
25	T	1269	CDL	C19-C18	-2.98	1.34	1.51
25	P	1270	CDL	C79-C78	-2.94	1.34	1.51
19	B	521	TGL	C20-CA9	-2.93	1.34	1.51
25	C	270	CDL	C62-C61	-2.93	1.34	1.51
25	P	1270	CDL	C39-C38	-2.85	1.35	1.51
25	C	270	CDL	C82-C81	-2.83	1.35	1.51
25	P	1270	CDL	C22-C21	-2.83	1.35	1.51
19	A	523	TGL	C10-CB9	-2.82	1.35	1.51
23	B	1085	CHD	C13-C14	-2.82	1.50	1.55
25	C	270	CDL	C22-C21	-2.81	1.35	1.51
19	A	523	TGL	C20-CA9	-2.79	1.35	1.51
25	P	1270	CDL	C82-C81	-2.79	1.35	1.51
19	N	1521	TGL	C20-CA9	-2.78	1.35	1.51
26	Z	1526	DMU	C3-C4	-2.76	1.45	1.52
19	L	522	TGL	C10-CB9	-2.76	1.35	1.51
14	N	515	HEA	C3C-C2C	-2.75	1.36	1.40
25	C	270	CDL	C19-C18	-2.75	1.35	1.51
25	T	1269	CDL	C39-C38	-2.75	1.35	1.51
23	B	1085	CHD	C10-C5	-2.74	1.50	1.55
25	P	1270	CDL	C19-C18	-2.72	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	1269	CDL	C79-C78	-2.70	1.35	1.51
19	A	523	TGL	C15-CC9	-2.66	1.36	1.51
25	G	269	CDL	C79-C78	-2.59	1.36	1.51
19	N	1523	TGL	C20-CA9	-2.58	1.36	1.51
25	T	1269	CDL	C22-C21	-2.58	1.36	1.51
25	G	269	CDL	C22-C21	-2.56	1.36	1.51
25	T	1269	CDL	C82-C81	-2.54	1.36	1.51
28	T	1264	PEK	O01-C02	-2.54	1.40	1.46
28	T	1264	PEK	O03-C01	-2.53	1.39	1.45
14	A	515	HEA	C1A-NA	-2.52	1.33	1.36
25	P	1270	CDL	C42-C41	-2.49	1.37	1.51
23	P	1525	CHD	C13-C14	-2.47	1.51	1.55
28	G	264	PEK	O01-C02	-2.46	1.40	1.46
25	G	269	CDL	C19-C18	-2.46	1.37	1.51
19	N	1521	TGL	OG1-CG1	-2.45	1.39	1.45
25	G	269	CDL	C39-C38	-2.44	1.37	1.51
19	L	522	TGL	C15-CC9	-2.41	1.37	1.51
19	N	1523	TGL	C15-CC9	-2.40	1.37	1.51
25	G	269	CDL	C82-C81	-2.40	1.37	1.51
25	C	270	CDL	OB6-CB4	-2.36	1.40	1.46
19	N	1521	TGL	OC1-CC1	-2.34	1.15	1.22
25	G	269	CDL	C42-C41	-2.31	1.38	1.51
19	N	1522	TGL	C15-CC9	-2.31	1.38	1.51
19	B	521	TGL	OG1-CG1	-2.23	1.40	1.45
23	C	271	CHD	C10-C9	-2.16	1.51	1.56
19	B	521	TGL	C15-CC9	-2.13	1.39	1.51
14	N	516	HEA	CMB-C2B	-2.07	1.47	1.51
23	O	229	CHD	C13-C17	-2.05	1.51	1.55
26	C	272	DMU	C3-C4	-2.01	1.47	1.52
23	C	525	CHD	C13-C14	-2.00	1.52	1.55
28	G	264	PEK	C2-C1	2.01	1.56	1.50
25	C	270	CDL	CB2-C1	2.03	1.59	1.51
26	Z	1526	DMU	O1-C10	2.03	1.47	1.41
19	L	522	TGL	CG1-CG2	2.04	1.56	1.50
14	N	515	HEA	C3C-CAC	2.05	1.52	1.47
20	A	524	PGV	C03-C02	2.05	1.56	1.50
23	C	525	CHD	C19-C10	2.07	1.58	1.54
28	G	265	PEK	P-O12	2.07	1.68	1.59
25	C	270	CDL	PB2-OB2	2.07	1.68	1.59
19	L	522	TGL	OG2-CG2	2.08	1.51	1.46
20	A	524	PGV	P-O11	2.08	1.68	1.59
14	N	516	HEA	C4D-CHA	2.08	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	516	HEA	C22-C23	2.09	1.38	1.32
26	C	272	DMU	O5-C6	2.09	1.47	1.41
19	N	1521	TGL	C18-C17	2.10	1.63	1.51
28	T	1264	PEK	O03-C21	2.11	1.39	1.33
25	P	1270	CDL	CA6-CA4	2.14	1.56	1.50
14	A	515	HEA	CAD-C3D	2.14	1.55	1.52
28	G	1263	PEK	C03-C02	2.18	1.56	1.50
14	A	515	HEA	O11-C11	2.20	1.47	1.42
28	G	1263	PEK	P-O12	2.21	1.69	1.59
25	T	1269	CDL	CB3-CB4	2.23	1.57	1.50
26	T	1272	DMU	O1-C10	2.23	1.47	1.41
23	P	1525	CHD	C11-C9	2.23	1.57	1.53
14	A	515	HEA	C1B-CHB	2.25	1.46	1.39
25	G	269	CDL	CB3-CB4	2.25	1.57	1.50
14	A	516	HEA	C1C-CHC	2.25	1.46	1.39
14	N	516	HEA	O11-C11	2.34	1.48	1.42
23	O	229	CHD	C11-C9	2.34	1.57	1.53
14	A	516	HEA	C1B-CHB	2.35	1.46	1.39
26	T	1272	DMU	O5-C6	2.35	1.47	1.41
28	T	263	PEK	C03-C02	2.45	1.57	1.50
14	A	515	HEA	C3A-C2A	2.45	1.43	1.40
28	G	264	PEK	O03-C21	2.47	1.40	1.33
28	G	265	PEK	C7-C8	2.51	1.64	1.51
20	A	521	PGV	O03-C01	2.51	1.50	1.45
19	N	1522	TGL	CG3-CG2	2.54	1.57	1.50
19	N	1521	TGL	C17-C16	2.55	1.66	1.51
26	C	272	DMU	C8-C7	2.56	1.59	1.52
14	N	515	HEA	C4C-CHD	2.56	1.46	1.39
20	N	1266	PGV	O03-C19	2.58	1.41	1.33
19	N	1523	TGL	C17-C16	2.59	1.66	1.51
23	O	229	CHD	C4-C3	2.60	1.56	1.51
14	A	515	HEA	C20-C19	2.62	1.57	1.51
20	C	267	PGV	O03-C19	2.63	1.41	1.33
19	L	522	TGL	CC2-CC1	2.64	1.58	1.50
19	L	522	TGL	CG3-CG2	2.65	1.58	1.50
14	N	515	HEA	C1A-NA	2.69	1.40	1.36
14	A	516	HEA	C14-C15	2.69	1.38	1.33
23	B	1085	CHD	C4-C3	2.73	1.57	1.51
28	T	263	PEK	C01-C02	2.84	1.58	1.50
28	G	1263	PEK	C01-C02	2.84	1.58	1.50
26	C	272	DMU	O1-C10	2.90	1.49	1.41
25	C	270	CDL	C37-C36	2.91	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	267	PGV	O01-C1	2.93	1.43	1.34
23	P	1271	CHD	C20-C17	2.94	1.59	1.54
14	A	515	HEA	CMB-C2B	2.95	1.57	1.51
20	P	1267	PGV	O01-C1	3.08	1.43	1.34
14	N	515	HEA	C4D-CHA	3.16	1.48	1.39
19	B	521	TGL	OG3-CC1	3.18	1.42	1.33
28	T	1264	PEK	O01-C1	3.19	1.43	1.34
26	Z	1526	DMU	O16-C6	3.22	1.45	1.40
20	A	521	PGV	O03-C19	3.33	1.43	1.33
25	C	270	CDL	C40-C39	3.35	1.70	1.51
20	N	1266	PGV	O01-C1	3.41	1.44	1.34
28	G	265	PEK	C6-C5	3.44	1.51	1.31
28	G	264	PEK	O01-C1	3.51	1.44	1.34
28	G	265	PEK	O03-C21	3.74	1.44	1.33
26	M	526	DMU	O16-C6	3.75	1.46	1.40
20	P	1267	PGV	O03-C19	3.85	1.44	1.33
14	N	516	HEA	C18-C19	3.90	1.40	1.33
14	A	515	HEA	C13-C14	3.93	1.61	1.50
25	C	270	CDL	OA8-CA7	4.00	1.45	1.33
19	N	1523	TGL	OG1-CA1	4.01	1.45	1.33
25	C	270	CDL	OB6-CB5	4.07	1.46	1.34
19	N	1521	TGL	OG3-CC1	4.08	1.45	1.33
20	A	524	PGV	O01-C1	4.14	1.46	1.34
19	A	523	TGL	OG1-CA1	4.15	1.45	1.33
22	R	1229	PSC	C13-C12	4.20	1.56	1.31
22	B	229	PSC	C13-C12	4.21	1.56	1.31
19	N	1521	TGL	OG2-CB1	4.23	1.47	1.34
25	C	270	CDL	OB8-CB7	4.27	1.46	1.33
25	G	269	CDL	OA8-CA7	4.29	1.46	1.33
20	P	1268	PGV	O03-C19	4.36	1.46	1.33
19	B	521	TGL	OG2-CB1	4.46	1.47	1.34
23	B	1085	CHD	C18-C13	4.46	1.61	1.54
26	C	272	DMU	O16-C6	4.46	1.48	1.40
22	B	229	PSC	O03-C19	4.47	1.46	1.33
25	P	1270	CDL	OB6-CB5	4.48	1.47	1.34
22	R	1229	PSC	O03-C19	4.58	1.47	1.33
25	P	1270	CDL	OB8-CB7	4.59	1.47	1.33
28	G	1263	PEK	O01-C1	4.61	1.48	1.34
25	G	269	CDL	OB8-CB7	4.64	1.47	1.33
20	N	1524	PGV	O01-C1	4.68	1.48	1.34
20	C	268	PGV	O03-C19	4.83	1.47	1.33
19	N	1521	TGL	OG1-CA1	4.85	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	1269	CDL	OA8-CA7	4.88	1.48	1.33
19	B	521	TGL	OG1-CA1	4.88	1.48	1.33
19	A	523	TGL	OG3-CC1	4.88	1.48	1.33
28	G	265	PEK	C17-C16	4.94	1.71	1.52
25	G	269	CDL	OA6-CA5	4.94	1.49	1.34
19	N	1523	TGL	OG3-CC1	4.95	1.48	1.33
22	R	1229	PSC	O01-C1	4.95	1.49	1.34
23	C	525	CHD	C18-C13	4.96	1.62	1.54
25	P	1270	CDL	OA6-CA5	5.00	1.49	1.34
28	S	1265	PEK	O03-C21	5.00	1.48	1.33
25	C	270	CDL	OA6-CA5	5.01	1.49	1.34
25	T	1269	CDL	OB6-CB5	5.02	1.49	1.34
25	T	1269	CDL	OA6-CA5	5.02	1.49	1.34
20	N	1524	PGV	O03-C19	5.02	1.48	1.33
28	G	265	PEK	O01-C1	5.03	1.49	1.34
26	T	1272	DMU	O16-C6	5.03	1.49	1.40
25	P	1270	CDL	OA8-CA7	5.05	1.48	1.33
28	T	263	PEK	O01-C1	5.05	1.49	1.34
28	S	1265	PEK	O01-C1	5.06	1.49	1.34
19	N	1522	TGL	OG1-CA1	5.06	1.48	1.33
19	N	1522	TGL	OG3-CC1	5.15	1.48	1.33
19	L	522	TGL	OG3-CC1	5.17	1.48	1.33
25	G	269	CDL	OB6-CB5	5.25	1.50	1.34
22	B	229	PSC	O01-C1	5.26	1.50	1.34
25	T	1269	CDL	OB8-CB7	5.28	1.49	1.33
19	L	522	TGL	OG1-CA1	5.32	1.49	1.33
28	G	265	PEK	C7-C6	5.58	1.81	1.51
20	A	524	PGV	O03-C19	5.59	1.50	1.33
19	N	1523	TGL	OG2-CB1	5.60	1.51	1.34
19	A	523	TGL	OG2-CB1	5.63	1.51	1.34
28	T	263	PEK	O03-C21	6.16	1.51	1.33
28	G	1263	PEK	O03-C21	6.23	1.52	1.33
20	P	1268	PGV	O01-C1	6.67	1.54	1.34
20	C	268	PGV	O01-C1	6.78	1.54	1.34
19	N	1522	TGL	OG2-CB1	7.03	1.55	1.34
19	L	522	TGL	OG2-CB1	7.17	1.55	1.34

All (683) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C18-C13-C12	-12.07	97.32	109.09
23	O	229	CHD	C18-C13-C12	-12.07	97.32	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C18-C13-C12	-10.27	99.07	109.09
23	O	229	CHD	C19-C10-C9	-9.69	96.65	111.18
23	C	525	CHD	O12-C12-C13	-9.36	95.93	111.11
14	N	515	HEA	C13-C12-C11	-9.31	102.14	114.51
23	P	1271	CHD	C18-C13-C12	-8.72	100.58	109.09
23	P	1525	CHD	C19-C10-C9	-8.70	98.13	111.18
23	C	525	CHD	C18-C13-C12	-8.70	100.61	109.09
14	A	515	HEA	C4B-C3B-C11	-8.43	117.85	127.01
14	A	515	HEA	CAA-CBA-CGA	-8.13	97.85	112.75
23	W	1059	CHD	C6-C5-C4	-8.00	102.11	111.05
23	P	1525	CHD	C18-C13-C14	-7.35	99.63	111.22
23	J	60	CHD	C6-C5-C4	-7.33	102.86	111.05
23	C	271	CHD	C18-C13-C12	-7.29	101.98	109.09
23	W	1059	CHD	C1-C10-C9	-7.22	99.81	111.45
23	O	229	CHD	O12-C12-C13	-7.06	99.67	111.11
23	B	1085	CHD	C6-C5-C4	-7.05	103.17	111.05
23	O	229	CHD	C6-C5-C4	-7.00	103.23	111.05
23	P	1271	CHD	C18-C13-C17	-6.99	100.20	111.22
23	B	1085	CHD	O12-C12-C13	-6.82	100.05	111.11
14	N	516	HEA	CAD-C3D-C4D	-6.74	119.69	127.01
23	O	229	CHD	C18-C13-C17	-6.61	100.79	111.22
14	A	515	HEA	C13-C12-C11	-6.43	105.96	114.51
23	B	1085	CHD	C18-C13-C14	-6.42	101.08	111.22
20	A	521	PGV	O03-C19-O04	-6.35	107.10	123.49
23	C	525	CHD	C19-C10-C9	-6.34	101.68	111.18
23	J	60	CHD	O7-C7-C6	-6.30	94.64	110.06
23	B	1085	CHD	C19-C10-C9	-6.29	101.75	111.18
14	N	515	HEA	C4B-C3B-C11	-6.27	120.20	127.01
23	P	1271	CHD	O7-C7-C6	-6.23	94.80	110.06
23	C	271	CHD	C19-C10-C9	-6.22	101.86	111.18
19	B	521	TGL	OG3-CG3-CG2	-6.20	92.01	108.69
23	B	1085	CHD	C23-C22-C20	-6.08	107.59	114.75
23	C	525	CHD	C23-C22-C20	-5.94	107.75	114.75
23	P	1525	CHD	C18-C13-C12	-5.93	103.31	109.09
23	C	271	CHD	O7-C7-C6	-5.86	95.71	110.06
23	B	1085	CHD	C18-C13-C17	-5.78	102.11	111.22
14	A	516	HEA	CAD-CBD-CGD	-5.75	102.20	112.75
23	P	1525	CHD	C6-C5-C4	-5.70	104.68	111.05
23	P	1271	CHD	C23-C22-C20	-5.64	108.10	114.75
23	P	1271	CHD	C19-C10-C9	-5.63	102.73	111.18
28	G	264	PEK	O03-C01-C02	-5.62	93.56	108.69
14	A	516	HEA	CAA-CBA-CGA	-5.61	102.46	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	O12-C12-C13	-5.58	102.06	111.11
23	C	271	CHD	C23-C22-C20	-5.20	108.62	114.75
23	W	1059	CHD	O12-C12-C11	-5.18	98.46	109.06
28	T	1264	PEK	O03-C01-C02	-5.15	94.83	108.69
26	M	526	DMU	O7-C10-C5	-4.92	96.13	108.10
23	C	525	CHD	C6-C5-C4	-4.88	105.60	111.05
23	J	60	CHD	C1-C10-C9	-4.78	103.74	111.45
20	N	1266	PGV	O03-C19-O04	-4.77	111.17	123.49
23	W	1059	CHD	O7-C7-C6	-4.77	98.37	110.06
23	C	525	CHD	C18-C13-C17	-4.73	103.75	111.22
23	W	1059	CHD	C18-C13-C12	-4.73	104.48	109.09
19	L	522	TGL	OG3-CC1-OC1	-4.72	111.30	123.49
19	B	521	TGL	OG1-CA1-OA1	-4.59	111.65	123.49
23	P	1525	CHD	O7-C7-C6	-4.57	98.86	110.06
23	W	1059	CHD	C18-C13-C14	-4.48	104.14	111.22
23	C	271	CHD	C6-C5-C4	-4.47	106.06	111.05
23	C	525	CHD	O7-C7-C6	-4.46	99.13	110.06
14	A	516	HEA	C1A-C2A-C3A	-4.35	102.72	107.07
23	J	60	CHD	O12-C12-C11	-4.35	100.17	109.06
23	J	60	CHD	C18-C13-C14	-4.34	104.37	111.22
23	P	1271	CHD	C6-C5-C4	-4.24	106.31	111.05
14	A	516	HEA	C20-C19-C18	-4.20	113.08	121.05
14	A	515	HEA	C27-C19-C18	-4.15	115.34	123.50
23	O	229	CHD	C1-C10-C9	-4.13	104.78	111.45
23	P	1525	CHD	O12-C12-C11	-4.13	100.61	109.06
14	A	515	HEA	C13-C14-C15	-4.10	118.85	127.76
19	N	1521	TGL	CG1-OG1-CA1	-4.08	105.44	116.85
19	N	1522	TGL	OG3-CC1-OC1	-4.08	112.97	123.49
23	C	525	CHD	C18-C13-C14	-4.06	104.82	111.22
23	O	229	CHD	O7-C7-C6	-4.05	100.14	110.06
23	P	1525	CHD	C18-C13-C17	-4.00	104.91	111.22
20	A	524	PGV	C4-C3-C2	-3.93	98.87	113.29
23	C	525	CHD	C22-C20-C17	-3.92	102.00	110.24
19	B	521	TGL	CG3-CG2-CG1	-3.87	103.03	112.07
23	P	1271	CHD	O12-C12-C11	-3.85	101.18	109.06
28	G	265	PEK	C7-C6-C5	-3.84	101.25	125.00
23	C	271	CHD	O12-C12-C13	-3.83	104.91	111.11
26	M	526	DMU	C22-C19-C18	-3.80	96.47	113.47
14	N	516	HEA	OMA-CMA-C3A	-3.79	117.45	125.11
23	C	271	CHD	C18-C13-C17	-3.76	105.28	111.22
23	P	1525	CHD	C23-C22-C20	-3.74	110.35	114.75
14	N	516	HEA	C1A-C2A-C3A	-3.71	103.36	107.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	521	TGL	CG1-OG1-CA1	-3.66	106.60	116.85
14	N	515	HEA	CAD-C3D-C4D	-3.66	123.03	127.01
14	A	515	HEA	C26-C15-C16	-3.63	109.86	115.41
23	B	1085	CHD	C19-C10-C5	-3.63	103.84	110.25
20	C	267	PGV	C22-C21-C20	-3.61	100.06	113.29
23	J	60	CHD	C19-C10-C5	-3.59	103.91	110.25
23	O	229	CHD	C22-C20-C17	-3.58	102.72	110.24
14	N	515	HEA	C26-C15-C14	-3.54	116.56	123.50
23	B	1085	CHD	C1-C10-C9	-3.50	105.80	111.45
23	P	1525	CHD	C1-C10-C9	-3.46	105.88	111.45
28	G	264	PEK	O01-C1-O02	-3.42	114.49	123.67
25	C	270	CDL	CB4-OB6-CB5	-3.41	109.72	117.89
23	C	525	CHD	C1-C10-C9	-3.36	106.03	111.45
25	C	270	CDL	C52-C51-CB5	-3.33	100.49	113.59
25	C	270	CDL	OB8-CB7-OB9	-3.32	114.92	123.49
19	B	521	TGL	OG3-CC1-OC1	-3.30	114.97	123.49
19	N	1521	TGL	OG1-CA1-OA1	-3.26	115.08	123.49
28	G	265	PEK	O03-C21-O04	-3.25	115.11	123.49
28	G	265	PEK	C8-C7-C6	-3.24	101.21	112.00
20	A	521	PGV	C02-O01-C1	-3.24	110.11	117.89
23	C	525	CHD	C21-C20-C22	-3.23	104.97	110.35
14	N	515	HEA	CMB-C2B-C1B	-3.22	123.03	128.36
25	C	270	CDL	OA8-CA7-OA9	-3.20	115.22	123.49
19	L	522	TGL	OB1-CB1-CB2	-3.19	110.96	123.72
28	G	264	PEK	C24-C23-C22	-3.18	101.62	113.29
20	P	1267	PGV	O03-C19-O04	-3.18	115.29	123.49
14	A	516	HEA	CMB-C2B-C1B	-3.17	123.12	128.36
20	C	267	PGV	C27-C26-C25	-3.15	98.29	114.53
28	T	1264	PEK	C32-C31-C30	-3.14	98.29	114.53
20	P	1268	PGV	O04-C19-C20	-3.14	111.14	123.72
20	C	268	PGV	O04-C19-C20	-3.14	111.17	123.72
23	C	271	CHD	C19-C10-C1	-3.12	102.96	108.20
14	N	516	HEA	C20-C19-C18	-3.09	115.19	121.05
19	N	1523	TGL	OG1-CA1-OA1	-3.09	115.53	123.49
19	N	1522	TGL	OB1-CB1-CB2	-3.08	111.40	123.72
28	G	264	PEK	O01-C02-C03	-3.08	97.52	108.36
23	O	229	CHD	C18-C13-C14	-3.05	106.41	111.22
19	L	522	TGL	CA5-CA4-CA3	-3.02	98.93	114.53
23	B	1085	CHD	O7-C7-C8	-3.02	102.60	109.26
14	N	516	HEA	CMC-C2C-C1C	-3.01	123.39	128.36
28	T	1264	PEK	O01-C1-O02	-3.01	115.60	123.67
20	C	268	PGV	O02-C1-C2	-2.97	111.86	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	S	1265	PEK	O03-C21-O04	-2.95	115.87	123.49
14	N	516	HEA	C26-C15-C14	-2.95	117.71	123.50
20	P	1268	PGV	C03-C02-C01	-2.95	105.18	112.07
23	C	271	CHD	O12-C12-C11	-2.93	103.07	109.06
23	B	1085	CHD	C21-C20-C17	-2.92	108.10	112.96
23	C	525	CHD	C19-C10-C5	-2.92	105.10	110.25
23	P	1271	CHD	O12-C12-C13	-2.91	106.39	111.11
28	G	264	PEK	O01-C02-C01	-2.91	98.10	108.36
25	T	1269	CDL	CB2-C1-CA2	-2.90	103.55	112.92
19	N	1523	TGL	CG3-CG2-CG1	-2.87	105.35	112.07
28	G	264	PEK	C27-C26-C25	-2.87	99.70	114.53
19	N	1522	TGL	CA4-CA3-CA2	-2.87	102.76	113.29
14	N	515	HEA	CAD-CBD-CGD	-2.87	107.49	112.75
14	A	516	HEA	CMC-C2C-C1C	-2.86	123.64	128.36
25	P	1270	CDL	OA6-CA5-OA7	-2.85	116.02	123.67
19	A	523	TGL	CG3-CG2-CG1	-2.84	105.42	112.07
23	P	1271	CHD	C1-C10-C9	-2.84	106.88	111.45
28	S	1265	PEK	C03-C02-C01	-2.83	105.46	112.07
19	N	1521	TGL	OG2-CB1-OB1	-2.82	116.10	123.67
23	C	525	CHD	O12-C12-C11	-2.81	103.31	109.06
23	B	1085	CHD	O7-C7-C6	-2.81	103.18	110.06
23	W	1059	CHD	C19-C10-C9	-2.81	106.97	111.18
26	M	526	DMU	O2-C8-C7	-2.80	104.02	110.34
22	R	1229	PSC	C32-C31-C30	-2.80	100.08	114.53
22	B	229	PSC	C32-C31-C30	-2.73	100.44	114.53
19	L	522	TGL	CA8-CA7-CA6	-2.72	100.49	114.53
23	W	1059	CHD	C23-C22-C20	-2.71	111.56	114.75
25	P	1270	CDL	C58-C57-C56	-2.70	100.57	114.53
20	C	267	PGV	O03-C19-O04	-2.69	116.56	123.49
19	A	523	TGL	OB1-CB1-CB2	-2.68	113.00	123.72
22	B	229	PSC	C03-C02-C01	-2.66	105.84	112.07
23	P	1525	CHD	C19-C10-C5	-2.66	105.55	110.25
25	P	1270	CDL	C54-C53-C52	-2.64	100.92	114.53
20	A	524	PGV	O03-C19-O04	-2.63	116.70	123.49
20	N	1266	PGV	O01-C1-O02	-2.62	116.64	123.67
28	G	264	PEK	C25-C24-C23	-2.60	101.11	114.53
14	A	516	HEA	C13-C14-C15	-2.59	122.12	127.76
20	C	267	PGV	C8-C9-C10	-2.59	103.76	113.86
20	C	268	PGV	C03-C02-C01	-2.55	106.10	112.07
28	G	264	PEK	C3-C2-C1	-2.54	103.62	113.59
28	G	265	PEK	C03-C02-C01	-2.52	106.18	112.07
14	N	516	HEA	C3C-CAC-CBC	-2.52	121.17	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	521	PGV	C4-C3-C2	-2.51	104.08	113.29
20	A	521	PGV	O01-C1-O02	-2.51	116.94	123.67
28	G	265	PEK	O01-C1-O02	-2.50	116.97	123.67
20	N	1266	PGV	C15-C14-C13	-2.50	104.12	113.86
19	N	1522	TGL	C26-C25-C24	-2.49	101.66	114.53
14	N	515	HEA	C13-C14-C15	-2.48	122.37	127.76
14	A	515	HEA	O11-C11-C3B	-2.44	104.62	111.82
25	C	270	CDL	C38-C37-C36	-2.44	101.94	114.53
20	P	1267	PGV	C27-C26-C25	-2.44	101.94	114.53
28	G	1263	PEK	O04-C21-C22	-2.43	114.01	123.72
26	M	526	DMU	C25-C28-C31	-2.41	102.09	114.53
19	B	521	TGL	OB1-CB1-CB2	-2.39	114.14	123.72
25	P	1270	CDL	OB8-CB7-OB9	-2.38	117.34	123.49
25	C	270	CDL	C53-C52-C51	-2.38	104.55	113.29
25	P	1270	CDL	C56-C55-C54	-2.38	102.24	114.53
26	Z	1526	DMU	O49-C1-C6	-2.37	104.83	110.02
20	P	1268	PGV	O02-C1-C2	-2.36	114.28	123.72
19	L	522	TGL	CA4-CA3-CA2	-2.35	104.66	113.29
23	W	1059	CHD	O7-C7-C8	-2.35	104.07	109.26
25	T	1269	CDL	OA6-CA5-OA7	-2.35	117.37	123.67
19	A	523	TGL	OG1-CA1-OA1	-2.34	117.45	123.49
25	T	1269	CDL	OB5-PB2-OB3	-2.32	100.62	109.62
28	T	1264	PEK	C30-C29-C28	-2.30	102.67	114.53
23	W	1059	CHD	O3-C3-C2	-2.28	103.58	110.05
22	B	229	PSC	C29-C28-C27	-2.28	102.74	114.53
28	T	1264	PEK	C24-C23-C22	-2.27	104.97	113.29
23	W	1059	CHD	O3-C3-C4	-2.27	105.36	109.86
25	P	1270	CDL	OA8-CA7-OA9	-2.26	117.65	123.49
20	A	521	PGV	C25-C24-C23	-2.25	102.89	114.53
28	T	263	PEK	O04-C21-C22	-2.24	114.75	123.72
28	G	265	PEK	C2-C3-C4	-2.24	108.83	113.30
23	P	1525	CHD	O7-C7-C8	-2.23	104.33	109.26
19	N	1522	TGL	CA8-CA7-CA6	-2.23	102.99	114.53
25	G	269	CDL	OB5-PB2-OB3	-2.23	100.95	109.62
25	C	270	CDL	OA6-CA5-OA7	-2.22	117.71	123.67
28	G	264	PEK	C29-C28-C27	-2.20	103.15	114.53
23	J	60	CHD	C19-C10-C9	-2.20	107.89	111.18
20	N	1266	PGV	C01-O03-C19	-2.19	110.71	116.85
20	N	1524	PGV	C3-C2-C1	-2.19	104.97	113.59
28	G	265	PEK	C23-C22-C21	-2.18	105.04	113.59
28	T	1264	PEK	O01-C02-C01	-2.17	100.71	108.36
14	A	515	HEA	C26-C15-C14	-2.17	119.24	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	1268	PGV	O03-C19-O04	-2.16	117.91	123.49
26	Z	1526	DMU	O2-C8-C7	-2.15	105.49	110.34
23	J	60	CHD	C18-C13-C17	-2.14	107.84	111.22
20	C	268	PGV	O12-P-O13	-2.14	101.31	109.62
14	N	515	HEA	CAA-C2A-C3A	-2.11	122.64	128.66
20	A	521	PGV	C03-C02-C01	-2.08	107.20	112.07
19	A	523	TGL	OG3-CC1-OC1	-2.07	118.14	123.49
23	P	1271	CHD	O7-C7-C8	-2.07	104.70	109.26
22	R	1229	PSC	C29-C28-C27	-2.06	103.88	114.53
19	L	522	TGL	CA3-CA2-CA1	-2.06	105.51	113.59
20	P	1268	PGV	O12-P-O13	-2.05	101.64	109.62
14	N	515	HEA	C21-C20-C19	-2.05	106.04	112.71
25	C	270	CDL	CA6-CA4-CA3	-2.05	107.28	112.07
28	S	1265	PEK	O04-C21-C22	-2.05	115.54	123.72
23	P	1525	CHD	C4-C5-C10	-2.04	110.40	112.66
28	T	1264	PEK	C28-C27-C26	-2.04	104.00	114.53
28	T	263	PEK	C18-C17-C16	-2.03	105.92	113.86
28	G	1263	PEK	O01-C1-O02	-2.03	118.22	123.67
23	O	229	CHD	O7-C7-C8	-2.01	104.82	109.26
23	O	229	CHD	C4-C5-C10	-2.00	110.45	112.66
28	G	1263	PEK	C02-O01-C1	2.00	122.70	117.89
28	G	264	PEK	C01-O03-C21	2.00	122.46	116.85
19	N	1521	TGL	CC3-CC2-CC1	2.01	121.48	113.59
19	N	1521	TGL	C16-C15-CC9	2.01	124.93	114.53
20	C	267	PGV	O03-C19-C20	2.02	118.04	111.90
20	C	268	PGV	O01-C02-C01	2.02	115.47	108.36
19	N	1523	TGL	OG3-CG3-CG2	2.02	114.13	108.69
19	N	1523	TGL	C21-C20-CA9	2.02	124.97	114.53
20	P	1268	PGV	C01-O03-C19	2.02	122.51	116.85
14	A	516	HEA	C21-C20-C19	2.03	119.32	112.71
25	C	270	CDL	C20-C19-C18	2.04	125.06	114.53
19	N	1521	TGL	C21-C20-CA9	2.05	125.10	114.53
26	T	1272	DMU	O4-C7-C5	2.05	114.95	110.34
20	C	267	PGV	O01-C1-C2	2.05	115.99	111.53
28	T	1264	PEK	O01-C1-C2	2.06	116.00	111.53
14	A	516	HEA	CBD-CAD-C3D	2.06	116.22	112.53
25	G	269	CDL	C39-C38-C37	2.06	125.18	114.53
22	B	229	PSC	O03-C19-C20	2.07	118.20	111.90
14	A	515	HEA	C12-C11-C3B	2.08	116.89	112.59
19	N	1522	TGL	CG1-OG1-CA1	2.09	122.70	116.85
14	N	516	HEA	CMD-C2D-C3D	2.10	129.62	125.24
25	G	269	CDL	C79-C78-C77	2.10	125.36	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	1263	PEK	O01-C02-C01	2.10	115.76	108.36
19	A	523	TGL	OG2-CG2-CG3	2.11	115.80	108.36
25	T	1269	CDL	C82-C81-C80	2.11	125.44	114.53
20	C	267	PGV	C01-O03-C19	2.11	122.76	116.85
19	N	1523	TGL	OG2-CG2-CG3	2.12	115.84	108.36
25	T	1269	CDL	OB8-CB6-CB4	2.14	114.44	108.69
23	P	1525	CHD	C9-C11-C12	2.15	117.08	114.36
25	T	1269	CDL	CA6-OA8-CA7	2.16	122.88	116.85
25	P	1270	CDL	C42-C41-C40	2.16	125.70	114.53
25	C	270	CDL	C39-C38-C37	2.17	125.74	114.53
25	G	269	CDL	C82-C81-C80	2.17	125.75	114.53
20	P	1267	PGV	O03-C19-C20	2.18	118.54	111.90
23	C	525	CHD	C11-C9-C10	2.19	116.07	113.79
23	W	1059	CHD	C13-C14-C8	2.20	117.59	114.75
20	P	1267	PGV	C01-O03-C19	2.20	123.01	116.85
19	B	521	TGL	C16-C15-CC9	2.21	125.94	114.53
25	G	269	CDL	CA6-OA8-CA7	2.23	123.08	116.85
19	L	522	TGL	C15-CC9-CC8	2.25	126.14	114.53
23	J	60	CHD	C9-C10-C5	2.25	112.00	108.67
25	C	270	CDL	O1-C1-CB2	2.27	117.99	109.35
23	O	229	CHD	C15-C14-C8	2.27	121.61	118.32
23	O	229	CHD	C21-C20-C22	2.29	114.17	110.35
14	N	516	HEA	CBD-CAD-C3D	2.30	116.65	112.53
26	Z	1526	DMU	O3-C5-C7	2.30	115.52	110.34
19	L	522	TGL	OG1-CG1-CG2	2.31	114.91	108.69
19	A	523	TGL	CB4-CB3-CB2	2.31	121.77	113.29
20	N	1524	PGV	C01-O03-C19	2.35	123.42	116.85
25	G	269	CDL	OA6-CA4-CA6	2.36	116.68	108.36
19	N	1522	TGL	OG2-CG2-CG3	2.36	116.69	108.36
19	N	1523	TGL	C20-CA9-CA8	2.37	126.78	114.53
25	G	269	CDL	C23-C22-C21	2.39	126.86	114.53
25	G	269	CDL	C19-C18-C17	2.40	126.90	114.53
25	G	269	CDL	C40-C39-C38	2.40	126.90	114.53
23	P	1525	CHD	C2-C1-C10	2.40	117.11	112.84
25	T	1269	CDL	C80-C79-C78	2.40	126.95	114.53
19	N	1522	TGL	C15-CC9-CC8	2.45	127.16	114.53
19	N	1522	TGL	OG1-CA1-CA2	2.45	119.37	111.90
26	C	272	DMU	O16-C18-C19	2.45	119.64	109.88
19	N	1522	TGL	OG3-CG3-CG2	2.46	115.32	108.69
23	B	1085	CHD	C5-C6-C7	2.47	117.19	114.44
19	N	1521	TGL	OG2-CG2-CG1	2.47	117.07	108.36
14	A	516	HEA	O11-C11-C12	2.48	115.80	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	521	PGV	O03-C01-C02	2.49	115.39	108.69
26	Z	1526	DMU	O16-C18-C19	2.49	119.80	109.88
26	T	1272	DMU	C10-C5-C7	2.50	114.90	109.97
14	A	515	HEA	CMB-C2B-C3B	2.52	130.30	125.14
23	P	1525	CHD	C1-C2-C3	2.55	114.58	110.43
23	B	1085	CHD	C4-C3-C2	2.56	113.78	110.52
28	S	1265	PEK	C14-C13-C12	2.56	120.51	112.00
26	Z	1526	DMU	C11-C9-C8	2.56	119.33	113.02
25	G	269	CDL	C43-C42-C41	2.57	127.80	114.53
26	C	272	DMU	C11-C9-C8	2.57	119.36	113.02
26	M	526	DMU	O3-C5-C7	2.58	116.16	110.34
28	G	264	PEK	O01-C1-C2	2.59	117.15	111.53
14	N	516	HEA	C4B-C3B-C11	2.59	129.82	127.01
23	P	1525	CHD	O3-C3-C4	2.59	115.01	109.86
25	C	270	CDL	C42-C41-C40	2.60	127.95	114.53
19	N	1522	TGL	OG1-CG1-CG2	2.61	115.72	108.69
19	L	522	TGL	C16-C15-CC9	2.62	128.06	114.53
20	A	524	PGV	O01-C02-C03	2.62	117.60	108.36
23	B	1085	CHD	C19-C10-C1	2.63	112.63	108.20
20	P	1268	PGV	C02-O01-C1	2.63	124.21	117.89
20	N	1524	PGV	O01-C02-C03	2.64	117.67	108.36
25	T	1269	CDL	C83-C82-C81	2.65	128.23	114.53
26	T	1272	DMU	O61-C57-C4	2.66	120.12	111.33
23	B	1085	CHD	C15-C14-C8	2.67	122.20	118.32
20	N	1524	PGV	O03-C01-C02	2.69	115.94	108.69
25	G	269	CDL	C83-C82-C81	2.70	128.49	114.53
26	T	1272	DMU	O7-C3-C4	2.71	116.45	109.32
26	T	1272	DMU	O5-C6-O16	2.72	116.60	110.05
19	N	1522	TGL	C16-C15-CC9	2.72	128.60	114.53
25	T	1269	CDL	OA6-CA4-CA6	2.73	117.97	108.36
22	B	229	PSC	O03-C01-C02	2.74	116.06	108.69
22	B	229	PSC	C02-O01-C1	2.74	124.46	117.89
28	T	1264	PEK	C01-O03-C21	2.74	124.53	116.85
23	C	271	CHD	C9-C10-C5	2.75	112.74	108.67
25	G	269	CDL	C80-C79-C78	2.75	128.72	114.53
25	G	269	CDL	C42-C41-C40	2.75	128.73	114.53
14	A	516	HEA	C27-C19-C18	2.76	128.92	123.50
26	Z	1526	DMU	C6-O5-C4	2.77	119.12	113.75
25	G	269	CDL	C22-C21-C20	2.77	128.83	114.53
19	N	1521	TGL	OG1-CG1-CG2	2.77	116.15	108.69
23	O	229	CHD	C21-C20-C17	2.79	117.60	112.96
23	O	229	CHD	C6-C7-C8	2.80	114.44	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	1524	PGV	O01-C1-C2	2.81	117.64	111.53
25	P	1270	CDL	CA4-OA6-CA5	2.81	124.64	117.89
28	T	1264	PEK	C2-C3-C4	2.82	118.91	113.30
23	J	60	CHD	C23-C22-C20	2.84	118.10	114.75
23	C	525	CHD	C16-C17-C13	2.85	106.43	103.60
23	C	271	CHD	C13-C17-C20	2.85	122.98	119.50
26	C	272	DMU	C18-O16-C6	2.87	118.95	113.94
19	N	1522	TGL	CC3-CC2-CC1	2.88	124.91	113.59
26	T	1272	DMU	C57-C4-C3	2.88	121.62	113.25
19	A	523	TGL	OG1-CA1-CA2	2.90	120.72	111.90
14	A	515	HEA	C27-C19-C20	2.90	119.83	115.41
14	N	515	HEA	C20-C19-C18	2.91	126.56	121.05
19	N	1522	TGL	CG3-OG3-CC1	2.95	125.11	116.85
14	A	515	HEA	C3C-C4C-NC	2.96	113.04	109.21
23	O	229	CHD	C2-C1-C10	2.96	118.13	112.84
23	C	525	CHD	C14-C8-C7	2.99	115.88	111.74
20	C	268	PGV	C01-O03-C19	2.99	125.20	116.85
28	T	263	PEK	O01-C1-C2	2.99	118.03	111.53
19	L	522	TGL	OG1-CA1-CA2	2.99	121.02	111.90
25	P	1270	CDL	OA8-CA7-C31	3.03	121.12	111.90
23	C	271	CHD	C21-C20-C17	3.03	118.00	112.96
19	B	521	TGL	C15-CC9-CC8	3.03	130.19	114.53
26	C	272	DMU	O7-C3-C2	3.04	115.01	107.17
23	C	525	CHD	C9-C11-C12	3.04	118.20	114.36
26	M	526	DMU	C1-C2-C3	3.06	116.33	109.60
28	T	263	PEK	C01-O03-C21	3.07	125.44	116.85
26	Z	1526	DMU	C10-O1-C9	3.08	119.72	113.75
25	P	1270	CDL	CA6-OA8-CA7	3.08	125.48	116.85
23	J	60	CHD	C14-C8-C9	3.11	113.90	109.62
23	P	1525	CHD	C16-C17-C20	3.12	117.61	112.05
23	B	1085	CHD	C2-C1-C10	3.12	118.40	112.84
26	T	1272	DMU	C11-C9-C8	3.13	120.73	113.02
14	N	516	HEA	C27-C19-C18	3.13	129.64	123.50
23	B	1085	CHD	C22-C20-C17	3.13	116.82	110.24
23	P	1271	CHD	C13-C17-C20	3.14	123.33	119.50
19	N	1523	TGL	OG3-CC1-CC2	3.16	121.51	111.90
20	A	524	PGV	O03-C01-C02	3.16	117.19	108.69
23	C	525	CHD	C9-C8-C7	3.17	115.67	111.92
20	N	1266	PGV	O03-C01-C02	3.17	117.22	108.69
19	N	1521	TGL	OG3-CC1-CC2	3.17	121.57	111.90
23	B	1085	CHD	C15-C16-C17	3.17	111.52	105.12
20	N	1524	PGV	O03-C19-C20	3.19	121.62	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	524	PGV	C02-O01-C1	3.21	125.58	117.89
26	T	1272	DMU	C10-O1-C9	3.23	120.02	113.75
26	C	272	DMU	C10-O1-C9	3.25	120.05	113.75
23	C	525	CHD	C1-C2-C3	3.25	115.70	110.43
25	C	270	CDL	OB8-CB7-C71	3.29	121.93	111.90
26	C	272	DMU	O5-C6-O16	3.30	118.00	110.05
23	O	229	CHD	C11-C12-C13	3.34	114.59	111.20
26	Z	1526	DMU	C10-C5-C7	3.34	116.56	109.97
19	L	522	TGL	OG2-CG2-CG3	3.35	120.17	108.36
19	N	1523	TGL	OG1-CA1-CA2	3.35	122.12	111.90
14	N	515	HEA	CMD-C2D-C3D	3.36	132.27	125.24
25	G	269	CDL	CB6-OB8-CB7	3.37	126.28	116.85
20	C	268	PGV	O03-C01-C02	3.38	117.78	108.69
26	C	272	DMU	O61-C57-C4	3.39	122.55	111.33
14	A	516	HEA	CMC-C2C-C3C	3.40	131.74	125.09
26	C	272	DMU	O7-C3-C4	3.43	118.33	109.32
20	N	1524	PGV	C02-O01-C1	3.44	126.14	117.89
23	C	271	CHD	C17-C13-C14	3.45	103.54	100.05
14	N	515	HEA	CBA-CAA-C2A	3.45	118.72	112.53
26	M	526	DMU	C6-O5-C4	3.46	120.45	113.75
14	N	515	HEA	CAA-C2A-C1A	3.46	130.76	127.01
26	Z	1526	DMU	C1-C2-C3	3.47	117.21	109.60
14	N	516	HEA	CMC-C2C-C3C	3.50	131.93	125.09
23	O	229	CHD	C16-C17-C13	3.50	107.08	103.60
26	M	526	DMU	O16-C18-C19	3.53	123.91	109.88
14	N	516	HEA	C12-C11-C3B	3.53	119.89	112.59
23	C	525	CHD	O3-C3-C4	3.57	116.95	109.86
23	P	1525	CHD	C13-C17-C20	3.57	123.85	119.50
23	B	1085	CHD	C11-C12-C13	3.60	114.86	111.20
23	J	60	CHD	C13-C14-C8	3.60	119.40	114.75
19	A	523	TGL	CG1-OG1-CA1	3.61	126.94	116.85
23	P	1525	CHD	C5-C4-C3	3.63	118.31	112.91
26	Z	1526	DMU	O5-C6-O16	3.63	118.80	110.05
26	C	272	DMU	C1-C2-C3	3.64	117.59	109.60
26	T	1272	DMU	C18-O16-C6	3.66	120.34	113.94
25	P	1270	CDL	OB8-CB7-C71	3.67	123.09	111.90
25	C	270	CDL	OA8-CA7-C31	3.68	123.11	111.90
23	B	1085	CHD	C11-C9-C8	3.69	115.97	110.73
26	M	526	DMU	C10-C5-C7	3.69	117.25	109.97
23	P	1525	CHD	C17-C13-C14	3.70	103.79	100.05
26	M	526	DMU	C7-C8-C9	3.71	116.66	110.20
25	T	1269	CDL	OA8-CA7-C31	3.71	123.20	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	CC3-CC2-CC1	3.72	128.20	113.59
20	A	524	PGV	C01-O03-C19	3.74	127.31	116.85
23	W	1059	CHD	C16-C17-C20	3.75	118.73	112.05
19	B	521	TGL	OG3-CC1-CC2	3.75	123.34	111.90
19	A	523	TGL	CG3-OG3-CC1	3.77	127.39	116.85
19	A	523	TGL	OG3-CC1-CC2	3.78	123.42	111.90
14	N	515	HEA	CMB-C2B-C3B	3.79	132.89	125.14
23	B	1085	CHD	C9-C8-C7	3.79	116.40	111.92
28	S	1265	PEK	O01-C1-C2	3.80	119.79	111.53
19	N	1522	TGL	OG3-CC1-CC2	3.82	123.53	111.90
19	N	1523	TGL	CG3-OG3-CC1	3.82	127.53	116.85
22	R	1229	PSC	O03-C19-C20	3.83	123.57	111.90
26	Z	1526	DMU	C2-C3-C4	3.84	119.53	110.84
23	O	229	CHD	C9-C11-C12	3.85	119.22	114.36
28	T	263	PEK	O03-C21-C22	3.89	123.75	111.90
19	B	521	TGL	OG2-CG2-CG1	3.89	122.08	108.36
26	T	1272	DMU	C2-C3-C4	3.90	119.66	110.84
28	T	263	PEK	O03-C01-C02	3.91	119.21	108.69
22	B	229	PSC	O01-C1-C2	3.93	120.06	111.53
23	C	271	CHD	C9-C11-C12	3.93	119.33	114.36
26	Z	1526	DMU	C6-C1-C2	3.94	117.74	109.97
26	T	1272	DMU	C6-O5-C4	3.94	121.39	113.75
26	M	526	DMU	O5-C6-O16	3.97	119.61	110.05
26	C	272	DMU	C6-O5-C4	3.97	121.46	113.75
23	J	60	CHD	C4-C5-C10	3.99	117.06	112.66
26	M	526	DMU	C6-C1-C2	4.00	117.86	109.97
25	T	1269	CDL	CB6-OB8-CB7	4.04	128.13	116.85
25	G	269	CDL	OA6-CA5-C11	4.05	120.34	111.53
19	L	522	TGL	OG3-CC1-CC2	4.06	124.25	111.90
26	C	272	DMU	C6-C1-C2	4.07	117.99	109.97
19	B	521	TGL	OG1-CG1-CG2	4.08	119.66	108.69
26	M	526	DMU	O7-C3-C2	4.08	117.71	107.17
28	G	1263	PEK	C01-O03-C21	4.09	128.28	116.85
23	J	60	CHD	C22-C20-C17	4.09	118.84	110.24
23	W	1059	CHD	C9-C10-C5	4.09	114.73	108.67
22	R	1229	PSC	O01-C1-C2	4.10	120.44	111.53
20	A	524	PGV	O03-C19-C20	4.12	124.44	111.90
23	W	1059	CHD	C1-C2-C3	4.13	117.14	110.43
23	P	1525	CHD	C15-C14-C8	4.16	124.36	118.32
26	T	1272	DMU	C1-C2-C3	4.19	118.80	109.60
23	C	525	CHD	C13-C17-C20	4.20	124.62	119.50
26	T	1272	DMU	O5-C4-C57	4.25	117.09	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C9-C10-C5	4.26	114.97	108.67
23	P	1271	CHD	C15-C14-C13	4.26	107.83	103.60
23	J	60	CHD	C17-C13-C14	4.26	104.36	100.05
23	O	229	CHD	C1-C2-C3	4.32	117.43	110.43
19	N	1521	TGL	OG2-CG2-CG3	4.32	123.58	108.36
23	C	525	CHD	C14-C8-C9	4.33	115.58	109.62
23	O	229	CHD	C11-C9-C10	4.34	118.30	113.79
23	C	271	CHD	C14-C8-C7	4.35	117.77	111.74
26	T	1272	DMU	O7-C10-C5	4.35	118.69	108.10
23	P	1525	CHD	C16-C17-C13	4.37	107.95	103.60
26	T	1272	DMU	C7-C8-C9	4.38	117.83	110.20
26	T	1272	DMU	O1-C9-C11	4.38	117.44	106.36
23	C	525	CHD	C5-C6-C7	4.39	119.33	114.44
23	P	1271	CHD	C21-C20-C17	4.40	120.29	112.96
19	B	521	TGL	OG2-CB1-CB2	4.40	121.10	111.53
23	C	525	CHD	C15-C14-C13	4.40	107.98	103.60
23	P	1271	CHD	C9-C11-C12	4.41	119.93	114.36
26	C	272	DMU	O5-C4-C3	4.41	119.06	109.75
23	J	60	CHD	C16-C17-C13	4.43	108.00	103.60
23	O	229	CHD	C17-C13-C14	4.43	104.53	100.05
28	G	265	PEK	O01-C1-C2	4.44	121.19	111.53
23	O	229	CHD	C5-C6-C7	4.50	119.45	114.44
23	C	271	CHD	C4-C3-C2	4.50	116.26	110.52
19	L	522	TGL	CG3-OG3-CC1	4.52	129.50	116.85
23	W	1059	CHD	C4-C5-C10	4.52	117.64	112.66
19	N	1522	TGL	OG2-CB1-CB2	4.53	121.37	111.53
26	T	1272	DMU	O5-C6-C1	4.55	119.60	110.28
26	Z	1526	DMU	C8-C7-C5	4.56	119.30	110.79
23	W	1059	CHD	C22-C20-C17	4.58	119.87	110.24
20	N	1266	PGV	O03-C19-C20	4.60	125.92	111.90
26	T	1272	DMU	C6-C1-C2	4.63	119.09	109.97
19	N	1523	TGL	OG2-CB1-CB2	4.66	121.66	111.53
23	J	60	CHD	C16-C17-C20	4.67	120.38	112.05
23	J	60	CHD	C1-C2-C3	4.68	118.03	110.43
28	G	1263	PEK	O03-C21-C22	4.70	126.21	111.90
26	Z	1526	DMU	O5-C4-C57	4.70	118.23	106.36
23	C	525	CHD	C2-C1-C10	4.77	121.36	112.84
23	P	1271	CHD	C16-C17-C13	4.79	108.36	103.60
26	Z	1526	DMU	C7-C8-C9	4.80	118.56	110.20
14	N	515	HEA	C26-C15-C16	4.83	122.78	115.41
23	P	1271	CHD	C11-C12-C13	4.83	116.11	111.20
26	M	526	DMU	C8-C7-C5	4.84	119.83	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C11-C9-C8	4.85	117.62	110.73
23	C	271	CHD	C17-C13-C12	4.86	121.99	117.68
23	P	1271	CHD	C14-C8-C7	4.88	118.50	111.74
23	B	1085	CHD	C15-C14-C13	4.89	108.47	103.60
19	L	522	TGL	OG2-CB1-CB2	4.90	122.19	111.53
23	C	271	CHD	C2-C1-C10	4.93	121.63	112.84
23	C	271	CHD	C1-C10-C5	4.93	115.92	107.81
23	O	229	CHD	C9-C8-C7	4.95	117.77	111.92
26	M	526	DMU	C2-C3-C4	4.97	122.08	110.84
26	Z	1526	DMU	O1-C9-C11	4.98	118.93	106.36
23	J	60	CHD	C15-C14-C13	4.98	108.55	103.60
28	G	1263	PEK	O01-C1-C2	5.00	122.39	111.53
23	B	1085	CHD	C9-C11-C12	5.01	120.69	114.36
23	J	60	CHD	C14-C8-C7	5.02	118.70	111.74
19	N	1521	TGL	OG1-CA1-CA2	5.02	127.19	111.90
26	C	272	DMU	C7-C8-C9	5.02	118.95	110.20
23	P	1525	CHD	C14-C8-C9	5.03	116.55	109.62
23	O	229	CHD	C14-C8-C9	5.05	116.56	109.62
26	T	1272	DMU	C8-C7-C5	5.06	120.23	110.79
28	G	1263	PEK	O03-C01-C02	5.08	122.36	108.69
26	C	272	DMU	C2-C3-C4	5.10	122.37	110.84
14	A	515	HEA	C16-C15-C14	5.11	130.75	121.05
28	G	265	PEK	O03-C21-C22	5.16	127.63	111.90
23	O	229	CHD	C11-C9-C8	5.20	118.11	110.73
19	N	1522	TGL	CG2-OG2-CB1	5.28	130.55	117.89
23	W	1059	CHD	C9-C11-C12	5.29	121.04	114.36
23	P	1525	CHD	C11-C9-C10	5.31	119.31	113.79
26	C	272	DMU	C8-C7-C5	5.32	120.72	110.79
25	G	269	CDL	OB6-CB5-C51	5.37	123.20	111.53
23	P	1271	CHD	C2-C1-C10	5.37	122.43	112.84
26	M	526	DMU	O5-C6-C1	5.38	121.31	110.28
26	C	272	DMU	O5-C6-C1	5.38	121.32	110.28
23	C	271	CHD	C14-C13-C12	5.39	112.21	107.39
23	W	1059	CHD	C17-C13-C12	5.39	122.46	117.68
20	P	1268	PGV	O01-C1-C2	5.40	123.28	111.53
19	B	521	TGL	OG1-CA1-CA2	5.41	128.39	111.90
23	W	1059	CHD	C11-C12-C13	5.41	116.70	111.20
26	T	1272	DMU	O5-C4-C3	5.46	121.28	109.75
23	C	525	CHD	C11-C9-C8	5.46	118.50	110.73
28	S	1265	PEK	O03-C21-C22	5.48	128.59	111.90
23	J	60	CHD	C5-C6-C7	5.49	120.56	114.44
26	C	272	DMU	O1-C9-C8	5.52	120.03	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C5-C4-C3	5.57	121.20	112.91
23	C	525	CHD	C15-C14-C8	5.62	126.48	118.32
26	C	272	DMU	O1-C9-C11	5.64	120.60	106.36
20	C	268	PGV	O03-C19-C20	5.64	129.09	111.90
23	P	1271	CHD	C1-C10-C5	5.65	117.09	107.81
23	P	1525	CHD	C11-C9-C8	5.65	118.76	110.73
23	P	1271	CHD	C6-C5-C10	5.67	118.90	112.66
23	J	60	CHD	C15-C14-C8	5.67	126.56	118.32
23	P	1525	CHD	C9-C8-C7	5.68	118.63	111.92
23	P	1271	CHD	C5-C4-C3	5.69	121.38	112.91
23	P	1271	CHD	C1-C2-C3	5.70	119.69	110.43
23	P	1271	CHD	C17-C13-C14	5.71	105.83	100.05
26	M	526	DMU	O1-C9-C11	5.73	120.83	106.36
23	C	525	CHD	C17-C13-C14	5.74	105.85	100.05
26	M	526	DMU	O5-C4-C3	5.75	121.89	109.75
19	B	521	TGL	OG2-CG2-CG3	5.76	128.65	108.36
19	L	522	TGL	CG2-OG2-CB1	5.80	131.81	117.89
25	T	1269	CDL	OA6-CA5-C11	5.85	124.24	111.53
23	B	1085	CHD	C6-C7-C8	5.85	117.68	111.47
23	O	229	CHD	C16-C17-C20	5.86	122.50	112.05
23	C	271	CHD	C5-C4-C3	5.87	121.64	112.91
23	J	60	CHD	C2-C1-C10	5.87	123.32	112.84
14	N	516	HEA	C20-C21-C22	5.89	127.12	111.69
23	W	1059	CHD	C15-C14-C8	5.93	126.93	118.32
23	W	1059	CHD	C2-C1-C10	5.94	123.45	112.84
23	W	1059	CHD	C5-C6-C7	6.02	121.15	114.44
14	A	516	HEA	C20-C21-C22	6.04	127.51	111.69
23	B	1085	CHD	C11-C9-C10	6.04	120.07	113.79
23	W	1059	CHD	C14-C8-C7	6.05	120.13	111.74
23	J	60	CHD	C9-C11-C12	6.07	122.03	114.36
23	B	1085	CHD	C14-C8-C9	6.10	118.01	109.62
20	A	521	PGV	O03-C19-C20	6.18	130.74	111.90
26	Z	1526	DMU	O5-C6-C1	6.21	123.02	110.28
23	C	525	CHD	C6-C7-C8	6.21	118.06	111.47
26	C	272	DMU	O5-C4-C57	6.22	122.08	106.36
23	W	1059	CHD	C11-C9-C8	6.22	119.58	110.73
23	J	60	CHD	C4-C3-C2	6.23	118.47	110.52
20	P	1268	PGV	O03-C19-C20	6.25	130.94	111.90
25	T	1269	CDL	OB6-CB5-C51	6.29	125.21	111.53
23	W	1059	CHD	C5-C4-C3	6.33	122.32	112.91
25	C	270	CDL	OA6-CA5-C11	6.33	125.29	111.53
26	M	526	DMU	O5-C4-C57	6.34	122.39	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	1526	DMU	O5-C4-C3	6.37	123.20	109.75
23	C	271	CHD	C16-C17-C20	6.38	123.43	112.05
23	P	1271	CHD	C5-C6-C7	6.41	121.59	114.44
26	Z	1526	DMU	O1-C9-C8	6.42	121.73	109.68
26	T	1272	DMU	O1-C9-C8	6.44	121.78	109.68
23	P	1525	CHD	C6-C7-C8	6.46	118.33	111.47
23	C	271	CHD	C5-C6-C7	6.47	121.65	114.44
23	C	271	CHD	C15-C14-C13	6.48	110.04	103.60
23	J	60	CHD	C14-C13-C12	6.48	113.20	107.39
23	O	229	CHD	C5-C4-C3	6.50	122.58	112.91
20	C	268	PGV	O01-C1-C2	6.51	125.68	111.53
23	B	1085	CHD	C1-C2-C3	6.63	121.19	110.43
23	B	1085	CHD	C16-C17-C20	6.64	123.90	112.05
23	W	1059	CHD	C6-C5-C10	6.68	120.01	112.66
23	C	271	CHD	C11-C9-C8	6.70	120.25	110.73
26	Z	1526	DMU	O1-C10-C5	6.70	124.03	110.28
23	W	1059	CHD	C1-C10-C5	6.72	118.86	107.81
23	P	1271	CHD	C4-C3-C2	6.74	119.11	110.52
23	P	1271	CHD	C4-C5-C10	6.74	120.08	112.66
19	N	1521	TGL	CG3-OG3-CC1	6.77	135.78	116.85
23	J	60	CHD	C1-C10-C5	6.78	118.95	107.81
23	P	1271	CHD	C15-C14-C8	6.80	128.19	118.32
23	W	1059	CHD	C15-C14-C13	6.87	110.43	103.60
23	C	271	CHD	C11-C12-C13	6.92	118.23	111.20
25	P	1270	CDL	OA6-CA5-C11	6.93	126.60	111.53
26	M	526	DMU	O1-C10-C5	6.94	124.51	110.28
23	J	60	CHD	C11-C12-C13	6.99	118.30	111.20
23	C	525	CHD	C17-C13-C12	7.00	123.88	117.68
23	W	1059	CHD	C14-C13-C12	7.06	113.71	107.39
23	C	271	CHD	C16-C17-C13	7.11	110.67	103.60
26	T	1272	DMU	O1-C10-C5	7.17	124.98	110.28
23	W	1059	CHD	C16-C17-C13	7.17	110.73	103.60
23	O	229	CHD	C4-C3-C2	7.21	119.71	110.52
23	P	1271	CHD	C11-C9-C8	7.22	121.00	110.73
23	P	1525	CHD	C11-C12-C13	7.23	118.54	111.20
19	N	1521	TGL	OG2-CB1-CB2	7.24	127.27	111.53
23	C	271	CHD	C6-C5-C10	7.25	120.65	112.66
23	J	60	CHD	C5-C4-C3	7.32	123.80	112.91
23	C	525	CHD	C11-C12-C13	7.46	118.78	111.20
23	C	271	CHD	C1-C2-C3	7.50	122.61	110.43
23	P	1271	CHD	C16-C17-C20	7.54	125.50	112.05
26	T	1272	DMU	O16-C6-C1	7.57	117.60	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C15-C14-C13	7.67	111.22	103.60
23	P	1525	CHD	C10-C9-C8	7.67	120.30	111.88
26	M	526	DMU	O1-C9-C8	7.69	124.12	109.68
23	C	525	CHD	C4-C3-C2	7.80	120.46	110.52
23	C	271	CHD	C15-C14-C8	7.80	129.65	118.32
23	W	1059	CHD	C13-C17-C20	7.81	129.01	119.50
23	W	1059	CHD	C4-C3-C2	7.82	120.49	110.52
19	A	523	TGL	OG2-CB1-CB2	7.86	128.60	111.53
26	C	272	DMU	O1-C10-C5	7.88	126.45	110.28
23	B	1085	CHD	C17-C13-C12	7.92	124.70	117.68
23	P	1271	CHD	C17-C13-C12	7.94	124.72	117.68
23	C	271	CHD	C6-C7-C8	7.99	119.95	111.47
26	Z	1526	DMU	O16-C6-C1	8.00	118.15	108.04
23	O	229	CHD	C15-C14-C13	8.01	111.56	103.60
23	C	271	CHD	C4-C5-C10	8.01	121.48	112.66
26	M	526	DMU	O16-C6-C1	8.27	118.48	108.04
23	J	60	CHD	C6-C5-C10	8.32	121.83	112.66
23	P	1271	CHD	C14-C13-C12	8.37	114.88	107.39
23	J	60	CHD	C13-C17-C20	8.40	129.73	119.50
23	W	1059	CHD	C6-C7-C8	8.56	120.55	111.47
23	B	1085	CHD	C17-C13-C14	8.88	109.03	100.05
23	P	1525	CHD	C14-C13-C12	8.94	115.40	107.39
23	C	525	CHD	C1-C10-C5	8.96	122.55	107.81
19	B	521	TGL	CG2-OG2-CB1	8.99	139.47	117.89
23	J	60	CHD	C6-C7-C8	9.02	121.04	111.47
23	C	525	CHD	C14-C13-C12	9.02	115.47	107.39
23	O	229	CHD	C17-C13-C12	9.06	125.71	117.68
23	B	1085	CHD	C5-C4-C3	9.11	126.46	112.91
19	N	1521	TGL	CG2-OG2-CB1	9.15	139.85	117.89
23	J	60	CHD	C17-C13-C12	9.33	125.94	117.68
23	P	1271	CHD	C6-C7-C8	9.35	121.39	111.47
19	B	521	TGL	CG3-OG3-CC1	9.38	143.07	116.85
23	O	229	CHD	C10-C9-C8	9.55	122.36	111.88
23	P	1525	CHD	C17-C13-C12	9.57	126.16	117.68
23	B	1085	CHD	C1-C10-C5	9.65	123.67	107.81
26	C	272	DMU	O16-C6-C1	9.76	120.36	108.04
23	B	1085	CHD	C10-C9-C8	9.88	122.73	111.88
23	C	525	CHD	C6-C5-C10	9.99	123.66	112.66
23	O	229	CHD	C1-C10-C5	10.45	125.00	107.81
23	C	525	CHD	C10-C9-C8	10.48	123.39	111.88
23	B	1085	CHD	C14-C13-C12	10.93	117.17	107.39
23	P	1525	CHD	C1-C10-C5	11.30	126.39	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1525	CHD	C4-C3-C2	11.41	125.07	110.52
23	O	229	CHD	C6-C5-C10	11.59	125.42	112.66
23	O	229	CHD	C14-C13-C12	12.39	118.48	107.39
23	W	1059	CHD	C10-C9-C8	12.57	125.67	111.88
23	P	1271	CHD	C10-C9-C8	12.59	125.70	111.88
23	B	1085	CHD	C6-C5-C10	12.92	126.90	112.66
23	C	271	CHD	C10-C9-C8	13.32	126.50	111.88
23	J	60	CHD	C10-C9-C8	13.63	126.83	111.88
23	P	1525	CHD	C6-C5-C10	14.23	128.34	112.66

All (40) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	M	526	DMU	C2
26	M	526	DMU	C4
26	M	526	DMU	C6
26	M	526	DMU	C9
26	M	526	DMU	C5
26	T	1272	DMU	C5
26	T	1272	DMU	C6
26	T	1272	DMU	C9
26	T	1272	DMU	C4
26	T	1272	DMU	C2
26	T	1272	DMU	C10
26	Z	1526	DMU	C2
26	Z	1526	DMU	C4
26	Z	1526	DMU	C6
26	Z	1526	DMU	C9
26	Z	1526	DMU	C5
23	B	1085	CHD	C9
26	C	272	DMU	C2
26	C	272	DMU	C4
26	C	272	DMU	C6
26	C	272	DMU	C9
26	C	272	DMU	C5
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB
23	O	229	CHD	C9
23	J	60	CHD	C9
14	A	515	HEA	ND
14	A	515	HEA	NA

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Mol	Chain	Res	Type	Atom
14	A	515	HEA	NB
23	W	1059	CHD	C17
23	W	1059	CHD	C9
23	P	1271	CHD	C9
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
23	C	271	CHD	C9

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C02-O01-C1-C2
25	C	270	CDL	CA4-OA6-CA5-C11
25	P	1270	CDL	CA4-OA6-CA5-C11
20	A	524	PGV	C02-O01-C1-C2
20	A	524	PGV	P-O11-C03-C02

There are no ring outliers.

40 monomers are involved in 272 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	3	0
14	A	516	HEA	1	0
20	A	521	PGV	1	0
19	A	523	TGL	3	0
20	A	524	PGV	12	0
23	B	1085	CHD	3	0
22	B	229	PSC	17	0
19	B	521	TGL	9	0
20	C	267	PGV	7	0
25	C	270	CDL	22	0
23	C	271	CHD	2	0
26	C	272	DMU	2	0
23	C	525	CHD	1	0
28	G	1263	PEK	10	0
28	G	264	PEK	4	0
28	G	265	PEK	8	0
25	G	269	CDL	24	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J	60	CHD	2	0
19	L	522	TGL	19	0
20	N	1266	PGV	1	0
19	N	1521	TGL	10	0
19	N	1522	TGL	6	0
19	N	1523	TGL	5	0
20	N	1524	PGV	8	0
14	N	515	HEA	5	0
14	N	516	HEA	2	0
23	O	229	CHD	1	0
20	P	1267	PGV	5	0
20	P	1268	PGV	2	0
25	P	1270	CDL	16	0
23	P	1271	CHD	3	0
23	P	1525	CHD	1	0
22	R	1229	PSC	16	0
28	S	1265	PEK	6	0
28	T	1264	PEK	4	0
25	T	1269	CDL	23	0
26	T	1272	DMU	6	0
28	T	263	PEK	15	0
23	W	1059	CHD	3	0
26	Z	1526	DMU	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.04	17 (3%) 50 49	36, 42, 52, 84	0
1	N	513/514 (99%)	-0.12	12 (2%) 64 63	43, 51, 63, 92	0
2	B	226/227 (99%)	-0.40	1 (0%) 93 93	36, 48, 78, 111	0
2	O	226/227 (99%)	-0.06	9 (3%) 42 41	49, 61, 93, 120	0
3	C	259/261 (99%)	0.09	21 (8%) 15 14	38, 45, 59, 86	0
3	P	259/261 (99%)	0.43	27 (10%) 8 8	44, 51, 68, 88	0
4	D	144/147 (97%)	-0.54	2 (1%) 78 77	43, 51, 75, 91	0
4	Q	144/147 (97%)	0.77	17 (11%) 6 6	55, 69, 96, 132	0
5	E	105/109 (96%)	-0.31	0 100 100	43, 51, 83, 118	0
5	R	105/109 (96%)	0.78	9 (8%) 13 12	51, 63, 92, 123	0
6	F	98/98 (100%)	-0.11	7 (7%) 19 18	40, 53, 112, 143	0
6	S	98/98 (100%)	-0.14	7 (7%) 19 18	49, 61, 113, 144	0
7	G	83/85 (97%)	0.54	16 (19%) 2 1	42, 55, 123, 129	0
7	T	83/85 (97%)	0.74	16 (19%) 2 1	46, 62, 121, 133	0
8	H	79/85 (92%)	0.03	3 (3%) 44 43	46, 58, 119, 129	0
8	U	79/85 (92%)	-0.30	2 (2%) 61 60	54, 69, 120, 127	0
9	I	72/73 (98%)	0.26	6 (8%) 14 13	48, 60, 105, 112	0
9	V	72/73 (98%)	1.01	12 (16%) 2 2	52, 74, 109, 112	0
10	J	58/59 (98%)	0.20	4 (6%) 20 19	45, 58, 86, 119	0
10	W	58/59 (98%)	0.47	7 (12%) 6 5	54, 66, 88, 120	0
11	K	49/56 (87%)	-0.38	0 100 100	45, 57, 75, 83	0
11	X	49/56 (87%)	0.91	10 (20%) 1 1	62, 69, 85, 99	0
12	L	46/47 (97%)	-0.34	1 (2%) 65 64	43, 48, 70, 100	0
12	Y	46/47 (97%)	-0.09	3 (6%) 22 22	53, 61, 82, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.29	1 (2%) 64 63	44, 51, 88, 120	0
13	Z	43/46 (93%)	0.51	7 (16%) 2 2	57, 65, 96, 121	0
All	All	3550/3614 (98%)	0.07	217 (6%) 25 24	36, 53, 92, 144	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	15.2
4	Q	5	VAL	11.5
7	T	1	ALA	10.9
6	F	1	ALA	10.5
4	Q	7	LYS	10.3
7	G	1	ALA	10.0
4	Q	8	SER	9.8
7	G	8	HIS	9.4
6	S	1	ALA	8.1
10	J	58	LYS	8.1
7	T	3	ALA	7.9
9	V	30	GLY	7.9
9	I	30	GLY	7.8
13	Z	43	SER	7.4
10	W	58	LYS	7.2
6	S	2	SER	6.9
6	F	96	LEU	6.9
6	F	97	ALA	6.5
8	H	46	LYS	6.4
6	S	96	LEU	6.4
7	T	40	GLY	6.3
7	G	2	SER	6.2
9	I	29	LEU	6.2
4	Q	4	SER	5.9
7	T	8	HIS	5.9
6	F	98	HIS	5.8
6	S	97	ALA	5.8
10	W	52	TRP	5.7
7	G	40	GLY	5.5
12	L	2	HIS	5.5
6	F	2	SER	5.5
7	G	5	LYS	5.4
9	V	29	LEU	5.4
7	T	4	ALA	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	R	109	VAL	5.0
7	G	9	GLY	5.0
9	I	37	PHE	4.9
3	P	247	VAL	4.7
10	J	1	PHE	4.7
6	S	98	HIS	4.7
4	Q	147	LYS	4.7
7	T	5	LYS	4.7
13	M	43	SER	4.7
13	Z	42	LYS	4.5
11	X	13	TYR	4.4
9	V	25	PHE	4.4
3	P	92	LEU	4.4
9	V	37	PHE	4.3
10	W	48	TYR	4.3
7	G	3	ALA	4.3
3	P	91	VAL	4.3
7	G	36	TRP	4.2
10	W	57	HIS	4.2
7	T	36	TRP	4.1
7	G	84	LYS	4.0
3	P	254	VAL	4.0
3	P	259	TRP	4.0
1	A	285	PHE	3.9
3	P	248	VAL	3.9
5	R	108	LYS	3.9
3	P	251	PHE	3.9
11	X	31	TYR	3.9
3	P	258	TRP	3.9
5	R	5	HIS	3.8
11	X	7	PRO	3.7
3	C	92	LEU	3.7
1	N	196	LEU	3.7
7	T	41	HIS	3.7
3	P	98	PHE	3.7
8	H	45	ALA	3.7
8	U	7	LYS	3.6
7	T	2	SER	3.6
1	A	197	LEU	3.6
4	Q	51	LEU	3.6
1	N	197	LEU	3.6
3	P	95	THR	3.6

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Mol	Chain	Res	Type	RSRZ
3	P	84	ILE	3.5
6	S	95	GLN	3.5
1	A	193	VAL	3.5
1	N	201	VAL	3.5
3	P	252	LEU	3.5
9	V	2	THR	3.5
3	C	88	ILE	3.5
3	P	88	ILE	3.5
7	T	84	LYS	3.5
7	G	39	SER	3.5
7	T	39	SER	3.4
9	V	19	PHE	3.4
11	X	9	PHE	3.4
10	J	57	HIS	3.4
4	Q	111	PHE	3.4
3	C	91	VAL	3.4
2	O	5	MET	3.4
9	V	33	THR	3.3
1	A	237	PHE	3.3
2	O	131	GLY	3.3
3	C	251	PHE	3.3
3	C	95	THR	3.2
13	Z	32	TRP	3.2
3	P	244	PHE	3.2
9	V	26	MET	3.2
2	O	90	ILE	3.2
8	U	48	GLY	3.1
5	R	106	LEU	3.1
3	P	94	PHE	3.1
9	I	25	PHE	3.1
7	G	6	GLY	3.1
1	A	201	VAL	3.1
3	P	99	TRP	3.1
1	A	194	LEU	3.0
9	I	33	THR	3.0
7	G	42	ARG	3.0
3	P	87	ILE	3.0
3	P	96	GLY	3.0
1	A	286	ILE	3.0
9	V	68	ILE	3.0
1	N	200	PRO	3.0
4	Q	136	ALA	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	Q	140	TYR	2.9
3	P	138	LEU	2.9
3	C	248	VAL	2.9
1	A	282	PHE	2.9
1	N	285	PHE	2.9
3	C	254	VAL	2.9
2	O	74	ILE	2.9
3	C	250	LEU	2.8
13	Z	39	ASN	2.8
3	P	250	LEU	2.8
11	X	34	THR	2.8
3	C	102	TYR	2.8
13	Z	35	TYR	2.8
6	F	95	GLN	2.8
7	T	6	GLY	2.7
3	C	87	ILE	2.7
2	O	59	GLN	2.7
3	C	255	SER	2.7
4	Q	102	TYR	2.7
1	N	237	PHE	2.7
2	O	133	LEU	2.7
3	P	102	TYR	2.7
7	T	12	GLY	2.7
6	S	94	HIS	2.7
1	A	284	GLY	2.7
11	X	35	GLN	2.6
7	G	4	ALA	2.6
7	G	10	GLY	2.6
9	V	3	ALA	2.6
4	Q	60	TYR	2.6
1	A	241	PRO	2.6
1	A	288	TRP	2.5
3	P	134	THR	2.5
1	N	447	TYR	2.5
7	T	7	ASP	2.5
4	Q	49	SER	2.5
4	Q	50	SER	2.5
7	T	42	ARG	2.5
4	Q	46	ALA	2.5
2	O	193	TYR	2.5
1	N	193	VAL	2.5
11	X	33	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	94	HIS	2.4
3	C	259	TRP	2.4
11	X	30	VAL	2.4
10	W	30	ILE	2.4
4	D	147	LYS	2.4
4	Q	134	PHE	2.4
3	C	252	LEU	2.4
3	C	245	VAL	2.4
3	P	89	SER	2.4
3	P	97	PHE	2.4
11	X	16	ALA	2.4
4	D	102	TYR	2.4
3	C	99	TRP	2.4
3	P	93	PHE	2.4
12	Y	47	LYS	2.4
3	C	98	PHE	2.3
9	I	19	PHE	2.3
5	R	15	TRP	2.3
9	V	53	ASN	2.3
1	A	283	LEU	2.3
5	R	93	LEU	2.3
13	Z	37	LEU	2.3
3	P	255	SER	2.3
8	H	44	THR	2.3
13	Z	41	LYS	2.3
3	P	85	LEU	2.3
3	C	84	ILE	2.3
10	J	4	ARG	2.3
3	C	89	SER	2.3
11	X	40	TRP	2.3
3	C	96	GLY	2.2
7	G	7	ASP	2.2
5	R	89	LEU	2.2
3	C	247	VAL	2.2
7	T	9	GLY	2.2
1	A	196	LEU	2.2
5	R	29	LEU	2.2
9	V	4	LEU	2.2
12	Y	38	PHE	2.2
5	R	52	LEU	2.2
1	N	192	ALA	2.1
7	G	41	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	161	ALA	2.1
1	A	287	VAL	2.1
1	N	452	THR	2.1
1	A	192	ALA	2.1
1	A	200	PRO	2.1
1	A	198	SER	2.1
3	C	106	LEU	2.1
4	Q	124	LEU	2.1
12	Y	3	TYR	2.1
1	N	234	LEU	2.1
2	B	58	ALA	2.1
2	O	3	TYR	2.0
2	O	130	PRO	2.0
10	W	26	ALA	2.0
10	W	33	ARG	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
1	FME	N	1	10/11	0.87	0.46	-	77,82,105,107	0
9	SAC	V	1	9/10	0.50	0.62	-	110,112,114,115	0
2	FME	B	1	10/11	0.98	0.10	-	46,48,51,61	0
9	SAC	I	1	9/10	0.58	0.54	-	99,103,106,106	0
2	FME	O	1	10/11	0.94	0.25	-	59,59,64,64	0
7	TPO	T	11	11/12	0.34	0.41	-	97,105,129,130	0
7	TPO	G	11	11/12	0.50	0.46	-	93,102,125,127	0
1	FME	A	1	10/11	0.94	0.21	-	63,70,93,102	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
20	PGV	A	524	51/51	0.78	0.27	12.63	62,101,132,135	0
25	CDL	P	1270	100/100	0.76	0.38	9.59	69,119,136,137	0
25	CDL	C	270	100/100	0.83	0.34	8.36	56,112,137,139	0
26	DMU	C	272	33/33	0.62	0.28	6.61	96,129,132,134	0
26	DMU	T	1272	33/33	0.60	0.37	5.75	111,140,141,141	0
19	TGL	N	1522	63/63	0.64	0.30	5.38	72,95,111,112	0
19	TGL	L	522	63/63	0.77	0.25	4.89	57,89,109,113	0
18	NA	N	519	1/1	0.87	0.24	4.86	58,58,58,58	0
20	PGV	N	1524	51/51	0.73	0.39	4.82	67,106,139,140	0
19	TGL	B	521	63/63	0.86	0.18	4.75	54,96,118,120	0
22	PSC	B	229	52/52	0.63	0.32	4.62	70,117,150,150	0
19	TGL	A	523	63/63	0.78	0.21	4.40	78,102,131,132	0
22	PSC	R	1229	52/52	0.56	0.35	4.38	73,120,150,150	0
23	CHD	J	60	29/29	0.85	0.34	4.03	103,112,119,120	0
19	TGL	N	1523	63/63	0.77	0.34	3.99	84,111,131,133	0
25	CDL	G	269	100/100	0.60	0.40	3.98	89,118,138,141	0
25	CDL	T	1269	100/100	0.58	0.44	3.75	92,117,138,143	0
23	CHD	W	1059	29/29	0.77	0.37	3.41	110,117,120,122	0
28	PEK	G	1263	53/53	0.40	0.68	3.07	83,126,150,150	0
17	MG	A	518	1/1	0.95	0.17	3.03	40,40,40,40	0
19	TGL	N	1521	63/63	0.88	0.22	2.84	69,101,120,123	0
20	PGV	C	268	51/51	0.65	0.66	2.75	78,103,119,120	0
27	ZN	F	99	1/1	0.99	0.15	2.48	48,48,48,48	0
20	PGV	P	1268	51/51	0.73	0.58	2.29	78,108,125,126	0
28	PEK	T	263	53/53	0.55	0.51	2.17	78,123,145,149	0
23	CHD	P	1525	29/29	0.96	0.27	2.14	48,54,57,59	0
23	CHD	C	525	29/29	0.96	0.29	1.85	38,50,57,65	0
26	DMU	Z	1526	33/33	0.90	0.28	1.81	73,80,94,96	0
21	CUA	B	228	2/2	0.99	0.15	1.62	41,41,41,42	0
20	PGV	P	1267	51/51	0.96	0.19	0.98	45,56,102,106	0
14	HEA	N	516	60/60	0.99	0.14	0.87	42,48,69,74	0
14	HEA	N	515	60/60	0.98	0.12	0.74	47,52,65,66	0
23	CHD	C	271	29/29	0.94	0.20	0.65	86,97,99,99	0
28	PEK	T	1264	53/53	0.95	0.17	0.62	49,70,109,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
28	PEK	S	1265	53/53	0.72	0.26	0.59	75,112,133,136	0
28	PEK	G	264	53/53	0.96	0.14	0.58	44,65,107,109	0
20	PGV	C	267	51/51	0.97	0.14	0.42	38,52,95,97	0
20	PGV	A	521	51/51	0.97	0.15	0.38	36,53,77,79	0
17	MG	N	518	1/1	0.92	0.11	0.36	50,50,50,50	0
28	PEK	G	265	53/53	0.74	0.23	0.35	70,109,135,138	0
23	CHD	P	1271	29/29	0.94	0.13	0.35	98,101,103,104	0
27	ZN	S	99	1/1	1.00	0.11	0.22	56,56,56,56	0
26	DMU	M	526	33/33	0.94	0.14	0.16	52,63,87,91	0
20	PGV	N	1266	51/51	0.96	0.15	0.10	45,60,81,84	0
15	CMO	N	520	2/2	1.00	0.14	0.00	47,47,47,48	0
21	CUA	O	228	2/2	0.98	0.11	-0.11	52,52,52,54	0
14	HEA	A	516	60/60	0.99	0.14	-0.24	32,40,56,64	0
14	HEA	A	515	60/60	0.99	0.12	-0.27	33,40,54,68	0
23	CHD	B	1085	29/29	0.97	0.14	-0.27	46,50,53,59	0
23	CHD	O	229	29/29	0.96	0.13	-0.29	45,49,56,62	0
16	CU	A	517	1/1	1.00	0.20	-0.88	40,40,40,40	0
15	CMO	A	520	2/2	0.99	0.15	-1.37	39,39,39,41	0
18	NA	A	519	1/1	0.96	0.06	-4.41	47,47,47,47	0
24	UNX	C	262	1/1	0.39	0.65	-	75,75,75,75	0
24	UNX	P	262	1/1	0.69	0.68	-	75,75,75,75	0
16	CU	N	517	1/1	1.00	0.18	-	49,49,49,49	0

## 6.5 Other polymers

There are no such residues in this entry.