



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2018 – 07:14 pm GMT

PDB ID : 1V54
Title : Bovine heart cytochrome c oxidase at the fully oxidized state
Authors : Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.
Deposited on : 2003-11-21
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

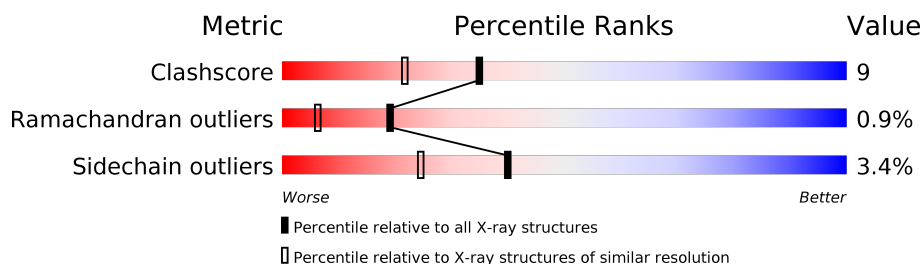
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	122078	6075 (1.80-1.80)
Ramachandran outliers	120005	6009 (1.80-1.80)
Sidechain outliers	119972	6008 (1.80-1.80)









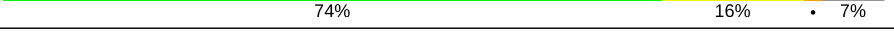


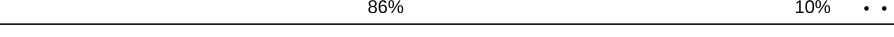
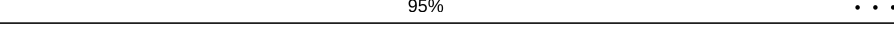
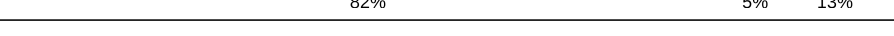


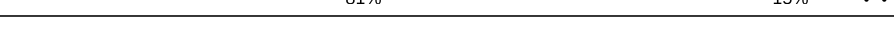

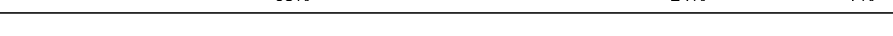
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	

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Mol	Chain	Length	Quality of chain
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
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
18	TGL	L	3522	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHD	C	3271	X	-	-	-
21	CHD	J	3060	X	-	-	-
21	CHD	P	4271	X	-	-	-
21	CHD	W	4060	X	-	-	-
25	PSC	O	4230	-	-	X	-
27	DMU	M	3526	X	-	-	-
27	DMU	Z	4526	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32636 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 polypeptide I.

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 polypeptide II.

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 polypeptide III.

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 IV 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 polypeptide Va.

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 polypeptide Vb.

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 polypeptide VIa-heart.

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 polypeptide VIb.

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 polypeptide VIc.

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 VIIa-heart.

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 polypeptide VIIb.

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 polypeptide VIIc.

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

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

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

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

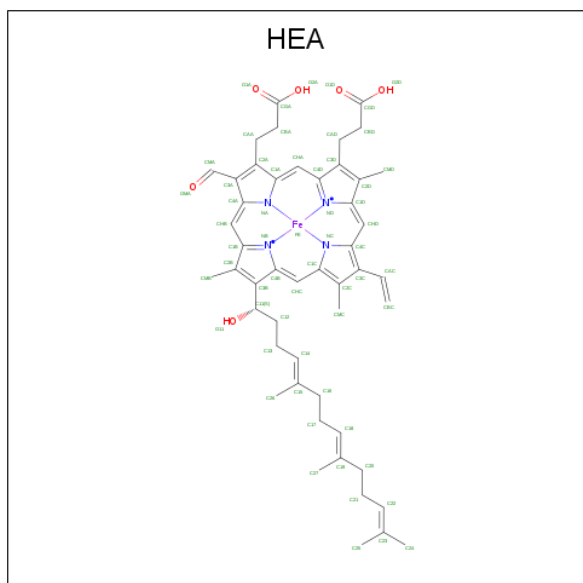
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

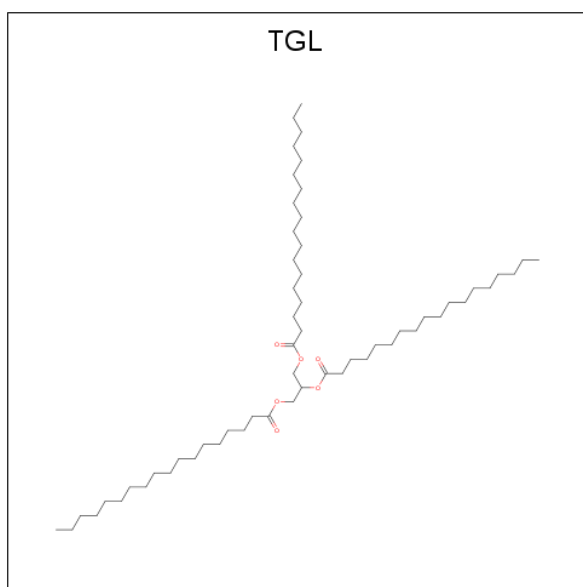
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



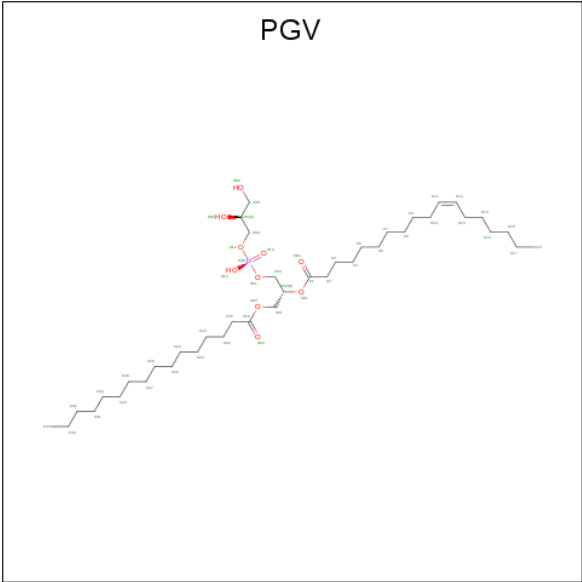
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



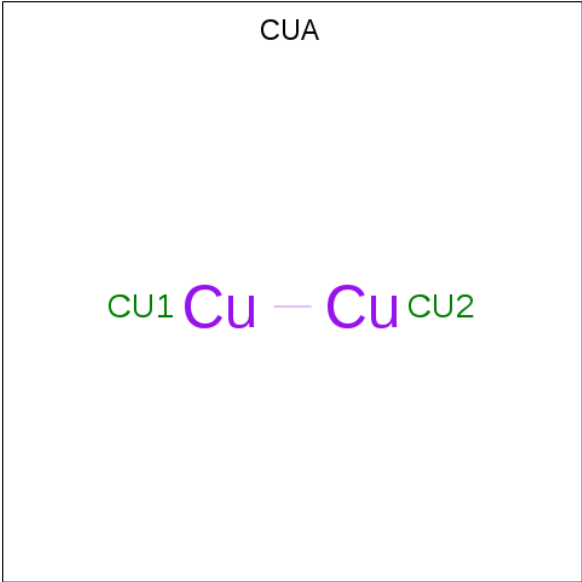
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



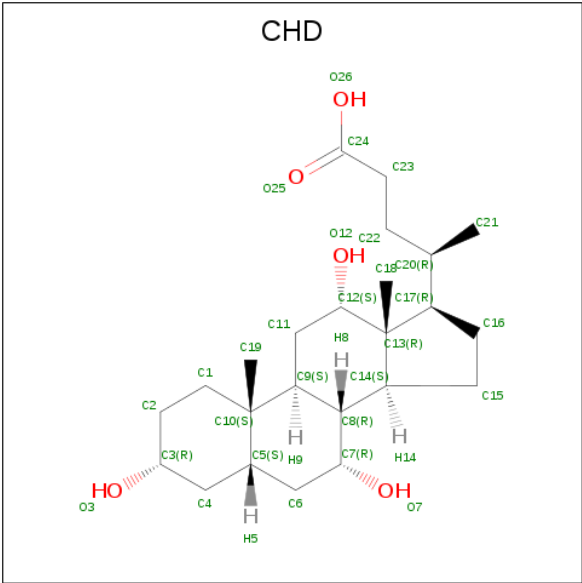
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 21 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



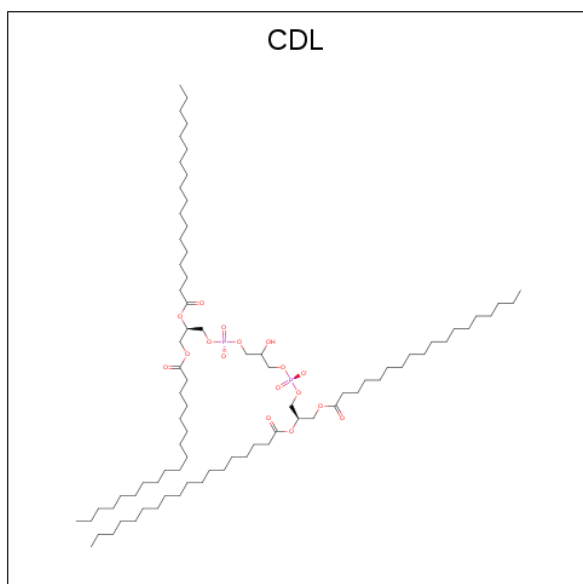
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			29	24	5		
21	C	1	Total	C	O	0	0
			29	24	5		

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

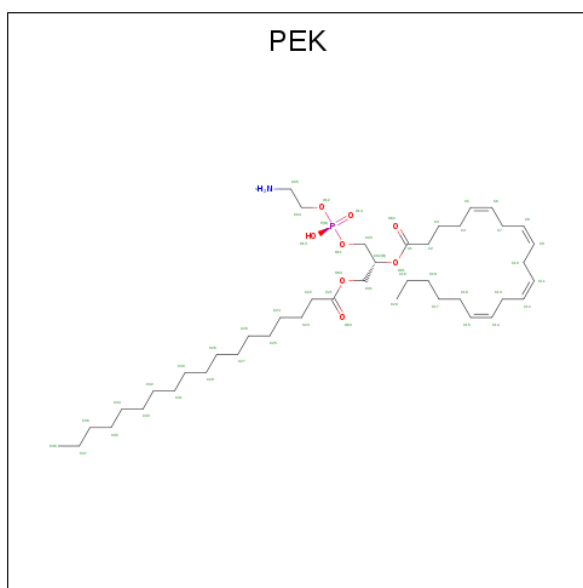
- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 23 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: $C_{43}H_{78}NO_8P$).

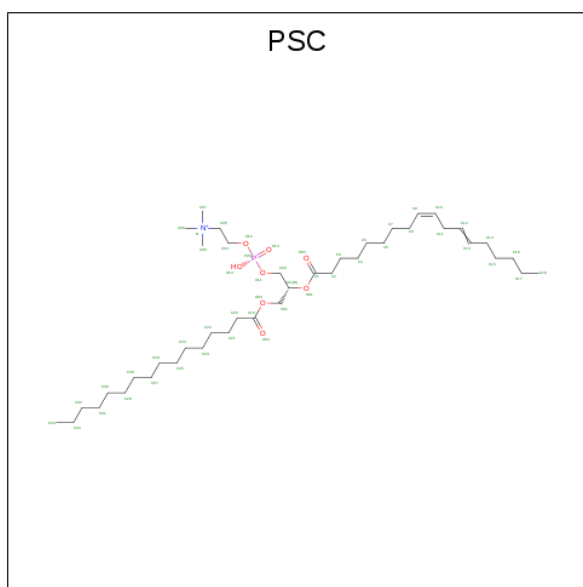


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

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

- Molecule 25 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

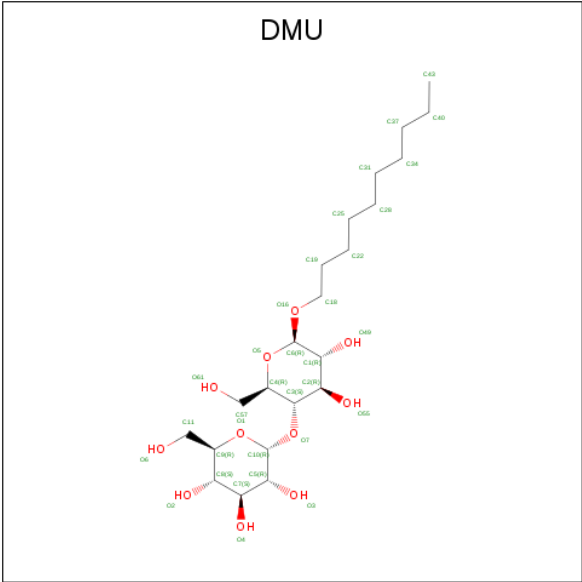


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	227	Total	O	0	0
			227	227		
28	B	180	Total	O	0	0
			180	180		
28	C	116	Total	O	0	0
			116	116		
28	D	109	Total	O	0	0
			109	109		
28	E	68	Total	O	0	0
			68	68		
28	F	80	Total	O	0	0
			80	80		
28	G	59	Total	O	0	0
			59	59		
28	H	71	Total	O	0	0
			71	71		
28	I	61	Total	O	0	0
			61	61		
28	J	21	Total	O	0	0
			21	21		

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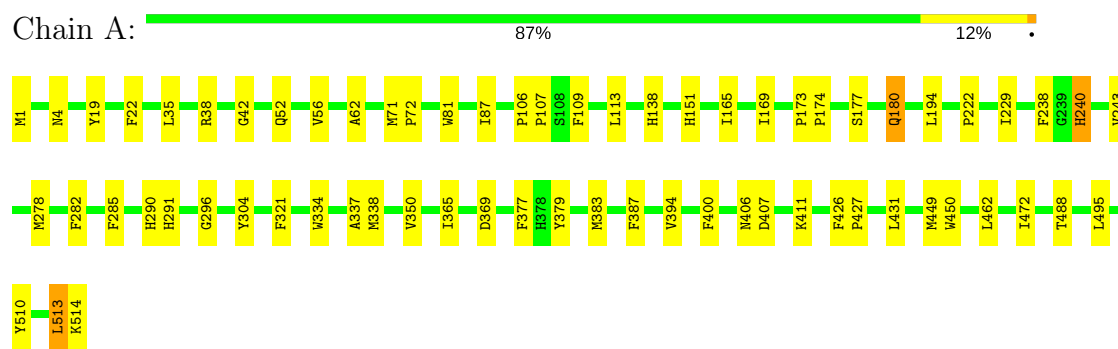
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	37	Total 37	O 37	0	0
28	L	23	Total 23	O 23	0	0
28	M	32	Total 32	O 32	0	0
28	N	217	Total 217	O 217	0	0
28	O	146	Total 146	O 146	0	0
28	P	120	Total 120	O 120	0	0
28	Q	73	Total 73	O 73	0	0
28	R	32	Total 32	O 32	0	0
28	S	54	Total 54	O 54	0	0
28	T	58	Total 58	O 58	0	0
28	U	65	Total 65	O 65	0	0
28	V	36	Total 36	O 36	0	0
28	W	13	Total 13	O 13	0	0
28	X	29	Total 29	O 29	0	0
28	Y	25	Total 25	O 25	0	0
28	Z	18	Total 18	O 18	0	0

3 Residue-property plots [i](#)

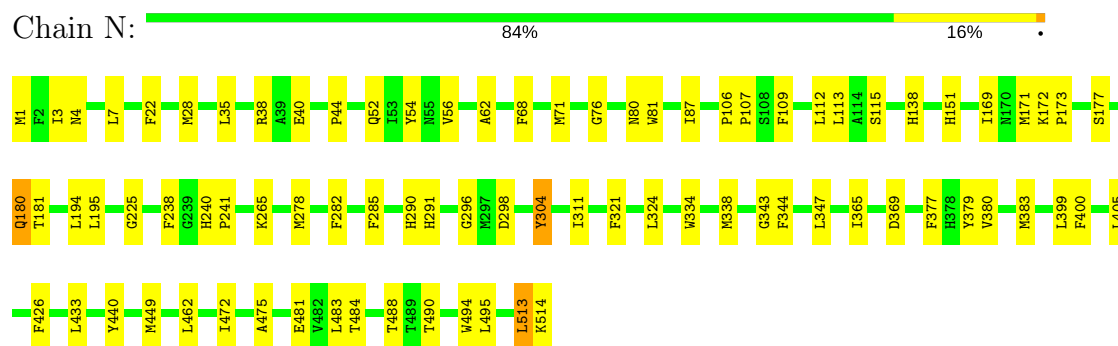
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

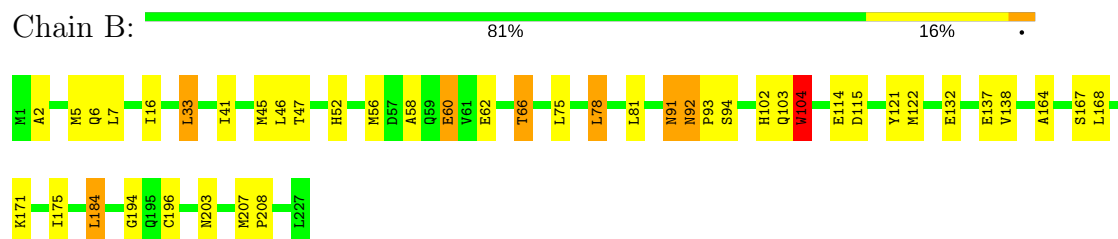
• Molecule 1: Cytochrome c oxidase polypeptide I



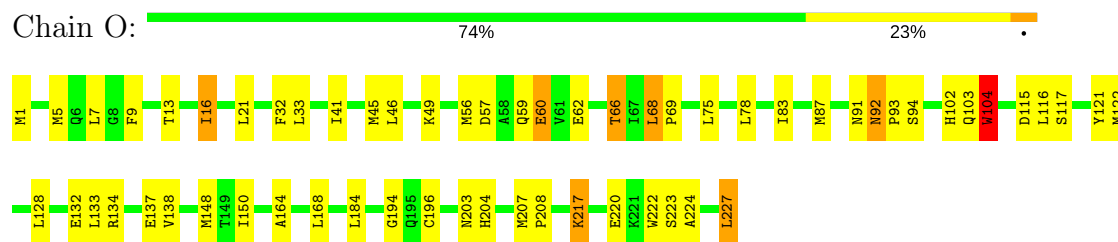
• Molecule 1: Cytochrome c oxidase polypeptide I



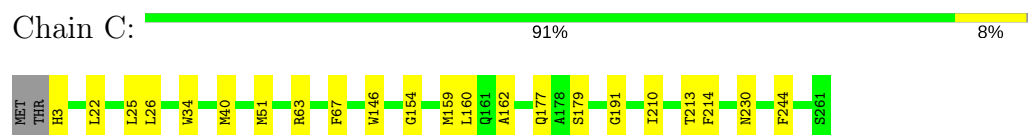
• Molecule 2: Cytochrome c oxidase polypeptide II



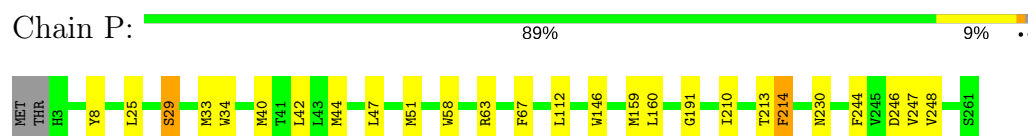
• Molecule 2: Cytochrome c oxidase polypeptide II



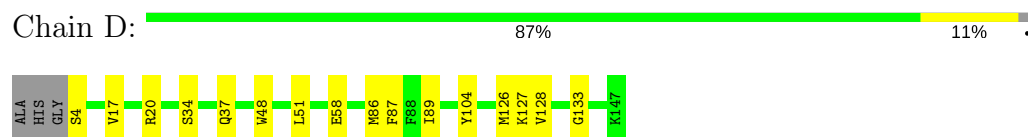
- Molecule 3: Cytochrome c oxidase polypeptide III



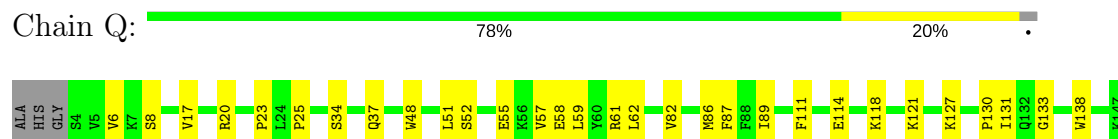
- Molecule 3: Cytochrome c oxidase polypeptide III



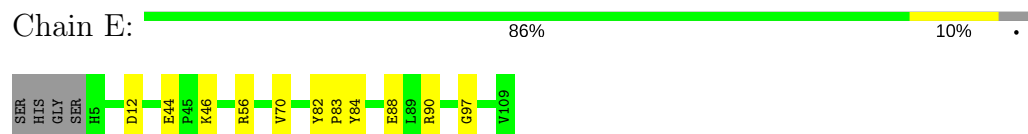
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1



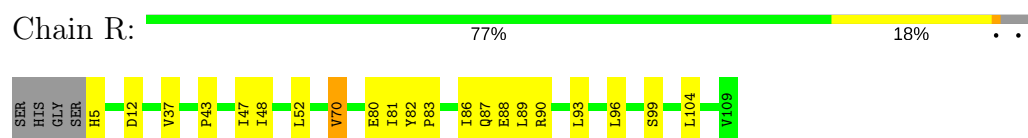
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1




- Molecule 5: Cytochrome c oxidase polypeptide Va



- Molecule 5: Cytochrome c oxidase polypeptide Va




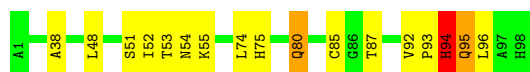
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  78% 19% ..



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  83% 14% ..



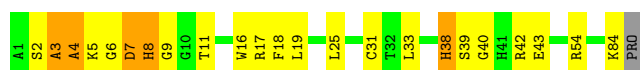
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  69% 21% 8% •




- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  72% 21% 6% •



- Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain H:  82% 9% 7% •




- Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain U:  74% 16% 7% •




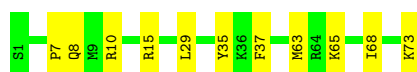
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  85% 14% •



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  85% 15%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J: 86% 10% ..



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W: 95% ...



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K: 82% 5% 13%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X: 77% 9% 13%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L: 87% 11% .



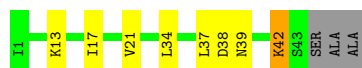
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y: 81% 15% ..

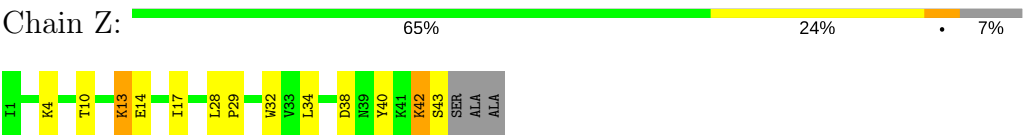


- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M: 76% 15% 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32636	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/4156	0.68	0/5678
1	N	0.50	0/4156	0.67	0/5678
2	B	0.48	0/1860	0.79	3/2534 (0.1%)
2	O	0.52	0/1860	0.82	3/2534 (0.1%)
3	C	0.51	0/2197	0.59	0/3005
3	P	0.48	0/2197	0.61	0/3005
4	D	0.48	0/1229	0.66	1/1658 (0.1%)
4	Q	0.51	0/1229	0.66	1/1658 (0.1%)
5	E	0.49	0/871	0.66	0/1182
5	R	0.50	0/871	0.68	0/1182
6	F	0.48	0/765	0.81	2/1038 (0.2%)
6	S	0.51	0/765	0.82	2/1038 (0.2%)
7	G	0.52	0/690	0.69	0/937
7	T	0.55	0/690	0.73	1/937 (0.1%)
8	H	0.47	0/682	0.68	0/921
8	U	0.49	0/682	0.67	0/921
9	I	0.53	0/605	0.60	0/802
9	V	0.53	0/605	0.62	0/802
10	J	0.47	0/471	0.60	0/636
10	W	0.48	0/471	0.64	0/636
11	K	0.50	0/398	0.67	0/546
11	X	0.49	0/398	0.66	0/546
12	L	0.50	0/393	0.56	0/526
12	Y	0.54	0/393	0.58	0/526
13	M	0.47	0/345	0.62	0/470
13	Z	0.43	0/345	0.61	0/470
All	All	0.50	0/29324	0.68	13/39866 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
8	U	0	1
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.25	127.89	111.00
2	B	103	GLN	CA-C-N	-6.20	103.55	117.20
6	F	94	HIS	N-CA-C	5.99	127.18	111.00
7	T	33	LEU	CA-CB-CG	5.91	128.88	115.30
2	O	103	GLN	CA-C-N	-5.82	104.40	117.20
2	B	184	LEU	CA-CB-CG	5.72	128.46	115.30
6	F	93	PRO	N-CA-C	5.69	126.90	112.10
4	D	133	GLY	N-CA-C	5.63	127.17	113.10
2	B	104	TRP	N-CA-C	5.47	125.78	111.00
4	Q	133	GLY	N-CA-C	5.43	126.67	113.10
2	O	227	LEU	CA-CB-CG	5.40	127.72	115.30
6	S	93	PRO	N-CA-C	5.33	125.94	112.10
2	O	104	TRP	N-CA-C	5.27	125.23	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
8	U	11	TYR	Sidechain

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	62	0
1	N	4027	0	4001	72	0
2	B	1824	0	1833	33	0
2	O	1824	0	1833	49	0
3	C	2110	0	2027	17	0
3	P	2110	0	2027	24	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	25	0
5	E	852	0	845	6	0
5	R	852	0	845	11	0
6	F	748	0	728	16	0
6	S	748	0	728	12	0
7	G	675	0	644	25	0
7	T	675	0	644	21	0
8	H	662	0	623	5	0
8	U	662	0	623	8	0
9	I	601	0	613	8	0
9	V	601	0	613	11	0
10	J	460	0	459	6	0
10	W	460	0	459	2	0
11	K	384	0	366	2	0
11	X	384	0	366	8	0
12	L	380	0	380	13	0
12	Y	380	0	380	10	0
13	M	335	0	352	5	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	4	0
17	N	120	0	108	3	0
18	A	63	0	110	11	0
18	D	63	0	110	15	0
18	L	63	0	110	25	0
18	N	126	0	220	38	0
18	Q	63	0	110	15	0
19	A	102	0	152	7	0
19	C	102	0	152	7	0
19	N	102	0	152	5	0
19	P	102	0	152	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	1	0
21	C	58	0	78	3	0
21	J	29	0	39	2	0
21	O	29	0	39	1	0
21	P	58	0	78	2	0
21	W	29	0	39	2	0
22	C	100	0	156	14	0
22	G	100	0	156	14	0
22	P	100	0	156	18	0
22	T	100	0	156	15	0
23	C	106	0	154	7	0
23	G	53	0	77	10	0
23	P	106	0	154	6	0
23	T	53	0	77	9	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	E	52	0	80	13	0
25	O	52	0	80	21	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	36	0	0
27	Z	33	0	36	0	0
28	A	227	0	0	2	0
28	B	180	0	0	8	0
28	C	116	0	0	1	0
28	D	109	0	0	3	0
28	E	68	0	0	2	0
28	F	80	0	0	2	0
28	G	59	0	0	3	0
28	H	71	0	0	1	0
28	I	61	0	0	2	0
28	J	21	0	0	0	0
28	K	37	0	0	0	0
28	L	23	0	0	1	0
28	M	32	0	0	0	0
28	N	217	0	0	5	0
28	O	146	0	0	1	0
28	P	120	0	0	1	0
28	Q	73	0	0	5	0
28	R	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	S	54	0	0	3	0
28	T	58	0	0	2	0
28	U	65	0	0	1	0
28	V	36	0	0	2	0
28	W	13	0	0	0	0
28	X	29	0	0	1	0
28	Y	25	0	0	1	0
28	Z	18	0	0	0	0
All	All	32636	0	31222	551	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 (551) 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)
7:G:84:LYS:HD2	7:G:84:LYS:H	1.14	1.08
22:C:3270:CDL:H662	19:C:3267:PGV:H182	1.41	1.03
3:P:63:ARG:HE	22:P:4270:CDL:HA22	1.24	1.03
7:T:84:LYS:H	7:T:84:LYS:HD2	1.23	1.02
3:C:63:ARG:HE	22:C:3270:CDL:HA22	1.23	1.01
10:W:33:ARG:HG2	21:W:4060:CHD:H152	1.46	0.94
18:N:4522:TGL:HC31	12:Y:13:PHE:HA	1.51	0.93
4:D:34:SER:H	4:D:37:GLN:HE21	1.16	0.89
23:C:3264:PEK:H161	23:C:3264:PEK:H102	1.55	0.89
4:Q:114:GLU:HB3	28:Q:2622:HOH:O	1.73	0.89
6:S:94:HIS:CD2	6:S:95:GLN:H	1.93	0.87
9:I:5:ALA:HB2	28:I:2536:HOH:O	1.73	0.86
6:F:85:CYS:SG	6:F:87:THR:HG23	2.15	0.86
22:P:4270:CDL:H242	22:P:4270:CDL:H661	1.59	0.84
18:N:4521:TGL:H101	18:N:4521:TGL:H271	1.58	0.84
18:A:3521:TGL:H241	18:A:3521:TGL:HA91	1.60	0.83
7:T:5:LYS:HD2	23:T:3263:PEK:H382	1.61	0.83
22:C:3270:CDL:H242	22:C:3270:CDL:H661	1.60	0.82
22:P:4270:CDL:H662	19:P:4267:PGV:H182	1.61	0.81
25:O:4230:PSC:H21	25:O:4230:PSC:H222	1.64	0.80
12:L:20:ARG:HH12	18:L:3522:TGL:HC61	1.45	0.80
3:P:67:PHE:HE1	22:P:4270:CDL:H1	1.45	0.80
25:E:3230:PSC:H21	25:E:3230:PSC:H222	1.65	0.79
4:Q:114:GLU:HG2	28:Q:1465:HOH:O	1.81	0.79
2:O:224:ALA:O	2:O:227:LEU:HG	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:CE1	18:A:3521:TGL:H282	2.19	0.77
23:P:4264:PEK:H161	23:P:4264:PEK:H102	1.64	0.77
1:N:113:LEU:CD1	18:N:4522:TGL:H292	2.16	0.76
2:O:49:LYS:NZ	18:Q:4523:TGL:HC71	2.00	0.76
19:N:4524:PGV:H321	19:N:4524:PGV:H162	1.68	0.76
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.69	0.75
18:N:4521:TGL:H241	18:N:4521:TGL:HA91	1.67	0.74
2:O:56:MET:HA	25:O:4230:PSC:H202	1.70	0.74
1:N:433:LEU:HD11	18:N:4521:TGL:OB1	1.88	0.74
19:A:3524:PGV:H321	19:A:3524:PGV:H162	1.70	0.74
3:P:210:ILE:HG23	19:P:4267:PGV:H102	1.70	0.74
10:J:33:ARG:HG2	21:J:3060:CHD:H152	1.68	0.74
12:L:13:PHE:HA	18:L:3522:TGL:HC31	1.68	0.74
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.68	0.74
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.69	0.73
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.70	0.73
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.68	0.73
22:C:3270:CDL:C66	19:C:3267:PGV:H182	2.18	0.72
28:B:4263:HOH:O	18:D:3523:TGL:HC52	1.89	0.72
1:N:1:FME:HCN	1:N:4:ASN:H	1.55	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.72
4:D:34:SER:H	4:D:37:GLN:NE2	1.88	0.71
3:C:67:PHE:HE1	22:C:3270:CDL:H1	1.55	0.71
18:D:3523:TGL:HA81	18:D:3523:TGL:H242	1.73	0.71
6:S:85:CYS:SG	6:S:87:THR:HG23	2.31	0.70
18:Q:4523:TGL:HG12	18:Q:4523:TGL:HC21	1.73	0.70
6:S:94:HIS:CG	6:S:95:GLN:H	2.09	0.70
18:N:4521:TGL:H101	18:N:4521:TGL:C27	2.20	0.70
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.27	0.69
22:P:4270:CDL:H662	19:P:4267:PGV:C18	2.21	0.69
3:C:210:ILE:HG23	19:C:3267:PGV:H102	1.75	0.69
1:A:334:TRP:HZ3	18:D:3523:TGL:HA62	1.57	0.68
3:P:246:ASP:HB2	28:P:1524:HOH:O	1.91	0.68
7:T:38:HIS:NE2	22:T:4269:CDL:H111	2.09	0.68
7:G:5:LYS:HB3	1:N:278:MET:SD	2.33	0.68
19:P:4267:PGV:H161	19:P:4267:PGV:H12	1.76	0.68
18:D:3523:TGL:HC31	28:D:3613:HOH:O	1.93	0.67
1:N:334:TRP:CZ3	18:Q:4523:TGL:HA42	2.30	0.67
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.76	0.67
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.77	0.67
1:N:472:ILE:HD13	18:N:4522:TGL:HA92	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:HD2	7:G:84:LYS:N	1.99	0.67
7:T:84:LYS:H	7:T:84:LYS:CD	2.03	0.66
6:S:94:HIS:CD2	6:S:95:GLN:N	2.63	0.66
9:V:10:ARG:HD2	28:V:2590:HOH:O	1.94	0.66
12:L:20:ARG:NH2	18:L:3522:TGL:HC32	2.11	0.66
25:E:3230:PSC:C07	9:I:10:ARG:HH21	2.09	0.66
2:O:41:ILE:HD13	25:O:4230:PSC:H342	1.79	0.65
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.77	0.65
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.65
22:C:3270:CDL:H812	19:C:3267:PGV:H181	1.79	0.65
2:B:92:ASN:HB3	28:B:4260:HOH:O	1.97	0.64
18:A:3521:TGL:H283	18:A:3521:TGL:HB92	1.79	0.64
4:D:58:GLU:HG3	28:D:3555:HOH:O	1.98	0.63
18:N:4521:TGL:HB91	2:O:32:PHE:CE2	2.33	0.63
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.80	0.63
18:Q:4523:TGL:H122	18:Q:4523:TGL:HB82	1.79	0.63
5:R:89:LEU:O	5:R:93:LEU:HG	1.99	0.63
18:D:3523:TGL:H122	18:D:3523:TGL:HB82	1.80	0.63
18:Q:4523:TGL:HA81	18:Q:4523:TGL:H242	1.80	0.62
6:S:75:HIS:H	6:S:80:GLN:HE22	1.46	0.62
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.64	0.62
6:F:92:VAL:O	6:F:92:VAL:HG23	1.99	0.62
2:O:68:LEU:HD22	25:O:4230:PSC:H171	1.82	0.62
28:N:2197:HOH:O	18:Q:4523:TGL:HG2	1.98	0.62
19:C:3267:PGV:H12	19:C:3267:PGV:H161	1.81	0.61
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.00	0.61
1:N:449:MET:SD	2:O:5:MET:HG2	2.40	0.61
28:B:4247:HOH:O	18:D:3523:TGL:H352	2.00	0.61
1:N:472:ILE:HG21	18:N:4522:TGL:HA81	1.83	0.60
1:A:334:TRP:CZ3	18:D:3523:TGL:HA42	2.37	0.60
2:O:49:LYS:HZ2	18:Q:4523:TGL:HC71	1.65	0.60
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.66	0.59
2:B:41:ILE:HD13	25:E:3230:PSC:H342	1.84	0.59
1:N:472:ILE:HG21	18:N:4522:TGL:CA8	2.32	0.59
3:P:160:LEU:HD13	21:P:4271:CHD:H181	1.84	0.59
25:O:4230:PSC:C07	9:V:10:ARG:HE	2.15	0.59
9:V:65:LYS:O	11:X:54:ARG:NH1	2.35	0.59
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.67	0.59
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.02	0.59
1:A:151:HIS:CD2	23:C:3264:PEK:H382	2.38	0.59
1:N:112:LEU:HG	28:N:1389:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:20:ARG:NH1	18:L:3522:TGL:HC61	2.17	0.58
1:A:407:ASP:O	1:A:411:LYS:HG3	2.04	0.58
7:G:8:HIS:HD2	23:G:4263:PEK:H252	1.66	0.58
18:N:4521:TGL:H281	18:N:4521:TGL:HB81	1.83	0.58
8:U:50:VAL:HG21	28:U:2545:HOH:O	2.02	0.58
1:A:1:FME:HCN	1:A:4:ASN:H	1.68	0.58
25:E:3230:PSC:H072	9:I:10:ARG:HH21	1.67	0.58
12:L:24:MET:HG3	28:L:2411:HOH:O	2.04	0.58
1:N:81:TRP:HZ2	18:N:4522:TGL:C28	2.17	0.58
12:Y:20:ARG:NH1	28:Y:1514:HOH:O	2.36	0.58
22:P:4270:CDL:H812	19:P:4267:PGV:H181	1.86	0.57
1:A:426:PHE:CD1	18:A:3521:TGL:H282	2.38	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.39	0.57
12:L:11:ILE:HG22	18:L:3522:TGL:H271	1.86	0.57
1:A:449:MET:SD	2:B:5:MET:HG2	2.45	0.57
2:O:41:ILE:CD1	25:O:4230:PSC:H342	2.34	0.57
1:N:113:LEU:HD13	18:N:4522:TGL:H292	1.84	0.57
22:G:3269:CDL:HB32	1:N:304:TYR:HD1	1.69	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.35	0.57
1:A:321:PHE:CD2	25:E:3230:PSC:H341	2.40	0.57
7:G:8:HIS:CD2	23:G:4263:PEK:H252	2.39	0.57
7:G:5:LYS:HD2	23:G:4263:PEK:H382	1.87	0.56
22:T:4269:CDL:HA62	22:T:4269:CDL:H322	1.87	0.56
9:I:5:ALA:O	9:I:7:PRO:HD3	2.04	0.56
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.87	0.56
19:A:3524:PGV:H141	4:D:87:PHE:CD2	2.41	0.56
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.05	0.56
2:O:59:GLN:HG3	2:O:59:GLN:O	2.06	0.56
22:G:3269:CDL:HA62	22:G:3269:CDL:H322	1.87	0.56
1:N:22:PHE:HA	18:N:4522:TGL:HB72	1.88	0.56
3:C:213:THR:HG23	22:C:3270:CDL:H762	1.88	0.55
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.88	0.55
23:C:3264:PEK:C16	23:C:3264:PEK:H102	2.34	0.55
7:T:5:LYS:CD	23:T:3263:PEK:H382	2.35	0.55
4:D:17:VAL:HG12	28:D:3556:HOH:O	2.06	0.55
5:E:84:TYR:O	5:E:88:GLU:HG2	2.07	0.55
3:C:160:LEU:HD13	21:C:3271:CHD:H181	1.88	0.55
1:A:334:TRP:CZ3	18:D:3523:TGL:HA62	2.41	0.54
1:A:472:ILE:HG21	18:L:3522:TGL:HA81	1.90	0.54
13:M:17:ILE:O	13:M:21:VAL:HG23	2.07	0.54
1:N:151:HIS:CD2	23:P:4264:PEK:H382	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.54
1:N:54:TYR:HB2	28:N:1075:HOH:O	2.07	0.54
4:D:127:LYS:HD2	28:I:371:HOH:O	2.07	0.54
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.07	0.54
2:B:56:MET:HG2	25:E:3230:PSC:H211	1.89	0.54
19:N:4524:PGV:H41	19:N:4524:PGV:H232	1.90	0.54
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.90	0.54
2:B:102:HIS:O	2:B:104:TRP:N	2.41	0.53
1:A:222:PRO:HD2	28:B:4240:HOH:O	2.07	0.53
18:A:3521:TGL:HC52	2:B:7:LEU:HD12	1.90	0.53
7:G:17:ARG:HD2	28:G:289:HOH:O	2.06	0.53
10:J:40:LEU:HD12	21:J:3060:CHD:H183	1.89	0.53
28:B:4144:HOH:O	18:D:3523:TGL:HC72	2.08	0.53
7:G:8:HIS:CE1	23:G:4263:PEK:H331	2.44	0.53
3:C:3:HIS:HE1	6:F:31:TYR:OH	1.90	0.53
7:G:19:LEU:HD21	23:G:4263:PEK:H362	1.90	0.53
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.90	0.53
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.22	0.53
18:A:3521:TGL:CB9	18:A:3521:TGL:H283	2.38	0.53
4:Q:118:LYS:HG3	28:Q:1465:HOH:O	2.08	0.53
1:A:81:TRP:HZ2	18:L:3522:TGL:H282	1.74	0.53
2:O:150:ILE:HD12	2:O:184:LEU:HD22	1.91	0.53
22:T:4269:CDL:H392	22:T:4269:CDL:H161	1.90	0.53
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.91	0.53
22:P:4270:CDL:C66	19:P:4267:PGV:H182	2.36	0.52
11:X:24:PHE:O	11:X:28:VAL:HG12	2.10	0.52
7:G:3:ALA:O	7:G:4:ALA:HB2	2.09	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.92	0.52
8:H:49:ASP:O	8:H:52:VAL:HG22	2.10	0.52
12:L:20:ARG:HH12	18:L:3522:TGL:CC6	2.16	0.52
22:G:3269:CDL:H392	22:G:3269:CDL:H161	1.92	0.52
1:N:265:LYS:HE3	28:S:2510:HOH:O	2.08	0.52
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.09	0.52
1:A:1:FME:HE2	1:A:1:FME:HA	1.90	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.91	0.52
1:N:52:GLN:O	1:N:56:VAL:HG23	2.10	0.52
28:B:4241:HOH:O	23:P:4265:PEK:H031	2.09	0.52
18:Q:4523:TGL:CG1	18:Q:4523:TGL:HC21	2.39	0.52
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.09	0.51
23:G:4263:PEK:H132	3:P:247:VAL:HG11	1.93	0.51
18:N:4521:TGL:HB91	2:O:32:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:MET:HG2	25:O:4230:PSC:H211	1.92	0.51
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.75	0.51
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.45	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.45	0.51
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.45	0.51
19:A:3524:PGV:H41	19:A:3524:PGV:H232	1.90	0.51
3:P:213:THR:HG23	22:P:4270:CDL:H762	1.92	0.51
1:N:113:LEU:HD12	18:N:4522:TGL:H292	1.93	0.51
12:L:20:ARG:HH22	18:L:3522:TGL:HC32	1.74	0.51
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.39	0.51
12:L:13:PHE:HB3	18:L:3522:TGL:HG12	1.93	0.51
6:F:25:ARG:HD2	28:F:154:HOH:O	2.10	0.51
6:F:64:GLU:O	6:F:65:ASP:HB2	2.11	0.51
3:C:191:GLY:HA3	28:G:143:HOH:O	2.11	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.12	0.50
17:A:515:HEA:HMC1	17:A:515:HEA:HBC1	1.93	0.50
7:G:37:LEU:HD21	22:G:3269:CDL:H361	1.93	0.50
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.50
7:T:3:ALA:O	7:T:4:ALA:HB2	2.11	0.50
18:N:4522:TGL:CG1	12:Y:13:PHE:HB3	2.41	0.50
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.41	0.50
1:A:472:ILE:HG21	18:L:3522:TGL:CA8	2.41	0.50
1:N:488:THR:HB	1:N:495:LEU:HD13	1.92	0.50
3:P:34:TRP:CD1	3:P:40:MET:HG2	2.47	0.50
1:A:177:SER:H	1:A:180:GLN:NE2	2.10	0.50
6:S:51:SER:O	6:S:94:HIS:N	2.45	0.50
22:T:4269:CDL:H511	22:T:4269:CDL:H172	1.93	0.50
7:T:5:LYS:HB2	23:T:3263:PEK:H372	1.94	0.50
23:G:4263:PEK:H9	3:P:244:PHE:HA	1.94	0.50
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.42	0.50
6:S:87:THR:HG21	28:S:1319:HOH:O	2.12	0.50
3:C:244:PHE:HA	23:T:3263:PEK:H9	1.93	0.50
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.25	0.50
22:G:3269:CDL:H511	22:G:3269:CDL:H172	1.92	0.50
18:L:3522:TGL:HC62	18:L:3522:TGL:HC22	1.93	0.50
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.93	0.50
23:C:3264:PEK:H32	23:C:3264:PEK:H71	1.93	0.50
8:U:7:LYS:O	8:U:8:ILE:HG22	2.12	0.50
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.00	0.49
2:O:102:HIS:O	2:O:104:TRP:N	2.45	0.49
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:3269:CDL:H522	22:G:3269:CDL:H202	1.95	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.49
1:A:81:TRP:HZ2	18:L:3522:TGL:C28	2.26	0.49
7:T:8:HIS:CD2	23:T:3263:PEK:H252	2.48	0.49
1:N:379:TYR:O	1:N:383:MET:HB2	2.12	0.49
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.13	0.49
7:G:34:ASN:HD22	22:G:3269:CDL:H151	1.78	0.49
1:N:514:LYS:HE2	28:S:1319:HOH:O	2.12	0.49
4:Q:89:ILE:HD12	18:Q:4523:TGL:H311	1.95	0.49
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.95	0.49
22:P:4270:CDL:H602	22:P:4270:CDL:H632	1.59	0.49
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.48
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.95	0.48
22:C:3270:CDL:HA61	28:C:3618:HOH:O	2.11	0.48
18:N:4521:TGL:OB1	18:N:4521:TGL:HB42	2.13	0.48
1:A:87:ILE:O	1:A:173:PRO:HD3	2.13	0.48
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.48	0.48
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.78	0.48
6:S:92:VAL:HG23	6:S:92:VAL:O	2.13	0.48
28:O:2266:HOH:O	8:U:61:LYS:HD3	2.12	0.48
25:O:4230:PSC:H071	9:V:10:ARG:HE	1.77	0.48
2:B:78:LEU:HD12	22:T:4269:CDL:H351	1.94	0.48
1:A:304:TYR:HD1	22:T:4269:CDL:HB32	1.79	0.48
1:A:472:ILE:HD13	18:L:3522:TGL:HA92	1.95	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
8:H:23:GLN:HG3	28:H:2167:HOH:O	2.12	0.48
25:O:4230:PSC:H212	25:O:4230:PSC:O01	2.14	0.48
2:O:49:LYS:HZ3	18:Q:4523:TGL:HC71	1.76	0.48
10:W:50:LEU:HD22	10:W:50:LEU:O	2.14	0.48
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.62	0.48
1:A:427:PRO:HG3	18:A:3521:TGL:H351	1.95	0.48
2:B:41:ILE:O	2:B:45:MET:HG2	2.14	0.48
2:O:104:TRP:HA	2:O:207:MET:SD	2.54	0.48
18:N:4521:TGL:HB91	2:O:32:PHE:HE2	1.75	0.48
19:N:4524:PGV:H141	4:Q:87:PHE:CD2	2.49	0.48
1:A:81:TRP:CZ2	18:L:3522:TGL:H282	2.49	0.47
2:B:114:GLU:HB3	28:B:4162:HOH:O	2.14	0.47
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.96	0.47
7:G:34:ASN:ND2	22:G:3269:CDL:H151	2.28	0.47
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.48	0.47
1:A:52:GLN:O	1:A:56:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.96	0.47
3:P:67:PHE:CE1	22:P:4270:CDL:H1	2.37	0.47
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.28	0.47
2:B:81:LEU:HD13	22:T:4269:CDL:H122	1.96	0.47
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.50	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.44	0.47
18:N:4521:TGL:HC52	2:O:7:LEU:HD12	1.97	0.47
3:P:25:LEU:O	3:P:29:SER:HB2	2.15	0.47
22:T:4269:CDL:H152	22:T:4269:CDL:H181	1.62	0.47
1:A:278:MET:SD	7:T:5:LYS:HB3	2.54	0.47
18:D:3523:TGL:HC91	18:D:3523:TGL:HC62	1.75	0.47
25:E:3230:PSC:H62	25:E:3230:PSC:H241	1.97	0.47
1:A:365:ILE:HD11	28:A:3732:HOH:O	2.14	0.47
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.95	0.47
2:B:58:ALA:O	2:B:62:GLU:HG3	2.15	0.47
21:W:4060:CHD:H161	21:W:4060:CHD:H212	1.74	0.47
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.46
1:A:379:TYR:O	1:A:383:MET:HB2	2.14	0.46
18:N:4521:TGL:H301	18:N:4521:TGL:HA92	1.96	0.46
18:N:4521:TGL:H283	18:N:4521:TGL:HB92	1.96	0.46
23:T:3263:PEK:H371	23:T:3263:PEK:H332	1.98	0.46
7:G:39:SER:HB3	28:G:2466:HOH:O	2.15	0.46
10:J:50:LEU:HD22	10:J:50:LEU:O	2.15	0.46
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.97	0.46
25:O:4230:PSC:H072	9:V:10:ARG:HE	1.81	0.46
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.81	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.98	0.46
18:A:3521:TGL:HG11	2:B:7:LEU:HB3	1.98	0.46
22:C:3270:CDL:H632	22:C:3270:CDL:H602	1.55	0.46
22:C:3270:CDL:H652	22:C:3270:CDL:H621	1.56	0.46
3:C:210:ILE:HD13	19:C:3267:PGV:H301	1.98	0.46
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.96	0.46
1:N:347:LEU:HD13	1:N:383:MET:SD	2.54	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.98	0.46
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.16	0.46
19:N:4524:PGV:H141	4:Q:87:PHE:CE2	2.51	0.46
18:N:4522:TGL:H181	18:N:4522:TGL:OA1	2.15	0.46
22:T:4269:CDL:H202	22:T:4269:CDL:H522	1.98	0.46
28:Q:1465:HOH:O	11:X:51:LYS:HD3	2.16	0.46
12:Y:20:ARG:HH21	12:Y:24:MET:CG	2.29	0.46
19:A:3524:PGV:H141	4:D:87:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.51	0.46
1:A:22:PHE:HA	18:L:3522:TGL:HB72	1.98	0.46
2:O:1:FME:SD	2:O:133:LEU:CD1	3.04	0.46
2:O:57:ASP:H	25:O:4230:PSC:H201	1.80	0.46
1:N:426:PHE:CE1	18:N:4521:TGL:H282	2.50	0.45
1:N:343:GLY:HA2	18:Q:4523:TGL:H202	1.98	0.45
3:P:191:GLY:HA3	28:T:1143:HOH:O	2.16	0.45
22:P:4270:CDL:H642	22:P:4270:CDL:H191	1.98	0.45
4:D:89:ILE:CD1	18:D:3523:TGL:H311	2.46	0.45
23:G:4263:PEK:H15	3:P:248:VAL:HG22	1.99	0.45
11:K:24:PHE:O	11:K:28:VAL:HG12	2.17	0.45
13:M:42:LYS:CE	13:M:42:LYS:HA	2.38	0.45
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.99	0.45
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.45
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.82	0.45
2:O:57:ASP:H	25:O:4230:PSC:C20	2.29	0.45
22:P:4270:CDL:CB3	22:P:4270:CDL:HB21	2.46	0.45
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.64	0.45
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.99	0.45
1:A:1:FME:HA	1:A:1:FME:CE	2.47	0.45
22:G:3269:CDL:H551	22:G:3269:CDL:H582	1.69	0.45
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.16	0.45
22:C:3270:CDL:H191	22:C:3270:CDL:H642	1.99	0.45
22:C:3270:CDL:HB21	22:C:3270:CDL:CB3	2.47	0.45
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.51	0.45
1:N:28:MET:HE2	17:N:515:HEA:H271	1.97	0.45
18:L:3522:TGL:OA1	18:L:3522:TGL:H181	2.17	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.17	0.45
1:N:321:PHE:CD2	25:O:4230:PSC:H341	2.52	0.45
1:N:365:ILE:HD11	28:N:2145:HOH:O	2.16	0.45
22:T:4269:CDL:H582	22:T:4269:CDL:H551	1.68	0.45
2:B:47:THR:HB	18:D:3523:TGL:H332	1.99	0.44
3:C:22:LEU:O	3:C:26:LEU:HG	2.17	0.44
6:F:92:VAL:O	6:F:92:VAL:CG2	2.63	0.44
18:L:3522:TGL:H122	18:L:3522:TGL:H291	1.66	0.44
25:O:4230:PSC:H221	25:O:4230:PSC:H251	1.75	0.44
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.70	0.44
2:B:91:ASN:HD22	2:B:92:ASN:N	2.15	0.44
18:N:4521:TGL:H222	18:N:4521:TGL:HA91	1.57	0.44
21:P:4271:CHD:H112	21:P:4271:CHD:H12A	1.65	0.44
4:Q:17:VAL:HG12	28:Q:2237:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.65	0.44
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.52	0.44
9:V:15:ARG:HD2	28:V:2350:HOH:O	2.17	0.44
19:A:3524:PGV:H81	19:A:3524:PGV:H262	2.00	0.44
2:B:94:SER:HB2	28:B:4194:HOH:O	2.17	0.44
4:D:126:MET:HA	9:I:68:ILE:HD13	2.00	0.44
18:N:4522:TGL:HG12	12:Y:13:PHE:HB3	1.98	0.44
18:L:3522:TGL:HG12	18:L:3522:TGL:CC1	2.48	0.44
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.99	0.44
23:G:4263:PEK:H332	23:G:4263:PEK:H371	2.00	0.44
1:N:344:PHE:C	1:N:344:PHE:CD1	2.91	0.44
4:Q:86:MET:HG2	18:Q:4523:TGL:H312	1.98	0.44
23:C:3265:PEK:H131	23:C:3265:PEK:H102	1.79	0.44
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.83	0.44
18:N:4521:TGL:HB81	18:N:4521:TGL:C28	2.48	0.44
1:N:400:PHE:HB3	18:N:4522:TGL:H282	1.99	0.44
18:N:4522:TGL:HB52	18:N:4522:TGL:HB81	1.65	0.44
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.17	0.44
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.53	0.44
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.48	0.44
5:R:87:GLN:HG2	5:R:88:GLU:N	2.32	0.44
1:A:350:VAL:HG21	18:A:3521:TGL:H271	2.00	0.44
4:D:34:SER:N	4:D:37:GLN:HE21	1.99	0.44
25:E:3230:PSC:H232	25:E:3230:PSC:H201	1.85	0.44
18:N:4521:TGL:CA9	18:N:4521:TGL:H241	2.41	0.44
2:O:56:MET:HA	25:O:4230:PSC:C20	2.44	0.44
2:O:62:GLU:O	2:O:66:THR:HB	2.18	0.44
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.17	0.44
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.99	0.44
2:B:104:TRP:HA	2:B:207:MET:SD	2.58	0.44
25:O:4230:PSC:H241	25:O:4230:PSC:H62	1.98	0.44
3:P:47:LEU:O	3:P:51:MET:HG2	2.18	0.44
22:T:4269:CDL:H631	22:T:4269:CDL:H662	1.85	0.44
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.45	0.44
1:A:383:MET:O	1:A:387:PHE:HB2	2.18	0.43
1:A:488:THR:HB	1:A:495:LEU:HD13	2.00	0.43
6:F:52:ILE:HA	6:F:94:HIS:HA	1.99	0.43
22:G:3269:CDL:H212	1:N:311:ILE:HD12	2.00	0.43
12:L:11:ILE:CG2	18:L:3522:TGL:H271	2.48	0.43
19:N:4524:PGV:H032	19:N:4524:PGV:O05	2.18	0.43
7:T:19:LEU:HD21	23:T:3263:PEK:H362	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.53	0.43
2:B:62:GLU:O	2:B:66:THR:HB	2.19	0.43
18:N:4521:TGL:H283	18:N:4521:TGL:CB9	2.49	0.43
25:E:3230:PSC:O01	25:E:3230:PSC:H212	2.17	0.43
7:G:7:ASP:O	7:G:9:GLY:N	2.51	0.43
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.00	0.43
4:D:86:MET:HG2	18:D:3523:TGL:H312	2.00	0.43
18:L:3522:TGL:HB81	18:L:3522:TGL:HB52	1.63	0.43
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.82	0.43
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.19	0.43
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.01	0.43
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.43
5:R:82:TYR:N	5:R:83:PRO:CD	2.81	0.43
6:S:52:ILE:O	6:S:94:HIS:ND1	2.52	0.43
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.99	0.43
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.43
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.53	0.43
7:G:44:ARG:HD2	7:G:82:TYR:CE1	2.54	0.43
22:T:4269:CDL:H601	22:T:4269:CDL:H571	1.70	0.43
23:C:3265:PEK:H383	22:G:3269:CDL:H272	2.01	0.43
2:O:1:FME:SD	2:O:133:LEU:HD13	2.58	0.43
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.34	0.43
5:E:97:GLY:HA2	28:E:3252:HOH:O	2.19	0.43
1:N:81:TRP:CZ2	18:N:4522:TGL:C28	3.00	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.43
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.18	0.43
22:T:4269:CDL:H732	22:T:4269:CDL:H762	1.94	0.43
18:N:4522:TGL:HA41	12:Y:25:MET:HG2	1.99	0.43
1:A:400:PHE:HB2	18:L:3522:TGL:H252	2.00	0.43
2:B:56:MET:HA	25:E:3230:PSC:H202	2.01	0.43
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.19	0.43
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.02	0.43
2:B:52:HIS:HE1	25:E:3230:PSC:H02	1.83	0.42
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.42
13:M:42:LYS:HE3	13:M:42:LYS:CA	2.46	0.42
2:O:220:GLU:O	2:O:223:SER:HB2	2.18	0.42
1:N:334:TRP:HZ3	18:Q:4523:TGL:HA62	1.83	0.42
1:N:324:LEU:HD13	2:O:41:ILE:HG22	2.01	0.42
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.89	0.42
3:P:58:TRP:CZ3	19:P:4267:PGV:H81	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:63:ARG:HE	22:P:4270:CDL:CA2	2.11	0.42
4:Q:89:ILE:CD1	18:Q:4523:TGL:H311	2.49	0.42
1:A:240:HIS:O	1:A:243:VAL:HG22	2.19	0.42
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.35	0.42
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.55	0.42
6:S:94:HIS:CG	6:S:95:GLN:N	2.84	0.42
1:A:165:ILE:O	1:A:169:ILE:HG12	2.18	0.42
18:A:3521:TGL:OB1	18:A:3521:TGL:HB42	2.18	0.42
18:D:3523:TGL:HB21	18:D:3523:TGL:OG1	2.19	0.42
1:N:112:LEU:HD23	1:N:112:LEU:C	2.40	0.42
2:O:121:TYR:O	2:O:138:VAL:HA	2.18	0.42
12:Y:20:ARG:HH21	12:Y:24:MET:HG3	1.85	0.42
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.42
25:E:3230:PSC:C14	25:E:3230:PSC:H343	2.49	0.42
7:G:7:ASP:O	1:N:169:ILE:HD12	2.20	0.42
2:O:116:LEU:HD12	2:O:117:SER:N	2.35	0.42
23:C:3265:PEK:H232	7:G:21:PHE:CD2	2.54	0.42
6:F:25:ARG:HB3	28:F:145:HOH:O	2.19	0.42
7:G:5:LYS:HB2	23:G:4263:PEK:H372	2.02	0.42
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.01	0.42
1:A:426:PHE:HE1	18:A:3521:TGL:H282	1.74	0.42
12:L:13:PHE:HB3	18:L:3522:TGL:CG1	2.49	0.42
5:R:48:ILE:O	5:R:52:LEU:HG	2.20	0.42
25:O:4230:PSC:H201	25:O:4230:PSC:H232	1.84	0.42
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.82	0.42
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.42
25:E:3230:PSC:H221	25:E:3230:PSC:H251	1.73	0.42
22:G:3269:CDL:H152	22:G:3269:CDL:H181	1.63	0.42
18:N:4522:TGL:H232	18:N:4522:TGL:H272	2.02	0.42
7:T:7:ASP:O	7:T:9:GLY:N	2.52	0.42
5:E:46:LYS:HG2	28:E:3281:HOH:O	2.19	0.41
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.01	0.41
2:B:92:ASN:HA	2:B:93:PRO:HD2	1.92	0.41
22:C:3270:CDL:H312	22:C:3270:CDL:H151	2.02	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.92	0.41
1:N:3:ILE:HG23	1:N:7:LEU:HD22	2.02	0.41
22:P:4270:CDL:H312	22:P:4270:CDL:H151	2.03	0.41
1:A:174:PRO:HB2	6:F:35:ALA:HB2	2.02	0.41
21:C:3271:CHD:H222	21:C:3271:CHD:H162	1.79	0.41
28:A:3739:HOH:O	4:D:20:ARG:HG3	2.21	0.41
9:I:65:LYS:O	11:K:54:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.02	0.41
21:O:3085:CHD:H212	21:O:3085:CHD:H12	2.01	0.41
22:P:4270:CDL:H372	22:P:4270:CDL:H192	2.02	0.41
7:T:2:SER:O	7:T:3:ALA:HB3	2.21	0.41
11:X:8:ASP:HB2	28:X:2472:HOH:O	2.19	0.41
21:C:3271:CHD:H112	21:C:3271:CHD:H12A	1.63	0.41
18:D:3523:TGL:HA52	18:D:3523:TGL:HB71	2.03	0.41
1:N:426:PHE:CD1	18:N:4521:TGL:H282	2.56	0.41
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.37	0.41
9:V:35:TYR:C	9:V:37:PHE:H	2.24	0.41
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.21	0.41
1:A:514:LYS:HA	6:F:38:ALA:HB3	2.03	0.41
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.20	0.41
12:L:20:ARG:HH22	18:L:3522:TGL:CC6	2.33	0.41
2:O:116:LEU:HD21	2:O:222:TRP:CH2	2.55	0.41
23:P:4264:PEK:H71	23:P:4264:PEK:H32	2.01	0.41
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.88	0.41
19:A:3524:PGV:H032	19:A:3524:PGV:O05	2.19	0.41
1:A:406:ASN:HD21	19:A:3524:PGV:C3	2.34	0.41
3:C:51:MET:SD	22:C:3270:CDL:H622	2.61	0.41
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.02	0.41
1:A:510:TYR:CD2	6:F:49:VAL:HG13	2.56	0.41
22:G:3269:CDL:HB32	1:N:304:TYR:CD1	2.51	0.41
18:Q:4523:TGL:HB31	18:Q:4523:TGL:HA32	2.03	0.41
7:T:8:HIS:CE1	23:T:3263:PEK:H331	2.56	0.41
18:N:4522:TGL:H342	12:Y:28:PHE:HA	2.03	0.41
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.41
19:C:3268:PGV:H202	19:C:3268:PGV:H231	1.83	0.41
25:O:4230:PSC:H343	25:O:4230:PSC:C14	2.51	0.41
8:U:9:LYS:HB3	8:U:10:ASN:H	1.57	0.41
2:B:121:TYR:O	2:B:138:VAL:HA	2.21	0.41
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.21	0.41
1:N:177:SER:H	1:N:180:GLN:NE2	2.19	0.41
18:N:4521:TGL:H101	18:N:4521:TGL:C28	2.50	0.41
2:O:13:THR:HB	2:O:168:LEU:HD23	2.03	0.41
22:P:4270:CDL:H561	22:P:4270:CDL:H532	1.83	0.41
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.03	0.41
22:G:3269:CDL:H601	22:G:3269:CDL:H571	1.71	0.41
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.50	0.41
18:N:4522:TGL:CC6	18:N:4522:TGL:HC22	2.51	0.41
1:N:76:GLY:O	1:N:80:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:214:PHE:CD1	19:P:4267:PGV:H71	2.55	0.41
23:P:4265:PEK:H383	22:T:4269:CDL:H272	2.03	0.41
3:P:51:MET:SD	22:P:4270:CDL:H622	2.61	0.41
9:V:73:LYS:HE3	9:V:73:LYS:HB3	1.86	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.95	0.41
1:A:426:PHE:HB3	1:A:427:PRO:HD3	2.03	0.41
21:B:4085:CHD:H12	21:B:4085:CHD:H212	2.03	0.41
25:O:4230:PSC:H042	25:O:4230:PSC:H062	1.86	0.41
7:T:17:ARG:HD3	28:T:1289:HOH:O	2.21	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.98	0.41
9:I:35:TYR:C	9:I:37:PHE:H	2.25	0.41
25:O:4230:PSC:H212	25:O:4230:PSC:C02	2.51	0.41
3:P:40:MET:O	3:P:44:MET:HG2	2.21	0.41
4:Q:51:LEU:HD21	4:Q:59:LEU:CD1	2.51	0.41
13:Z:42:LYS:HE3	13:Z:43:SER:N	2.36	0.41
6:F:51:SER:O	6:F:94:HIS:N	2.54	0.40
23:P:4264:PEK:C16	23:P:4264:PEK:H102	2.43	0.40
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.56	0.40
25:O:4230:PSC:H343	25:O:4230:PSC:C13	2.51	0.40
8:U:50:VAL:O	8:U:50:VAL:HG12	2.21	0.40
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.56	0.40
1:A:113:LEU:CD1	18:L:3522:TGL:H292	2.51	0.40
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.85	0.40
22:P:4270:CDL:H641	22:P:4270:CDL:H231	2.02	0.40
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.89	0.40
7:T:31:CYS:SG	22:T:4269:CDL:H532	2.61	0.40
7:T:8:HIS:CD2	23:T:3263:PEK:H231	2.55	0.40
1:A:513:LEU:HA	1:A:513:LEU:HD22	1.81	0.40
17:A:515:HEA:HMB1	17:A:515:HEA:H11	1.98	0.40
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.57	0.40
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.04	0.40
2:O:68:LEU:HB3	2:O:69:PRO:HD3	2.04	0.40
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.84	0.40
1:N:298:ASP:HB3	28:N:1369:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	496 (97%)	16 (3%)	0	100	100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	B	225/227 (99%)	208 (92%)	14 (6%)	3 (1%)	13	3
2	O	225/227 (99%)	206 (92%)	16 (7%)	3 (1%)	13	3
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
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%)	89 (93%)	4 (4%)	3 (3%)	4	0
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
7	G	81/85 (95%)	68 (84%)	6 (7%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	6	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	6	1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	124 (4%)	30 (1%)	19	6

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	60	GLU
6	F	94	HIS
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
2	O	104	TRP
7	T	3	ALA
8	U	8	ILE
2	B	104	TRP
2	O	60	GLU
7	T	40	GLY
6	F	96	LEU
8	H	46	LYS
6	S	96	LEU
7	G	6	GLY
7	T	6	GLY
8	U	46	LYS
2	O	92	ASN
2	B	92	ASN

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	418 (98%)	8 (2%)	60	49
1	N	426/426 (100%)	415 (97%)	11 (3%)	49	35
2	B	210/210 (100%)	200 (95%)	10 (5%)	28	13
2	O	210/210 (100%)	197 (94%)	13 (6%)	20	7
3	C	224/226 (99%)	220 (98%)	4 (2%)	62	51
3	P	224/226 (99%)	219 (98%)	5 (2%)	55	42
4	D	128/129 (99%)	126 (98%)	2 (2%)	65	57
4	Q	128/129 (99%)	126 (98%)	2 (2%)	65	57
5	E	92/95 (97%)	90 (98%)	2 (2%)	55	42
5	R	92/95 (97%)	88 (96%)	4 (4%)	32	16
6	F	81/81 (100%)	79 (98%)	2 (2%)	50	37
6	S	81/81 (100%)	77 (95%)	4 (5%)	27	12
7	G	67/68 (98%)	61 (91%)	6 (9%)	10	3
7	T	67/68 (98%)	62 (92%)	5 (8%)	15	4
8	H	71/75 (95%)	69 (97%)	2 (3%)	47	33
8	U	71/75 (95%)	67 (94%)	4 (6%)	23	9
9	I	57/57 (100%)	53 (93%)	4 (7%)	16	5
9	V	57/57 (100%)	55 (96%)	2 (4%)	39	23
10	J	49/50 (98%)	48 (98%)	1 (2%)	58	46
10	W	49/50 (98%)	48 (98%)	1 (2%)	58	46
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	49	35
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	37 (95%)	2 (5%)	26	11
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	7	1
All	All	3040/3082 (99%)	2936 (97%)	104 (3%)	40	24

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	104	TRP
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	42	ARG
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU
13	M	13	LYS
13	M	34	LEU

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Mol	Chain	Res	Type
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	338	MET
1	N	369	ASP
1	N	484	THR
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	104	TRP
2	O	115	ASP
2	O	148	MET
2	O	217	LYS
3	P	29	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	121	LYS
5	R	5	HIS
5	R	70	VAL
5	R	80	GLU
5	R	90	ARG
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN

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Mol	Chain	Res	Type
7	T	18	PHE
7	T	38	HIS
7	T	42	ARG
7	T	43	GLU
7	T	54	ARG
8	U	9	LYS
8	U	21	PRO
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	29	LEU
10	W	50	LEU
11	X	54	ARG
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 (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	8	HIS
7	G	34	ASN
9	I	8	GLN
11	K	35	GLN
1	N	80	ASN

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Mol	Chain	Res	Type
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
9	V	8	GLN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	9,9,10	0.84	0	7,9,11	1.25	2 (28%)
2	FME	B	1	2	9,9,10	0.90	0	7,9,11	2.04	1 (14%)
7	TPO	G	11	7	9,10,11	2.06	2 (22%)	11,14,16	1.06	1 (9%)
9	SAC	I	1	9	8,8,9	2.54	3 (37%)	7,9,11	2.85	2 (28%)
1	FME	N	1	1	9,9,10	0.85	0	7,9,11	1.89	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	9,9,10	0.73	0	7,9,11	1.42	1 (14%)
7	TPO	T	11	7	9,10,11	2.04	2 (22%)	11,14,16	1.09	1 (9%)
9	SAC	V	1	9	8,8,9	2.73	3 (37%)	7,9,11	3.26	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	-	0/5/9/11	0/0/0/0
2	FME	B	1	2	-	0/5/9/11	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	-	0/5/9/11	0/0/0/0
2	FME	O	1	2	-	0/5/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-C	2.56	1.53	1.50
7	G	11	TPO	CB-CA	2.97	1.59	1.53
7	T	11	TPO	CB-CA	3.32	1.59	1.53
9	V	1	SAC	CA-C	3.34	1.54	1.50
9	I	1	SAC	CA-N	4.24	1.52	1.46
9	V	1	SAC	CA-N	4.35	1.52	1.46
7	T	11	TPO	CA-C	4.48	1.56	1.50
7	G	11	TPO	CA-C	4.50	1.56	1.50
9	I	1	SAC	OAC-C1A	4.97	1.34	1.23
9	V	1	SAC	OAC-C1A	5.05	1.35	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-7.13	110.25	123.24
9	I	1	SAC	CA-N-C1A	-5.82	112.62	123.24
2	B	1	FME	CA-N-CN	-4.79	115.46	122.82
1	N	1	FME	CA-N-CN	-4.24	116.30	122.82
2	O	1	FME	CA-N-CN	-2.96	118.27	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.46	119.35	125.09
9	V	1	SAC	OAC-C1A-C2A	-2.25	118.00	122.07
7	T	11	TPO	O-C-CA	-2.19	119.98	125.09
1	A	1	FME	CA-N-CN	-2.17	119.48	122.82
1	A	1	FME	O-C-CA	-2.16	120.05	125.09
7	G	11	TPO	O-C-CA	-2.04	120.33	125.09
9	V	1	SAC	CB-CA-N	2.52	116.36	110.61
9	V	1	SAC	C2A-C1A-N	2.78	120.97	116.10
9	I	1	SAC	CB-CA-N	3.63	118.90	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 42 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	A	3266	-	50,50,50	0.91	1 (2%)	53,56,56	0.82	2 (3%)
18	TGL	A	3521	-	62,62,62	0.98	4 (6%)	65,65,65	1.14	7 (10%)
19	PGV	A	3524	-	50,50,50	1.12	6 (12%)	53,56,56	1.25	7 (13%)
17	HEA	A	515	1	43,67,67	1.16	3 (6%)	37,103,103	1.50	8 (21%)
17	HEA	A	516	1	43,67,67	1.24	4 (9%)	37,103,103	1.38	6 (16%)
20	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	CHD	B	4085	-	29,32,32	0.71	0	47,51,51	1.90	14 (29%)
23	PEK	C	3264	-	52,52,52	1.52	4 (7%)	55,57,57	1.31	7 (12%)
23	PEK	C	3265	-	52,52,52	1.70	11 (21%)	55,57,57	1.15	6 (10%)
19	PGV	C	3267	-	50,50,50	0.81	1 (2%)	53,56,56	0.94	3 (5%)
19	PGV	C	3268	-	50,50,50	1.12	4 (8%)	53,56,56	0.66	0
22	CDL	C	3270	-	99,99,99	0.79	3 (3%)	105,111,111	0.91	5 (4%)
21	CHD	C	3271	-	29,32,32	0.78	1 (3%)	47,51,51	3.70	22 (46%)
21	CHD	C	3525	-	29,32,32	0.79	0	47,51,51	1.62	11 (23%)
18	TGL	D	3523	-	62,62,62	1.16	3 (4%)	65,65,65	1.13	9 (13%)
25	PSC	E	3230	-	51,51,51	1.26	4 (7%)	57,59,59	1.10	4 (7%)
22	CDL	G	3269	-	99,99,99	0.97	5 (5%)	105,111,111	0.91	7 (6%)
23	PEK	G	4263	-	52,52,52	1.74	9 (17%)	55,57,57	1.09	3 (5%)
21	CHD	J	3060	-	29,32,32	0.85	1 (3%)	47,51,51	3.34	24 (51%)
18	TGL	L	3522	-	62,62,62	1.38	7 (11%)	65,65,65	1.26	5 (7%)
27	DMU	M	3526	-	34,34,34	3.20	8 (23%)	45,45,45	4.29	19 (42%)
19	PGV	N	4266	-	50,50,50	1.03	3 (6%)	53,56,56	1.09	4 (7%)
18	TGL	N	4521	-	62,62,62	1.00	4 (6%)	65,65,65	1.11	3 (4%)
18	TGL	N	4522	-	62,62,62	1.42	7 (11%)	65,65,65	1.17	5 (7%)
19	PGV	N	4524	-	50,50,50	1.12	4 (8%)	53,56,56	1.19	7 (13%)
17	HEA	N	515	1	43,67,67	1.22	4 (9%)	37,103,103	1.56	12 (32%)
17	HEA	N	516	1	43,67,67	1.22	5 (11%)	37,103,103	1.36	6 (16%)
20	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
21	CHD	O	3085	-	29,32,32	0.74	0	47,51,51	1.92	18 (38%)
25	PSC	O	4230	-	51,51,51	1.22	3 (5%)	57,59,59	1.11	4 (7%)
23	PEK	P	4264	-	52,52,52	1.52	5 (9%)	55,57,57	1.41	12 (21%)
23	PEK	P	4265	-	52,52,52	1.74	12 (23%)	55,57,57	1.13	6 (10%)
19	PGV	P	4267	-	50,50,50	1.00	2 (4%)	53,56,56	1.09	5 (9%)
19	PGV	P	4268	-	50,50,50	1.13	4 (8%)	53,56,56	0.68	0
22	CDL	P	4270	-	99,99,99	0.81	4 (4%)	105,111,111	0.89	5 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CHD	P	4271	-	29,32,32	0.75	0	47,51,51	3.63	21 (44%)
21	CHD	P	4525	-	29,32,32	0.82	1 (3%)	47,51,51	1.67	9 (19%)
18	TGL	Q	4523	-	62,62,62	1.14	3 (4%)	65,65,65	1.07	5 (7%)
23	PEK	T	3263	-	52,52,52	1.74	11 (21%)	55,57,57	1.07	3 (5%)
22	CDL	T	4269	-	99,99,99	0.93	4 (4%)	105,111,111	0.92	7 (6%)
21	CHD	W	4060	-	29,32,32	0.93	2 (6%)	47,51,51	3.30	25 (53%)
27	DMU	Z	4526	-	34,34,34	3.18	8 (23%)	45,45,45	4.25	19 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	A	3266	-	-	0/55/55/55	0/0/0/0
18	TGL	A	3521	-	-	0/65/65/65	0/0/0/0
19	PGV	A	3524	-	-	0/55/55/55	0/0/0/0
17	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
20	CUA	B	228	2	-	0/0/0/0	0/0/0/0
21	CHD	B	4085	-	-	0/7/74/74	0/4/4/4
23	PEK	C	3264	-	-	0/56/56/56	0/0/0/0
23	PEK	C	3265	-	-	0/56/56/56	0/0/0/0
19	PGV	C	3267	-	-	0/55/55/55	0/0/0/0
19	PGV	C	3268	-	-	0/55/55/55	0/0/0/0
22	CDL	C	3270	-	-	0/110/110/110	0/0/0/0
21	CHD	C	3271	-	5/5/12/12	0/7/74/74	0/4/4/4
21	CHD	C	3525	-	-	0/7/74/74	0/4/4/4
18	TGL	D	3523	-	-	2/65/65/65	0/0/0/0
25	PSC	E	3230	-	-	0/55/55/55	0/0/0/0
22	CDL	G	3269	-	-	0/110/110/110	0/0/0/0
23	PEK	G	4263	-	-	0/56/56/56	0/0/0/0
21	CHD	J	3060	-	5/5/12/12	0/7/74/74	0/4/4/4
18	TGL	L	3522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	3526	-	5/5/10/10	0/19/59/59	0/2/2/2
19	PGV	N	4266	-	-	0/55/55/55	0/0/0/0
18	TGL	N	4521	-	-	0/65/65/65	0/0/0/0
18	TGL	N	4522	-	-	0/65/65/65	0/0/0/0
19	PGV	N	4524	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
17	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
20	CUA	O	228	2	-	0/0/0/0	0/0/0/0
21	CHD	O	3085	-	-	0/7/74/74	0/4/4/4
25	PSC	O	4230	-	-	0/55/55/55	0/0/0/0
23	PEK	P	4264	-	-	0/56/56/56	0/0/0/0
23	PEK	P	4265	-	-	0/56/56/56	0/0/0/0
19	PGV	P	4267	-	-	0/55/55/55	0/0/0/0
19	PGV	P	4268	-	-	0/55/55/55	0/0/0/0
22	CDL	P	4270	-	-	0/110/110/110	0/0/0/0
21	CHD	P	4271	-	5/5/12/12	0/7/74/74	0/4/4/4
21	CHD	P	4525	-	-	0/7/74/74	0/4/4/4
18	TGL	Q	4523	-	-	1/65/65/65	0/0/0/0
23	PEK	T	3263	-	-	0/56/56/56	0/0/0/0
22	CDL	T	4269	-	-	0/110/110/110	0/0/0/0
21	CHD	W	4060	-	5/5/12/12	0/7/74/74	0/4/4/4
27	DMU	Z	4526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	3526	DMU	O7-C3	-8.12	1.22	1.43
27	Z	4526	DMU	O7-C3	-7.93	1.22	1.43
27	Z	4526	DMU	O16-C6	-7.42	1.27	1.40
27	M	3526	DMU	O1-C9	-7.01	1.27	1.44
27	M	3526	DMU	O16-C6	-6.99	1.28	1.40
27	Z	4526	DMU	O1-C9	-6.93	1.27	1.44
27	M	3526	DMU	O5-C4	-6.70	1.27	1.44
27	M	3526	DMU	O16-C18	-6.41	1.25	1.43
27	Z	4526	DMU	O5-C4	-6.32	1.28	1.44
27	Z	4526	DMU	O7-C10	-6.11	1.24	1.41
27	M	3526	DMU	O7-C10	-6.06	1.24	1.41
27	Z	4526	DMU	O16-C18	-5.99	1.26	1.43
27	Z	4526	DMU	O1-C10	-5.82	1.26	1.41
27	M	3526	DMU	O1-C10	-5.58	1.27	1.41
27	M	3526	DMU	O5-C6	-4.54	1.30	1.41
27	Z	4526	DMU	O5-C6	-4.37	1.30	1.41
17	N	516	HEA	C3A-CMA	-3.45	1.38	1.46
17	A	516	HEA	C3C-C2C	-3.38	1.35	1.40
17	A	516	HEA	C3A-C2A	-3.37	1.35	1.40
17	N	515	HEA	C3A-CMA	-3.21	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C3A-C2A	-3.21	1.35	1.40
17	A	516	HEA	C3A-CMA	-3.06	1.39	1.46
17	A	515	HEA	C3A-CMA	-2.94	1.39	1.46
17	N	516	HEA	C3A-C2A	-2.83	1.36	1.40
18	N	4521	TGL	OG1-CG1	-2.67	1.39	1.45
18	A	3521	TGL	OG1-CG1	-2.50	1.39	1.45
23	P	4264	PEK	O03-C01	-2.27	1.40	1.45
21	C	3271	CHD	C10-C9	-2.11	1.52	1.56
23	T	3263	PEK	O01-C1	2.01	1.40	1.34
17	N	515	HEA	C4D-ND	2.01	1.40	1.36
21	W	4060	CHD	C20-C17	2.01	1.58	1.54
17	N	516	HEA	C1B-NB	2.03	1.40	1.36
22	P	4270	CDL	C31-CA7	2.04	1.56	1.50
19	A	3524	PGV	O03-C19	2.04	1.39	1.33
25	E	3230	PSC	C01-C02	2.06	1.56	1.50
18	N	4522	TGL	CG3-CG2	2.06	1.56	1.50
19	A	3524	PGV	P-O12	2.07	1.67	1.59
17	N	516	HEA	C1D-C2D	2.08	1.47	1.42
21	P	4525	CHD	C8-C9	2.10	1.58	1.53
19	C	3268	PGV	C03-C02	2.14	1.56	1.50
19	N	4524	PGV	C01-C02	2.14	1.56	1.50
22	P	4270	CDL	OA8-CA7	2.15	1.39	1.33
22	C	3270	CDL	OA8-CA7	2.15	1.39	1.33
23	C	3265	PEK	P-O12	2.16	1.68	1.59
23	C	3265	PEK	O01-C1	2.16	1.40	1.34
19	P	4267	PGV	O03-C19	2.18	1.39	1.33
19	P	4268	PGV	C03-C02	2.20	1.57	1.50
18	L	3522	TGL	CG3-CG2	2.20	1.57	1.50
19	A	3524	PGV	C01-C02	2.22	1.57	1.50
17	A	516	HEA	C4D-ND	2.22	1.40	1.36
23	P	4265	PEK	C22-C21	2.23	1.57	1.50
23	G	4263	PEK	P-O11	2.24	1.68	1.59
19	N	4266	PGV	O03-C19	2.24	1.39	1.33
17	N	515	HEA	C1C-NC	2.24	1.40	1.36
18	L	3522	TGL	CC2-CC1	2.25	1.57	1.50
23	T	3263	PEK	C2-C1	2.26	1.57	1.50
22	C	3270	CDL	CA3-CA4	2.27	1.57	1.50
22	G	3269	CDL	CA6-CA4	2.27	1.57	1.50
25	O	4230	PSC	C2-C1	2.29	1.57	1.50
19	A	3524	PGV	C20-C19	2.30	1.57	1.50
22	P	4270	CDL	CA3-CA4	2.31	1.57	1.50
19	N	4266	PGV	C01-C02	2.32	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	3265	PEK	C2-C1	2.37	1.57	1.50
18	L	3522	TGL	OG3-CG3	2.38	1.50	1.45
19	N	4524	PGV	C20-C19	2.39	1.57	1.50
23	P	4265	PEK	O01-C1	2.40	1.41	1.34
17	A	515	HEA	C3C-CAC	2.40	1.52	1.47
22	T	4269	CDL	OA6-CA5	2.41	1.41	1.34
22	T	4269	CDL	C11-CA5	2.41	1.57	1.50
18	L	3522	TGL	OG2-CG2	2.41	1.52	1.46
23	C	3265	PEK	P-O11	2.43	1.69	1.59
18	N	4522	TGL	CC2-CC1	2.43	1.57	1.50
22	G	3269	CDL	C11-CA5	2.45	1.57	1.50
23	P	4265	PEK	P-O12	2.45	1.69	1.59
18	N	4522	TGL	CB2-CB1	2.46	1.57	1.50
25	E	3230	PSC	C2-C1	2.48	1.57	1.50
22	C	3270	CDL	CA6-CA4	2.48	1.57	1.50
23	T	3263	PEK	P-O11	2.50	1.69	1.59
22	T	4269	CDL	CB3-CB4	2.50	1.57	1.50
23	P	4265	PEK	C2-C1	2.56	1.58	1.50
19	C	3268	PGV	O01-C1	2.57	1.41	1.34
18	N	4522	TGL	OG3-CG3	2.58	1.50	1.45
17	N	516	HEA	C4D-ND	2.59	1.41	1.36
22	G	3269	CDL	CB3-CB4	2.59	1.58	1.50
23	C	3265	PEK	C01-C02	2.61	1.58	1.50
23	P	4265	PEK	P-O11	2.61	1.69	1.59
19	P	4268	PGV	O01-C1	2.64	1.41	1.34
23	P	4265	PEK	C01-C02	2.65	1.58	1.50
23	T	3263	PEK	C22-C21	2.71	1.58	1.50
19	N	4524	PGV	P-O11	2.71	1.70	1.59
19	A	3524	PGV	P-O11	2.71	1.70	1.59
21	J	3060	CHD	C13-C17	2.74	1.60	1.55
22	P	4270	CDL	CA6-CA4	2.76	1.58	1.50
19	C	3268	PGV	C2-C1	2.86	1.58	1.50
23	G	4263	PEK	C22-C21	2.87	1.58	1.50
18	N	4521	TGL	OG3-CC1	2.91	1.41	1.33
23	C	3265	PEK	O03-C21	2.92	1.41	1.33
18	A	3521	TGL	OG3-CC1	2.96	1.41	1.33
19	P	4268	PGV	C2-C1	2.97	1.59	1.50
22	G	3269	CDL	OA6-CA5	2.99	1.42	1.34
23	P	4265	PEK	C03-C02	3.01	1.59	1.50
19	C	3267	PGV	C12-C11	3.01	1.48	1.31
23	T	3263	PEK	C01-C02	3.06	1.59	1.50
21	W	4060	CHD	C13-C17	3.09	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	515	HEA	C4D-ND	3.10	1.42	1.36
23	C	3265	PEK	C03-C02	3.14	1.59	1.50
18	N	4521	TGL	OG1-CA1	3.18	1.42	1.33
23	G	4263	PEK	O03-C21	3.24	1.42	1.33
22	G	3269	CDL	CB6-CB4	3.33	1.60	1.50
23	P	4265	PEK	O03-C21	3.38	1.43	1.33
23	G	4263	PEK	C01-C02	3.41	1.60	1.50
18	A	3521	TGL	OG1-CA1	3.42	1.43	1.33
23	T	3263	PEK	C03-C02	3.50	1.60	1.50
18	D	3523	TGL	OG2-CB1	3.53	1.44	1.34
22	T	4269	CDL	CB6-CB4	3.54	1.60	1.50
18	A	3521	TGL	OG2-CB1	3.61	1.44	1.34
23	T	3263	PEK	O03-C21	3.61	1.43	1.33
23	G	4263	PEK	C03-C02	3.63	1.61	1.50
19	P	4267	PGV	C12-C11	3.79	1.52	1.31
18	Q	4523	TGL	OG3-CC1	3.90	1.44	1.33
18	N	4521	TGL	OG2-CB1	4.02	1.45	1.34
19	N	4266	PGV	C12-C11	4.09	1.54	1.31
18	L	3522	TGL	OG3-CC1	4.12	1.45	1.33
23	P	4265	PEK	C15-C14	4.13	1.54	1.31
23	P	4264	PEK	C6-C5	4.17	1.54	1.31
18	Q	4523	TGL	OG2-CB1	4.21	1.46	1.34
23	C	3265	PEK	C15-C14	4.21	1.55	1.31
19	A	3524	PGV	C12-C11	4.22	1.55	1.31
23	G	4263	PEK	C9-C8	4.23	1.55	1.31
23	P	4264	PEK	C9-C8	4.24	1.55	1.31
19	A	3266	PGV	C12-C11	4.24	1.55	1.31
23	C	3264	PEK	C9-C8	4.27	1.55	1.31
19	N	4524	PGV	C12-C11	4.27	1.55	1.31
25	E	3230	PSC	C13-C12	4.28	1.55	1.31
23	C	3264	PEK	C6-C5	4.29	1.55	1.31
23	T	3263	PEK	C15-C14	4.33	1.55	1.31
23	T	3263	PEK	C9-C8	4.33	1.55	1.31
23	C	3265	PEK	C9-C8	4.35	1.55	1.31
23	P	4265	PEK	C9-C8	4.38	1.56	1.31
23	G	4263	PEK	C15-C14	4.38	1.56	1.31
18	D	3523	TGL	OG3-CC1	4.40	1.46	1.33
19	C	3268	PGV	C12-C11	4.40	1.56	1.31
23	P	4265	PEK	C6-C5	4.43	1.56	1.31
25	E	3230	PSC	C10-C9	4.44	1.56	1.31
23	C	3265	PEK	C12-C11	4.45	1.56	1.31
23	G	4263	PEK	C6-C5	4.46	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	O	4230	PSC	C13-C12	4.48	1.56	1.31
18	N	4522	TGL	OG3-CC1	4.49	1.46	1.33
23	P	4265	PEK	C12-C11	4.49	1.56	1.31
23	C	3265	PEK	C6-C5	4.51	1.56	1.31
19	P	4268	PGV	C12-C11	4.52	1.56	1.31
23	T	3263	PEK	C6-C5	4.52	1.56	1.31
25	O	4230	PSC	C10-C9	4.55	1.57	1.31
18	Q	4523	TGL	OG1-CA1	4.56	1.46	1.33
23	T	3263	PEK	C12-C11	4.64	1.57	1.31
18	L	3522	TGL	OG1-CA1	4.71	1.47	1.33
23	C	3264	PEK	C12-C11	4.73	1.58	1.31
23	P	4264	PEK	C15-C14	4.76	1.58	1.31
23	G	4263	PEK	C12-C11	4.85	1.58	1.31
23	C	3264	PEK	C15-C14	4.86	1.58	1.31
23	P	4264	PEK	C12-C11	4.98	1.59	1.31
18	D	3523	TGL	OG1-CA1	5.07	1.48	1.33
18	N	4522	TGL	OG1-CA1	5.15	1.48	1.33
18	N	4522	TGL	OG2-CB1	5.31	1.49	1.34
18	L	3522	TGL	OG2-CB1	5.68	1.50	1.34

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	3271	CHD	C17-C13-C12	-9.86	108.56	117.67
21	P	4271	CHD	C17-C13-C12	-9.75	108.66	117.67
21	C	3271	CHD	C19-C10-C9	-8.24	99.50	111.17
27	M	3526	DMU	C8-C7-C5	-7.89	96.98	110.83
27	Z	4526	DMU	C8-C7-C5	-7.87	97.03	110.83
21	P	4271	CHD	C19-C10-C9	-7.51	100.53	111.17
21	W	4060	CHD	C15-C14-C8	-5.52	110.54	118.33
21	J	3060	CHD	C15-C14-C8	-5.52	110.54	118.33
19	N	4266	PGV	C01-O03-C19	-5.21	101.55	117.13
21	P	4271	CHD	C15-C14-C8	-5.12	111.11	118.33
21	C	3271	CHD	C15-C14-C8	-5.11	111.12	118.33
21	J	3060	CHD	C18-C13-C14	-4.98	103.38	111.23
21	C	3271	CHD	C19-C10-C1	-4.82	100.41	108.25
21	P	4271	CHD	C19-C10-C1	-4.80	100.44	108.25
21	W	4060	CHD	C18-C13-C14	-4.72	103.79	111.23
21	J	3060	CHD	C17-C13-C12	-3.90	114.07	117.67
21	B	4085	CHD	C16-C17-C13	-3.89	99.68	103.57
23	C	3264	PEK	O03-C21-C22	-3.85	100.78	111.92
21	B	4085	CHD	C15-C14-C8	-3.68	113.14	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	4085	CHD	C15-C14-C13	-3.64	99.93	103.57
21	P	4525	CHD	C15-C14-C8	-3.61	113.24	118.33
21	W	4060	CHD	C17-C13-C12	-3.60	114.34	117.67
21	O	3085	CHD	C16-C17-C13	-3.60	99.97	103.57
21	O	3085	CHD	C15-C14-C8	-3.59	113.26	118.33
21	B	4085	CHD	O3-C3-C4	-3.56	102.74	109.86
19	P	4267	PGV	C9-C10-C11	-3.46	93.69	112.48
21	J	3060	CHD	C19-C10-C9	-3.44	106.29	111.17
23	P	4264	PEK	O03-C21-C22	-3.42	102.03	111.92
23	C	3264	PEK	C30-C29-C28	-3.38	96.05	114.41
25	O	4230	PSC	C01-O03-C19	-3.35	107.11	117.13
22	P	4270	CDL	CB6-OB8-CB7	-3.33	107.18	117.13
25	E	3230	PSC	C01-O03-C19	-3.29	107.30	117.13
21	C	3525	CHD	C15-C14-C8	-3.21	113.80	118.33
21	C	3525	CHD	C14-C13-C12	-3.20	104.34	107.39
21	B	4085	CHD	C14-C13-C12	-3.15	104.39	107.39
22	C	3270	CDL	CB6-OB8-CB7	-3.14	107.74	117.13
23	P	4264	PEK	C30-C29-C28	-3.13	97.41	114.41
19	A	3266	PGV	C01-O03-C19	-3.06	107.98	117.13
21	P	4525	CHD	C14-C8-C9	-3.05	105.48	109.64
21	W	4060	CHD	C19-C10-C9	-3.04	106.86	111.17
21	O	3085	CHD	C14-C13-C12	-2.97	104.56	107.39
23	P	4264	PEK	C3-C2-C1	-2.94	103.00	113.60
21	O	3085	CHD	C15-C14-C13	-2.94	100.63	103.57
22	C	3270	CDL	OB6-CB5-C51	-2.94	105.36	111.55
17	N	515	HEA	C27-C19-C18	-2.92	116.02	123.70
27	Z	4526	DMU	C2-C3-C4	-2.91	104.18	110.93
19	C	3267	PGV	C9-C10-C11	-2.84	97.05	112.48
17	A	515	HEA	C27-C19-C18	-2.84	116.25	123.70
21	C	3525	CHD	C14-C8-C9	-2.81	105.81	109.64
27	M	3526	DMU	C2-C3-C4	-2.79	104.45	110.93
21	B	4085	CHD	C19-C10-C1	-2.77	103.74	108.25
21	O	3085	CHD	O3-C3-C4	-2.75	104.35	109.86
19	P	4267	PGV	O01-C1-C2	-2.75	105.76	111.55
19	A	3524	PGV	C3-C2-C1	-2.73	103.74	113.60
21	C	3271	CHD	C18-C13-C14	-2.71	106.95	111.23
21	B	4085	CHD	C14-C8-C9	-2.69	105.98	109.64
21	O	3085	CHD	C14-C8-C9	-2.68	105.99	109.64
17	N	515	HEA	CMB-C2B-C1B	-2.68	124.35	128.46
23	C	3264	PEK	C27-C26-C25	-2.64	100.11	114.41
17	N	515	HEA	C17-C18-C19	-2.63	121.14	127.66
17	N	516	HEA	CMB-C2B-C1B	-2.62	124.43	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	4267	PGV	C14-C13-C12	-2.61	98.30	112.48
18	L	3522	TGL	OG3-CC1-OC1	-2.60	117.25	123.58
21	O	3085	CHD	C19-C10-C1	-2.58	104.05	108.25
17	A	516	HEA	C4B-C3B-C2B	-2.53	105.10	106.87
23	C	3264	PEK	C3-C2-C1	-2.51	104.54	113.60
21	W	4060	CHD	C19-C10-C5	-2.51	106.00	110.35
19	N	4524	PGV	C3-C2-C1	-2.51	104.54	113.60
17	N	515	HEA	C4B-C3B-C2B	-2.50	105.12	106.87
17	A	515	HEA	C17-C18-C19	-2.50	121.49	127.66
23	P	4264	PEK	C32-C31-C30	-2.49	100.89	114.41
18	N	4522	TGL	OG3-CC1-OC1	-2.48	117.53	123.58
17	A	515	HEA	CMB-C2B-C1B	-2.47	124.67	128.46
23	C	3264	PEK	C32-C31-C30	-2.46	101.05	114.41
23	P	4264	PEK	O03-C01-C02	-2.44	102.56	108.64
18	N	4521	TGL	OG3-CC1-OC1	-2.43	117.65	123.58
18	A	3521	TGL	OG3-CC1-OC1	-2.41	117.69	123.58
21	P	4271	CHD	C18-C13-C14	-2.41	107.42	111.23
22	C	3270	CDL	C52-C51-CB5	-2.41	104.91	113.60
23	P	4264	PEK	C34-C33-C32	-2.40	101.36	114.41
21	C	3525	CHD	C19-C10-C9	-2.38	107.80	111.17
19	N	4266	PGV	C3-C2-C1	-2.32	105.22	113.60
22	P	4270	CDL	OB6-CB5-C51	-2.31	106.68	111.55
19	A	3524	PGV	O01-C1-C2	-2.31	106.69	111.55
19	A	3266	PGV	O01-C1-C2	-2.31	106.69	111.55
17	A	516	HEA	CMC-C2C-C1C	-2.30	124.93	128.46
22	P	4270	CDL	C52-C51-CB5	-2.30	105.31	113.60
19	C	3267	PGV	C3-C2-C1	-2.29	105.34	113.60
18	N	4521	TGL	CG3-OG3-CC1	-2.29	110.29	117.13
21	J	3060	CHD	C19-C10-C5	-2.29	106.39	110.35
19	N	4524	PGV	O01-C1-C2	-2.28	106.74	111.55
23	P	4264	PEK	C25-C24-C23	-2.28	102.04	114.41
19	C	3267	PGV	O01-C1-C2	-2.27	106.76	111.55
22	T	4269	CDL	OB8-CB7-C71	-2.25	105.39	111.92
17	N	516	HEA	C4B-C3B-C2B	-2.25	105.30	106.87
23	C	3264	PEK	C25-C24-C23	-2.24	102.25	114.41
23	P	4264	PEK	C27-C26-C25	-2.24	102.28	114.41
18	Q	4523	TGL	OG3-CC1-OC1	-2.23	118.14	123.58
18	A	3521	TGL	CG3-OG3-CC1	-2.20	110.56	117.13
17	N	515	HEA	C26-C15-C14	-2.18	117.96	123.70
17	A	515	HEA	C21-C20-C19	-2.16	105.70	112.85
23	P	4264	PEK	C28-C27-C26	-2.14	102.81	114.41
22	G	3269	CDL	OB8-CB7-C71	-2.13	105.75	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	3523	TGL	CG3-OG3-CC1	-2.13	110.77	117.13
19	P	4267	PGV	C8-C9-C10	-2.12	105.60	113.70
17	N	515	HEA	C13-C14-C15	-2.11	122.44	127.66
17	N	515	HEA	CMC-C2C-C1C	-2.11	125.22	128.46
21	C	3525	CHD	C16-C17-C13	-2.10	101.47	103.57
21	C	3525	CHD	O12-C12-C13	-2.09	107.56	111.08
17	A	515	HEA	C13-C14-C15	-2.09	122.49	127.66
17	N	516	HEA	C20-C19-C18	-2.07	116.89	121.10
17	N	515	HEA	C21-C20-C19	-2.06	106.05	112.85
17	A	516	HEA	CMB-C2B-C1B	-2.04	125.33	128.46
19	P	4267	PGV	C01-O03-C19	-2.04	111.03	117.13
18	D	3523	TGL	OG2-CB1-OB1	-2.04	118.66	123.69
18	Q	4523	TGL	CG3-OG3-CC1	-2.04	111.04	117.13
18	D	3523	TGL	OG3-CC1-OC1	-2.04	118.61	123.58
21	O	3085	CHD	C4-C5-C10	-2.03	110.47	112.66
21	O	3085	CHD	C18-C13-C12	-2.01	106.99	109.07
21	O	3085	CHD	C13-C17-C20	-2.00	117.06	119.50
25	O	4230	PSC	P-O12-C04	2.00	131.44	121.59
17	N	516	HEA	C1B-C2B-C3B	2.01	108.39	107.00
18	A	3521	TGL	CB5-CB4-CB3	2.01	125.34	114.41
18	Q	4523	TGL	CB6-CB5-CB4	2.02	125.40	114.41
22	T	4269	CDL	C80-C79-C78	2.03	125.45	114.41
22	G	3269	CDL	C80-C79-C78	2.04	125.47	114.41
21	W	4060	CHD	C13-C14-C8	2.04	117.39	114.77
22	P	4270	CDL	OB6-CB5-OB7	2.05	128.74	123.69
18	A	3521	TGL	CC6-CC5-CC4	2.05	125.54	114.41
21	O	3085	CHD	C18-C13-C14	2.05	114.47	111.23
17	N	515	HEA	C16-C15-C14	2.06	125.29	121.10
21	C	3271	CHD	C9-C10-C5	2.06	111.58	108.61
25	E	3230	PSC	P-O12-C04	2.06	131.75	121.59
19	N	4266	PGV	C22-C21-C20	2.07	120.76	113.23
21	C	3525	CHD	C2-C1-C10	2.08	116.40	112.79
21	B	4085	CHD	C5-C6-C7	2.08	116.75	114.44
22	G	3269	CDL	C23-C22-C21	2.09	125.75	114.41
18	D	3523	TGL	CB5-CB4-CB3	2.09	125.77	114.41
23	P	4264	PEK	C8-C7-C6	2.10	118.98	111.84
18	L	3522	TGL	OG1-CG1-CG2	2.11	113.89	108.64
22	T	4269	CDL	C20-C19-C18	2.11	125.86	114.41
21	O	3085	CHD	C9-C11-C12	2.11	117.12	114.33
21	P	4525	CHD	C17-C13-C12	2.12	119.64	117.67
21	B	4085	CHD	C17-C13-C14	2.13	102.27	100.08
23	P	4265	PEK	C14-C13-C12	2.15	119.14	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	3521	TGL	CB6-CB5-CB4	2.16	126.15	114.41
21	O	3085	CHD	C1-C10-C9	2.17	114.81	111.36
18	D	3523	TGL	OG1-CG1-CG2	2.18	114.08	108.64
21	B	4085	CHD	C9-C11-C12	2.18	117.22	114.33
22	T	4269	CDL	C23-C22-C21	2.19	126.30	114.41
22	G	3269	CDL	C20-C19-C18	2.20	126.35	114.41
19	N	4266	PGV	O03-C01-C02	2.20	114.12	108.64
18	D	3523	TGL	OG3-CC1-CC2	2.21	118.32	111.92
21	J	3060	CHD	C4-C5-C10	2.22	115.06	112.66
18	D	3523	TGL	OG1-CA1-CA2	2.23	118.36	111.92
21	W	4060	CHD	C4-C5-C10	2.24	115.09	112.66
23	C	3265	PEK	C14-C13-C12	2.25	119.49	111.84
18	D	3523	TGL	CB6-CB5-CB4	2.27	126.73	114.41
23	C	3265	PEK	P-O12-C04	2.27	132.77	121.59
17	A	516	HEA	C1B-C2B-C3B	2.27	108.58	107.00
22	P	4270	CDL	OA8-CA6-CA4	2.28	114.33	108.64
22	T	4269	CDL	C22-C21-C20	2.29	126.82	114.41
23	P	4265	PEK	P-O12-C04	2.29	132.86	121.59
17	A	515	HEA	C20-C19-C18	2.29	125.76	121.10
18	Q	4523	TGL	OG1-CA1-CA2	2.30	118.57	111.92
21	J	3060	CHD	C14-C8-C7	2.31	114.92	111.80
22	C	3270	CDL	OB6-CB5-OB7	2.31	129.40	123.69
22	G	3269	CDL	C22-C21-C20	2.32	126.99	114.41
21	C	3525	CHD	C10-C9-C8	2.33	114.37	111.87
23	P	4264	PEK	O03-C21-O04	2.33	129.27	123.58
18	N	4522	TGL	OG1-CG1-CG2	2.35	114.48	108.64
21	W	4060	CHD	C14-C8-C7	2.37	115.00	111.80
17	A	515	HEA	CMC-C2C-C3C	2.38	129.21	124.88
22	G	3269	CDL	OB8-CB6-CB4	2.39	114.59	108.64
19	A	3524	PGV	O01-C02-C03	2.42	117.18	108.43
21	P	4271	CHD	C14-C8-C7	2.42	115.07	111.80
27	Z	4526	DMU	C10-O7-C3	2.44	124.06	117.97
21	W	4060	CHD	C6-C5-C4	2.44	113.90	111.13
17	N	515	HEA	CMD-C2D-C3D	2.44	129.54	124.94
19	N	4524	PGV	O01-C02-C03	2.46	117.33	108.43
23	C	3264	PEK	O03-C21-O04	2.49	129.66	123.58
22	C	3270	CDL	OA8-CA6-CA4	2.49	114.85	108.64
22	T	4269	CDL	OB8-CB6-CB4	2.49	114.85	108.64
21	P	4271	CHD	O12-C12-C13	2.51	115.30	111.08
17	N	515	HEA	C20-C19-C18	2.51	126.21	121.10
17	A	515	HEA	CMD-C2D-C3D	2.52	129.69	124.94
22	G	3269	CDL	C19-C18-C17	2.53	128.12	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	4264	PEK	C11-C10-C9	2.53	120.43	111.84
22	T	4269	CDL	C19-C18-C17	2.54	128.21	114.41
18	L	3522	TGL	OG1-CA1-CA2	2.54	119.27	111.92
25	E	3230	PSC	C15-C14-C13	2.55	126.31	112.48
21	C	3271	CHD	C14-C8-C7	2.55	115.25	111.80
21	W	4060	CHD	C14-C13-C12	2.56	109.82	107.39
21	P	4271	CHD	C16-C15-C14	2.56	110.24	105.13
21	C	3525	CHD	C5-C6-C7	2.57	117.28	114.44
23	G	4263	PEK	C03-C02-C01	2.58	117.67	111.86
18	A	3521	TGL	OG3-CC1-CC2	2.60	119.43	111.92
17	N	515	HEA	CMC-C2C-C3C	2.60	129.62	124.88
18	N	4522	TGL	OG1-CA1-CA2	2.61	119.48	111.92
17	N	516	HEA	C3C-C4C-NC	2.62	112.59	109.21
21	P	4271	CHD	C1-C2-C3	2.62	113.79	110.45
21	P	4525	CHD	C9-C11-C12	2.62	117.80	114.33
21	C	3271	CHD	O12-C12-C13	2.65	115.53	111.08
21	P	4525	CHD	C6-C5-C10	2.66	115.54	112.66
21	C	3271	CHD	C5-C6-C7	2.66	117.38	114.44
21	O	3085	CHD	C1-C10-C5	2.66	111.85	107.77
21	J	3060	CHD	C14-C13-C12	2.67	109.92	107.39
27	M	3526	DMU	O7-C10-O1	2.67	118.22	110.66
21	C	3271	CHD	C15-C16-C17	2.68	110.47	105.13
21	W	4060	CHD	C15-C16-C17	2.69	110.48	105.13
21	C	3525	CHD	C1-C10-C5	2.69	111.89	107.77
25	O	4230	PSC	C15-C14-C13	2.70	127.10	112.48
21	C	3271	CHD	C16-C15-C14	2.70	110.50	105.13
21	J	3060	CHD	C6-C5-C4	2.72	114.21	111.13
21	B	4085	CHD	C5-C4-C3	2.72	116.85	112.83
23	T	3263	PEK	C03-C02-C01	2.73	118.02	111.86
21	P	4271	CHD	C6-C5-C10	2.74	115.62	112.66
21	C	3271	CHD	C1-C2-C3	2.74	113.94	110.45
21	P	4525	CHD	C1-C2-C3	2.74	113.94	110.45
21	C	3271	CHD	C6-C5-C10	2.76	115.64	112.66
23	P	4265	PEK	O03-C01-C02	2.76	115.51	108.64
21	P	4271	CHD	C15-C16-C17	2.78	110.68	105.13
21	O	3085	CHD	C1-C2-C3	2.79	114.01	110.45
21	J	3060	CHD	C15-C16-C17	2.79	110.70	105.13
21	B	4085	CHD	C1-C10-C5	2.81	112.08	107.77
21	C	3271	CHD	C5-C4-C3	2.83	117.01	112.83
23	C	3265	PEK	O03-C01-C02	2.87	115.80	108.64
17	A	516	HEA	CMC-C2C-C3C	2.88	130.13	124.88
21	J	3060	CHD	C16-C15-C14	2.92	110.94	105.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	4271	CHD	C1-C10-C9	2.92	116.01	111.36
23	C	3265	PEK	C8-C7-C6	2.93	121.80	111.84
21	B	4085	CHD	C10-C9-C8	2.96	115.05	111.87
19	N	4524	PGV	C03-C02-C01	2.96	118.54	111.86
19	N	4524	PGV	C02-O01-C1	2.97	124.89	117.88
19	A	3524	PGV	C03-C02-C01	2.97	118.55	111.86
27	Z	4526	DMU	O7-C10-O1	2.98	119.11	110.66
23	T	3263	PEK	O03-C01-C02	2.99	116.09	108.64
21	P	4271	CHD	C5-C4-C3	3.01	117.28	112.83
19	N	4524	PGV	P-O12-C04	3.03	139.42	121.68
21	P	4525	CHD	C1-C10-C5	3.03	112.42	107.77
23	P	4265	PEK	C8-C7-C6	3.04	122.19	111.84
21	W	4060	CHD	C16-C15-C14	3.05	111.20	105.13
17	A	516	HEA	C27-C19-C20	3.06	120.57	115.29
21	P	4525	CHD	C5-C6-C7	3.07	117.84	114.44
21	C	3271	CHD	C1-C10-C9	3.10	116.29	111.36
19	A	3524	PGV	P-O12-C04	3.13	140.05	121.68
21	P	4271	CHD	C5-C6-C7	3.14	117.92	114.44
23	P	4265	PEK	C11-C10-C9	3.19	122.68	111.84
21	W	4060	CHD	C1-C2-C3	3.19	114.52	110.45
25	O	4230	PSC	C16-C15-C14	3.19	125.93	113.70
27	M	3526	DMU	C10-O7-C3	3.19	125.95	117.97
23	G	4263	PEK	O03-C01-C02	3.20	116.61	108.64
21	J	3060	CHD	C1-C2-C3	3.21	114.55	110.45
23	C	3265	PEK	C11-C10-C9	3.24	122.86	111.84
23	P	4265	PEK	P-O11-C03	3.25	140.76	121.68
21	J	3060	CHD	C5-C4-C3	3.26	117.64	112.83
21	W	4060	CHD	C11-C9-C10	3.27	117.19	113.74
19	N	4524	PGV	P-O11-C03	3.31	141.06	121.68
17	N	516	HEA	C27-C19-C20	3.31	121.00	115.29
23	C	3265	PEK	P-O11-C03	3.32	141.13	121.68
21	J	3060	CHD	C11-C9-C10	3.36	117.28	113.74
25	E	3230	PSC	C16-C15-C14	3.38	126.67	113.70
19	A	3524	PGV	P-O11-C03	3.40	141.60	121.68
21	W	4060	CHD	C5-C4-C3	3.45	117.93	112.83
21	B	4085	CHD	C1-C2-C3	3.46	114.86	110.45
21	O	3085	CHD	C5-C4-C3	3.48	117.97	112.83
23	G	4263	PEK	P-O11-C03	3.52	142.34	121.68
21	O	3085	CHD	C5-C6-C7	3.55	118.37	114.44
21	P	4271	CHD	C14-C13-C12	3.56	110.77	107.39
19	A	3524	PGV	C02-O01-C1	3.60	126.38	117.88
18	N	4522	TGL	OG2-CB1-CB2	3.61	119.16	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	3060	CHD	C2-C1-C10	3.62	119.06	112.79
23	T	3263	PEK	P-O11-C03	3.67	143.22	121.68
21	O	3085	CHD	C10-C9-C8	3.70	115.85	111.87
21	C	3271	CHD	C14-C13-C12	3.78	110.98	107.39
21	W	4060	CHD	C2-C1-C10	3.80	119.37	112.79
27	Z	4526	DMU	O7-C10-C5	3.88	118.37	108.08
21	C	3525	CHD	C13-C17-C20	3.93	124.28	119.50
27	M	3526	DMU	O7-C10-C5	3.94	118.52	108.08
21	P	4271	CHD	C4-C3-C2	3.98	115.42	110.56
27	Z	4526	DMU	O16-C6-C1	3.98	114.68	108.24
18	L	3522	TGL	OG2-CB1-CB2	4.14	120.28	111.55
18	Q	4523	TGL	OG2-CB1-CB2	4.17	120.35	111.55
27	M	3526	DMU	O7-C3-C4	4.20	121.05	109.42
21	P	4525	CHD	C13-C17-C20	4.21	124.61	119.50
21	J	3060	CHD	C5-C6-C7	4.26	119.16	114.44
21	C	3271	CHD	C4-C3-C2	4.29	115.80	110.56
21	W	4060	CHD	C1-C10-C5	4.40	114.52	107.77
18	N	4522	TGL	OG3-CG3-CG2	4.50	119.85	108.64
27	Z	4526	DMU	O7-C3-C4	4.54	121.99	109.42
21	W	4060	CHD	C5-C6-C7	4.54	119.47	114.44
18	A	3521	TGL	OG2-CB1-CB2	4.57	121.19	111.55
21	J	3060	CHD	C1-C10-C5	4.67	114.93	107.77
21	W	4060	CHD	C4-C3-C2	4.73	116.34	110.56
18	N	4521	TGL	OG2-CB1-CB2	4.75	121.55	111.55
18	D	3523	TGL	OG2-CB1-CB2	4.76	121.57	111.55
21	P	4271	CHD	C4-C5-C10	4.79	117.83	112.66
27	M	3526	DMU	O16-C6-C1	4.82	116.04	108.24
21	J	3060	CHD	C11-C12-C13	4.86	116.27	111.23
18	L	3522	TGL	OG3-CG3-CG2	4.97	121.02	108.64
21	W	4060	CHD	C9-C8-C7	5.09	117.89	111.92
27	M	3526	DMU	O5-C6-C1	5.12	121.35	110.34
27	M	3526	DMU	O5-C6-O16	5.17	122.18	109.96
21	J	3060	CHD	C9-C8-C7	5.19	118.01	111.92
21	C	3271	CHD	C4-C5-C10	5.20	118.28	112.66
21	W	4060	CHD	C11-C12-C13	5.26	116.69	111.23
21	J	3060	CHD	C6-C5-C10	5.26	118.35	112.66
21	J	3060	CHD	C4-C3-C2	5.30	117.03	110.56
27	Z	4526	DMU	O5-C6-C1	5.32	121.77	110.34
21	W	4060	CHD	C6-C5-C10	5.34	118.44	112.66
27	Z	4526	DMU	O5-C6-O16	5.60	123.21	109.96
27	Z	4526	DMU	C18-O16-C6	5.63	123.46	113.85
21	P	4271	CHD	C9-C8-C7	5.74	118.65	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	3271	CHD	C9-C8-C7	5.81	118.73	111.92
27	Z	4526	DMU	O7-C3-C2	5.95	123.27	107.27
27	M	3526	DMU	O7-C3-C2	6.03	123.47	107.27
21	C	3271	CHD	C1-C10-C5	6.18	117.25	107.77
27	M	3526	DMU	C18-O16-C6	6.27	124.56	113.85
21	P	4271	CHD	C1-C10-C5	6.33	117.48	107.77
21	J	3060	CHD	C10-C9-C8	6.46	118.82	111.87
21	W	4060	CHD	C10-C9-C8	6.55	118.91	111.87
27	Z	4526	DMU	O5-C4-C57	6.77	123.45	106.43
21	J	3060	CHD	C13-C17-C20	6.84	127.82	119.50
21	W	4060	CHD	C13-C17-C20	6.87	127.84	119.50
27	M	3526	DMU	O5-C4-C57	6.89	123.75	106.43
27	M	3526	DMU	O1-C9-C11	6.99	124.00	106.43
27	Z	4526	DMU	C7-C8-C9	7.02	122.79	110.24
27	M	3526	DMU	O5-C4-C3	7.09	124.81	109.76
27	M	3526	DMU	C7-C8-C9	7.16	123.06	110.24
27	Z	4526	DMU	O1-C9-C8	7.19	122.90	109.69
27	Z	4526	DMU	O1-C9-C11	7.26	124.68	106.43
27	Z	4526	DMU	O5-C4-C3	7.33	125.34	109.76
27	M	3526	DMU	O1-C9-C8	7.48	123.43	109.69
27	Z	4526	DMU	C6-O5-C4	8.04	129.56	113.71
27	M	3526	DMU	C6-O5-C4	8.37	130.20	113.71
21	W	4060	CHD	C17-C13-C14	9.16	109.46	100.08
21	J	3060	CHD	C17-C13-C14	9.50	109.81	100.08
21	C	3271	CHD	C10-C9-C8	9.77	122.37	111.87
27	M	3526	DMU	C1-C2-C3	9.90	132.43	109.68
21	P	4271	CHD	C17-C13-C14	9.90	110.22	100.08
27	Z	4526	DMU	C1-C2-C3	9.93	132.50	109.68
21	P	4271	CHD	C10-C9-C8	10.15	122.78	111.87
21	C	3271	CHD	C17-C13-C14	10.31	110.64	100.08
27	Z	4526	DMU	C10-C5-C7	10.40	131.73	109.98
27	M	3526	DMU	C10-C5-C7	10.50	131.95	109.98

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	Z	4526	DMU	C4
27	Z	4526	DMU	C6
27	Z	4526	DMU	C5
27	Z	4526	DMU	C2
27	Z	4526	DMU	C9
21	C	3271	CHD	C12

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Mol	Chain	Res	Type	Atom
21	C	3271	CHD	C8
21	C	3271	CHD	C3
21	C	3271	CHD	C9
21	C	3271	CHD	C14
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB
27	M	3526	DMU	C4
27	M	3526	DMU	C6
27	M	3526	DMU	C5
27	M	3526	DMU	C2
27	M	3526	DMU	C9
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB
21	W	4060	CHD	C12
21	W	4060	CHD	C8
21	W	4060	CHD	C9
21	W	4060	CHD	C14
21	W	4060	CHD	C17
21	P	4271	CHD	C12
21	P	4271	CHD	C8
21	P	4271	CHD	C3
21	P	4271	CHD	C9
21	P	4271	CHD	C14
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
21	J	3060	CHD	C12
21	J	3060	CHD	C8
21	J	3060	CHD	C9
21	J	3060	CHD	C14
21	J	3060	CHD	C17

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	Q	4523	TGL	CG2-OG2-CB1-CB2
18	D	3523	TGL	CG2-OG2-CB1-OB1

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Mol	Chain	Res	Type	Atoms
18	D	3523	TGL	CG2-OG2-CB1-CB2

There are no ring outliers.

32 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	3521	TGL	11	0
19	A	3524	PGV	7	0
17	A	515	HEA	3	0
17	A	516	HEA	1	0
21	B	4085	CHD	1	0
23	C	3264	PEK	4	0
23	C	3265	PEK	3	0
19	C	3267	PGV	6	0
19	C	3268	PGV	1	0
22	C	3270	CDL	14	0
21	C	3271	CHD	3	0
18	D	3523	TGL	15	0
25	E	3230	PSC	13	0
22	G	3269	CDL	14	0
23	G	4263	PEK	10	0
21	J	3060	CHD	2	0
18	L	3522	TGL	25	0
18	N	4521	TGL	19	0
18	N	4522	TGL	19	0
19	N	4524	PGV	5	0
17	N	515	HEA	3	0
21	O	3085	CHD	1	0
25	O	4230	PSC	21	0
23	P	4264	PEK	4	0
23	P	4265	PEK	2	0
19	P	4267	PGV	8	0
22	P	4270	CDL	18	0
21	P	4271	CHD	2	0
18	Q	4523	TGL	15	0
23	T	3263	PEK	9	0
22	T	4269	CDL	15	0
21	W	4060	CHD	2	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.