



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:34 am GMT

PDB ID : 3AG2
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 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

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

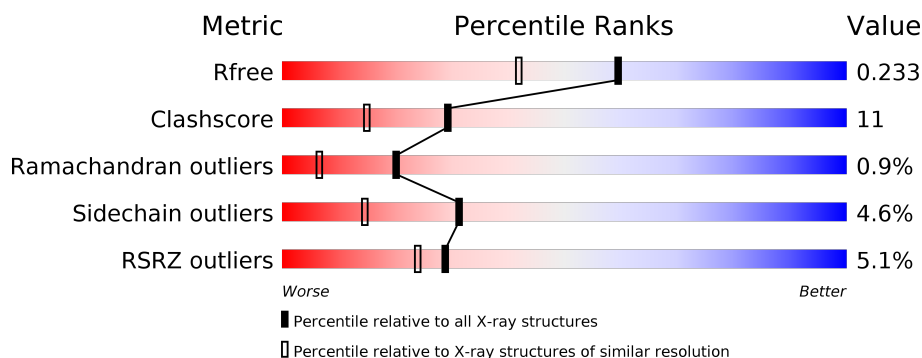
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>0.5%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>0.5%</div> </div> </div>
1	N	514	<div> <div>0.5%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>0.5%</div> </div> </div>
2	B	227	<div> <div></div> <div> <div></div> <div>74%</div> <div>21%</div> <div>6%</div> </div> </div>
2	O	227	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>1%</div> </div> </div>
3	C	261	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>0.5%</div> </div> </div>
3	P	261	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>0.5%</div> </div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	515	X	-	-	-
14	HEA	A	516	X	-	-	-
14	HEA	N	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	516	X	-	-	-
19	TGL	A	523	-	-	-	X
19	TGL	B	521	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	N	1523	-	-	-	X
19	TGL	O	1521	-	-	-	X
20	PGV	A	524	-	-	-	X
20	PGV	C	268	-	-	-	X
20	PGV	N	1524	-	-	-	X
21	CHD	C	271	X	-	-	X
21	CHD	J	60	X	-	-	X
21	CHD	P	1271	X	-	-	X
21	CHD	W	1059	X	-	-	X
23	PSC	B	229	-	-	-	X
23	PSC	R	1229	-	-	-	X
25	PEK	G	1263	-	-	-	X
25	PEK	T	263	-	-	X	-
26	CDL	C	270	-	-	-	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	X	X
26	CDL	T	1269	-	-	X	X
27	DMU	C	272	X	-	-	X
27	DMU	M	526	X	-	-	-
27	DMU	P	1272	X	-	-	X
27	DMU	Z	1526	X	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32400 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

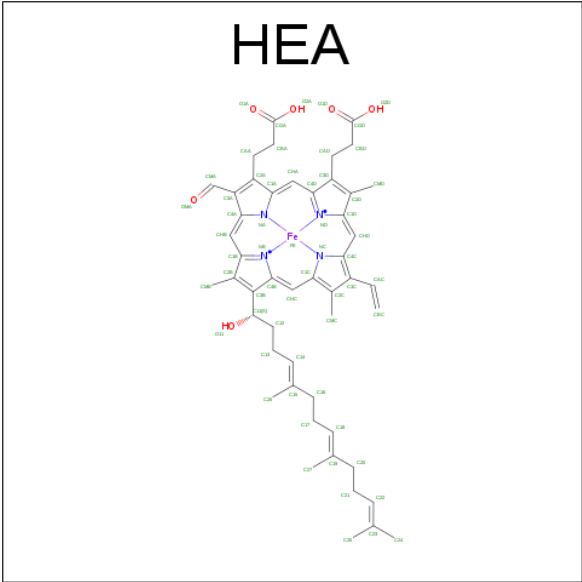
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).

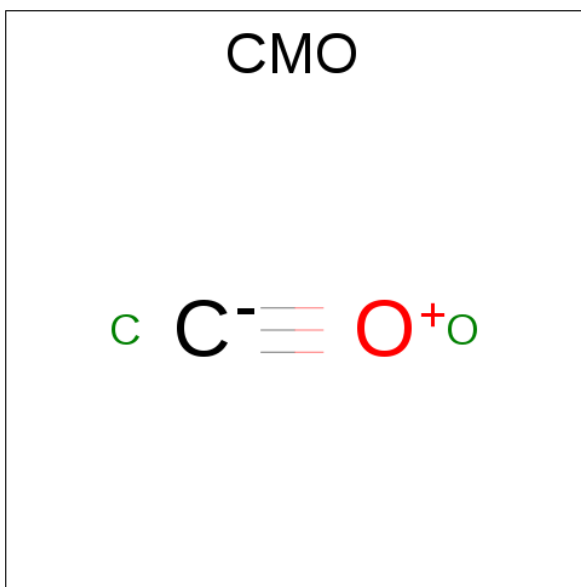


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

- Molecule 16 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

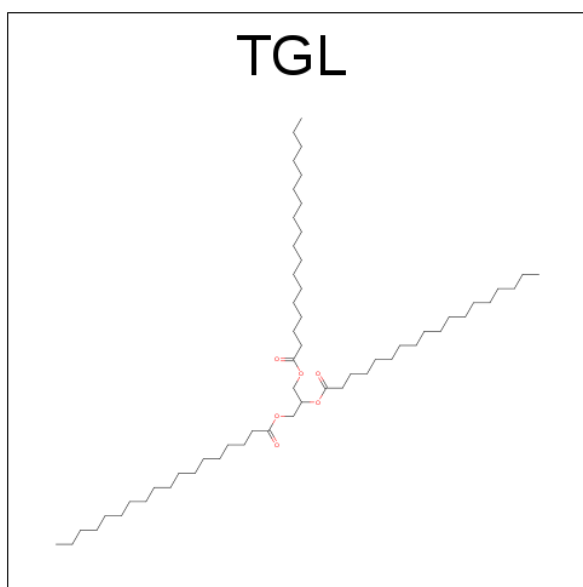
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

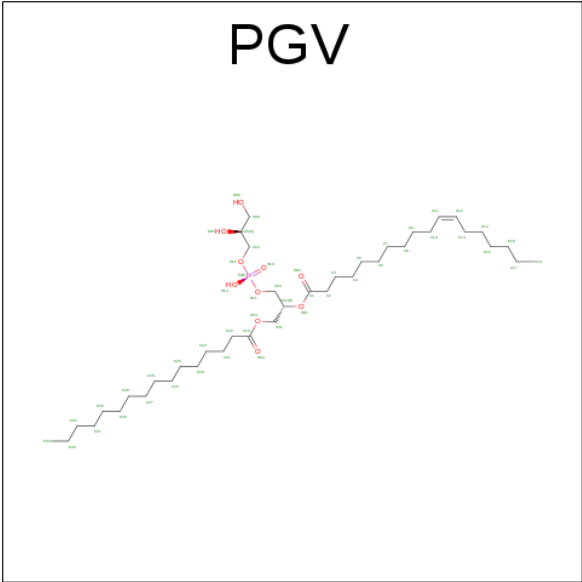
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



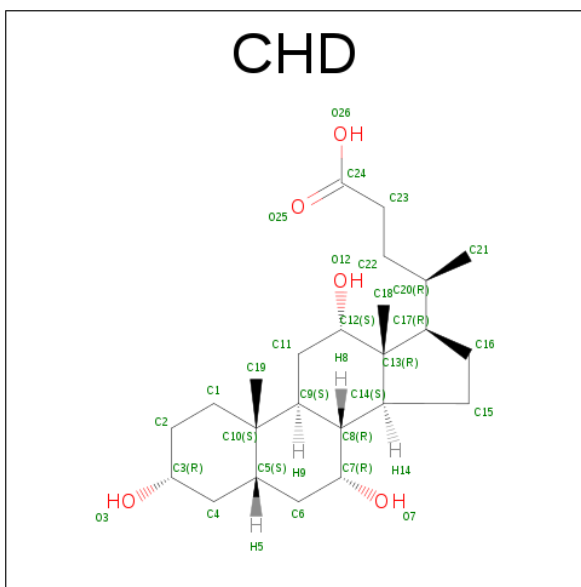
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



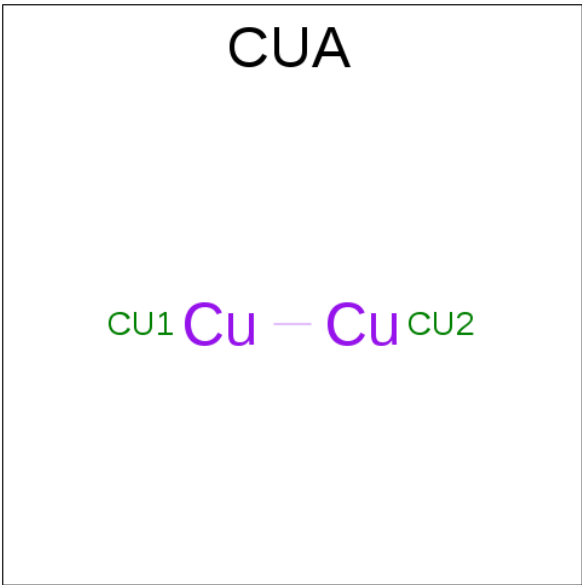
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	G	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0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

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



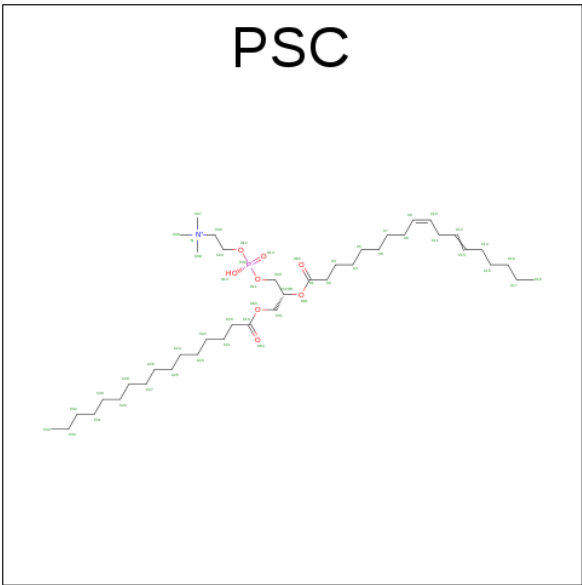
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C O 29 24 5	0	0
21	B	1	Total C O 29 24 5	0	0
21	C	1	Total C O 29 24 5	0	0
21	G	1	Total C O 29 24 5	0	0
21	J	1	Total C O 29 24 5	0	0
21	P	1	Total C O 29 24 5	0	0
21	P	1	Total C O 29 24 5	0	0
21	W	1	Total C O 29 24 5	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



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

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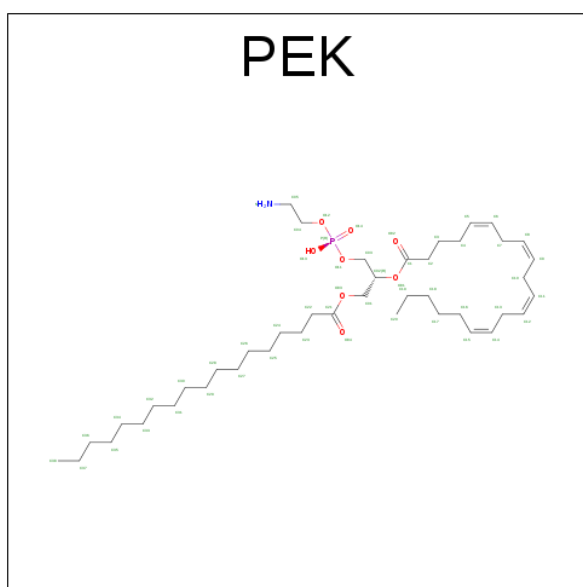
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- 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 (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



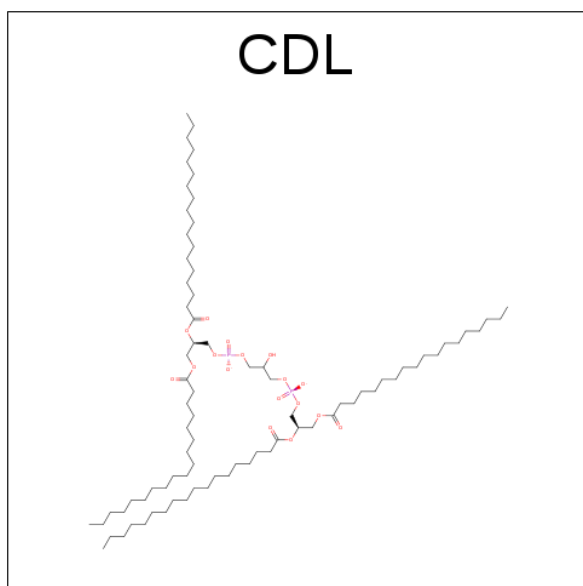
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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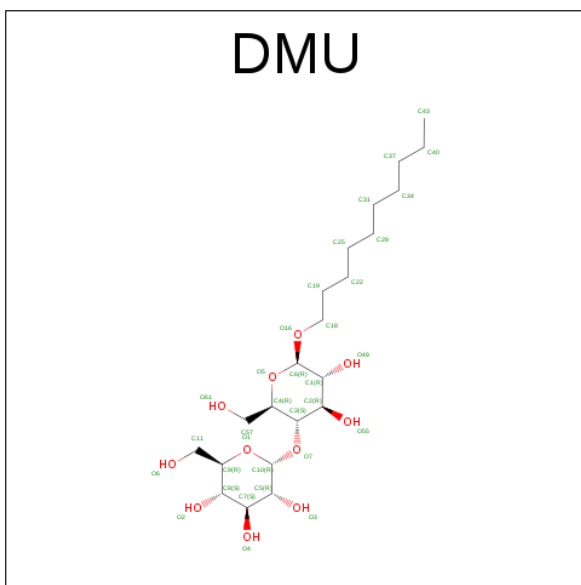
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 27 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



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

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	213	Total O 213 213	0	0
29	B	135	Total O 135 135	0	0
29	C	109	Total O 109 109	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	D	93	Total O 93 93	0	0
29	E	61	Total O 61 61	0	0
29	F	80	Total O 80 80	0	0
29	G	56	Total O 56 56	0	0
29	H	53	Total O 53 53	0	0
29	I	35	Total O 35 35	0	0
29	J	16	Total O 16 16	0	0
29	K	21	Total O 21 21	0	0
29	L	28	Total O 28 28	0	0
29	M	24	Total O 24 24	0	0
29	N	205	Total O 205 205	0	0
29	O	106	Total O 106 106	0	0
29	P	106	Total O 106 106	0	0
29	Q	51	Total O 51 51	0	0
29	R	39	Total O 39 39	0	0
29	S	62	Total O 62 62	0	0
29	T	47	Total O 47 47	0	0
29	U	50	Total O 50 50	0	0
29	V	21	Total O 21 21	0	0
29	W	15	Total O 15 15	0	0
29	X	19	Total O 19 19	0	0

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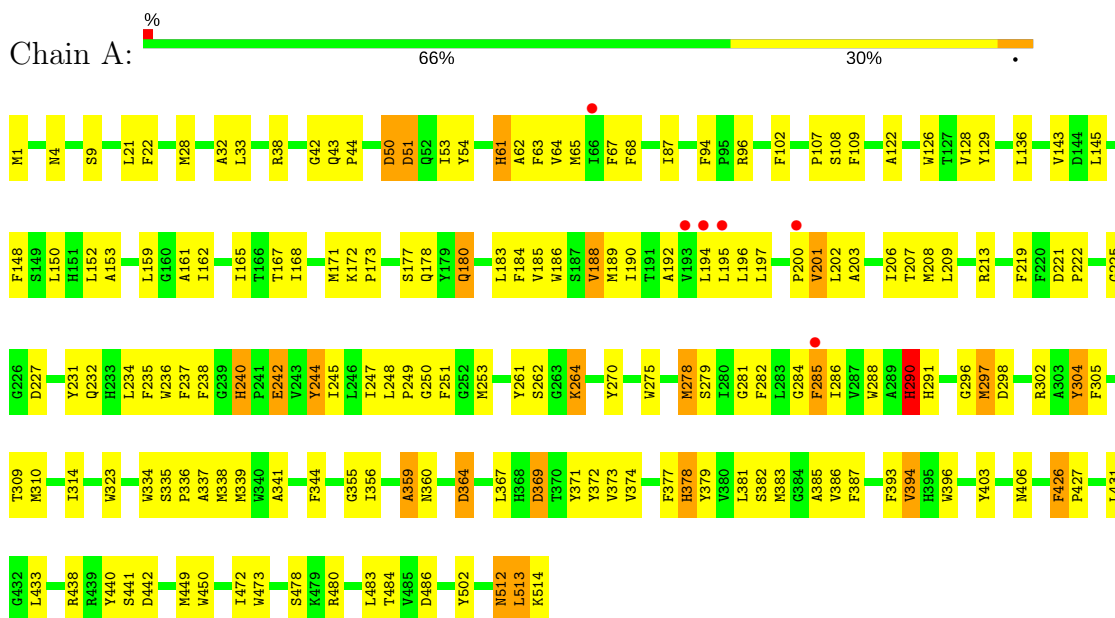
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	12	Total 12	O 12	0	0
29	Z	7	Total 7	O 7	0	0

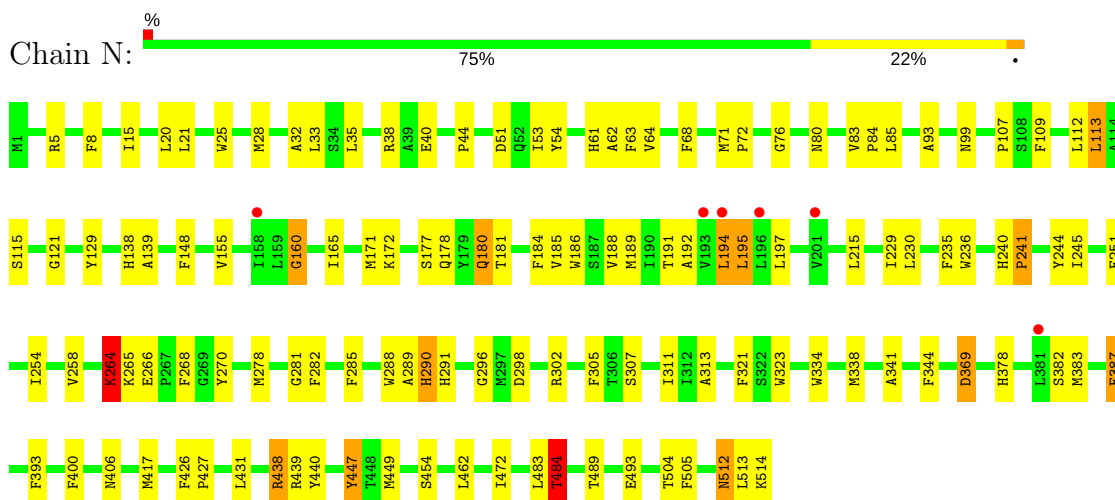
3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1

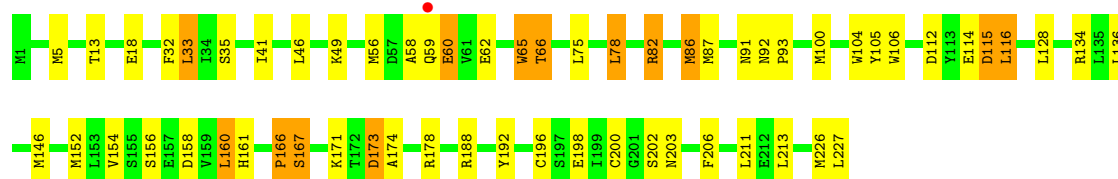


• Molecule 1: Cytochrome c oxidase subunit 1



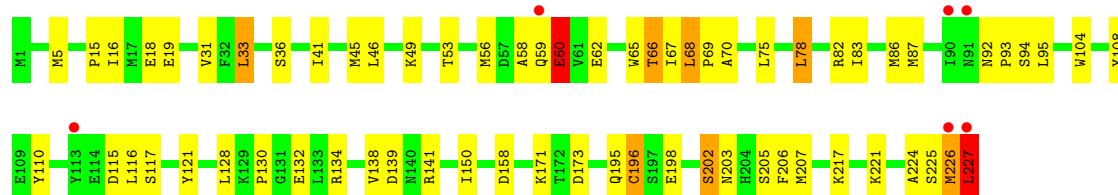
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 




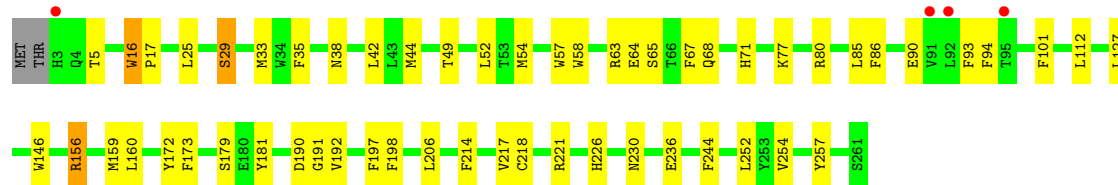
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 




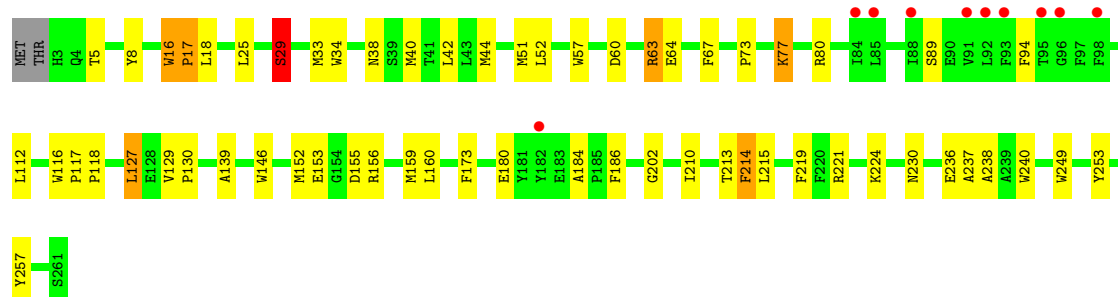
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 




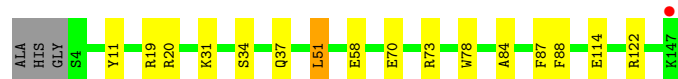
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 

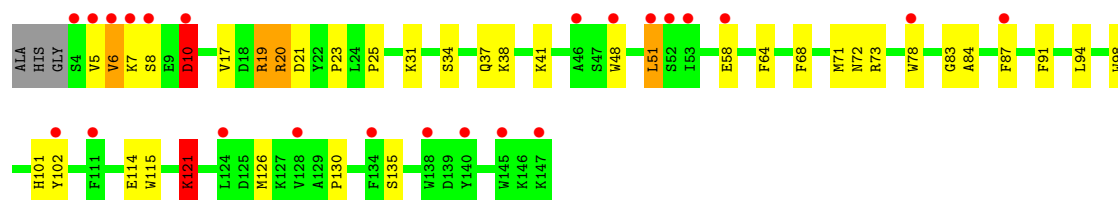
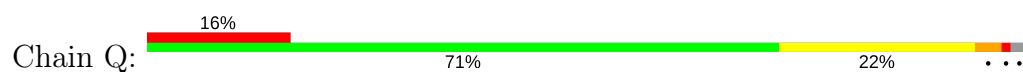


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

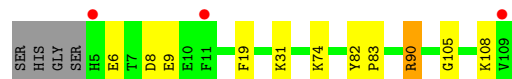
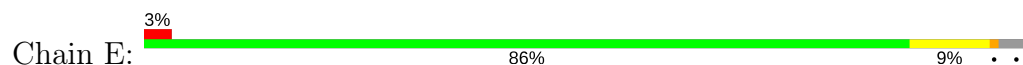
Chain D: 



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



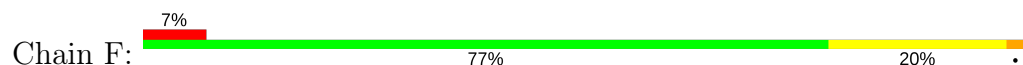
• Molecule 5: Cytochrome c oxidase subunit 5A



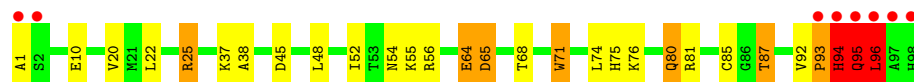
• Molecule 5: Cytochrome c oxidase subunit 5A



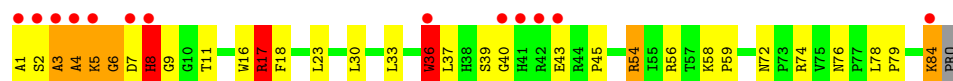
• Molecule 6: Cytochrome c oxidase subunit 5B



• Molecule 6: Cytochrome c oxidase subunit 5B

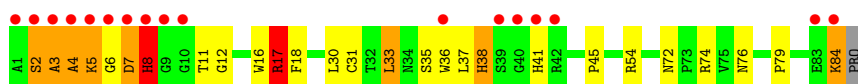


• Molecule 7: Cytochrome c oxidase subunit 6A2

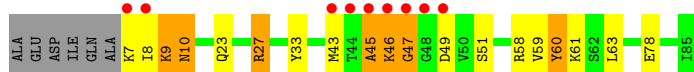


• Molecule 7: Cytochrome c oxidase subunit 6A2

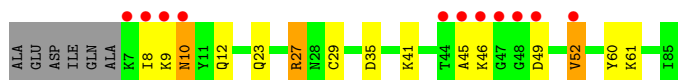
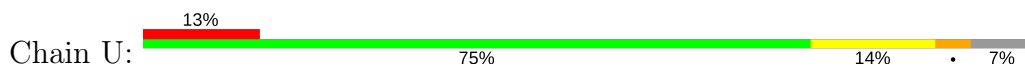




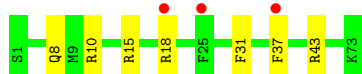
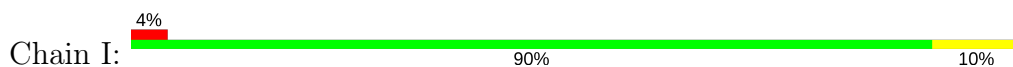
• Molecule 8: Cytochrome c oxidase subunit 6B1



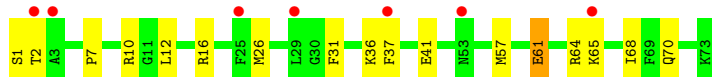
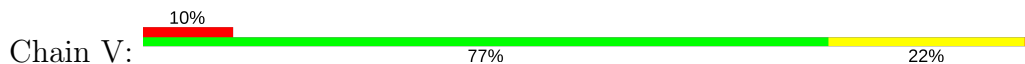
• Molecule 8: Cytochrome c oxidase subunit 6B1



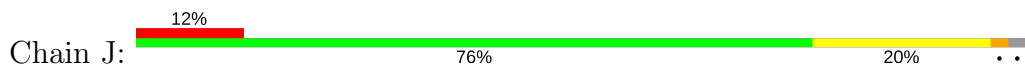
• Molecule 9: Cytochrome c oxidase subunit 6C



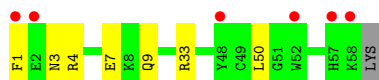
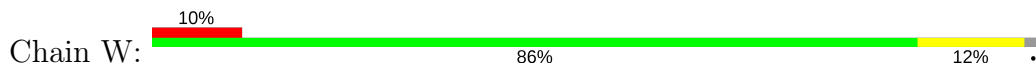
• Molecule 9: Cytochrome c oxidase subunit 6C



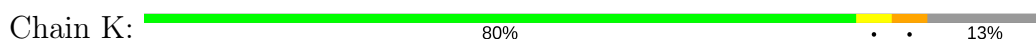
• Molecule 10: Cytochrome c oxidase polypeptide 7A1



• Molecule 10: Cytochrome c oxidase polypeptide 7A1

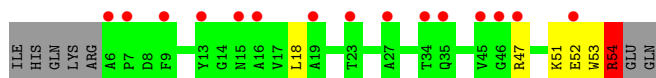
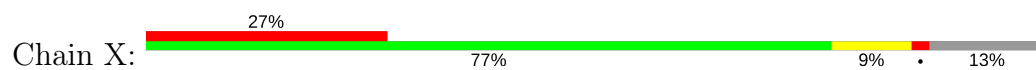


• Molecule 11: Cytochrome c oxidase subunit 7B

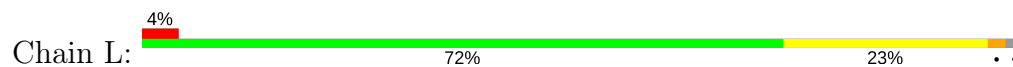




- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 12: Cytochrome c oxidase subunit 7C



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.83Å 206.93Å 178.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 80.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 99.6 (80.36-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.192 , 0.223 0.204 , 0.233	Depositor DCC
R_{free} test set	30375 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32400	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.97	92/4156 (2.2%)	1.70	92/5678 (1.6%)
1	N	1.62	41/4156 (1.0%)	1.37	33/5678 (0.6%)
2	B	1.61	20/1860 (1.1%)	1.41	19/2534 (0.7%)
2	O	1.31	9/1860 (0.5%)	1.20	11/2534 (0.4%)
3	C	1.62	22/2197 (1.0%)	1.31	19/3005 (0.6%)
3	P	1.52	17/2197 (0.8%)	1.29	19/3005 (0.6%)
4	D	1.46	6/1229 (0.5%)	1.22	7/1658 (0.4%)
4	Q	1.24	8/1229 (0.7%)	1.01	3/1658 (0.2%)
5	E	1.29	2/871 (0.2%)	1.04	2/1182 (0.2%)
5	R	1.16	0/871	0.97	3/1182 (0.3%)
6	F	1.43	4/765 (0.5%)	1.19	3/1038 (0.3%)
6	S	1.37	4/765 (0.5%)	1.29	8/1038 (0.8%)
7	G	1.38	3/690 (0.4%)	1.29	8/937 (0.9%)
7	T	1.41	3/690 (0.4%)	1.37	5/937 (0.5%)
8	H	1.37	1/682 (0.1%)	1.18	4/921 (0.4%)
8	U	1.19	0/682	1.04	1/921 (0.1%)
9	I	1.26	0/605	1.03	0/802
9	V	1.20	0/605	1.02	2/802 (0.2%)
10	J	1.30	2/471 (0.4%)	1.08	1/636 (0.2%)
10	W	1.22	2/471 (0.4%)	1.06	0/636
11	K	1.42	1/398 (0.3%)	1.14	1/546 (0.2%)
11	X	1.17	1/398 (0.3%)	0.98	1/546 (0.2%)
12	L	1.53	1/393 (0.3%)	1.19	0/526
12	Y	1.45	2/393 (0.5%)	1.14	1/526 (0.2%)
13	M	1.46	2/345 (0.6%)	1.31	2/470 (0.4%)
13	Z	1.12	0/345	1.01	0/470
All	All	1.53	243/29324 (0.8%)	1.31	245/39866 (0.6%)

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	5
2	B	0	2
6	S	0	2
10	J	0	1
All	All	0	10

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	TYR	CD2-CE2	14.73	1.61	1.39
1	A	394	VAL	CB-CG2	-11.76	1.28	1.52
1	A	438	ARG	CB-CG	-10.50	1.24	1.52
1	A	371	TYR	CE1-CZ	-10.20	1.25	1.38
1	A	203	ALA	N-CA	9.97	1.66	1.46
3	P	29	SER	CB-OG	-9.88	1.29	1.42
1	N	270	TYR	CD2-CE2	9.87	1.54	1.39
7	T	36	TRP	CB-CG	9.70	1.67	1.50
3	C	94	PHE	CD1-CE1	9.46	1.58	1.39
1	A	364	ASP	C-O	9.45	1.41	1.23
1	A	371	TYR	CD1-CE1	9.37	1.53	1.39
7	G	36	TRP	CB-CG	9.07	1.66	1.50
2	B	196	CYS	CB-SG	9.00	1.97	1.82
1	A	201	VAL	CA-CB	8.88	1.73	1.54
1	A	379	TYR	CE1-CZ	8.86	1.50	1.38
1	A	242	GLU	CG-CD	8.63	1.65	1.51
7	T	5	LYS	CB-CG	8.59	1.75	1.52
1	N	235	PHE	CE1-CZ	8.57	1.53	1.37
1	A	129	TYR	CE2-CZ	-8.38	1.27	1.38
1	A	219	PHE	CE2-CZ	8.35	1.53	1.37
2	B	106	TRP	CE3-CZ3	8.30	1.52	1.38
6	S	54	ASN	CB-CG	-8.15	1.32	1.51
1	A	270	TYR	CD2-CE2	8.05	1.51	1.39
1	A	279	SER	CB-OG	-8.05	1.31	1.42
1	A	378	HIS	CB-CG	7.93	1.64	1.50
1	A	192	ALA	N-CA	7.91	1.62	1.46
6	S	71	TRP	CB-CG	7.90	1.64	1.50
2	B	200	CYS	CB-SG	7.78	1.95	1.82
3	C	35	PHE	CG-CD2	7.77	1.50	1.38
1	N	139	ALA	CA-CB	7.69	1.68	1.52
1	N	505	PHE	CD2-CE2	7.58	1.54	1.39
1	N	484	THR	CB-CG2	7.48	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	270	TYR	CB-CG	7.45	1.62	1.51
3	C	192	VAL	CB-CG2	-7.42	1.37	1.52
1	A	143	VAL	CB-CG1	7.39	1.68	1.52
1	N	270	TYR	CE2-CZ	-7.24	1.29	1.38
3	C	29	SER	CB-OG	-7.23	1.32	1.42
1	N	288	TRP	CE3-CZ3	7.19	1.50	1.38
1	A	9	SER	CB-OG	7.18	1.51	1.42
1	N	192	ALA	N-CA	7.08	1.60	1.46
2	B	59	GLN	CG-CD	7.08	1.67	1.51
1	A	61	HIS	CB-CG	6.99	1.62	1.50
2	B	202	SER	CB-OG	-6.99	1.33	1.42
1	N	258	VAL	C-O	6.98	1.36	1.23
2	B	115	ASP	CB-CG	6.95	1.66	1.51
1	A	281	GLY	N-CA	6.93	1.56	1.46
1	A	264	LYS	CG-CD	-6.91	1.28	1.52
1	A	440	TYR	CD2-CE2	6.86	1.49	1.39
1	A	128	VAL	N-CA	6.86	1.60	1.46
1	A	231	TYR	CG-CD2	6.85	1.48	1.39
1	N	454	SER	CB-OG	6.84	1.51	1.42
2	O	19	GLU	CB-CG	-6.84	1.39	1.52
1	A	355	GLY	N-CA	6.75	1.56	1.46
1	N	438	ARG	CB-CG	-6.71	1.34	1.52
13	M	4	LYS	CB-CG	-6.71	1.34	1.52
1	N	288	TRP	CB-CG	6.71	1.62	1.50
1	A	279	SER	CA-CB	6.69	1.62	1.52
5	E	9	GLU	CG-CD	6.66	1.61	1.51
3	P	57	TRP	CD1-NE1	6.63	1.49	1.38
2	O	198	GLU	C-O	6.60	1.35	1.23
1	N	63	PHE	CE2-CZ	6.60	1.49	1.37
1	A	184	PHE	CE2-CZ	6.56	1.49	1.37
1	N	195	LEU	C-O	6.55	1.35	1.23
1	A	162	ILE	CB-CG2	6.54	1.73	1.52
1	A	304	TYR	CE1-CZ	6.52	1.47	1.38
1	N	236	TRP	CE3-CZ3	6.52	1.49	1.38
1	A	206	ILE	CB-CG2	6.50	1.73	1.52
2	B	192	TYR	CE2-CZ	6.49	1.47	1.38
7	G	5	LYS	CB-CG	6.46	1.70	1.52
1	A	403	TYR	CD1-CE1	-6.45	1.29	1.39
1	A	372	TYR	CD1-CE1	6.44	1.49	1.39
1	A	238	PHE	CD1-CE1	6.42	1.52	1.39
1	A	42	GLY	N-CA	6.41	1.55	1.46
1	A	371	TYR	CZ-OH	6.40	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	87	PHE	CD2-CE2	6.39	1.52	1.39
1	A	297	MET	CB-CG	6.38	1.71	1.51
2	B	166	PRO	CB-CG	6.35	1.81	1.50
1	N	155	VAL	CA-CB	6.33	1.68	1.54
3	P	238	ALA	CA-CB	6.33	1.65	1.52
3	P	89	SER	CB-OG	6.33	1.50	1.42
1	A	373	VAL	CB-CG2	6.30	1.66	1.52
11	K	39	GLU	CB-CG	6.30	1.64	1.52
12	Y	4	GLU	CG-CD	6.30	1.61	1.51
3	C	93	PHE	CE2-CZ	6.26	1.49	1.37
1	A	284	GLY	CA-C	6.25	1.61	1.51
4	D	19	ARG	CZ-NH2	6.19	1.41	1.33
2	B	154	VAL	CB-CG2	6.19	1.65	1.52
11	X	52	GLU	CG-CD	6.18	1.61	1.51
4	Q	64	PHE	CE1-CZ	6.15	1.49	1.37
3	P	180	GLU	CD-OE1	6.13	1.32	1.25
1	A	314	ILE	C-N	6.13	1.45	1.34
1	N	8	PHE	CD1-CE1	6.12	1.51	1.39
1	A	387	PHE	CD2-CE2	6.11	1.51	1.39
13	M	26	PHE	CE1-CZ	6.10	1.49	1.37
1	N	447	TYR	CD2-CE2	6.10	1.48	1.39
4	Q	58	GLU	CG-CD	6.09	1.61	1.51
1	A	275	TRP	CB-CG	6.07	1.61	1.50
3	C	101	PHE	CG-CD2	6.05	1.47	1.38
1	A	244	TYR	CB-CG	-6.03	1.42	1.51
3	C	58	TRP	CE3-CZ3	6.03	1.48	1.38
4	D	87	PHE	CE1-CZ	6.02	1.48	1.37
1	N	165	ILE	N-CA	6.00	1.58	1.46
4	Q	87	PHE	CD1-CE1	5.99	1.51	1.39
1	A	186	TRP	CA-CB	5.98	1.67	1.53
1	A	153	ALA	CA-CB	5.96	1.65	1.52
3	C	172	TYR	CD1-CE1	5.96	1.48	1.39
3	P	64	GLU	CG-CD	5.96	1.60	1.51
4	D	11	TYR	CB-CG	5.93	1.60	1.51
1	N	251	PHE	CE1-CZ	5.92	1.48	1.37
1	A	359	ALA	CA-CB	5.92	1.64	1.52
2	B	18	GLU	CD-OE1	5.92	1.32	1.25
1	A	94	PHE	N-CA	5.91	1.58	1.46
1	A	285	PHE	CD2-CE2	5.91	1.51	1.39
3	P	236	GLU	CD-OE1	5.90	1.32	1.25
3	C	197	PHE	CE1-CZ	5.89	1.48	1.37
1	N	323	TRP	CE3-CZ3	5.89	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	TRP	CA-CB	5.88	1.66	1.53
1	N	393	PHE	CE2-CZ	5.87	1.48	1.37
3	P	16	TRP	CE3-CZ3	5.87	1.48	1.38
1	A	304	TYR	CD1-CE1	5.85	1.48	1.39
3	C	198	PHE	CE1-CZ	5.85	1.48	1.37
1	A	203	ALA	C-O	5.83	1.34	1.23
2	B	174	ALA	CA-CB	5.83	1.64	1.52
3	P	153	GLU	CG-CD	5.82	1.60	1.51
2	B	35	SER	CA-CB	5.81	1.61	1.52
12	L	13	PHE	CE1-CZ	5.81	1.48	1.37
3	P	219	PHE	CE2-CZ	5.81	1.48	1.37
3	C	173	PHE	CE1-CZ	5.78	1.48	1.37
1	N	387	PHE	CE2-CZ	5.75	1.48	1.37
2	B	32	PHE	CD2-CE2	5.74	1.50	1.39
8	H	59	VAL	CB-CG2	5.74	1.64	1.52
1	A	235	PHE	CD1-CE1	5.72	1.50	1.39
1	A	236	TRP	CE3-CZ3	5.71	1.48	1.38
12	Y	13	PHE	CE1-CZ	5.70	1.48	1.37
1	A	262	SER	C-O	5.69	1.34	1.23
1	A	129	TYR	CG-CD2	5.69	1.46	1.39
2	B	105	TYR	CD1-CE1	5.69	1.47	1.39
1	A	261	TYR	CE2-CZ	5.68	1.46	1.38
6	F	1	ALA	C-O	5.67	1.34	1.23
1	A	440	TYR	CG-CD1	5.67	1.46	1.39
1	N	235	PHE	CD2-CE2	5.67	1.50	1.39
3	C	244	PHE	CE2-CZ	5.66	1.48	1.37
1	A	237	PHE	CE1-CZ	5.66	1.48	1.37
1	A	148	PHE	CG-CD2	5.64	1.47	1.38
1	A	285	PHE	CG-CD2	-5.64	1.30	1.38
3	C	57	TRP	CB-CG	5.63	1.60	1.50
1	A	251	PHE	CG-CD2	5.63	1.47	1.38
1	N	344	PHE	CE1-CZ	5.63	1.48	1.37
1	A	64	VAL	CB-CG1	5.61	1.64	1.52
1	N	188	VAL	CB-CG1	5.60	1.64	1.52
1	A	386	VAL	CB-CG2	5.58	1.64	1.52
3	C	244	PHE	CD2-CE2	5.58	1.50	1.39
2	O	60	GLU	CB-CG	5.58	1.62	1.52
10	W	7	GLU	CB-CG	-5.58	1.41	1.52
1	A	67	PHE	CE2-CZ	5.58	1.48	1.37
1	A	278	MET	C-O	-5.57	1.12	1.23
1	N	505	PHE	CB-CG	5.57	1.60	1.51
1	A	480	ARG	CZ-NH2	5.56	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	244	TYR	CG-CD1	5.55	1.46	1.39
1	A	126	TRP	CE3-CZ3	5.54	1.47	1.38
10	J	48	TYR	CG-CD2	5.53	1.46	1.39
4	Q	121	LYS	CD-CE	5.53	1.65	1.51
1	A	203	ALA	CA-CB	5.53	1.64	1.52
4	D	58	GLU	CD-OE2	5.52	1.31	1.25
1	N	184	PHE	CE2-CZ	5.52	1.47	1.37
4	Q	121	LYS	CE-NZ	5.52	1.62	1.49
1	N	313	ALA	CA-CB	5.51	1.64	1.52
3	C	257	TYR	CE2-CZ	5.50	1.45	1.38
6	F	64	GLU	CD-OE2	5.50	1.31	1.25
3	P	94	PHE	CD1-CE1	5.50	1.50	1.39
1	A	286	ILE	CA-CB	5.49	1.67	1.54
1	A	128	VAL	CB-CG1	5.49	1.64	1.52
4	D	87	PHE	CD1-CE1	5.49	1.50	1.39
3	P	240	TRP	CE3-CZ3	5.46	1.47	1.38
3	C	16	TRP	CB-CG	5.46	1.60	1.50
1	A	396	TRP	CE3-CZ3	5.45	1.47	1.38
2	O	18	GLU	CD-OE1	5.44	1.31	1.25
5	E	19	PHE	CE1-CZ	5.43	1.47	1.37
1	N	281	GLY	N-CA	5.43	1.54	1.46
2	B	206	PHE	CE1-CZ	5.42	1.47	1.37
1	A	426	PHE	CE1-CZ	5.41	1.47	1.37
6	F	2	SER	N-CA	5.41	1.57	1.46
1	A	63	PHE	CE2-CZ	5.40	1.47	1.37
1	A	473	TRP	CG-CD1	5.40	1.44	1.36
6	F	73	TRP	CE3-CZ3	5.40	1.47	1.38
1	A	108	SER	CB-OG	5.39	1.49	1.42
1	A	68	PHE	CD2-CE2	5.39	1.50	1.39
4	Q	5	VAL	CA-CB	5.37	1.66	1.54
1	N	64	VAL	CB-CG2	5.37	1.64	1.52
6	S	20	VAL	CB-CG2	5.37	1.64	1.52
3	C	90	GLU	CD-OE2	5.36	1.31	1.25
4	Q	10	ASP	CB-CG	5.35	1.62	1.51
1	A	385	ALA	CA-CB	5.34	1.63	1.52
7	T	17	ARG	CD-NE	-5.33	1.37	1.46
1	N	186	TRP	CG-CD1	5.33	1.44	1.36
1	A	122	ALA	CA-CB	5.33	1.63	1.52
1	A	393	PHE	CE1-CZ	5.32	1.47	1.37
2	B	59	GLN	CB-CG	5.30	1.66	1.52
2	B	160	LEU	N-CA	5.30	1.56	1.46
1	A	344	PHE	CE1-CZ	5.30	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	TRP	C-O	5.30	1.33	1.23
1	N	270	TYR	CD1-CE1	5.29	1.47	1.39
3	C	33	MET	CG-SD	5.28	1.94	1.81
6	S	65	ASP	CB-CG	5.27	1.62	1.51
3	P	253	TYR	CG-CD1	5.26	1.46	1.39
1	A	167	THR	CB-OG1	5.23	1.53	1.43
1	A	341	ALA	CA-CB	5.23	1.63	1.52
1	A	323	TRP	CZ3-CH2	5.20	1.48	1.40
2	O	59	GLN	CG-CD	5.20	1.63	1.51
3	P	139	ALA	CA-CB	5.20	1.63	1.52
3	P	237	ALA	CA-CB	5.20	1.63	1.52
4	Q	6	VAL	CA-CB	5.19	1.65	1.54
1	N	188	VAL	N-CA	5.19	1.56	1.46
1	A	234	LEU	N-CA	-5.18	1.35	1.46
1	N	264	LYS	C-O	5.16	1.33	1.23
2	B	18	GLU	CG-CD	5.16	1.59	1.51
1	A	148	PHE	CE1-CZ	5.16	1.47	1.37
2	B	32	PHE	CG-CD1	5.16	1.46	1.38
1	A	248	LEU	CA-CB	5.15	1.65	1.53
2	B	161	HIS	CB-CG	5.15	1.59	1.50
3	C	236	GLU	CD-OE1	5.14	1.31	1.25
2	O	108	TYR	CE2-CZ	5.14	1.45	1.38
2	O	196	CYS	CB-SG	5.14	1.91	1.82
2	O	132	GLU	CD-OE2	5.12	1.31	1.25
10	W	1	PHE	CE1-CZ	5.12	1.47	1.37
1	A	186	TRP	CE3-CZ3	5.11	1.47	1.38
1	N	99	ASN	CG-ND2	5.11	1.45	1.32
1	A	249	PRO	N-CA	-5.10	1.38	1.47
3	C	38	ASN	CB-CG	5.10	1.62	1.51
1	N	129	TYR	CD2-CE2	5.10	1.47	1.39
1	N	185	VAL	CB-CG1	5.09	1.63	1.52
3	P	184	ALA	CA-CB	5.09	1.63	1.52
7	G	17	ARG	CD-NE	-5.09	1.37	1.46
1	A	502	TYR	C-O	5.06	1.32	1.23
10	J	34	VAL	CB-CG2	5.05	1.63	1.52
1	N	148	PHE	CD1-CE1	5.03	1.49	1.39
3	C	221	ARG	CB-CG	5.03	1.66	1.52
3	P	186	PHE	CE2-CZ	5.02	1.46	1.37
3	C	86	PHE	CD2-CE2	5.02	1.49	1.39
1	A	393	PHE	CG-CD1	5.01	1.46	1.38
1	A	290	HIS	C-O	-5.01	1.13	1.23
2	O	31	VAL	CB-CG1	5.01	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	VAL	CB-CG2	5.00	1.63	1.52

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	17	ARG	NE-CZ-NH1	15.38	127.99	120.30
7	T	17	ARG	NE-CZ-NH2	-12.64	113.98	120.30
3	P	63	ARG	NE-CZ-NH1	12.31	126.45	120.30
4	D	20	ARG	NE-CZ-NH2	-12.09	114.25	120.30
3	C	221	ARG	NE-CZ-NH1	-12.06	114.27	120.30
1	N	244	TYR	CG-CD2-CE2	11.48	130.49	121.30
7	G	17	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	A	208	MET	CG-SD-CE	11.06	117.90	100.20
4	D	19	ARG	NE-CZ-NH1	-10.85	114.88	120.30
1	A	244	TYR	CG-CD1-CE1	-10.69	112.75	121.30
4	D	20	ARG	NE-CZ-NH1	10.39	125.50	120.30
6	S	45	ASP	CB-CG-OD1	-10.33	109.00	118.30
1	N	194	LEU	CB-CG-CD2	10.19	128.33	111.00
3	P	63	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	A	136	LEU	CB-CG-CD2	-9.73	94.46	111.00
1	A	129	TYR	CB-CG-CD1	-9.36	115.38	121.00
1	A	183	LEU	CB-CG-CD1	-9.15	95.45	111.00
1	A	244	TYR	CG-CD2-CE2	9.07	128.56	121.30
3	P	155	ASP	CB-CG-OD1	9.05	126.44	118.30
1	N	270	TYR	CB-CG-CD1	-9.02	115.59	121.00
1	A	244	TYR	CD1-CE1-CZ	8.97	127.87	119.80
1	A	298	ASP	CB-CG-OD2	8.85	126.26	118.30
1	A	244	TYR	CB-CG-CD1	-8.73	115.76	121.00
1	N	244	TYR	CG-CD1-CE1	-8.64	114.39	121.30
3	C	94	PHE	CB-CG-CD2	-8.61	114.77	120.80
1	N	244	TYR	CZ-CE2-CD2	-8.59	112.07	119.80
7	G	54	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	A	102	PHE	CZ-CE2-CD2	8.17	129.90	120.10
1	A	235	PHE	CB-CG-CD1	8.15	126.51	120.80
1	A	188	VAL	CG1-CB-CG2	-8.15	97.86	110.90
1	A	136	LEU	CA-CB-CG	8.14	134.03	115.30
2	O	139	ASP	CB-CG-OD2	8.13	125.62	118.30
4	Q	20	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	N	270	TYR	CZ-CE2-CD2	-8.07	112.54	119.80
1	A	278	MET	CA-CB-CG	-8.06	99.60	113.30
1	N	302	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	244	TYR	CB-CG-CD2	8.03	125.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	244	TYR	CZ-CE2-CD2	-7.95	112.64	119.80
3	C	252	LEU	CB-CG-CD1	-7.95	97.49	111.00
3	P	60	ASP	CB-CG-OD1	7.89	125.40	118.30
8	H	63	LEU	CB-CG-CD2	7.85	124.34	111.00
1	A	288	TRP	N-CA-CB	-7.82	96.53	110.60
3	C	190	ASP	CB-CG-OD2	7.74	125.26	118.30
5	E	74	LYS	CD-CE-NZ	-7.68	94.04	111.70
1	A	28	MET	CG-SD-CE	7.62	112.40	100.20
1	A	196	LEU	CB-CG-CD1	-7.59	98.10	111.00
1	A	202	LEU	O-C-N	7.51	134.71	122.70
1	A	227	ASP	CB-CG-OD1	-7.49	111.56	118.30
1	A	373	VAL	CA-CB-CG2	-7.46	99.71	110.90
3	P	221	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	A	129	TYR	CG-CD2-CE2	-7.45	115.34	121.30
3	P	80	ARG	CG-CD-NE	-7.41	96.24	111.80
1	N	244	TYR	CD1-CE1-CZ	7.29	126.36	119.80
1	A	302	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	305	PHE	CD1-CE1-CZ	-7.24	111.41	120.10
5	E	90	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	202	LEU	CB-CA-C	-7.19	96.54	110.20
2	B	82	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	N	369	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	242	GLU	OE1-CD-OE2	-7.12	114.75	123.30
1	N	129	TYR	CB-CG-CD1	-7.06	116.76	121.00
1	A	54	TYR	CB-CG-CD1	-7.02	116.79	121.00
3	P	257	TYR	CG-CD2-CE2	7.00	126.90	121.30
1	A	221	ASP	CB-CG-OD2	-6.93	112.06	118.30
3	P	214	PHE	CB-CG-CD1	6.92	125.64	120.80
6	S	54	ASN	CB-CA-C	-6.89	96.62	110.40
7	G	54	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	129	TYR	CZ-CE2-CD2	-6.85	113.63	119.80
11	K	54	ARG	NE-CZ-NH1	-6.83	116.89	120.30
7	G	17	ARG	NE-CZ-NH1	6.78	123.69	120.30
2	B	188	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	184	PHE	CG-CD1-CE1	6.75	128.23	120.80
3	P	127	LEU	CA-CB-CG	6.73	130.78	115.30
1	N	505	PHE	CB-CG-CD1	-6.73	116.09	120.80
2	B	211	LEU	CB-CG-CD1	-6.70	99.61	111.00
1	A	438	ARG	CB-CA-C	-6.62	97.16	110.40
3	P	80	ARG	NE-CZ-NH1	-6.61	117.00	120.30
2	B	202	SER	CB-CA-C	-6.59	97.58	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	93	PHE	CG-CD1-CE1	6.58	128.04	120.80
2	O	19	GLU	N-CA-CB	-6.58	98.76	110.60
13	M	34	LEU	CB-CG-CD1	6.57	122.16	111.00
1	A	207	THR	CA-CB-CG2	-6.55	103.22	112.40
12	Y	24	MET	CB-CA-C	-6.54	97.32	110.40
3	C	94	PHE	CD1-CE1-CZ	-6.53	112.27	120.10
2	B	65	TRP	CB-CA-C	6.53	123.46	110.40
1	A	54	TYR	CZ-CE2-CD2	-6.52	113.93	119.80
1	A	189	MET	CA-CB-CG	-6.51	102.23	113.30
3	P	155	ASP	CB-CG-OD2	-6.50	112.45	118.30
7	T	33	LEU	CA-CB-CG	6.50	130.24	115.30
4	Q	20	ARG	NE-CZ-NH1	6.48	123.54	120.30
4	Q	10	ASP	CB-CG-OD1	6.44	124.10	118.30
4	D	51	LEU	CB-CG-CD1	6.44	121.94	111.00
1	A	387	PHE	CB-CG-CD2	6.39	125.27	120.80
1	A	64	VAL	CA-CB-CG2	-6.38	101.33	110.90
1	A	201	VAL	CA-CB-CG1	-6.37	101.34	110.90
2	B	152	MET	CG-SD-CE	6.37	110.39	100.20
3	P	152	MET	CG-SD-CE	6.33	110.33	100.20
1	A	383	MET	CA-CB-CG	-6.33	102.55	113.30
1	N	113	LEU	CB-CG-CD1	6.30	121.71	111.00
1	N	298	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	339	MET	CG-SD-CE	-6.26	90.18	100.20
2	O	227	LEU	CB-CG-CD1	-6.26	100.36	111.00
1	N	270	TYR	CE1-CZ-CE2	6.25	129.80	119.80
1	A	145	LEU	CA-CB-CG	-6.22	100.99	115.30
6	S	56	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	51	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	285	PHE	CB-CG-CD1	-6.18	116.47	120.80
3	C	29	SER	CB-CA-C	-6.17	98.37	110.10
2	B	161	HIS	N-CA-C	-6.17	94.35	111.00
3	C	80	ARG	CG-CD-NE	-6.16	98.86	111.80
1	A	270	TYR	CG-CD2-CE2	-6.11	116.41	121.30
1	A	129	TYR	CE1-CZ-CE2	6.10	129.56	119.80
1	N	188	VAL	CG1-CB-CG2	-6.09	101.16	110.90
2	B	136	LEU	CB-CG-CD1	-6.07	100.69	111.00
1	A	285	PHE	O-C-N	-6.06	113.01	122.70
2	O	139	ASP	CB-CG-OD1	-6.02	112.88	118.30
1	A	150	LEU	CB-CG-CD2	-6.02	100.77	111.00
6	S	25	ARG	NE-CZ-NH2	-6.01	117.29	120.30
3	C	93	PHE	CD1-CE1-CZ	-6.01	112.89	120.10
1	N	230	LEU	CB-CG-CD2	-6.01	100.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	298	ASP	CB-CG-OD1	-5.98	112.92	118.30
7	G	56	ARG	NE-CZ-NH1	5.95	123.28	120.30
9	V	16	ARG	NE-CZ-NH1	-5.93	117.33	120.30
3	C	254	VAL	CA-CB-CG1	-5.92	102.02	110.90
3	P	94	PHE	CB-CG-CD2	-5.91	116.66	120.80
1	A	184	PHE	CG-CD2-CE2	-5.91	114.30	120.80
1	A	253	MET	CA-CB-CG	-5.89	103.29	113.30
3	C	44	MET	CG-SD-CE	5.89	109.62	100.20
6	S	45	ASP	CB-CG-OD2	5.88	123.59	118.30
11	X	54	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	N	189	MET	CG-SD-CE	-5.85	90.84	100.20
1	N	197	LEU	CB-CG-CD1	-5.85	101.06	111.00
3	P	214	PHE	CB-CG-CD2	-5.83	116.72	120.80
3	C	190	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	96	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	201	VAL	CA-CB-CG2	-5.81	102.18	110.90
5	R	53	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	129	TYR	CB-CA-C	-5.76	98.87	110.40
1	A	279	SER	CA-CB-OG	-5.74	95.71	111.20
1	N	160	GLY	N-CA-C	-5.74	98.76	113.10
1	N	438	ARG	CB-CA-C	-5.73	98.93	110.40
1	A	371	TYR	CA-CB-CG	-5.73	102.51	113.40
1	A	22	PHE	CG-CD2-CE2	5.72	127.10	120.80
8	H	27	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	N	251	PHE	CB-CG-CD1	-5.72	116.80	120.80
3	C	218	CYS	CA-CB-SG	-5.72	103.71	114.00
2	O	173	ASP	CB-CG-OD1	5.70	123.43	118.30
2	B	198	GLU	CA-C-N	-5.70	104.67	117.20
1	A	235	PHE	CZ-CE2-CD2	5.69	126.93	120.10
1	A	374	VAL	CG1-CB-CG2	5.68	120.00	110.90
1	A	512	ASN	CB-CA-C	-5.68	99.05	110.40
2	O	82	ARG	NE-CZ-NH2	-5.66	117.47	120.30
10	J	28	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	240	HIS	CA-CB-CG	-5.64	104.01	113.60
5	R	60	ASP	CB-CG-OD2	5.64	123.37	118.30
7	T	17	ARG	CB-CG-CD	-5.63	96.96	111.60
2	B	156	SER	CB-CA-C	-5.63	99.41	110.10
2	O	158	ASP	CB-CG-OD1	5.61	123.35	118.30
2	O	65	TRP	CA-CB-CG	5.59	124.33	113.70
3	C	206	LEU	CB-CG-CD1	-5.58	101.52	111.00
2	B	158	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	202	LEU	N-CA-C	-5.55	96.01	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	100	MET	CA-CB-CG	-5.55	103.86	113.30
6	S	81	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	209	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	A	192	ALA	O-C-N	-5.53	113.86	122.70
1	A	102	PHE	CG-CD1-CE1	5.52	126.88	120.80
1	A	251	PHE	O-C-N	-5.52	113.82	123.20
6	S	54	ASN	N-CA-CB	-5.49	100.71	110.60
1	N	268	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	A	38	ARG	CG-CD-NE	5.48	123.30	111.80
1	A	442	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	433	LEU	CB-CG-CD1	-5.47	101.69	111.00
2	B	158	ASP	CB-CG-OD1	5.47	123.22	118.30
6	S	94	HIS	N-CA-C	5.47	125.77	111.00
3	P	215	LEU	CB-CG-CD1	-5.47	101.71	111.00
1	A	235	PHE	CG-CD1-CE1	5.45	126.80	120.80
1	A	242	GLU	CG-CD-OE2	5.43	129.17	118.30
1	A	38	ARG	NE-CZ-NH1	5.43	123.02	120.30
8	U	35	ASP	CB-CG-OD1	5.43	123.18	118.30
1	A	285	PHE	CZ-CE2-CD2	-5.41	113.61	120.10
1	A	159	LEU	CB-CG-CD2	5.40	120.18	111.00
8	H	58	ARG	NE-CZ-NH1	-5.40	117.60	120.30
6	F	21	MET	CG-SD-CE	5.35	108.77	100.20
3	P	29	SER	CB-CA-C	-5.35	99.93	110.10
7	G	6	GLY	N-CA-C	5.35	126.47	113.10
8	H	33	TYR	CD1-CE1-CZ	-5.35	114.99	119.80
2	O	68	LEU	CA-CB-CG	-5.34	103.01	115.30
1	A	278	MET	CG-SD-CE	-5.32	91.70	100.20
1	N	15	ILE	CA-CB-CG1	-5.32	100.90	111.00
1	N	512	ASN	CB-CA-C	-5.31	99.77	110.40
2	B	173	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	168	ILE	CG1-CB-CG2	-5.29	99.77	111.40
3	C	85	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	A	438	ARG	N-CA-C	-5.28	96.75	111.00
1	A	200	PRO	O-C-N	-5.27	114.26	122.70
7	T	8	HIS	N-CA-C	5.27	125.23	111.00
1	N	5	ARG	CG-CD-NE	-5.27	100.74	111.80
4	D	20	ARG	CB-CA-C	-5.26	99.88	110.40
2	B	161	HIS	C-N-CA	-5.25	108.58	121.70
3	P	33	MET	CG-SD-CE	5.24	108.58	100.20
4	D	122	ARG	NE-CZ-NH1	5.23	122.92	120.30
7	G	23	LEU	CB-CG-CD1	5.23	119.89	111.00
1	A	197	LEU	CA-CB-CG	-5.23	103.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	LEU	CB-CG-CD1	-5.23	102.11	111.00
2	B	178	ARG	NE-CZ-NH2	5.22	122.91	120.30
3	C	181	TYR	CZ-CE2-CD2	-5.22	115.11	119.80
1	A	189	MET	CG-SD-CE	-5.21	91.86	100.20
1	A	355	GLY	N-CA-C	-5.21	100.08	113.10
3	P	18	LEU	CB-CG-CD1	-5.20	102.15	111.00
1	A	369	ASP	CB-CG-OD1	5.20	122.98	118.30
3	C	33	MET	CG-SD-CE	5.20	108.51	100.20
1	A	264	LYS	CD-CE-NZ	5.19	123.64	111.70
2	B	112	ASP	CB-CG-OD1	5.17	122.96	118.30
9	V	57	MET	CG-SD-CE	5.16	108.45	100.20
1	A	102	PHE	CD1-CE1-CZ	-5.15	113.92	120.10
1	N	38	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	B	86	MET	CA-CB-CG	5.15	122.05	113.30
1	N	191	THR	N-CA-C	-5.14	97.11	111.00
6	F	93	PRO	C-N-CA	5.12	134.50	121.70
3	C	156	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	N	28	MET	CG-SD-CE	5.11	108.38	100.20
5	R	73	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	N	229	ILE	CG1-CB-CG2	-5.11	100.16	111.40
1	N	244	TYR	CB-CG-CD2	5.09	124.06	121.00
2	B	116	LEU	CB-CG-CD2	-5.07	102.38	111.00
6	F	95	GLN	N-CA-C	5.07	124.70	111.00
1	A	250	GLY	N-CA-C	-5.06	100.46	113.10
1	A	261	TYR	CB-CG-CD1	-5.06	117.97	121.00
13	M	26	PHE	CB-CA-C	-5.05	100.30	110.40
1	N	230	LEU	CB-CG-CD1	5.05	119.58	111.00
1	A	171	MET	CA-CB-CG	-5.04	104.73	113.30
2	O	65	TRP	N-CA-C	5.04	124.60	111.00
3	P	257	TYR	CZ-CE2-CD2	-5.04	115.27	119.80
2	O	226	MET	CG-SD-CE	5.03	108.25	100.20
1	A	379	TYR	CD1-CE1-CZ	-5.03	115.28	119.80
1	A	480	ARG	CD-NE-CZ	5.02	130.63	123.60
1	N	189	MET	CA-CB-CG	-5.02	104.77	113.30
1	N	505	PHE	CZ-CE2-CD2	-5.02	114.08	120.10
4	D	51	LEU	CA-CB-CG	5.01	126.83	115.30
7	G	8	HIS	N-CA-C	5.01	124.53	111.00
1	A	50	ASP	CB-CG-OD2	5.00	122.80	118.30
1	A	206	ILE	O-C-N	5.00	130.70	122.70
3	C	49	THR	CA-CB-CG2	-5.00	105.40	112.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	VAL	Mainchain
1	A	201	VAL	Mainchain
1	A	232	GLN	Mainchain
1	A	247	ILE	Mainchain
1	A	65	MET	Mainchain
2	B	160	LEU	Mainchain
2	B	173	ASP	Mainchain
10	J	57	HIS	Peptide
6	S	93	PRO	Peptide
6	S	95	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	65	0
1	N	4027	0	4001	79	0
2	B	1824	0	1833	23	0
2	O	1824	0	1833	37	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	6	0
4	Q	1195	0	1183	27	0
5	E	852	0	845	3	0
5	R	852	0	845	11	0
6	F	748	0	728	17	0
6	S	748	0	728	28	0
7	G	675	0	643	38	0
7	T	675	0	643	56	0
8	H	662	0	623	11	0
8	U	662	0	623	9	0
9	I	601	0	613	6	0
9	V	601	0	613	13	0
10	J	460	0	459	7	0
10	W	460	0	459	4	0
11	K	384	0	366	2	0
11	X	384	0	366	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	380	0	380	12	0
12	Y	380	0	380	9	0
13	M	335	0	352	8	0
13	Z	335	0	352	6	0
14	A	120	0	109	14	0
14	N	120	0	108	3	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	2	0	0	1	0
16	N	2	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	12	0
19	B	63	0	110	7	0
19	L	63	0	110	12	0
19	N	126	0	220	18	0
19	O	63	0	110	9	0
20	A	102	0	152	11	0
20	C	102	0	152	7	0
20	G	51	0	76	2	0
20	N	102	0	152	10	0
20	P	51	0	76	6	0
21	A	29	0	37	0	0
21	B	29	0	35	1	0
21	C	29	0	35	8	0
21	G	29	0	37	1	0
21	J	29	0	35	1	0
21	P	58	0	71	10	0
21	W	29	0	35	2	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	17	0
23	R	52	0	80	15	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	53	0	77	5	0
25	G	106	0	154	29	0
25	P	106	0	154	21	0
25	T	53	0	77	24	0
26	C	100	0	156	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	G	100	0	156	39	0
26	P	100	0	156	21	0
26	T	100	0	156	35	0
27	C	33	0	38	2	0
27	M	33	0	38	0	0
27	P	33	0	38	4	0
27	Z	33	0	39	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	213	0	0	2	0
29	B	135	0	0	5	0
29	C	109	0	0	1	0
29	D	93	0	0	2	0
29	E	61	0	0	1	0
29	F	80	0	0	2	0
29	G	56	0	0	6	0
29	H	53	0	0	1	0
29	I	35	0	0	1	0
29	J	16	0	0	1	0
29	K	21	0	0	1	0
29	L	28	0	0	3	0
29	M	24	0	0	1	0
29	N	205	0	0	6	0
29	O	106	0	0	1	0
29	P	106	0	0	3	0
29	Q	51	0	0	3	0
29	R	39	0	0	0	0
29	S	62	0	0	4	0
29	T	47	0	0	10	0
29	U	50	0	0	1	0
29	V	21	0	0	0	0
29	W	15	0	0	0	0
29	X	19	0	0	0	0
29	Y	12	0	0	0	0
29	Z	7	0	0	0	0
All	All	32400	0	31275	668	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 11.

All (668) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:484:THR:CG2	1:N:484:THR:CB	1.77	1.63
26:G:269:CDL:C15	26:G:269:CDL:C16	1.76	1.62
7:T:5:LYS:CG	7:T:5:LYS:CB	1.75	1.56
1:A:297:MET:SD	1:A:297:MET:CE	2.02	1.46
7:G:5:LYS:HD2	25:G:1263:PEK:C38	1.50	1.42
2:B:166:PRO:CB	2:B:166:PRO:CG	1.81	1.41
27:P:1272:DMU:C2	27:P:1272:DMU:O55	1.67	1.39
6:S:52:ILE:O	6:S:94:HIS:CE1	1.82	1.30
7:T:5:LYS:HD2	25:T:263:PEK:C38	1.73	1.16
7:T:5:LYS:CD	25:T:263:PEK:H383	1.74	1.16
3:P:160:LEU:HD13	21:P:1271:CHD:C18	1.75	1.15
25:P:1265:PEK:H383	26:T:1269:CDL:C27	1.75	1.15
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.62	1.14
25:C:264:PEK:H102	25:C:264:PEK:H161	1.15	1.13
7:G:5:LYS:HD2	25:G:1263:PEK:H383	1.15	1.13
23:R:1229:PSC:H142	23:R:1229:PSC:H343	1.13	1.11
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.15	1.09
19:N:1523:TGL:HC21	19:N:1523:TGL:HG11	1.32	1.09
20:C:267:PGV:H182	26:C:270:CDL:H662	1.14	1.08
25:P:1265:PEK:H383	26:T:1269:CDL:H272	1.19	1.08
25:P:1265:PEK:C38	26:T:1269:CDL:C27	2.31	1.07
3:C:160:LEU:HD13	21:C:271:CHD:C18	1.85	1.07
23:R:1229:PSC:C34	23:R:1229:PSC:H142	1.83	1.07
6:S:85:CYS:SG	6:S:87:THR:HG23	1.96	1.05
6:F:1:ALA:N	25:G:265:PEK:H041	1.72	1.04
12:L:20:ARG:HH22	19:L:522:TGL:HC32	0.96	1.03
25:P:1265:PEK:C38	26:T:1269:CDL:H273	1.89	1.03
10:W:33:ARG:HG2	21:W:1059:CHD:H152	1.38	1.01
7:T:5:LYS:CD	25:T:263:PEK:C38	2.36	1.00
26:G:269:CDL:H541	26:G:269:CDL:H231	1.45	0.98
7:G:5:LYS:CD	25:G:1263:PEK:H383	1.94	0.98
23:R:1229:PSC:H343	23:R:1229:PSC:C14	1.92	0.98
7:G:5:LYS:HD2	25:G:1263:PEK:H381	1.40	0.98
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.45	0.98
7:T:5:LYS:HD2	25:T:263:PEK:H383	1.35	0.98
25:P:1265:PEK:H041	6:S:1:ALA:H2	1.30	0.97
7:G:5:LYS:HG2	1:N:278:MET:HB3	1.47	0.96
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.27	0.96
7:G:5:LYS:CD	25:G:1263:PEK:C38	2.43	0.96
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.46	0.96
8:U:49:ASP:O	8:U:52:VAL:HG22	1.64	0.95
20:C:268:PGV:H21	20:C:268:PGV:H62	1.47	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:265:PEK:H381	26:G:269:CDL:H273	1.47	0.95
7:T:72:ASN:H	7:T:76:ASN:HD22	1.15	0.94
25:P:1265:PEK:H041	6:S:1:ALA:N	1.82	0.94
26:T:1269:CDL:H571	26:T:1269:CDL:H782	1.46	0.94
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.49	0.94
3:P:160:LEU:HD13	21:P:1271:CHD:H181	1.46	0.94
7:T:5:LYS:HD2	25:T:263:PEK:H381	1.47	0.94
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.32	0.94
1:A:278:MET:HB3	7:T:5:LYS:HG2	1.47	0.94
7:T:2:SER:OG	25:T:263:PEK:H301	1.67	0.94
6:S:52:ILE:O	6:S:94:HIS:HE1	1.42	0.93
7:T:84:LYS:H	7:T:84:LYS:HD2	1.32	0.92
7:T:5:LYS:CG	25:T:263:PEK:H383	2.00	0.92
7:G:36:TRP:HB3	29:G:4858:HOH:O	1.69	0.91
19:B:521:TGL:H281	19:B:521:TGL:H102	1.50	0.91
10:J:33:ARG:HG2	21:J:60:CHD:H152	1.48	0.91
6:F:85:CYS:SG	6:F:87:THR:HG23	2.11	0.91
20:N:1524:PGV:H311	13:Z:19:LEU:HD23	1.52	0.90
7:G:72:ASN:H	7:G:76:ASN:HD22	1.17	0.90
25:P:1265:PEK:H381	26:T:1269:CDL:H273	1.53	0.90
25:G:265:PEK:C38	26:G:269:CDL:C27	2.50	0.90
6:F:1:ALA:H2	25:G:265:PEK:H041	1.33	0.89
26:G:269:CDL:C23	26:G:269:CDL:H541	2.04	0.88
19:B:521:TGL:C28	19:B:521:TGL:H102	2.03	0.88
7:G:84:LYS:HD2	7:G:84:LYS:H	1.36	0.88
20:C:267:PGV:C18	26:C:270:CDL:H662	2.04	0.87
23:B:229:PSC:C07	9:I:10:ARG:HH21	1.87	0.87
25:G:265:PEK:C38	26:G:269:CDL:H273	2.03	0.87
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.54	0.87
3:C:160:LEU:HD13	21:C:271:CHD:H181	1.56	0.87
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.08	0.86
20:A:524:PGV:H311	13:M:19:LEU:HD23	1.57	0.86
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.40	0.85
23:B:229:PSC:O01	23:B:229:PSC:H212	1.76	0.84
20:A:524:PGV:C01	20:A:524:PGV:H221	2.08	0.83
23:R:1229:PSC:O01	23:R:1229:PSC:H212	1.77	0.83
25:G:265:PEK:H381	26:G:269:CDL:C27	2.10	0.82
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.45	0.81
26:G:269:CDL:C14	26:G:269:CDL:C16	2.58	0.81
26:G:269:CDL:C15	26:G:269:CDL:H182	2.10	0.81
26:C:270:CDL:H231	26:C:270:CDL:H661	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:34:SER:H	4:D:37:GLN:HE21	1.28	0.81
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.15	0.81
13:M:39:ASN:O	13:M:43:SER:HB2	1.81	0.80
20:A:524:PGV:H221	20:A:524:PGV:H012	1.62	0.80
6:S:52:ILE:C	6:S:94:HIS:CE1	2.55	0.80
26:G:269:CDL:C24	26:G:269:CDL:H541	2.11	0.80
26:T:1269:CDL:H571	26:T:1269:CDL:C78	2.13	0.79
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.63	0.79
7:G:30:LEU:CD2	26:G:269:CDL:H461	2.13	0.78
20:P:1267:PGV:H182	26:P:1270:CDL:H662	1.66	0.78
25:C:264:PEK:C10	25:C:264:PEK:H161	2.08	0.77
26:P:1270:CDL:OB9	26:P:1270:CDL:H522	1.85	0.77
7:T:30:LEU:HD21	26:T:1269:CDL:H461	1.66	0.77
6:F:1:ALA:H1	25:G:265:PEK:H041	1.49	0.77
7:T:72:ASN:H	7:T:76:ASN:ND2	1.83	0.77
7:T:5:LYS:HB2	25:T:263:PEK:C36	2.14	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.66	0.76
26:G:269:CDL:H571	26:G:269:CDL:H792	1.67	0.76
11:X:54:ARG:NH2	11:X:54:ARG:HG3	1.96	0.76
7:T:84:LYS:H	7:T:84:LYS:CD	1.98	0.76
7:G:84:LYS:H	7:G:84:LYS:CD	1.99	0.75
26:G:269:CDL:H241	26:G:269:CDL:H541	1.69	0.75
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.99	0.75
7:G:5:LYS:HB3	1:N:278:MET:SD	2.26	0.75
19:O:1521:TGL:H221	19:O:1521:TGL:H362	1.69	0.75
25:P:1264:PEK:H161	25:P:1264:PEK:H101	1.67	0.75
7:T:2:SER:O	25:T:263:PEK:H322	1.86	0.75
7:T:84:LYS:N	7:T:84:LYS:HD2	1.99	0.75
20:P:1267:PGV:H182	26:P:1270:CDL:C66	2.17	0.75
2:B:41:ILE:HD13	23:B:229:PSC:H342	1.67	0.74
8:H:45:ALA:O	8:H:47:GLY:N	2.21	0.74
19:N:1522:TGL:HC62	19:N:1522:TGL:HC22	1.70	0.74
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.68	0.74
21:C:271:CHD:O25	21:C:271:CHD:H20	1.88	0.73
2:O:141:ARG:H	9:V:70:GLN:HE22	1.36	0.73
19:A:523:TGL:HG12	19:A:523:TGL:HC21	1.71	0.73
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.02	0.73
19:N:1522:TGL:HC62	19:N:1522:TGL:CC2	2.19	0.73
3:P:210:ILE:HD13	20:P:1267:PGV:H301	1.71	0.73
1:N:514:LYS:HE2	29:S:3514:HOH:O	1.87	0.72
6:S:95:GLN:HB2	29:S:4477:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.37	0.72
26:G:269:CDL:C54	26:G:269:CDL:H241	2.19	0.72
26:G:269:CDL:HA21	26:G:269:CDL:H111	1.71	0.72
25:P:1265:PEK:C38	26:T:1269:CDL:H272	2.02	0.72
7:T:8:HIS:CD2	25:T:263:PEK:H232	2.24	0.72
25:C:264:PEK:H32	25:C:264:PEK:H71	1.70	0.71
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.36	0.71
3:C:160:LEU:CD1	21:C:271:CHD:H181	2.20	0.71
7:T:3:ALA:CB	25:T:263:PEK:H382	2.20	0.71
6:F:95:GLN:OE1	6:F:95:GLN:HA	1.90	0.71
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.11	0.71
26:G:269:CDL:C15	26:G:269:CDL:C17	2.69	0.71
8:H:46:LYS:HB2	8:U:52:VAL:HG12	1.72	0.71
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.73	0.71
6:S:64:GLU:O	6:S:65:ASP:HB2	1.90	0.70
6:F:1:ALA:N	25:G:265:PEK:C04	2.52	0.70
3:P:160:LEU:CD1	21:P:1271:CHD:H181	2.19	0.70
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.57	0.70
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.73	0.70
26:P:1270:CDL:H242	26:P:1270:CDL:H661	1.73	0.70
7:G:30:LEU:HD23	26:G:269:CDL:H461	1.73	0.69
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	1.92	0.69
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.74	0.69
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.92	0.69
1:N:513:LEU:O	1:N:514:LYS:HB2	1.93	0.69
26:G:269:CDL:H201	1:N:311:ILE:CD1	2.22	0.69
1:N:472:ILE:HG21	19:N:1522:TGL:HA91	1.73	0.69
7:T:5:LYS:CB	25:T:263:PEK:H362	2.19	0.69
1:N:417:MET:CE	29:N:3166:HOH:O	2.41	0.69
1:A:513:LEU:O	1:A:514:LYS:HB2	1.93	0.69
7:G:72:ASN:H	7:G:76:ASN:ND2	1.90	0.69
25:P:1264:PEK:H161	25:P:1264:PEK:C10	2.22	0.68
19:A:523:TGL:HC61	29:B:2562:HOH:O	1.92	0.68
6:S:94:HIS:CD2	6:S:95:GLN:H	2.10	0.68
26:T:1269:CDL:H541	26:T:1269:CDL:H241	1.76	0.68
20:C:267:PGV:H182	26:C:270:CDL:C66	2.09	0.68
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.74	0.68
1:A:177:SER:H	1:A:180:GLN:HE21	1.41	0.68
25:G:265:PEK:H383	26:G:269:CDL:H272	1.77	0.67
8:H:9:LYS:O	8:H:10:ASN:HB2	1.92	0.67
20:A:524:PGV:H302	20:A:524:PGV:H132	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:226:HIS:CE1	26:C:270:CDL:HB31	2.30	0.67
26:G:269:CDL:HA21	26:G:269:CDL:C11	2.25	0.66
6:S:75:HIS:H	6:S:80:GLN:HE22	1.44	0.66
26:G:269:CDL:C15	26:G:269:CDL:C18	2.73	0.66
20:N:1524:PGV:H221	20:N:1524:PGV:C01	2.25	0.66
19:N:1523:TGL:HG11	19:N:1523:TGL:CC2	2.17	0.66
25:G:265:PEK:C38	26:G:269:CDL:H272	2.26	0.66
2:O:49:LYS:HE2	29:Q:3076:HOH:O	1.95	0.66
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.93	0.66
6:F:97:ALA:HB2	29:F:4597:HOH:O	1.96	0.66
23:B:229:PSC:H072	9:I:10:ARG:HH21	1.60	0.65
10:J:4:ARG:HD2	10:J:7:GLU:OE2	1.96	0.65
1:A:177:SER:H	1:A:180:GLN:NE2	1.95	0.65
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.77	0.65
26:P:1270:CDL:HB22	26:P:1270:CDL:PA1	2.36	0.65
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.78	0.65
20:A:521:PGV:H302	29:C:4771:HOH:O	1.96	0.65
3:C:67:PHE:CE1	26:C:270:CDL:H1	2.20	0.65
1:A:484:THR:HB	13:M:2:THR:OG1	1.97	0.65
19:L:522:TGL:CC6	19:L:522:TGL:HC22	2.25	0.65
26:G:269:CDL:OA7	26:G:269:CDL:H342	1.98	0.64
7:G:45:PRO:HD2	29:G:2099:HOH:O	1.98	0.64
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.85	0.64
1:N:53:ILE:HG12	29:N:3704:HOH:O	1.98	0.64
1:A:297:MET:CB	1:A:297:MET:CE	2.76	0.64
4:D:34:SER:H	4:D:37:GLN:NE2	1.94	0.64
25:P:1265:PEK:C04	6:S:1:ALA:N	2.59	0.64
23:B:229:PSC:H231	23:B:229:PSC:H42	1.80	0.63
1:N:417:MET:HE3	29:N:3166:HOH:O	1.98	0.63
26:T:1269:CDL:H111	26:T:1269:CDL:HA21	1.80	0.63
26:G:269:CDL:H151	26:G:269:CDL:H182	1.80	0.63
6:F:1:ALA:H1	25:G:265:PEK:C04	2.09	0.62
19:O:1521:TGL:H241	19:O:1521:TGL:H201	1.80	0.62
1:N:484:THR:CG2	1:N:484:THR:HB	2.16	0.62
1:N:449:MET:SD	2:O:5:MET:HG2	2.40	0.62
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.34	0.62
26:G:269:CDL:H201	1:N:311:ILE:HD11	1.79	0.62
1:A:278:MET:SD	7:T:5:LYS:HB3	2.40	0.61
7:G:30:LEU:HD21	26:G:269:CDL:H461	1.81	0.61
10:J:52:TRP:O	10:J:57:HIS:HE1	1.82	0.61
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:8:ASP:HA	23:R:1229:PSC:H071	1.83	0.61
6:S:95:GLN:NE2	6:S:95:GLN:HA	2.14	0.61
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.65	0.61
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.36	0.61
20:A:524:PGV:H011	20:A:524:PGV:H221	1.83	0.61
6:S:85:CYS:SG	6:S:87:THR:CG2	2.84	0.60
1:N:514:LYS:NZ	29:N:3645:HOH:O	2.33	0.60
26:T:1269:CDL:C11	26:T:1269:CDL:HA21	2.31	0.60
25:C:264:PEK:H261	27:C:272:DMU:H11	1.82	0.60
21:C:271:CHD:O25	21:C:271:CHD:C20	2.49	0.60
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.66	0.60
1:A:21:LEU:HD23	19:L:522:TGL:H211	1.83	0.60
19:N:1523:TGL:HB22	4:Q:78:TRP:HA	1.83	0.59
21:P:1271:CHD:H211	21:P:1271:CHD:O25	2.02	0.59
7:T:7:ASP:HB3	29:T:4509:HOH:O	2.01	0.59
3:P:160:LEU:HD13	21:P:1271:CHD:H182	1.80	0.59
20:A:524:PGV:H062	29:M:2126:HOH:O	2.02	0.59
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	2.02	0.59
8:U:9:LYS:HG3	8:U:10:ASN:H	1.68	0.59
9:V:65:LYS:O	11:X:54:ARG:NH1	2.36	0.59
23:R:1229:PSC:H322	23:R:1229:PSC:H12	1.84	0.58
6:S:55:LYS:HA	6:S:74:LEU:O	2.04	0.58
1:N:177:SER:H	1:N:180:GLN:HE21	1.51	0.58
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.85	0.58
3:C:156:ARG:HE	21:C:271:CHD:C24	2.16	0.58
23:B:229:PSC:H32	23:B:229:PSC:H011	1.85	0.58
2:B:56:MET:HG2	23:B:229:PSC:H211	1.85	0.58
26:T:1269:CDL:H171	29:T:4750:HOH:O	2.03	0.58
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.86	0.57
8:U:9:LYS:O	8:U:10:ASN:HB2	2.04	0.57
20:C:268:PGV:C6	20:C:268:PGV:H21	2.25	0.57
3:P:63:ARG:HE	26:P:1270:CDL:CA2	2.12	0.57
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.19	0.57
12:Y:22:LEU:O	12:Y:26:THR:HB	2.04	0.57
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.85	0.57
2:O:56:MET:HA	23:R:1229:PSC:H202	1.86	0.57
1:A:310:MET:HE1	1:A:360:ASN:HD21	1.68	0.57
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.87	0.57
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.87	0.57
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.87	0.57
7:T:17:ARG:HD2	29:T:3446:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:229:PSC:H322	23:B:229:PSC:H12	1.87	0.57
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.69	0.57
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.85	0.57
23:B:229:PSC:H071	9:I:10:ARG:HH21	1.67	0.56
12:L:9:LYS:HG3	29:L:4884:HOH:O	2.05	0.56
19:O:1521:TGL:HA71	19:O:1521:TGL:H112	1.88	0.56
7:T:2:SER:OG	25:T:263:PEK:C30	2.49	0.56
6:S:92:VAL:HG23	6:S:92:VAL:O	2.06	0.56
8:H:43:MET:HE3	8:H:49:ASP:N	2.21	0.56
6:F:64:GLU:O	6:F:65:ASP:HB2	2.03	0.56
1:N:177:SER:H	1:N:180:GLN:NE2	2.02	0.56
20:G:1268:PGV:H11	21:P:1525:CHD:H152	1.88	0.56
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.89	0.56
20:P:1267:PGV:H182	26:P:1270:CDL:C67	2.36	0.56
7:T:72:ASN:N	7:T:76:ASN:HD22	1.95	0.56
19:O:1521:TGL:H101	19:O:1521:TGL:C28	2.36	0.55
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.36	0.55
27:P:1272:DMU:O1	27:P:1272:DMU:H30	2.06	0.55
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.71	0.55
6:F:26:LYS:HE3	29:F:4625:HOH:O	2.06	0.55
26:T:1269:CDL:H562	26:T:1269:CDL:H762	1.89	0.55
3:C:226:HIS:HE1	26:C:270:CDL:HB31	1.68	0.55
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	2.37	0.55
3:P:160:LEU:HD13	21:P:1271:CHD:H183	1.83	0.55
26:C:270:CDL:H772	26:C:270:CDL:H642	1.90	0.54
7:G:5:LYS:HG2	1:N:278:MET:CB	2.30	0.54
26:T:1269:CDL:C24	26:T:1269:CDL:H541	2.38	0.54
25:G:265:PEK:C37	26:G:269:CDL:H273	2.36	0.54
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.89	0.54
1:N:514:LYS:HA	6:S:38:ALA:CB	2.36	0.54
23:R:1229:PSC:C07	9:V:10:ARG:HH21	2.21	0.54
7:T:31:CYS:SG	26:T:1269:CDL:H551	2.48	0.54
2:O:83:ILE:O	2:O:87:MET:HG3	2.07	0.54
25:P:1265:PEK:H041	6:S:1:ALA:H1	1.70	0.54
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.73	0.54
2:B:62:GLU:O	2:B:66:THR:HB	2.07	0.54
19:A:523:TGL:HB22	4:D:78:TRP:HB3	1.90	0.54
7:T:5:LYS:CB	25:T:263:PEK:H383	2.38	0.54
8:U:27:ARG:NH1	29:U:3431:HOH:O	2.41	0.54
9:V:1:SAC:OAC	9:V:1:SAC:HB3	2.06	0.54
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.96	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:229:PSC:C07	9:I:10:ARG:NH2	2.67	0.53
3:C:217:VAL:HG22	26:C:270:CDL:H732	1.89	0.53
20:N:1524:PGV:H012	20:N:1524:PGV:H221	1.89	0.53
7:G:5:LYS:CG	25:G:1263:PEK:H383	2.38	0.53
7:G:1:ALA:HB2	20:G:1268:PGV:H321	1.90	0.53
26:T:1269:CDL:OA7	26:T:1269:CDL:H311	2.09	0.53
29:H:4877:HOH:O	8:U:46:LYS:HD2	2.08	0.53
7:G:84:LYS:HD2	7:G:84:LYS:N	2.15	0.53
26:C:270:CDL:H231	26:C:270:CDL:H641	1.91	0.53
8:H:43:MET:CE	8:H:49:ASP:N	2.72	0.53
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.57	0.53
19:L:522:TGL:C23	19:L:522:TGL:HA92	2.32	0.53
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.73	0.52
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.91	0.52
7:T:17:ARG:CD	29:T:3446:HOH:O	2.57	0.52
1:A:335:SER:HB2	1:A:336:PRO:HD2	1.91	0.52
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.91	0.52
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.44	0.52
6:S:94:HIS:CG	6:S:95:GLN:H	2.26	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.52
25:P:1265:PEK:H381	26:T:1269:CDL:C27	2.21	0.52
1:A:240:HIS:CD2	1:A:240:HIS:C	2.83	0.52
1:A:297:MET:HE3	1:A:297:MET:HB3	1.92	0.52
3:C:160:LEU:HD13	21:C:271:CHD:H183	1.83	0.52
8:H:60:TYR:C	8:H:60:TYR:CD1	2.82	0.52
19:A:523:TGL:HC72	2:B:49:LYS:HD3	1.92	0.52
1:N:33:LEU:HB3	1:N:61:HIS:HB2	1.93	0.51
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.28	0.51
1:A:426:PHE:HB3	1:A:427:PRO:HD3	1.92	0.51
19:N:1522:TGL:CC6	19:N:1522:TGL:CC2	2.88	0.51
1:A:377:PHE:CD1	14:A:516:HEA:HAD1	2.45	0.51
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.40	0.51
3:P:112:LEU:HD13	3:P:118:PRO:HG3	1.92	0.51
7:T:45:PRO:HD2	29:T:3099:HOH:O	2.09	0.51
1:A:152:LEU:N	1:A:152:LEU:HD23	2.24	0.51
4:Q:102:TYR:CD1	13:Z:35:TYR:HE1	2.29	0.51
1:N:265:LYS:HE3	29:N:4362:HOH:O	2.11	0.51
13:M:39:ASN:O	13:M:43:SER:CB	2.57	0.51
2:O:68:LEU:HB2	2:O:69:PRO:HD3	1.92	0.51
27:C:272:DMU:O1	27:C:272:DMU:H30	2.10	0.51
8:H:9:LYS:O	8:H:10:ASN:CB	2.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:52:GLU:HG3	29:K:4847:HOH:O	2.10	0.51
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.94	0.50
2:O:33:LEU:CD1	9:V:31:PHE:CD1	2.94	0.50
19:A:523:TGL:HA32	19:A:523:TGL:HB42	1.93	0.50
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.50
1:A:382:SER:OG	14:A:515:HEA:H121	2.12	0.50
7:T:5:LYS:HD3	25:T:263:PEK:C38	2.36	0.50
7:T:8:HIS:HD2	25:T:263:PEK:H232	1.72	0.50
20:P:1267:PGV:H182	26:P:1270:CDL:H671	1.94	0.50
1:N:484:THR:CG2	1:N:484:THR:C	2.80	0.50
4:Q:72:ASN:HB3	29:Q:3076:HOH:O	2.12	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.50
2:B:13:THR:OG1	2:B:167:SER:HB2	2.12	0.49
5:R:67:ILE:O	5:R:71:VAL:HG23	2.12	0.49
2:B:82:ARG:HG2	2:B:86:MET:HE3	1.92	0.49
23:B:229:PSC:H071	9:I:10:ARG:NH2	2.27	0.49
1:A:483:LEU:HD21	13:M:4:LYS:HD3	1.94	0.49
29:A:4282:HOH:O	23:B:229:PSC:H21	2.11	0.49
19:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.95	0.49
2:B:114:GLU:HB3	29:B:4709:HOH:O	2.13	0.49
26:G:269:CDL:OA7	26:G:269:CDL:H311	2.13	0.49
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.52	0.49
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.22	0.49
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.95	0.49
23:B:229:PSC:C02	23:B:229:PSC:H212	2.42	0.49
20:N:1524:PGV:H011	20:N:1524:PGV:H221	1.93	0.49
1:A:297:MET:CE	1:A:297:MET:HB3	2.41	0.49
2:O:121:TYR:O	2:O:138:VAL:HA	2.12	0.49
26:P:1270:CDL:HB21	26:P:1270:CDL:OB6	2.13	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.94	0.49
23:R:1229:PSC:H343	23:R:1229:PSC:C13	2.41	0.49
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.46	0.49
19:A:523:TGL:CG3	19:A:523:TGL:OB1	2.61	0.49
27:P:1272:DMU:H28	27:P:1272:DMU:C2	2.11	0.49
3:P:25:LEU:O	3:P:29:SER:HB2	2.13	0.49
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.13	0.48
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.47	0.48
7:G:3:ALA:O	7:G:4:ALA:CB	2.61	0.48
25:P:1265:PEK:C04	6:S:1:ALA:H1	2.25	0.48
19:B:521:TGL:H241	19:B:521:TGL:H201	1.95	0.48
19:A:523:TGL:HG12	19:A:523:TGL:CC2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.13	0.48
26:G:269:CDL:H351	2:O:78:LEU:HD12	1.96	0.48
6:S:87:THR:HG21	29:S:3514:HOH:O	2.12	0.48
26:T:1269:CDL:H202	26:T:1269:CDL:H511	1.95	0.48
12:L:24:MET:HE3	29:L:4798:HOH:O	2.14	0.48
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.94	0.48
25:T:263:PEK:H351	29:T:4509:HOH:O	2.12	0.48
19:A:523:TGL:HG32	19:A:523:TGL:OB1	2.14	0.48
26:G:269:CDL:H1	26:G:269:CDL:OB4	2.14	0.48
1:N:83:VAL:N	1:N:84:PRO:CD	2.76	0.48
3:P:52:LEU:HD21	26:P:1270:CDL:H412	1.95	0.48
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.14	0.48
1:A:50:ASP:HB3	1:A:53:ILE:HD12	1.94	0.48
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.49	0.48
7:T:5:LYS:HB2	25:T:263:PEK:H383	1.95	0.48
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.28	0.48
23:R:1229:PSC:H072	9:V:10:ARG:HH21	1.78	0.48
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.79	0.48
2:B:146:MET:HA	2:B:213:LEU:HD12	1.96	0.47
1:N:76:GLY:O	1:N:80:ASN:HB2	2.14	0.47
2:O:95:LEU:HD23	2:O:150:ILE:HG12	1.96	0.47
6:S:22:LEU:HD12	29:S:4465:HOH:O	2.13	0.47
10:W:33:ARG:CG	21:W:1059:CHD:H152	2.27	0.47
12:L:22:LEU:O	12:L:26:THR:HB	2.13	0.47
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.79	0.47
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.13	0.47
1:A:240:HIS:CE1	1:A:244:TYR:OH	2.68	0.47
1:A:51:ASP:OD1	1:A:441:SER:OG	2.25	0.47
3:C:52:LEU:HD23	26:C:270:CDL:H362	1.96	0.47
1:N:489:THR:HA	6:S:71:TRP:O	2.14	0.47
7:T:37:LEU:CD2	26:T:1269:CDL:H361	2.45	0.47
19:B:521:TGL:C28	19:B:521:TGL:C10	2.86	0.47
25:T:263:PEK:H312	25:T:263:PEK:H282	1.59	0.47
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.66	0.47
7:T:3:ALA:O	7:T:4:ALA:HB2	2.15	0.47
8:H:43:MET:CE	8:H:49:ASP:H	2.27	0.47
1:N:426:PHE:N	1:N:427:PRO:CD	2.77	0.47
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.13	0.47
5:R:8:ASP:HA	23:R:1229:PSC:C07	2.44	0.47
7:T:33:LEU:O	7:T:37:LEU:HB2	2.14	0.47
1:A:364:ASP:OD2	14:A:516:HEA:O1A	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:523:TGL:HA52	19:A:523:TGL:HB62	1.95	0.47
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.14	0.47
6:F:55:LYS:HA	6:F:74:LEU:O	2.14	0.47
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.39	0.47
26:G:269:CDL:H511	26:G:269:CDL:H202	1.96	0.46
19:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.97	0.46
14:N:515:HEA:H212	14:N:515:HEA:H271	1.73	0.46
26:C:270:CDL:H192	26:C:270:CDL:C64	2.45	0.46
26:T:1269:CDL:C17	29:T:4750:HOH:O	2.62	0.46
26:G:269:CDL:H241	26:G:269:CDL:H542	1.95	0.46
19:N:1522:TGL:HA82	12:Y:29:PHE:HZ	1.80	0.46
25:P:1264:PEK:C3	25:P:1264:PEK:H71	2.42	0.46
3:P:16:TRP:N	3:P:17:PRO:CD	2.79	0.46
1:N:195:LEU:HD23	1:N:245:ILE:HD13	1.96	0.46
25:P:1265:PEK:C37	26:T:1269:CDL:H273	2.44	0.46
21:B:1085:CHD:H212	21:B:1085:CHD:H12	1.96	0.46
23:B:229:PSC:H251	23:B:229:PSC:H221	1.59	0.46
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.80	0.46
19:N:1522:TGL:HC31	12:Y:14:SER:H	1.81	0.46
1:N:93:ALA:HA	1:N:171:MET:SD	2.56	0.46
1:N:172:LYS:HB2	1:N:172:LYS:HE2	1.76	0.46
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.51	0.46
1:A:378:HIS:HE1	14:A:515:HEA:C1A	2.29	0.46
3:C:54:MET:HE3	26:C:270:CDL:H612	1.97	0.46
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.98	0.46
1:N:21:LEU:HD23	19:N:1522:TGL:H211	1.97	0.46
19:O:1521:TGL:HA82	19:O:1521:TGL:H252	1.98	0.46
23:R:1229:PSC:H212	23:R:1229:PSC:C02	2.46	0.46
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.50	0.46
9:V:37:PHE:HA	9:V:41:GLU:HB2	1.97	0.46
19:B:521:TGL:H252	19:B:521:TGL:HA91	1.98	0.46
4:D:114:GLU:OE1	11:K:51:LYS:NZ	2.48	0.46
4:D:70:GLU:O	4:D:73:ARG:NH1	2.49	0.46
7:G:2:SER:OG	25:G:1263:PEK:C29	2.64	0.46
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.73	0.46
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.63	0.46
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.97	0.46
5:R:80:GLU:CD	5:R:80:GLU:H	2.19	0.46
7:G:17:ARG:CD	29:G:2446:HOH:O	2.64	0.46
7:G:5:LYS:HD2	25:G:1263:PEK:C37	2.36	0.45
1:N:215:LEU:HD11	25:P:1264:PEK:H271	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:1229:PSC:H142	23:R:1229:PSC:H341	1.88	0.45
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.98	0.45
20:N:1524:PGV:H312	13:Z:16:ALA:HA	1.98	0.45
1:A:449:MET:SD	2:B:5:MET:HG2	2.56	0.45
20:C:267:PGV:H312	20:C:267:PGV:H282	1.72	0.45
7:G:11:TPO:CG2	7:G:11:TPO:O	2.65	0.45
20:N:1524:PGV:H92	4:Q:84:ALA:HB2	1.97	0.45
26:G:269:CDL:H152	1:N:307:SER:CB	2.46	0.45
2:O:226:MET:HG3	2:O:226:MET:O	2.16	0.45
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.48	0.45
19:N:1522:TGL:H251	19:N:1522:TGL:H282	1.62	0.45
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.51	0.45
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.45
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.47	0.45
1:N:378:HIS:O	1:N:382:SER:HB3	2.16	0.45
1:N:438:ARG:O	1:N:439:ARG:HB2	2.16	0.45
26:T:1269:CDL:H222	26:T:1269:CDL:H531	1.98	0.45
1:A:310:MET:CE	1:A:360:ASN:HD21	2.30	0.45
8:H:45:ALA:C	8:H:47:GLY:H	2.16	0.45
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.52	0.45
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.98	0.45
21:P:1271:CHD:C20	21:P:1271:CHD:O25	2.65	0.45
3:P:224:LYS:HD3	26:P:1270:CDL:HB31	1.98	0.45
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.99	0.45
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.99	0.45
1:N:321:PHE:CD2	23:R:1229:PSC:H341	2.52	0.45
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.98	0.45
7:T:37:LEU:HD23	26:T:1269:CDL:H361	1.99	0.45
1:A:334:TRP:HB2	19:A:523:TGL:HG11	1.99	0.45
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.99	0.45
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.54	0.45
26:P:1270:CDL:H532	26:P:1270:CDL:H561	1.59	0.45
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.30	0.44
10:J:7:GLU:HG3	29:J:4784:HOH:O	2.16	0.44
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.93	0.44
3:P:40:MET:O	3:P:44:MET:HG2	2.18	0.44
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.00	0.44
26:C:270:CDL:H192	26:C:270:CDL:C63	2.47	0.44
5:R:52:LEU:O	5:R:55:CYS:HB2	2.17	0.44
20:A:524:PGV:C1	20:A:524:PGV:O13	2.65	0.44
23:B:229:PSC:H042	29:E:2664:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:63:SER:O	5:R:67:ILE:HG13	2.18	0.44
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.98	0.44
25:G:265:PEK:H371	26:G:269:CDL:C27	2.47	0.44
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.83	0.44
26:T:1269:CDL:H552	26:T:1269:CDL:H521	1.59	0.44
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.51	0.44
1:A:161:ALA:O	1:A:165:ILE:HG13	2.17	0.44
1:A:478:SER:HA	13:M:8:THR:O	2.18	0.44
19:N:1523:TGL:HC21	19:N:1523:TGL:CG1	2.23	0.44
25:G:265:PEK:C37	26:G:269:CDL:C27	2.95	0.44
7:T:8:HIS:ND1	25:T:263:PEK:H312	2.32	0.44
14:A:515:HEA:H212	14:A:515:HEA:H271	1.83	0.44
2:B:128:LEU:HD11	2:B:134:ARG:HA	2.00	0.44
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.36	0.44
3:P:34:TRP:HZ2	27:P:1272:DMU:H29	1.82	0.44
1:N:383:MET:O	1:N:387:PHE:HB2	2.17	0.44
12:Y:20:ARG:NH2	12:Y:24:MET:SD	2.91	0.44
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.99	0.43
1:A:309:THR:HG22	14:A:516:HEA:HMB2	2.00	0.43
12:L:2:HIS:CG	12:L:3:TYR:H	2.36	0.43
26:T:1269:CDL:H592	26:T:1269:CDL:H561	1.29	0.43
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.53	0.43
5:E:105:GLY:O	5:E:108:LYS:HG2	2.17	0.43
4:Q:68:PHE:HA	4:Q:71:MET:HG2	1.99	0.43
23:B:229:PSC:H081	5:E:8:ASP:OD1	2.18	0.43
19:B:521:TGL:HC22	29:I:2606:HOH:O	2.17	0.43
2:B:87:MET:HE2	29:B:4459:HOH:O	2.16	0.43
6:F:92:VAL:O	6:F:92:VAL:HG23	2.18	0.43
2:O:15:PRO:HD2	29:O:3080:HOH:O	2.19	0.43
3:P:156:ARG:HE	21:P:1271:CHD:C24	2.31	0.43
7:G:2:SER:OG	25:G:1263:PEK:H291	2.18	0.43
12:L:26:THR:CG2	29:L:4690:HOH:O	2.67	0.43
1:N:115:SER:O	1:N:121:GLY:HA2	2.19	0.43
26:P:1270:CDL:H232	26:P:1270:CDL:H262	1.64	0.43
4:Q:34:SER:O	4:Q:38:LYS:HG3	2.19	0.43
26:T:1269:CDL:H252	26:T:1269:CDL:H221	1.61	0.43
7:T:2:SER:CB	25:T:263:PEK:H301	2.47	0.43
1:A:1:FME:CE	1:A:4:ASN:HD22	2.31	0.43
26:G:269:CDL:H451	2:O:70:ALA:HB1	2.00	0.43
2:O:36:SER:HB3	19:O:1521:TGL:H131	2.01	0.43
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:LYS:O	8:U:10:ASN:CB	2.67	0.43
14:A:515:HEA:H122	29:A:2378:HOH:O	2.19	0.43
2:O:116:LEU:HD12	2:O:117:SER:N	2.33	0.43
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.40	0.43
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.00	0.43
14:A:515:HEA:HHD	14:A:515:HEA:HAC	1.90	0.43
14:A:516:HEA:ND	16:A:520:CMO:C	2.82	0.43
7:G:8:HIS:O	7:G:9:GLY:C	2.57	0.43
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.67	0.43
1:N:85:LEU:HB3	1:N:493:GLU:HA	2.00	0.43
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.54	0.43
25:P:1265:PEK:H311	25:P:1265:PEK:H282	1.92	0.43
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.99	0.43
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.16	0.43
1:A:33:LEU:HB3	1:A:61:HIS:HB2	2.00	0.43
20:C:268:PGV:H241	20:C:268:PGV:H11	2.00	0.43
25:G:265:PEK:H371	26:G:269:CDL:H273	2.00	0.43
1:N:240:HIS:C	1:N:240:HIS:CD2	2.92	0.43
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.99	0.43
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.01	0.43
1:N:484:THR:CG2	1:N:484:THR:CA	2.83	0.43
26:P:1270:CDL:H121	29:P:4619:HOH:O	2.18	0.43
3:P:202:GLY:HA3	25:P:1264:PEK:H21	2.01	0.43
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.19	0.42
26:P:1270:CDL:HB22	26:P:1270:CDL:OA5	2.19	0.42
26:C:270:CDL:CB2	26:C:270:CDL:PA1	3.06	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.42
4:Q:91:PHE:O	4:Q:94:LEU:HB2	2.19	0.42
7:T:33:LEU:HD13	7:T:37:LEU:HD22	2.01	0.42
2:B:116:LEU:CD1	2:B:226:MET:HB3	2.49	0.42
25:G:265:PEK:H383	26:G:269:CDL:C27	2.32	0.42
5:R:78:HIS:CD2	9:V:12:LEU:HD13	2.54	0.42
1:A:222:PRO:HD2	29:B:4745:HOH:O	2.18	0.42
1:A:378:HIS:CE1	14:A:515:HEA:C1A	3.03	0.42
2:B:166:PRO:CG	29:B:2318:HOH:O	2.68	0.42
8:H:78:GLU:HG2	8:H:78:GLU:O	2.18	0.42
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.01	0.42
7:T:38:HIS:HD1	7:T:38:HIS:N	2.18	0.42
8:U:9:LYS:CG	8:U:10:ASN:H	2.29	0.42
1:A:310:MET:HE2	1:A:356:ILE:HG23	2.01	0.42
1:A:377:PHE:O	1:A:381:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:O:1521:TGL:H101	19:O:1521:TGL:H281	2.02	0.42
6:S:92:VAL:CG2	6:S:92:VAL:O	2.67	0.42
19:A:523:TGL:HG31	29:D:4320:HOH:O	2.19	0.42
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.84	0.42
1:N:266:GLU:OE1	6:S:68:THR:OG1	2.28	0.42
4:Q:114:GLU:HG3	11:X:51:LYS:HZ2	1.84	0.42
19:A:523:TGL:CG3	29:D:4320:HOH:O	2.67	0.42
3:P:67:PHE:HA	10:W:9:GLN:HG2	2.01	0.42
14:A:516:HEA:HAA1	14:A:516:HEA:HMA	1.86	0.42
2:B:58:ALA:O	2:B:62:GLU:HG3	2.20	0.42
1:N:20:LEU:HB3	19:N:1522:TGL:H221	2.01	0.42
1:N:431:LEU:HD22	1:N:447:TYR:HB3	2.02	0.42
3:P:129:VAL:N	3:P:130:PRO:CD	2.83	0.42
21:P:1525:CHD:H112	21:P:1525:CHD:H12A	1.59	0.42
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.20	0.42
26:T:1269:CDL:OA7	26:T:1269:CDL:H342	2.20	0.42
1:A:310:MET:HE1	1:A:360:ASN:ND2	2.34	0.42
20:N:1266:PGV:H42	20:N:1266:PGV:H71	1.92	0.42
1:N:160:GLY:HA2	29:N:3450:HOH:O	2.20	0.42
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.18	0.42
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.51	0.41
20:A:524:PGV:O02	20:A:524:PGV:O13	2.37	0.41
19:B:521:TGL:HA72	19:B:521:TGL:H301	2.01	0.41
2:B:92:ASN:HA	2:B:93:PRO:HD2	1.83	0.41
12:L:46:LYS:O	12:L:47:LYS:HB2	2.20	0.41
20:N:1266:PGV:H302	29:P:4757:HOH:O	2.20	0.41
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.50	0.41
1:N:513:LEU:O	1:N:514:LYS:CB	2.60	0.41
3:P:173:PHE:CD2	3:P:173:PHE:C	2.94	0.41
10:W:3:ASN:OD1	10:W:3:ASN:C	2.58	0.41
1:A:337:ALA:HB2	1:A:394:VAL:HG23	2.01	0.41
20:A:524:PGV:H02	20:A:524:PGV:O14	2.21	0.41
3:C:16:TRP:N	3:C:17:PRO:CD	2.83	0.41
3:C:191:GLY:HA3	29:G:2132:HOH:O	2.20	0.41
7:G:17:ARG:HD3	29:G:2446:HOH:O	2.20	0.41
1:N:264:LYS:HE2	2:O:53:THR:HA	2.02	0.41
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.20	0.41
23:R:1229:PSC:H232	23:R:1229:PSC:H201	1.51	0.41
7:T:72:ASN:N	7:T:76:ASN:ND2	2.62	0.41
21:C:271:CHD:H212	21:C:271:CHD:O12	2.20	0.41
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:HD12	2:O:68:LEU:N	2.36	0.41
7:T:12:GLY:CA	29:T:3372:HOH:O	2.68	0.41
19:O:1521:TGL:H201	19:O:1521:TGL:C24	2.48	0.41
7:T:79:PRO:HD2	29:T:3063:HOH:O	2.19	0.41
4:Q:98:TRP:CD2	27:Z:1526:DMU:H10	2.55	0.41
1:A:472:ILE:HG21	19:L:522:TGL:HA91	2.02	0.41
19:O:1521:TGL:HC22	29:Q:3606:HOH:O	2.21	0.41
1:A:43:GLN:HB2	1:A:44:PRO:HD2	2.01	0.41
1:A:359:ALA:HA	14:A:516:HEA:OMA	2.20	0.41
7:G:3:ALA:HB1	25:G:1263:PEK:H382	2.03	0.41
2:O:225:SER:C	2:O:227:LEU:H	2.23	0.41
3:P:116:TRP:HA	3:P:117:PRO:C	2.40	0.41
4:Q:126:MET:HA	9:V:68:ILE:HD13	2.01	0.41
4:D:84:ALA:O	4:D:88:PHE:HD1	2.04	0.41
21:G:86:CHD:H212	21:G:86:CHD:H12	2.02	0.41
10:J:56:PRO:HB2	10:J:58:LYS:HD3	2.02	0.41
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.56	0.41
2:O:67:ILE:HD13	2:O:67:ILE:HA	1.93	0.41
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.56	0.41
20:P:1267:PGV:H12	20:P:1267:PGV:H152	1.64	0.41
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.53	0.41
7:T:3:ALA:HB3	25:T:263:PEK:H382	2.03	0.41
1:A:514:LYS:HA	6:F:38:ALA:CB	2.47	0.41
2:B:41:ILE:CD1	23:B:229:PSC:H342	2.44	0.41
12:L:14:SER:H	19:L:522:TGL:HC31	1.85	0.41
1:N:25:TRP:CE3	19:N:1522:TGL:HB91	2.56	0.41
1:N:68:PHE:HE2	1:N:112:LEU:HD12	1.85	0.41
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	0.41
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.63	0.41
5:R:105:GLY:O	5:R:108:LYS:HG2	2.20	0.41
1:A:512:ASN:HD22	1:A:512:ASN:HA	1.63	0.41
2:B:227:LEU:HA	2:B:227:LEU:HD23	1.84	0.41
1:A:190:ILE:H	1:A:190:ILE:HG13	1.64	0.40
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.79	0.40
26:C:270:CDL:H412	26:C:270:CDL:H382	1.75	0.40
4:Q:83:GLY:HA3	11:X:18:LEU:HA	2.03	0.40
7:T:35:SER:C	7:T:37:LEU:H	2.22	0.40
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.02	0.40
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.85	0.40
7:T:11:TPO:O	7:T:11:TPO:CG2	2.69	0.40
13:M:17:ILE:O	13:M:21:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:ARG:HD2	29:G:2446:HOH:O	2.21	0.40
7:G:58:LYS:HG3	7:G:59:PRO:HD2	2.04	0.40
1:N:254:ILE:HD12	1:N:341:ALA:HA	2.04	0.40
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.56	0.40
1:N:71:MET:N	1:N:72:PRO:CD	2.85	0.40
4:Q:41:LYS:HE3	4:Q:41:LYS:HB3	1.85	0.40
14:A:516:HEA:HBC1	14:A:516:HEA:HMC1	2.03	0.40
25:G:265:PEK:H301	2:O:66:THR:CG2	2.51	0.40
1:N:240:HIS:O	1:N:241:PRO:C	2.57	0.40
3:P:249:TRP:HD1	29:P:3165:HOH:O	2.04	0.40
7:T:12:GLY:HA3	29:T:3372:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	496 (97%)	16 (3%)	0	100	100
2	B	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	38	23
2	O	225/227 (99%)	215 (96%)	8 (4%)	2 (1%)	20	6
3	C	257/261 (98%)	250 (97%)	7 (3%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	38	23
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
5	E	103/109 (94%)	101 (98%)	1 (1%)	1 (1%)	18	5
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	18	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	5	0
7	G	81/85 (95%)	68 (84%)	5 (6%)	8 (10%)	1	0
7	T	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2	0
8	H	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	0
8	U	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	3 (4%)	1 (1%)	13	3
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	7	1
All	All	3504/3614 (97%)	3352 (96%)	121 (4%)	31 (1%)	20	6

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	39	SER
8	H	8	ILE
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
8	U	8	ILE
8	U	10	ASN
13	Z	41	LYS
2	B	60	GLU
7	G	6	GLY
7	G	8	HIS

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Mol	Chain	Res	Type
7	G	37	LEU
7	G	40	GLY
8	H	47	GLY
3	P	38	ASN
6	S	95	GLN
7	T	8	HIS
7	G	3	ALA
2	O	60	GLU
7	T	6	GLY
8	U	45	ALA
2	O	224	ALA
6	S	96	LEU
9	V	36	LYS
5	E	6	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	418 (98%)	8 (2%)	62	50
1	N	426/426 (100%)	414 (97%)	12 (3%)	49	34
2	B	210/210 (100%)	200 (95%)	10 (5%)	30	13
2	O	210/210 (100%)	194 (92%)	16 (8%)	15	4
3	C	224/226 (99%)	218 (97%)	6 (3%)	50	35
3	P	224/226 (99%)	216 (96%)	8 (4%)	40	23
4	D	128/129 (99%)	126 (98%)	2 (2%)	68	58
4	Q	128/129 (99%)	121 (94%)	7 (6%)	25	10
5	E	92/95 (97%)	90 (98%)	2 (2%)	57	44
5	R	92/95 (97%)	91 (99%)	1 (1%)	78	72
6	F	81/81 (100%)	78 (96%)	3 (4%)	39	22
6	S	81/81 (100%)	74 (91%)	7 (9%)	12	3
7	G	67/68 (98%)	59 (88%)	8 (12%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	61 (91%)	6 (9%)	11	3
8	H	71/75 (95%)	64 (90%)	7 (10%)	9	2
8	U	71/75 (95%)	64 (90%)	7 (10%)	9	2
9	I	57/57 (100%)	52 (91%)	5 (9%)	12	3
9	V	57/57 (100%)	54 (95%)	3 (5%)	26	11
10	J	49/50 (98%)	48 (98%)	1 (2%)	60	48
10	W	49/50 (98%)	47 (96%)	2 (4%)	35	18
11	K	39/46 (85%)	37 (95%)	2 (5%)	28	12
11	X	39/46 (85%)	37 (95%)	2 (5%)	28	12
12	L	39/40 (98%)	38 (97%)	1 (3%)	51	36
12	Y	39/40 (98%)	37 (95%)	2 (5%)	28	12
13	M	37/38 (97%)	30 (81%)	7 (19%)	2	0
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	1
All	All	3040/3082 (99%)	2900 (95%)	140 (5%)	31	15

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	180	GLN
1	A	264	LYS
1	A	290	HIS
1	A	338	MET
1	A	369	ASP
1	A	486	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
3	C	77	LYS

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Mol	Chain	Res	Type
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	31	LYS
4	D	51	LEU
5	E	31	LYS
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU
6	F	95	GLN
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	10	ASN
8	H	27	ARG
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	8	GLN
9	I	15	ARG
9	I	18	ARG
9	I	37	PHE
9	I	43	ARG
10	J	50	LEU
11	K	51	LYS
11	K	54	ARG
12	L	26	THR
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS

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Mol	Chain	Res	Type
13	M	43	SER
1	N	44	PRO
1	N	109	PHE
1	N	138	HIS
1	N	180	GLN
1	N	241	PRO
1	N	264	LYS
1	N	290	HIS
1	N	338	MET
1	N	369	ASP
1	N	484	THR
1	N	504	THR
1	N	512	ASN
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	86	MET
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	171	LYS
2	O	202	SER
2	O	205	SER
2	O	217	LYS
2	O	221	LYS
2	O	227	LEU
3	P	17	PRO
3	P	29	SER
3	P	73	PRO
3	P	77	LYS
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	10	ASP
4	Q	19	ARG
4	Q	31	LYS
4	Q	51	LEU

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Mol	Chain	Res	Type
4	Q	73	ARG
4	Q	121	LYS
5	R	79	LYS
6	S	37	LYS
6	S	48	LEU
6	S	64	GLU
6	S	80	GLN
6	S	87	THR
6	S	94	HIS
6	S	96	LEU
7	T	2	SER
7	T	17	ARG
7	T	18	PHE
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	12	GLN
8	U	27	ARG
8	U	29	CYS
8	U	41	LYS
8	U	52	VAL
8	U	60	TYR
8	U	61	LYS
9	V	2	THR
9	V	26	MET
9	V	61	GLU
10	W	4	ARG
10	W	50	LEU
11	X	47	ARG
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	39	ASN
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN

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Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	360	ASN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
4	D	29	HIS
4	D	37	GLN
4	D	143	ASN
5	E	94	ASN
7	G	76	ASN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	68	GLN
3	P	76	GLN
3	P	161	GLN
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
5	R	78	HIS
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
6	S	98	HIS
7	T	76	ASN
9	V	8	GLN

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Mol	Chain	Res	Type
9	V	70	GLN
10	W	57	HIS
11	X	35	GLN

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	1.40	2 (22%)	7,9,11	6.13	5 (71%)
2	FME	B	1	2	9,9,10	1.93	3 (33%)	7,9,11	6.21	4 (57%)
7	TPO	G	11	7	9,10,11	3.22	5 (55%)	10,14,16	1.53	2 (20%)
9	SAC	I	1	9	8,8,9	2.61	3 (37%)	6,9,11	0.98	0
1	FME	N	1	1	9,9,10	1.22	1 (11%)	7,9,11	6.01	2 (28%)
2	FME	O	1	2	9,9,10	1.24	1 (11%)	7,9,11	6.24	3 (42%)
7	TPO	T	11	7	9,10,11	2.97	5 (55%)	10,14,16	1.89	3 (30%)
9	SAC	V	1	9	8,8,9	4.18	3 (37%)	6,9,11	2.70	5 (83%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0

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

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.08	1.10	1.22
2	O	1	FME	O1-CN	-2.71	1.14	1.22
2	B	1	FME	CG-SD	-2.43	1.67	1.81
1	N	1	FME	O1-CN	-2.22	1.15	1.22
1	A	1	FME	O1-CN	-2.14	1.16	1.22
7	T	11	TPO	P-O2P	2.16	1.63	1.54
7	G	11	TPO	P-O3P	2.22	1.63	1.54
2	B	1	FME	CB-CG	2.25	1.60	1.51
7	G	11	TPO	P-O2P	2.43	1.64	1.54
7	T	11	TPO	P-O3P	2.69	1.65	1.54
9	I	1	SAC	CA-C	2.97	1.54	1.50
1	A	1	FME	CA-C	3.02	1.54	1.50
7	G	11	TPO	P-O1P	3.42	1.62	1.50
7	T	11	TPO	P-O1P	3.63	1.63	1.50
7	G	11	TPO	CA-C	4.33	1.55	1.50
9	I	1	SAC	CA-N	4.44	1.52	1.46
7	T	11	TPO	CA-C	4.54	1.56	1.50
9	I	1	SAC	OAC-C1A	4.63	1.34	1.23
7	T	11	TPO	P-OG1	4.91	1.68	1.59
9	V	1	SAC	OAC-C1A	6.05	1.37	1.23
7	G	11	TPO	P-OG1	6.56	1.71	1.59
9	V	1	SAC	CA-C	6.82	1.59	1.50
9	V	1	SAC	CA-N	6.95	1.56	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-15.70	98.67	122.82
1	N	1	FME	CA-N-CN	-15.42	99.10	122.82
2	B	1	FME	CA-N-CN	-15.42	99.11	122.82
1	A	1	FME	CA-N-CN	-14.65	100.30	122.82
2	B	1	FME	O1-CN-N	-3.66	115.00	125.20
1	A	1	FME	CG-CB-CA	-3.33	103.32	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	O-C-CA	-3.30	117.45	125.15
9	V	1	SAC	OAC-C1A-C2A	-3.07	116.47	122.06
7	T	11	TPO	O-C-CA	-3.04	118.07	125.15
7	G	11	TPO	O-C-CA	-2.90	118.38	125.15
2	O	1	FME	CG-CB-CA	-2.87	104.66	112.97
2	B	1	FME	CB-CG-SD	-2.84	99.68	113.26
9	V	1	SAC	CB-CA-N	-2.49	104.80	110.60
1	A	1	FME	O-C-CA	-2.33	119.72	125.15
2	B	1	FME	CG-CB-CA	-2.04	107.07	112.97
1	A	1	FME	CB-CA-C	2.00	114.95	111.65
7	T	11	TPO	O3P-P-OG1	2.03	115.24	106.00
9	V	1	SAC	OG-CB-CA	2.18	116.55	111.02
7	G	11	TPO	O2P-P-OG1	2.52	117.46	106.00
1	N	1	FME	O1-CN-N	2.71	132.75	125.20
2	O	1	FME	O1-CN-N	2.84	133.11	125.20
9	V	1	SAC	OAC-C1A-N	3.47	128.60	121.92
7	T	11	TPO	CG2-CB-CA	4.42	121.41	113.22
1	A	1	FME	CE-SD-CG	5.26	119.22	100.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1	SAC	CB-CA-N-C1A
2	B	1	FME	O1-CN-N-CA
1	N	1	FME	O1-CN-N-CA
1	A	1	FME	O1-CN-N-CA
2	O	1	FME	O1-CN-N-CA

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
7	G	11	TPO	2	0
7	T	11	TPO	2	0
9	V	1	SAC	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	515	1	44,67,67	1.48	9 (20%)	37,103,103	3.91	18 (48%)
14	HEA	A	516	1	44,67,67	2.55	8 (18%)	37,103,103	3.14	14 (37%)
16	CMO	A	520	15	0,1,1	0.00	-	0,0,0	0.00	-
20	PGV	A	521	-	50,50,50	1.32	5 (10%)	51,56,56	1.70	13 (25%)
19	TGL	A	523	-	62,62,62	1.45	7 (11%)	65,65,65	1.47	11 (16%)
20	PGV	A	524	-	50,50,50	1.41	4 (8%)	51,56,56	1.55	9 (17%)
21	CHD	A	525	-	29,32,32	1.62	7 (24%)	47,51,51	5.64	34 (72%)
21	CHD	B	1085	-	29,32,32	1.76	8 (27%)	47,51,51	5.79	32 (68%)
22	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	PSC	B	229	-	51,51,51	1.36	3 (5%)	56,59,59	1.32	6 (10%)
19	TGL	B	521	-	62,62,62	1.34	6 (9%)	65,65,65	2.06	15 (23%)
25	PEK	C	264	-	52,52,52	1.01	1 (1%)	54,57,57	1.84	14 (25%)
20	PGV	C	267	-	50,50,50	0.97	2 (4%)	51,56,56	1.60	10 (19%)
20	PGV	C	268	-	50,50,50	1.34	2 (4%)	51,56,56	1.63	7 (13%)
26	CDL	C	270	-	99,99,99	1.44	12 (12%)	101,111,111	1.57	17 (16%)
21	CHD	C	271	-	29,32,32	0.84	0	47,51,51	5.02	28 (59%)
27	DMU	C	272	-	34,34,34	1.99	5 (14%)	45,45,45	3.41	24 (53%)
25	PEK	G	1263	-	52,52,52	1.39	4 (7%)	54,57,57	1.56	5 (9%)
20	PGV	G	1268	-	50,50,50	1.41	3 (6%)	51,56,56	1.89	9 (17%)
25	PEK	G	265	-	52,52,52	1.46	5 (9%)	54,57,57	1.52	6 (11%)
26	CDL	G	269	-	99,99,99	1.62	16 (16%)	101,111,111	1.70	20 (19%)
21	CHD	G	86	-	29,32,32	1.50	6 (20%)	47,51,51	5.49	35 (74%)
21	CHD	J	60	-	29,32,32	1.41	5 (17%)	47,51,51	5.17	31 (65%)
19	TGL	L	522	-	62,62,62	1.60	10 (16%)	65,65,65	2.23	18 (27%)
27	DMU	M	526	-	34,34,34	0.91	1 (2%)	45,45,45	3.51	29 (64%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	N	1266	-	50,50,50	1.26	5 (10%)	51,56,56	1.73	12 (23%)
19	TGL	N	1522	-	62,62,62	1.83	10 (16%)	65,65,65	2.04	18 (27%)
19	TGL	N	1523	-	62,62,62	1.46	6 (9%)	65,65,65	1.67	12 (18%)
20	PGV	N	1524	-	50,50,50	1.22	2 (4%)	51,56,56	1.53	8 (15%)
14	HEA	N	515	1	44,67,67	1.31	4 (9%)	37,103,103	3.19	19 (51%)
14	HEA	N	516	1	44,67,67	1.42	9 (20%)	37,103,103	2.69	13 (35%)
16	CMO	N	520	15	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	O	1521	-	62,62,62	1.36	6 (9%)	65,65,65	1.89	10 (15%)
22	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
25	PEK	P	1264	-	52,52,52	0.95	4 (7%)	54,57,57	1.84	11 (20%)
25	PEK	P	1265	-	52,52,52	1.38	4 (7%)	54,57,57	1.51	6 (11%)
20	PGV	P	1267	-	50,50,50	0.92	2 (4%)	51,56,56	1.52	8 (15%)
26	CDL	P	1270	-	99,99,99	1.42	15 (15%)	101,111,111	1.61	22 (21%)
21	CHD	P	1271	-	29,32,32	0.85	1 (3%)	47,51,51	4.90	33 (70%)
27	DMU	P	1272	-	34,34,34	2.38	7 (20%)	45,45,45	3.45	23 (51%)
21	CHD	P	1525	-	29,32,32	1.27	5 (17%)	47,51,51	5.93	37 (78%)
23	PSC	R	1229	-	51,51,51	1.39	5 (9%)	56,59,59	1.31	5 (8%)
26	CDL	T	1269	-	99,99,99	1.41	13 (13%)	101,111,111	1.62	18 (17%)
25	PEK	T	263	-	52,52,52	1.50	6 (11%)	54,57,57	1.55	9 (16%)
21	CHD	W	1059	-	29,32,32	1.43	6 (20%)	47,51,51	5.37	32 (68%)
27	DMU	Z	1526	-	34,34,34	1.07	2 (5%)	45,45,45	3.31	22 (48%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	516	1	3/3/7/16	0/24/76/76	0/0/8/8
16	CMO	A	520	15	-	0/0/0/0	0/0/0/0
20	PGV	A	521	-	-	0/55/55/55	0/0/0/0
19	TGL	A	523	-	-	0/65/65/65	0/0/0/0
20	PGV	A	524	-	-	1/55/55/55	0/0/0/0
21	CHD	A	525	-	-	0/7/74/74	0/4/4/4
21	CHD	B	1085	-	-	0/7/74/74	0/4/4/4
22	CUA	B	228	2	-	0/0/0/0	0/0/0/0
23	PSC	B	229	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	B	521	-	-	0/65/65/65	0/0/0/0
25	PEK	C	264	-	-	0/56/56/56	0/0/0/0
20	PGV	C	267	-	-	0/55/55/55	0/0/0/0
20	PGV	C	268	-	-	0/55/55/55	0/0/0/0
26	CDL	C	270	-	-	0/110/110/110	0/0/0/0
21	CHD	C	271	-	2/2/12/12	0/7/74/74	0/4/4/4
27	DMU	C	272	-	5/5/10/10	0/19/59/59	0/2/2/2
25	PEK	G	1263	-	-	0/56/56/56	0/0/0/0
20	PGV	G	1268	-	-	0/55/55/55	0/0/0/0
25	PEK	G	265	-	-	0/56/56/56	0/0/0/0
26	CDL	G	269	-	-	0/110/110/110	0/0/0/0
21	CHD	G	86	-	-	0/7/74/74	0/4/4/4
21	CHD	J	60	-	1/1/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
27	DMU	M	526	-	5/5/10/10	0/19/59/59	0/2/2/2
20	PGV	N	1266	-	-	0/55/55/55	0/0/0/0
19	TGL	N	1522	-	-	0/65/65/65	0/0/0/0
19	TGL	N	1523	-	-	0/65/65/65	0/0/0/0
20	PGV	N	1524	-	-	2/55/55/55	0/0/0/0
14	HEA	N	515	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	N	516	1	3/3/7/16	0/24/76/76	0/0/8/8
16	CMO	N	520	15	-	0/0/0/0	0/0/0/0
19	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
22	CUA	O	228	2	-	0/0/0/0	0/0/0/0
25	PEK	P	1264	-	-	0/56/56/56	0/0/0/0
25	PEK	P	1265	-	-	0/56/56/56	0/0/0/0
20	PGV	P	1267	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
21	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
27	DMU	P	1272	-	5/5/10/10	0/19/59/59	0/2/2/2
21	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
23	PSC	R	1229	-	-	0/55/55/55	0/0/0/0
26	CDL	T	1269	-	-	0/110/110/110	0/0/0/0
25	PEK	T	263	-	-	0/56/56/56	0/0/0/0
21	CHD	W	1059	-	1/1/12/12	0/7/74/74	0/4/4/4
27	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1085	CHD	C10-C5	-4.33	1.48	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	515	HEA	C1A-NA	-4.19	1.31	1.36
14	A	516	HEA	CAA-C2A	-3.72	1.45	1.52
21	B	1085	CHD	C13-C14	-3.67	1.49	1.55
19	L	522	TGL	C10-CB9	-3.61	1.31	1.51
26	P	1270	CDL	C59-C58	-3.50	1.31	1.51
26	C	270	CDL	C59-C58	-3.47	1.31	1.51
19	L	522	TGL	C20-CA9	-3.44	1.32	1.51
26	G	269	CDL	C59-C58	-3.41	1.32	1.51
19	N	1522	TGL	C10-CB9	-3.41	1.32	1.51
26	T	1269	CDL	C59-C58	-3.37	1.32	1.51
19	N	1522	TGL	C20-CA9	-3.34	1.32	1.51
26	C	270	CDL	C62-C61	-3.28	1.32	1.51
14	N	515	HEA	CAA-C2A	-3.18	1.46	1.52
26	T	1269	CDL	C62-C61	-3.17	1.33	1.51
19	O	1521	TGL	C10-CB9	-3.10	1.33	1.51
26	T	1269	CDL	C42-C41	-3.09	1.34	1.51
27	Z	1526	DMU	C3-C4	-3.06	1.44	1.52
26	C	270	CDL	C79-C78	-3.06	1.34	1.51
21	G	86	CHD	C10-C5	-3.05	1.50	1.55
26	P	1270	CDL	C62-C61	-3.05	1.34	1.51
19	B	521	TGL	C20-CA9	-2.99	1.34	1.51
27	M	526	DMU	C3-C4	-2.95	1.45	1.52
26	P	1270	CDL	C19-C18	-2.95	1.34	1.51
19	N	1523	TGL	C10-CB9	-2.94	1.34	1.51
21	B	1085	CHD	C8-C14	-2.94	1.48	1.53
26	G	269	CDL	C62-C61	-2.93	1.34	1.51
26	C	270	CDL	C19-C18	-2.93	1.34	1.51
26	P	1270	CDL	C79-C78	-2.87	1.35	1.51
26	G	269	CDL	C39-C38	-2.85	1.35	1.51
26	G	269	CDL	C42-C41	-2.85	1.35	1.51
21	A	525	CHD	C11-C12	-2.85	1.48	1.53
19	A	523	TGL	C10-CB9	-2.84	1.35	1.51
26	P	1270	CDL	C22-C21	-2.82	1.35	1.51
19	A	523	TGL	C15-CC9	-2.80	1.35	1.51
26	T	1269	CDL	C79-C78	-2.80	1.35	1.51
14	N	516	HEA	C4B-NB	-2.79	1.33	1.36
19	N	1523	TGL	C20-CA9	-2.77	1.35	1.51
21	G	86	CHD	C15-C14	-2.76	1.48	1.54
26	C	270	CDL	C39-C38	-2.74	1.36	1.51
19	N	1523	TGL	C15-CC9	-2.73	1.36	1.51
19	A	523	TGL	C20-CA9	-2.72	1.36	1.51
25	P	1264	PEK	O03-C01	-2.72	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	525	CHD	C1-C10	-2.71	1.49	1.54
26	P	1270	CDL	C82-C81	-2.68	1.36	1.51
19	B	521	TGL	C10-CB9	-2.66	1.36	1.51
26	C	270	CDL	C22-C21	-2.66	1.36	1.51
19	O	1521	TGL	C20-CA9	-2.66	1.36	1.51
14	N	515	HEA	C3C-CAC	-2.65	1.42	1.47
26	C	270	CDL	C82-C81	-2.63	1.36	1.51
20	A	521	PGV	O01-C02	-2.60	1.39	1.46
26	T	1269	CDL	C39-C38	-2.59	1.36	1.51
26	T	1269	CDL	C19-C18	-2.58	1.36	1.51
21	A	525	CHD	C6-C7	-2.58	1.48	1.52
21	P	1525	CHD	C6-C7	-2.58	1.48	1.52
26	G	269	CDL	C22-C21	-2.57	1.36	1.51
25	P	1264	PEK	O01-C02	-2.53	1.40	1.46
26	G	269	CDL	C82-C81	-2.52	1.37	1.51
26	G	269	CDL	C19-C18	-2.47	1.37	1.51
19	O	1521	TGL	C15-CC9	-2.40	1.37	1.51
26	P	1270	CDL	C39-C38	-2.39	1.37	1.51
26	T	1269	CDL	C82-C81	-2.38	1.38	1.51
14	A	515	HEA	C3B-C2B	-2.38	1.33	1.41
19	L	522	TGL	C15-CC9	-2.37	1.38	1.51
26	G	269	CDL	C79-C78	-2.36	1.38	1.51
26	T	1269	CDL	C22-C21	-2.35	1.38	1.51
26	C	270	CDL	C42-C41	-2.35	1.38	1.51
19	N	1522	TGL	C15-CC9	-2.34	1.38	1.51
14	A	515	HEA	CAA-C2A	-2.32	1.48	1.52
21	G	86	CHD	C1-C10	-2.31	1.49	1.54
21	B	1085	CHD	C13-C12	-2.30	1.50	1.54
21	A	525	CHD	C10-C5	-2.28	1.51	1.55
26	P	1270	CDL	C42-C41	-2.26	1.38	1.51
21	P	1525	CHD	C1-C10	-2.20	1.50	1.54
19	B	521	TGL	C15-CC9	-2.15	1.39	1.51
21	A	525	CHD	C15-C14	-2.12	1.49	1.54
21	B	1085	CHD	C20-C17	-2.07	1.50	1.54
21	P	1525	CHD	C13-C12	-2.06	1.51	1.54
25	G	265	PEK	C03-C02	2.00	1.56	1.50
26	P	1270	CDL	CA6-CA4	2.00	1.56	1.50
27	P	1272	DMU	O7-C10	2.01	1.47	1.41
20	A	524	PGV	P-O11	2.01	1.67	1.59
27	C	272	DMU	C8-C7	2.01	1.57	1.52
14	N	516	HEA	C4A-NA	2.01	1.39	1.36
21	J	60	CHD	C20-C17	2.02	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	60	CHD	C8-C7	2.03	1.57	1.53
23	R	1229	PSC	P-O12	2.03	1.67	1.59
21	P	1271	CHD	C11-C9	2.03	1.57	1.53
25	T	263	PEK	P-O12	2.04	1.67	1.59
19	L	522	TGL	OG2-CG2	2.04	1.51	1.46
27	P	1272	DMU	O7-C3	2.05	1.48	1.43
20	N	1266	PGV	C5-C4	2.06	1.63	1.51
21	P	1525	CHD	O12-C12	2.06	1.47	1.43
14	A	515	HEA	C13-C14	2.06	1.57	1.50
27	P	1272	DMU	C8-C7	2.07	1.57	1.52
26	P	1270	CDL	PB2-OB3	2.08	1.58	1.50
21	W	1059	CHD	C20-C17	2.09	1.58	1.54
21	W	1059	CHD	C8-C7	2.09	1.57	1.53
21	J	60	CHD	C8-C14	2.10	1.58	1.53
21	W	1059	CHD	C8-C14	2.11	1.58	1.53
21	B	1085	CHD	O12-C12	2.13	1.47	1.43
14	N	516	HEA	C20-C19	2.15	1.56	1.51
26	T	1269	CDL	CB6-CB4	2.17	1.56	1.50
21	G	86	CHD	C11-C9	2.20	1.57	1.53
14	A	515	HEA	O11-C11	2.21	1.48	1.42
14	N	516	HEA	C18-C19	2.21	1.38	1.33
14	A	515	HEA	C4B-NB	2.21	1.39	1.36
20	A	524	PGV	C03-C02	2.22	1.57	1.50
19	A	523	TGL	OB1-CB1	2.23	1.29	1.22
27	C	272	DMU	C2-C1	2.23	1.58	1.52
21	P	1525	CHD	C16-C15	2.23	1.60	1.54
14	A	515	HEA	C1D-ND	2.26	1.39	1.36
21	B	1085	CHD	C18-C13	2.26	1.58	1.54
20	N	1266	PGV	C3-C2	2.27	1.60	1.52
20	A	521	PGV	C01-C02	2.28	1.57	1.50
20	A	521	PGV	C3-C2	2.29	1.60	1.52
26	G	269	CDL	C17-C16	2.32	1.64	1.51
19	L	522	TGL	CG3-CG2	2.32	1.57	1.50
14	N	516	HEA	C14-C15	2.32	1.38	1.33
25	P	1264	PEK	C2-C1	2.33	1.57	1.50
26	P	1270	CDL	PB2-OB2	2.34	1.69	1.59
14	N	515	HEA	CMD-C2D	2.35	1.56	1.51
19	N	1522	TGL	CC2-CC1	2.36	1.57	1.50
20	P	1267	PGV	O01-C1	2.36	1.41	1.34
25	P	1264	PEK	O01-C1	2.38	1.41	1.34
20	G	1268	PGV	P-O11	2.38	1.69	1.59
21	W	1059	CHD	C11-C12	2.39	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	265	PEK	P-O12	2.40	1.69	1.59
27	P	1272	DMU	C2-C1	2.45	1.58	1.52
19	N	1522	TGL	OG2-CG2	2.46	1.53	1.46
21	J	60	CHD	C8-C9	2.46	1.58	1.53
26	G	269	CDL	C11-CA5	2.46	1.57	1.50
23	R	1229	PSC	C2-C1	2.47	1.57	1.50
25	T	263	PEK	P-O11	2.48	1.69	1.59
21	W	1059	CHD	C8-C9	2.52	1.58	1.53
25	G	1263	PEK	P-O11	2.54	1.70	1.59
25	T	263	PEK	C01-C02	2.55	1.57	1.50
19	N	1522	TGL	CG1-CG2	2.60	1.58	1.50
25	P	1265	PEK	P-O12	2.61	1.70	1.59
14	A	516	HEA	C14-C15	2.61	1.39	1.33
25	G	1263	PEK	C03-C02	2.61	1.58	1.50
21	G	86	CHD	O12-C12	2.62	1.48	1.43
25	P	1265	PEK	P-O11	2.63	1.70	1.59
14	N	516	HEA	O11-C11	2.69	1.49	1.42
19	L	522	TGL	CG1-CG2	2.70	1.58	1.50
14	N	516	HEA	C3C-C2C	2.76	1.44	1.40
21	G	86	CHD	O7-C7	2.78	1.49	1.43
25	G	265	PEK	P-O11	2.79	1.71	1.59
25	T	263	PEK	C03-C02	2.80	1.58	1.50
19	L	522	TGL	CC2-CC1	2.82	1.58	1.50
14	N	516	HEA	C4C-CHD	2.82	1.47	1.40
20	C	267	PGV	O01-C1	2.87	1.42	1.34
19	N	1522	TGL	CG3-CG2	2.90	1.58	1.50
21	A	525	CHD	C18-C13	2.92	1.59	1.54
14	A	516	HEA	OMA-CMA	3.04	1.32	1.21
14	A	515	HEA	C3C-C2C	3.09	1.44	1.40
14	N	516	HEA	C1C-CHC	3.11	1.48	1.40
14	A	515	HEA	C12-C13	3.15	1.63	1.53
20	C	267	PGV	O03-C19	3.28	1.43	1.33
27	Z	1526	DMU	O16-C6	3.37	1.46	1.40
19	L	522	TGL	OG3-CC1	3.37	1.43	1.33
26	G	269	CDL	C15-C14	3.38	1.70	1.51
21	J	60	CHD	C11-C9	3.42	1.59	1.53
20	P	1267	PGV	O03-C19	3.59	1.43	1.33
27	P	1272	DMU	O1-C10	3.72	1.51	1.41
21	B	1085	CHD	C1-C2	3.73	1.61	1.53
27	C	272	DMU	O1-C10	3.73	1.51	1.41
20	N	1266	PGV	C01-C02	3.76	1.61	1.50
14	A	516	HEA	C3C-C2C	3.76	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	525	CHD	O12-C12	3.83	1.50	1.43
19	B	521	TGL	OG3-CC1	3.89	1.44	1.33
14	A	516	HEA	C1D-ND	3.89	1.41	1.36
26	C	270	CDL	OB6-CB5	3.89	1.45	1.34
20	N	1524	PGV	O01-C1	3.90	1.45	1.34
26	P	1270	CDL	OB8-CB7	3.90	1.44	1.33
14	A	515	HEA	C4C-CHD	3.94	1.50	1.40
27	C	272	DMU	O16-C6	4.07	1.47	1.40
26	P	1270	CDL	OA6-CA5	4.12	1.46	1.34
21	W	1059	CHD	C11-C9	4.13	1.60	1.53
26	C	270	CDL	OA6-CA5	4.13	1.46	1.34
23	B	229	PSC	C13-C12	4.15	1.55	1.31
20	N	1266	PGV	O01-C1	4.16	1.46	1.34
20	G	1268	PGV	O03-C19	4.16	1.45	1.33
26	T	1269	CDL	OB8-CB7	4.19	1.45	1.33
20	C	268	PGV	O03-C19	4.26	1.45	1.33
20	A	521	PGV	O03-C19	4.27	1.45	1.33
26	C	270	CDL	OB8-CB7	4.32	1.46	1.33
26	P	1270	CDL	OB6-CB5	4.33	1.46	1.34
26	G	269	CDL	C16-C15	4.34	1.76	1.51
23	R	1229	PSC	C13-C12	4.38	1.56	1.31
25	C	264	PEK	O01-C1	4.41	1.47	1.34
19	O	1521	TGL	OG1-CA1	4.43	1.46	1.33
20	N	1266	PGV	O03-C19	4.45	1.46	1.33
27	P	1272	DMU	O16-C6	4.46	1.48	1.40
19	B	521	TGL	OG2-CB1	4.52	1.47	1.34
23	R	1229	PSC	O03-C19	4.59	1.46	1.33
20	A	524	PGV	O01-C1	4.62	1.47	1.34
19	A	523	TGL	OG3-CC1	4.63	1.47	1.33
23	B	229	PSC	O01-C1	4.66	1.47	1.34
19	O	1521	TGL	OG3-CC1	4.66	1.47	1.33
26	G	269	CDL	OB8-CB7	4.72	1.47	1.33
23	R	1229	PSC	O01-C1	4.73	1.48	1.34
19	A	523	TGL	OG1-CA1	4.78	1.47	1.33
26	T	1269	CDL	OB6-CB5	4.83	1.48	1.34
19	N	1523	TGL	OG1-CA1	4.83	1.47	1.33
19	N	1523	TGL	OG3-CC1	4.89	1.47	1.33
26	G	269	CDL	OA8-CA7	4.90	1.47	1.33
25	G	1263	PEK	O01-C1	4.92	1.48	1.34
23	B	229	PSC	O03-C19	4.92	1.47	1.33
20	N	1524	PGV	O03-C19	5.00	1.48	1.33
26	T	1269	CDL	OA6-CA5	5.05	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	1269	CDL	OA8-CA7	5.12	1.48	1.33
19	N	1522	TGL	OG3-CC1	5.12	1.48	1.33
25	T	263	PEK	O01-C1	5.16	1.49	1.34
25	P	1265	PEK	O01-C1	5.20	1.49	1.34
25	P	1265	PEK	O03-C21	5.22	1.48	1.33
19	L	522	TGL	OG1-CA1	5.23	1.48	1.33
19	O	1521	TGL	OG2-CB1	5.29	1.49	1.34
20	A	521	PGV	O01-C1	5.36	1.49	1.34
26	G	269	CDL	OB6-CB5	5.38	1.49	1.34
25	G	265	PEK	O01-C1	5.46	1.50	1.34
20	A	524	PGV	O03-C19	5.47	1.49	1.33
26	P	1270	CDL	OA8-CA7	5.56	1.49	1.33
19	B	521	TGL	OG1-CA1	5.57	1.49	1.33
19	A	523	TGL	OG2-CB1	5.59	1.50	1.34
26	G	269	CDL	OA6-CA5	5.62	1.50	1.34
19	N	1523	TGL	OG2-CB1	5.75	1.51	1.34
25	G	265	PEK	O03-C21	5.83	1.50	1.33
25	G	1263	PEK	O03-C21	5.86	1.50	1.33
14	A	516	HEA	CMB-C2B	5.87	1.63	1.51
26	C	270	CDL	OA8-CA7	6.00	1.51	1.33
20	C	268	PGV	O01-C1	6.22	1.52	1.34
19	L	522	TGL	OG2-CB1	6.41	1.52	1.34
25	T	263	PEK	O03-C21	6.66	1.53	1.33
19	N	1522	TGL	OG1-CA1	6.69	1.53	1.33
20	G	1268	PGV	O01-C1	7.10	1.54	1.34
14	A	516	HEA	C3A-C2A	7.38	1.50	1.40
19	N	1522	TGL	OG2-CB1	7.48	1.56	1.34
27	C	272	DMU	O55-C2	8.42	1.62	1.43
14	A	516	HEA	CMD-C2D	10.35	1.73	1.51
27	P	1272	DMU	O55-C2	10.74	1.67	1.43

All (723) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	C13-C12-C11	-15.12	91.56	114.46
21	B	1085	CHD	C18-C13-C12	-11.59	97.29	109.08
21	A	525	CHD	C19-C10-C9	-11.30	94.99	111.16
21	G	86	CHD	C18-C13-C12	-11.17	97.71	109.08
21	B	1085	CHD	C19-C10-C9	-11.04	95.36	111.16
14	N	515	HEA	C13-C12-C11	-10.93	97.91	114.46
21	G	86	CHD	C19-C10-C9	-10.85	95.64	111.16
21	P	1525	CHD	C18-C13-C12	-9.92	98.98	109.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	525	CHD	O12-C12-C13	-8.94	96.20	111.12
19	L	522	TGL	OG3-CC1-OC1	-8.69	101.97	123.55
21	A	525	CHD	C23-C22-C20	-8.48	103.29	114.72
21	P	1525	CHD	C19-C10-C9	-8.42	99.12	111.16
21	B	1085	CHD	C18-C13-C17	-7.94	98.69	111.23
21	W	1059	CHD	C6-C5-C4	-7.49	102.63	111.13
21	G	86	CHD	C6-C5-C4	-7.48	102.64	111.13
14	A	516	HEA	C20-C19-C18	-7.07	106.63	121.10
21	G	86	CHD	O12-C12-C13	-7.03	99.39	111.12
21	P	1525	CHD	C18-C13-C14	-6.81	100.47	111.23
21	B	1085	CHD	C6-C5-C4	-6.81	103.40	111.13
21	A	525	CHD	C6-C5-C4	-6.74	103.48	111.13
21	C	271	CHD	C19-C10-C1	-6.70	97.23	108.24
21	P	1525	CHD	C6-C5-C4	-6.69	103.53	111.13
21	A	525	CHD	C18-C13-C14	-6.68	100.68	111.23
14	A	515	HEA	CAA-CBA-CGA	-6.28	101.93	112.66
14	N	515	HEA	C1B-C2B-C3B	-6.22	102.67	107.00
21	P	1525	CHD	C22-C20-C17	-6.10	97.44	110.26
21	W	1059	CHD	C18-C13-C12	-5.85	103.12	109.08
14	N	516	HEA	C13-C12-C11	-5.85	105.60	114.46
21	P	1525	CHD	C19-C10-C5	-5.72	100.44	110.30
19	N	1523	TGL	CG3-CG2-CG1	-5.68	99.05	111.86
25	P	1264	PEK	O03-C01-C02	-5.65	94.46	108.66
20	N	1266	PGV	O01-C1-O02	-5.61	109.69	123.68
14	A	515	HEA	C26-C15-C14	-5.60	108.74	123.69
27	M	526	DMU	O7-C10-C5	-5.60	95.50	108.11
14	A	515	HEA	C20-C19-C18	-5.59	109.65	121.10
14	A	515	HEA	CAD-CBD-CGD	-5.56	103.15	112.66
14	A	516	HEA	C13-C12-C11	-5.55	106.06	114.46
21	J	60	CHD	C6-C5-C4	-5.54	104.84	111.13
14	N	516	HEA	OMA-CMA-C3A	-5.52	112.40	125.08
21	C	271	CHD	C6-C5-C4	-5.50	104.88	111.13
21	G	86	CHD	C18-C13-C14	-5.49	102.55	111.23
21	A	525	CHD	C18-C13-C12	-5.43	103.55	109.08
14	N	516	HEA	CMC-C2C-C1C	-5.34	120.26	128.46
21	B	1085	CHD	O12-C12-C13	-5.32	102.23	111.12
21	A	525	CHD	C22-C20-C17	-5.29	99.14	110.26
21	J	60	CHD	C18-C13-C12	-5.27	103.71	109.08
25	P	1264	PEK	O01-C1-O02	-5.17	110.78	123.68
14	A	515	HEA	C1B-C2B-C3B	-5.16	103.41	107.00
14	N	515	HEA	CAD-CBD-CGD	-5.04	104.05	112.66
21	P	1271	CHD	C19-C10-C1	-4.87	100.25	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1085	CHD	O7-C7-C6	-4.75	98.53	110.02
21	P	1525	CHD	O7-C7-C6	-4.63	98.82	110.02
26	C	270	CDL	OB8-CB7-OB9	-4.59	112.16	123.55
27	Z	1526	DMU	O7-C10-C5	-4.58	97.78	108.11
21	P	1525	CHD	C1-C10-C9	-4.57	104.09	111.39
21	P	1525	CHD	O12-C12-C11	-4.57	99.73	109.11
21	W	1059	CHD	C19-C10-C5	-4.53	102.49	110.30
19	N	1522	TGL	OG3-CC1-OC1	-4.53	112.31	123.55
20	G	1268	PGV	C03-C02-C01	-4.47	101.77	111.86
21	P	1525	CHD	C21-C20-C22	-4.42	103.38	110.35
19	B	521	TGL	OG3-CC1-OC1	-4.37	112.70	123.55
20	P	1267	PGV	C8-C9-C10	-4.35	97.03	113.74
21	C	271	CHD	C23-C22-C20	-4.29	108.94	114.72
21	B	1085	CHD	C18-C13-C14	-4.28	104.47	111.23
21	P	1525	CHD	C23-C22-C20	-4.26	108.98	114.72
21	P	1271	CHD	C19-C10-C9	-4.21	105.14	111.16
21	A	525	CHD	C18-C13-C17	-4.08	104.77	111.23
25	P	1265	PEK	O03-C21-O04	-4.06	113.47	123.55
14	N	515	HEA	C26-C15-C14	-4.03	112.94	123.69
25	C	264	PEK	C24-C23-C22	-4.03	98.47	113.24
14	N	516	HEA	C1B-C2B-C3B	-3.99	104.22	107.00
26	P	1270	CDL	OB8-CB7-OB9	-3.98	113.67	123.55
21	G	86	CHD	C4-C5-C10	-3.84	108.46	112.66
20	C	267	PGV	C9-C10-C11	-3.84	91.60	112.50
21	W	1059	CHD	C19-C10-C1	-3.80	102.00	108.24
19	B	521	TGL	CB3-CB2-CB1	-3.79	99.76	113.58
20	A	521	PGV	O01-C1-O02	-3.79	114.23	123.68
21	G	86	CHD	O7-C7-C6	-3.78	100.87	110.02
27	M	526	DMU	O7-C10-O1	-3.77	101.53	110.70
21	J	60	CHD	C19-C10-C5	-3.76	103.81	110.30
20	N	1524	PGV	C4-C3-C2	-3.74	99.52	113.24
25	C	264	PEK	O03-C21-C22	-3.74	101.01	111.90
25	C	264	PEK	O03-C01-C02	-3.71	99.33	108.66
21	A	525	CHD	O7-C7-C6	-3.71	101.04	110.02
21	P	1525	CHD	C18-C13-C17	-3.70	105.38	111.23
21	P	1525	CHD	C16-C15-C14	-3.68	97.77	105.12
20	A	521	PGV	O03-C19-O04	-3.68	114.42	123.55
14	A	516	HEA	CAA-C2A-C3A	-3.66	118.11	128.59
14	N	516	HEA	C20-C19-C18	-3.60	113.73	121.10
26	P	1270	CDL	CB6-CB4-CB3	-3.58	103.78	111.86
25	C	264	PEK	C25-C24-C23	-3.56	96.11	114.45
20	A	521	PGV	C03-C02-C01	-3.52	103.93	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	1525	CHD	O12-C12-C13	-3.49	105.29	111.12
26	G	269	CDL	C16-C15-C14	-3.49	96.45	114.45
20	P	1267	PGV	C27-C26-C25	-3.42	96.81	114.45
20	G	1268	PGV	O02-C1-C2	-3.42	110.16	123.68
21	B	1085	CHD	C1-C10-C9	-3.42	105.94	111.39
19	O	1521	TGL	OG1-CA1-OA1	-3.38	115.17	123.55
14	A	516	HEA	OMA-CMA-C3A	-3.37	117.32	125.08
20	N	1266	PGV	O03-C19-O04	-3.36	115.20	123.55
21	P	1271	CHD	C18-C13-C12	-3.35	105.67	109.08
21	G	86	CHD	C1-C10-C9	-3.34	106.06	111.39
14	N	515	HEA	CMB-C2B-C1B	-3.33	123.35	128.46
20	C	267	PGV	C8-C9-C10	-3.30	101.05	113.74
20	A	521	PGV	C22-C21-C20	-3.30	101.13	113.24
26	P	1270	CDL	C55-C54-C53	-3.25	97.70	114.45
19	N	1522	TGL	CA4-CA3-CA2	-3.21	101.47	113.24
20	A	524	PGV	O03-C19-O04	-3.20	115.61	123.55
20	N	1266	PGV	C4-C3-C2	-3.18	101.57	113.24
26	G	269	CDL	OA6-CA5-OA7	-3.18	115.75	123.68
26	G	269	CDL	OA8-CA7-OA9	-3.16	115.70	123.55
19	A	523	TGL	OG3-CC1-OC1	-3.16	115.71	123.55
21	G	86	CHD	O12-C12-C11	-3.13	102.67	109.11
14	N	515	HEA	OMA-CMA-C3A	-3.10	117.95	125.08
20	G	1268	PGV	O03-C19-O04	-3.09	115.87	123.55
20	P	1267	PGV	O01-C1-O02	-3.09	115.97	123.68
20	N	1524	PGV	O03-C19-O04	-3.07	115.93	123.55
20	C	267	PGV	O01-C02-C03	-3.06	97.32	108.44
25	P	1264	PEK	O03-C21-C22	-3.04	103.05	111.90
14	A	516	HEA	C4B-C3B-C2B	-3.04	104.74	106.87
25	C	264	PEK	O01-C1-O02	-3.01	116.16	123.68
21	A	525	CHD	C1-C10-C9	-3.01	106.58	111.39
25	G	265	PEK	O03-C21-O04	-3.00	116.11	123.55
21	P	1271	CHD	C18-C13-C17	-2.99	106.51	111.23
14	A	516	HEA	C16-C15-C14	-2.98	115.00	121.10
26	P	1270	CDL	OA6-CA5-OA7	-2.98	116.25	123.68
19	N	1522	TGL	CA9-CA8-CA7	-2.96	99.18	114.45
23	B	229	PSC	O01-C1-O02	-2.95	116.33	123.68
21	W	1059	CHD	C18-C13-C14	-2.94	106.59	111.23
20	N	1266	PGV	C03-C02-C01	-2.92	105.26	111.86
21	G	86	CHD	C18-C13-C17	-2.92	106.61	111.23
25	C	264	PEK	C27-C26-C25	-2.91	99.45	114.45
21	W	1059	CHD	O3-C3-C4	-2.90	104.08	109.87
20	C	268	PGV	C03-C02-C01	-2.89	105.34	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	515	HEA	O11-C11-C3B	-2.87	103.58	111.83
26	T	1269	CDL	OA6-CA5-OA7	-2.87	116.53	123.68
20	C	268	PGV	O03-C19-O04	-2.84	116.50	123.55
14	A	515	HEA	CMB-C2B-C1B	-2.84	124.10	128.46
26	C	270	CDL	C61-C60-C59	-2.83	99.87	114.45
26	T	1269	CDL	OB8-CB7-OB9	-2.82	116.54	123.55
23	R	1229	PSC	O01-C1-O02	-2.82	116.64	123.68
19	A	523	TGL	CG3-CG2-CG1	-2.81	105.52	111.86
21	W	1059	CHD	C1-C10-C9	-2.77	106.98	111.39
26	C	270	CDL	CB4-OB6-CB5	-2.76	111.34	117.88
19	L	522	TGL	CB9-CB8-CB7	-2.75	100.30	114.45
14	A	516	HEA	CMD-C2D-C3D	-2.73	119.79	124.94
21	J	60	CHD	C18-C13-C14	-2.73	106.91	111.23
19	B	521	TGL	CA5-CA4-CA3	-2.68	100.63	114.45
25	C	264	PEK	C26-C25-C24	-2.68	100.63	114.45
26	C	270	CDL	OA6-CA5-OA7	-2.68	116.99	123.68
25	T	263	PEK	O04-C21-C22	-2.66	113.18	123.68
20	A	524	PGV	C3-C2-C1	-2.65	103.89	113.58
14	N	515	HEA	C17-C18-C19	-2.64	121.04	127.68
20	C	267	PGV	C27-C26-C25	-2.64	100.85	114.45
19	B	521	TGL	OB1-CB1-CB2	-2.64	113.27	123.68
21	A	525	CHD	C9-C10-C5	-2.63	104.84	108.63
19	L	522	TGL	CA5-CA4-CA3	-2.60	101.06	114.45
21	A	525	CHD	C16-C15-C14	-2.59	99.96	105.12
25	P	1265	PEK	O11-P-O14	-2.59	98.82	109.25
20	A	521	PGV	C4-C3-C2	-2.58	103.80	113.24
19	N	1523	TGL	OG3-CC1-OC1	-2.57	117.16	123.55
20	A	521	PGV	C3-C2-C1	-2.57	104.19	113.58
21	J	60	CHD	C19-C10-C1	-2.57	104.01	108.24
20	A	521	PGV	O01-C02-C01	-2.56	99.12	108.44
21	J	60	CHD	C1-C10-C9	-2.56	107.31	111.39
20	P	1267	PGV	C9-C8-C7	-2.56	101.27	114.45
19	L	522	TGL	CB4-CB3-CB2	-2.56	103.87	113.24
26	C	270	CDL	C57-C56-C55	-2.55	101.30	114.45
26	G	269	CDL	CB6-CB4-CB3	-2.55	106.11	111.86
20	C	267	PGV	C5-C4-C3	-2.55	101.33	114.45
20	A	521	PGV	C23-C22-C21	-2.54	101.36	114.45
21	C	271	CHD	C18-C13-C17	-2.53	107.23	111.23
14	N	515	HEA	CAA-CBA-CGA	-2.53	108.34	112.66
19	N	1523	TGL	OG1-CA1-OA1	-2.53	117.27	123.55
19	O	1521	TGL	CG3-CG2-CG1	-2.52	106.16	111.86
19	N	1522	TGL	OB1-CB1-CB2	-2.50	113.78	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	1271	CHD	C14-C8-C9	-2.49	106.24	109.64
26	C	270	CDL	C53-C52-C51	-2.48	104.16	113.24
25	C	264	PEK	O01-C02-C01	-2.46	99.48	108.44
25	P	1264	PEK	C30-C29-C28	-2.45	101.84	114.45
21	P	1271	CHD	C23-C22-C20	-2.44	111.44	114.72
20	N	1266	PGV	C23-C22-C21	-2.43	101.92	114.45
27	M	526	DMU	C22-C19-C18	-2.43	102.57	113.48
14	N	515	HEA	C27-C19-C18	-2.42	117.24	123.69
25	G	265	PEK	C2-C3-C4	-2.40	109.00	113.29
19	A	523	TGL	OG1-CA1-OA1	-2.40	117.60	123.55
19	L	522	TGL	C24-C23-C22	-2.39	102.12	114.45
26	G	269	CDL	OB8-CB7-OB9	-2.37	117.66	123.55
20	C	267	PGV	O03-C19-O04	-2.37	117.66	123.55
19	L	522	TGL	OA1-CA1-CA2	-2.37	114.33	123.68
14	A	516	HEA	CMB-C2B-C3B	-2.35	120.40	124.92
25	P	1264	PEK	C26-C25-C24	-2.34	102.38	114.45
19	L	522	TGL	CA9-CA8-CA7	-2.34	102.39	114.45
14	A	515	HEA	CBA-CAA-C2A	-2.34	108.00	112.47
21	B	1085	CHD	O12-C12-C11	-2.34	104.31	109.11
21	P	1271	CHD	C19-C10-C5	-2.33	106.28	110.30
25	C	264	PEK	O11-P-O14	-2.29	99.99	109.25
25	C	264	PEK	C29-C28-C27	-2.29	102.66	114.45
19	L	522	TGL	CA7-CA6-CA5	-2.29	102.67	114.45
26	C	270	CDL	C54-C53-C52	-2.29	102.67	114.45
25	T	263	PEK	O01-C1-O02	-2.28	117.98	123.68
19	O	1521	TGL	OG3-CC1-OC1	-2.28	117.88	123.55
14	N	515	HEA	O11-C11-C3B	-2.28	105.27	111.83
19	L	522	TGL	CA3-CA2-CA1	-2.28	105.27	113.58
20	A	521	PGV	C25-C24-C23	-2.27	102.73	114.45
20	C	268	PGV	O02-C1-C2	-2.25	114.78	123.68
14	N	515	HEA	CMC-C2C-C1C	-2.25	125.01	128.46
21	B	1085	CHD	C19-C10-C1	-2.25	104.55	108.24
26	P	1270	CDL	OB4-PB2-OB5	-2.23	97.59	108.14
26	T	1269	CDL	CB6-CB4-CB3	-2.22	106.84	111.86
23	R	1229	PSC	C07-N-C06	-2.22	103.36	108.98
26	P	1270	CDL	OA8-CA7-OA9	-2.20	118.08	123.55
20	N	1266	PGV	C8-C9-C10	-2.20	105.31	113.74
20	C	267	PGV	C14-C13-C12	-2.20	100.54	112.50
19	N	1522	TGL	CB9-CB8-CB7	-2.19	103.19	114.45
27	M	526	DMU	C25-C28-C31	-2.18	103.24	114.45
20	P	1267	PGV	O12-P-O13	-2.17	100.50	109.25
20	C	268	PGV	O04-C19-C20	-2.17	115.12	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	521	PGV	C6-C5-C4	-2.16	103.31	114.45
19	N	1522	TGL	OA1-CA1-CA2	-2.16	115.13	123.68
26	T	1269	CDL	OA8-CA7-OA9	-2.16	118.19	123.55
26	G	269	CDL	OB7-CB5-C51	-2.16	115.14	123.68
20	P	1267	PGV	O03-C19-O04	-2.16	118.19	123.55
25	C	264	PEK	C3-C2-C1	-2.15	105.73	113.58
25	T	263	PEK	C18-C17-C16	-2.13	105.58	113.74
25	P	1264	PEK	C03-C02-C01	-2.12	107.07	111.86
19	L	522	TGL	C26-C25-C24	-2.12	103.53	114.45
26	T	1269	CDL	C14-C13-C12	-2.12	103.54	114.45
20	N	1524	PGV	C8-C9-C10	-2.12	105.61	113.74
20	G	1268	PGV	O12-P-O13	-2.10	100.76	109.25
26	P	1270	CDL	C57-C56-C55	-2.09	103.71	114.45
20	N	1266	PGV	C5-C4-C3	-2.08	103.72	114.45
20	N	1266	PGV	C15-C14-C13	-2.08	105.74	113.74
26	P	1270	CDL	CB6-OB8-CB7	-2.07	110.91	117.13
20	N	1266	PGV	C01-O03-C19	-2.06	110.93	117.13
27	P	1272	DMU	C19-C22-C25	-2.06	103.85	114.45
20	G	1268	PGV	O04-C19-C20	-2.05	115.58	123.68
14	N	516	HEA	C25-C23-C22	-2.05	116.47	122.65
27	Z	1526	DMU	O4-C7-C8	-2.05	105.91	110.36
20	A	521	PGV	C21-C20-C19	-2.04	106.12	113.58
20	N	1266	PGV	O01-C02-C01	-2.04	101.03	108.44
27	P	1272	DMU	O2-C8-C9	-2.01	104.22	109.28
19	B	521	TGL	CB7-CB6-CB5	-2.01	104.11	114.45
20	A	524	PGV	C22-C21-C20	2.01	120.62	113.24
27	C	272	DMU	O4-C7-C5	2.02	114.75	110.36
26	P	1270	CDL	C22-C21-C20	2.02	124.87	114.45
14	A	515	HEA	C27-C19-C20	2.02	118.80	115.29
26	T	1269	CDL	C40-C39-C38	2.03	124.91	114.45
25	P	1264	PEK	O01-C1-C2	2.03	115.77	111.55
26	C	270	CDL	OA2-PA1-OA3	2.03	117.45	109.25
19	L	522	TGL	OG2-CB1-OB1	2.03	128.75	123.68
21	B	1085	CHD	C15-C14-C8	2.05	121.22	118.32
27	M	526	DMU	C10-O1-C9	2.06	117.60	113.72
14	N	515	HEA	C12-C13-C14	2.08	117.79	112.33
26	C	270	CDL	C72-C71-CB7	2.08	121.17	113.58
20	C	268	PGV	C32-C31-C30	2.08	125.18	114.45
20	A	524	PGV	O01-C1-C2	2.09	115.88	111.55
27	P	1272	DMU	C10-C5-C7	2.09	113.86	109.98
21	J	60	CHD	C13-C14-C8	2.09	117.46	114.77
14	N	516	HEA	C21-C20-C19	2.09	120.00	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1522	TGL	OG2-CB1-OB1	2.10	128.90	123.68
25	P	1265	PEK	C24-C23-C22	2.11	120.97	113.24
19	B	521	TGL	C33-C19-C18	2.12	125.38	114.45
27	M	526	DMU	O55-C2-C1	2.12	114.97	110.36
19	A	523	TGL	CB3-CB2-CB1	2.13	121.36	113.58
20	C	267	PGV	O14-P-O13	2.13	123.32	112.28
14	N	515	HEA	C3C-C4C-NC	2.14	111.97	109.21
26	G	269	CDL	C72-C71-CB7	2.16	121.45	113.58
26	P	1270	CDL	C43-C42-C41	2.16	125.58	114.45
14	A	515	HEA	CMC-C2C-C1C	2.16	131.78	128.46
26	T	1269	CDL	C80-C79-C78	2.16	125.58	114.45
26	P	1270	CDL	C32-C31-CA7	2.16	121.48	113.58
19	N	1523	TGL	CG2-OG2-CB1	2.18	123.03	117.88
26	P	1270	CDL	C40-C39-C38	2.18	125.70	114.45
23	B	229	PSC	C02-O01-C1	2.18	123.03	117.88
21	W	1059	CHD	C11-C9-C8	2.20	114.01	110.82
21	P	1525	CHD	C2-C1-C10	2.21	116.66	112.80
19	L	522	TGL	OG2-CG2-CG3	2.21	116.48	108.44
23	B	229	PSC	O01-C02-C03	2.22	116.52	108.44
26	P	1270	CDL	C83-C82-C81	2.23	125.95	114.45
26	G	269	CDL	CB4-OB6-CB5	2.23	123.15	117.88
19	B	521	TGL	OG2-CG2-CG3	2.25	116.61	108.44
25	P	1265	PEK	C01-O03-C21	2.25	123.91	117.13
20	C	267	PGV	O03-C19-C20	2.26	118.47	111.90
27	Z	1526	DMU	C11-C9-C8	2.26	118.28	113.00
21	C	271	CHD	C11-C9-C10	2.26	116.13	113.74
20	A	524	PGV	O03-C01-C02	2.26	114.34	108.66
20	N	1524	PGV	C02-O01-C1	2.27	123.24	117.88
27	M	526	DMU	O49-C1-C6	2.27	114.77	110.03
26	P	1270	CDL	OA8-CA6-CA4	2.27	114.36	108.66
26	T	1269	CDL	C85-C84-C83	2.29	126.24	114.45
26	G	269	CDL	C82-C81-C80	2.30	126.29	114.45
19	A	523	TGL	C21-C20-CA9	2.32	126.42	114.45
26	T	1269	CDL	C82-C81-C80	2.34	126.50	114.45
19	N	1522	TGL	C16-C15-CC9	2.35	126.55	114.45
27	M	526	DMU	O5-C6-O16	2.37	115.64	110.02
19	N	1523	TGL	C24-C23-C22	2.37	126.65	114.45
26	G	269	CDL	C23-C22-C21	2.38	126.70	114.45
25	P	1264	PEK	C8-C7-C6	2.39	119.98	111.84
19	B	521	TGL	OG3-CG3-CG2	2.40	114.68	108.66
23	B	229	PSC	C3-C2-C1	2.42	122.41	113.58
21	A	525	CHD	C14-C8-C9	2.42	112.93	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	C20-C19-C18	2.43	126.95	114.45
19	N	1523	TGL	C16-C15-CC9	2.43	126.97	114.45
19	N	1523	TGL	OG1-CA1-CA2	2.43	118.98	111.90
25	T	263	PEK	C2-C3-C4	2.44	117.64	113.29
26	T	1269	CDL	CA6-OA8-CA7	2.44	124.46	117.13
26	G	269	CDL	C83-C82-C81	2.44	127.04	114.45
19	O	1521	TGL	C15-CC9-CC8	2.44	127.05	114.45
27	C	272	DMU	O7-C3-C2	2.45	113.08	107.19
27	M	526	DMU	O4-C7-C8	2.45	115.69	110.36
25	P	1264	PEK	O02-C1-C2	2.45	133.37	123.68
21	P	1271	CHD	C11-C9-C10	2.46	116.35	113.74
21	P	1525	CHD	C15-C14-C8	2.46	121.81	118.32
27	C	272	DMU	O5-C6-O16	2.49	115.92	110.02
21	G	86	CHD	C13-C14-C8	2.49	117.98	114.77
26	C	270	CDL	C39-C38-C37	2.49	127.30	114.45
25	G	265	PEK	C03-C02-C01	2.49	117.48	111.86
21	P	1525	CHD	C17-C13-C14	2.49	102.62	100.08
21	B	1085	CHD	C11-C9-C8	2.54	114.50	110.82
27	M	526	DMU	C6-O5-C4	2.57	118.55	113.72
23	B	229	PSC	O03-C19-C20	2.57	119.37	111.90
14	A	516	HEA	C17-C18-C19	2.57	134.14	127.68
26	T	1269	CDL	C39-C38-C37	2.58	127.73	114.45
27	Z	1526	DMU	C10-O1-C9	2.58	118.58	113.72
20	P	1267	PGV	O01-C1-C2	2.59	116.93	111.55
26	C	270	CDL	C42-C41-C40	2.60	127.86	114.45
21	G	86	CHD	C13-C17-C20	2.60	122.65	119.49
26	P	1270	CDL	OA8-CA7-C31	2.60	119.48	111.90
27	C	272	DMU	C10-O1-C9	2.60	118.62	113.72
19	A	523	TGL	OG2-CB1-CB2	2.61	116.98	111.55
14	N	516	HEA	C26-C15-C16	2.62	119.83	115.29
19	L	522	TGL	C15-CC9-CC8	2.62	127.98	114.45
19	N	1522	TGL	C15-CC9-CC8	2.63	127.98	114.45
25	C	264	PEK	O01-C1-C2	2.63	117.02	111.55
26	C	270	CDL	C82-C81-C80	2.64	128.06	114.45
26	P	1270	CDL	CA6-OA8-CA7	2.64	125.07	117.13
20	A	521	PGV	O01-C02-C03	2.64	118.04	108.44
26	P	1270	CDL	OB6-CB4-CB6	2.64	118.05	108.44
26	T	1269	CDL	C19-C18-C17	2.65	128.11	114.45
27	M	526	DMU	C11-C9-C8	2.66	119.24	113.00
21	P	1271	CHD	C18-C13-C14	2.67	115.45	111.23
27	C	272	DMU	C10-C5-C7	2.69	114.98	109.98
19	N	1522	TGL	OG2-CB1-CB2	2.70	117.17	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	270	CDL	OA8-CA7-C31	2.71	119.77	111.90
25	P	1264	PEK	O04-C21-C22	2.71	134.41	123.68
21	W	1059	CHD	O12-C12-C11	2.73	114.72	109.11
26	T	1269	CDL	C23-C22-C21	2.74	128.59	114.45
14	N	515	HEA	CMD-C2D-C3D	2.74	130.12	124.94
19	A	523	TGL	OG1-CA1-CA2	2.75	119.90	111.90
26	G	269	CDL	CA6-OA8-CA7	2.75	125.41	117.13
26	T	1269	CDL	C83-C82-C81	2.81	128.92	114.45
21	P	1271	CHD	O7-C7-C8	2.81	115.61	109.33
26	G	269	CDL	C79-C78-C77	2.81	128.95	114.45
27	Z	1526	DMU	C6-C1-C2	2.85	115.28	109.98
26	P	1270	CDL	C42-C41-C40	2.85	129.15	114.45
21	B	1085	CHD	C16-C15-C14	2.86	110.83	105.12
14	A	515	HEA	C27-C19-C18	2.88	131.39	123.69
26	G	269	CDL	C80-C79-C78	2.88	129.32	114.45
19	A	523	TGL	CG3-OG3-CC1	2.90	125.84	117.13
27	M	526	DMU	O49-C1-C2	2.90	116.66	110.36
21	G	86	CHD	C9-C11-C12	2.90	118.14	114.32
25	T	263	PEK	C02-O01-C1	2.91	124.74	117.88
19	N	1522	TGL	OG1-CG1-CG2	2.91	115.96	108.66
25	G	1263	PEK	O03-C01-C02	2.92	116.00	108.66
21	P	1271	CHD	O7-C7-C6	2.93	117.11	110.02
27	Z	1526	DMU	C57-C4-C3	2.93	121.24	113.24
21	G	86	CHD	C1-C2-C3	2.93	114.16	110.42
20	N	1266	PGV	O02-C1-C2	2.94	135.31	123.68
26	P	1270	CDL	C39-C38-C37	2.95	129.64	114.45
21	G	86	CHD	C15-C16-C17	2.95	111.02	105.12
25	C	264	PEK	O04-C21-C22	2.97	135.44	123.68
26	P	1270	CDL	C82-C81-C80	3.01	129.98	114.45
20	G	1268	PGV	O01-C02-C03	3.01	119.39	108.44
21	A	525	CHD	C14-C13-C12	3.02	110.25	107.39
27	P	1272	DMU	O7-C3-C4	3.05	116.84	109.34
20	N	1524	PGV	O03-C19-C20	3.05	120.78	111.90
21	G	86	CHD	C2-C1-C10	3.05	118.12	112.80
27	M	526	DMU	O55-C2-C3	3.05	116.82	109.87
21	G	86	CHD	O3-C3-C2	3.06	117.51	110.10
23	R	1229	PSC	C3-C2-C1	3.06	124.75	113.58
27	M	526	DMU	C10-C5-C7	3.06	115.67	109.98
23	R	1229	PSC	O03-C19-C20	3.08	120.86	111.90
20	A	524	PGV	C01-O03-C19	3.09	126.44	117.13
27	M	526	DMU	C1-C2-C3	3.10	116.03	109.61
20	N	1524	PGV	C01-O03-C19	3.10	126.46	117.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	C19-C18-C17	3.11	130.46	114.45
27	P	1272	DMU	C11-C9-C8	3.12	120.31	113.00
27	C	272	DMU	C18-O16-C6	3.13	119.23	113.87
19	N	1523	TGL	OG2-CG2-CG3	3.13	119.81	108.44
14	N	516	HEA	CMC-C2C-C3C	3.16	130.76	124.89
14	N	515	HEA	C4B-C3B-C2B	3.16	109.08	106.87
19	B	521	TGL	CG1-OG1-CA1	3.18	126.69	117.13
19	N	1522	TGL	OG2-CG2-CG3	3.19	120.03	108.44
14	A	515	HEA	C12-C13-C14	3.19	120.72	112.33
26	C	270	CDL	OA8-CA6-CA4	3.22	116.74	108.66
27	P	1272	DMU	C18-O16-C6	3.22	119.39	113.87
20	G	1268	PGV	C02-O01-C1	3.24	125.52	117.88
21	J	60	CHD	C11-C9-C8	3.25	115.53	110.82
20	P	1267	PGV	O14-P-O13	3.26	129.15	112.28
19	B	521	TGL	C15-CC9-CC8	3.29	131.38	114.45
19	N	1522	TGL	OG1-CA1-CA2	3.29	121.48	111.90
21	B	1085	CHD	C5-C6-C7	3.31	118.10	114.44
27	C	272	DMU	C6-C1-C2	3.31	116.13	109.98
19	A	523	TGL	CG1-OG1-CA1	3.32	127.12	117.13
19	O	1521	TGL	OG3-CC1-CC2	3.34	121.62	111.90
27	C	272	DMU	O61-C57-C4	3.35	122.61	111.34
21	B	1085	CHD	C15-C14-C13	3.36	106.92	103.57
14	N	516	HEA	C13-C14-C15	3.38	136.18	127.68
21	A	525	CHD	C5-C4-C3	3.39	117.84	112.87
21	A	525	CHD	C19-C10-C1	3.41	113.85	108.24
27	Z	1526	DMU	C10-C5-C7	3.42	116.33	109.98
19	A	523	TGL	C10-CB9-CB8	3.42	132.08	114.45
27	M	526	DMU	O7-C3-C2	3.42	115.43	107.19
26	C	270	CDL	CA6-OA8-CA7	3.43	127.44	117.13
27	P	1272	DMU	C6-C1-C2	3.43	116.36	109.98
27	Z	1526	DMU	O3-C5-C7	3.44	117.84	110.36
21	A	525	CHD	C2-C1-C10	3.44	118.79	112.80
21	B	1085	CHD	C5-C4-C3	3.45	117.93	112.87
27	M	526	DMU	C57-C4-C3	3.46	122.68	113.24
25	G	1263	PEK	C01-O03-C21	3.46	127.55	117.13
21	P	1525	CHD	C16-C17-C20	3.47	117.69	112.14
20	N	1524	PGV	O01-C02-C03	3.50	121.16	108.44
19	N	1523	TGL	OG1-CG1-CG2	3.50	117.46	108.66
21	P	1271	CHD	C13-C17-C20	3.52	123.77	119.49
27	P	1272	DMU	C10-O1-C9	3.53	120.37	113.72
27	M	526	DMU	O16-C6-C1	3.55	114.02	108.23
27	M	526	DMU	O3-C5-C7	3.56	118.10	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1523	TGL	OG3-CC1-CC2	3.56	122.26	111.90
14	A	515	HEA	CMB-C2B-C3B	3.60	131.82	124.92
27	P	1272	DMU	O61-C57-C4	3.61	123.49	111.34
26	T	1269	CDL	CB6-OB8-CB7	3.61	128.00	117.13
27	Z	1526	DMU	C18-O16-C6	3.62	120.07	113.87
21	C	271	CHD	C9-C10-C5	3.62	113.86	108.63
25	T	263	PEK	C01-O03-C21	3.65	128.12	117.13
21	G	86	CHD	C11-C9-C10	3.67	117.63	113.74
27	M	526	DMU	C18-O16-C6	3.67	120.17	113.87
21	P	1525	CHD	C15-C16-C17	3.68	112.47	105.12
20	A	524	PGV	O01-C02-C03	3.69	121.85	108.44
20	A	524	PGV	C02-O01-C1	3.69	126.60	117.88
21	P	1525	CHD	C13-C17-C20	3.69	123.97	119.49
14	A	516	HEA	C26-C15-C16	3.71	121.72	115.29
27	C	272	DMU	C11-C9-C8	3.73	121.73	113.00
21	B	1085	CHD	C16-C17-C20	3.74	118.12	112.14
21	A	525	CHD	C13-C14-C8	3.75	119.60	114.77
19	N	1523	TGL	CG3-OG3-CC1	3.79	128.55	117.13
14	A	515	HEA	O11-C11-C12	3.80	124.16	110.21
21	G	86	CHD	C21-C20-C22	3.82	116.36	110.35
27	P	1272	DMU	O5-C4-C57	3.83	115.58	106.41
20	C	267	PGV	O01-C1-C2	3.87	119.58	111.55
27	C	272	DMU	O5-C4-C57	3.87	115.68	106.41
19	N	1522	TGL	CG1-OG1-CA1	3.87	128.78	117.13
19	N	1522	TGL	OG3-CC1-CC2	3.88	123.19	111.90
19	B	521	TGL	OG3-CC1-CC2	3.88	123.20	111.90
21	P	1525	CHD	C19-C10-C1	3.89	114.63	108.24
21	A	525	CHD	C17-C13-C14	3.94	104.09	100.08
19	O	1521	TGL	OG1-CA1-CA2	3.94	123.38	111.90
21	C	271	CHD	C9-C8-C7	3.95	116.57	111.92
19	B	521	TGL	OG1-CA1-CA2	3.98	123.47	111.90
21	P	1525	CHD	C11-C9-C10	3.99	117.97	113.74
21	A	525	CHD	C1-C2-C3	4.00	115.52	110.42
21	W	1059	CHD	C17-C13-C12	4.00	121.35	117.67
27	C	272	DMU	O7-C3-C4	4.01	119.21	109.34
19	A	523	TGL	OG3-CC1-CC2	4.05	123.68	111.90
25	G	1263	PEK	O03-C21-C22	4.07	123.75	111.90
27	C	272	DMU	O1-C9-C11	4.10	116.22	106.41
27	M	526	DMU	C7-C8-C9	4.12	117.48	110.22
21	P	1271	CHD	C9-C10-C5	4.12	114.58	108.63
27	P	1272	DMU	C2-C3-C4	4.13	119.64	110.88
20	N	1266	PGV	O03-C19-C20	4.14	123.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1085	CHD	C13-C14-C8	4.14	120.10	114.77
21	C	271	CHD	O7-C7-C8	4.14	118.57	109.33
21	A	525	CHD	O3-C3-C4	4.15	118.15	109.87
25	T	263	PEK	O03-C01-C02	4.15	119.09	108.66
27	C	272	DMU	C2-C3-C4	4.17	119.71	110.88
19	L	522	TGL	OG1-CA1-CA2	4.18	124.05	111.90
19	B	521	TGL	CG3-OG3-CC1	4.19	129.74	117.13
19	N	1522	TGL	CG3-OG3-CC1	4.19	129.75	117.13
20	A	524	PGV	O03-C19-C20	4.20	124.12	111.90
27	Z	1526	DMU	C7-C8-C9	4.20	117.62	110.22
21	B	1085	CHD	C6-C7-C8	4.22	115.99	111.50
21	A	525	CHD	C9-C8-C7	4.22	116.89	111.92
27	Z	1526	DMU	O5-C6-O16	4.23	120.06	110.02
20	A	521	PGV	O03-C19-C20	4.24	124.23	111.90
25	T	263	PEK	O01-C1-C2	4.25	120.37	111.55
25	T	263	PEK	O03-C21-C22	4.26	124.29	111.90
21	G	86	CHD	C15-C14-C8	4.27	124.36	118.32
14	N	515	HEA	C26-C15-C16	4.28	122.72	115.29
14	N	515	HEA	C27-C19-C20	4.29	122.73	115.29
21	C	271	CHD	C16-C17-C20	4.32	119.05	112.14
21	W	1059	CHD	C22-C20-C17	4.34	119.38	110.26
27	P	1272	DMU	O5-C4-C3	4.34	118.64	109.75
14	A	515	HEA	C3C-C4C-NC	4.36	114.85	109.21
25	G	265	PEK	C01-O03-C21	4.40	130.35	117.13
27	C	272	DMU	O5-C4-C3	4.40	118.75	109.75
26	T	1269	CDL	OA8-CA7-C31	4.42	124.75	111.90
19	L	522	TGL	OG1-CG1-CG2	4.43	119.78	108.66
21	P	1271	CHD	C16-C17-C20	4.47	119.29	112.14
27	Z	1526	DMU	C2-C3-C4	4.47	120.37	110.88
27	M	526	DMU	O5-C4-C3	4.50	118.97	109.75
19	O	1521	TGL	OG2-CB1-CB2	4.51	120.91	111.55
27	C	272	DMU	C57-C4-C3	4.51	125.53	113.24
27	C	272	DMU	C7-C8-C9	4.51	118.17	110.22
27	M	526	DMU	O1-C9-C11	4.52	117.25	106.41
21	G	86	CHD	C16-C17-C20	4.53	119.40	112.14
21	P	1525	CHD	C14-C8-C9	4.53	115.81	109.64
26	G	269	CDL	OA8-CA7-C31	4.55	125.13	111.90
20	N	1524	PGV	O01-C1-C2	4.55	121.01	111.55
19	N	1522	TGL	CC3-CC2-CC1	4.56	130.22	113.58
21	P	1271	CHD	C14-C13-C12	4.56	111.72	107.39
25	G	1263	PEK	C02-O01-C1	4.57	128.68	117.88
27	P	1272	DMU	C57-C4-C3	4.58	125.73	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Z	1526	DMU	C1-C2-C3	4.61	119.17	109.61
25	G	265	PEK	O01-C1-C2	4.62	121.14	111.55
14	A	515	HEA	CMD-C2D-C3D	4.63	133.66	124.94
14	N	515	HEA	CMB-C2B-C3B	4.63	133.81	124.92
21	P	1271	CHD	C4-C5-C10	4.65	117.73	112.66
21	C	271	CHD	C13-C17-C20	4.66	125.14	119.49
27	P	1272	DMU	C7-C8-C9	4.69	118.48	110.22
26	G	269	CDL	CB6-OB8-CB7	4.70	131.28	117.13
26	C	270	CDL	OB8-CB7-C71	4.73	125.65	111.90
21	B	1085	CHD	C14-C8-C9	4.74	116.09	109.64
27	P	1272	DMU	O7-C10-C5	4.74	118.80	108.11
27	Z	1526	DMU	C6-O5-C4	4.76	122.68	113.72
21	B	1085	CHD	C9-C8-C7	4.78	117.53	111.92
14	A	516	HEA	CBD-CAD-C3D	4.78	121.62	112.48
21	P	1271	CHD	C9-C11-C12	4.78	120.62	114.32
21	P	1525	CHD	C5-C6-C7	4.78	119.73	114.44
14	A	516	HEA	C3C-C4C-NC	4.80	115.41	109.21
25	P	1265	PEK	O03-C21-C22	4.81	125.89	111.90
23	R	1229	PSC	O01-C1-C2	4.84	121.59	111.55
27	C	272	DMU	C6-O5-C4	4.86	122.87	113.72
27	M	526	DMU	C8-C7-C5	4.88	119.45	110.84
21	C	271	CHD	C11-C9-C8	4.90	117.93	110.82
19	O	1521	TGL	OG2-CG2-CG3	4.91	126.27	108.44
14	N	515	HEA	CMC-C2C-C3C	4.91	134.00	124.89
27	Z	1526	DMU	O5-C4-C3	4.95	119.88	109.75
21	P	1525	CHD	C5-C4-C3	4.96	120.14	112.87
27	M	526	DMU	O5-C4-C57	4.98	118.33	106.41
25	P	1265	PEK	O01-C1-C2	4.98	121.89	111.55
21	P	1525	CHD	O3-C3-C4	4.98	119.82	109.87
21	G	86	CHD	C11-C9-C8	4.99	118.06	110.82
19	N	1523	TGL	OG2-CB1-CB2	5.00	121.94	111.55
21	P	1525	CHD	C10-C9-C8	5.01	117.27	111.87
25	G	265	PEK	O03-C21-C22	5.03	126.53	111.90
14	N	516	HEA	C27-C19-C20	5.03	124.02	115.29
21	J	60	CHD	C9-C8-C7	5.04	117.84	111.92
21	A	525	CHD	C15-C16-C17	5.04	115.19	105.12
26	G	269	CDL	OA6-CA5-C11	5.05	122.04	111.55
21	P	1525	CHD	C1-C2-C3	5.06	116.86	110.42
27	Z	1526	DMU	C8-C7-C5	5.07	119.77	110.84
27	P	1272	DMU	C6-O5-C4	5.07	123.26	113.72
21	A	525	CHD	C11-C9-C8	5.09	118.20	110.82
19	L	522	TGL	OG3-CC1-CC2	5.12	126.79	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	1270	CDL	OB8-CB7-C71	5.14	126.85	111.90
21	W	1059	CHD	C9-C10-C5	5.14	116.05	108.63
14	N	516	HEA	C3C-C4C-NC	5.14	115.85	109.21
27	Z	1526	DMU	O1-C9-C11	5.18	118.81	106.41
27	C	272	DMU	C1-C2-C3	5.19	120.36	109.61
27	Z	1526	DMU	O5-C4-C57	5.20	118.86	106.41
25	C	264	PEK	C2-C3-C4	5.20	122.57	113.29
27	P	1272	DMU	O1-C9-C11	5.20	118.88	106.41
19	L	522	TGL	CG2-OG2-CB1	5.21	130.19	117.88
21	J	60	CHD	C22-C20-C17	5.23	121.24	110.26
14	N	516	HEA	CBD-CAD-C3D	5.23	122.48	112.48
21	P	1271	CHD	C11-C9-C8	5.23	118.41	110.82
19	O	1521	TGL	CG3-OG3-CC1	5.25	132.92	117.13
21	P	1271	CHD	C11-C12-C13	5.26	116.67	111.22
21	W	1059	CHD	C9-C8-C7	5.27	118.11	111.92
21	P	1271	CHD	C9-C8-C7	5.27	118.12	111.92
27	P	1272	DMU	C1-C2-C3	5.28	120.56	109.61
21	J	60	CHD	C1-C10-C5	5.28	115.98	107.79
21	C	271	CHD	C14-C13-C12	5.30	112.42	107.39
21	W	1059	CHD	C2-C1-C10	5.31	122.05	112.80
21	J	60	CHD	C9-C10-C5	5.35	116.36	108.63
21	G	86	CHD	C9-C8-C7	5.36	118.22	111.92
26	T	1269	CDL	OA6-CA5-C11	5.37	122.71	111.55
21	J	60	CHD	C11-C9-C10	5.37	119.43	113.74
27	C	272	DMU	C8-C7-C5	5.37	120.32	110.84
21	W	1059	CHD	C1-C10-C5	5.38	116.13	107.79
21	G	86	CHD	C14-C8-C9	5.42	117.01	109.64
14	A	516	HEA	CAA-CBA-CGA	5.52	122.10	112.66
21	C	271	CHD	C9-C11-C12	5.54	121.63	114.32
27	Z	1526	DMU	O16-C6-C1	5.56	117.30	108.23
27	C	272	DMU	O7-C10-C5	5.56	120.64	108.11
21	J	60	CHD	C4-C3-C2	5.58	117.48	110.55
21	G	86	CHD	C15-C14-C13	5.59	109.13	103.57
23	B	229	PSC	O01-C1-C2	5.60	123.17	111.55
21	A	525	CHD	C13-C17-C20	5.65	126.34	119.49
21	G	86	CHD	C5-C6-C7	5.65	120.69	114.44
21	B	1085	CHD	C17-C13-C14	5.66	105.84	100.08
20	C	268	PGV	O03-C19-C20	5.66	128.37	111.90
21	G	86	CHD	C17-C13-C14	5.67	105.86	100.08
21	W	1059	CHD	C5-C4-C3	5.67	121.20	112.87
21	A	525	CHD	C9-C11-C12	5.70	121.84	114.32
20	G	1268	PGV	O03-C19-C20	5.72	128.55	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	1263	PEK	O01-C1-C2	5.72	123.44	111.55
27	P	1272	DMU	O5-C6-C1	5.76	121.41	110.30
21	J	60	CHD	C14-C13-C12	5.78	112.88	107.39
21	C	271	CHD	C1-C10-C5	5.80	116.78	107.79
21	C	271	CHD	C2-C1-C10	5.81	122.92	112.80
21	C	271	CHD	C11-C12-C13	5.83	117.25	111.22
14	A	515	HEA	C26-C15-C16	5.84	125.42	115.29
26	C	270	CDL	OA6-CA5-C11	5.85	123.69	111.55
21	W	1059	CHD	C14-C13-C12	5.86	112.95	107.39
21	B	1085	CHD	C9-C11-C12	6.01	122.24	114.32
27	C	272	DMU	O5-C6-C1	6.03	121.92	110.30
21	W	1059	CHD	C6-C7-C8	6.03	117.91	111.50
27	P	1272	DMU	O1-C9-C8	6.03	120.77	109.66
21	J	60	CHD	C9-C11-C12	6.04	122.29	114.32
19	B	521	TGL	OG2-CB1-CB2	6.05	124.11	111.55
25	P	1264	PEK	C2-C3-C4	6.06	124.10	113.29
21	A	525	CHD	C11-C12-C13	6.07	117.51	111.22
19	L	522	TGL	CC3-CC2-CC1	6.08	135.78	113.58
26	T	1269	CDL	OB6-CB5-C51	6.08	124.18	111.55
26	P	1270	CDL	OA6-CA5-C11	6.08	124.19	111.55
27	P	1272	DMU	C8-C7-C5	6.09	121.57	110.84
21	J	60	CHD	C2-C1-C10	6.12	123.47	112.80
21	J	60	CHD	C15-C14-C8	6.14	127.01	118.32
21	G	86	CHD	C5-C4-C3	6.18	121.94	112.87
21	J	60	CHD	C17-C13-C12	6.21	123.38	117.67
21	P	1271	CHD	C5-C6-C7	6.21	121.31	114.44
21	P	1271	CHD	C1-C10-C5	6.24	117.45	107.79
26	G	269	CDL	OB6-CB5-C51	6.26	124.55	111.55
20	C	268	PGV	O01-C1-C2	6.26	124.56	111.55
21	C	271	CHD	C5-C4-C3	6.29	122.09	112.87
27	Z	1526	DMU	O5-C6-C1	6.30	122.45	110.30
21	C	271	CHD	C4-C3-C2	6.31	118.39	110.55
21	P	1271	CHD	C2-C1-C10	6.39	123.94	112.80
21	P	1271	CHD	C1-C2-C3	6.40	118.58	110.42
21	B	1085	CHD	C1-C2-C3	6.42	118.61	110.42
21	W	1059	CHD	C11-C12-C13	6.45	117.90	111.22
21	P	1525	CHD	C11-C12-C13	6.45	117.90	111.22
21	J	60	CHD	C6-C5-C10	6.51	119.77	112.66
21	W	1059	CHD	C4-C3-C2	6.51	118.64	110.55
21	W	1059	CHD	C6-C5-C10	6.56	119.83	112.66
21	W	1059	CHD	C11-C9-C10	6.57	120.70	113.74
21	W	1059	CHD	C9-C11-C12	6.58	122.99	114.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	526	DMU	C2-C3-C4	6.58	124.84	110.88
21	J	60	CHD	C6-C7-C8	6.62	118.54	111.50
21	J	60	CHD	C4-C5-C10	6.63	119.90	112.66
21	P	1271	CHD	C4-C3-C2	6.65	118.80	110.55
27	C	272	DMU	O1-C9-C8	6.66	121.93	109.66
21	W	1059	CHD	C15-C14-C13	6.81	110.35	103.57
21	J	60	CHD	C5-C4-C3	6.87	122.95	112.87
21	G	86	CHD	C11-C12-C13	6.88	118.35	111.22
21	J	60	CHD	C11-C12-C13	6.89	118.35	111.22
21	C	271	CHD	C5-C6-C7	6.89	122.06	114.44
21	P	1271	CHD	C15-C14-C8	6.97	128.18	118.32
21	C	271	CHD	C4-C5-C10	7.01	120.31	112.66
21	C	271	CHD	C1-C2-C3	7.01	119.36	110.42
21	P	1271	CHD	C5-C4-C3	7.12	123.31	112.87
27	Z	1526	DMU	O1-C9-C8	7.15	122.84	109.66
21	P	1271	CHD	C6-C7-C8	7.16	119.11	111.50
21	B	1085	CHD	C16-C17-C13	7.22	110.76	103.57
19	N	1522	TGL	CG2-OG2-CB1	7.23	134.95	117.88
19	B	521	TGL	CG2-OG2-CB1	7.34	135.22	117.88
27	P	1272	DMU	O1-C10-C5	7.42	124.61	110.30
27	Z	1526	DMU	O1-C10-C5	7.43	124.63	110.30
20	G	1268	PGV	O01-C1-C2	7.47	127.06	111.55
27	M	526	DMU	O1-C9-C8	7.47	123.42	109.66
21	C	271	CHD	C6-C7-C8	7.53	119.51	111.50
21	W	1059	CHD	C15-C14-C8	7.54	128.99	118.32
21	J	60	CHD	C1-C2-C3	7.61	120.12	110.42
27	C	272	DMU	O16-C6-C1	7.62	120.67	108.23
27	C	272	DMU	O1-C10-C5	7.71	125.17	110.30
21	G	86	CHD	C14-C13-C12	7.72	114.72	107.39
21	P	1525	CHD	C9-C8-C7	7.79	121.08	111.92
21	C	271	CHD	C15-C14-C13	7.83	111.36	103.57
21	B	1085	CHD	C14-C13-C12	7.93	114.91	107.39
21	W	1059	CHD	C4-C5-C10	7.95	121.34	112.66
21	P	1525	CHD	C11-C9-C8	7.95	122.34	110.82
21	J	60	CHD	C5-C6-C7	7.95	123.24	114.44
21	W	1059	CHD	C1-C2-C3	7.95	120.56	110.42
21	B	1085	CHD	C11-C9-C10	7.96	122.17	113.74
21	A	525	CHD	C15-C14-C13	7.97	111.50	103.57
19	O	1521	TGL	CG2-OG2-CB1	7.98	136.74	117.88
27	M	526	DMU	O1-C10-C5	7.99	125.71	110.30
21	G	86	CHD	C4-C3-C2	8.00	120.49	110.55
21	B	1085	CHD	C4-C3-C2	8.05	120.55	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	1525	CHD	C4-C3-C2	8.08	120.58	110.55
21	P	1271	CHD	C16-C17-C13	8.10	111.63	103.57
21	P	1271	CHD	C6-C5-C10	8.19	121.61	112.66
21	A	525	CHD	C6-C5-C10	8.27	121.70	112.66
21	J	60	CHD	C15-C14-C13	8.29	111.82	103.57
21	C	271	CHD	C14-C8-C7	8.30	123.06	111.80
21	J	60	CHD	C14-C8-C7	8.31	123.06	111.80
21	P	1271	CHD	C14-C8-C7	8.31	123.06	111.80
21	C	271	CHD	C6-C5-C10	8.38	121.82	112.66
21	A	525	CHD	C4-C3-C2	8.39	120.97	110.55
21	C	271	CHD	C15-C14-C8	8.58	130.46	118.32
21	B	1085	CHD	C10-C9-C8	8.67	121.22	111.87
21	W	1059	CHD	C5-C6-C7	8.73	124.10	114.44
21	P	1525	CHD	C17-C13-C12	8.83	125.79	117.67
27	P	1272	DMU	O16-C6-C1	8.86	122.68	108.23
21	W	1059	CHD	C14-C8-C7	8.95	123.93	111.80
21	C	271	CHD	C16-C17-C13	9.01	112.54	103.57
21	J	60	CHD	C16-C17-C13	9.04	112.57	103.57
27	M	526	DMU	O5-C6-C1	9.13	127.91	110.30
21	G	86	CHD	C17-C13-C12	9.24	126.17	117.67
21	A	525	CHD	C5-C6-C7	9.29	124.72	114.44
21	G	86	CHD	C10-C9-C8	9.56	122.18	111.87
21	J	60	CHD	C13-C17-C20	9.96	131.57	119.49
14	A	516	HEA	C27-C19-C20	10.07	132.77	115.29
21	W	1059	CHD	C16-C17-C13	10.28	113.81	103.57
21	W	1059	CHD	C13-C17-C20	10.36	132.05	119.49
21	J	60	CHD	C10-C9-C8	10.46	123.14	111.87
21	A	525	CHD	C1-C10-C5	10.48	124.04	107.79
21	W	1059	CHD	C10-C9-C8	10.55	123.24	111.87
21	P	1271	CHD	C10-C9-C8	11.30	124.05	111.87
21	P	1271	CHD	C15-C14-C13	11.31	114.83	103.57
21	G	86	CHD	C1-C10-C5	11.52	125.65	107.79
21	P	1525	CHD	C6-C5-C10	11.67	125.41	112.66
21	P	1525	CHD	C1-C10-C5	11.69	125.91	107.79
21	B	1085	CHD	C6-C5-C10	11.78	125.53	112.66
21	A	525	CHD	C10-C9-C8	11.98	124.78	111.87
21	C	271	CHD	C10-C9-C8	12.11	124.93	111.87
21	G	86	CHD	C6-C5-C10	12.50	126.31	112.66
21	P	1525	CHD	C14-C13-C12	12.89	119.62	107.39
21	A	525	CHD	C17-C13-C12	13.20	129.81	117.67
21	B	1085	CHD	C1-C10-C5	13.66	128.97	107.79
21	P	1525	CHD	C15-C14-C13	13.88	117.39	103.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1085	CHD	C17-C13-C12	13.88	130.43	117.67

All (37) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
21	P	1271	CHD	C9
21	C	271	CHD	C14
21	C	271	CHD	C9
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
27	P	1272	DMU	C2
27	P	1272	DMU	C4
27	P	1272	DMU	C6
27	P	1272	DMU	C9
27	P	1272	DMU	C5
27	M	526	DMU	C2
27	M	526	DMU	C4
27	M	526	DMU	C6
27	M	526	DMU	C9
27	M	526	DMU	C5
21	J	60	CHD	C17
27	Z	1526	DMU	C2
27	Z	1526	DMU	C4
27	Z	1526	DMU	C6
27	Z	1526	DMU	C9
27	Z	1526	DMU	C5
27	C	272	DMU	C2
27	C	272	DMU	C4
27	C	272	DMU	C6
27	C	272	DMU	C9
27	C	272	DMU	C5
21	W	1059	CHD	C17

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C02-O01-C1-C2
20	N	1524	PGV	C02-O01-C1-O02
20	N	1524	PGV	C02-O01-C1-C2

There are no ring outliers.

40 monomers are involved in 339 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	7	0
14	A	516	HEA	7	0
16	A	520	CMO	1	0
20	A	521	PGV	1	0
19	A	523	TGL	12	0
20	A	524	PGV	10	0
21	B	1085	CHD	1	0
23	B	229	PSC	17	0
19	B	521	TGL	7	0
25	C	264	PEK	5	0
20	C	267	PGV	4	0
20	C	268	PGV	3	0
26	C	270	CDL	20	0
21	C	271	CHD	8	0
27	C	272	DMU	2	0
25	G	1263	PEK	12	0
20	G	1268	PGV	2	0
25	G	265	PEK	17	0
26	G	269	CDL	39	0
21	G	86	CHD	1	0
21	J	60	CHD	1	0
19	L	522	TGL	12	0
20	N	1266	PGV	2	0
19	N	1522	TGL	14	0
19	N	1523	TGL	4	0
20	N	1524	PGV	8	0
14	N	515	HEA	3	0
19	O	1521	TGL	9	0
25	P	1264	PEK	7	0
25	P	1265	PEK	14	0
20	P	1267	PGV	6	0
26	P	1270	CDL	21	0
21	P	1271	CHD	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	P	1272	DMU	4	0
21	P	1525	CHD	2	0
23	R	1229	PSC	15	0
26	T	1269	CDL	35	0
25	T	263	PEK	24	0
21	W	1059	CHD	2	0
27	Z	1526	DMU	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.12	6 (1%) 79 77	19, 26, 35, 62	0
1	N	513/514 (99%)	0.03	6 (1%) 79 77	23, 31, 39, 66	0
2	B	226/227 (99%)	-0.39	1 (0%) 92 90	19, 31, 55, 77	0
2	O	226/227 (99%)	-0.16	6 (2%) 55 50	28, 38, 66, 85	0
3	C	259/261 (99%)	-0.28	4 (1%) 74 70	23, 29, 41, 64	0
3	P	259/261 (99%)	-0.14	10 (3%) 40 35	25, 31, 43, 67	0
4	D	144/147 (97%)	-0.41	1 (0%) 87 86	27, 35, 52, 69	0
4	Q	144/147 (97%)	1.20	23 (15%) 2 1	35, 47, 73, 118	0
5	E	105/109 (96%)	0.13	3 (2%) 52 47	29, 35, 62, 99	0
5	R	105/109 (96%)	0.63	6 (5%) 24 20	33, 40, 69, 104	0
6	F	98/98 (100%)	0.36	7 (7%) 17 13	27, 37, 82, 128	0
6	S	98/98 (100%)	0.08	8 (8%) 12 10	29, 39, 86, 121	0
7	G	83/85 (97%)	0.78	13 (15%) 2 2	27, 36, 101, 109	0
7	T	83/85 (97%)	0.89	17 (20%) 1 1	26, 36, 98, 111	0
8	H	79/85 (92%)	0.21	9 (11%) 6 4	27, 37, 89, 111	0
8	U	79/85 (92%)	0.28	11 (13%) 3 2	35, 42, 92, 112	0
9	I	72/73 (98%)	0.02	3 (4%) 37 31	28, 44, 66, 73	0
9	V	72/73 (98%)	0.77	7 (9%) 8 7	33, 51, 67, 90	0
10	J	58/59 (98%)	0.54	7 (12%) 5 4	30, 38, 70, 96	0
10	W	58/59 (98%)	0.44	6 (10%) 7 6	31, 39, 72, 108	0
11	K	49/56 (87%)	-0.29	0 100 100	30, 37, 51, 64	0
11	X	49/56 (87%)	1.68	15 (30%) 0 0	39, 46, 64, 79	0
12	L	46/47 (97%)	-0.29	2 (4%) 36 30	25, 32, 46, 77	0
12	Y	46/47 (97%)	-0.17	1 (2%) 62 58	32, 37, 59, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.04	3 (6%) 17 14	28, 31, 75, 106	0
13	Z	43/46 (93%)	0.51	7 (16%) 2 1	35, 39, 92, 117	0
All	All	3550/3614 (98%)	0.12	182 (5%) 29 24	19, 34, 65, 128	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	35.5
4	Q	4	SER	22.2
4	Q	6	VAL	18.1
6	F	98	HIS	12.6
6	F	97	ALA	11.5
6	S	97	ALA	11.1
6	F	96	LEU	11.0
13	Z	43	SER	10.1
7	G	2	SER	9.1
5	R	109	VAL	8.6
10	J	1	PHE	8.0
6	F	1	ALA	7.7
5	R	5	HIS	7.6
7	G	1	ALA	7.4
4	Q	8	SER	7.2
6	F	2	SER	7.0
7	G	3	ALA	7.0
6	S	1	ALA	6.9
8	H	7	LYS	6.9
8	U	8	ILE	6.8
8	H	46	LYS	6.8
8	H	44	THR	6.6
8	H	47	GLY	6.5
7	T	42	ARG	6.4
7	T	1	ALA	6.4
8	U	7	LYS	6.3
7	G	42	ARG	6.1
8	H	45	ALA	6.0
7	T	36	TRP	6.0
7	T	84	LYS	5.9
7	G	5	LYS	5.8
13	Z	42	LYS	5.8
9	V	2	THR	5.6
6	S	98	HIS	5.5

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Mol	Chain	Res	Type	RSRZ
7	G	4	ALA	5.3
7	T	8	HIS	5.3
6	S	96	LEU	5.3
7	T	40	GLY	5.2
13	M	43	SER	5.2
4	Q	147	LYS	5.1
9	I	37	PHE	5.1
6	S	2	SER	5.1
5	E	5	HIS	5.0
6	S	94	HIS	5.0
2	O	90	ILE	4.9
7	T	5	LYS	4.9
10	J	58	LYS	4.9
7	T	2	SER	4.8
11	X	7	PRO	4.7
7	T	4	ALA	4.7
13	Z	40	TYR	4.7
10	W	1	PHE	4.6
11	X	6	ALA	4.6
7	T	39	SER	4.5
10	W	58	LYS	4.4
8	U	45	ALA	4.4
13	Z	41	LYS	4.3
11	X	13	TYR	4.3
8	U	48	GLY	4.2
9	V	37	PHE	4.2
4	Q	7	LYS	4.1
7	G	41	HIS	4.1
8	U	44	THR	4.0
7	G	8	HIS	4.0
7	G	84	LYS	4.0
8	U	46	LYS	4.0
8	H	48	GLY	3.9
2	O	226	MET	3.9
2	O	113	TYR	3.9
11	X	23	THR	3.9
12	Y	47	LYS	3.8
11	X	46	GLY	3.8
13	M	42	LYS	3.8
5	E	109	VAL	3.8
7	T	3	ALA	3.8
6	F	95	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
3	P	91	VAL	3.6
7	G	40	GLY	3.6
5	R	96	LEU	3.5
13	Z	39	ASN	3.4
4	D	147	LYS	3.4
2	O	91	ASN	3.4
12	L	2	HIS	3.4
4	Q	51	LEU	3.3
11	X	16	ALA	3.3
10	W	57	HIS	3.3
10	W	48	TYR	3.3
8	U	47	GLY	3.2
7	T	10	GLY	3.2
10	J	2	GLU	3.2
4	Q	102	TYR	3.2
5	R	52	LEU	3.1
4	Q	138	TRP	3.1
11	X	47	ARG	3.1
6	S	95	GLN	3.1
4	Q	145	TRP	3.1
10	W	2	GLU	3.0
11	X	27	ALA	3.0
7	G	36	TRP	3.0
6	S	93	PRO	3.0
11	X	34	THR	2.9
13	M	40	TYR	2.9
5	R	108	LYS	2.9
9	V	25	PHE	2.9
4	Q	140	TYR	2.9
10	J	48	TYR	2.9
11	X	52	GLU	2.9
1	N	158	ILE	2.8
7	T	41	HIS	2.8
9	V	3	ALA	2.8
8	U	49	ASP	2.8
9	V	65	LYS	2.7
4	Q	111	PHE	2.7
6	F	94	HIS	2.7
11	X	19	ALA	2.7
3	P	88	ILE	2.6
8	H	8	ILE	2.6
10	W	52	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
4	Q	58	GLU	2.6
2	O	227	LEU	2.6
3	C	92	LEU	2.6
4	Q	134	PHE	2.6
10	J	52	TRP	2.6
3	P	85	LEU	2.5
8	U	10	ASN	2.5
4	Q	53	ILE	2.5
8	H	43	MET	2.5
5	R	48	ILE	2.5
7	T	7	ASP	2.5
2	B	59	GLN	2.5
4	Q	48	TRP	2.5
8	U	9	LYS	2.5
1	A	195	LEU	2.5
4	Q	124	LEU	2.5
11	X	15	ASN	2.4
3	P	92	LEU	2.4
9	V	29	LEU	2.4
1	N	201	VAL	2.4
3	C	91	VAL	2.4
10	J	57	HIS	2.4
5	E	11	PHE	2.4
2	O	59	GLN	2.4
13	Z	35	TYR	2.4
7	T	9	GLY	2.4
10	J	30	ILE	2.4
12	L	47	LYS	2.3
3	C	3	HIS	2.3
1	A	66	ILE	2.3
8	H	49	ASP	2.3
4	Q	52	SER	2.3
1	A	194	LEU	2.3
9	I	25	PHE	2.3
3	C	95	THR	2.3
7	G	43	GLU	2.3
7	T	6	GLY	2.3
1	A	285	PHE	2.2
3	P	93	PHE	2.2
11	X	45	VAL	2.2
3	P	84	ILE	2.2
4	Q	10	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
4	Q	78	TRP	2.2
3	P	95	THR	2.2
7	T	83	GLU	2.2
9	I	18	ARG	2.2
3	P	98	PHE	2.2
3	P	96	GLY	2.2
4	Q	87	PHE	2.2
7	G	7	ASP	2.1
3	P	182	TYR	2.1
9	V	53	ASN	2.1
11	X	35	GLN	2.1
13	Z	32	TRP	2.1
4	Q	46	ALA	2.1
1	A	193	VAL	2.1
1	N	193	VAL	2.1
8	U	52	VAL	2.1
4	Q	128	VAL	2.0
1	A	200	PRO	2.0
1	N	194	LEU	2.0
1	N	196	LEU	2.0
11	X	9	PHE	2.0
1	N	381	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FME	O	1	10/11	0.96	0.16	-	36,38,46,49	0
7	TPO	T	11	11/12	0.46	0.35	-	75,83,108,109	0
2	FME	B	1	10/11	0.96	0.11	-	30,32,39,53	0
9	SAC	I	1	9/10	0.76	0.30	-	81,85,88,89	0
1	FME	N	1	10/11	0.94	0.17	-	45,50,74,74	0
9	SAC	V	1	9/10	0.23	0.66	-	96,98,100,100	0
1	FME	A	1	10/11	0.93	0.15	-	44,48,66,75	0
7	TPO	G	11	11/12	0.51	0.31	-	72,80,107,107	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
21	CHD	W	1059	29/29	0.41	0.51	16.08	103,122,124,124	0
20	PGV	A	524	51/51	0.78	0.24	11.39	39,75,118,121	0
27	DMU	C	272	33/33	0.48	0.32	10.66	79,115,119,122	0
21	CHD	J	60	29/29	0.47	0.45	10.44	107,123,126,126	0
26	CDL	P	1270	100/100	0.71	0.33	8.41	41,95,114,116	0
20	PGV	N	1524	51/51	0.69	0.32	5.16	50,78,121,124	0
26	CDL	C	270	100/100	0.71	0.34	4.98	45,95,113,114	0
19	TGL	N	1522	63/63	0.64	0.26	4.72	49,72,85,88	0
27	DMU	P	1272	33/33	0.50	0.33	4.62	84,116,120,121	0
19	TGL	L	522	63/63	0.78	0.23	3.73	37,62,79,81	0
21	CHD	P	1271	29/29	0.76	0.34	3.17	95,109,114,115	0
19	TGL	O	1521	63/63	0.83	0.17	3.06	49,74,94,99	0
19	TGL	A	523	63/63	0.80	0.18	3.01	52,75,91,93	0
21	CHD	C	271	29/29	0.76	0.47	2.95	95,110,116,117	0
19	TGL	B	521	63/63	0.83	0.18	2.80	51,70,96,101	0
19	TGL	N	1523	63/63	0.66	0.23	2.70	54,79,93,95	0
23	PSC	R	1229	52/52	0.62	0.33	2.48	48,100,130,134	0
20	PGV	C	268	51/51	0.72	0.36	2.45	54,89,113,114	0
23	PSC	B	229	52/52	0.67	0.29	2.41	52,101,130,132	0
26	CDL	G	269	100/100	0.58	0.29	2.35	60,88,121,127	0
27	DMU	Z	1526	33/33	0.83	0.24	2.29	43,57,73,75	0
26	CDL	T	1269	100/100	0.62	0.28	2.22	58,90,120,122	0
20	PGV	G	1268	51/51	0.69	0.36	1.99	69,93,110,113	0
25	PEK	T	263	53/53	0.52	0.39	1.96	49,96,124,125	0
28	ZN	F	99	1/1	0.99	0.09	1.89	32,32,32,32	0
17	MG	N	518	1/1	0.95	0.13	1.84	30,30,30,30	0
25	PEK	G	1263	53/53	0.59	0.43	1.66	53,99,127,128	0
25	PEK	P	1265	53/53	0.56	0.31	1.43	46,87,117,120	0
17	MG	A	518	1/1	0.98	0.11	1.34	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	DMU	M	526	33/33	0.87	0.13	1.24	34,46,66,68	0
21	CHD	A	525	29/29	0.96	0.15	0.95	23,31,37,39	0
21	CHD	P	1525	29/29	0.95	0.14	0.71	28,33,38,42	0
20	PGV	P	1267	51/51	0.97	0.12	0.66	27,39,76,78	0
14	HEA	N	516	60/60	0.98	0.13	0.62	21,29,40,42	0
20	PGV	N	1266	51/51	0.97	0.15	0.61	23,39,64,65	0
20	PGV	C	267	51/51	0.96	0.11	0.55	26,35,69,73	0
25	PEK	G	265	53/53	0.49	0.23	0.55	57,87,115,119	0
28	ZN	S	99	1/1	0.99	0.08	0.45	35,35,35,35	0
25	PEK	P	1264	53/53	0.95	0.13	0.45	30,48,75,77	0
25	PEK	C	264	53/53	0.96	0.11	0.37	24,42,72,74	0
20	PGV	A	521	51/51	0.97	0.12	0.34	23,32,57,60	0
18	NA	N	519	1/1	0.97	0.10	0.17	36,36,36,36	0
22	CUA	B	228	2/2	0.99	0.11	0.14	23,23,23,24	0
22	CUA	O	228	2/2	0.97	0.09	0.08	31,31,31,31	0
14	HEA	N	515	60/60	0.98	0.11	0.01	23,30,47,55	0
21	CHD	G	86	29/29	0.95	0.10	-0.36	22,28,34,35	0
14	HEA	A	516	60/60	0.98	0.12	-0.38	14,23,34,36	0
21	CHD	B	1085	29/29	0.95	0.08	-0.43	22,28,33,38	0
14	HEA	A	515	60/60	0.98	0.12	-0.52	17,24,43,60	0
16	CMO	N	520	2/2	0.94	0.12	-1.51	30,30,30,30	0
18	NA	A	519	1/1	0.97	0.05	-2.09	30,30,30,30	0
15	CU	N	517	1/1	0.99	0.14	-	29,29,29,29	0
15	CU	A	517	1/1	0.99	0.13	-	22,22,22,22	0
16	CMO	A	520	2/2	0.92	0.12	-	25,25,25,25	0
24	UNX	C	262	1/1	0.55	0.60	-	69,69,69,69	0
24	UNX	P	262	1/1	0.70	0.62	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.