



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AG3
Title : Bovine Heart Cytochrome c Oxidase in the Nitric Oxide-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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

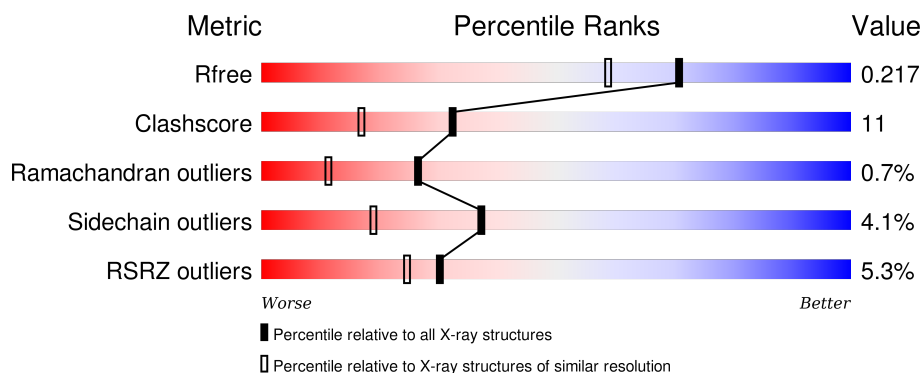
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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></div> <div>76%21%..</div> </div>
1	N	514	<div> <div>%</div> <div>76%20%..</div> </div>
2	B	227	<div> <div></div> <div>70%25%..</div> </div>
2	O	227	<div> <div>3%</div> <div>73%22%..</div> </div>
3	C	261	<div> <div>%</div> <div>78%20%..</div> </div>

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	515	X	-	-	-
14	HEA	N	516	X	-	-	-
17	MG	N	518	-	-	-	X
19	TGL	A	521	-	-	-	X
19	TGL	D	523	-	-	-	X
19	TGL	L	522	-	-	-	X
19	TGL	N	1522	-	-	-	X
19	TGL	O	1521	-	-	-	X
19	TGL	Q	1523	-	-	-	X
20	PGV	C	268	-	-	-	X
20	PGV	M	524	-	-	-	X
20	PGV	N	1524	-	-	-	X
20	PGV	P	1268	-	-	-	X
22	PSC	B	229	-	-	X	X
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	P	1271	X	-	-	-
23	CHD	W	1059	X	-	-	X
25	PEK	G	1263	-	-	X	X
25	PEK	T	263	-	-	X	-
26	CDL	C	270	-	-	X	X
26	CDL	G	269	-	-	X	X
26	CDL	P	1270	-	-	X	X
26	CDL	T	1269	-	-	X	X
28	DMU	G	272	X	-	-	X
28	DMU	M	526	X	-	-	X
28	DMU	P	1272	X	-	-	X
28	DMU	Z	1526	X	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32545 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	5	0
			4060	2712	628	684	36			
1	N	514	Total	C	N	O	S	0	5	0
			4060	2712	628	684	36			

- 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 675	C 431	N 129	O 113	P 1	S 1	0	0	0
7	T	84	Total 675	C 431	N 129	O 113	P 1	S 1	0	0	0

- 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			

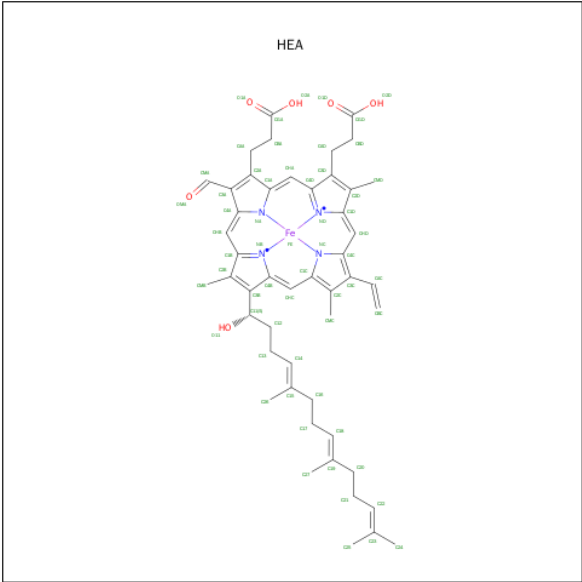
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C.

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.

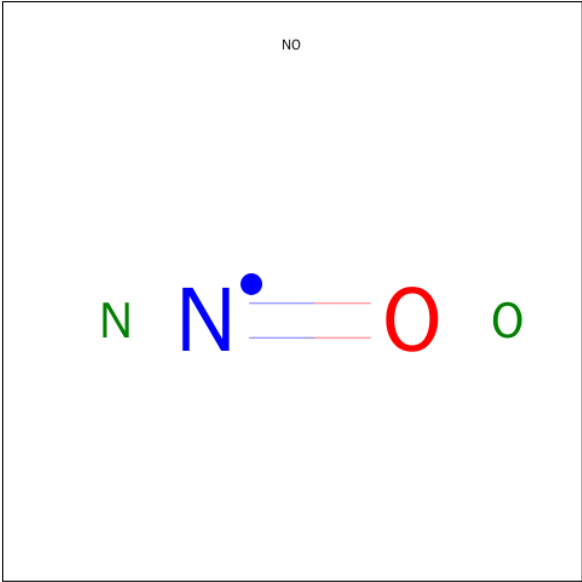
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

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



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

- Molecule 15 is NITRIC OXIDE (three-letter code: NO) (formula: NO).



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

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

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

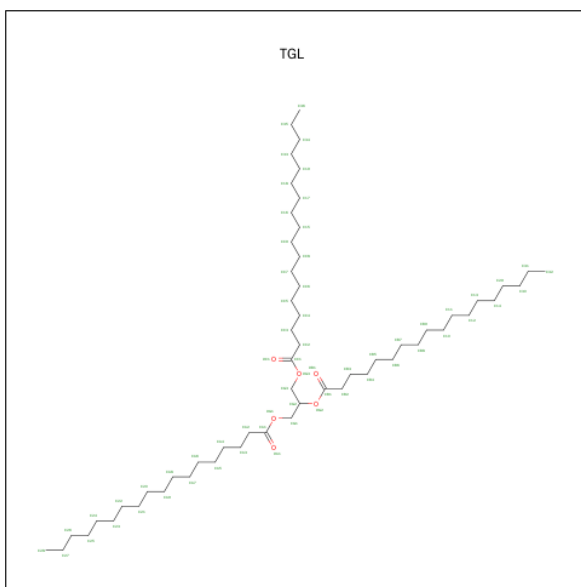
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

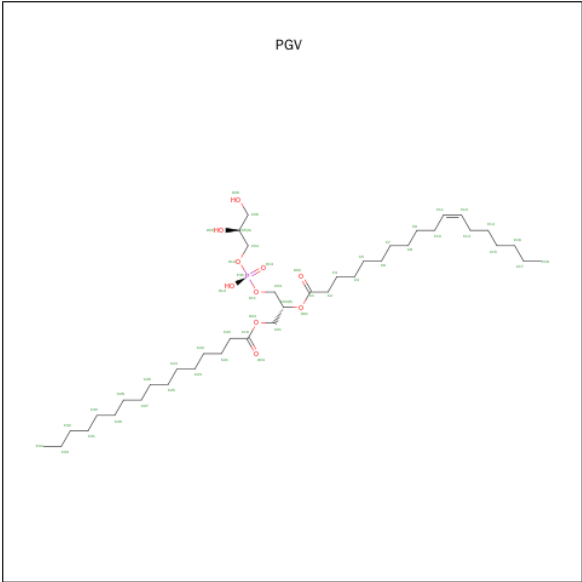
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total Na 1 1	0	0
18	N	1	Total Na 1 1	0	0

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



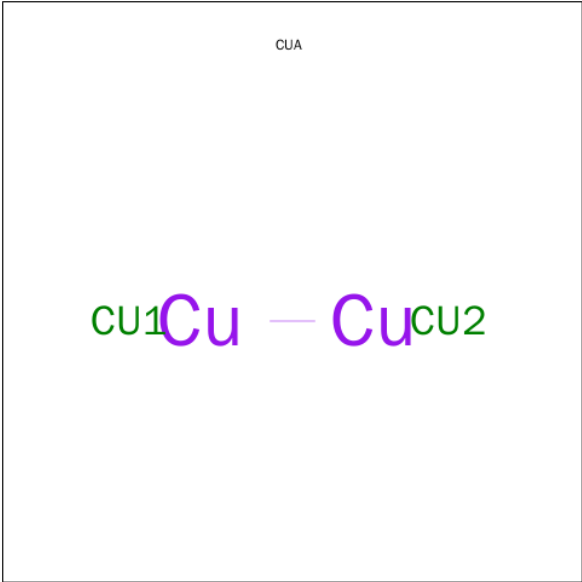
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

- 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).



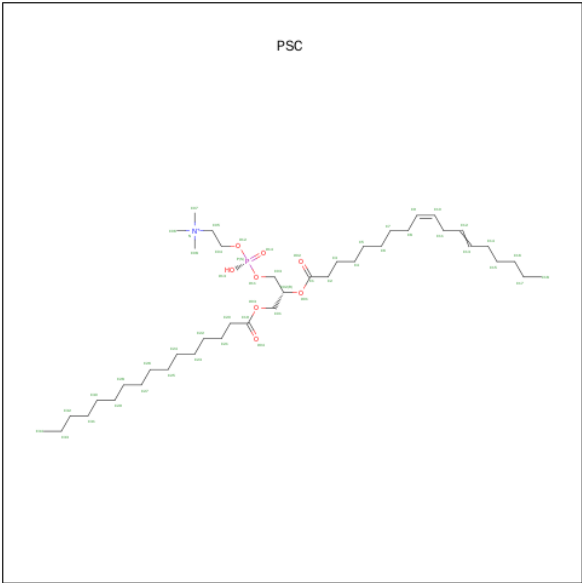
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	M	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



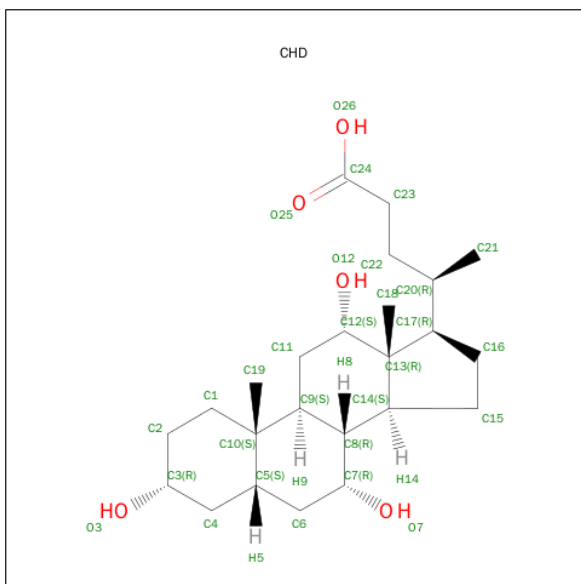
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

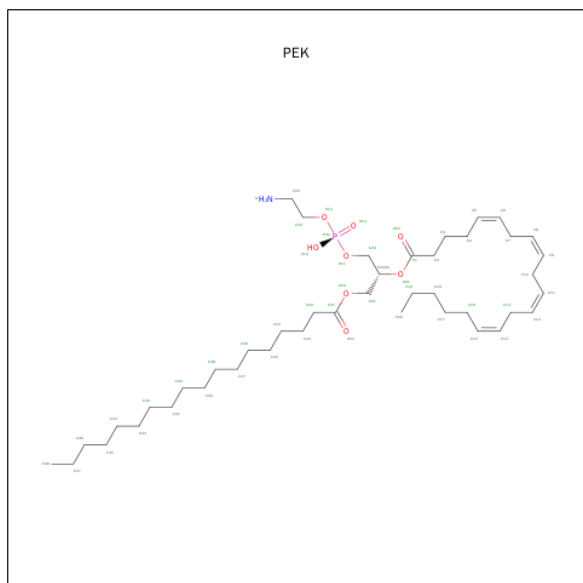


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total 29	C 24	O 5	0	0
23	C	1	Total 29	C 24	O 5	0	0
23	C	1	Total 29	C 24	O 5	0	0
23	J	1	Total 29	C 24	O 5	0	0
23	O	1	Total 29	C 24	O 5	0	0
23	P	1	Total 29	C 24	O 5	0	0
23	P	1	Total 29	C 24	O 5	0	0
23	W	1	Total 29	C 24	O 5	0	0

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

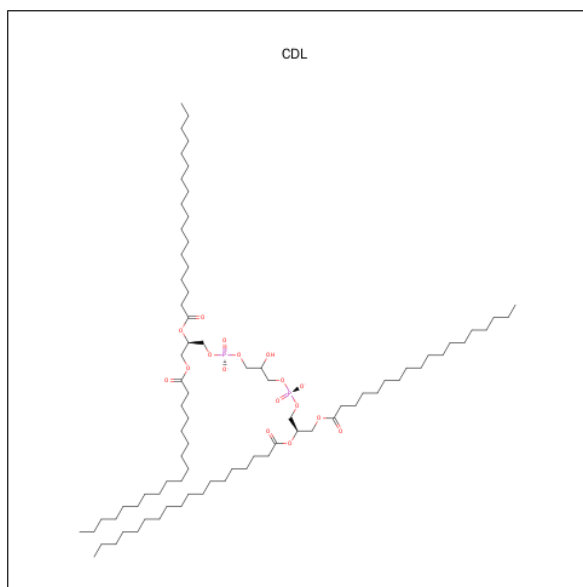
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



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

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).

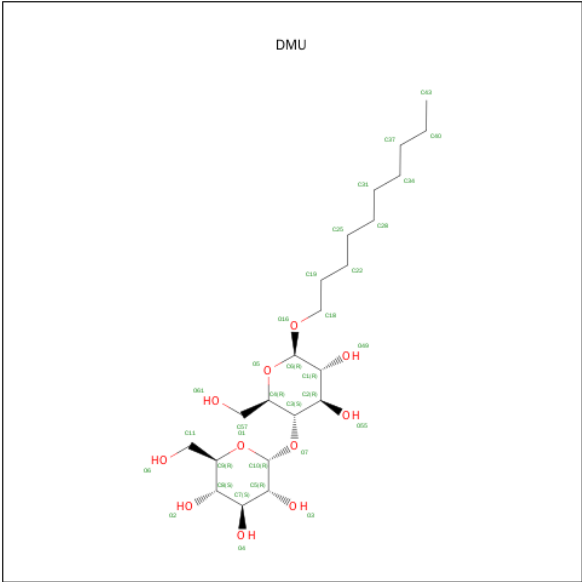


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

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

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

- Molecule 28 is SUGAR (DECYL-BETA-D-MALTOPYRANOSIDE) (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	218	Total	O	0	0
			218	218		
29	B	143	Total	O	0	0
			143	143		
29	C	116	Total	O	0	0
			116	116		
29	D	80	Total	O	0	0
			80	80		
29	E	49	Total	O	0	0
			49	49		
29	F	61	Total	O	0	0
			61	61		
29	G	45	Total	O	0	0
			45	45		
29	H	51	Total	O	0	0
			51	51		

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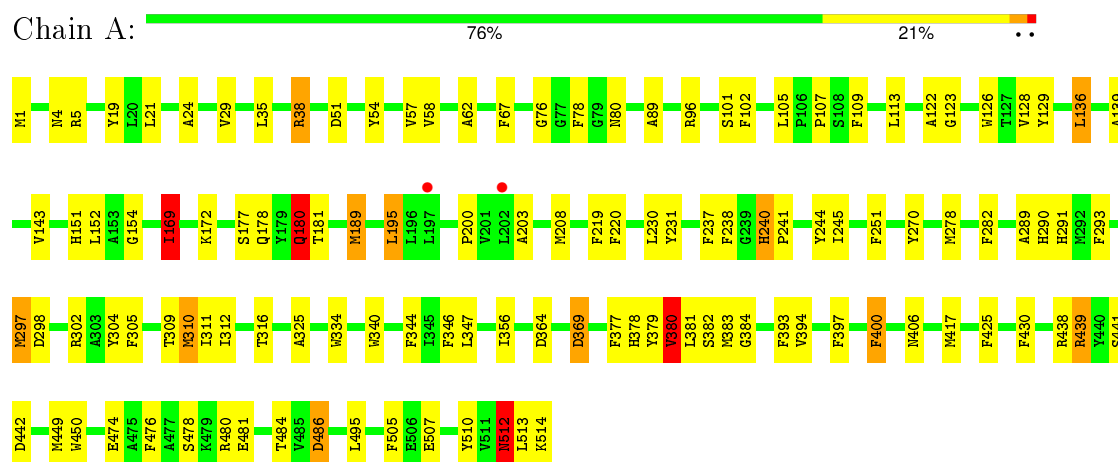
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	37	Total O 37 37	0	0
29	J	24	Total O 24 24	0	0
29	K	29	Total O 29 29	0	0
29	L	23	Total O 23 23	0	0
29	M	31	Total O 31 31	0	0
29	N	222	Total O 222 222	0	0
29	O	137	Total O 137 137	0	0
29	P	102	Total O 102 102	0	0
29	Q	65	Total O 65 65	0	0
29	R	47	Total O 47 47	0	0
29	S	64	Total O 64 64	0	0
29	T	47	Total O 47 47	0	0
29	U	49	Total O 49 49	0	0
29	V	27	Total O 27 27	0	0
29	W	19	Total O 19 19	0	0
29	X	22	Total O 22 22	0	0
29	Y	21	Total O 21 21	0	0
29	Z	14	Total O 14 14	0	0

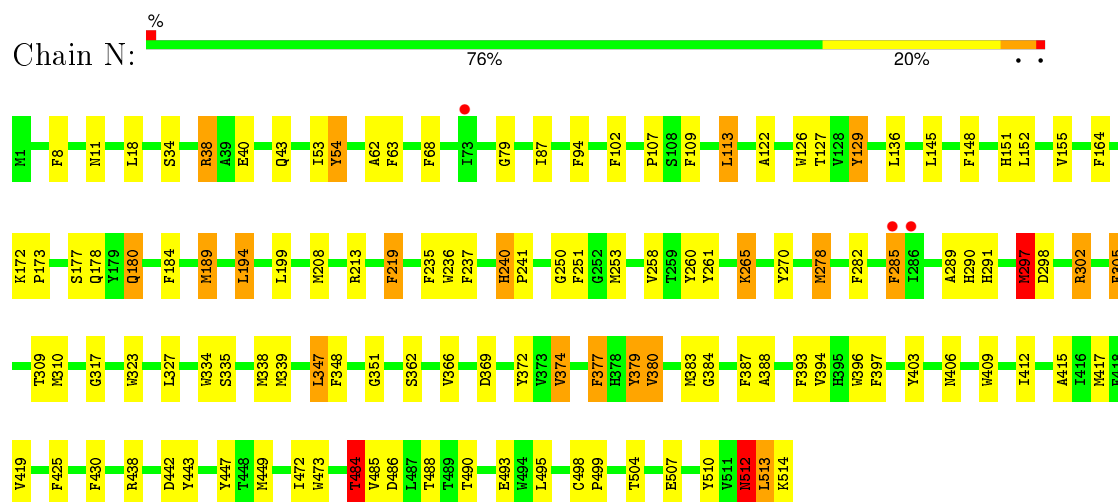
3 Residue-property plots

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

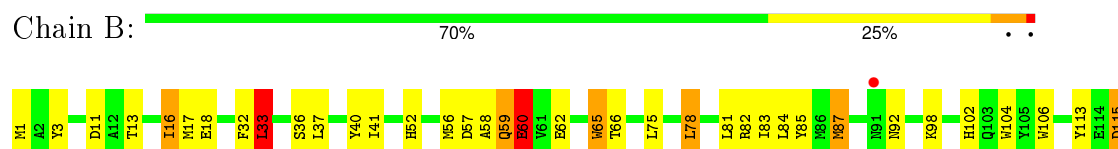
• Molecule 1: Cytochrome c oxidase subunit 1



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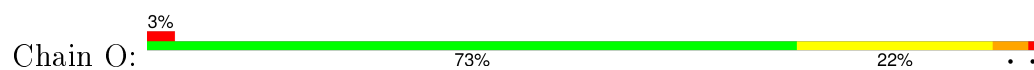


• Molecule 2: Cytochrome c oxidase subunit 2

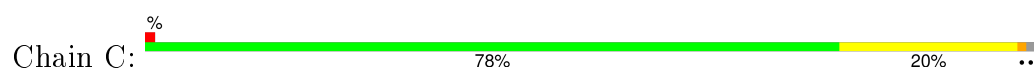




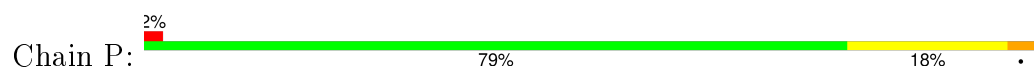
• Molecule 2: Cytochrome c oxidase subunit 2



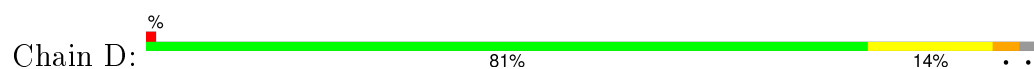
• Molecule 3: Cytochrome c oxidase subunit 3



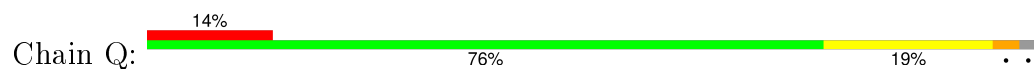
• Molecule 3: Cytochrome c oxidase subunit 3

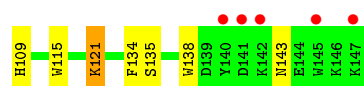


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

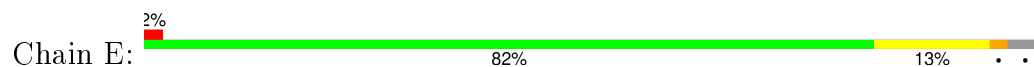


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

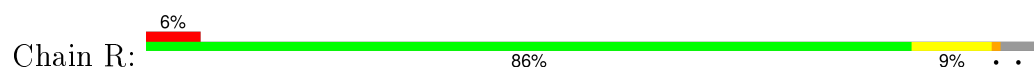




- Molecule 5: Cytochrome c oxidase subunit 5A



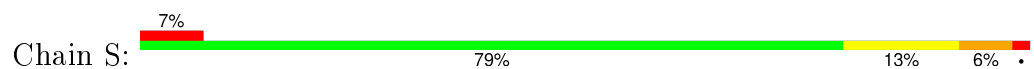
- Molecule 5: Cytochrome c oxidase subunit 5A



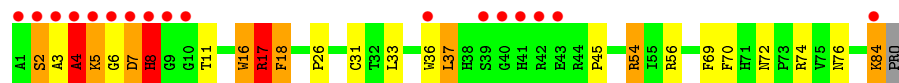
- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 7: Cytochrome c oxidase subunit 6A2

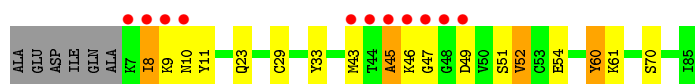


- Molecule 7: Cytochrome c oxidase subunit 6A2

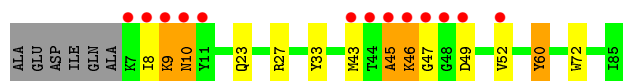
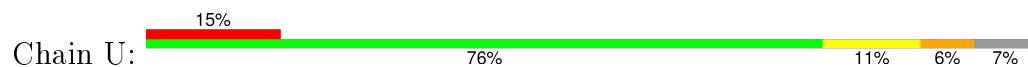


- Molecule 8: Cytochrome c oxidase subunit 6B1

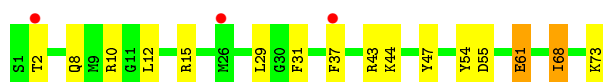
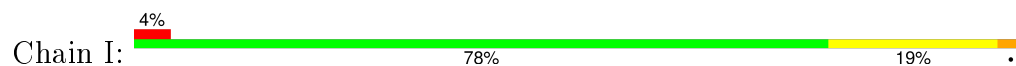




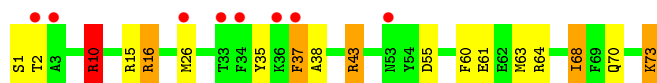
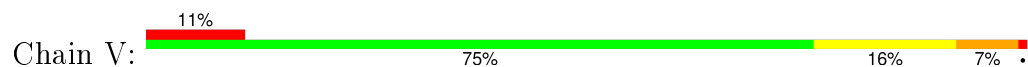
- Molecule 8: Cytochrome c oxidase subunit 6B1



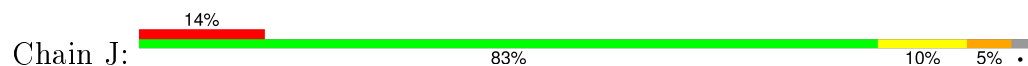
- Molecule 9: Cytochrome c oxidase subunit 6C



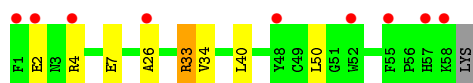
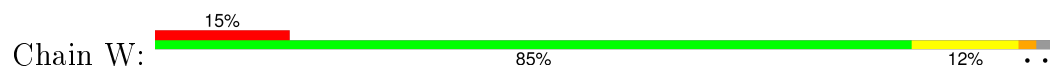
- Molecule 9: Cytochrome c oxidase subunit 6C



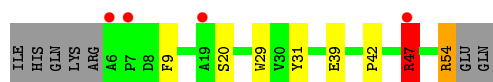
- Molecule 10: Cytochrome c oxidase polypeptide 7A1



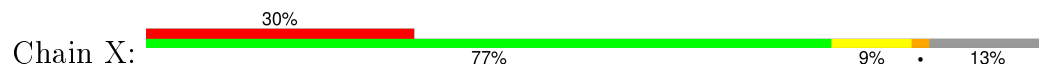
- Molecule 10: Cytochrome c oxidase polypeptide 7A1

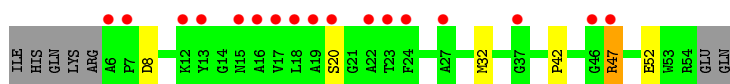


- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B





- Molecule 12: Cytochrome c oxidase subunit 7C



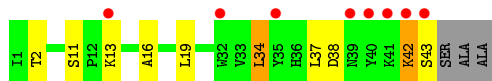
- Molecule 12: Cytochrome c oxidase subunit 7C



- 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	182.29Å 208.36Å 177.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80 83.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.80) 99.6 (83.50-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.3	Depositor
R, R_{free}	0.175 , 0.203 0.190 , 0.217	Depositor DCC
R_{free} test set	30650 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 63.7	EDS
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 617373 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32545	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PEK, ZN, CHD, HEA, SAC, CDL, PSC, NO, 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	1.80	66/4189 (1.6%)	1.47	43/5722 (0.8%)
1	N	1.81	63/4189 (1.5%)	1.38	35/5722 (0.6%)
2	B	1.84	41/1860 (2.2%)	1.48	19/2534 (0.7%)
2	O	1.61	21/1860 (1.1%)	1.31	14/2534 (0.6%)
3	C	1.66	26/2197 (1.2%)	1.33	18/3005 (0.6%)
3	P	1.68	21/2197 (1.0%)	1.33	18/3005 (0.6%)
4	D	1.65	12/1229 (1.0%)	1.46	16/1658 (1.0%)
4	Q	1.53	10/1229 (0.8%)	1.30	10/1658 (0.6%)
5	E	1.56	4/871 (0.5%)	1.35	8/1182 (0.7%)
5	R	1.39	3/871 (0.3%)	1.13	2/1182 (0.2%)
6	F	1.66	8/765 (1.0%)	1.32	5/1038 (0.5%)
6	S	1.62	4/765 (0.5%)	1.42	4/1038 (0.4%)
7	G	1.69	10/690 (1.4%)	1.68	8/937 (0.9%)
7	T	1.59	4/690 (0.6%)	1.64	8/937 (0.9%)
8	H	1.59	5/682 (0.7%)	1.21	2/921 (0.2%)
8	U	1.33	2/682 (0.3%)	1.11	0/921
9	I	1.56	4/605 (0.7%)	1.20	4/802 (0.5%)
9	V	1.44	0/605	1.25	6/802 (0.7%)
10	J	1.40	1/471 (0.2%)	1.19	4/636 (0.6%)
10	W	1.55	5/471 (1.1%)	1.20	2/636 (0.3%)
11	K	1.63	5/398 (1.3%)	1.26	3/546 (0.5%)
11	X	1.27	1/398 (0.3%)	1.05	1/546 (0.2%)
12	L	1.68	6/393 (1.5%)	1.27	2/526 (0.4%)
12	Y	1.75	9/393 (2.3%)	1.24	0/526
13	M	1.64	5/345 (1.4%)	1.32	4/470 (0.9%)
13	Z	1.40	2/345 (0.6%)	1.16	3/470 (0.6%)
All	All	1.67	338/29390 (1.2%)	1.36	239/39954 (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	1
2	B	1	0
6	F	0	1
6	S	0	1
All	All	1	3

All (338) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	167	SER	CB-OG	-12.15	1.26	1.42
7	T	36	TRP	CB-CG	11.41	1.70	1.50
7	G	36	TRP	CB-CG	11.12	1.70	1.50
6	S	54	ASN	CB-CG	-10.52	1.26	1.51
4	Q	121	LYS	CE-NZ	10.12	1.74	1.49
3	P	29	SER	CB-OG	-9.97	1.29	1.42
1	N	189	MET	CB-CG	9.80	1.82	1.51
2	B	132	GLU	CD-OE2	9.61	1.36	1.25
11	K	29	TRP	CE3-CZ3	9.40	1.54	1.38
3	C	29	SER	CA-CB	9.34	1.67	1.52
1	N	380[A]	VAL	CB-CG1	-9.06	1.33	1.52
1	N	380[B]	VAL	CB-CG1	-9.06	1.33	1.52
1	A	189	MET	CG-SD	-8.97	1.57	1.81
9	I	61	GLU	CG-CD	-8.96	1.38	1.51
2	B	192	TYR	CE2-CZ	8.87	1.50	1.38
1	A	512	ASN	CB-CG	-8.76	1.30	1.51
2	B	65	TRP	CB-CG	-8.75	1.34	1.50
4	D	104	TYR	CD1-CE1	8.57	1.52	1.39
5	E	55	CYS	CB-SG	8.49	1.96	1.82
4	D	100	LYS	CE-NZ	8.49	1.70	1.49
2	B	59	GLN	CG-CD	8.46	1.70	1.51
3	C	181	TYR	CD1-CE1	8.45	1.52	1.39
1	A	302	ARG	CZ-NH1	8.34	1.43	1.33
7	T	17	ARG	CD-NE	-8.27	1.32	1.46
2	B	87	MET	CG-SD	8.21	2.02	1.81
7	G	17	ARG	CD-NE	-8.12	1.32	1.46
2	O	132	GLU	CD-OE2	8.05	1.34	1.25
7	G	16	TRP	CE3-CZ3	7.98	1.52	1.38
1	A	297	MET	CG-SD	7.93	2.01	1.81
2	B	157	GLU	CB-CG	7.92	1.67	1.52
3	P	46	GLY	N-CA	7.91	1.57	1.46
1	A	346	PHE	CD1-CE1	7.83	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	TRP	CZ3-CH2	7.76	1.52	1.40
3	P	20	GLY	N-CA	7.75	1.57	1.46
1	N	148	PHE	CE1-CZ	7.74	1.52	1.37
1	N	473	TRP	CE3-CZ3	7.71	1.51	1.38
3	P	230	ASN	CB-CG	-7.65	1.33	1.51
3	C	29	SER	CB-OG	-7.61	1.32	1.42
2	O	106	TRP	CE3-CZ3	7.58	1.51	1.38
3	C	181	TYR	CD2-CE2	7.58	1.50	1.39
9	I	54	TYR	CD2-CE2	7.57	1.50	1.39
1	N	484	THR	CB-CG2	7.54	1.77	1.52
1	N	285	PHE	CD1-CE1	7.53	1.54	1.39
5	E	84	TYR	CG-CD1	7.51	1.49	1.39
2	B	40	TYR	CD1-CE1	7.50	1.50	1.39
1	A	394	VAL	CB-CG2	-7.48	1.37	1.52
6	F	56	ARG	CZ-NH1	7.45	1.42	1.33
1	A	129	TYR	CD2-CE2	7.41	1.50	1.39
2	O	59	GLN	CG-CD	7.41	1.68	1.51
1	N	512	ASN	CA-CB	7.34	1.72	1.53
2	B	218	TYR	CD1-CE1	7.34	1.50	1.39
1	N	335	SER	CB-OG	7.33	1.51	1.42
6	F	73	TRP	CE3-CZ3	7.25	1.50	1.38
2	O	60	GLU	CB-CG	7.25	1.66	1.52
1	A	244	TYR	CD1-CE1	7.22	1.50	1.39
2	B	18	GLU	CD-OE1	7.21	1.33	1.25
2	O	60	GLU	CG-CD	7.17	1.62	1.51
3	C	81	TYR	CD1-CE1	7.12	1.50	1.39
1	N	374	VAL	CB-CG2	7.12	1.67	1.52
1	A	346	PHE	CD2-CE2	7.09	1.53	1.39
1	N	394	VAL	CB-CG2	-7.05	1.38	1.52
1	N	403	TYR	CE1-CZ	-7.04	1.29	1.38
13	M	4	LYS	CD-CE	-7.03	1.33	1.51
1	N	425	PHE	CD1-CE1	-7.03	1.25	1.39
7	T	5	LYS	CB-CG	7.03	1.71	1.52
3	P	181	TYR	CD1-CE1	7.01	1.49	1.39
8	H	61	LYS	CE-NZ	6.98	1.66	1.49
1	N	447	TYR	CE1-CZ	6.94	1.47	1.38
2	B	115	ASP	CB-CG	6.92	1.66	1.51
1	N	297	MET	CG-SD	6.92	1.99	1.81
7	G	5	LYS	CB-CG	6.89	1.71	1.52
11	K	39	GLU	CB-CG	6.88	1.65	1.52
4	Q	87	PHE	CG-CD1	6.88	1.49	1.38
1	A	129	TYR	CE2-CZ	-6.83	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	87	PHE	CD1-CE1	6.83	1.52	1.39
1	N	260	TYR	CD1-CE1	6.79	1.49	1.39
3	P	218	CYS	CB-SG	6.78	1.93	1.82
1	N	94	PHE	CE2-CZ	6.76	1.50	1.37
2	B	60	GLU	CG-CD	6.74	1.62	1.51
5	R	9	GLU	CG-CD	6.73	1.62	1.51
1	A	122	ALA	CA-CB	6.72	1.66	1.52
4	Q	9	GLU	CB-CG	6.64	1.64	1.52
1	N	236	TRP	CE3-CZ3	6.62	1.49	1.38
1	A	101	SER	CB-OG	6.60	1.50	1.42
2	O	65	TRP	CB-CG	-6.60	1.38	1.50
6	S	71	TRP	CE3-CZ3	6.55	1.49	1.38
2	B	92	ASN	CB-CG	6.53	1.66	1.51
2	O	196	CYS	CB-SG	6.53	1.93	1.82
1	N	397	PHE	CE2-CZ	6.52	1.49	1.37
2	O	202	SER	CA-CB	6.52	1.62	1.52
1	A	293	PHE	CB-CG	6.51	1.62	1.51
6	F	1	ALA	CA-CB	6.51	1.66	1.52
1	A	154	GLY	N-CA	6.50	1.55	1.46
10	J	7	GLU	CG-CD	6.48	1.61	1.51
9	I	47	TYR	CD2-CE2	6.47	1.49	1.39
13	Z	16	ALA	CA-CB	6.47	1.66	1.52
1	A	298	ASP	CG-OD2	6.46	1.40	1.25
1	A	89	ALA	CA-CB	6.45	1.66	1.52
3	P	86	PHE	CD1-CE1	6.44	1.52	1.39
12	Y	20	ARG	CG-CD	6.43	1.68	1.51
2	B	147	GLU	CG-CD	6.42	1.61	1.51
1	A	231	TYR	CG-CD1	6.39	1.47	1.39
1	A	38	ARG	CZ-NH2	6.39	1.41	1.33
3	C	253	TYR	CG-CD1	6.39	1.47	1.39
1	A	507	GLU	CG-CD	6.38	1.61	1.51
2	B	192	TYR	CG-CD1	6.38	1.47	1.39
6	F	92	VAL	CB-CG2	-6.38	1.39	1.52
12	Y	13	PHE	CD2-CE2	6.38	1.52	1.39
6	F	1	ALA	C-O	6.38	1.35	1.23
5	R	75	ALA	CA-CB	6.36	1.65	1.52
1	A	238	PHE	CD1-CE1	6.35	1.51	1.39
2	O	202	SER	CB-OG	-6.34	1.34	1.42
1	N	415	ALA	CA-CB	6.33	1.65	1.52
2	B	85	TYR	CD1-CE1	6.30	1.48	1.39
2	O	60	GLU	CD-OE2	6.29	1.32	1.25
12	Y	46	LYS	CD-CE	-6.26	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	21	VAL	CB-CG2	6.25	1.66	1.52
3	P	8	TYR	CD2-CE2	6.24	1.48	1.39
1	N	155	VAL	CB-CG2	6.24	1.66	1.52
1	N	348	PHE	CD1-CE1	6.20	1.51	1.39
10	W	26	ALA	CA-CB	6.19	1.65	1.52
1	A	298	ASP	CB-CG	6.17	1.64	1.51
1	N	302	ARG	CZ-NH1	6.15	1.41	1.33
2	B	18	GLU	CD-OE2	6.13	1.32	1.25
1	A	19	TYR	CE2-CZ	6.13	1.46	1.38
7	T	50	TYR	CD2-CE2	6.12	1.48	1.39
5	E	9	GLU	CG-CD	6.12	1.61	1.51
3	P	172	TYR	CG-CD1	6.10	1.47	1.39
1	A	379	TYR	CD1-CE1	6.09	1.48	1.39
12	L	5	GLU	CD-OE2	-6.09	1.19	1.25
2	B	218	TYR	CD2-CE2	6.07	1.48	1.39
1	N	164	PHE	CD2-CE2	6.07	1.51	1.39
3	P	193	TYR	CG-CD2	6.07	1.47	1.39
1	N	79	GLY	N-CA	6.05	1.55	1.46
3	P	77	LYS	CA-CB	-6.03	1.40	1.53
10	W	7	GLU	CD-OE1	6.02	1.32	1.25
2	O	3	TYR	CD2-CE2	6.02	1.48	1.39
6	S	31	TYR	CG-CD2	6.00	1.47	1.39
12	L	13	PHE	CG-CD1	5.98	1.47	1.38
1	A	123	GLY	C-O	5.98	1.33	1.23
1	A	128	VAL	CB-CG1	5.97	1.65	1.52
6	S	1	ALA	CA-CB	5.97	1.65	1.52
4	D	87	PHE	CE2-CZ	5.96	1.48	1.37
4	Q	17	VAL	CB-CG1	-5.95	1.40	1.52
3	C	172	TYR	CG-CD1	5.95	1.46	1.39
3	P	251	PHE	CD1-CE1	5.95	1.51	1.39
1	A	113	LEU	CB-CG	5.94	1.69	1.52
1	A	24	ALA	CA-CB	5.93	1.64	1.52
2	O	192	TYR	CD2-CE2	5.92	1.48	1.39
1	N	122	ALA	CA-CB	5.91	1.64	1.52
3	P	64	GLU	CG-CD	5.90	1.60	1.51
4	D	138	TRP	CE3-CZ3	5.90	1.48	1.38
1	A	439	ARG	CD-NE	5.90	1.56	1.46
2	O	193	TYR	CD1-CE1	5.88	1.48	1.39
4	D	100	LYS	CD-CE	5.88	1.66	1.51
1	A	430	PHE	CD1-CE1	5.87	1.50	1.39
1	A	244	TYR	CD2-CE2	5.85	1.48	1.39
6	F	76	LYS	CD-CE	5.85	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	372	TYR	CD2-CE2	5.85	1.48	1.39
1	N	235	PHE	CD2-CE2	5.84	1.50	1.39
13	M	32	TRP	CG-CD1	5.83	1.45	1.36
3	C	146	TRP	CE3-CZ3	5.82	1.48	1.38
11	K	9	PHE	CE2-CZ	5.82	1.48	1.37
1	A	380[A]	VAL	CB-CG1	-5.80	1.40	1.52
1	A	380[B]	VAL	CB-CG1	-5.80	1.40	1.52
2	B	210	VAL	CB-CG2	5.80	1.65	1.52
1	N	397	PHE	CG-CD1	5.80	1.47	1.38
2	O	65	TRP	CE3-CZ3	5.80	1.48	1.38
2	B	65	TRP	CD1-NE1	5.79	1.47	1.38
1	N	297	MET	CB-CG	5.78	1.69	1.51
3	C	227	PHE	CE1-CZ	5.78	1.48	1.37
1	A	450	TRP	CB-CG	5.78	1.60	1.50
2	B	120	SER	CB-OG	5.77	1.49	1.42
1	A	305	PHE	CE2-CZ	5.77	1.48	1.37
1	A	340	TRP	CD2-CE2	5.75	1.48	1.41
2	B	118	PHE	CG-CD1	5.74	1.47	1.38
1	N	113	LEU	CG-CD1	5.74	1.73	1.51
1	N	63	PHE	CE2-CZ	5.73	1.48	1.37
1	A	54	TYR	CD2-CE2	5.73	1.48	1.39
1	A	57	VAL	CB-CG1	5.73	1.64	1.52
3	C	186	PHE	CE1-CZ	5.73	1.48	1.37
2	O	127	GLU	CD-OE2	5.72	1.31	1.25
1	A	113	LEU	CG-CD1	5.72	1.73	1.51
4	Q	88	PHE	CE1-CZ	5.72	1.48	1.37
12	L	37	PHE	CD1-CE1	5.72	1.50	1.39
1	A	476	PHE	CE2-CZ	5.71	1.48	1.37
3	C	214	PHE	CE2-CZ	5.71	1.48	1.37
1	N	251	PHE	CE2-CZ	5.71	1.48	1.37
1	N	235	PHE	CD1-CE1	5.68	1.50	1.39
1	N	113	LEU	CB-CG	5.68	1.69	1.52
2	B	3	TYR	CD2-CE2	-5.67	1.30	1.39
13	M	32	TRP	CB-CG	5.67	1.60	1.50
3	C	161	GLN	CG-CD	5.67	1.64	1.51
8	H	33	TYR	CD1-CE1	5.67	1.47	1.39
1	N	270	TYR	CD2-CE2	5.65	1.47	1.39
3	C	81	TYR	CD2-CE2	5.65	1.47	1.39
11	K	31	TYR	CD2-CE2	5.64	1.47	1.39
5	E	70	VAL	CB-CG2	5.64	1.64	1.52
2	O	92	ASN	CB-CG	5.64	1.64	1.51
1	A	19	TYR	CG-CD1	5.63	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	35	PHE	CE1-CZ	5.62	1.48	1.37
1	A	251	PHE	CG-CD2	5.62	1.47	1.38
2	O	59	GLN	CB-CG	5.60	1.67	1.52
3	P	195	SER	CB-OG	5.60	1.49	1.42
12	Y	5	GLU	CD-OE2	-5.60	1.19	1.25
3	P	233	PHE	CD1-CE1	5.60	1.50	1.39
4	Q	138	TRP	CE3-CZ3	5.60	1.48	1.38
3	C	90	GLU	CD-OE1	5.59	1.31	1.25
12	Y	33	PHE	CE2-CZ	5.59	1.48	1.37
7	G	70	PHE	CD2-CE2	5.58	1.50	1.39
2	B	60	GLU	CB-CG	5.58	1.62	1.52
2	B	59	GLN	CB-CG	5.58	1.67	1.52
1	N	237	PHE	CD1-CE1	5.56	1.50	1.39
1	N	261	TYR	CE2-CZ	5.56	1.45	1.38
2	O	212	GLU	CD-OE1	5.56	1.31	1.25
5	R	84	TYR	CG-CD1	5.55	1.46	1.39
1	A	143	VAL	CB-CG1	5.55	1.64	1.52
1	A	480	ARG	CZ-NH2	5.54	1.40	1.33
2	B	155	SER	CA-CB	5.54	1.61	1.52
1	N	261	TYR	CG-CD1	5.54	1.46	1.39
10	W	7	GLU	CB-CG	-5.54	1.41	1.52
2	B	106	TRP	CB-CG	5.54	1.60	1.50
3	C	33	MET	CG-SD	5.53	1.95	1.81
1	N	219	PHE	CE1-CZ	5.51	1.47	1.37
1	A	379	TYR	CD2-CE2	5.49	1.47	1.39
7	G	56	ARG	CZ-NH1	5.49	1.40	1.33
2	O	105	TYR	CG-CD2	5.49	1.46	1.39
1	N	258	VAL	CB-CG1	-5.47	1.41	1.52
1	N	184	PHE	CE1-CZ	5.47	1.47	1.37
8	U	33	TYR	CE2-CZ	5.47	1.45	1.38
1	A	425	PHE	CD2-CE2	5.46	1.50	1.39
1	N	419	VAL	CA-CB	5.46	1.66	1.54
2	B	147	GLU	CD-OE1	-5.46	1.19	1.25
2	B	36	SER	CA-CB	5.45	1.61	1.52
4	D	4	SER	N-CA	5.45	1.57	1.46
7	G	70	PHE	CG-CD2	5.45	1.47	1.38
1	N	510	TYR	CD2-CE2	5.45	1.47	1.39
1	A	344	PHE	CD2-CE2	5.44	1.50	1.39
1	A	510	TYR	CE2-CZ	5.44	1.45	1.38
1	N	396	TRP	CE3-CZ3	5.43	1.47	1.38
1	N	323	TRP	CZ3-CH2	5.43	1.48	1.40
3	P	33	MET	CG-SD	5.43	1.95	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	W	34	VAL	CB-CG2	5.43	1.64	1.52
2	B	200	CYS	CB-SG	5.42	1.91	1.82
1	A	474	GLU	CG-CD	5.40	1.60	1.51
2	B	151	ARG	CB-CG	5.40	1.67	1.52
1	N	11	ASN	C-O	5.40	1.33	1.23
4	Q	134	PHE	CE1-CZ	5.40	1.47	1.37
8	H	23	GLN	CG-CD	5.39	1.63	1.51
3	C	91	VAL	CB-CG1	5.39	1.64	1.52
1	N	236	TRP	CG-CD1	5.38	1.44	1.36
1	A	505	PHE	CE2-CZ	5.36	1.47	1.37
1	A	67	PHE	CG-CD2	5.36	1.46	1.38
1	A	438	ARG	CG-CD	5.36	1.65	1.51
4	D	19	ARG	CZ-NH2	5.36	1.40	1.33
1	A	293	PHE	CG-CD1	5.35	1.46	1.38
12	L	35	ALA	CA-CB	5.35	1.63	1.52
1	N	126	TRP	CE3-CZ3	5.35	1.47	1.38
9	I	61	GLU	CB-CG	-5.35	1.42	1.52
1	N	447	TYR	CD2-CE2	5.35	1.47	1.39
8	H	70	SER	CB-OG	-5.34	1.35	1.42
3	C	64	GLU	CG-CD	5.34	1.59	1.51
8	U	72	TRP	CB-CG	5.34	1.59	1.50
2	B	143	VAL	CB-CG2	5.33	1.64	1.52
12	Y	20	ARG	CB-CG	5.32	1.67	1.52
3	P	172	TYR	CE2-CZ	5.32	1.45	1.38
3	P	253	TYR	CD2-CE2	5.32	1.47	1.39
1	N	388	ALA	CA-CB	5.32	1.63	1.52
3	C	230	ASN	CB-CG	-5.30	1.38	1.51
2	O	105	TYR	CE1-CZ	5.29	1.45	1.38
3	C	258	TRP	CE3-CZ3	5.29	1.47	1.38
7	G	18	PHE	CE2-CZ	-5.28	1.27	1.37
1	N	393	PHE	CG-CD2	5.27	1.46	1.38
3	C	197	PHE	CE1-CZ	5.27	1.47	1.37
3	C	254	VAL	CB-CG2	5.27	1.64	1.52
4	D	104	TYR	CG-CD2	5.27	1.46	1.39
1	N	317	GLY	N-CA	5.26	1.53	1.46
2	B	106	TRP	CD1-NE1	5.26	1.46	1.38
1	A	139	ALA	CA-CB	5.26	1.63	1.52
3	P	220	PHE	CE2-CZ	5.26	1.47	1.37
2	B	197	SER	CB-OG	5.26	1.49	1.42
8	H	54	GLU	CB-CG	5.25	1.62	1.52
4	D	20	ARG	CD-NE	-5.24	1.37	1.46
1	A	29	VAL	CB-CG1	5.24	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	233	PHE	CD1-CE1	5.23	1.49	1.39
1	N	493	GLU	CB-CG	5.23	1.62	1.52
13	M	3	ALA	CA-CB	5.23	1.63	1.52
13	Z	11	SER	C-O	5.22	1.33	1.23
2	B	192	TYR	CD1-CE1	5.21	1.47	1.39
4	Q	60	TYR	CE2-CZ	5.21	1.45	1.38
4	Q	64	PHE	CE1-CZ	5.21	1.47	1.37
2	B	32	PHE	CG-CD1	5.21	1.46	1.38
1	A	270	TYR	CB-CG	5.20	1.59	1.51
1	N	54	TYR	CD2-CE2	5.20	1.47	1.39
6	F	92	VAL	CA-CB	5.18	1.65	1.54
1	N	219	PHE	CE2-CZ	5.18	1.47	1.37
1	A	78	PHE	CG-CD1	5.18	1.46	1.38
4	Q	115	TRP	CG-CD1	5.18	1.44	1.36
11	K	54	ARG	CZ-NH1	5.17	1.39	1.33
12	Y	32	GLY	N-CA	5.16	1.53	1.46
4	D	87	PHE	CG-CD1	5.16	1.46	1.38
3	C	80	ARG	CG-CD	5.15	1.64	1.51
1	A	58	VAL	CB-CG1	5.14	1.63	1.52
1	A	67	PHE	CE1-CZ	5.14	1.47	1.37
1	N	305	PHE	CG-CD2	5.14	1.46	1.38
12	Y	4	GLU	CG-CD	5.14	1.59	1.51
2	B	152	MET	CB-CG	-5.14	1.34	1.51
11	X	52	GLU	CD-OE1	5.13	1.31	1.25
6	F	55	LYS	CD-CE	5.12	1.64	1.51
3	P	180	GLU	CD-OE1	5.12	1.31	1.25
7	G	4	ALA	CA-CB	-5.12	1.41	1.52
1	N	379	TYR	CD1-CE1	5.11	1.47	1.39
2	B	17	MET	CG-SD	5.11	1.94	1.81
1	A	154	GLY	C-O	-5.10	1.15	1.23
1	N	8	PHE	CD2-CE2	5.10	1.49	1.39
2	O	97	VAL	CB-CG1	5.09	1.63	1.52
2	B	98	LYS	CD-CE	5.08	1.64	1.51
1	A	289	ALA	CA-CB	5.08	1.63	1.52
3	C	193	TYR	CE1-CZ	5.08	1.45	1.38
1	N	129	TYR	CG-CD2	5.07	1.45	1.39
1	A	393	PHE	CD2-CE2	5.07	1.49	1.39
1	N	377	PHE	CG-CD1	5.07	1.46	1.38
3	P	214	PHE	CE1-CZ	5.06	1.47	1.37
7	G	18	PHE	CD2-CE2	5.06	1.49	1.39
2	B	187	SER	CB-OG	5.05	1.48	1.42
12	L	3	TYR	CE1-CZ	5.05	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	46	LYS	CD-CE	-5.04	1.38	1.51
3	C	225	PHE	CE2-CZ	5.04	1.47	1.37
1	N	43	GLN	CG-CD	5.04	1.62	1.51
1	A	203	ALA	N-CA	5.04	1.56	1.46
4	D	17	VAL	CB-CG2	-5.03	1.42	1.52
1	N	507	GLU	CG-CD	5.03	1.59	1.51
12	Y	28	PHE	CE1-CZ	5.03	1.46	1.37
10	W	33	ARG	CG-CD	5.02	1.64	1.51
2	B	113	TYR	N-CA	5.02	1.56	1.46
1	A	54	TYR	CE2-CZ	5.02	1.45	1.38
1	A	400	PHE	CE1-CZ	5.01	1.46	1.37
1	A	220	PHE	CE2-CZ	5.01	1.46	1.37

All (239) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	17	ARG	NE-CZ-NH1	23.02	131.81	120.30
7	G	17	ARG	NE-CZ-NH2	-22.34	109.13	120.30
7	G	17	ARG	NE-CZ-NH1	22.31	131.46	120.30
7	T	17	ARG	NE-CZ-NH2	-21.59	109.50	120.30
4	D	20	ARG	NE-CZ-NH2	-21.22	109.69	120.30
4	Q	20	ARG	NE-CZ-NH2	-18.22	111.19	120.30
4	D	20	ARG	NE-CZ-NH1	17.80	129.20	120.30
4	Q	20	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	N	278	MET	CG-SD-CE	-12.57	80.08	100.20
1	A	136	LEU	CB-CG-CD2	-11.98	90.63	111.00
5	E	90	ARG	NE-CZ-NH2	-11.90	114.35	120.30
4	D	19	ARG	NE-CZ-NH1	-11.30	114.65	120.30
6	S	54	ASN	CB-CA-C	-11.14	88.11	110.40
1	N	310	MET	CG-SD-CE	-10.53	83.34	100.20
5	E	40	ASP	CB-CG-OD2	10.46	127.71	118.30
2	B	37	LEU	CB-CG-CD1	-10.40	93.32	111.00
5	E	90	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	A	189	MET	CG-SD-CE	-9.98	84.23	100.20
1	A	297	MET	CG-SD-CE	-9.48	85.03	100.20
1	N	298	ASP	CB-CG-OD2	9.34	126.70	118.30
11	K	47	ARG	NE-CZ-NH2	9.32	124.96	120.30
3	P	156	ARG	NE-CZ-NH1	-9.31	115.64	120.30
7	T	14	ARG	NE-CZ-NH2	-9.19	115.71	120.30
7	G	33	LEU	CA-CB-CG	9.13	136.30	115.30
2	O	82	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	A	298	ASP	CB-CG-OD2	8.89	126.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	82	ARG	CG-CD-NE	-8.61	93.73	111.80
2	B	65	TRP	CB-CA-C	8.47	127.33	110.40
3	C	221	ARG	NE-CZ-NH1	-8.17	116.22	120.30
3	P	221	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	A	5	ARG	NE-CZ-NH2	-8.13	116.23	120.30
11	K	54	ARG	NE-CZ-NH2	-7.88	116.36	120.30
2	B	87	MET	CA-CB-CG	7.87	126.67	113.30
3	P	80	ARG	CG-CD-NE	-7.83	95.35	111.80
3	C	94	PHE	CB-CG-CD2	-7.79	115.35	120.80
13	M	34	LEU	CB-CG-CD1	7.69	124.07	111.00
5	E	60	ASP	CB-CG-OD2	7.66	125.19	118.30
7	G	17	ARG	CB-CG-CD	-7.61	91.81	111.60
1	N	442	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	N	113	LEU	CB-CG-CD1	7.49	123.74	111.00
1	A	417	MET	CG-SD-CE	-7.40	88.36	100.20
1	A	136	LEU	CA-CB-CG	7.37	132.24	115.30
1	A	510	TYR	CB-CG-CD2	-7.32	116.61	121.00
9	I	68	ILE	CG1-CB-CG2	7.26	127.37	111.40
3	P	155	ASP	CB-CG-OD1	7.22	124.80	118.30
3	P	63	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	189	MET	CA-CB-CG	-7.18	101.08	113.30
7	G	54	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	N	145	LEU	CA-CB-CG	-7.18	98.79	115.30
2	B	60	GLU	N-CA-C	-7.13	91.74	111.00
4	Q	20	ARG	CD-NE-CZ	7.12	133.57	123.60
11	X	32	MET	CG-SD-CE	7.07	111.51	100.20
7	T	17	ARG	CB-CG-CD	-7.06	93.25	111.60
1	A	380[A]	VAL	CB-CA-C	-7.01	98.07	111.40
1	A	380[B]	VAL	CB-CA-C	-7.01	98.07	111.40
4	D	4	SER	N-CA-CB	6.97	120.96	110.50
13	Z	19	LEU	CB-CG-CD2	-6.94	99.19	111.00
9	I	55	ASP	CB-CG-OD1	6.94	124.54	118.30
1	N	145	LEU	CB-CG-CD1	-6.89	99.29	111.00
2	B	82	ARG	NE-CZ-NH2	-6.86	116.87	120.30
4	D	19	ARG	NE-CZ-NH2	6.83	123.71	120.30
10	W	40	LEU	CB-CG-CD2	6.79	122.54	111.00
1	N	278	MET	CA-CB-CG	-6.77	101.79	113.30
1	N	298	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	N	438	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	A	512	ASN	CB-CA-C	-6.69	97.02	110.40
1	N	38	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	O	36	SER	CB-CA-C	6.68	122.79	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	ARG	NE-CZ-NH1	-6.67	116.96	120.30
6	F	48	LEU	CB-CG-CD1	6.67	122.34	111.00
1	N	194	LEU	CB-CG-CD2	6.63	122.28	111.00
5	R	106	LEU	CB-CG-CD1	6.63	122.27	111.00
1	A	302	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	N	512	ASN	CB-CA-C	-6.57	97.25	110.40
2	B	66	THR	OG1-CB-CG2	6.57	125.11	110.00
3	C	176	LEU	CB-CG-CD1	-6.53	99.89	111.00
3	P	152	MET	CA-CB-CG	-6.53	102.20	113.30
2	O	75	LEU	CB-CG-CD1	6.53	122.10	111.00
3	C	29	SER	CA-CB-OG	-6.53	93.58	111.20
3	C	233	PHE	CB-CG-CD2	-6.50	116.25	120.80
2	O	66	THR	OG1-CB-CG2	6.48	124.91	110.00
4	D	36	SER	N-CA-CB	6.47	120.21	110.50
1	A	129	TYR	CB-CG-CD1	-6.46	117.13	121.00
1	N	366	VAL	CG1-CB-CG2	-6.45	100.58	110.90
4	D	21	ASP	CB-CG-OD2	6.43	124.09	118.30
1	A	442	ASP	CB-CG-OD1	-6.43	112.51	118.30
4	D	20	ARG	CA-CB-CG	6.43	127.54	113.40
1	A	169	ILE	CG1-CB-CG2	-6.42	97.28	111.40
4	D	94	LEU	CB-CG-CD2	6.42	121.91	111.00
9	V	73	LYS	CD-CE-NZ	6.35	126.30	111.70
9	V	16	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	152	LEU	CB-CG-CD1	-6.28	100.33	111.00
1	A	439	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	N	486	ASP	CB-CG-OD1	6.19	123.87	118.30
1	N	253	MET	CA-CB-CG	-6.16	102.82	113.30
3	C	102	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	A	310	MET	CG-SD-CE	-6.14	90.38	100.20
2	B	36	SER	CB-CA-C	6.14	121.76	110.10
4	D	20	ARG	CD-NE-CZ	6.12	132.17	123.60
12	L	24	MET	CA-CB-CG	6.09	123.66	113.30
9	V	64	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	N	189	MET	CA-CB-CG	-6.07	102.98	113.30
13	Z	34	LEU	CB-CG-CD1	6.05	121.29	111.00
1	N	152	LEU	CB-CG-CD2	6.05	121.28	111.00
2	O	65	TRP	CB-CA-C	6.05	122.49	110.40
4	Q	79	LYS	CD-CE-NZ	-6.04	97.80	111.70
10	W	40	LEU	CB-CG-CD1	-6.01	100.77	111.00
5	E	90	ARG	CG-CD-NE	-6.00	99.19	111.80
7	T	33	LEU	CB-CG-CD1	6.00	121.20	111.00
7	T	33	LEU	CA-CB-CG	5.99	129.08	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	52	VAL	CB-CA-C	-5.99	100.02	111.40
3	C	80	ARG	CG-CD-NE	-5.99	99.23	111.80
1	A	369	ASP	CB-CG-OD1	5.98	123.68	118.30
4	D	31	LYS	CB-CG-CD	-5.98	96.06	111.60
3	C	40	MET	CA-CB-CG	-5.98	103.14	113.30
1	N	113	LEU	CB-CG-CD2	5.97	121.16	111.00
1	N	213	ARG	NE-CZ-NH2	-5.92	117.34	120.30
6	F	92	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	A	195	LEU	CB-CG-CD1	-5.90	100.97	111.00
3	P	80	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	219	PHE	CB-CG-CD2	-5.88	116.69	120.80
6	F	81	ARG	NE-CZ-NH1	-5.88	117.36	120.30
2	O	112	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	312	ILE	CA-CB-CG1	-5.84	99.91	111.00
8	H	61	LYS	CD-CE-NZ	5.83	125.12	111.70
9	V	10	ARG	NE-CZ-NH2	-5.82	117.39	120.30
9	I	12	LEU	CB-CG-CD2	-5.81	101.12	111.00
3	C	151	LEU	CB-CG-CD2	-5.80	101.13	111.00
1	A	311	ILE	CA-CB-CG1	-5.76	100.05	111.00
2	O	132	GLU	CG-CD-OE1	-5.75	106.79	118.30
1	A	208	MET	CG-SD-CE	5.75	109.40	100.20
3	P	60	ASP	CB-CG-OD1	5.75	123.47	118.30
2	O	170	LEU	CB-CG-CD1	-5.74	101.24	111.00
4	Q	17	VAL	CG1-CB-CG2	-5.70	101.78	110.90
3	P	163	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	A	230	LEU	CB-CG-CD2	-5.68	101.34	111.00
5	R	60	ASP	CB-CG-OD2	5.68	123.41	118.30
7	G	8	HIS	N-CA-C	5.66	126.28	111.00
3	C	43	LEU	CB-CG-CD1	-5.65	101.39	111.00
3	P	253	TYR	CB-CG-CD2	-5.64	117.61	121.00
3	P	44	MET	CG-SD-CE	5.64	109.22	100.20
3	P	102	TYR	CB-CG-CD2	-5.62	117.63	121.00
3	C	203	PHE	CB-CG-CD2	-5.62	116.87	120.80
1	A	244	TYR	CA-CB-CG	-5.62	102.73	113.40
4	Q	61	ARG	NE-CZ-NH2	5.61	123.10	120.30
4	Q	92	THR	CA-CB-CG2	-5.60	104.56	112.40
1	A	397	PHE	CB-CG-CD2	-5.57	116.90	120.80
3	C	224	LYS	CD-CE-NZ	-5.56	98.92	111.70
1	N	302	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	O	202	SER	CB-CA-C	-5.55	99.56	110.10
1	A	180	GLN	CA-CB-CG	-5.54	101.21	113.40
2	B	170	LEU	CB-CG-CD2	-5.53	101.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	68	ILE	CG1-CB-CG2	5.52	123.54	111.40
1	A	298	ASP	CB-CG-OD1	-5.51	113.34	118.30
2	B	3	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
1	N	485	VAL	N-CA-CB	-5.51	99.39	111.50
1	A	231	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	N	513	LEU	C-N-CA	-5.49	107.98	121.70
1	A	237	PHE	CB-CG-CD1	-5.49	116.96	120.80
13	M	14	GLU	OE1-CD-OE2	-5.49	116.72	123.30
3	C	155	ASP	CB-CG-OD1	5.48	123.23	118.30
1	N	240	HIS	CA-CB-CG	-5.45	104.34	113.60
3	P	156	ARG	NH1-CZ-NH2	5.45	125.39	119.40
4	D	123	MET	CA-CB-CG	-5.44	104.04	113.30
1	A	495	LEU	CB-CG-CD2	-5.44	101.75	111.00
2	B	157	GLU	CA-CB-CG	-5.43	101.45	113.40
6	S	81	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	B	33	LEU	CB-CG-CD1	5.42	120.21	111.00
9	I	73	LYS	CD-CE-NZ	-5.42	99.25	111.70
1	A	486	ASP	CB-CA-C	-5.41	99.57	110.40
1	N	250	GLY	N-CA-C	-5.41	99.57	113.10
1	N	270	TYR	CD1-CE1-CZ	-5.39	114.95	119.80
3	P	216	ILE	CG1-CB-CG2	-5.39	99.55	111.40
4	Q	51	LEU	CA-CB-CG	5.38	127.67	115.30
3	C	90	GLU	OE1-CD-OE2	5.37	129.75	123.30
7	T	17	ARG	CD-NE-CZ	5.36	131.10	123.60
4	D	51	LEU	CB-CG-CD1	5.36	120.11	111.00
1	A	35	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	N	339	MET	CA-CB-CG	-5.34	104.22	113.30
6	S	54	ASN	CB-CG-OD1	-5.33	110.94	121.60
1	A	102	PHE	CG-CD1-CE1	5.31	126.64	120.80
11	K	20	SER	CB-CA-C	-5.31	100.01	110.10
2	B	11	ASP	CB-CG-OD2	5.31	123.08	118.30
3	P	94	PHE	CB-CG-CD2	-5.31	117.08	120.80
2	O	33	LEU	CB-CG-CD1	5.29	119.99	111.00
2	B	188	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	96	ARG	NE-CZ-NH1	-5.28	117.66	120.30
12	L	5	GLU	C-N-CA	-5.26	111.24	122.30
5	E	14	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	240	HIS	CA-CB-CG	-5.26	104.66	113.60
3	C	254	VAL	CA-CB-CG2	-5.26	103.01	110.90
13	M	26	PHE	CB-CA-C	-5.25	99.89	110.40
2	B	158	ASP	CB-CG-OD2	-5.25	113.57	118.30
3	P	92	LEU	CB-CG-CD2	-5.25	102.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	147	GLU	OE1-CD-OE2	-5.24	117.01	123.30
4	D	51	LEU	CA-CB-CG	5.24	127.35	115.30
2	B	128	LEU	CB-CG-CD1	-5.24	102.09	111.00
2	B	139	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	113	LEU	CB-CG-CD1	5.21	119.86	111.00
2	O	87	MET	CG-SD-CE	5.21	108.53	100.20
3	C	193	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	A	449	MET	CA-CB-CG	-5.19	104.47	113.30
1	N	213	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	316	THR	CA-CB-CG2	-5.18	105.14	112.40
2	B	16	ILE	CA-CB-CG1	-5.18	101.16	111.00
2	O	139	ASP	CB-CG-OD2	5.17	122.96	118.30
9	V	55	ASP	CB-CG-OD1	5.17	122.95	118.30
13	M	38	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	N	347	LEU	CB-CG-CD1	-5.16	102.22	111.00
1	N	102	PHE	CG-CD1-CE1	5.15	126.47	120.80
6	F	22	LEU	CB-CG-CD2	5.15	119.75	111.00
1	N	164	PHE	CB-CG-CD2	-5.15	117.20	120.80
13	Z	37	LEU	CB-CG-CD1	-5.14	102.25	111.00
3	P	85	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	N	68	PHE	CB-CG-CD1	-5.14	117.20	120.80
4	D	79	LYS	CD-CE-NZ	-5.13	99.89	111.70
1	N	327	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	N	251	PHE	CB-CA-C	-5.12	100.17	110.40
10	J	28	ASP	CB-CG-OD1	5.10	122.89	118.30
4	D	17	VAL	CB-CA-C	-5.10	101.71	111.40
4	Q	19	ARG	NE-CZ-NH1	-5.09	117.75	120.30
2	B	84	LEU	CB-CG-CD1	-5.09	102.35	111.00
7	G	16	TRP	CA-CB-CG	-5.09	104.03	113.70
3	C	245	VAL	CA-CB-CG2	-5.09	103.27	110.90
6	S	6	VAL	CG1-CB-CG2	-5.08	102.77	110.90
5	E	108	LYS	CB-CA-C	5.08	120.56	110.40
10	J	57	HIS	CB-CA-C	5.07	120.55	110.40
10	J	50	LEU	CB-CG-CD1	5.07	119.62	111.00
1	A	105	LEU	CB-CG-CD1	-5.07	102.38	111.00
6	F	29	ASP	CB-CG-OD2	-5.06	113.74	118.30
7	G	7	ASP	N-CA-C	5.05	124.64	111.00
4	Q	135	SER	CA-CB-OG	-5.05	97.55	111.20
3	C	102	TYR	CZ-CE2-CD2	-5.05	115.25	119.80
2	O	66	THR	CA-CB-CG2	5.05	119.47	112.40
10	J	35	THR	CA-CB-CG2	-5.04	105.35	112.40
7	T	8	HIS	N-CA-C	5.02	124.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	199	LEU	CB-CG-CD1	-5.01	102.48	111.00
3	P	181	TYR	CG-CD1-CE1	-5.01	117.29	121.30
5	E	14	ARG	NE-CZ-NH2	-5.00	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	66	THR	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	TYR	Sidechain
6	F	93	PRO	Peptide
6	S	93	PRO	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	4060	0	4037	59	0
1	N	4060	0	4037	67	0
2	B	1824	0	1833	29	0
2	O	1824	0	1833	34	1
3	C	2110	0	2027	30	0
3	P	2110	0	2027	31	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	10	0
5	E	852	0	845	8	0
5	R	852	0	845	8	1
6	F	748	0	728	17	0
6	S	748	0	728	19	1
7	G	675	0	643	43	0
7	T	675	0	643	51	0
8	H	662	0	623	13	0
8	U	662	0	623	11	0
9	I	601	0	613	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	601	0	613	14	0
10	J	460	0	459	5	0
10	W	460	0	459	6	0
11	K	384	0	366	1	0
11	X	384	0	366	4	0
12	L	380	0	380	10	0
12	Y	380	0	380	8	0
13	M	335	0	352	10	0
13	Z	335	0	352	2	0
14	A	120	0	107	9	0
14	N	120	0	108	8	0
15	A	2	0	0	0	0
15	N	2	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	N	1	0	0	0	0
19	A	63	0	110	8	0
19	D	63	0	110	8	0
19	L	63	0	110	15	0
19	N	63	0	110	15	0
19	O	63	0	110	10	0
19	Q	63	0	110	12	0
20	A	51	0	76	0	0
20	C	102	0	152	8	0
20	M	51	0	76	15	0
20	N	102	0	152	9	0
20	P	102	0	152	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	26	0
22	R	52	0	80	15	0
23	B	29	0	36	2	0
23	C	58	0	73	4	0
23	J	29	0	36	1	0
23	O	29	0	39	3	0
23	P	58	0	73	6	0
23	W	29	0	36	1	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	53	0	77	8	0
25	G	106	0	154	43	0
25	P	106	0	154	24	0
25	T	53	0	77	21	0
26	C	100	0	156	26	0
26	G	100	0	156	30	0
26	P	100	0	156	25	0
26	T	100	0	156	27	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	37	4	0
28	M	33	0	37	0	0
28	P	33	0	39	6	0
28	Z	33	0	38	2	0
29	A	218	0	0	5	0
29	B	143	0	0	7	0
29	C	116	0	0	3	0
29	D	80	0	0	3	0
29	E	49	0	0	0	0
29	F	61	0	0	2	0
29	G	45	0	0	2	0
29	H	51	0	0	1	0
29	I	37	0	0	2	0
29	J	24	0	0	0	0
29	K	29	0	0	0	0
29	L	23	0	0	1	0
29	M	31	0	0	2	0
29	N	222	0	0	7	0
29	O	137	0	0	5	0
29	P	102	0	0	0	0
29	Q	65	0	0	3	0
29	R	47	0	0	0	0
29	S	64	0	0	0	0
29	T	47	0	0	2	0
29	U	49	0	0	2	0
29	V	27	0	0	2	0
29	W	19	0	0	0	0
29	X	22	0	0	2	0
29	Y	21	0	0	1	0
29	Z	14	0	0	1	0
All	All	32545	0	31351	653	2

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 (653) 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)
25:P:1265:PEK:H383	26:T:1269:CDL:C27	1.21	1.67
1:N:484:THR:CG2	1:N:484:THR:CB	1.77	1.60
4:D:100:LYS:CE	4:D:100:LYS:NZ	1.70	1.55
1:N:189:MET:CB	1:N:189:MET:CG	1.82	1.52
4:Q:121:LYS:CE	4:Q:121:LYS:NZ	1.74	1.50
2:B:87:MET:CG	2:B:87:MET:SD	2.02	1.47
1:A:297:MET:SD	1:A:297:MET:CG	2.01	1.47
25:P:1265:PEK:C38	26:T:1269:CDL:C27	2.06	1.32
22:B:229:PSC:H142	22:B:229:PSC:H343	1.23	1.18
1:N:513:LEU:O	1:N:514:LYS:HB2	1.41	1.16
7:T:84:LYS:HD2	7:T:84:LYS:H	1.09	1.16
25:P:1265:PEK:C38	26:T:1269:CDL:H273	1.69	1.15
1:A:513:LEU:O	1:A:514:LYS:HB2	1.37	1.15
22:B:229:PSC:C14	22:B:229:PSC:H343	1.78	1.14
22:R:1229:PSC:C34	22:R:1229:PSC:H142	1.79	1.13
20:M:524:PGV:H011	20:M:524:PGV:H22	1.12	1.11
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.16	1.10
7:T:2:SER:O	25:T:263:PEK:H331	1.52	1.08
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.31	1.07
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.70	1.06
6:F:85:CYS:SG	6:F:87:THR:HG23	1.96	1.05
20:C:267:PGV:H172	26:C:270:CDL:H662	1.33	1.05
7:G:84:LYS:N	7:G:84:LYS:HD2	1.69	1.04
22:B:229:PSC:H072	9:I:10:ARG:HH21	1.20	1.04
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.41	1.02
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.42	1.01
25:P:1265:PEK:C38	26:T:1269:CDL:H272	1.81	1.00
2:O:227:LEU:HD21	29:O:4852:HOH:O	1.60	0.99
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.43	0.99
7:G:84:LYS:HD2	7:G:84:LYS:H	0.83	0.99
7:G:84:LYS:H	7:G:84:LYS:CD	1.76	0.98
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.44	0.98
25:P:1264:PEK:H12	25:P:1264:PEK:H242	1.46	0.98
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.29	0.97
25:P:1265:PEK:H383	26:T:1269:CDL:H272	0.98	0.97
6:F:97:ALA:HB2	29:F:4812:HOH:O	1.61	0.97
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.06	0.96
22:B:229:PSC:H142	22:B:229:PSC:C34	1.96	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.26	0.94
20:M:524:PGV:C2	20:M:524:PGV:H011	1.97	0.94
13:M:39:ASN:O	13:M:43:SER:OG	1.86	0.94
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.48	0.94
22:R:1229:PSC:H142	22:R:1229:PSC:H343	1.48	0.93
25:C:264:PEK:H101	25:C:264:PEK:H161	1.52	0.92
8:H:9:LYS:O	8:H:10:ASN:HB2	1.69	0.92
1:A:513:LEU:O	1:A:514:LYS:CB	2.09	0.91
20:M:524:PGV:C01	20:M:524:PGV:H22	2.01	0.91
6:S:85:CYS:SG	6:S:87:THR:HG23	2.11	0.91
1:A:406:ASN:HD21	20:M:524:PGV:H21	1.36	0.90
1:A:297:MET:CE	1:A:297:MET:CG	2.50	0.90
19:A:521:TGL:H111	19:A:521:TGL:H283	1.52	0.89
25:P:1265:PEK:H381	26:T:1269:CDL:H273	1.49	0.89
7:T:5:LYS:CD	25:T:263:PEK:H371	2.03	0.88
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.56	0.88
1:N:417:MET:CE	29:N:3166:HOH:O	2.22	0.88
7:G:3:ALA:CB	25:G:1263:PEK:H382	2.03	0.87
8:H:9:LYS:HG3	8:H:10:ASN:H	1.38	0.87
7:T:5:LYS:HD2	25:T:263:PEK:C37	2.05	0.86
25:G:265:PEK:H371	26:G:269:CDL:C27	2.05	0.86
7:G:2:SER:OG	25:G:1263:PEK:C29	2.23	0.86
3:P:224:LYS:HE3	26:P:1270:CDL:HB31	1.58	0.86
20:N:1524:PGV:H011	20:N:1524:PGV:H22	1.57	0.86
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.38	0.85
10:W:2:GLU:HB2	10:W:4:ARG:NH1	1.90	0.85
13:M:19:LEU:HD23	20:M:524:PGV:H311	1.57	0.84
3:P:34:TRP:HE1	28:P:1272:DMU:H29	1.40	0.84
1:N:513:LEU:O	1:N:514:LYS:CB	2.14	0.84
7:G:72:ASN:H	7:G:76:ASN:HD22	1.23	0.84
8:H:9:LYS:HG3	8:H:10:ASN:N	1.92	0.83
26:T:1269:CDL:H111	26:T:1269:CDL:HA21	1.60	0.83
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.03	0.83
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.61	0.83
7:T:84:LYS:H	7:T:84:LYS:CD	1.89	0.83
22:R:1229:PSC:H343	22:R:1229:PSC:C14	2.09	0.82
3:P:224:LYS:CD	26:P:1270:CDL:HB32	2.09	0.82
7:T:84:LYS:HD2	7:T:84:LYS:N	1.93	0.82
29:A:4501:HOH:O	25:C:264:PEK:H381	1.80	0.81
9:V:1:SAC:OAC	9:V:1:SAC:HB3	1.79	0.81
1:A:1:FME:CE	1:A:4:ASN:HD22	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:417:MET:HE1	29:N:3166:HOH:O	1.78	0.81
1:A:297:MET:CE	1:A:297:MET:CB	2.59	0.81
26:C:270:CDL:H522	26:C:270:CDL:OB9	1.80	0.81
22:B:229:PSC:O02	22:B:229:PSC:H032	1.80	0.80
19:A:521:TGL:H201	19:A:521:TGL:H241	1.64	0.79
8:U:27:ARG:HG2	29:U:4871:HOH:O	1.79	0.79
20:C:267:PGV:C17	26:C:270:CDL:H662	2.12	0.79
25:P:1265:PEK:H383	26:T:1269:CDL:H271	1.58	0.79
26:P:1270:CDL:HB22	26:P:1270:CDL:PA1	2.15	0.78
26:G:269:CDL:H201	26:G:269:CDL:H511	1.65	0.78
29:A:4740:HOH:O	3:C:77:LYS:HE2	1.84	0.78
19:N:1522:TGL:H231	19:N:1522:TGL:HA92	1.65	0.78
25:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.28	0.77
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.66	0.77
7:G:2:SER:OG	25:G:1263:PEK:H291	1.84	0.77
25:C:264:PEK:HN2	7:G:76:ASN:HD21	1.32	0.77
26:P:1270:CDL:H192	26:P:1270:CDL:H231	1.65	0.76
7:T:5:LYS:HD2	25:T:263:PEK:C38	2.15	0.76
7:T:72:ASN:H	7:T:76:ASN:HD22	1.34	0.76
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.66	0.75
19:O:1521:TGL:H241	19:O:1521:TGL:H201	1.67	0.75
26:C:270:CDL:H672	26:C:270:CDL:H252	1.68	0.75
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.67	0.75
19:A:521:TGL:HA92	19:A:521:TGL:H252	1.70	0.74
26:G:269:CDL:H352	2:O:78:LEU:HD12	1.70	0.74
22:B:229:PSC:C34	22:B:229:PSC:C14	2.59	0.73
26:P:1270:CDL:H242	26:P:1270:CDL:H661	1.70	0.73
25:G:265:PEK:H371	26:G:269:CDL:H272	1.68	0.73
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.53	0.73
25:C:264:PEK:H71	25:C:264:PEK:H32	1.69	0.73
25:G:265:PEK:C38	26:G:269:CDL:C27	2.66	0.73
1:N:189:MET:CA	1:N:189:MET:CG	2.65	0.73
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.71	0.73
28:G:272:DMU:O1	28:G:272:DMU:H29	1.89	0.73
25:G:265:PEK:C37	26:G:269:CDL:C27	2.67	0.73
1:N:383[B]:MET:O	1:N:387:PHE:HB2	1.89	0.73
25:G:265:PEK:H371	26:G:269:CDL:H273	1.69	0.73
6:F:1:ALA:H1	25:G:265:PEK:H042	1.53	0.72
26:G:269:CDL:H562	26:G:269:CDL:H782	1.70	0.72
7:G:69:PHE:HZ	28:G:272:DMU:H1	1.54	0.72
3:P:224:LYS:HE3	26:P:1270:CDL:CB3	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:351:GLY:HA3	1:N:380[A]:VAL:HG13	1.70	0.72
4:Q:100:LYS:HE2	29:Q:4794:HOH:O	1.88	0.72
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.71	0.71
22:R:1229:PSC:C07	9:V:10:ARG:HH21	2.03	0.71
22:B:229:PSC:H072	9:I:10:ARG:NH2	2.02	0.71
19:O:1521:TGL:H101	19:O:1521:TGL:C28	2.20	0.71
22:B:229:PSC:C07	9:I:10:ARG:HH21	2.00	0.71
26:T:1269:CDL:H561	26:T:1269:CDL:H762	1.73	0.71
25:G:265:PEK:C37	26:G:269:CDL:H272	2.21	0.71
19:N:1522:TGL:H362	29:Y:4638:HOH:O	1.91	0.71
22:R:1229:PSC:C34	22:R:1229:PSC:C14	2.64	0.70
8:U:23:GLN:HG3	29:U:4345:HOH:O	1.91	0.70
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.71	0.70
7:G:5:LYS:CD	25:G:1263:PEK:H371	2.21	0.70
3:C:246:ASP:HB2	29:C:4099:HOH:O	1.91	0.70
2:B:81:LEU:HD12	26:T:1269:CDL:H351	1.73	0.70
8:H:45:ALA:O	8:H:47:GLY:N	2.24	0.70
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.93	0.69
19:L:522:TGL:HC62	19:L:522:TGL:CC2	2.19	0.69
1:N:189:MET:CB	1:N:189:MET:SD	2.79	0.69
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.73	0.69
3:P:34:TRP:NE1	28:P:1272:DMU:H29	2.09	0.68
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.75	0.68
9:I:44:LYS:HE2	29:I:4840:HOH:O	1.94	0.68
22:B:229:PSC:H141	22:B:229:PSC:H343	1.70	0.68
29:N:4526:HOH:O	2:O:87:MET:SD	2.52	0.68
20:N:1524:PGV:H22	20:N:1524:PGV:C01	2.23	0.68
7:G:11:TPO:CG2	7:G:11:TPO:O	2.42	0.67
1:N:177:SER:H	1:N:180:GLN:HE21	1.43	0.67
25:P:1265:PEK:H042	6:S:1:ALA:N	2.08	0.67
10:W:2:GLU:CB	10:W:4:ARG:NH1	2.57	0.66
8:U:45:ALA:O	8:U:47:GLY:N	2.28	0.66
25:C:264:PEK:C10	25:C:264:PEK:H161	2.25	0.66
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.59	0.66
14:A:515:HEA:HMC1	14:A:515:HEA:HBC1	1.76	0.66
3:P:63:ARG:HE	26:P:1270:CDL:CA2	2.08	0.66
1:A:484:THR:HB	13:M:2:THR:OG1	1.95	0.66
9:V:73:LYS:CA	9:V:73:LYS:HE3	2.25	0.66
23:O:229:CHD:H212	23:O:229:CHD:H12	1.76	0.66
12:L:46:LYS:O	12:L:47:LYS:HB2	1.96	0.66
6:S:53:THR:HG22	6:S:54:ASN:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:1271:CHD:H162	23:P:1271:CHD:H232	1.77	0.65
9:V:73:LYS:HA	9:V:73:LYS:HE3	1.77	0.65
8:U:9:LYS:O	8:U:10:ASN:HB2	1.95	0.65
12:Y:22:LEU:O	12:Y:26:THR:HB	1.95	0.65
25:G:265:PEK:H383	26:G:269:CDL:C27	2.25	0.65
1:A:282:PHE:HA	7:T:4:ALA:CB	2.26	0.65
29:A:4197:HOH:O	22:B:229:PSC:H21	1.97	0.65
1:A:484:THR:HG22	29:A:4618:HOH:O	1.96	0.65
26:T:1269:CDL:H331	26:T:1269:CDL:OA8	1.97	0.64
20:P:1267:PGV:H172	26:P:1270:CDL:H652	1.80	0.64
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.07	0.64
14:N:515:HEA:HMC1	14:N:515:HEA:HBC1	1.80	0.64
4:Q:7:LYS:O	4:Q:10:ASP:HB2	1.98	0.64
7:T:5:LYS:HB2	25:T:263:PEK:C36	2.24	0.64
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.28	0.64
6:S:94:HIS:O	6:S:95:GLN:HB2	1.96	0.64
7:G:3:ALA:HB1	25:G:1263:PEK:C38	2.28	0.64
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.62	0.64
2:O:49:LYS:HD2	29:Q:3076:HOH:O	1.98	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.98	0.63
8:H:52:VAL:HG12	8:U:46:LYS:HB2	1.79	0.63
19:N:1522:TGL:HA92	19:N:1522:TGL:C23	2.28	0.63
19:O:1521:TGL:H101	19:O:1521:TGL:H281	1.79	0.63
22:R:1229:PSC:H071	9:V:10:ARG:HH21	1.64	0.63
8:H:9:LYS:HA	29:H:4747:HOH:O	1.97	0.63
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.63	0.63
3:P:224:LYS:CE	26:P:1270:CDL:HB31	2.28	0.63
1:A:297:MET:HE3	1:A:297:MET:HB3	1.80	0.62
6:F:1:ALA:N	25:G:265:PEK:H042	2.13	0.62
25:P:1265:PEK:H042	6:S:1:ALA:H1	1.65	0.62
19:Q:1523:TGL:HG12	19:Q:1523:TGL:HC21	1.82	0.62
3:P:224:LYS:HD2	26:P:1270:CDL:HB32	1.80	0.62
28:G:272:DMU:C10	28:G:272:DMU:H29	2.29	0.62
2:B:13:THR:OG1	2:B:167:SER:HB2	2.00	0.62
8:H:9:LYS:CG	8:H:10:ASN:H	2.08	0.62
7:T:2:SER:OG	25:T:263:PEK:C29	2.48	0.62
19:O:1521:TGL:H201	19:O:1521:TGL:C24	2.30	0.62
25:P:1265:PEK:C04	6:S:1:ALA:N	2.62	0.61
26:T:1269:CDL:H201	26:T:1269:CDL:H511	1.82	0.61
7:G:17:ARG:HD2	29:O:2446:HOH:O	1.98	0.61
19:Q:1523:TGL:OB1	19:Q:1523:TGL:HG32	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.82	0.61
6:F:1:ALA:N	25:G:265:PEK:C04	2.64	0.61
8:U:9:LYS:HG3	8:U:10:ASN:H	1.65	0.61
2:O:42:ILE:HG21	19:Q:1523:TGL:H231	1.81	0.61
20:C:267:PGV:H172	26:C:270:CDL:C66	2.22	0.61
26:C:270:CDL:PA1	26:C:270:CDL:HB21	2.40	0.61
1:A:51:ASP:OD1	1:A:441:SER:OG	2.15	0.61
7:G:3:ALA:CB	25:G:1263:PEK:C38	2.77	0.61
10:W:2:GLU:CB	10:W:4:ARG:HH11	2.14	0.61
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.30	0.61
1:A:297:MET:HE2	1:A:297:MET:CB	2.30	0.60
22:B:229:PSC:O02	22:B:229:PSC:C03	2.50	0.60
3:C:210:ILE:HD13	20:C:267:PGV:H301	1.82	0.60
7:G:69:PHE:CZ	28:G:272:DMU:H1	2.36	0.60
1:N:177:SER:H	1:N:180:GLN:NE2	1.98	0.60
7:G:2:SER:O	25:G:1263:PEK:H331	2.01	0.60
10:W:2:GLU:HB2	10:W:4:ARG:HH12	1.66	0.60
2:B:78:LEU:HD12	26:T:1269:CDL:H352	1.84	0.60
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.65	0.60
1:A:297:MET:HE3	1:A:297:MET:CB	2.31	0.60
7:G:5:LYS:CB	25:G:1263:PEK:H362	2.19	0.60
7:G:5:LYS:HD2	25:G:1263:PEK:C37	2.31	0.60
10:J:52:TRP:O	10:J:57:HIS:HE1	1.85	0.60
4:Q:109:HIS:HD2	29:Q:3122:HOH:O	1.85	0.59
2:B:78:LEU:CD1	26:T:1269:CDL:H352	2.33	0.59
3:C:224:LYS:CD	26:C:270:CDL:HB32	2.33	0.59
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.14	0.59
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.85	0.59
20:C:268:PGV:H031	29:C:4819:HOH:O	2.02	0.59
7:G:5:LYS:HB3	1:N:278:MET:SD	2.43	0.59
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.37	0.58
1:N:449:MET:SD	2:O:5:MET:HG2	2.43	0.58
29:B:3446:HOH:O	7:T:17:ARG:CD	2.51	0.58
1:N:189:MET:CB	1:N:189:MET:CE	2.80	0.58
7:G:37:LEU:HD11	26:G:269:CDL:H361	1.84	0.58
2:O:89:GLU:O	2:O:91:ASN:ND2	2.36	0.58
4:Q:95:LEU:HD22	28:Z:1526:DMU:H13	1.86	0.58
2:O:226:MET:O	2:O:227:LEU:C	2.41	0.58
2:O:84:LEU:HA	2:O:87:MET:HE2	1.84	0.58
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.86	0.58
3:C:210:ILE:HG12	20:C:267:PGV:H132	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:11:TPO:HG22	7:T:11:TPO:O	2.04	0.58
19:N:1522:TGL:H231	19:N:1522:TGL:CA9	2.32	0.57
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	2.03	0.57
7:T:36:TRP:HB3	29:T:4707:HOH:O	2.03	0.57
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.40	0.57
20:M:524:PGV:H141	20:M:524:PGV:C30	2.35	0.57
7:T:2:SER:OG	25:T:263:PEK:H291	2.04	0.57
22:B:229:PSC:H071	5:E:8:ASP:HA	1.85	0.57
22:R:1229:PSC:O01	22:R:1229:PSC:H212	2.05	0.57
7:T:8:HIS:CD2	25:T:263:PEK:H232	2.39	0.57
1:A:1:FME:HE1	1:A:4:ASN:HD22	1.69	0.57
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.02	0.57
1:A:297:MET:HE3	1:A:297:MET:CG	2.35	0.57
19:L:522:TGL:C23	19:L:522:TGL:HA92	2.20	0.57
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.68	0.57
7:G:2:SER:OG	25:G:1263:PEK:H301	2.05	0.57
8:U:43:MET:HE3	8:U:49:ASP:N	2.20	0.57
7:T:3:ALA:CB	25:T:263:PEK:H382	2.34	0.57
25:P:1265:PEK:C37	26:T:1269:CDL:H272	2.34	0.57
25:G:1263:PEK:H132	3:P:247:VAL:HG12	1.86	0.57
3:P:34:TRP:CZ2	28:P:1272:DMU:O5	2.58	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.39	0.57
28:P:1272:DMU:H30	7:T:62:TRP:HB3	1.87	0.56
1:N:351:GLY:CA	1:N:380[A]:VAL:HG13	2.34	0.56
8:U:49:ASP:O	8:U:52:VAL:HG22	2.06	0.56
29:B:3446:HOH:O	7:T:17:ARG:HD3	2.04	0.56
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.22	0.56
26:G:269:CDL:H241	26:G:269:CDL:H531	1.87	0.56
4:D:34:SER:H	4:D:37:GLN:NE2	2.03	0.56
25:P:1265:PEK:H8	29:T:4897:HOH:O	2.05	0.56
19:Q:1523:TGL:HA91	19:Q:1523:TGL:H242	1.86	0.56
3:C:95:THR:HG21	20:C:268:PGV:H282	1.85	0.56
3:P:224:LYS:CE	26:P:1270:CDL:CB3	2.84	0.56
25:P:1265:PEK:H041	7:T:17:ARG:HH22	1.69	0.56
7:T:5:LYS:CB	25:T:263:PEK:H362	2.26	0.56
1:A:297:MET:CE	1:A:297:MET:HB3	2.32	0.56
6:F:64:GLU:O	6:F:65:ASP:HB2	2.06	0.56
1:N:309:THR:HG22	14:N:516:HEA:HMB2	1.86	0.56
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.41	0.55
26:C:270:CDL:HA4	26:C:270:CDL:H122	1.87	0.55
26:G:269:CDL:H201	26:G:269:CDL:C51	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:1522:TGL:OC1	19:N:1522:TGL:HC51	2.06	0.55
19:Q:1523:TGL:HC21	19:Q:1523:TGL:CG1	2.37	0.55
7:G:2:SER:O	25:G:1263:PEK:H322	2.07	0.55
7:G:3:ALA:O	7:G:4:ALA:HB2	2.05	0.55
7:G:17:ARG:CD	29:O:2446:HOH:O	2.54	0.55
4:D:34:SER:H	4:D:37:GLN:HE21	1.55	0.55
26:C:270:CDL:OA5	26:C:270:CDL:HB21	2.06	0.55
1:A:62:ALA:HB2	14:A:515:HEA:HBD1	1.88	0.55
3:P:224:LYS:CD	26:P:1270:CDL:CB3	2.84	0.55
26:G:269:CDL:H352	2:O:78:LEU:CD1	2.35	0.55
1:N:297:MET:CE	1:N:302:ARG:HG2	2.37	0.55
1:A:177:SER:H	1:A:180:GLN:HE21	1.55	0.55
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.88	0.55
20:P:1267:PGV:C18	26:P:1270:CDL:H662	2.36	0.55
26:G:269:CDL:H451	2:O:70:ALA:HB1	1.89	0.55
2:O:32:PHE:CE2	19:O:1521:TGL:HA51	2.41	0.55
1:N:409:TRP:HA	1:N:412:ILE:HD12	1.89	0.55
25:P:1265:PEK:C04	6:S:1:ALA:H2	2.19	0.54
3:C:224:LYS:HE3	26:C:270:CDL:HB32	1.88	0.54
19:A:521:TGL:H363	19:A:521:TGL:H221	1.89	0.54
22:B:229:PSC:H071	5:E:8:ASP:OD1	2.07	0.54
29:N:3132:HOH:O	3:P:191:GLY:HA3	2.07	0.54
13:M:19:LEU:HD23	20:M:524:PGV:C31	2.32	0.54
1:A:377:PHE:HA	1:A:380[B]:VAL:HG22	1.90	0.54
20:M:524:PGV:H062	29:M:2126:HOH:O	2.07	0.54
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.38	0.54
7:G:3:ALA:O	7:G:4:ALA:CB	2.55	0.54
19:A:521:TGL:C11	19:A:521:TGL:H283	2.32	0.54
1:A:334:TRP:CE3	19:D:523:TGL:HA31	2.43	0.54
1:A:478:SER:O	13:M:6:ALA:HB1	2.08	0.54
26:G:269:CDL:H561	26:G:269:CDL:H762	1.89	0.54
19:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.90	0.53
7:G:11:TPO:HG22	7:G:11:TPO:O	2.08	0.53
22:R:1229:PSC:O01	22:R:1229:PSC:C21	2.57	0.53
26:G:269:CDL:H351	2:O:81:LEU:HD12	1.89	0.53
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.53
7:G:2:SER:OG	25:G:1263:PEK:C30	2.56	0.53
7:T:83:GLU:HA	7:T:84:LYS:NZ	2.23	0.53
7:T:37:LEU:HD21	26:T:1269:CDL:H361	1.90	0.53
1:N:113:LEU:HD12	19:N:1522:TGL:H141	1.89	0.53
2:O:226:MET:O	2:O:227:LEU:OXT	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:MET:HE3	8:H:49:ASP:N	2.24	0.53
1:A:21:LEU:HD23	19:L:522:TGL:H211	1.90	0.53
1:N:62:ALA:HB2	14:N:515:HEA:HBD1	1.91	0.53
19:Q:1523:TGL:OB1	19:Q:1523:TGL:CG3	2.57	0.53
2:B:56:MET:HB3	22:B:229:PSC:H211	1.91	0.53
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.23	0.53
1:N:309:THR:CG2	14:N:516:HEA:HMB2	2.39	0.52
5:R:108:LYS:O	5:R:108:LYS:HG2	2.09	0.52
26:P:1270:CDL:C24	26:P:1270:CDL:H661	2.38	0.52
20:N:1524:PGV:H011	20:N:1524:PGV:H221	1.91	0.52
2:O:66:THR:HG21	23:O:229:CHD:H3	1.91	0.52
2:O:13:THR:HB	2:O:168:LEU:HD23	1.91	0.52
2:B:1:FME:HCN	2:B:193:TYR:HB2	1.92	0.52
1:N:136:LEU:HD12	29:N:4821:HOH:O	2.08	0.52
26:T:1269:CDL:OA7	26:T:1269:CDL:H331	2.08	0.52
7:T:11:TPO:CG2	7:T:11:TPO:O	2.57	0.52
5:E:31:LYS:HE2	6:F:83:PRO:O	2.09	0.52
7:T:37:LEU:CD2	26:T:1269:CDL:H361	2.40	0.52
7:T:38:HIS:CE1	26:T:1269:CDL:H122	2.45	0.52
2:O:227:LEU:CD2	29:O:4852:HOH:O	2.34	0.52
25:G:265:PEK:H292	29:O:4943:HOH:O	2.09	0.52
25:G:265:PEK:C37	26:G:269:CDL:H273	2.37	0.52
23:P:1271:CHD:C16	23:P:1271:CHD:H232	2.38	0.52
1:N:484:THR:CG2	1:N:484:THR:C	2.79	0.52
7:G:72:ASN:H	7:G:76:ASN:ND2	1.99	0.52
3:P:34:TRP:HE1	28:P:1272:DMU:C57	2.18	0.52
2:B:1:FME:CN	2:B:193:TYR:H	2.23	0.52
1:N:53:ILE:HG12	29:N:3704:HOH:O	2.08	0.52
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.44	0.52
8:H:45:ALA:C	8:H:47:GLY:H	2.13	0.51
13:M:13:LYS:HE3	29:M:4807:HOH:O	2.09	0.51
12:L:14:SER:H	19:L:522:TGL:HC31	1.75	0.51
7:G:5:LYS:HD2	25:G:1263:PEK:C38	2.40	0.51
26:G:269:CDL:HA21	26:G:269:CDL:H112	1.93	0.51
7:T:38:HIS:HE2	26:T:1269:CDL:H122	1.75	0.51
2:B:41:ILE:HD13	22:B:229:PSC:H342	1.93	0.51
20:M:524:PGV:H141	20:M:524:PGV:H302	1.91	0.51
20:P:1267:PGV:H172	26:P:1270:CDL:C65	2.40	0.51
14:N:516:HEA:HBC1	14:N:516:HEA:HMC1	1.92	0.51
26:G:269:CDL:HA21	26:G:269:CDL:C11	2.41	0.51
20:N:1524:PGV:H221	20:N:1524:PGV:C01	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:1266:PGV:H183	25:P:1264:PEK:H332	1.93	0.51
26:C:270:CDL:H772	26:C:270:CDL:H651	1.92	0.51
19:O:1521:TGL:C20	19:O:1521:TGL:H241	2.38	0.51
20:M:524:PGV:O13	20:M:524:PGV:O01	2.29	0.51
10:W:2:GLU:HB3	10:W:4:ARG:HH11	1.75	0.51
7:T:84:LYS:N	7:T:84:LYS:CD	2.64	0.50
3:C:67:PHE:CE1	26:C:270:CDL:H1	2.39	0.50
23:O:229:CHD:H212	23:O:229:CHD:C12	2.41	0.50
3:P:40:MET:O	3:P:44:MET:HG2	2.11	0.50
11:X:8:ASP:HB2	29:X:4890:HOH:O	2.11	0.50
7:T:2:SER:O	25:T:263:PEK:C33	2.43	0.50
3:P:224:LYS:HD3	26:P:1270:CDL:HB32	1.91	0.50
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.77	0.50
5:R:107:ASP:N	5:R:107:ASP:OD2	2.45	0.50
26:G:269:CDL:H771	29:G:4678:HOH:O	2.12	0.50
19:N:1522:TGL:HA62	12:Y:25:MET:HG2	1.94	0.50
2:O:58:ALA:O	2:O:62:GLU:HG3	2.12	0.50
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.94	0.50
3:C:224:LYS:CE	26:C:270:CDL:HB32	2.42	0.50
8:H:43:MET:CE	8:H:49:ASP:H	2.23	0.50
12:L:24:MET:SD	19:L:522:TGL:H161	2.51	0.50
25:T:263:PEK:O04	25:T:263:PEK:H242	2.11	0.50
22:B:229:PSC:H222	22:B:229:PSC:O04	2.11	0.50
2:B:58:ALA:O	2:B:62:GLU:HG3	2.12	0.50
25:G:265:PEK:H383	26:G:269:CDL:H271	1.93	0.50
1:N:113:LEU:HD12	19:N:1522:TGL:C14	2.42	0.50
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.41	0.50
5:E:21:LYS:HE2	5:E:24:ILE:HA	1.93	0.50
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.42	0.50
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.00	0.49
7:T:38:HIS:NE2	26:T:1269:CDL:H122	2.27	0.49
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.93	0.49
7:T:3:ALA:O	7:T:4:ALA:HB2	2.12	0.49
1:A:278:MET:SD	7:T:5:LYS:HB3	2.53	0.49
20:P:1267:PGV:H182	26:P:1270:CDL:H662	1.94	0.49
12:L:2:HIS:CG	12:L:3:TYR:H	2.30	0.49
1:N:484:THR:HB	13:Z:2:THR:OG1	2.12	0.49
7:T:7:ASP:OD1	7:T:8:HIS:N	2.45	0.49
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.48	0.49
6:S:55:LYS:HA	6:S:74:LEU:O	2.12	0.49
1:A:189:MET:HG3	1:A:189:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD23	1:A:245:ILE:HD13	1.95	0.49
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.94	0.49
1:N:34:SER:HB2	14:N:515:HEA:C2B	2.43	0.49
1:A:347:LEU:HD13	1:A:383[B]:MET:HB3	1.95	0.49
1:N:113:LEU:HD12	19:N:1522:TGL:C13	2.43	0.48
19:N:1522:TGL:CC3	12:Y:20:ARG:HH21	2.25	0.48
2:B:57:ASP:H	22:B:229:PSC:H201	1.77	0.48
7:G:17:ARG:HH22	25:G:265:PEK:H041	1.79	0.48
8:U:9:LYS:O	8:U:10:ASN:CB	2.61	0.48
1:A:325:ALA:HA	22:B:229:PSC:H291	1.96	0.48
2:O:84:LEU:HA	2:O:87:MET:CE	2.43	0.48
8:U:9:LYS:HG3	8:U:10:ASN:N	2.28	0.48
3:C:103:HIS:HA	20:C:268:PGV:H012	1.95	0.48
11:X:8:ASP:HB3	29:X:4788:HOH:O	2.13	0.48
26:G:269:CDL:H782	26:G:269:CDL:C56	2.40	0.48
25:P:1265:PEK:C04	6:S:1:ALA:H1	2.27	0.48
19:A:521:TGL:H111	19:A:521:TGL:C28	2.34	0.48
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.95	0.48
1:A:1:FME:HE2	1:A:4:ASN:HD22	1.78	0.48
3:P:63:ARG:HE	26:P:1270:CDL:HA21	1.78	0.48
1:N:334:TRP:CZ3	19:Q:1523:TGL:HA51	2.48	0.48
7:T:2:SER:OG	25:T:263:PEK:H292	2.14	0.47
22:R:1229:PSC:H142	22:R:1229:PSC:H341	1.82	0.47
26:C:270:CDL:HB22	10:J:8:LYS:NZ	2.29	0.47
1:A:377:PHE:CD1	14:A:516:HEA:HAD1	2.49	0.47
3:C:122:HIS:HD2	29:C:4553:HOH:O	1.95	0.47
3:C:207:HIS:HD2	3:C:241:TYR:OH	1.97	0.47
25:G:1263:PEK:H132	3:P:247:VAL:CG1	2.44	0.47
25:G:265:PEK:C38	26:G:269:CDL:H273	2.44	0.47
7:G:8:HIS:HE1	25:G:1263:PEK:H321	1.80	0.47
1:A:334:TRP:CZ3	19:D:523:TGL:HA52	2.49	0.47
5:R:41:LEU:CD2	22:R:1229:PSC:H041	2.45	0.47
6:F:1:ALA:N	25:G:265:PEK:H041	2.30	0.47
1:N:18:LEU:CD2	19:N:1522:TGL:HB21	2.44	0.47
14:N:516:HEA:CBC	14:N:516:HEA:HMC1	2.44	0.47
2:B:1:FME:HCN	2:B:193:TYR:H	1.80	0.47
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.47
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.95	0.47
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.13	0.47
7:G:5:LYS:HG3	25:G:1263:PEK:C38	2.32	0.47
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:MET:HE2	1:A:297:MET:HB2	1.96	0.47
22:B:229:PSC:H322	22:B:229:PSC:C28	2.45	0.47
23:C:271:CHD:H162	23:C:271:CHD:H232	1.97	0.47
3:C:3:HIS:HE1	6:F:96:LEU:CD2	2.28	0.47
19:L:522:TGL:OA1	19:L:522:TGL:H182	2.15	0.46
6:F:1:ALA:H2	25:G:265:PEK:C04	2.28	0.46
14:A:516:HEA:HMC1	14:A:516:HEA:HBC1	1.96	0.46
22:B:229:PSC:C07	5:E:8:ASP:HA	2.46	0.46
25:P:1264:PEK:C7	25:P:1264:PEK:H32	2.35	0.46
19:A:521:TGL:HC22	29:D:2606:HOH:O	2.16	0.46
29:B:3446:HOH:O	7:T:17:ARG:HD2	2.14	0.46
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.45	0.46
2:O:217:LYS:HE2	2:O:220:GLU:OE2	2.16	0.46
26:C:270:CDL:CB2	10:J:8:LYS:HZ2	2.28	0.46
26:P:1270:CDL:HB22	26:P:1270:CDL:OA5	2.15	0.46
1:N:351:GLY:C	1:N:380[A]:VAL:HG13	2.35	0.46
7:T:38:HIS:ND1	7:T:38:HIS:N	2.63	0.46
26:G:269:CDL:H562	26:G:269:CDL:C78	2.41	0.46
9:V:15:ARG:HD2	29:V:4529:HOH:O	2.16	0.46
12:L:20:ARG:HH22	19:L:522:TGL:HC61	1.80	0.46
1:A:334:TRP:CD1	19:D:523:TGL:HC41	2.51	0.46
1:A:309:THR:HG22	14:A:516:HEA:HMB2	1.97	0.46
1:N:488:THR:HB	1:N:495:LEU:HD13	1.97	0.46
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.50	0.46
3:P:210:ILE:HG12	20:P:1267:PGV:H132	1.98	0.46
1:A:400:PHE:HB3	19:L:522:TGL:H283	1.98	0.45
19:Q:1523:TGL:H351	9:V:16:ARG:HH21	1.81	0.45
2:B:56:MET:HA	22:B:229:PSC:H202	1.97	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.45
23:B:1085:CHD:H112	23:B:1085:CHD:H12A	1.82	0.45
11:X:42:PRO:HG2	11:X:47:ARG:NE	2.31	0.45
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.77	0.45
6:S:53:THR:CG2	6:S:54:ASN:H	2.19	0.45
23:P:1271:CHD:C16	23:P:1271:CHD:C23	2.95	0.45
10:J:4:ARG:HD3	10:J:7:GLU:OE2	2.17	0.45
25:P:1265:PEK:H041	6:S:1:ALA:N	2.31	0.45
5:R:11:PHE:HB3	22:R:1229:PSC:H073	1.99	0.45
3:C:202:GLY:HA3	25:C:264:PEK:H21	1.98	0.45
1:N:18:LEU:HD22	19:N:1522:TGL:HB21	1.98	0.45
26:G:269:CDL:H182	26:G:269:CDL:H152	1.60	0.45
26:G:269:CDL:C56	26:G:269:CDL:H762	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.68	0.45
1:A:364:ASP:OD2	14:A:516:HEA:O1A	2.35	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.45
3:P:202:GLY:HA3	25:P:1264:PEK:H21	1.99	0.45
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.52	0.45
1:N:380[B]:VAL:O	1:N:384[B]:GLY:HA3	2.17	0.45
3:P:156:ARG:HE	23:P:1271:CHD:C24	2.29	0.44
1:A:382[B]:SER:OG	14:A:515:HEA:H121	2.18	0.44
5:R:80:GLU:CD	5:R:80:GLU:H	2.20	0.44
29:L:4824:HOH:O	13:M:32:TRP:HH2	1.99	0.44
26:G:269:CDL:H561	26:G:269:CDL:H592	1.29	0.44
19:O:1521:TGL:H252	19:O:1521:TGL:H282	1.73	0.44
28:Z:1526:DMU:H9	28:Z:1526:DMU:H15	1.33	0.44
8:H:43:MET:HE3	8:H:49:ASP:H	1.80	0.44
23:B:1085:CHD:H212	23:B:1085:CHD:H12	1.99	0.44
4:D:109:HIS:HB3	29:D:4632:HOH:O	2.18	0.44
8:H:9:LYS:HD2	8:H:11:TYR:HB2	1.97	0.44
1:A:240:HIS:CD2	1:A:240:HIS:C	2.90	0.44
26:C:270:CDL:OB7	26:C:270:CDL:OA3	2.36	0.44
7:T:7:ASP:CG	7:T:8:HIS:N	2.71	0.44
10:J:33:ARG:HG2	23:J:60:CHD:C15	2.48	0.44
3:C:67:PHE:HE1	26:C:270:CDL:C1	2.27	0.44
1:N:347:LEU:HD13	1:N:383[B]:MET:SD	2.58	0.44
1:N:62:ALA:HB1	14:N:515:HEA:HMD3	2.00	0.44
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.44
1:N:87:ILE:O	1:N:173:PRO:HD3	2.18	0.44
2:B:59:GLN:O	2:B:60:GLU:HG3	2.17	0.44
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.60	0.44
22:B:229:PSC:C07	9:I:10:ARG:NH2	2.72	0.43
22:R:1229:PSC:H251	22:R:1229:PSC:H221	1.67	0.43
1:N:362:SER:OG	2:O:87:MET:HE2	2.18	0.43
11:X:42:PRO:HG2	11:X:47:ARG:HE	1.83	0.43
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.99	0.43
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.47	0.43
4:D:101:HIS:HD2	4:D:102:TYR:CZ	2.36	0.43
20:M:524:PGV:H061	20:M:524:PGV:P	2.58	0.43
1:N:379:TYR:O	1:N:383[A]:MET:HB2	2.18	0.43
4:D:70:GLU:O	4:D:73:ARG:NH1	2.52	0.43
20:M:524:PGV:C2	20:M:524:PGV:C01	2.75	0.43
1:N:472:ILE:HG21	19:N:1522:TGL:HA91	2.01	0.43
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:O	1:A:381[A]:LEU:HB3	2.19	0.43
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.16	0.43
19:O:1521:TGL:H101	19:O:1521:TGL:H283	1.98	0.43
6:S:94:HIS:CD2	6:S:95:GLN:H	2.37	0.43
20:M:524:PGV:C14	20:M:524:PGV:H302	2.48	0.43
28:P:1272:DMU:H1	7:T:69:PHE:HZ	1.84	0.43
19:Q:1523:TGL:HA91	19:Q:1523:TGL:C24	2.48	0.43
6:F:1:ALA:H1	25:G:265:PEK:C04	2.21	0.43
25:G:1263:PEK:H331	25:G:1263:PEK:H361	1.86	0.43
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.49	0.43
1:N:53:ILE:HD13	1:N:53:ILE:HG21	1.74	0.43
2:B:16:ILE:HG13	29:B:4955:HOH:O	2.19	0.43
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.43
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.93	0.42
22:R:1229:PSC:H072	9:V:10:ARG:HH21	1.83	0.42
26:P:1270:CDL:H652	26:P:1270:CDL:H622	1.33	0.42
1:N:351:GLY:C	1:N:380[A]:VAL:CG1	2.87	0.42
2:O:146:MET:HA	2:O:213:LEU:HD12	2.01	0.42
5:E:105:GLY:O	5:E:108:LYS:HE2	2.18	0.42
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.42
1:N:417:MET:HE2	29:N:3166:HOH:O	2.03	0.42
9:V:35:TYR:C	9:V:37:PHE:H	2.21	0.42
26:T:1269:CDL:C56	26:T:1269:CDL:H782	2.48	0.42
3:C:224:LYS:HE3	26:C:270:CDL:CB3	2.49	0.42
1:A:136:LEU:HD12	29:A:4591:HOH:O	2.18	0.42
4:D:87:PHE:CZ	20:M:524:PGV:H152	2.54	0.42
22:B:229:PSC:H141	22:B:229:PSC:C34	2.37	0.42
22:B:229:PSC:H041	5:E:41:LEU:HD23	2.02	0.42
7:G:2:SER:OG	25:G:1263:PEK:H292	2.15	0.42
26:C:270:CDL:H672	26:C:270:CDL:C25	2.45	0.42
20:N:1524:PGV:H062	29:Z:4423:HOH:O	2.19	0.42
26:C:270:CDL:H192	26:C:270:CDL:H642	2.00	0.42
19:A:521:TGL:H201	19:A:521:TGL:C24	2.43	0.42
6:S:95:GLN:NE2	6:S:95:GLN:HA	2.32	0.42
7:T:35:SER:C	7:T:37:LEU:H	2.23	0.42
4:D:109:HIS:HD2	29:D:2122:HOH:O	2.03	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.42
23:P:1525:CHD:H12A	23:P:1525:CHD:H112	1.86	0.42
10:W:33:ARG:HG2	23:W:1059:CHD:C15	2.50	0.42
3:C:230:ASN:HB2	29:F:2400:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:1269:CDL:H241	26:T:1269:CDL:H542	2.01	0.42
3:C:51:MET:HB3	26:C:270:CDL:H381	2.02	0.42
3:C:156:ARG:HE	23:C:271:CHD:C24	2.33	0.42
8:U:60:TYR:C	8:U:60:TYR:CD1	2.92	0.42
1:A:512:ASN:HD22	1:A:512:ASN:HA	1.51	0.42
2:B:87:MET:HE2	29:B:4235:HOH:O	2.19	0.42
1:N:430:PHE:HE1	19:O:1521:TGL:HB21	1.85	0.42
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.84	0.42
1:A:380[B]:VAL:O	1:A:384[B]:GLY:HA3	2.20	0.42
1:N:208:MET:HG2	1:N:219:PHE:CE1	2.54	0.42
1:N:240:HIS:C	1:N:240:HIS:CD2	2.93	0.42
20:N:1524:PGV:C15	20:N:1524:PGV:H321	2.49	0.42
2:O:32:PHE:HE2	19:O:1521:TGL:HA51	1.84	0.42
5:R:23:ASP:N	5:R:23:ASP:OD2	2.49	0.42
4:D:127:LYS:HD2	29:I:2618:HOH:O	2.20	0.42
26:G:269:CDL:C24	26:G:269:CDL:H542	2.50	0.41
2:B:102:HIS:O	2:B:104:TRP:HA	2.20	0.41
23:C:271:CHD:H212	23:C:271:CHD:H12	2.01	0.41
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.20	0.41
7:T:5:LYS:CD	25:T:263:PEK:C38	2.94	0.41
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.44	0.41
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.41
29:B:2562:HOH:O	19:D:523:TGL:HC72	2.19	0.41
3:C:109:THR:HB	3:C:110:PRO:HD2	2.02	0.41
19:D:523:TGL:H231	19:D:523:TGL:H201	1.34	0.41
3:C:207:HIS:CD2	3:C:241:TYR:OH	2.73	0.41
3:C:3:HIS:CE1	6:F:96:LEU:CD2	3.04	0.41
26:C:270:CDL:H252	26:C:270:CDL:C67	2.45	0.41
13:M:42:LYS:HD2	13:M:42:LYS:HA	1.60	0.41
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.18	0.41
13:M:16:ALA:HA	20:M:524:PGV:H312	2.03	0.41
7:G:5:LYS:CG	25:G:1263:PEK:H383	2.35	0.41
7:G:31:CYS:SG	26:G:269:CDL:H532	2.61	0.41
1:A:378:HIS:HA	1:A:382[A]:SER:OG	2.20	0.41
9:V:15:ARG:HB2	29:V:4529:HOH:O	2.19	0.41
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.55	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.93	0.41
2:B:128:LEU:HD11	2:B:134:ARG:HA	2.02	0.41
2:B:217:LYS:CE	29:B:4805:HOH:O	2.68	0.41
12:L:47:LYS:HE2	12:L:47:LYS:HB2	1.86	0.41
14:A:516:HEA:HMC1	14:A:516:HEA:CBC	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:41:LYS:HE3	4:Q:41:LYS:HB3	1.82	0.41
1:N:127:THR:HB	1:N:129:TYR:CE2	2.55	0.41
2:B:56:MET:HA	22:B:229:PSC:C20	2.51	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.77	0.41
26:P:1270:CDL:CB2	26:P:1270:CDL:PA1	2.97	0.41
19:Q:1523:TGL:H122	19:Q:1523:TGL:HB92	1.79	0.41
1:N:297:MET:HE2	1:N:302:ARG:HG2	2.02	0.41
7:G:45:PRO:HD2	29:G:2099:HOH:O	2.21	0.41
1:A:439:ARG:HD3	2:B:199:ILE:HB	2.03	0.41
1:A:169:ILE:HD13	1:A:169:ILE:N	2.34	0.41
6:S:37:LYS:HA	6:S:37:LYS:HD2	1.91	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.72	0.41
3:C:105:SER:HA	3:C:116:TRP:CE3	2.56	0.41
2:B:52:HIS:HE1	22:B:229:PSC:H212	1.85	0.41
7:T:5:LYS:HD2	25:T:263:PEK:H381	2.00	0.41
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.56	0.41
1:A:107:PRO:HB3	3:C:25:LEU:HB2	2.03	0.41
5:E:48:ILE:HD13	5:E:48:ILE:HA	1.91	0.41
1:N:512:ASN:HA	1:N:512:ASN:HD22	1.63	0.41
13:Z:42:LYS:HA	13:Z:42:LYS:HD2	1.96	0.41
20:P:1268:PGV:H21	20:P:1268:PGV:H51	1.82	0.41
5:R:11:PHE:CB	22:R:1229:PSC:H073	2.50	0.40
25:C:264:PEK:C7	25:C:264:PEK:H32	2.40	0.40
6:F:1:ALA:H2	25:G:265:PEK:H041	1.85	0.40
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.03	0.40
2:O:227:LEU:HA	2:O:227:LEU:HD23	1.34	0.40
19:N:1522:TGL:HC32	12:Y:20:ARG:HH21	1.86	0.40
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.57	0.40
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.04	0.40
1:A:310:MET:CE	1:A:356:ILE:HG23	2.51	0.40
5:R:41:LEU:HD23	22:R:1229:PSC:H041	2.02	0.40
7:T:3:ALA:HB3	25:T:263:PEK:H361	2.02	0.40
14:A:515:HEA:HHD	14:A:515:HEA:HAC	1.93	0.40
2:O:62:GLU:O	2:O:66:THR:HB	2.21	0.40
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.03	0.40
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.56	0.40
2:B:83:ILE:O	2:B:87:MET:HG3	2.22	0.40
7:T:3:ALA:HB3	25:T:263:PEK:H382	2.03	0.40
9:V:37:PHE:CD1	9:V:38:ALA:N	2.90	0.40
1:A:76:GLY:O	1:A:80:ASN:HB2	2.22	0.40
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:OG1	5:R:80:GLU:OE1[3_647]	1.64	0.56
2:O:126:SER:O	6:S:94:HIS:CB[2_684]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/514 (101%)	504 (98%)	13 (2%)	0	100	100
1	N	517/514 (101%)	501 (97%)	16 (3%)	0	100	100
2	B	225/227 (99%)	220 (98%)	4 (2%)	1 (0%)	39	23
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	39	23
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	135 (95%)	6 (4%)	1 (1%)	26	11
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5	0
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	5	0
7	G	81/85 (95%)	67 (83%)	9 (11%)	5 (6%)	2	0
7	T	81/85 (95%)	69 (85%)	8 (10%)	4 (5%)	3	0
8	H	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2	0
8	U	77/85 (91%)	69 (90%)	4 (5%)	4 (5%)	2	0
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	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%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3514/3614 (97%)	3380 (96%)	108 (3%)	26 (1%)	26	11

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
8	H	45	ALA
8	H	46	LYS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	45	ALA
8	U	46	LYS
2	B	60	GLU
8	H	8	ILE
2	O	60	GLU
6	S	94	HIS
8	U	8	ILE
8	U	10	ASN
6	F	96	LEU
7	G	6	GLY
8	H	51	SER
4	Q	35	ALA
7	G	37	LEU
6	S	96	LEU
7	T	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/426 (101%)	419 (97%)	11 (3%)	54	37
1	N	430/426 (101%)	418 (97%)	12 (3%)	51	35
2	B	210/210 (100%)	201 (96%)	9 (4%)	35	17
2	O	210/210 (100%)	198 (94%)	12 (6%)	25	10
3	C	224/226 (99%)	222 (99%)	2 (1%)	84	80
3	P	224/226 (99%)	218 (97%)	6 (3%)	52	36
4	D	128/129 (99%)	125 (98%)	3 (2%)	58	42
4	Q	128/129 (99%)	122 (95%)	6 (5%)	32	14
5	E	92/95 (97%)	91 (99%)	1 (1%)	80	74
5	R	92/95 (97%)	91 (99%)	1 (1%)	80	74
6	F	81/81 (100%)	78 (96%)	3 (4%)	41	23
6	S	81/81 (100%)	75 (93%)	6 (7%)	17	5
7	G	67/68 (98%)	60 (90%)	7 (10%)	9	2
7	T	67/68 (98%)	59 (88%)	8 (12%)	6	1
8	H	71/75 (95%)	68 (96%)	3 (4%)	36	18
8	U	71/75 (95%)	69 (97%)	2 (3%)	51	35
9	I	57/57 (100%)	50 (88%)	7 (12%)	6	1
9	V	57/57 (100%)	50 (88%)	7 (12%)	6	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	63	49
10	W	49/50 (98%)	48 (98%)	1 (2%)	63	49
11	K	39/46 (85%)	37 (95%)	2 (5%)	29	12
11	X	39/46 (85%)	37 (95%)	2 (5%)	29	12
12	L	39/40 (98%)	38 (97%)	1 (3%)	54	37
12	Y	39/40 (98%)	36 (92%)	3 (8%)	16	5
13	M	37/38 (97%)	32 (86%)	5 (14%)	5	1
13	Z	37/38 (97%)	32 (86%)	5 (14%)	5	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3048/3082 (99%)	2922 (96%)	126 (4%)	37 19

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	169	ILE
1	A	180	GLN
1	A	200	PRO
1	A	241	PRO
1	A	369	ASP
1	A	380[A]	VAL
1	A	380[B]	VAL
1	A	486	ASP
1	A	512	ASN
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
2	B	217	LYS
3	C	159	MET
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
4	D	58	GLU
5	E	90	ARG
6	F	48	LEU
6	F	50	PRO
6	F	96	LEU
7	G	2	SER
7	G	17	ARG
7	G	18	PHE
7	G	26	PRO
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	8	ILE

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Mol	Chain	Res	Type
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	29	LEU
9	I	37	PHE
9	I	43	ARG
9	I	61	GLU
9	I	68	ILE
10	J	50	LEU
11	K	47	ARG
11	K	54	ARG
12	L	26	THR
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	241	PRO
1	N	265	LYS
1	N	297	MET
1	N	338	MET
1	N	369	ASP
1	N	443	TYR
1	N	484	THR
1	N	504	THR
1	N	512	ASN
2	O	33	LEU
2	O	60	GLU
2	O	61	VAL
2	O	65	TRP
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	171	LYS
2	O	203	ASN
2	O	217	LYS

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Mol	Chain	Res	Type
3	P	23	SER
3	P	77	LYS
3	P	110	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	7	LYS
4	Q	9	GLU
4	Q	31	LYS
4	Q	51	LEU
4	Q	143	ASN
5	R	108	LYS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	2	SER
7	T	17	ARG
7	T	18	PHE
7	T	36	TRP
7	T	38	HIS
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	9	LYS
8	U	60	TYR
9	V	2	THR
9	V	10	ARG
9	V	26	MET
9	V	37	PHE
9	V	43	ARG
9	V	61	GLU
9	V	70	GLN
10	W	50	LEU
11	X	20	SER
11	X	47	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR

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Mol	Chain	Res	Type
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS
13	Z	43	SER

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
3	C	161	GLN
3	C	207	HIS
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
7	G	8	HIS
7	G	76	ASN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
1	N	99	ASN
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

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Mol	Chain	Res	Type
3	P	207	HIS
4	Q	37	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	94	HIS
7	T	76	ASN
8	U	23	GLN
10	W	29	ASN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	A	1	1	8,9,10	2.32	2 (25%)	6,9,11	10.18	3 (50%)
2	FME	B	1	2	8,9,10	3.80	5 (62%)	6,9,11	11.14	4 (66%)
7	TPO	G	11	7	8,10,11	2.40	5 (62%)	7,14,16	1.66	2 (28%)
9	SAC	I	1	9	7,8,9	2.85	3 (42%)	7,9,11	1.46	2 (28%)
1	FME	N	1	1	8,9,10	1.24	1 (12%)	6,9,11	9.52	3 (50%)
2	FME	O	1	2	8,9,10	2.04	3 (37%)	6,9,11	7.10	4 (66%)
7	TPO	T	11	7	8,10,11	2.48	4 (50%)	7,14,16	1.68	2 (28%)
9	SAC	V	1	9	7,8,9	3.12	2 (28%)	7,9,11	1.52	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-6.01	1.03	1.22
2	O	1	FME	O1-CN	-4.53	1.08	1.22
1	A	1	FME	O1-CN	-3.08	1.13	1.22
2	B	1	FME	CG-SD	-2.95	1.64	1.81
2	O	1	FME	CG-SD	-2.23	1.68	1.81
2	O	1	FME	CB-CG	2.18	1.60	1.51
7	G	11	TPO	CG2-CB	2.19	1.56	1.51
7	T	11	TPO	P-O2P	2.22	1.62	1.54
7	G	11	TPO	P-O3P	2.25	1.62	1.54
1	N	1	FME	CA-N	2.48	1.49	1.46
7	G	11	TPO	P-O2P	2.61	1.64	1.54
9	I	1	SAC	CB-CA	2.64	1.58	1.52
7	T	11	TPO	P-O3P	2.74	1.64	1.54
2	B	1	FME	CB-CA	2.99	1.58	1.53
7	G	11	TPO	P-OG1	3.23	1.69	1.60
7	T	11	TPO	P-O1P	3.38	1.62	1.51
7	T	11	TPO	P-OG1	3.96	1.72	1.60
7	G	11	TPO	P-O1P	4.00	1.64	1.51
9	I	1	SAC	CA-N	4.35	1.52	1.46
2	B	1	FME	CA-N	4.67	1.53	1.46
9	V	1	SAC	OAC-C1A	4.99	1.34	1.23
9	I	1	SAC	OAC-C1A	5.02	1.34	1.23
1	A	1	FME	CA-N	5.53	1.54	1.46
2	B	1	FME	CN-N	5.89	1.55	1.33
9	V	1	SAC	CA-N	6.10	1.55	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	O1-CN-N	-23.08	91.52	124.76
1	A	1	FME	CA-N-CN	-22.50	88.22	122.82
1	N	1	FME	CA-N-CN	-19.41	92.96	122.82
2	O	1	FME	CA-N-CN	-16.83	96.94	122.82
2	B	1	FME	CA-N-CN	-13.91	101.44	122.82
2	B	1	FME	CG-CB-CA	-3.39	103.10	113.06
7	T	11	TPO	OG1-P-O1P	-2.98	99.65	107.11
7	G	11	TPO	O-C-CA	-2.87	117.85	125.44
7	T	11	TPO	O-C-CA	-2.78	118.11	125.44
9	V	1	SAC	O-C-CA	-2.52	118.79	125.44
2	O	1	FME	CG-CB-CA	-2.50	105.72	113.06
2	O	1	FME	O-C-CA	-2.34	119.27	125.44
2	B	1	FME	O-C-CA	-2.22	119.59	125.44
9	I	1	SAC	C2A-C1A-N	-2.12	112.05	116.11
2	O	1	FME	CB-CG-SD	-2.02	104.67	113.17
9	V	1	SAC	CA-N-C1A	2.05	128.32	121.37
9	I	1	SAC	CB-CA-N	2.13	115.27	110.60
7	G	11	TPO	CG2-CB-CA	2.48	118.22	113.17
1	N	1	FME	CE-SD-CG	3.19	111.27	100.37
1	A	1	FME	CE-SD-CG	5.42	118.87	100.37
1	A	1	FME	O1-CN-N	8.86	137.52	124.76
1	N	1	FME	O1-CN-N	12.31	142.48	124.76

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	3	0
2	B	1	FME	3	0
7	G	11	TPO	3	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, 2 are unknown and 8 are monoatomic - leaving 46 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	515	1	40,67,67	1.31	5 (12%)	41,103,103	2.79	20 (48%)
14	HEA	A	516	1,15	40,67,67	1.49	7 (17%)	41,103,103	2.50	13 (31%)
15	NO	A	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	A	521	-	62,62,62	1.32	6 (9%)	65,65,65	1.83	13 (20%)
20	PGV	A	522	-	50,50,50	1.18	5 (10%)	51,56,56	1.50	10 (19%)
23	CHD	B	1085	-	29,32,32	2.15	9 (31%)	48,51,51	5.30	33 (68%)
21	CUA	B	228	2	0,1,1	0.00	-	0,0,0	0.00	-
22	PSC	B	229	-	51,51,51	1.23	3 (5%)	55,59,59	1.30	7 (12%)
25	PEK	C	264	-	51,52,52	1.13	4 (7%)	52,57,57	2.35	11 (21%)
20	PGV	C	267	-	50,50,50	0.89	1 (2%)	51,56,56	1.39	12 (23%)
20	PGV	C	268	-	50,50,50	1.30	4 (8%)	51,56,56	1.67	5 (9%)
26	CDL	C	270	-	99,99,99	1.44	15 (15%)	101,111,111	1.82	18 (17%)
23	CHD	C	271	-	29,32,32	0.99	1 (3%)	48,51,51	5.12	32 (66%)
23	CHD	C	525	-	29,32,32	1.56	5 (17%)	48,51,51	5.20	33 (68%)
19	TGL	D	523	-	62,62,62	1.55	7 (11%)	65,65,65	1.74	15 (23%)
25	PEK	G	1263	-	51,52,52	1.43	4 (7%)	52,57,57	1.52	7 (13%)
25	PEK	G	265	-	51,52,52	1.45	4 (7%)	52,57,57	1.66	8 (15%)
26	CDL	G	269	-	99,99,99	1.43	14 (14%)	101,111,111	1.64	22 (21%)
28	DMU	G	272	-	34,34,34	1.42	6 (17%)	45,45,45	3.68	24 (53%)
23	CHD	J	60	-	29,32,32	1.05	2 (6%)	48,51,51	5.16	34 (70%)
19	TGL	L	522	-	62,62,62	1.64	7 (11%)	65,65,65	2.13	16 (24%)
20	PGV	M	524	-	50,50,50	1.17	2 (4%)	51,56,56	1.58	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DMU	M	526	-	34,34,34	1.21	4 (11%)	45,45,45	3.67	27 (60%)
20	PGV	N	1266	-	50,50,50	1.20	4 (8%)	51,56,56	1.56	8 (15%)
19	TGL	N	1522	-	62,62,62	1.62	10 (16%)	65,65,65	1.96	17 (26%)
20	PGV	N	1524	-	50,50,50	1.28	4 (8%)	51,56,56	1.43	8 (15%)
14	HEA	N	515	1	40,67,67	1.16	2 (5%)	41,103,103	2.59	16 (39%)
14	HEA	N	516	1,15	40,67,67	1.31	7 (17%)	41,103,103	2.33	18 (43%)
15	NO	N	520	14,16	0,1,1	0.00	-	0,0,0	0.00	-
19	TGL	O	1521	-	62,62,62	1.38	6 (9%)	65,65,65	1.81	12 (18%)
21	CUA	O	228	2	0,1,1	0.00	-	0,0,0	0.00	-
23	CHD	O	229	-	29,32,32	1.98	10 (34%)	48,51,51	5.54	33 (68%)
25	PEK	P	1264	-	51,52,52	0.93	2 (3%)	52,57,57	2.42	12 (23%)
25	PEK	P	1265	-	51,52,52	1.43	6 (11%)	52,57,57	1.54	9 (17%)
20	PGV	P	1267	-	50,50,50	1.04	2 (4%)	51,56,56	1.65	12 (23%)
20	PGV	P	1268	-	50,50,50	1.41	3 (6%)	51,56,56	1.75	9 (17%)
26	CDL	P	1270	-	99,99,99	1.45	14 (14%)	101,111,111	1.88	23 (22%)
23	CHD	P	1271	-	29,32,32	0.88	1 (3%)	48,51,51	5.33	34 (70%)
28	DMU	P	1272	-	34,34,34	1.65	6 (17%)	45,45,45	3.53	28 (62%)
23	CHD	P	1525	-	29,32,32	1.95	12 (41%)	48,51,51	5.64	35 (72%)
19	TGL	Q	1523	-	62,62,62	1.49	7 (11%)	65,65,65	1.51	10 (15%)
22	PSC	R	1229	-	51,51,51	1.38	3 (5%)	55,59,59	1.33	6 (10%)
26	CDL	T	1269	-	99,99,99	1.34	12 (12%)	101,111,111	1.70	19 (18%)
25	PEK	T	263	-	51,52,52	1.26	4 (7%)	52,57,57	1.45	8 (15%)
23	CHD	W	1059	-	29,32,32	0.90	1 (3%)	48,51,51	5.17	34 (70%)
28	DMU	Z	1526	-	34,34,34	1.13	4 (11%)	45,45,45	3.50	25 (55%)

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	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	NO	A	520	14,16	-	0/0/0/0	0/0/0/0
19	TGL	A	521	-	-	0/65/65/65	0/0/0/0
20	PGV	A	522	-	-	0/55/55/55	0/0/0/0
23	CHD	B	1085	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CUA	B	228	2	-	0/0/0/0	0/0/0/0
22	PSC	B	229	-	-	0/55/55/55	0/0/0/0
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
23	CHD	C	271	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
19	TGL	D	523	-	-	0/65/65/65	0/0/0/0
25	PEK	G	1263	-	-	0/56/56/56	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
28	DMU	G	272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	J	60	-	2/2/12/12	0/7/74/74	0/4/4/4
19	TGL	L	522	-	-	0/65/65/65	0/0/0/0
20	PGV	M	524	-	-	2/55/55/55	0/0/0/0
28	DMU	M	526	-	4/4/10/10	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
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	1,15	3/3/7/16	0/24/76/76	0/0/8/8
15	NO	N	520	14,16	-	0/0/0/0	0/0/0/0
19	TGL	O	1521	-	-	0/65/65/65	0/0/0/0
21	CUA	O	228	2	-	0/0/0/0	0/0/0/0
23	CHD	O	229	-	-	0/7/74/74	0/4/4/4
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
20	PGV	P	1268	-	-	0/55/55/55	0/0/0/0
26	CDL	P	1270	-	-	0/110/110/110	0/0/0/0
23	CHD	P	1271	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	P	1272	-	6/6/10/10	0/19/59/59	0/2/2/2
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	0/65/65/65	0/0/0/0
22	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
23	CHD	W	1059	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	Z	1526	-	5/5/10/10	0/19/59/59	0/2/2/2

All (235) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1085	CHD	C10-C5	-5.01	1.46	1.55
23	P	1525	CHD	C6-C5	-4.23	1.46	1.53
23	C	525	CHD	C11-C12	-3.77	1.46	1.53
23	B	1085	CHD	C8-C7	-3.67	1.47	1.53
19	L	522	TGL	C20-CA9	-3.66	1.30	1.51
23	O	229	CHD	C6-C7	-3.66	1.46	1.52
23	P	1525	CHD	C10-C5	-3.62	1.49	1.55
26	P	1270	CDL	C59-C58	-3.49	1.31	1.51
26	C	270	CDL	C59-C58	-3.38	1.32	1.51
26	C	270	CDL	C79-C78	-3.28	1.32	1.51
14	A	516	HEA	C4A-NA	-3.26	1.32	1.36
23	P	1525	CHD	C6-C7	-3.23	1.47	1.52
19	N	1522	TGL	C20-CA9	-3.23	1.32	1.51
26	G	269	CDL	C42-C41	-3.21	1.33	1.51
28	M	526	DMU	C3-C4	-3.19	1.44	1.52
28	Z	1526	DMU	C3-C4	-3.14	1.44	1.52
19	L	522	TGL	C10-CB9	-3.10	1.33	1.51
26	P	1270	CDL	C62-C61	-3.10	1.33	1.51
19	O	1521	TGL	C10-CB9	-3.03	1.34	1.51
26	T	1269	CDL	C59-C58	-3.03	1.34	1.51
19	N	1522	TGL	C10-CB9	-3.01	1.34	1.51
26	P	1270	CDL	C79-C78	-2.97	1.34	1.51
26	P	1270	CDL	C82-C81	-2.96	1.34	1.51
19	O	1521	TGL	C20-CA9	-2.95	1.34	1.51
23	P	1525	CHD	C1-C10	-2.95	1.48	1.54
26	G	269	CDL	C59-C58	-2.95	1.34	1.51
26	P	1270	CDL	C19-C18	-2.94	1.34	1.51
19	D	523	TGL	C20-CA9	-2.94	1.34	1.51
19	A	521	TGL	C10-CB9	-2.94	1.34	1.51
19	A	521	TGL	C20-CA9	-2.91	1.34	1.51
26	C	270	CDL	C62-C61	-2.91	1.34	1.51
23	C	525	CHD	C15-C14	-2.90	1.47	1.54
26	T	1269	CDL	C79-C78	-2.88	1.34	1.51
23	B	1085	CHD	C13-C14	-2.87	1.50	1.55
26	C	270	CDL	C82-C81	-2.86	1.35	1.51
23	C	525	CHD	C10-C5	-2.86	1.50	1.55
26	C	270	CDL	C19-C18	-2.82	1.35	1.51
26	T	1269	CDL	C42-C41	-2.82	1.35	1.51
26	T	1269	CDL	C19-C18	-2.80	1.35	1.51
19	Q	1523	TGL	C10-CB9	-2.80	1.35	1.51
26	P	1270	CDL	C22-C21	-2.78	1.35	1.51
26	G	269	CDL	C19-C18	-2.75	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	C62-C61	-2.74	1.35	1.51
19	Q	1523	TGL	C15-CC9	-2.74	1.35	1.51
26	G	269	CDL	C79-C78	-2.73	1.35	1.51
19	D	523	TGL	C15-CC9	-2.72	1.35	1.51
28	M	526	DMU	C6-C1	-2.69	1.44	1.52
26	C	270	CDL	C22-C21	-2.67	1.36	1.51
26	G	269	CDL	C39-C38	-2.67	1.36	1.51
26	G	269	CDL	C22-C21	-2.66	1.36	1.51
26	T	1269	CDL	C22-C21	-2.65	1.36	1.51
26	P	1270	CDL	C39-C38	-2.62	1.36	1.51
25	C	264	PEK	O03-C01	-2.60	1.39	1.45
19	Q	1523	TGL	C20-CA9	-2.60	1.36	1.51
23	O	229	CHD	C13-C12	-2.58	1.50	1.54
26	G	269	CDL	C82-C81	-2.58	1.36	1.51
26	T	1269	CDL	C62-C61	-2.53	1.36	1.51
26	C	270	CDL	C39-C38	-2.52	1.37	1.51
20	A	522	PGV	O01-C02	-2.50	1.40	1.46
26	T	1269	CDL	C39-C38	-2.48	1.37	1.51
23	O	229	CHD	C13-C14	-2.46	1.51	1.55
19	O	1521	TGL	C15-CC9	-2.45	1.37	1.51
23	B	1085	CHD	C13-C12	-2.42	1.50	1.54
26	T	1269	CDL	C82-C81	-2.41	1.37	1.51
19	L	522	TGL	C15-CC9	-2.35	1.37	1.51
26	C	270	CDL	C42-C41	-2.34	1.38	1.51
19	N	1522	TGL	C15-CC9	-2.33	1.38	1.51
20	N	1266	PGV	O01-C02	-2.33	1.40	1.46
20	C	268	PGV	O04-C19	-2.27	1.15	1.22
25	C	264	PEK	C23-C22	-2.24	1.43	1.52
19	A	521	TGL	C15-CC9	-2.18	1.38	1.51
23	P	1525	CHD	C13-C12	-2.17	1.51	1.54
23	C	271	CHD	C10-C9	-2.17	1.51	1.56
19	D	523	TGL	C10-CB9	-2.14	1.39	1.51
28	G	272	DMU	C3-C4	-2.13	1.47	1.52
28	M	526	DMU	C8-C9	-2.07	1.48	1.53
26	P	1270	CDL	C42-C41	-2.07	1.39	1.51
23	O	229	CHD	C10-C5	-2.04	1.51	1.55
14	N	516	HEA	CMB-C2B	2.01	1.55	1.51
28	G	272	DMU	C2-C1	2.02	1.57	1.52
23	P	1525	CHD	O7-C7	2.02	1.47	1.43
20	P	1267	PGV	O05-C05	2.03	1.49	1.43
20	A	522	PGV	C03-C02	2.04	1.56	1.50
14	N	515	HEA	O11-C11	2.07	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	1085	CHD	C4-C3	2.07	1.55	1.51
23	P	1525	CHD	C21-C20	2.08	1.58	1.53
20	N	1524	PGV	C03-C02	2.08	1.56	1.50
23	O	229	CHD	C4-C5	2.09	1.57	1.53
23	P	1525	CHD	C13-C17	2.09	1.59	1.55
26	P	1270	CDL	PB2-OB2	2.09	1.68	1.59
28	Z	1526	DMU	C2-C1	2.11	1.57	1.52
26	G	269	CDL	C17-C16	2.12	1.63	1.51
25	P	1264	PEK	O03-C21	2.12	1.39	1.33
14	N	516	HEA	O11-C11	2.12	1.47	1.42
26	G	269	CDL	CB6-CB4	2.12	1.56	1.50
14	N	516	HEA	C4C-CHD	2.13	1.45	1.39
23	B	1085	CHD	C21-C20	2.14	1.58	1.53
25	P	1265	PEK	C22-C21	2.16	1.57	1.50
23	J	60	CHD	C11-C9	2.17	1.57	1.53
28	G	272	DMU	O1-C10	2.18	1.47	1.41
23	J	60	CHD	C20-C17	2.19	1.58	1.54
20	N	1524	PGV	C21-C20	2.19	1.60	1.52
20	C	267	PGV	C03-C02	2.20	1.56	1.50
25	G	1263	PEK	P-O11	2.21	1.69	1.59
23	O	229	CHD	C19-C10	2.21	1.58	1.54
28	Z	1526	DMU	O16-C18	2.22	1.49	1.42
28	G	272	DMU	O7-C10	2.24	1.47	1.41
14	A	515	HEA	CAA-C2A	2.24	1.56	1.52
25	T	263	PEK	C01-C02	2.25	1.57	1.50
14	N	515	HEA	C12-C13	2.25	1.60	1.53
25	P	1265	PEK	C03-C02	2.26	1.57	1.50
25	T	263	PEK	C03-C02	2.27	1.57	1.50
19	N	1522	TGL	OG2-CG2	2.27	1.52	1.46
14	N	516	HEA	CAD-C3D	2.27	1.55	1.52
14	N	516	HEA	C18-C19	2.28	1.37	1.33
28	P	1272	DMU	O7-C10	2.29	1.47	1.41
28	Z	1526	DMU	O16-C6	2.31	1.44	1.40
19	N	1522	TGL	CG1-CG2	2.31	1.57	1.50
26	C	270	CDL	PB2-OB2	2.31	1.69	1.59
23	W	1059	CHD	C20-C17	2.32	1.58	1.54
14	A	516	HEA	C4D-CHA	2.32	1.46	1.39
28	M	526	DMU	O16-C6	2.33	1.44	1.40
23	P	1525	CHD	C19-C10	2.34	1.58	1.54
20	P	1268	PGV	P-O11	2.34	1.69	1.59
19	N	1522	TGL	OB1-CB1	2.36	1.29	1.22
23	O	229	CHD	O7-C7	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1265	PEK	P-O11	2.39	1.70	1.59
28	G	272	DMU	O5-C6	2.42	1.48	1.41
14	A	516	HEA	CAD-C3D	2.43	1.56	1.52
20	N	1266	PGV	C01-C02	2.43	1.57	1.50
14	N	516	HEA	C1D-ND	2.44	1.40	1.36
14	A	516	HEA	C1A-NA	2.45	1.40	1.36
23	B	1085	CHD	C4-C5	2.45	1.58	1.53
14	A	515	HEA	O11-C11	2.48	1.48	1.42
26	C	270	CDL	PA1-OA5	2.50	1.70	1.59
14	A	515	HEA	C21-C22	2.51	1.57	1.50
14	A	516	HEA	C14-C15	2.51	1.37	1.33
20	A	522	PGV	O03-C19	2.52	1.40	1.33
25	G	265	PEK	P-O11	2.52	1.70	1.59
25	P	1264	PEK	C2-C1	2.54	1.58	1.50
23	P	1525	CHD	C10-C9	2.56	1.61	1.56
28	P	1272	DMU	O5-C6	2.57	1.48	1.41
28	P	1272	DMU	C2-C1	2.59	1.59	1.52
25	C	264	PEK	O01-C1	2.62	1.42	1.34
20	C	268	PGV	P-O11	2.63	1.71	1.59
20	A	522	PGV	O01-C1	2.64	1.42	1.34
26	C	270	CDL	PB2-OB3	2.71	1.61	1.51
28	P	1272	DMU	O5-C4	2.71	1.51	1.44
23	O	229	CHD	O12-C12	2.74	1.48	1.43
23	O	229	CHD	C22-C20	2.75	1.62	1.54
23	P	1525	CHD	C11-C9	2.75	1.58	1.53
23	C	525	CHD	C18-C13	2.75	1.58	1.54
23	B	1085	CHD	O12-C12	2.82	1.48	1.43
14	A	515	HEA	C12-C13	2.86	1.63	1.53
14	A	516	HEA	C4B-NB	2.88	1.40	1.36
26	P	1270	CDL	OB6-CB5	2.89	1.42	1.34
28	P	1272	DMU	O1-C10	2.91	1.49	1.41
14	N	516	HEA	C16-C15	2.95	1.57	1.51
14	A	515	HEA	C22-C23	2.96	1.41	1.32
25	G	1263	PEK	C03-C02	3.00	1.59	1.50
23	P	1271	CHD	C20-C17	3.01	1.60	1.54
25	C	264	PEK	C2-C1	3.01	1.59	1.50
23	P	1525	CHD	O12-C12	3.10	1.49	1.43
14	A	516	HEA	O11-C11	3.10	1.50	1.42
25	G	265	PEK	P-O12	3.10	1.73	1.59
19	L	522	TGL	CC2-CC1	3.27	1.60	1.50
25	P	1265	PEK	P-O12	3.29	1.74	1.59
20	P	1267	PGV	C01-C02	3.31	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	1270	CDL	PB2-OB3	3.37	1.63	1.51
20	M	524	PGV	O01-C1	3.40	1.44	1.34
19	N	1522	TGL	CG3-CG2	3.42	1.60	1.50
23	C	525	CHD	C11-C9	3.50	1.59	1.53
20	N	1524	PGV	O01-C1	3.50	1.44	1.34
22	B	229	PSC	C13-C12	3.51	1.52	1.31
20	C	268	PGV	O03-C19	3.55	1.44	1.33
20	P	1268	PGV	O03-C19	3.55	1.44	1.33
26	C	270	CDL	OB6-CB5	3.66	1.45	1.34
20	N	1266	PGV	O01-C1	3.72	1.45	1.34
25	T	263	PEK	O01-C1	3.77	1.45	1.34
26	C	270	CDL	OA6-CA5	3.87	1.45	1.34
20	N	1266	PGV	O03-C19	3.90	1.45	1.33
20	A	522	PGV	C01-C02	3.92	1.61	1.50
19	D	523	TGL	OG3-CC1	4.00	1.45	1.33
26	G	269	CDL	OA8-CA7	4.09	1.45	1.33
26	T	1269	CDL	OB8-CB7	4.15	1.45	1.33
19	A	521	TGL	OG2-CB1	4.16	1.46	1.34
26	T	1269	CDL	OA8-CA7	4.24	1.46	1.33
19	L	522	TGL	OG3-CC1	4.25	1.46	1.33
22	R	1229	PSC	C13-C12	4.26	1.56	1.31
19	Q	1523	TGL	OG3-CC1	4.27	1.46	1.33
22	B	229	PSC	O03-C19	4.36	1.46	1.33
19	Q	1523	TGL	OB1-CB1	4.37	1.35	1.22
19	N	1522	TGL	OG1-CA1	4.41	1.46	1.33
19	N	1522	TGL	OG3-CC1	4.41	1.46	1.33
22	B	229	PSC	O01-C1	4.47	1.47	1.34
26	T	1269	CDL	OB6-CB5	4.52	1.47	1.34
19	A	521	TGL	OG3-CC1	4.52	1.46	1.33
26	P	1270	CDL	OA6-CA5	4.52	1.47	1.34
19	D	523	TGL	OG1-CA1	4.54	1.47	1.33
22	R	1229	PSC	O03-C19	4.55	1.47	1.33
19	O	1521	TGL	OG3-CC1	4.55	1.47	1.33
26	P	1270	CDL	OB8-CB7	4.61	1.47	1.33
19	O	1521	TGL	OG1-CA1	4.73	1.47	1.33
19	A	521	TGL	OG1-CA1	4.73	1.47	1.33
26	G	269	CDL	OB8-CB7	4.74	1.47	1.33
19	D	523	TGL	OG2-CB1	4.90	1.49	1.34
22	R	1229	PSC	O01-C1	4.98	1.49	1.34
19	Q	1523	TGL	OG2-CB1	4.98	1.49	1.34
26	T	1269	CDL	OA6-CA5	4.98	1.49	1.34
19	O	1521	TGL	OG2-CB1	5.00	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1265	PEK	O01-C1	5.01	1.49	1.34
19	L	522	TGL	OG1-CA1	5.06	1.48	1.33
26	P	1270	CDL	OA8-CA7	5.12	1.48	1.33
19	Q	1523	TGL	OG1-CA1	5.14	1.48	1.33
26	C	270	CDL	OB8-CB7	5.18	1.48	1.33
20	N	1524	PGV	O03-C19	5.26	1.49	1.33
26	G	269	CDL	OA6-CA5	5.26	1.50	1.34
26	C	270	CDL	OA8-CA7	5.27	1.49	1.33
20	M	524	PGV	O03-C19	5.29	1.49	1.33
26	G	269	CDL	OB6-CB5	5.33	1.50	1.34
28	G	272	DMU	O16-C6	5.37	1.49	1.40
25	G	1263	PEK	O01-C1	5.46	1.50	1.34
23	B	1085	CHD	C18-C13	5.50	1.63	1.54
23	O	229	CHD	C18-C13	5.53	1.63	1.54
25	G	265	PEK	O03-C21	5.54	1.50	1.33
25	G	265	PEK	O01-C1	5.63	1.51	1.34
19	D	523	TGL	OB1-CB1	5.65	1.39	1.22
25	P	1265	PEK	O03-C21	5.79	1.50	1.33
25	T	263	PEK	O03-C21	5.86	1.51	1.33
25	G	1263	PEK	O03-C21	5.87	1.51	1.33
28	P	1272	DMU	O16-C6	5.87	1.50	1.40
20	C	268	PGV	O01-C1	6.08	1.52	1.34
19	N	1522	TGL	OG2-CB1	6.88	1.54	1.34
19	L	522	TGL	OG2-CB1	7.08	1.55	1.34
20	P	1268	PGV	O01-C1	7.18	1.55	1.34

All (746) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C18-C13-C12	-11.11	98.26	109.09
23	P	1271	CHD	C23-C22-C20	-10.75	102.07	114.75
23	P	1525	CHD	C23-C22-C20	-10.58	102.27	114.75
23	P	1271	CHD	C18-C13-C12	-10.33	99.01	109.09
23	O	229	CHD	C19-C10-C9	-10.09	96.05	111.18
23	C	525	CHD	C23-C22-C20	-10.05	102.91	114.75
23	P	1525	CHD	C19-C10-C9	-9.96	96.25	111.18
23	J	60	CHD	C18-C13-C12	-9.79	99.54	109.09
23	C	525	CHD	C19-C10-C9	-9.67	96.68	111.18
23	C	271	CHD	C18-C13-C12	-9.55	99.77	109.09
23	B	1085	CHD	C18-C13-C12	-9.38	99.94	109.09
23	B	1085	CHD	C6-C5-C4	-9.29	100.67	111.05
23	W	1059	CHD	C18-C13-C12	-9.07	100.24	109.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1085	CHD	C18-C13-C17	-8.98	97.06	111.22
23	P	1525	CHD	C18-C13-C12	-8.86	100.44	109.09
23	C	271	CHD	O7-C7-C6	-8.40	89.49	110.06
23	B	1085	CHD	C19-C10-C9	-8.39	98.61	111.18
19	L	522	TGL	OG3-CC1-OC1	-8.13	102.51	123.49
23	C	525	CHD	O12-C12-C13	-7.68	98.67	111.11
23	O	229	CHD	C6-C5-C4	-7.62	102.53	111.05
23	C	525	CHD	C18-C13-C17	-7.55	99.31	111.22
23	P	1271	CHD	O7-C7-C6	-7.15	92.55	110.06
23	C	525	CHD	C18-C13-C14	-7.13	99.97	111.22
14	A	515	HEA	C13-C12-C11	-7.12	105.05	114.51
23	P	1525	CHD	C18-C13-C14	-7.00	100.17	111.22
26	C	270	CDL	CB4-OB6-CB5	-6.92	101.30	117.89
26	P	1270	CDL	CB4-OB6-CB5	-6.90	101.32	117.89
19	D	523	TGL	OG2-CB1-CB2	-6.37	97.67	111.53
23	B	1085	CHD	O12-C12-C13	-6.36	100.81	111.11
23	C	271	CHD	C19-C10-C9	-6.18	101.92	111.18
14	N	515	HEA	C13-C12-C11	-6.04	106.48	114.51
23	C	525	CHD	C22-C20-C17	-6.01	97.61	110.24
23	O	229	CHD	O12-C12-C13	-5.94	101.48	111.11
14	N	515	HEA	CAA-CBA-CGA	-5.93	101.87	112.75
23	O	229	CHD	C18-C13-C14	-5.91	101.89	111.22
14	N	515	HEA	C4B-C3B-C11	-5.81	120.70	127.01
23	P	1525	CHD	O12-C12-C13	-5.73	101.83	111.11
14	A	516	HEA	C16-C15-C14	-5.70	110.25	121.05
23	P	1525	CHD	C18-C13-C17	-5.65	102.31	111.22
14	N	516	HEA	C13-C12-C11	-5.59	107.08	114.51
23	P	1525	CHD	C22-C20-C17	-5.53	98.62	110.24
14	A	515	HEA	C4B-C3B-C11	-5.50	121.04	127.01
23	C	271	CHD	C23-C22-C20	-5.48	108.30	114.75
23	O	229	CHD	C21-C20-C17	-5.36	104.03	112.96
28	M	526	DMU	O7-C10-C5	-5.24	95.36	108.10
23	P	1271	CHD	O12-C12-C11	-5.22	98.39	109.06
23	P	1271	CHD	C19-C10-C1	-5.20	99.45	108.20
23	P	1271	CHD	C18-C13-C17	-5.11	103.16	111.22
19	N	1522	TGL	OG3-CC1-OC1	-4.99	110.60	123.49
23	J	60	CHD	C19-C10-C5	-4.98	101.45	110.25
20	N	1524	PGV	C4-C3-C2	-4.98	95.03	113.29
14	N	515	HEA	CAD-C3D-C4D	-4.91	121.68	127.01
23	P	1525	CHD	C4-C5-C10	-4.89	107.27	112.66
28	Z	1526	DMU	O7-C10-C5	-4.84	96.33	108.10
14	A	516	HEA	OMA-CMA-C3A	-4.69	115.63	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C6-C5-C4	-4.68	105.82	111.05
25	P	1264	PEK	O01-C1-O02	-4.67	111.13	123.67
23	O	229	CHD	O7-C7-C6	-4.67	98.62	110.06
26	P	1270	CDL	C52-C51-CB5	-4.63	95.38	113.59
23	W	1059	CHD	C19-C10-C5	-4.62	102.10	110.25
19	N	1522	TGL	CB4-CB3-CB2	-4.61	96.37	113.29
14	N	515	HEA	CMB-C2B-C1B	-4.61	120.74	128.36
25	G	265	PEK	O03-C21-O04	-4.51	111.86	123.49
23	B	1085	CHD	C4-C5-C10	-4.50	107.69	112.66
26	C	270	CDL	C52-C51-CB5	-4.49	95.95	113.59
25	C	264	PEK	O01-C1-O02	-4.47	111.67	123.67
14	A	515	HEA	C17-C18-C19	-4.37	118.26	127.76
23	P	1525	CHD	C6-C5-C4	-4.37	106.17	111.05
19	Q	1523	TGL	CG3-CG2-CG1	-4.37	101.85	112.07
25	C	264	PEK	O03-C01-C02	-4.28	97.17	108.69
20	P	1268	PGV	C03-C02-C01	-4.28	102.07	112.07
20	N	1266	PGV	O01-C1-O02	-4.25	112.27	123.67
23	P	1525	CHD	O12-C12-C11	-4.24	100.38	109.06
14	A	515	HEA	C13-C14-C15	-4.17	118.69	127.76
23	W	1059	CHD	C6-C5-C4	-4.17	106.39	111.05
25	C	264	PEK	C24-C23-C22	-4.15	98.08	113.29
19	L	522	TGL	CA4-CA3-CA2	-4.14	98.09	113.29
23	W	1059	CHD	C1-C10-C9	-4.06	104.90	111.45
14	A	515	HEA	O11-C11-C3B	-4.02	99.95	111.82
20	M	524	PGV	C8-C9-C10	-4.02	98.17	113.86
20	C	267	PGV	C22-C21-C20	-4.02	98.55	113.29
14	N	516	HEA	C1A-C2A-C3A	-3.95	103.12	107.07
26	G	269	CDL	CB6-CB4-CB3	-3.94	102.86	112.07
23	C	525	CHD	O7-C7-C6	-3.91	100.47	110.06
23	C	525	CHD	O7-C7-C8	-3.89	100.67	109.26
20	A	522	PGV	O01-C1-O02	-3.87	113.28	123.67
14	A	515	HEA	CAD-CBD-CGD	-3.84	105.71	112.75
23	J	60	CHD	C18-C13-C14	-3.78	105.25	111.22
23	C	525	CHD	C6-C5-C4	-3.78	106.82	111.05
23	J	60	CHD	C1-C10-C9	-3.76	105.39	111.45
19	L	522	TGL	C26-C25-C24	-3.74	95.24	114.53
23	P	1525	CHD	O7-C7-C6	-3.74	100.91	110.06
23	O	229	CHD	C9-C10-C5	-3.72	103.16	108.67
23	O	229	CHD	C18-C13-C17	-3.67	105.42	111.22
20	P	1267	PGV	C27-C26-C25	-3.66	95.63	114.53
22	B	229	PSC	C29-C28-C27	-3.65	95.70	114.53
23	B	1085	CHD	C19-C10-C5	-3.63	103.85	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	268	PGV	O04-C19-C20	-3.62	109.26	123.72
23	W	1059	CHD	O7-C7-C6	-3.62	101.20	110.06
25	C	264	PEK	C03-C02-C01	-3.58	103.69	112.07
20	N	1266	PGV	O01-C02-C01	-3.58	95.74	108.36
26	T	1269	CDL	OA8-CA7-OA9	-3.57	114.28	123.49
20	P	1267	PGV	O01-C1-O02	-3.55	114.14	123.67
23	W	1059	CHD	C18-C13-C14	-3.54	105.64	111.22
23	C	271	CHD	O12-C12-C11	-3.51	101.87	109.06
25	P	1264	PEK	O11-P-O14	-3.49	96.09	109.62
20	A	522	PGV	C23-C22-C21	-3.49	96.53	114.53
23	P	1271	CHD	C19-C10-C9	-3.48	105.96	111.18
26	T	1269	CDL	CB6-CB4-CB3	-3.44	104.03	112.07
25	P	1264	PEK	O03-C21-C22	-3.42	101.47	111.90
20	A	522	PGV	O03-C19-O04	-3.41	114.68	123.49
23	W	1059	CHD	O12-C12-C11	-3.41	102.09	109.06
25	C	264	PEK	C25-C24-C23	-3.39	97.03	114.53
14	N	515	HEA	CAD-CBD-CGD	-3.33	106.64	112.75
20	P	1267	PGV	O03-C01-C02	-3.33	99.72	108.69
23	P	1271	CHD	O12-C12-C13	-3.33	105.71	111.11
14	N	516	HEA	CMB-C2B-C1B	-3.33	122.86	128.36
25	P	1265	PEK	O03-C21-O04	-3.30	114.96	123.49
28	M	526	DMU	O7-C10-O1	-3.30	102.34	110.68
14	N	515	HEA	C13-C14-C15	-3.25	120.69	127.76
23	C	271	CHD	C11-C9-C10	-3.23	110.43	113.79
20	P	1268	PGV	O12-P-O13	-3.20	97.21	109.62
14	N	515	HEA	C25-C23-C24	-3.19	106.80	114.64
14	A	515	HEA	CAA-CBA-CGA	-3.17	106.94	112.75
23	O	229	CHD	O12-C12-C11	-3.13	102.65	109.06
22	B	229	PSC	C11-C12-C13	-3.13	105.65	125.00
14	A	515	HEA	CBD-CAD-C3D	-3.11	106.95	112.53
20	N	1524	PGV	O03-C19-O04	-3.09	115.51	123.49
23	C	525	CHD	C19-C10-C5	-3.09	104.80	110.25
25	P	1264	PEK	O03-C01-C02	-3.08	100.41	108.69
25	T	263	PEK	O01-C1-O02	-3.06	115.46	123.67
20	P	1268	PGV	O02-C1-C2	-3.06	111.49	123.72
26	C	270	CDL	OA6-CA5-OA7	-3.05	115.48	123.67
26	T	1269	CDL	OA6-CA5-OA7	-3.03	115.55	123.67
25	G	265	PEK	O11-P-O14	-3.01	97.92	109.62
23	P	1525	CHD	C1-C10-C9	-3.00	106.62	111.45
25	P	1264	PEK	C25-C24-C23	-2.98	99.13	114.53
25	P	1265	PEK	C35-C34-C33	-2.97	99.19	114.53
19	D	523	TGL	OG1-CA1-OA1	-2.97	115.83	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C18-C13-C17	-2.97	106.53	111.22
20	P	1267	PGV	O03-C19-O04	-2.95	115.87	123.49
25	T	263	PEK	C18-C17-C16	-2.94	102.37	113.86
19	N	1522	TGL	C26-C25-C24	-2.83	99.93	114.53
20	M	524	PGV	C4-C3-C2	-2.82	102.95	113.29
26	P	1270	CDL	C55-C54-C53	-2.79	100.10	114.53
19	A	521	TGL	OG3-CC1-OC1	-2.79	116.28	123.49
20	P	1268	PGV	O03-C19-O04	-2.78	116.32	123.49
20	M	524	PGV	O01-C1-O02	-2.77	116.23	123.67
23	C	525	CHD	C18-C13-C12	-2.77	106.39	109.09
28	P	1272	DMU	O49-C1-C6	-2.76	103.96	110.02
20	N	1266	PGV	O03-C19-O04	-2.75	116.40	123.49
14	N	516	HEA	CAD-CBD-CGD	-2.74	107.72	112.75
19	D	523	TGL	OG3-CC1-OC1	-2.74	116.42	123.49
23	J	60	CHD	O7-C7-C6	-2.74	103.35	110.06
26	C	270	CDL	OB8-CB7-OB9	-2.73	116.45	123.49
26	P	1270	CDL	OA6-CA5-OA7	-2.73	116.35	123.67
19	Q	1523	TGL	OG3-CC1-OC1	-2.72	116.47	123.49
25	T	263	PEK	C8-C7-C6	-2.69	103.07	112.00
26	T	1269	CDL	OB8-CB7-OB9	-2.68	116.57	123.49
19	L	522	TGL	CG3-CG2-CG1	-2.66	105.84	112.07
28	Z	1526	DMU	O7-C10-O1	-2.66	103.95	110.68
23	P	1525	CHD	C19-C10-C5	-2.65	105.57	110.25
26	P	1270	CDL	OA8-CA7-OA9	-2.65	116.66	123.49
20	C	268	PGV	O03-C19-O04	-2.64	116.67	123.49
14	A	515	HEA	C16-C15-C14	-2.64	116.05	121.05
14	N	515	HEA	CMC-C2C-C1C	-2.64	124.00	128.36
23	C	271	CHD	C19-C10-C5	-2.64	105.60	110.25
23	O	229	CHD	C4-C5-C10	-2.63	109.76	112.66
26	P	1270	CDL	OB9-CB7-C71	-2.62	113.26	123.72
19	A	521	TGL	CB7-CB6-CB5	-2.61	101.05	114.53
14	A	516	HEA	O11-C11-C3B	-2.60	104.15	111.82
19	A	521	TGL	OG1-CA1-OA1	-2.60	116.79	123.49
28	M	526	DMU	C25-C28-C31	-2.59	101.15	114.53
14	A	515	HEA	C20-C21-C22	-2.57	104.96	111.69
23	B	1085	CHD	C9-C10-C5	-2.57	104.88	108.67
20	N	1266	PGV	C03-C02-C01	-2.56	106.08	112.07
19	O	1521	TGL	OB1-CB1-CB2	-2.56	113.48	123.72
23	O	229	CHD	C22-C20-C17	-2.56	104.86	110.24
26	P	1270	CDL	CA6-CA4-CA3	-2.56	106.09	112.07
20	A	522	PGV	C8-C9-C10	-2.53	103.98	113.86
20	C	267	PGV	O03-C01-C02	-2.52	101.91	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	CB7-CB6-CB5	-2.51	101.57	114.53
23	P	1271	CHD	C6-C5-C4	-2.51	108.24	111.05
23	B	1085	CHD	C1-C10-C9	-2.51	107.40	111.45
25	C	264	PEK	C27-C26-C25	-2.50	101.62	114.53
26	P	1270	CDL	CB2-C1-CA2	-2.49	104.85	112.92
20	C	268	PGV	O12-P-O13	-2.47	100.04	109.62
20	M	524	PGV	C28-C27-C26	-2.46	101.85	114.53
23	C	271	CHD	O12-C12-C13	-2.45	107.13	111.11
20	C	267	PGV	C21-C20-C19	-2.45	103.95	113.59
22	R	1229	PSC	C27-C26-C25	-2.45	101.87	114.53
26	P	1270	CDL	C58-C57-C56	-2.45	101.90	114.53
23	B	1085	CHD	O12-C12-C11	-2.44	104.07	109.06
26	G	269	CDL	CA6-CA4-CA3	-2.43	106.39	112.07
23	B	1085	CHD	C18-C13-C14	-2.41	107.41	111.22
19	D	523	TGL	CG3-CG2-CG1	-2.41	106.44	112.07
28	M	526	DMU	C28-C31-C34	-2.41	102.11	114.53
26	C	270	CDL	OB9-CB7-C71	-2.39	114.16	123.72
28	M	526	DMU	O4-C7-C5	-2.38	104.98	110.34
20	P	1267	PGV	C9-C10-C11	-2.38	99.98	112.45
20	P	1267	PGV	C22-C21-C20	-2.37	104.58	113.29
25	C	264	PEK	C32-C31-C30	-2.36	102.33	114.53
20	C	267	PGV	C8-C9-C10	-2.36	104.65	113.86
14	A	515	HEA	OMA-CMA-C3A	-2.36	120.35	125.11
19	L	522	TGL	C25-C24-C23	-2.35	102.38	114.53
25	P	1264	PEK	C24-C23-C22	-2.34	104.70	113.29
14	A	516	HEA	C3C-CAC-CBC	-2.34	121.53	126.32
26	C	270	CDL	O1-C1-CA2	-2.33	100.47	109.35
19	A	521	TGL	OG1-CG1-CG2	-2.31	102.46	108.69
14	A	515	HEA	C3C-CAC-CBC	-2.30	121.61	126.32
28	M	526	DMU	C22-C19-C18	-2.30	103.19	113.47
14	N	516	HEA	CAD-C3D-C2D	-2.28	122.49	129.00
19	N	1522	TGL	C24-C23-C22	-2.28	102.78	114.53
19	L	522	TGL	C24-C23-C22	-2.27	102.78	114.53
25	P	1264	PEK	C32-C31-C30	-2.27	102.78	114.53
26	G	269	CDL	CB2-C1-CA2	-2.27	105.58	112.92
19	N	1522	TGL	CA8-CA7-CA6	-2.26	102.85	114.53
19	L	522	TGL	CA8-CA7-CA6	-2.26	102.85	114.53
20	C	267	PGV	C27-C26-C25	-2.26	102.89	114.53
26	G	269	CDL	OB7-CB5-C51	-2.25	114.71	123.72
20	P	1268	PGV	O04-C19-C20	-2.25	114.74	123.72
22	R	1229	PSC	C21-C20-C19	-2.24	104.78	113.59
23	B	1085	CHD	O7-C7-C6	-2.24	104.57	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	522	PGV	O05-C05-C04	-2.23	100.85	109.35
19	L	522	TGL	CC4-CC3-CC2	-2.23	105.11	113.29
20	A	522	PGV	C7-C6-C5	-2.23	103.02	114.53
26	T	1269	CDL	OB5-PB2-OB3	-2.22	100.98	109.62
20	N	1524	PGV	C5-C4-C3	-2.21	103.11	114.53
28	Z	1526	DMU	O4-C7-C8	-2.20	105.39	110.34
14	A	515	HEA	CBA-CAA-C2A	-2.19	108.60	112.53
22	B	229	PSC	C32-C31-C30	-2.19	103.21	114.53
20	C	267	PGV	O03-C19-O04	-2.19	117.85	123.49
25	T	263	PEK	O04-C21-C22	-2.18	115.00	123.72
14	N	515	HEA	C17-C18-C19	-2.18	123.03	127.76
14	A	516	HEA	CMC-C2C-C1C	-2.17	124.78	128.36
20	N	1266	PGV	C5-C4-C3	-2.16	103.36	114.53
28	P	1272	DMU	O3-C5-C10	-2.16	105.28	110.02
26	P	1270	CDL	OB8-CB7-OB9	-2.15	117.94	123.49
19	L	522	TGL	OA1-CA1-CA2	-2.14	115.16	123.72
14	A	515	HEA	CMB-C2B-C1B	-2.13	124.83	128.36
19	D	523	TGL	CC4-CC3-CC2	-2.13	105.49	113.29
23	J	60	CHD	C19-C10-C1	-2.12	104.64	108.20
26	G	269	CDL	OB5-PB2-OB3	-2.11	101.44	109.62
23	C	271	CHD	C18-C13-C14	-2.10	107.90	111.22
25	P	1264	PEK	C30-C29-C28	-2.10	103.70	114.53
19	N	1522	TGL	CA5-CA4-CA3	-2.10	103.70	114.53
20	C	267	PGV	C4-C3-C2	-2.09	105.61	113.29
23	W	1059	CHD	C19-C10-C9	-2.09	108.05	111.18
20	C	267	PGV	O01-C1-O02	-2.08	118.08	123.67
23	C	525	CHD	C22-C23-C24	-2.08	104.53	113.02
20	P	1267	PGV	C03-C02-C01	-2.08	107.21	112.07
28	P	1272	DMU	O55-C2-C3	-2.08	104.96	109.87
14	N	516	HEA	C26-C15-C14	-2.07	119.43	123.50
22	B	229	PSC	C27-C26-C25	-2.07	103.82	114.53
19	O	1521	TGL	OG3-CC1-OC1	-2.07	118.14	123.49
23	O	229	CHD	C23-C22-C20	-2.07	112.32	114.75
14	N	516	HEA	CMC-C2C-C3C	-2.04	121.09	125.09
23	P	1271	CHD	C19-C10-C5	-2.04	106.66	110.25
20	A	522	PGV	O01-C02-C01	-2.02	101.23	108.36
20	P	1267	PGV	C04-C05-C06	-2.02	102.93	111.08
19	Q	1523	TGL	CC4-CC3-CC2	-2.01	105.91	113.29
20	P	1267	PGV	C8-C9-C10	-2.01	106.03	113.86
26	G	269	CDL	OA6-CA5-OA7	-2.00	118.30	123.67
20	N	1524	PGV	C26-C25-C24	2.00	124.88	114.53
26	T	1269	CDL	C62-C61-C60	2.01	124.89	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	1267	PGV	C31-C30-C29	2.01	124.89	114.53
20	M	524	PGV	C15-C14-C13	2.01	121.70	113.86
26	T	1269	CDL	C13-C12-C11	2.02	120.69	113.29
28	M	526	DMU	O49-C1-C6	2.02	114.45	110.02
20	P	1267	PGV	C02-O01-C1	2.03	122.75	117.89
23	W	1059	CHD	C21-C20-C17	2.03	116.34	112.96
26	G	269	CDL	O1-C1-CB2	2.03	117.09	109.35
14	N	516	HEA	CMC-C2C-C1C	2.04	131.73	128.36
26	P	1270	CDL	C82-C81-C80	2.04	125.06	114.53
19	D	523	TGL	C16-C15-CC9	2.04	125.08	114.53
25	P	1265	PEK	C14-C13-C12	2.04	118.80	112.00
26	P	1270	CDL	C32-C31-CA7	2.04	121.63	113.59
20	C	267	PGV	C31-C30-C29	2.04	125.09	114.53
14	A	515	HEA	C26-C15-C16	2.05	118.54	115.41
23	O	229	CHD	C15-C16-C17	2.05	109.26	105.12
20	M	524	PGV	C7-C6-C5	2.05	125.14	114.53
22	B	229	PSC	C16-C15-C14	2.07	121.92	113.86
26	G	269	CDL	C39-C38-C37	2.07	125.20	114.53
25	C	264	PEK	O04-C21-C22	2.07	132.02	123.72
20	C	267	PGV	O14-P-O12	2.09	118.98	108.46
20	A	522	PGV	O01-C1-C2	2.09	116.07	111.53
28	Z	1526	DMU	O7-C3-C4	2.10	114.84	109.32
23	C	271	CHD	C21-C20-C22	2.11	113.86	110.35
14	N	515	HEA	C24-C23-C22	2.13	129.47	122.61
25	G	265	PEK	O13-P-O11	2.14	119.24	108.46
26	G	269	CDL	C62-C61-C60	2.15	125.62	114.53
14	A	516	HEA	CAA-C2A-C1A	2.15	129.34	127.01
25	G	265	PEK	C11-C10-C9	2.15	119.17	112.00
19	O	1521	TGL	C33-C19-C18	2.16	125.67	114.53
26	G	269	CDL	C42-C41-C40	2.16	125.68	114.53
20	C	267	PGV	C02-O01-C1	2.16	123.08	117.89
19	Q	1523	TGL	C24-C23-C22	2.17	125.73	114.53
26	T	1269	CDL	C23-C22-C21	2.17	125.74	114.53
26	C	270	CDL	CB6-CB4-CB3	2.17	117.16	112.07
19	A	521	TGL	CC3-CC2-CC1	2.19	122.18	113.59
26	T	1269	CDL	C22-C21-C20	2.20	125.92	114.53
23	C	525	CHD	C2-C1-C10	2.21	116.77	112.84
14	A	515	HEA	C12-C13-C14	2.21	118.59	112.40
19	N	1522	TGL	OG2-CB1-OB1	2.21	129.61	123.67
26	T	1269	CDL	C40-C39-C38	2.23	126.04	114.53
28	Z	1526	DMU	C10-O1-C9	2.24	118.09	113.75
14	N	515	HEA	C3C-C4C-NC	2.24	112.11	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	OB6-CB4-CB6	2.25	116.27	108.36
22	B	229	PSC	C3-C2-C1	2.25	122.44	113.59
26	G	269	CDL	C80-C79-C78	2.26	126.18	114.53
19	D	523	TGL	CG2-OG2-CB1	2.26	123.30	117.89
28	M	526	DMU	O5-C4-C3	2.26	114.52	109.75
28	G	272	DMU	O55-C2-C3	2.26	115.22	109.87
20	N	1524	PGV	O01-C02-C01	2.27	116.36	108.36
22	R	1229	PSC	C3-C2-C1	2.27	122.53	113.59
26	P	1270	CDL	OA6-CA4-CA3	2.28	116.38	108.36
26	G	269	CDL	CA4-OA6-CA5	2.28	123.37	117.89
19	Q	1523	TGL	CG1-OG1-CA1	2.29	123.25	116.85
19	N	1522	TGL	CB3-CB2-CB1	2.29	122.61	113.59
25	P	1265	PEK	C36-C35-C34	2.29	126.38	114.53
19	Q	1523	TGL	CG3-OG3-CC1	2.30	123.27	116.85
25	G	1263	PEK	C14-C13-C12	2.30	119.65	112.00
28	P	1272	DMU	O16-C18-C19	2.31	119.08	109.88
19	N	1522	TGL	C15-CC9-CC8	2.32	126.49	114.53
26	P	1270	CDL	C80-C79-C78	2.33	126.54	114.53
25	P	1265	PEK	C01-O03-C21	2.33	123.36	116.85
19	D	523	TGL	C25-C24-C23	2.33	126.57	114.53
14	N	516	HEA	C26-C15-C16	2.33	118.97	115.41
20	M	524	PGV	O03-C19-C20	2.35	119.05	111.90
26	G	269	CDL	CA6-OA8-CA7	2.35	123.41	116.85
26	G	269	CDL	C23-C22-C21	2.35	126.66	114.53
20	N	1524	PGV	O01-C02-C03	2.35	116.65	108.36
25	G	1263	PEK	O03-C01-C02	2.37	115.08	108.69
23	P	1525	CHD	C15-C16-C17	2.38	109.92	105.12
23	P	1271	CHD	C13-C17-C20	2.39	122.41	119.50
28	G	272	DMU	O5-C6-O16	2.39	115.81	110.05
23	J	60	CHD	C23-C22-C20	2.41	117.59	114.75
14	N	515	HEA	C20-C19-C18	2.41	125.62	121.05
19	N	1522	TGL	OG1-CG1-CG2	2.41	115.18	108.69
28	P	1272	DMU	O55-C2-C1	2.42	115.78	110.34
28	G	272	DMU	C11-C9-C8	2.43	119.00	113.02
26	T	1269	CDL	C82-C81-C80	2.43	127.07	114.53
25	P	1265	PEK	C24-C23-C22	2.45	122.28	113.29
14	N	516	HEA	C21-C20-C19	2.46	120.71	112.71
26	T	1269	CDL	OA6-CA4-CA6	2.49	117.14	108.36
28	Z	1526	DMU	O5-C6-O16	2.51	116.10	110.05
20	C	267	PGV	O01-C1-C2	2.51	116.99	111.53
28	P	1272	DMU	O7-C3-C4	2.53	115.96	109.32
26	C	270	CDL	C42-C41-C40	2.54	127.67	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	521	TGL	CG1-OG1-CA1	2.54	123.97	116.85
25	T	263	PEK	C01-O03-C21	2.55	123.97	116.85
23	O	229	CHD	C5-C4-C3	2.55	116.71	112.91
19	D	523	TGL	OG3-CC1-CC2	2.59	119.79	111.90
23	O	229	CHD	C11-C12-C13	2.59	113.83	111.20
20	N	1266	PGV	C9-C10-C11	2.59	126.05	112.45
28	Z	1526	DMU	O7-C3-C2	2.61	113.90	107.17
26	T	1269	CDL	C39-C38-C37	2.61	128.00	114.53
23	P	1525	CHD	C15-C14-C8	2.61	122.11	118.32
26	P	1270	CDL	CA6-OA8-CA7	2.62	124.19	116.85
26	G	269	CDL	CB4-OB6-CB5	2.62	124.19	117.89
23	B	1085	CHD	C16-C15-C14	2.63	110.41	105.12
19	Q	1523	TGL	OG2-CG2-CG1	2.63	117.63	108.36
26	G	269	CDL	C83-C82-C81	2.64	128.17	114.53
26	C	270	CDL	C40-C39-C38	2.65	128.20	114.53
23	B	1085	CHD	C16-C17-C20	2.66	116.80	112.05
20	N	1266	PGV	O01-C1-C2	2.66	117.32	111.53
28	Z	1526	DMU	C10-C5-C7	2.67	115.22	109.97
14	A	515	HEA	CMB-C2B-C3B	2.67	130.59	125.14
26	C	270	CDL	OA8-CA7-C31	2.67	120.03	111.90
23	P	1271	CHD	C13-C14-C8	2.67	118.19	114.75
26	C	270	CDL	CA4-OA6-CA5	2.67	124.31	117.89
28	M	526	DMU	O55-C2-C1	2.67	116.36	110.34
26	P	1270	CDL	OA8-CA6-CA4	2.68	115.89	108.69
28	P	1272	DMU	C10-C5-C7	2.68	115.26	109.97
14	N	516	HEA	C13-C14-C15	2.68	133.60	127.76
23	C	271	CHD	C14-C8-C7	2.74	115.54	111.74
23	C	525	CHD	C15-C14-C8	2.75	122.31	118.32
14	N	515	HEA	CMC-C2C-C3C	2.75	130.47	125.09
23	B	1085	CHD	C13-C17-C20	2.77	122.87	119.50
20	N	1524	PGV	C01-O03-C19	2.79	124.64	116.85
26	P	1270	CDL	CB6-OB8-CB7	2.79	124.67	116.85
23	P	1525	CHD	C19-C10-C1	2.80	112.91	108.20
14	N	516	HEA	C3C-C4C-NC	2.80	112.83	109.21
25	G	1263	PEK	O03-C21-C22	2.82	120.49	111.90
26	G	269	CDL	OA6-CA4-CA6	2.83	118.33	108.36
19	O	1521	TGL	OG2-CG2-CG3	2.83	118.33	108.36
25	P	1264	PEK	O04-C21-C22	2.84	135.08	123.72
26	C	270	CDL	OA6-CA4-CA3	2.85	118.39	108.36
26	C	270	CDL	O1-C1-CB2	2.85	120.22	109.35
19	O	1521	TGL	OG2-CG2-CG1	2.85	118.42	108.36
25	P	1264	PEK	O02-C1-C2	2.86	135.15	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	1523	TGL	OG1-CA1-CA2	2.86	120.60	111.90
28	P	1272	DMU	O5-C6-C1	2.86	116.14	110.28
26	P	1270	CDL	OA8-CA7-C31	2.86	120.61	111.90
19	D	523	TGL	C10-CB9-CB8	2.86	129.30	114.53
25	P	1264	PEK	C02-O01-C1	2.87	124.77	117.89
19	D	523	TGL	C21-C20-CA9	2.87	129.36	114.53
28	G	272	DMU	C10-C5-C7	2.88	115.64	109.97
19	N	1522	TGL	OG2-CG2-CG3	2.91	118.61	108.36
28	G	272	DMU	C10-O1-C9	2.91	119.40	113.75
14	A	516	HEA	CBD-CAD-C3D	2.91	117.75	112.53
20	P	1267	PGV	O14-P-O13	2.93	128.38	112.53
28	Z	1526	DMU	O49-C1-C2	2.93	116.94	110.34
14	A	516	HEA	C26-C15-C16	2.94	119.89	115.41
28	P	1272	DMU	C2-C3-C4	2.94	117.49	110.84
23	O	229	CHD	O3-C3-C4	2.95	115.73	109.86
25	P	1265	PEK	O03-C01-C02	2.95	116.63	108.69
25	G	265	PEK	C24-C23-C22	2.95	124.12	113.29
20	M	524	PGV	O01-C02-C01	2.96	118.79	108.36
14	A	515	HEA	CMD-C2D-C3D	2.96	131.43	125.24
14	A	516	HEA	C26-C15-C14	2.97	129.33	123.50
26	P	1270	CDL	C39-C38-C37	2.97	129.88	114.53
14	N	515	HEA	CMB-C2B-C3B	2.98	131.22	125.14
19	L	522	TGL	OG2-CG2-CG3	2.99	118.89	108.36
19	O	1521	TGL	C15-CC9-CC8	3.01	130.07	114.53
19	L	522	TGL	C15-CC9-CC8	3.01	130.08	114.53
28	P	1272	DMU	O49-C1-C2	3.01	117.11	110.34
26	T	1269	CDL	C80-C79-C78	3.01	130.09	114.53
19	A	521	TGL	C15-CC9-CC8	3.02	130.12	114.53
14	N	515	HEA	C26-C15-C16	3.02	120.03	115.41
22	R	1229	PSC	O01-C1-C2	3.03	118.12	111.53
19	N	1522	TGL	CC3-CC2-CC1	3.05	125.58	113.59
23	B	1085	CHD	C16-C17-C13	3.06	106.64	103.60
22	R	1229	PSC	O03-C19-C20	3.06	121.23	111.90
25	G	265	PEK	O03-C01-C02	3.07	116.95	108.69
28	M	526	DMU	C6-C1-C2	3.07	116.03	109.97
20	A	522	PGV	C8-C7-C6	3.08	130.44	114.53
23	B	1085	CHD	C15-C14-C8	3.08	122.79	118.32
28	Z	1526	DMU	O61-C57-C4	3.08	121.52	111.33
23	P	1525	CHD	C17-C13-C14	3.09	103.17	100.05
20	N	1266	PGV	O03-C19-C20	3.11	121.37	111.90
25	C	264	PEK	C01-O03-C21	3.12	125.57	116.85
23	P	1271	CHD	C21-C20-C17	3.12	118.16	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	522	PGV	O03-C19-C20	3.12	121.42	111.90
14	N	516	HEA	C20-C21-C22	3.12	119.87	111.69
19	A	521	TGL	OG3-CC1-CC2	3.16	121.52	111.90
19	N	1522	TGL	OG3-CG3-CG2	3.16	117.21	108.69
20	P	1268	PGV	C02-O01-C1	3.17	125.50	117.89
19	L	522	TGL	OG1-CA1-CA2	3.20	121.64	111.90
26	T	1269	CDL	C83-C82-C81	3.20	131.04	114.53
14	N	516	HEA	CAD-C3D-C4D	3.20	130.48	127.01
23	J	60	CHD	C9-C8-C7	3.21	115.71	111.92
28	M	526	DMU	C11-C9-C8	3.21	120.92	113.02
28	P	1272	DMU	O4-C7-C5	3.21	117.56	110.34
28	G	272	DMU	O4-C7-C5	3.22	117.59	110.34
19	D	523	TGL	CB3-CB2-CB1	3.22	126.27	113.59
14	N	516	HEA	CMB-C2B-C3B	3.25	131.79	125.14
23	C	271	CHD	C9-C11-C12	3.26	118.48	114.36
19	O	1521	TGL	CG1-OG1-CA1	3.27	125.98	116.85
23	C	525	CHD	C14-C8-C9	3.27	114.12	109.62
14	A	516	HEA	CAD-C3D-C4D	3.29	130.59	127.01
23	W	1059	CHD	C9-C8-C7	3.31	115.83	111.92
26	T	1269	CDL	CB6-OB8-CB7	3.31	126.10	116.85
22	B	229	PSC	O01-C1-C2	3.32	118.75	111.53
23	B	1085	CHD	C15-C14-C13	3.34	106.92	103.60
28	P	1272	DMU	O7-C10-C5	3.35	116.25	108.10
19	A	521	TGL	OG1-CA1-CA2	3.35	122.10	111.90
25	C	264	PEK	O02-C1-C2	3.36	137.17	123.72
20	P	1268	PGV	O01-C02-C03	3.38	120.26	108.36
23	J	60	CHD	C16-C17-C20	3.39	118.10	112.05
28	G	272	DMU	O7-C3-C4	3.39	118.24	109.32
26	C	270	CDL	C39-C38-C37	3.40	132.08	114.53
23	C	525	CHD	C15-C16-C17	3.40	111.98	105.12
28	G	272	DMU	C1-C2-C3	3.41	117.08	109.60
28	M	526	DMU	C57-C4-C3	3.41	123.17	113.25
23	P	1271	CHD	C5-C6-C7	3.41	118.24	114.44
22	R	1229	PSC	C02-O01-C1	3.42	126.10	117.89
23	W	1059	CHD	C13-C14-C8	3.43	119.18	114.75
23	B	1085	CHD	C1-C2-C3	3.44	116.02	110.43
19	O	1521	TGL	OG3-CC1-CC2	3.47	122.46	111.90
19	O	1521	TGL	OG1-CA1-CA2	3.47	122.47	111.90
28	M	526	DMU	O7-C3-C2	3.49	116.18	107.17
28	G	272	DMU	O7-C10-C5	3.50	116.61	108.10
26	G	269	CDL	OB8-CB6-CB4	3.50	118.11	108.69
28	Z	1526	DMU	C7-C8-C9	3.50	116.31	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1522	TGL	CG3-OG3-CC1	3.51	126.66	116.85
23	P	1525	CHD	C2-C1-C10	3.51	119.11	112.84
26	P	1270	CDL	C42-C41-C40	3.57	132.94	114.53
28	Z	1526	DMU	C1-C2-C3	3.57	117.45	109.60
19	Q	1523	TGL	OG3-CC1-CC2	3.59	122.83	111.90
20	M	524	PGV	C01-O03-C19	3.60	126.91	116.85
23	B	1085	CHD	C6-C7-C8	3.60	115.29	111.47
19	D	523	TGL	CG3-OG3-CC1	3.65	127.05	116.85
20	M	524	PGV	C02-O01-C1	3.69	126.74	117.89
19	A	521	TGL	OG2-CG2-CG3	3.69	121.37	108.36
19	N	1522	TGL	OG1-CA1-CA2	3.70	123.19	111.90
26	C	270	CDL	CB6-OB8-CB7	3.73	127.28	116.85
28	Z	1526	DMU	C57-C4-C3	3.77	124.20	113.25
19	D	523	TGL	OG2-CB1-OB1	3.77	133.78	123.67
25	T	263	PEK	O01-C1-C2	3.79	119.77	111.53
23	B	1085	CHD	C11-C9-C8	3.83	116.17	110.73
25	G	1263	PEK	C01-O03-C21	3.85	127.61	116.85
26	P	1270	CDL	CA4-OA6-CA5	3.87	127.17	117.89
25	T	263	PEK	O03-C01-C02	3.87	119.12	108.69
23	B	1085	CHD	C9-C11-C12	3.92	119.31	114.36
23	W	1059	CHD	C16-C17-C20	3.93	119.06	112.05
23	P	1271	CHD	C4-C5-C10	3.94	116.99	112.66
20	N	1524	PGV	O03-C19-C20	3.94	123.90	111.90
14	N	516	HEA	CBD-CAD-C3D	3.96	119.63	112.53
28	P	1272	DMU	C7-C8-C9	3.96	117.11	110.20
25	G	1263	PEK	C2-C3-C4	3.97	121.20	113.30
23	O	229	CHD	C15-C14-C8	3.97	124.08	118.32
23	P	1525	CHD	C9-C11-C12	3.97	119.38	114.36
23	C	271	CHD	C11-C12-C13	3.99	115.26	111.20
23	C	525	CHD	C5-C4-C3	4.00	118.86	112.91
23	C	271	CHD	C17-C13-C14	4.01	104.11	100.05
23	P	1271	CHD	C2-C1-C10	4.03	120.04	112.84
19	D	523	TGL	OG1-CA1-CA2	4.04	124.19	111.90
28	P	1272	DMU	O7-C10-O1	4.04	120.90	110.68
23	J	60	CHD	C11-C9-C10	4.04	118.00	113.79
28	Z	1526	DMU	O5-C4-C57	4.05	116.58	106.36
23	P	1525	CHD	C11-C12-C13	4.05	115.32	111.20
25	G	265	PEK	O01-C1-C2	4.07	120.38	111.53
28	G	272	DMU	O7-C3-C2	4.09	117.73	107.17
28	G	272	DMU	O5-C6-C1	4.09	118.68	110.28
23	B	1085	CHD	C14-C8-C9	4.10	115.25	109.62
28	P	1272	DMU	C10-O1-C9	4.11	121.72	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	270	CDL	CA6-OA8-CA7	4.14	128.41	116.85
28	M	526	DMU	O49-C1-C2	4.15	119.67	110.34
26	G	269	CDL	OB6-CB5-C51	4.16	120.57	111.53
23	B	1085	CHD	C11-C9-C10	4.18	118.14	113.79
28	G	272	DMU	O5-C4-C3	4.18	118.58	109.75
23	C	525	CHD	C13-C17-C20	4.19	124.61	119.50
28	G	272	DMU	C7-C8-C9	4.20	117.52	110.20
23	J	60	CHD	C22-C20-C17	4.21	119.08	110.24
28	Z	1526	DMU	O3-C5-C7	4.22	119.85	110.34
23	C	525	CHD	C6-C7-C8	4.23	115.96	111.47
14	A	516	HEA	C17-C18-C19	4.23	136.96	127.76
23	O	229	CHD	C14-C8-C9	4.23	115.44	109.62
19	N	1522	TGL	OG3-CC1-CC2	4.23	124.80	111.90
23	J	60	CHD	C11-C9-C8	4.24	116.75	110.73
23	O	229	CHD	C5-C6-C7	4.25	119.17	114.44
14	N	516	HEA	CAA-C2A-C1A	4.32	131.70	127.01
28	Z	1526	DMU	C6-O5-C4	4.34	122.17	113.75
28	M	526	DMU	C1-C2-C3	4.37	119.19	109.60
28	M	526	DMU	O1-C9-C11	4.37	117.39	106.36
23	J	60	CHD	C13-C14-C8	4.37	120.39	114.75
28	G	272	DMU	O1-C9-C11	4.38	117.43	106.36
23	P	1525	CHD	C14-C8-C9	4.39	115.65	109.62
28	G	272	DMU	C6-C1-C2	4.40	118.65	109.97
25	G	1263	PEK	C02-O01-C1	4.43	128.53	117.89
28	Z	1526	DMU	O5-C4-C3	4.45	119.15	109.75
25	T	263	PEK	O03-C21-C22	4.47	125.52	111.90
28	Z	1526	DMU	C18-O16-C6	4.49	121.79	113.94
23	W	1059	CHD	C22-C20-C17	4.50	119.69	110.24
23	C	271	CHD	C2-C1-C10	4.50	120.87	112.84
20	C	268	PGV	O01-C1-C2	4.50	121.32	111.53
28	G	272	DMU	O61-C57-C4	4.52	126.28	111.33
23	C	271	CHD	C4-C5-C10	4.55	117.67	112.66
25	P	1265	PEK	O03-C21-C22	4.56	125.78	111.90
23	P	1271	CHD	C9-C11-C12	4.57	120.13	114.36
23	C	525	CHD	C9-C11-C12	4.59	120.16	114.36
23	W	1059	CHD	C2-C1-C10	4.63	121.10	112.84
23	B	1085	CHD	C9-C8-C7	4.64	117.40	111.92
23	C	525	CHD	O3-C3-C4	4.64	119.10	109.86
23	P	1271	CHD	C17-C13-C14	4.65	104.75	100.05
23	P	1271	CHD	C14-C8-C7	4.67	118.22	111.74
19	A	521	TGL	CG3-OG3-CC1	4.68	129.94	116.85
14	A	515	HEA	CAD-C3D-C4D	4.68	132.09	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	1272	DMU	C18-O16-C6	4.71	122.17	113.94
23	P	1525	CHD	C5-C6-C7	4.71	119.69	114.44
28	M	526	DMU	O3-C5-C7	4.74	121.01	110.34
23	O	229	CHD	C1-C2-C3	4.76	118.16	110.43
28	P	1272	DMU	C1-C2-C3	4.77	120.08	109.60
25	P	1265	PEK	O01-C1-C2	4.78	121.92	111.53
23	C	525	CHD	C11-C9-C8	4.82	117.58	110.73
25	G	1263	PEK	O01-C1-C2	4.83	122.02	111.53
19	A	521	TGL	OG2-CB1-CB2	4.86	122.08	111.53
28	M	526	DMU	C7-C8-C9	4.86	118.67	110.20
28	P	1272	DMU	O61-C57-C4	4.86	127.39	111.33
23	P	1525	CHD	C11-C9-C8	4.87	117.64	110.73
19	O	1521	TGL	CG3-OG3-CC1	4.89	130.53	116.85
23	O	229	CHD	C11-C9-C8	4.91	117.71	110.73
26	G	269	CDL	CB6-OB8-CB7	4.91	130.59	116.85
23	C	271	CHD	C17-C13-C12	4.92	122.04	117.68
23	P	1525	CHD	C13-C17-C20	4.92	125.50	119.50
23	J	60	CHD	C9-C10-C5	4.92	115.96	108.67
23	B	1085	CHD	C5-C4-C3	4.93	120.25	112.91
28	P	1272	DMU	C6-O5-C4	4.96	123.36	113.75
28	G	272	DMU	C8-C7-C5	4.96	120.05	110.79
26	T	1269	CDL	OA8-CA7-C31	4.97	127.04	111.90
28	M	526	DMU	O5-C6-C1	5.00	120.53	110.28
23	C	525	CHD	C9-C8-C7	5.00	117.83	111.92
23	C	271	CHD	C1-C2-C3	5.03	118.59	110.43
14	N	516	HEA	C4B-C3B-C11	5.03	132.47	127.01
19	L	522	TGL	OG3-CC1-CC2	5.04	127.25	111.90
23	C	525	CHD	C11-C12-C13	5.05	116.33	111.20
28	M	526	DMU	O55-C2-C3	5.05	121.83	109.87
23	P	1525	CHD	C9-C8-C7	5.10	117.95	111.92
23	P	1271	CHD	C16-C17-C13	5.13	108.70	103.60
23	O	229	CHD	C17-C13-C12	5.14	122.23	117.68
19	L	522	TGL	CC3-CC2-CC1	5.14	133.81	113.59
23	O	229	CHD	C11-C9-C10	5.19	119.18	113.79
28	M	526	DMU	C8-C7-C5	5.19	120.48	110.79
23	J	60	CHD	C2-C1-C10	5.19	122.11	112.84
19	Q	1523	TGL	OG1-CG1-CG2	5.20	122.68	108.69
20	P	1268	PGV	O01-C1-C2	5.24	122.92	111.53
23	W	1059	CHD	C5-C4-C3	5.26	120.74	112.91
23	P	1525	CHD	C10-C9-C8	5.27	117.66	111.88
23	P	1525	CHD	O3-C3-C4	5.29	120.39	109.86
23	O	229	CHD	C17-C13-C14	5.29	105.40	100.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	272	DMU	C2-C3-C4	5.30	122.83	110.84
28	Z	1526	DMU	C2-C3-C4	5.31	122.86	110.84
23	C	271	CHD	C5-C4-C3	5.32	120.83	112.91
28	P	1272	DMU	O5-C4-C57	5.33	119.83	106.36
23	P	1271	CHD	C4-C3-C2	5.34	117.33	110.52
28	G	272	DMU	C6-O5-C4	5.36	124.14	113.75
23	J	60	CHD	C15-C14-C8	5.36	126.10	118.32
23	C	525	CHD	C17-C13-C14	5.37	105.48	100.05
19	L	522	TGL	CG2-OG2-CB1	5.40	130.84	117.89
28	P	1272	DMU	C6-C1-C2	5.42	120.66	109.97
28	M	526	DMU	C2-C3-C4	5.42	123.11	110.84
23	J	60	CHD	C4-C5-C10	5.45	118.66	112.66
23	O	229	CHD	C9-C11-C12	5.49	121.30	114.36
23	C	271	CHD	C5-C6-C7	5.50	120.57	114.44
28	Z	1526	DMU	O1-C9-C11	5.51	120.28	106.36
26	P	1270	CDL	OB8-CB7-C71	5.54	128.78	111.90
28	Z	1526	DMU	C8-C7-C5	5.56	121.17	110.79
20	P	1268	PGV	O03-C19-C20	5.58	128.90	111.90
23	W	1059	CHD	C15-C14-C8	5.60	126.45	118.32
23	P	1271	CHD	C15-C14-C13	5.61	109.18	103.60
23	C	525	CHD	C11-C9-C10	5.62	119.63	113.79
26	T	1269	CDL	OA6-CA5-C11	5.63	123.77	111.53
23	W	1059	CHD	C11-C9-C8	5.64	118.75	110.73
26	C	270	CDL	OB8-CB7-C71	5.74	129.38	111.90
28	P	1272	DMU	C8-C7-C5	5.74	121.51	110.79
28	P	1272	DMU	O5-C6-O16	5.76	123.92	110.05
23	P	1525	CHD	C5-C4-C3	5.78	121.51	112.91
23	J	60	CHD	C1-C2-C3	5.79	119.82	110.43
23	P	1525	CHD	C11-C9-C10	5.80	119.82	113.79
23	C	271	CHD	C16-C17-C20	5.86	122.51	112.05
23	O	229	CHD	C15-C14-C13	5.88	109.44	103.60
19	O	1521	TGL	CG2-OG2-CB1	5.88	132.00	117.89
23	J	60	CHD	C11-C12-C13	5.89	117.19	111.20
28	P	1272	DMU	O5-C4-C3	5.91	122.22	109.75
23	W	1059	CHD	C6-C5-C10	5.92	119.17	112.66
19	N	1522	TGL	CG2-OG2-CB1	5.95	132.17	117.89
28	P	1272	DMU	O1-C9-C8	5.97	120.88	109.68
28	P	1272	DMU	O1-C9-C11	6.00	121.52	106.36
23	W	1059	CHD	C9-C11-C12	6.01	121.95	114.36
19	A	521	TGL	CG2-OG2-CB1	6.01	132.31	117.89
23	C	271	CHD	C16-C17-C13	6.01	109.58	103.60
23	W	1059	CHD	C9-C10-C5	6.03	117.60	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C10-C9-C8	6.05	118.53	111.88
23	W	1059	CHD	C11-C12-C13	6.08	117.38	111.20
23	P	1271	CHD	C11-C12-C13	6.10	117.40	111.20
26	G	269	CDL	OA6-CA5-C11	6.11	124.80	111.53
28	P	1272	DMU	O1-C10-C5	6.11	122.81	110.28
28	M	526	DMU	C6-O5-C4	6.11	125.60	113.75
25	G	265	PEK	O03-C21-C22	6.14	130.62	111.90
19	O	1521	TGL	OG2-CB1-CB2	6.18	124.97	111.53
28	M	526	DMU	O5-C4-C57	6.19	122.01	106.36
26	C	270	CDL	OA6-CA5-C11	6.21	125.02	111.53
23	J	60	CHD	C15-C14-C13	6.25	109.82	103.60
23	W	1059	CHD	C1-C2-C3	6.26	120.59	110.43
23	C	525	CHD	C15-C14-C13	6.27	109.83	103.60
23	B	1085	CHD	C4-C3-C2	6.30	118.55	110.52
28	M	526	DMU	O1-C9-C8	6.32	121.55	109.68
14	A	516	HEA	C3C-C4C-NC	6.33	117.39	109.21
23	J	60	CHD	C5-C4-C3	6.33	122.33	112.91
23	W	1059	CHD	C1-C10-C5	6.35	118.25	107.81
23	B	1085	CHD	C17-C13-C14	6.36	106.48	100.05
23	J	60	CHD	C16-C17-C13	6.38	109.95	103.60
23	J	60	CHD	C1-C10-C5	6.38	118.30	107.81
26	T	1269	CDL	OB6-CB5-C51	6.42	125.48	111.53
26	P	1270	CDL	OA6-CA5-C11	6.45	125.56	111.53
23	J	60	CHD	C4-C3-C2	6.47	118.77	110.52
23	P	1271	CHD	C14-C13-C12	6.47	113.19	107.39
28	G	272	DMU	O1-C10-C5	6.49	123.59	110.28
23	W	1059	CHD	C4-C3-C2	6.51	118.82	110.52
23	P	1271	CHD	C5-C4-C3	6.53	122.62	112.91
23	W	1059	CHD	C16-C17-C13	6.54	110.10	103.60
23	P	1271	CHD	C16-C17-C20	6.54	123.72	112.05
23	J	60	CHD	C5-C6-C7	6.56	121.76	114.44
23	C	271	CHD	C15-C14-C13	6.57	110.13	103.60
23	P	1271	CHD	C17-C13-C12	6.59	123.52	117.68
23	W	1059	CHD	C5-C6-C7	6.60	121.80	114.44
23	P	1271	CHD	C1-C2-C3	6.62	121.18	110.43
28	G	272	DMU	C18-O16-C6	6.62	125.52	113.94
23	P	1271	CHD	C11-C9-C8	6.65	120.18	110.73
23	J	60	CHD	C6-C5-C10	6.71	120.05	112.66
23	P	1271	CHD	C15-C14-C8	6.73	128.10	118.32
28	P	1272	DMU	O16-C6-C1	6.74	116.55	108.04
28	G	272	DMU	O5-C4-C57	6.76	123.45	106.36
28	Z	1526	DMU	O5-C6-C1	6.95	124.53	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C17-C13-C12	6.98	123.87	117.68
23	W	1059	CHD	C4-C5-C10	6.99	120.35	112.66
23	C	271	CHD	C15-C14-C8	7.14	128.69	118.32
23	W	1059	CHD	C15-C14-C13	7.14	110.70	103.60
23	O	229	CHD	C10-C9-C8	7.15	119.73	111.88
23	J	60	CHD	C9-C11-C12	7.18	123.43	114.36
23	W	1059	CHD	C17-C13-C12	7.25	124.11	117.68
14	A	515	HEA	O11-C11-C12	7.26	127.47	109.73
20	C	268	PGV	O03-C19-C20	7.28	134.07	111.90
28	Z	1526	DMU	O1-C10-C5	7.35	125.36	110.28
23	C	271	CHD	C4-C3-C2	7.38	119.93	110.52
28	Z	1526	DMU	O1-C9-C8	7.39	123.56	109.68
28	G	272	DMU	O1-C9-C8	7.40	123.57	109.68
23	P	1525	CHD	C4-C3-C2	7.42	119.98	110.52
23	J	60	CHD	C17-C13-C12	7.47	124.30	117.68
23	C	271	CHD	C1-C10-C5	7.52	120.17	107.81
23	P	1271	CHD	C1-C10-C5	7.53	120.18	107.81
23	B	1085	CHD	C17-C13-C12	7.55	124.38	117.68
23	J	60	CHD	C14-C8-C7	7.64	122.33	111.74
23	O	229	CHD	C9-C8-C7	7.66	120.97	111.92
28	M	526	DMU	O16-C6-C1	7.69	117.75	108.04
14	A	516	HEA	C4B-C3B-C11	7.79	135.47	127.01
23	B	1085	CHD	C10-C9-C8	7.82	120.47	111.88
23	W	1059	CHD	C6-C7-C8	7.83	119.78	111.47
23	J	60	CHD	C6-C7-C8	7.96	119.92	111.47
23	C	271	CHD	C11-C9-C8	8.12	122.27	110.73
23	J	60	CHD	C14-C13-C12	8.35	114.87	107.39
23	O	229	CHD	C4-C3-C2	8.39	121.22	110.52
23	W	1059	CHD	C14-C13-C12	8.46	114.96	107.39
28	Z	1526	DMU	O16-C6-C1	8.56	118.85	108.04
23	W	1059	CHD	C14-C8-C7	8.70	123.81	111.74
23	C	271	CHD	C6-C7-C8	8.71	120.71	111.47
23	C	271	CHD	C6-C5-C10	8.71	122.25	112.66
23	P	1525	CHD	C15-C14-C13	8.72	112.28	103.60
28	M	526	DMU	O1-C10-C5	8.75	128.23	110.28
23	P	1271	CHD	C6-C7-C8	8.81	120.82	111.47
23	C	525	CHD	C4-C3-C2	8.97	121.96	110.52
23	C	525	CHD	C1-C10-C5	8.98	122.58	107.81
23	C	271	CHD	C14-C13-C12	9.01	115.46	107.39
23	W	1059	CHD	C13-C17-C20	9.01	130.48	119.50
23	J	60	CHD	C13-C17-C20	9.80	131.44	119.50
23	P	1525	CHD	C17-C13-C12	10.11	126.64	117.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C6-C5-C10	10.31	124.01	112.66
23	P	1525	CHD	C1-C10-C5	10.32	124.78	107.81
23	W	1059	CHD	C10-C9-C8	10.65	123.57	111.88
25	C	264	PEK	C2-C3-C4	10.66	134.54	113.30
28	G	272	DMU	O16-C6-C1	10.76	121.63	108.04
23	J	60	CHD	C10-C9-C8	10.98	123.93	111.88
23	O	229	CHD	C1-C10-C5	11.18	126.19	107.81
23	C	525	CHD	C14-C13-C12	11.36	117.56	107.39
23	B	1085	CHD	C14-C13-C12	11.58	117.76	107.39
23	C	525	CHD	C6-C5-C10	11.60	125.43	112.66
23	B	1085	CHD	C1-C10-C5	12.03	127.58	107.81
23	P	1525	CHD	C6-C5-C10	12.33	126.25	112.66
23	P	1271	CHD	C10-C9-C8	12.90	126.04	111.88
25	P	1264	PEK	C2-C3-C4	13.10	139.41	113.30
23	P	1525	CHD	C14-C13-C12	13.27	119.28	107.39
23	C	271	CHD	C10-C9-C8	13.59	126.80	111.88
23	O	229	CHD	C14-C13-C12	14.28	120.18	107.39
23	O	229	CHD	C6-C5-C10	14.88	129.05	112.66
23	B	1085	CHD	C6-C5-C10	15.05	129.24	112.66

All (38) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C5
28	P	1272	DMU	C6
28	P	1272	DMU	C9
28	P	1272	DMU	C4
28	P	1272	DMU	C2
28	P	1272	DMU	C10
14	A	516	HEA	ND
14	A	516	HEA	NA
14	A	516	HEA	NB
14	N	515	HEA	ND
14	N	515	HEA	NA
14	N	515	HEA	NB
23	C	271	CHD	C9
23	P	1271	CHD	C9
23	W	1059	CHD	C17
28	Z	1526	DMU	C2
28	Z	1526	DMU	C4
28	Z	1526	DMU	C6
28	Z	1526	DMU	C9

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Mol	Chain	Res	Type	Atom
28	Z	1526	DMU	C5
28	G	272	DMU	C5
28	G	272	DMU	C6
28	G	272	DMU	C9
28	G	272	DMU	C4
28	G	272	DMU	C2
28	G	272	DMU	C3
28	M	526	DMU	C2
28	M	526	DMU	C4
28	M	526	DMU	C9
28	M	526	DMU	C5
23	J	60	CHD	C17
23	J	60	CHD	C9
14	A	515	HEA	ND
14	A	515	HEA	NA
14	A	515	HEA	NB
14	N	516	HEA	ND
14	N	516	HEA	NA
14	N	516	HEA	NB

All (4) torsion outliers are listed below:

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

There are no ring outliers.

39 monomers are involved in 370 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	515	HEA	4	0
14	A	516	HEA	5	0
19	A	521	TGL	8	0
23	B	1085	CHD	2	0
22	B	229	PSC	26	0
25	C	264	PEK	8	0
20	C	267	PGV	5	0
20	C	268	PGV	3	0
26	C	270	CDL	26	0
23	C	271	CHD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	D	523	TGL	8	0
25	G	1263	PEK	24	0
25	G	265	PEK	19	0
26	G	269	CDL	30	0
28	G	272	DMU	4	0
23	J	60	CHD	1	0
19	L	522	TGL	15	0
20	M	524	PGV	15	0
20	N	1266	PGV	1	0
19	N	1522	TGL	15	0
20	N	1524	PGV	8	0
14	N	515	HEA	4	0
14	N	516	HEA	4	0
19	O	1521	TGL	10	0
23	O	229	CHD	3	0
25	P	1264	PEK	7	0
25	P	1265	PEK	17	0
20	P	1267	PGV	5	0
20	P	1268	PGV	1	0
26	P	1270	CDL	25	0
23	P	1271	CHD	5	0
28	P	1272	DMU	6	0
23	P	1525	CHD	1	0
19	Q	1523	TGL	12	0
22	R	1229	PSC	15	0
26	T	1269	CDL	27	0
25	T	263	PEK	21	0
23	W	1059	CHD	1	0
28	Z	1526	DMU	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.06	2 (0%) 93 91	21, 25, 33, 64	0
1	N	513/514 (99%)	0.04	3 (0%) 90 88	24, 28, 36, 63	0
2	B	226/227 (99%)	-0.32	1 (0%) 93 91	20, 30, 48, 68	0
2	O	226/227 (99%)	-0.25	7 (3%) 52 47	25, 34, 58, 80	0
3	C	259/261 (99%)	-0.34	2 (0%) 87 85	23, 27, 39, 61	0
3	P	259/261 (99%)	-0.16	6 (2%) 64 59	25, 30, 41, 58	0
4	D	144/147 (97%)	-0.39	1 (0%) 89 87	27, 34, 48, 64	0
4	Q	144/147 (97%)	0.87	21 (14%) 3 2	31, 40, 65, 115	0
5	E	105/109 (96%)	-0.08	2 (1%) 70 66	28, 33, 58, 98	0
5	R	105/109 (96%)	0.48	7 (6%) 21 17	29, 37, 58, 101	0
6	F	98/98 (100%)	0.38	8 (8%) 14 11	26, 35, 79, 127	0
6	S	98/98 (100%)	0.27	7 (7%) 19 15	27, 37, 85, 121	0
7	G	83/85 (97%)	0.82	17 (20%) 1 1	25, 33, 90, 108	0
7	T	83/85 (97%)	0.89	17 (20%) 1 1	26, 34, 91, 107	0
8	H	79/85 (92%)	0.26	11 (13%) 4 3	27, 37, 83, 109	0
8	U	79/85 (92%)	0.47	13 (16%) 2 2	30, 41, 88, 109	0
9	I	72/73 (98%)	0.20	3 (4%) 40 34	28, 40, 57, 67	0
9	V	72/73 (98%)	0.66	8 (11%) 7 5	30, 44, 61, 77	0
10	J	58/59 (98%)	0.41	8 (13%) 4 3	27, 35, 56, 97	0
10	W	58/59 (98%)	0.56	9 (15%) 3 2	29, 37, 57, 102	0
11	K	49/56 (87%)	0.31	4 (8%) 14 11	30, 37, 52, 66	0
11	X	49/56 (87%)	1.69	17 (34%) 0 0	34, 42, 56, 72	0
12	L	46/47 (97%)	-0.37	2 (4%) 39 32	25, 31, 48, 73	0
12	Y	46/47 (97%)	-0.26	1 (2%) 65 60	29, 34, 51, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.11	4 (9%) 11 8	27, 31, 69, 98	0
13	Z	43/46 (93%)	0.66	8 (18%) 2 1	32, 37, 79, 106	0
All	All	3550/3614 (98%)	0.11	189 (5%) 30 25	20, 31, 58, 127	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	15.6
4	Q	5	VAL	14.6
6	F	1	ALA	13.9
6	S	1	ALA	13.9
6	S	97	ALA	12.1
6	F	96	LEU	11.7
6	S	98	HIS	11.4
6	F	98	HIS	10.7
4	Q	4	SER	10.1
6	F	97	ALA	9.1
5	R	5	HIS	8.8
5	R	109	VAL	8.4
8	U	7	LYS	8.3
13	Z	42	LYS	8.2
13	Z	43	SER	7.9
6	S	2	SER	7.7
5	E	5	HIS	7.6
7	G	8	HIS	7.4
6	S	94	HIS	7.2
8	U	8	ILE	7.1
10	W	58	LYS	6.9
7	G	1	ALA	6.8
7	T	36	TRP	6.6
8	U	44	THR	6.5
6	F	95	GLN	6.4
10	J	1	PHE	6.3
6	F	2	SER	6.3
7	G	36	TRP	6.2
4	Q	51	LEU	6.1
7	T	3	ALA	6.1
8	H	47	GLY	5.9
7	T	8	HIS	5.9
4	Q	7	LYS	5.8
7	T	84	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
7	G	40	GLY	5.6
7	T	42	ARG	5.6
13	M	43	SER	5.5
8	H	7	LYS	5.5
8	U	45	ALA	5.4
7	T	40	GLY	5.2
9	V	2	THR	5.2
6	F	94	HIS	5.2
9	I	37	PHE	5.1
4	Q	8	SER	5.0
7	G	42	ARG	5.0
7	T	1	ALA	5.0
7	T	5	LYS	4.9
8	H	8	ILE	4.9
8	U	48	GLY	4.8
11	X	6	ALA	4.8
10	W	57	HIS	4.8
7	G	2	SER	4.6
13	Z	41	LYS	4.5
13	Z	40	TYR	4.5
8	H	45	ALA	4.5
5	E	109	VAL	4.5
8	H	48	GLY	4.5
8	U	10	ASN	4.5
4	Q	48	TRP	4.4
7	G	84	LYS	4.4
7	G	41	HIS	4.4
4	Q	147	LYS	4.4
10	W	52	TRP	4.3
7	G	10	GLY	4.3
11	X	7	PRO	4.3
2	O	226	MET	4.3
9	V	37	PHE	4.3
7	T	4	ALA	4.3
12	L	47	LYS	4.3
11	K	7	PRO	4.2
10	J	58	LYS	4.2
13	M	42	LYS	4.2
7	T	41	HIS	4.1
11	X	17	VAL	4.0
7	T	39	SER	4.0
8	H	44	THR	4.0

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Mol	Chain	Res	Type	RSRZ
4	Q	46	ALA	4.0
11	X	19	ALA	4.0
11	X	13	TYR	4.0
8	U	47	GLY	3.9
7	T	2	SER	3.8
2	O	113	TYR	3.7
11	X	16	ALA	3.7
6	S	96	LEU	3.7
7	G	6	GLY	3.6
4	D	147	LYS	3.6
7	G	3	ALA	3.6
10	W	1	PHE	3.6
7	G	5	LYS	3.5
7	T	10	GLY	3.5
13	Z	35	TYR	3.5
2	O	90	ILE	3.5
7	G	4	ALA	3.5
6	S	95	GLN	3.3
8	U	43	MET	3.3
7	G	7	ASP	3.3
10	J	57	HIS	3.3
5	R	108	LYS	3.3
4	Q	141	ASP	3.3
7	G	43	GLU	3.3
11	X	20	SER	3.2
11	X	47	ARG	3.1
12	Y	47	LYS	3.1
4	Q	102	TYR	3.1
7	G	39	SER	3.0
5	R	96	LEU	3.0
8	H	46	LYS	3.0
4	Q	53	ILE	3.0
8	U	46	LYS	3.0
4	Q	60	TYR	2.9
7	T	9	GLY	2.8
11	K	6	ALA	2.8
4	Q	145	TRP	2.8
13	Z	39	ASN	2.8
11	X	23	THR	2.8
2	O	227	LEU	2.8
10	W	4	ARG	2.8
8	U	52	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
13	M	40	TYR	2.7
8	U	49	ASP	2.7
8	H	43	MET	2.7
5	R	94	ASN	2.7
9	V	53	ASN	2.7
8	H	10	ASN	2.7
9	V	34	PHE	2.7
11	X	18	LEU	2.7
9	I	2	THR	2.7
13	M	39	ASN	2.7
7	T	6	GLY	2.7
3	P	91	VAL	2.6
5	R	93	LEU	2.6
4	Q	33	LEU	2.6
10	W	55	PHE	2.6
4	Q	49	SER	2.6
10	J	56	PRO	2.6
6	F	3	GLY	2.6
1	A	202	LEU	2.6
7	G	9	GLY	2.6
8	U	9	LYS	2.6
5	R	92	THR	2.5
10	J	52	TRP	2.5
9	V	33	THR	2.5
4	Q	140	TYR	2.5
8	U	11	TYR	2.5
10	W	48	TYR	2.5
2	O	59	GLN	2.4
7	T	7	ASP	2.4
3	C	38	ASN	2.4
8	H	49	ASP	2.4
3	P	88	ILE	2.4
12	L	2	HIS	2.4
10	W	2	GLU	2.4
13	Z	32	TRP	2.3
4	Q	58	GLU	2.3
11	X	15	ASN	2.3
1	N	286	ILE	2.3
3	P	37	PHE	2.3
8	H	9	LYS	2.3
4	Q	40	LEU	2.3
11	X	27	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
9	V	26	MET	2.2
11	X	12	LYS	2.2
13	Z	13	LYS	2.2
7	T	43	GLU	2.2
4	Q	142	LYS	2.2
9	V	3	ALA	2.2
11	X	24	PHE	2.2
1	N	73	ILE	2.2
10	J	2	GLU	2.1
9	V	36	LYS	2.1
10	J	48	TYR	2.1
3	P	38	ASN	2.1
10	W	26	ALA	2.1
2	O	60	GLU	2.1
2	B	91	ASN	2.1
1	A	197	LEU	2.1
4	Q	72	ASN	2.1
10	J	4	ARG	2.1
11	X	46	GLY	2.1
1	N	285	PHE	2.1
3	P	93	PHE	2.0
2	O	224	ALA	2.0
11	K	47	ARG	2.0
11	X	22	ALA	2.0
3	C	92	LEU	2.0
3	P	99	TRP	2.0
9	I	26	MET	2.0
11	K	19	ALA	2.0
11	X	37	GLY	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
9	SAC	V	1	9/10	0.63	0.55	-	83,86,88,88	0
7	TPO	G	11	11/12	0.50	0.31	-	66,75,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FME	B	1	10/11	0.97	0.11	-	20,30,40,52	0
2	FME	O	1	10/11	0.96	0.10	-	33,34,40,48	0
1	FME	N	1	10/11	0.91	0.13	-	42,48,77,80	0
7	TPO	T	11	11/12	0.43	0.35	-	71,80,101,104	0
9	SAC	I	1	9/10	0.87	0.30	-	63,66,69,73	0
1	FME	A	1	10/11	0.94	0.12	-	38,41,68,76	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
20	PGV	M	524	51/51	0.80	0.25	11.05	40,70,127,129	0
28	DMU	G	272	33/33	0.39	0.34	9.93	72,100,115,116	0
28	DMU	P	1272	33/33	0.40	0.35	9.06	72,106,119,121	0
23	CHD	W	1059	29/29	0.68	0.39	7.88	101,108,110,112	0
23	CHD	J	60	29/29	0.60	0.41	6.21	99,104,108,108	0
26	CDL	P	1270	100/100	0.71	0.28	5.84	36,86,117,120	0
19	TGL	N	1522	63/63	0.65	0.25	5.45	49,64,84,89	0
26	CDL	C	270	100/100	0.77	0.27	4.91	42,84,109,110	0
19	TGL	D	523	63/63	0.74	0.20	4.74	53,67,97,99	0
19	TGL	L	522	63/63	0.77	0.23	4.59	36,62,78,81	0
19	TGL	A	521	63/63	0.81	0.18	4.49	53,72,88,92	0
19	TGL	O	1521	63/63	0.80	0.17	3.81	53,75,88,92	0
19	TGL	Q	1523	63/63	0.72	0.22	3.81	56,74,100,102	0
20	PGV	N	1524	51/51	0.72	0.30	3.73	41,76,121,123	0
17	MG	N	518	1/1	0.97	0.12	2.66	29,29,29,29	0
20	PGV	C	268	51/51	0.73	0.31	2.59	51,79,108,111	0
28	DMU	M	526	33/33	0.91	0.14	2.55	35,44,61,65	0
26	CDL	T	1269	100/100	0.59	0.28	2.44	59,86,115,118	0
22	PSC	B	229	52/52	0.67	0.32	2.39	45,95,136,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
28	DMU	Z	1526	33/33	0.82	0.25	2.38	40,50,71,75	0
25	PEK	G	1263	53/53	0.55	0.43	2.31	51,96,123,124	0
26	CDL	G	269	100/100	0.62	0.25	2.06	58,86,116,120	0
20	PGV	P	1268	51/51	0.70	0.32	2.03	57,77,111,112	0
22	PSC	R	1229	52/52	0.58	0.30	1.77	49,95,129,135	0
21	CUA	B	228	2/2	1.00	0.12	1.37	23,23,23,23	0
25	PEK	T	263	53/53	0.60	0.32	1.30	48,94,121,122	0
20	PGV	C	267	51/51	0.96	0.11	1.27	22,33,73,74	0
17	MG	A	518	1/1	0.98	0.13	1.25	24,24,24,24	0
20	PGV	P	1267	51/51	0.94	0.13	1.22	23,37,80,82	0
23	CHD	P	1271	29/29	0.90	0.20	1.15	51,63,68,69	0
25	PEK	P	1264	53/53	0.93	0.14	1.15	25,49,81,82	0
25	PEK	P	1265	53/53	0.43	0.30	0.99	46,76,107,110	0
23	CHD	C	525	29/29	0.97	0.14	0.98	21,30,35,38	0
25	PEK	G	265	53/53	0.55	0.27	0.89	47,79,103,105	0
25	PEK	C	264	53/53	0.95	0.12	0.84	24,45,77,80	0
23	CHD	C	271	29/29	0.89	0.19	0.82	54,61,65,73	0
27	ZN	F	99	1/1	0.98	0.08	0.68	31,31,31,31	0
14	HEA	N	516	60/60	0.99	0.13	0.67	22,26,31,36	0
20	PGV	N	1266	51/51	0.95	0.13	0.63	23,36,59,64	0
23	CHD	P	1525	29/29	0.96	0.14	0.59	27,31,35,37	0
20	PGV	A	522	51/51	0.97	0.11	0.43	20,33,67,71	0
16	CU	A	517	1/1	1.00	0.14	0.20	24,24,24,24	0
27	ZN	S	99	1/1	0.99	0.09	0.11	33,33,33,33	0
21	CUA	O	228	2/2	0.99	0.09	-0.04	27,27,27,27	0
14	HEA	A	516	60/60	0.99	0.12	-0.23	19,22,30,34	0
14	HEA	N	515	60/60	0.98	0.10	-0.27	21,26,40,44	0
14	HEA	A	515	60/60	0.99	0.11	-0.29	19,23,38,41	0
23	CHD	B	1085	29/29	0.97	0.08	-0.35	23,26,31,37	0
23	CHD	O	229	29/29	0.97	0.08	-0.43	21,25,31,33	0
18	NA	N	519	1/1	0.96	0.07	-0.59	31,31,31,31	0
18	NA	A	519	1/1	0.98	0.07	-0.63	28,28,28,28	0
15	NO	A	520	2/2	0.98	0.10	-1.90	24,24,24,25	0
15	NO	N	520	2/2	0.99	0.08	-2.21	26,26,26,31	0
24	UNX	C	262	1/1	0.40	0.47	-	81,81,81,81	0
16	CU	N	517	1/1	1.00	0.15	-	26,26,26,26	0
24	UNX	P	262	1/1	0.66	0.42	-	82,82,82,82	0

6.5 Other polymers ⓘ

There are no such residues in this entry.