



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:20 PM UTC

PDB ID : 3G37 / pdb_00003g37
EMDB ID : EMD-1674
Title : Cryo-EM structure of actin filament in the presence of phosphate
Authors : Wakabayshi, T.; Murakami, K.; Yasunaga, T.; Noguchi, T.Q.; Uyeda, T.Q.
Deposited on : 2009-02-02
Resolution : 6.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

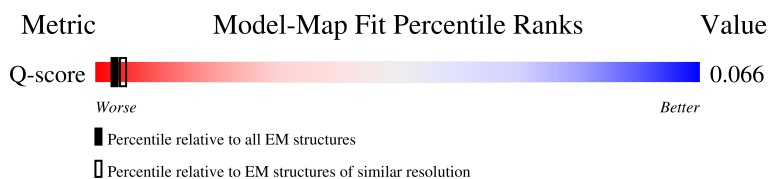
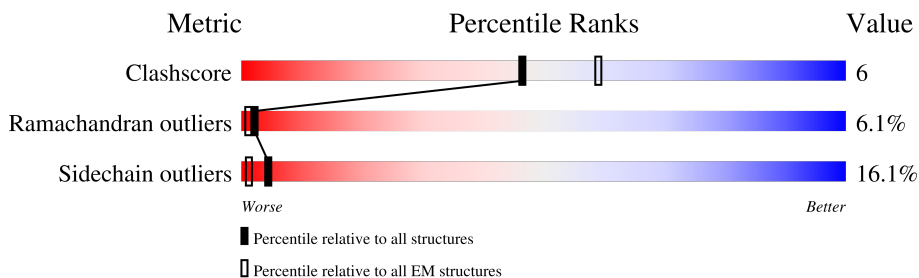
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.00 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	525 (5.50 - 6.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	376	
1	P	376	
1	Q	376	
1	R	376	

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Mol	Chain	Length	Quality of chain
1	S	376	
1	T	376	
1	U	376	
1	V	376	
1	W	376	
1	X	376	
1	Y	376	
1	Z	376	

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
3	PO4	O	803	-	X	-	-
3	PO4	P	803	-	X	-	-
3	PO4	R	803	-	X	-	-
3	PO4	S	803	-	X	-	-
3	PO4	T	803	-	X	-	-
3	PO4	U	802	-	X	-	-
3	PO4	V	803	-	X	-	-
3	PO4	X	803	-	X	-	-
3	PO4	Y	801	-	X	X	-
3	PO4	Y	803	-	X	-	-
3	PO4	Z	802	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35808 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	P	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Q	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	R	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	S	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	T	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	U	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	V	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	W	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	X	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Y	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		
1	Z	376	Total	C	N	O	S	0	0
			2936	1857	493	565	21		

There are 12 discrepancies between the modelled and reference sequences:

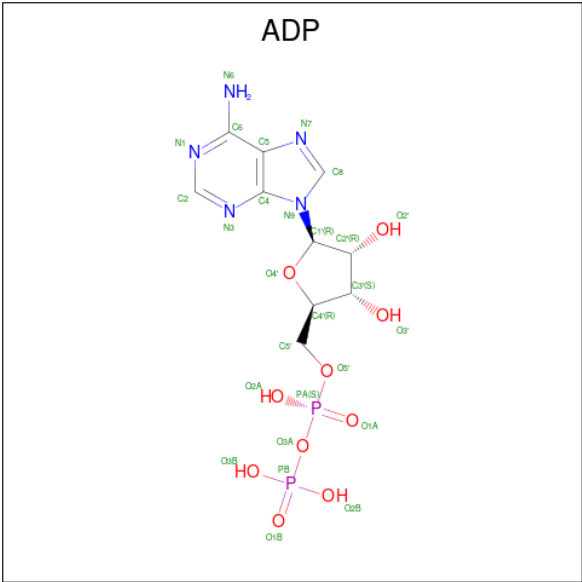
Chain	Residue	Modelled	Actual	Comment	Reference
O	0	ACE	-	acetylation	UNP P68135
P	0	ACE	-	acetylation	UNP P68135
Q	0	ACE	-	acetylation	UNP P68135
R	0	ACE	-	acetylation	UNP P68135
S	0	ACE	-	acetylation	UNP P68135
T	0	ACE	-	acetylation	UNP P68135

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Chain	Residue	Modelled	Actual	Comment	Reference
U	0	ACE	-	acetylation	UNP P68135
V	0	ACE	-	acetylation	UNP P68135
W	0	ACE	-	acetylation	UNP P68135
X	0	ACE	-	acetylation	UNP P68135
Y	0	ACE	-	acetylation	UNP P68135
Z	0	ACE	-	acetylation	UNP P68135

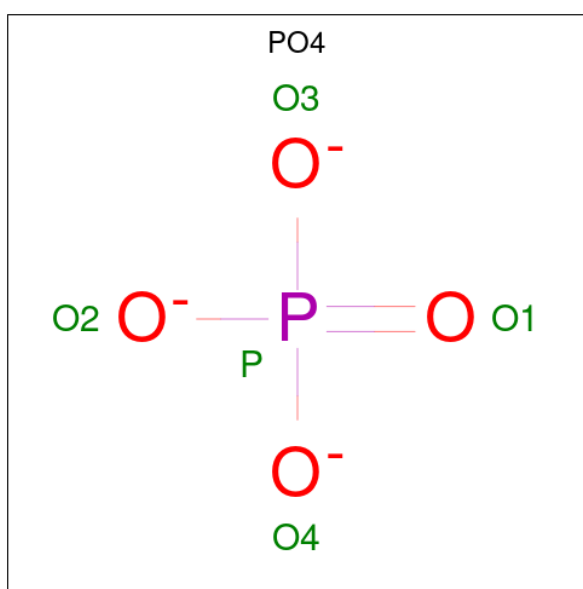
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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Mol	Chain	Residues	Atoms					AltConf
2	W	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	X	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Y	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	Z	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
3	O	1	Total	O	P	0
			5	4	1	
3	O	1	Total	O	P	0
			5	4	1	
3	O	1	Total	O	P	0
			5	4	1	
3	P	1	Total	O	P	0
			5	4	1	
3	P	1	Total	O	P	0
			5	4	1	
3	P	1	Total	O	P	0
			5	4	1	
3	Q	1	Total	O	P	0
			5	4	1	

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Mol	Chain	Residues	Atoms			AltConf
3	Q	1	Total	O	P	0
			5	4	1	
3	Q	1	Total	O	P	0
			5	4	1	
3	R	1	Total	O	P	0
			5	4	1	
3	R	1	Total	O	P	0
			5	4	1	
3	R	1	Total	O	P	0
			5	4	1	
3	S	1	Total	O	P	0
			5	4	1	
3	S	1	Total	O	P	0
			5	4	1	
3	S	1	Total	O	P	0
			5	4	1	
3	T	1	Total	O	P	0
			5	4	1	
3	T	1	Total	O	P	0
			5	4	1	
3	T	1	Total	O	P	0
			5	4	1	
3	T	1	Total	O	P	0
			5	4	1	
3	U	1	Total	O	P	0
			5	4	1	
3	U	1	Total	O	P	0
			5	4	1	
3	U	1	Total	O	P	0
			5	4	1	
3	V	1	Total	O	P	0
			5	4	1	
3	V	1	Total	O	P	0
			5	4	1	
3	W	1	Total	O	P	0
			5	4	1	
3	W	1	Total	O	P	0
			5	4	1	
3	W	1	Total	O	P	0
			5	4	1	
3	X	1	Total	O	P	0
			5	4	1	

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Mol	Chain	Residues	Atoms			AltConf
3	X	1	Total	O	P	0
			5	4	1	
3	X	1	Total	O	P	0
			5	4	1	
3	Y	1	Total	O	P	0
			5	4	1	
3	Y	1	Total	O	P	0
			5	4	1	
3	Y	1	Total	O	P	0
			5	4	1	
3	Z	1	Total	O	P	0
			5	4	1	
3	Z	1	Total	O	P	0
			5	4	1	
3	Z	1	Total	O	P	0
			5	4	1	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	O	6	Total	Mg	0
			6	6	
4	P	5	Total	Mg	0
			5	5	
4	Q	7	Total	Mg	0
			7	7	
4	R	6	Total	Mg	0
			6	6	
4	S	6	Total	Mg	0
			6	6	
4	T	6	Total	Mg	0
			6	6	
4	U	6	Total	Mg	0
			6	6	
4	V	6	Total	Mg	0
			6	6	
4	W	6	Total	Mg	0
			6	6	
4	X	6	Total	Mg	0
			6	6	
4	Y	6	Total	Mg	0
			6	6	

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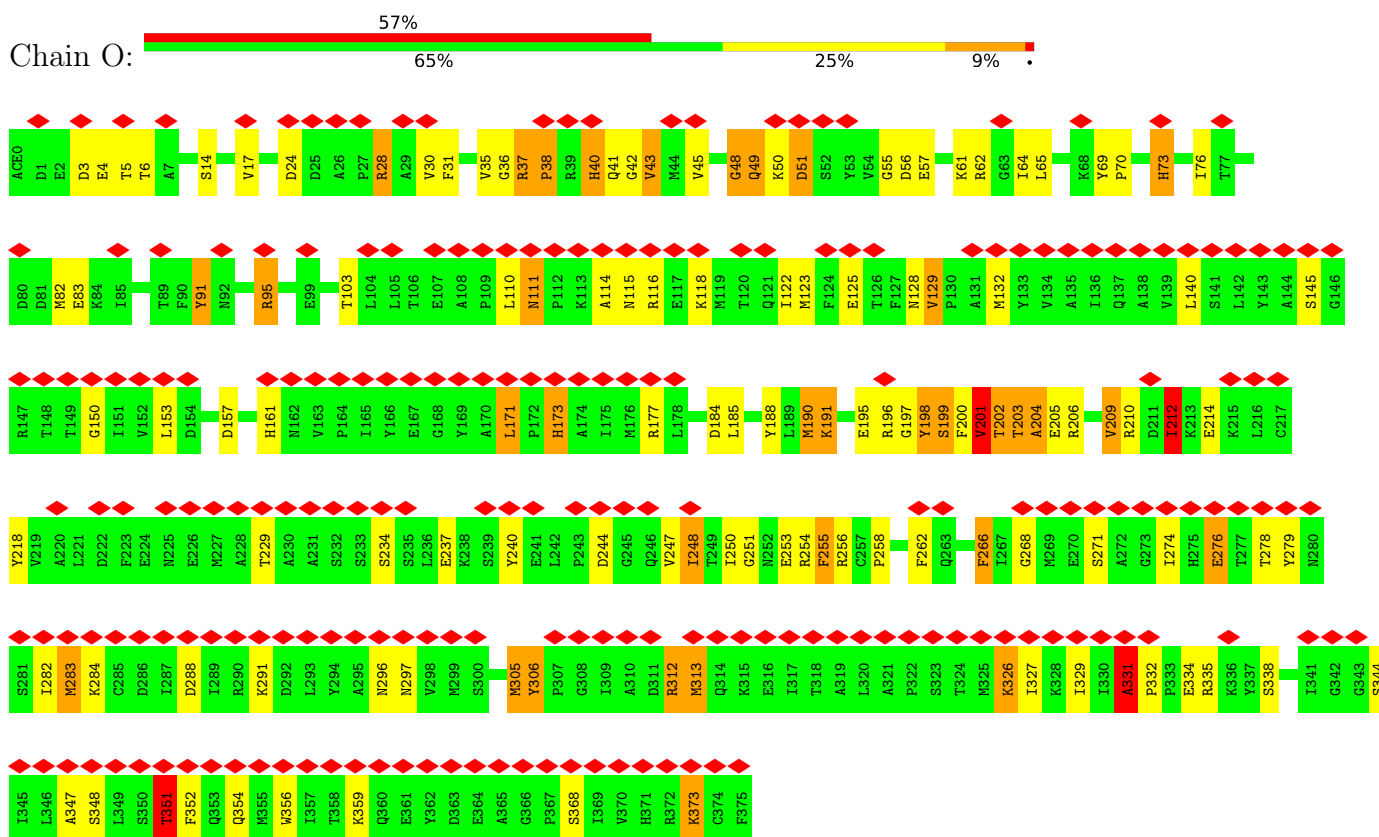
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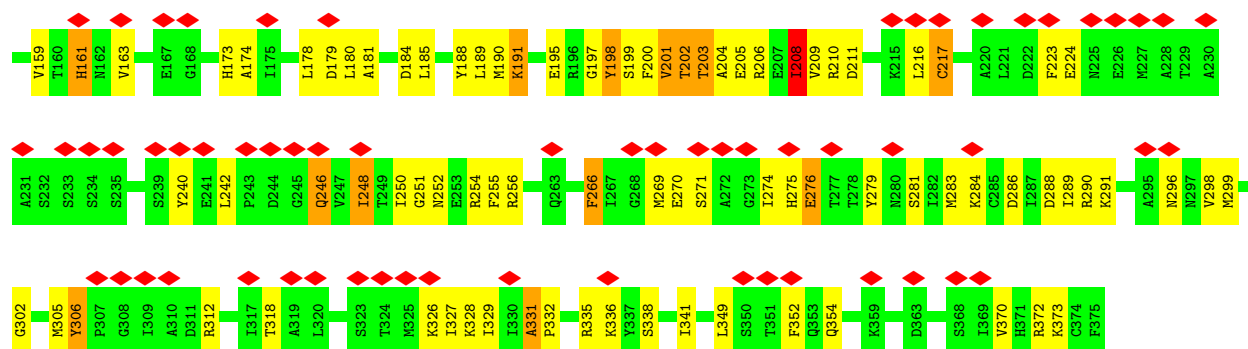
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	Z	6	6	6	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

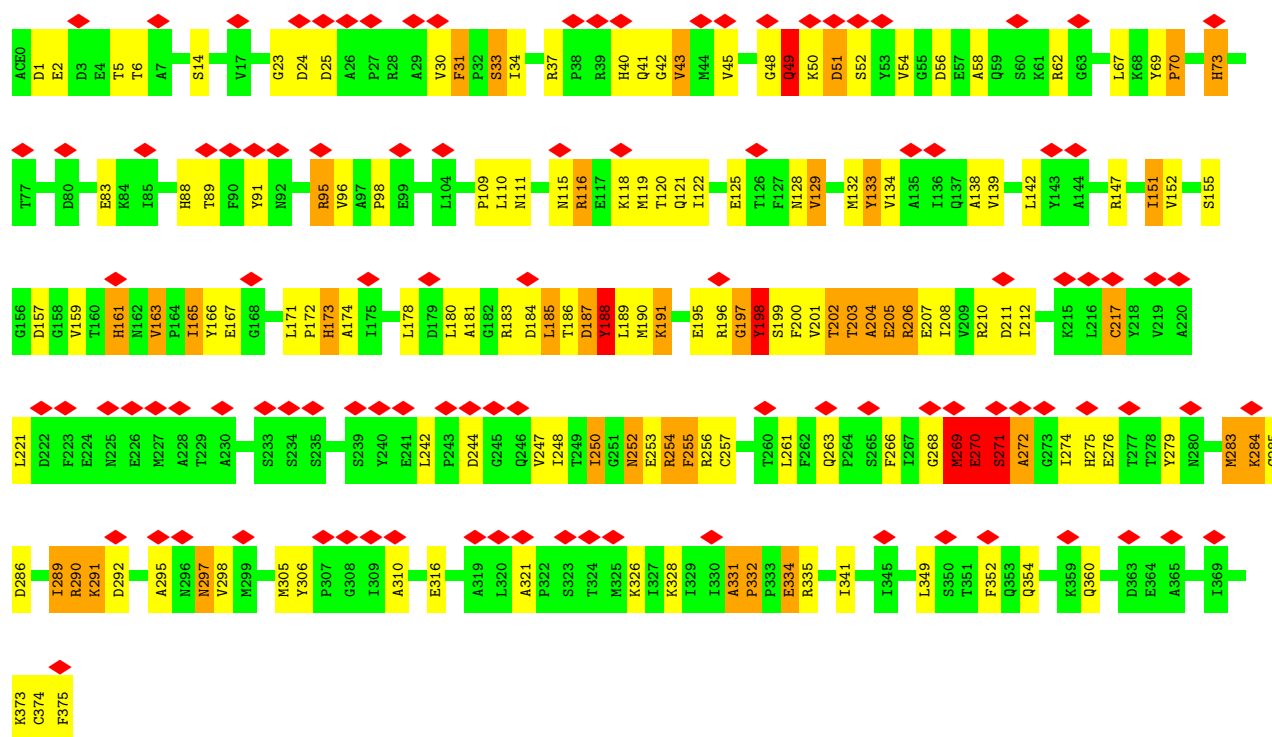
- Molecule 1: Actin, alpha skeletal muscle





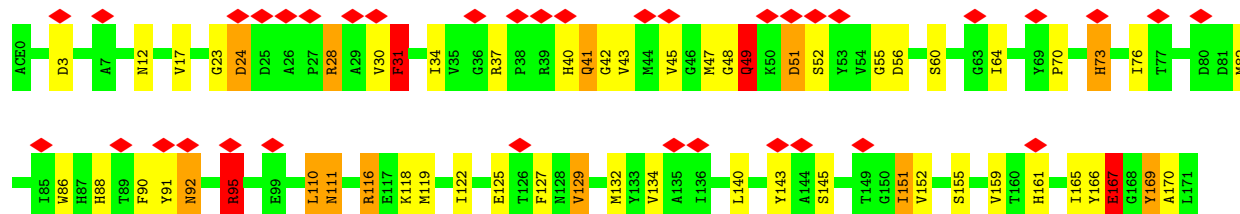
• Molecule 1: Actin, alpha skeletal muscle

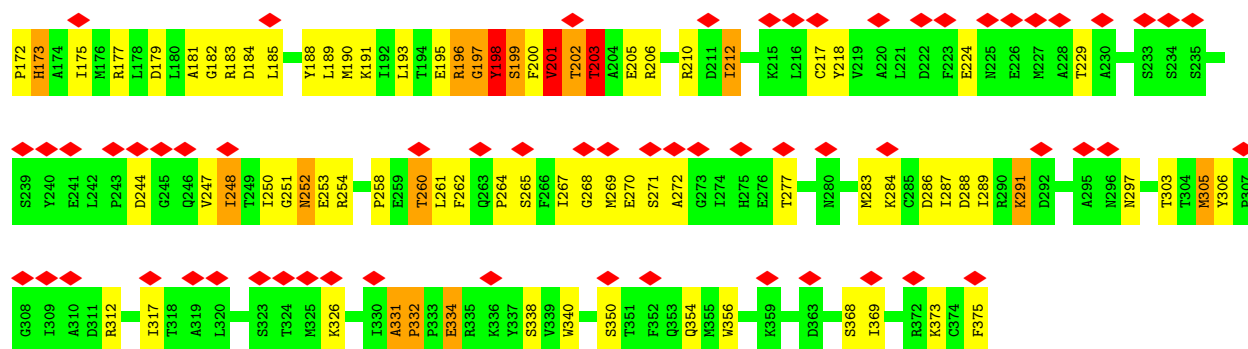
Chain Q: 27% 59% 30% 10%



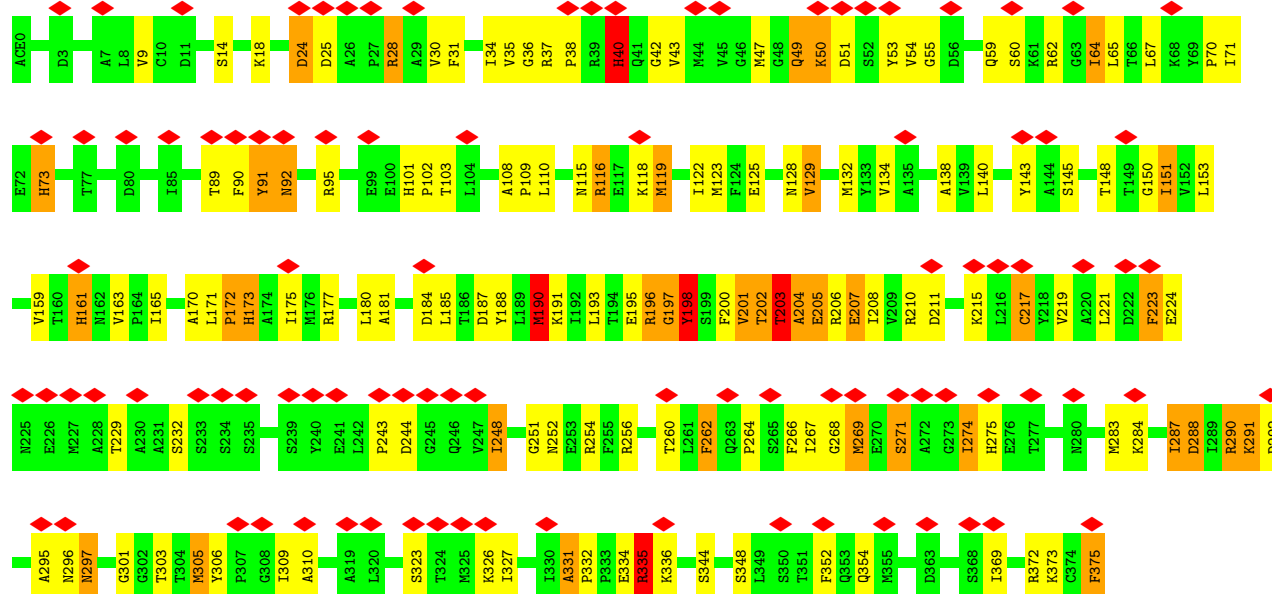
• Molecule 1: Actin, alpha skeletal muscle

Chain R: 26% 64% 28% 7%

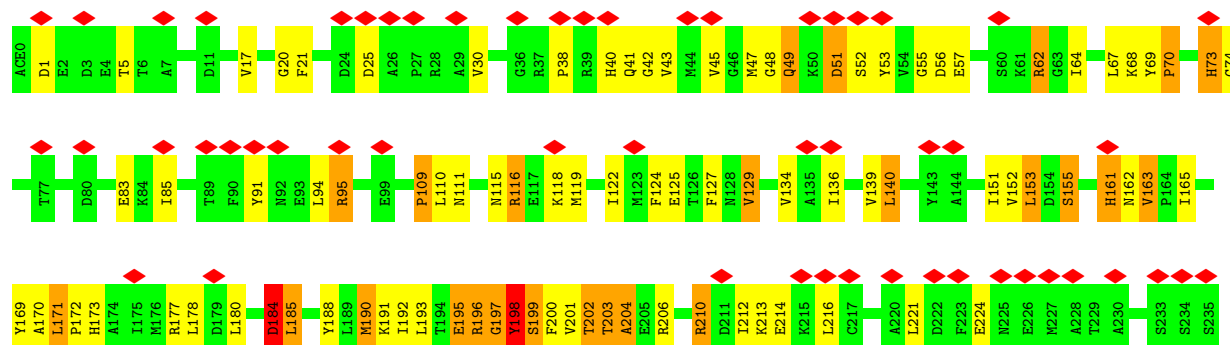


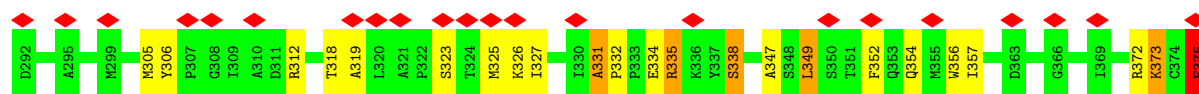


• Molecule 1: Actin, alpha skeletal muscle

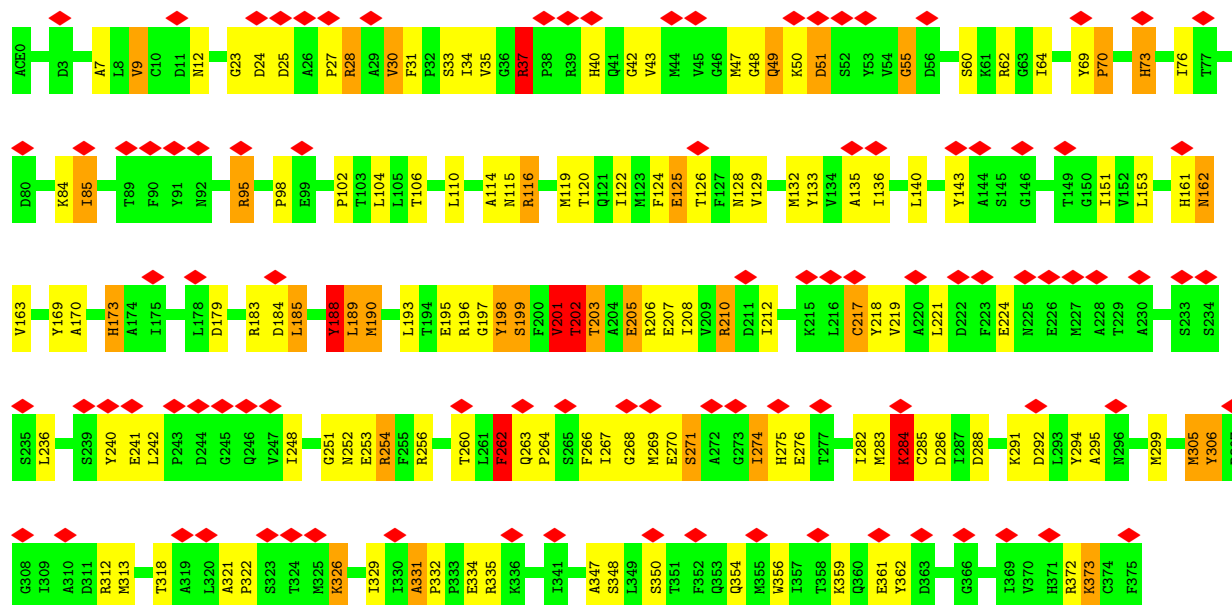


• Molecule 1: Actin, alpha skeletal muscle

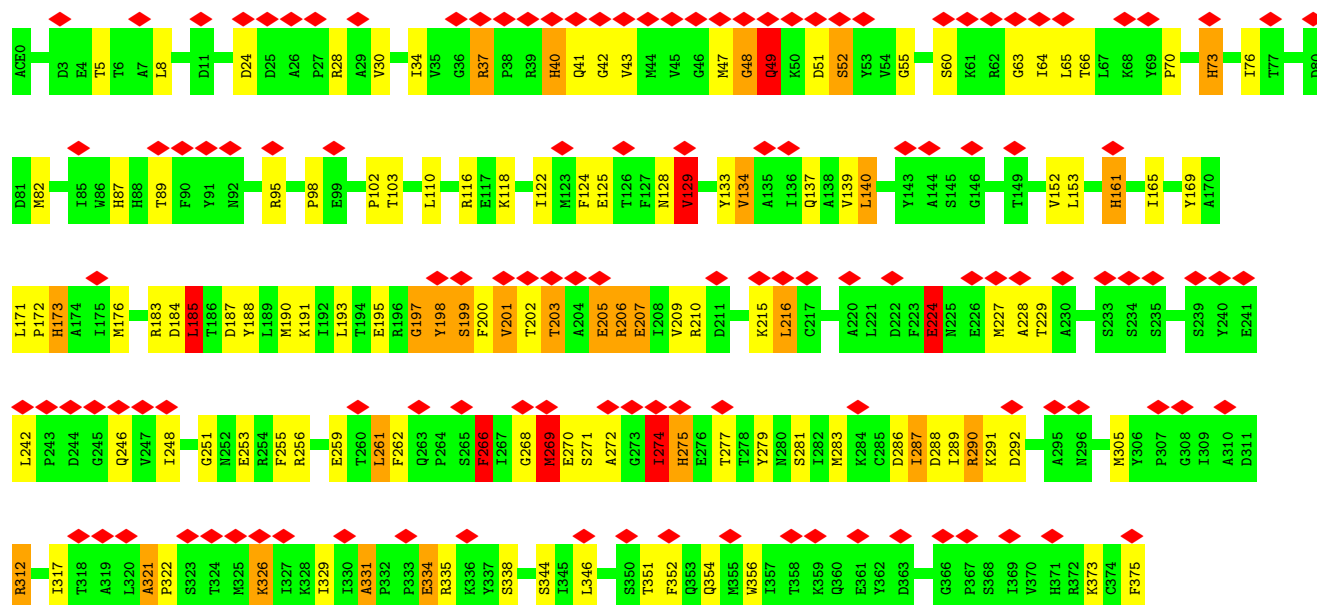




- Molecule 1: Actin, alpha skeletal muscle

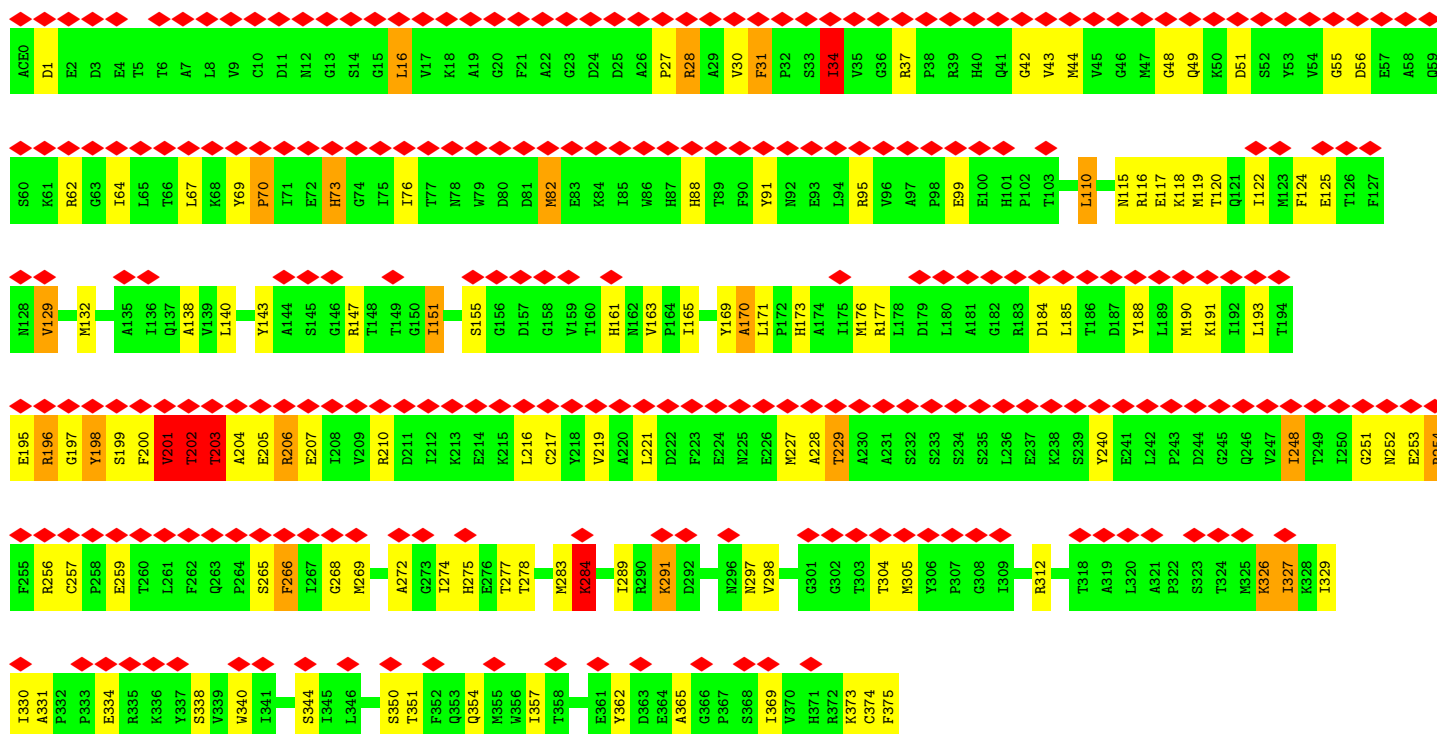


- Molecule 1: Actin, alpha skeletal muscle



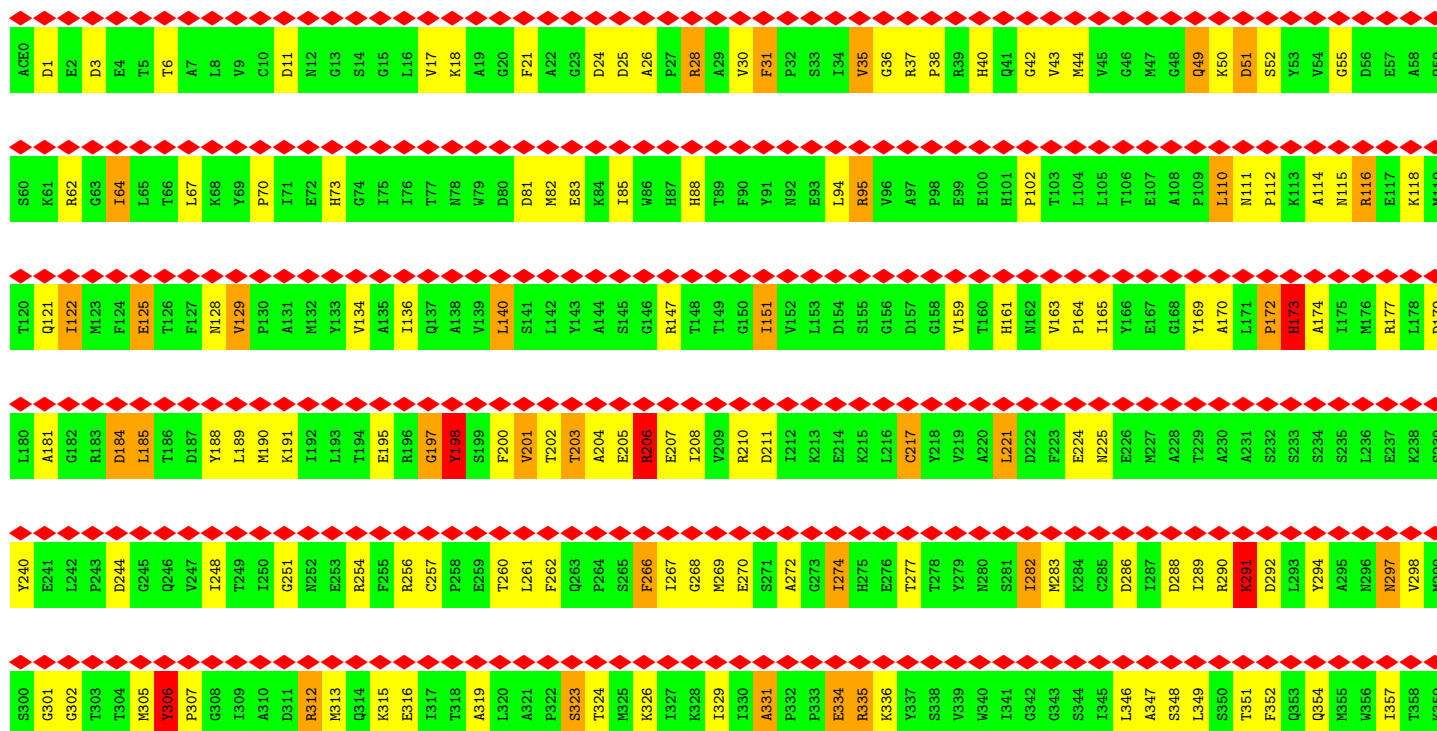
- Molecule 1: Actin, alpha skeletal muscle

Chain Y: 



• Molecule 1: Actin, alpha skeletal muscle

Chain Z: 



Q360	E361	Y362	D363	E364	A365	G366	P367	S368	I369	V370	H371	R372	K373	C374	F375
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of particles used	8000	Depositor
Resolution determination method	Not provided	
CTF correction method	FSC at 0.143 cut-off	Depositor
Microscope	HITACHI EF2000	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	100000	Depositor
Image detector	GENERIC CCD	Depositor
Maximum map value	105.405	Depositor
Minimum map value	-66.216	Depositor
Average map value	0.454	Depositor
Map value standard deviation	12.051	Depositor
Recommended contour level	33	Depositor
Map size (Å)	275.275, 275.275, 275.275	wwPDB
Map dimensions	121, 121, 121	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.275, 2.275, 2.275	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, PO4, HIC, MG, ACE

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	O	0.97	3/2984 (0.1%)	1.87	64/4042 (1.6%)
1	P	1.19	21/2984 (0.7%)	1.89	73/4042 (1.8%)
1	Q	1.05	8/2984 (0.3%)	1.88	70/4042 (1.7%)
1	R	1.04	10/2984 (0.3%)	1.91	75/4042 (1.9%)
1	S	0.97	4/2984 (0.1%)	1.87	56/4042 (1.4%)
1	T	0.99	3/2984 (0.1%)	1.87	47/4042 (1.2%)
1	U	0.96	3/2984 (0.1%)	1.83	58/4042 (1.4%)
1	V	0.94	3/2984 (0.1%)	1.83	62/4042 (1.5%)
1	W	0.98	3/2984 (0.1%)	1.87	63/4042 (1.6%)
1	X	0.96	4/2984 (0.1%)	1.83	52/4042 (1.3%)
1	Y	0.94	4/2984 (0.1%)	1.79	44/4042 (1.1%)
1	Z	0.96	3/2984 (0.1%)	1.87	73/4042 (1.8%)
All	All	1.00	69/35808 (0.2%)	1.86	737/48504 (1.5%)

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	O	0	18
1	P	0	17
1	Q	0	25
1	R	0	16
1	S	0	21
1	T	0	19
1	U	0	25
1	V	0	19
1	W	0	24
1	X	0	14
1	Y	0	22

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Z	0	23
All	All	0	243

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	62	ARG	C-N	14.70	1.55	1.33
1	P	62	ARG	CA-C	14.40	1.72	1.52
1	P	62	ARG	C-O	-12.83	1.07	1.24
1	P	61	LYS	CG-CD	12.44	1.89	1.52
1	Q	187	ASP	CG-OD2	-11.46	1.03	1.25
1	Q	187	ASP	CG-OD1	10.73	1.45	1.25
1	R	167	GLU	CD-OE1	-10.00	1.06	1.25
1	W	198	TYR	CA-C	-8.74	1.42	1.53
1	Q	203	THR	CA-C	8.38	1.64	1.52
1	S	198	TYR	CA-C	-7.90	1.42	1.52
1	S	203	THR	CA-C	7.90	1.63	1.52
1	O	198	TYR	CA-C	-7.81	1.43	1.52
1	R	167	GLU	CD-OE2	7.61	1.39	1.25
1	Q	270	GLU	CA-C	-7.58	1.44	1.52
1	P	201	VAL	C-O	-7.34	1.15	1.24
1	O	203	THR	CA-C	7.30	1.62	1.52
1	X	198	TYR	CA-C	-7.29	1.44	1.52
1	P	63	GLY	C-N	-6.98	1.24	1.33
1	P	61	LYS	CD-CE	6.95	1.73	1.52
1	P	64	ILE	N-CA	-6.85	1.38	1.46
1	Z	206	ARG	CA-C	6.80	1.59	1.53
1	U	203	THR	CA-C	6.74	1.61	1.52
1	P	61	LYS	C-N	-6.55	1.24	1.33
1	P	63	GLY	N-CA	-6.54	1.36	1.45
1	T	203	THR	CA-C	6.53	1.61	1.52
1	T	206	ARG	CA-C	6.51	1.60	1.52
1	Z	198	TYR	CA-C	-6.51	1.44	1.52
1	P	203	THR	CA-C	6.47	1.61	1.52
1	P	64	ILE	CA-CB	-6.44	1.46	1.54
1	X	206	ARG	CA-C	6.44	1.59	1.53
1	S	207	GLU	CA-CB	6.38	1.63	1.53
1	R	167	GLU	CA-C	-6.34	1.44	1.52
1	R	198	TYR	CA-C	-6.33	1.45	1.52
1	P	61	LYS	CB-CG	6.32	1.71	1.52
1	V	203	THR	CA-C	6.32	1.60	1.52
1	R	203	THR	CA-C	6.26	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	203	THR	CA-C	6.16	1.61	1.52
1	W	203	THR	CA-C	6.06	1.60	1.52
1	U	198	TYR	CA-C	-6.04	1.45	1.52
1	R	169	TYR	CA-CB	6.03	1.61	1.53
1	T	198	TYR	CA-C	-5.96	1.45	1.53
1	X	203	THR	CA-C	5.84	1.60	1.52
1	V	198	TYR	CA-C	-5.82	1.45	1.52
1	P	198	TYR	CA-C	-5.80	1.45	1.52
1	R	286	ASP	CG-OD1	5.71	1.36	1.25
1	P	60	SER	C-N	-5.69	1.26	1.33
1	P	202	THR	C-N	5.68	1.41	1.33
1	Y	198	TYR	CA-C	-5.67	1.45	1.52
1	R	167	GLU	CA-CB	5.63	1.62	1.53
1	X	201	VAL	CA-CB	-5.58	1.46	1.54
1	Q	183	ARG	CA-C	-5.58	1.48	1.53
1	U	206	ARG	CA-C	5.54	1.60	1.52
1	Q	111	ASN	N-CA	-5.45	1.42	1.46
1	Y	206	ARG	CA-C	5.43	1.60	1.52
1	R	206	ARG	CA-C	5.43	1.60	1.52
1	W	206	ARG	CA-C	5.41	1.59	1.52
1	Q	205	GLU	CA-C	5.40	1.59	1.52
1	O	206	ARG	CA-C	5.36	1.59	1.52
1	P	60	SER	CA-CB	5.30	1.62	1.53
1	Z	203	THR	CA-C	5.18	1.59	1.52
1	S	206	ARG	CA-C	5.17	1.59	1.52
1	Q	198	TYR	CA-C	-5.15	1.46	1.52
1	P	205	GLU	C-N	5.15	1.40	1.33
1	Y	205	GLU	CA-C	5.11	1.59	1.52
1	P	205	GLU	CA-C	5.08	1.59	1.52
1	P	206	ARG	CA-C	5.05	1.59	1.52
1	V	204	ALA	N-CA	5.02	1.52	1.46
1	P	61	LYS	CE-NZ	5.02	1.64	1.49
1	R	167	GLU	N-CA	5.00	1.52	1.46

All (737) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	206	ARG	N-CA-C	12.86	125.02	111.14
1	Q	269	MET	CG-SD-CE	-12.03	74.43	100.90
1	S	198	TYR	N-CA-CB	12.00	130.40	110.47
1	U	198	TYR	N-CA-CB	11.90	129.22	110.65
1	Q	198	TYR	N-CA-CB	11.82	129.11	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	286	ASP	CA-CB-CG	11.72	124.32	112.60
1	R	198	TYR	N-CA-CB	11.23	128.19	110.57
1	Y	272	ALA	N-CA-C	11.03	117.82	108.78
1	T	162	ASN	CA-C-N	11.01	130.09	122.60
1	T	162	ASN	C-N-CA	11.01	130.09	122.60
1	O	276	GLU	CB-CG-CD	10.99	131.29	112.60
1	W	206	ARG	N-CA-C	10.77	122.98	111.03
1	P	198	TYR	N-CA-CB	10.67	127.32	110.57
1	Z	198	TYR	N-CA-CB	10.62	128.11	110.47
1	O	198	TYR	N-CA-CB	10.44	127.79	110.47
1	P	204	ALA	N-CA-CB	-10.22	94.99	110.33
1	T	198	TYR	N-CA-CB	9.88	128.93	110.56
1	V	375	PHE	CA-CB-CG	9.72	123.52	113.80
1	P	61	LYS	N-CA-C	-9.62	92.72	108.41
1	P	204	ALA	N-CA-C	9.61	125.49	112.90
1	Z	266	PHE	CA-CB-CG	-9.18	104.62	113.80
1	P	203	THR	N-CA-CB	9.16	123.29	110.01
1	Q	161	HIS	CA-CB-CG	9.00	122.80	113.80
1	P	62	ARG	O-C-N	-8.96	110.67	122.59
1	P	61	LYS	CB-CG-CD	8.87	131.71	111.30
1	X	292	ASP	CA-CB-CG	-8.86	103.74	112.60
1	Z	286	ASP	CA-CB-CG	8.83	121.43	112.60
1	W	267	ILE	N-CA-C	-8.80	102.73	110.74
1	P	62	ARG	CB-CA-C	-8.78	92.95	110.42
1	P	61	LYS	N-CA-CB	-8.76	96.99	110.65
1	Q	306	TYR	N-CA-C	8.69	119.60	109.60
1	V	266	PHE	CA-CB-CG	-8.55	105.25	113.80
1	Y	198	TYR	N-CA-C	-8.53	95.50	109.40
1	Y	198	TYR	N-CA-CB	8.53	125.67	110.83
1	X	203	THR	N-CA-CB	8.38	122.75	110.26
1	Z	161	HIS	CA-CB-CG	8.30	122.10	113.80
1	W	203	THR	N-CA-CB	8.29	122.40	110.13
1	T	162	ASN	CA-CB-CG	-8.25	104.35	112.60
1	T	184	ASP	CA-CB-CG	-8.22	104.38	112.60
1	P	63	GLY	CA-C-N	8.14	133.12	121.55
1	P	63	GLY	C-N-CA	8.14	133.12	121.55
1	O	206	ARG	N-CA-C	8.13	123.32	113.41
1	R	262	PHE	CA-CB-CG	-8.09	105.71	113.80
1	P	161	HIS	CA-CB-CG	7.96	121.76	113.80
1	Q	297	ASN	CA-CB-CG	7.91	120.51	112.60
1	S	204	ALA	N-CA-CB	-7.86	100.45	110.90
1	O	173	HIS	CA-CB-CG	7.82	121.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	274	ILE	N-CA-C	7.81	118.56	110.36
1	X	161	HIS	CA-CB-CG	7.75	121.55	113.80
1	R	31	PHE	CA-CB-CG	7.75	121.55	113.80
1	V	198	TYR	N-CA-CB	7.70	123.08	110.69
1	R	92	ASN	CA-CB-CG	7.67	120.27	112.60
1	R	166	TYR	CA-C-N	7.66	136.17	121.54
1	R	166	TYR	C-N-CA	7.66	136.17	121.54
1	R	267	ILE	N-CA-C	-7.62	104.36	111.45
1	O	291	LYS	CA-C-N	7.61	131.24	120.28
1	O	291	LYS	C-N-CA	7.61	131.24	120.28
1	Y	88	HIS	CA-CB-CG	7.61	121.41	113.80
1	V	161	HIS	CA-CB-CG	7.60	121.40	113.80
1	P	51	ASP	CA-C-N	7.55	138.12	121.81
1	P	51	ASP	C-N-CA	7.55	138.12	121.81
1	X	183	ARG	N-CA-C	7.53	119.38	111.03
1	Q	297	ASN	CB-CA-C	-7.51	99.00	110.26
1	W	205	GLU	CB-CA-C	7.50	122.62	110.09
1	X	274	ILE	N-CA-C	7.48	117.60	110.42
1	S	206	ARG	N-CA-C	7.48	122.69	112.90
1	V	203	THR	N-CA-CB	7.44	121.17	110.16
1	R	332	PRO	N-CA-C	7.40	119.73	110.70
1	W	198	TYR	N-CA-C	-7.39	92.26	107.70
1	W	205	GLU	CA-C-N	7.34	130.61	120.63
1	W	205	GLU	C-N-CA	7.34	130.61	120.63
1	Y	351	THR	CA-C-N	7.33	131.08	120.38
1	Y	351	THR	C-N-CA	7.33	131.08	120.38
1	W	203	THR	CB-CA-C	-7.32	98.50	110.79
1	P	35	VAL	N-CA-C	-7.31	99.90	108.82
1	W	162	ASN	CA-CB-CG	-7.30	105.30	112.60
1	V	323	SER	CA-C-N	7.30	129.93	120.44
1	V	323	SER	C-N-CA	7.30	129.93	120.44
1	Q	91	TYR	N-CA-C	7.28	119.30	111.36
1	V	203	THR	O-C-N	-7.26	113.87	122.15
1	X	224	GLU	CA-C-N	7.24	129.98	120.28
1	X	224	GLU	C-N-CA	7.24	129.98	120.28
1	O	347	ALA	CA-C-N	7.23	130.94	120.38
1	O	347	ALA	C-N-CA	7.23	130.94	120.38
1	W	347	ALA	CA-C-N	7.21	130.66	120.28
1	W	347	ALA	C-N-CA	7.21	130.66	120.28
1	P	274	ILE	N-CA-C	7.20	118.51	111.67
1	T	329	ILE	N-CA-CB	7.20	119.63	110.99
1	W	34	ILE	N-CA-C	7.20	119.18	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	190	MET	CG-SD-CE	7.18	116.71	100.90
1	R	51	ASP	CA-C-N	7.15	134.91	121.69
1	R	51	ASP	C-N-CA	7.15	134.91	121.69
1	Q	271	SER	N-CA-CB	7.10	122.49	110.49
1	Y	274	ILE	N-CA-C	7.10	117.82	110.36
1	U	203	THR	O-C-N	-7.09	113.16	122.59
1	T	127	PHE	CA-CB-CG	-7.06	106.74	113.80
1	V	198	TYR	N-CA-C	-7.04	98.25	109.59
1	S	40	HIS	CA-CB-CG	7.02	120.82	113.80
1	R	201	VAL	CA-CB-CG1	6.99	122.28	110.40
1	U	129	VAL	N-CA-C	6.98	123.97	108.88
1	U	212	ILE	N-CA-C	6.98	117.09	110.53
1	X	375	PHE	CA-CB-CG	6.98	120.78	113.80
1	W	201	VAL	CA-CB-CG1	6.97	122.25	110.40
1	S	203	THR	N-CA-C	6.97	120.67	111.75
1	V	138	ALA	CA-C-N	6.96	129.34	120.56
1	V	138	ALA	C-N-CA	6.96	129.34	120.56
1	R	161	HIS	CA-CB-CG	6.92	120.72	113.80
1	V	205	GLU	CA-C-N	6.91	129.84	120.44
1	V	205	GLU	C-N-CA	6.91	129.84	120.44
1	V	332	PRO	N-CA-C	6.90	119.12	110.70
1	S	203	THR	N-CA-CB	6.89	121.03	110.14
1	S	65	LEU	CB-CA-C	-6.88	105.80	114.40
1	W	224	GLU	CA-C-N	6.88	129.49	120.28
1	W	224	GLU	C-N-CA	6.88	129.49	120.28
1	R	127	PHE	CA-CB-CG	-6.86	106.94	113.80
1	S	92	ASN	CA-CB-CG	6.85	119.45	112.60
1	P	62	ARG	CA-C-O	6.84	130.29	120.51
1	X	286	ASP	CA-CB-CG	6.84	119.44	112.60
1	T	202	THR	CA-CB-OG1	6.81	119.82	109.60
1	O	297	ASN	CA-CB-CG	-6.77	105.83	112.60
1	R	252	ASN	CA-CB-CG	6.77	119.37	112.60
1	Y	201	VAL	CA-CB-CG1	6.76	121.89	110.40
1	S	196	ARG	NE-CZ-NH2	6.75	125.28	119.20
1	O	335	ARG	N-CA-C	6.73	121.20	113.19
1	Q	31	PHE	CA-CB-CG	6.72	120.52	113.80
1	W	262	PHE	CA-CB-CG	-6.72	107.08	113.80
1	P	201	VAL	CA-CB-CG1	6.70	121.80	110.40
1	U	207	GLU	N-CA-C	6.70	121.16	113.19
1	T	163	VAL	O-C-N	-6.69	116.80	121.55
1	Z	24	ASP	N-CA-C	6.69	119.58	109.95
1	X	216	LEU	N-CA-CB	-6.68	101.67	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	301	GLY	N-CA-C	6.67	120.44	110.97
1	U	203	THR	N-CA-CB	6.66	121.75	110.49
1	X	321	ALA	N-CA-C	6.66	117.78	110.13
1	S	215	LYS	N-CA-C	6.64	119.35	111.71
1	V	184	ASP	CA-CB-CG	-6.63	105.97	112.60
1	S	187	ASP	CA-CB-CG	-6.62	105.98	112.60
1	V	286	ASP	CA-CB-CG	6.62	119.22	112.60
1	U	204	ALA	N-CA-CB	-6.62	101.75	110.88
1	V	217	CYS	N-CA-C	6.60	118.90	108.67
1	O	191	LYS	CA-CB-CG	6.60	127.29	114.10
1	Y	16	LEU	CA-C-N	6.60	129.95	120.98
1	Y	16	LEU	C-N-CA	6.60	129.95	120.98
1	Q	286	ASP	CA-CB-CG	6.58	119.18	112.60
1	S	163	VAL	N-CA-C	6.57	114.05	107.55
1	Q	270	GLU	CA-C-N	6.54	134.03	121.54
1	Q	270	GLU	C-N-CA	6.54	134.03	121.54
1	O	368	SER	CA-C-N	6.53	131.53	120.29
1	O	368	SER	C-N-CA	6.53	131.53	120.29
1	W	326	LYS	N-CA-C	6.53	119.36	108.13
1	V	127	PHE	CA-CB-CG	-6.53	107.28	113.80
1	O	128	ASN	CA-C-N	6.52	134.19	122.13
1	O	128	ASN	C-N-CA	6.52	134.19	122.13
1	S	203	THR	O-C-N	-6.51	114.78	122.20
1	Q	163	VAL	N-CA-C	6.51	113.48	107.56
1	U	323	SER	CA-C-N	6.50	129.52	120.29
1	U	323	SER	C-N-CA	6.50	129.52	120.29
1	Q	205	GLU	CB-CA-C	6.49	121.13	110.17
1	Z	301	GLY	N-CA-C	6.49	119.63	111.85
1	Z	128	ASN	CA-C-N	6.48	134.12	122.13
1	Z	128	ASN	C-N-CA	6.48	134.12	122.13
1	O	40	HIS	CA-CB-CG	6.48	120.28	113.80
1	T	347	ALA	CA-C-N	6.47	129.59	120.28
1	T	347	ALA	C-N-CA	6.47	129.59	120.28
1	W	206	ARG	O-C-N	-6.47	115.05	122.03
1	O	356	TRP	CA-CB-CG	6.46	125.87	113.60
1	V	253	GLU	CA-C-N	6.44	132.40	122.42
1	V	253	GLU	C-N-CA	6.44	132.40	122.42
1	W	266	PHE	CA-CB-CG	-6.42	107.38	113.80
1	S	287	ILE	N-CA-C	6.42	117.20	110.72
1	S	205	GLU	CB-CA-C	6.42	121.56	110.72
1	O	348	SER	N-CA-C	6.40	119.94	111.75
1	R	3	ASP	CA-CB-CG	-6.40	106.20	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	101	HIS	CA-CB-CG	6.39	120.19	113.80
1	Z	102	PRO	N-CA-C	6.39	121.38	111.21
1	Z	31	PHE	CA-CB-CG	6.38	120.18	113.80
1	Q	375	PHE	CA-CB-CG	6.38	120.18	113.80
1	X	198	TYR	N-CA-CB	6.37	120.95	110.69
1	R	166	TYR	CA-C-O	-6.36	113.83	120.70
1	W	31	PHE	O-C-N	-6.36	116.88	121.84
1	Z	297	ASN	CA-C-N	6.34	131.16	122.34
1	Z	297	ASN	C-N-CA	6.34	131.16	122.34
1	Q	203	THR	N-CA-CB	6.34	121.20	110.49
1	O	288	ASP	CA-CB-CG	-6.34	106.26	112.60
1	Z	291	LYS	CA-C-N	6.34	129.09	120.54
1	Z	291	LYS	C-N-CA	6.34	129.09	120.54
1	O	203	THR	N-CA-CB	6.33	121.19	110.49
1	W	161	HIS	CA-CB-CG	6.31	120.11	113.80
1	O	196	ARG	NE-CZ-NH2	6.30	124.87	119.20
1	P	191	LYS	CA-CB-CG	6.30	126.70	114.10
1	W	163	VAL	N-CA-C	6.30	114.12	107.76
1	X	129	VAL	N-CA-C	6.29	122.47	108.88
1	T	335	ARG	N-CA-CB	-6.29	101.33	110.70
1	T	204	ALA	N-CA-CB	6.28	119.39	110.67
1	V	279	TYR	CA-C-N	6.28	129.32	120.28
1	V	279	TYR	C-N-CA	6.28	129.32	120.28
1	Q	203	THR	O-C-N	-6.27	114.25	122.59
1	Q	23	GLY	N-CA-C	6.27	123.41	114.64
1	Z	267	ILE	N-CA-C	-6.26	105.63	111.45
1	U	128	ASN	CA-C-N	6.25	133.70	122.13
1	U	128	ASN	C-N-CA	6.25	133.70	122.13
1	P	332	PRO	N-CA-C	6.25	118.33	110.70
1	S	335	ARG	N-CA-C	6.25	124.11	110.80
1	R	248	ILE	N-CA-CB	6.24	118.99	111.31
1	R	291	LYS	CA-C-N	6.24	130.59	120.60
1	R	291	LYS	C-N-CA	6.24	130.59	120.60
1	Z	64	ILE	CA-CB-CG1	6.24	121.00	110.40
1	Q	49	GLN	N-CA-CB	6.23	121.02	110.49
1	P	37	ARG	O-C-N	-6.22	114.16	121.32
1	R	52	SER	N-CA-C	-6.22	98.48	108.55
1	Z	323	SER	CA-C-N	6.22	129.12	120.29
1	Z	323	SER	C-N-CA	6.22	129.12	120.29
1	R	202	THR	CA-CB-OG1	6.21	118.92	109.60
1	U	274	ILE	N-CA-C	6.21	118.86	111.09
1	O	282	ILE	CB-CA-C	-6.20	105.35	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	49	GLN	CB-CG-CD	6.19	123.13	112.60
1	Y	202	THR	CA-C-N	6.19	133.37	121.54
1	Y	202	THR	C-N-CA	6.19	133.37	121.54
1	Q	212	ILE	N-CA-C	6.19	116.82	110.82
1	Z	24	ASP	CA-C-N	6.19	129.07	121.64
1	Z	24	ASP	C-N-CA	6.19	129.07	121.64
1	Z	51	ASP	CA-C-N	6.18	133.34	121.54
1	Z	51	ASP	C-N-CA	6.18	133.34	121.54
1	V	128	ASN	CA-C-N	6.17	133.55	122.13
1	V	128	ASN	C-N-CA	6.17	133.55	122.13
1	X	351	THR	CA-C-N	6.17	128.55	120.28
1	X	351	THR	C-N-CA	6.17	128.55	120.28
1	O	161	HIS	CA-CB-CG	6.17	119.97	113.80
1	W	207	GLU	N-CA-C	6.17	120.81	113.16
1	O	212	ILE	N-CA-C	6.16	116.32	110.53
1	S	332	PRO	N-CA-C	6.16	118.22	110.70
1	R	368	SER	CA-C-N	6.14	130.70	120.62
1	R	368	SER	C-N-CA	6.14	130.70	120.62
1	X	206	ARG	CB-CA-C	6.14	121.16	111.39
1	X	279	TYR	CA-C-N	6.14	128.51	120.28
1	X	279	TYR	C-N-CA	6.14	128.51	120.28
1	R	12	ASN	CA-CB-CG	-6.14	106.46	112.60
1	T	51	ASP	CA-C-N	6.13	133.26	121.54
1	T	51	ASP	C-N-CA	6.13	133.26	121.54
1	R	132	MET	N-CA-C	6.13	119.19	109.50
1	Y	207	GLU	N-CA-C	6.13	120.45	113.15
1	P	266	PHE	CA-CB-CG	-6.12	107.68	113.80
1	X	65	LEU	CB-CA-C	-6.12	106.75	114.40
1	Z	204	ALA	N-CA-C	6.10	121.65	113.72
1	U	206	ARG	CB-CA-C	6.09	122.55	110.42
1	U	290	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	P	286	ASP	N-CA-CB	6.08	118.91	109.85
1	R	161	HIS	CB-CA-C	-6.08	98.25	109.37
1	P	60	SER	N-CA-C	6.07	123.74	110.80
1	Q	33	SER	N-CA-C	6.07	119.05	109.39
1	V	204	ALA	N-CA-CB	-6.07	102.51	110.59
1	P	279	TYR	CA-C-N	6.07	128.42	120.28
1	P	279	TYR	C-N-CA	6.07	128.42	120.28
1	U	275	HIS	CA-CB-CG	6.07	119.87	113.80
1	U	290	ARG	CA-C-N	6.07	129.23	120.79
1	U	290	ARG	C-N-CA	6.07	129.23	120.79
1	Q	334	GLU	CA-C-N	6.07	133.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	334	GLU	C-N-CA	6.07	133.13	121.54
1	S	274	ILE	N-CA-C	6.07	116.81	110.62
1	S	291	LYS	CA-C-N	6.05	129.51	120.31
1	S	291	LYS	C-N-CA	6.05	129.51	120.31
1	Q	129	VAL	N-CA-C	6.05	121.94	108.88
1	O	111	ASN	CA-CB-CG	-6.04	106.56	112.60
1	O	202	THR	CB-CA-C	6.04	122.43	110.42
1	P	290	ARG	CA-C-N	6.03	133.06	121.54
1	P	290	ARG	C-N-CA	6.03	133.06	121.54
1	Q	310	ALA	CA-C-N	6.01	128.83	120.29
1	Q	310	ALA	C-N-CA	6.01	128.83	120.29
1	V	228	ALA	CA-C-N	6.01	128.62	120.38
1	V	228	ALA	C-N-CA	6.01	128.62	120.38
1	R	331	ALA	N-CA-C	6.01	123.09	109.81
1	P	349	LEU	CA-C-N	6.00	129.82	120.82
1	P	349	LEU	C-N-CA	6.00	129.82	120.82
1	Y	196	ARG	NE-CZ-NH2	6.00	124.59	119.20
1	R	217	CYS	N-CA-C	5.99	118.54	107.99
1	Z	347	ALA	CA-C-N	5.99	128.59	120.38
1	Z	347	ALA	C-N-CA	5.99	128.59	120.38
1	R	305	MET	N-CA-C	5.99	118.57	111.33
1	U	161	HIS	CA-CB-CG	5.98	119.78	113.80
1	Q	274	ILE	N-CA-C	5.98	118.56	111.09
1	X	37	ARG	O-C-N	-5.98	115.82	121.20
1	S	248	ILE	CA-CB-CG1	5.97	120.56	110.40
1	Q	332	PRO	N-CA-C	5.97	117.98	110.70
1	U	163	VAL	CA-C-N	5.96	126.16	119.90
1	U	163	VAL	C-N-CA	5.96	126.16	119.90
1	Y	161	HIS	CA-CB-CG	5.96	119.76	113.80
1	U	205	GLU	CB-CA-C	5.95	120.34	109.99
1	W	198	TYR	N-CA-CB	5.95	120.56	110.87
1	Z	1	ASP	CA-CB-CG	-5.94	106.66	112.60
1	Z	121	GLN	N-CA-C	5.93	117.54	111.14
1	Q	206	ARG	CB-CA-C	5.93	122.22	110.42
1	Z	136	ILE	N-CA-C	5.93	116.34	107.51
1	O	203	THR	O-C-N	-5.92	114.71	122.59
1	V	201	VAL	CA-CB-CG1	5.92	120.47	110.40
1	Y	176	MET	CG-SD-CE	-5.92	87.87	100.90
1	Z	35	VAL	N-CA-C	-5.92	101.60	108.82
1	Y	31	PHE	O-C-N	-5.91	117.71	121.85
1	Q	167	GLU	N-CA-C	5.90	119.33	111.30
1	O	201	VAL	CA-CB-CG1	5.90	120.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	203	THR	CA-C-N	5.90	132.37	121.52
1	P	203	THR	C-N-CA	5.90	132.37	121.52
1	S	217	CYS	N-CA-C	5.89	118.50	110.55
1	S	202	THR	CB-CA-C	5.89	122.14	110.42
1	P	331	ALA	N-CA-C	5.88	122.81	109.81
1	X	82	MET	CG-SD-CE	-5.88	87.97	100.90
1	Q	96	VAL	N-CA-C	5.88	116.65	108.89
1	S	128	ASN	CA-C-N	5.86	132.97	122.13
1	S	128	ASN	C-N-CA	5.86	132.97	122.13
1	T	202	THR	CB-CA-C	5.85	122.07	110.42
1	O	266	PHE	CA-CB-CG	-5.85	107.95	113.80
1	R	350	SER	CA-C-N	5.85	128.44	120.54
1	R	350	SER	C-N-CA	5.85	128.44	120.54
1	P	151	ILE	N-CA-CB	5.84	118.71	111.41
1	Q	48	GLY	CA-C-N	5.82	132.66	121.54
1	Q	48	GLY	C-N-CA	5.82	132.66	121.54
1	Z	306	TYR	N-CA-C	5.82	122.67	109.81
1	Y	291	LYS	CA-C-N	5.81	130.43	120.72
1	Y	291	LYS	C-N-CA	5.81	130.43	120.72
1	V	192	ILE	N-CA-C	5.81	115.99	110.53
1	O	351	THR	CA-C-N	5.80	128.64	120.28
1	O	351	THR	C-N-CA	5.80	128.64	120.28
1	Z	44	MET	CA-C-N	5.80	128.09	120.60
1	Z	44	MET	C-N-CA	5.80	128.09	120.60
1	Y	205	GLU	CB-CA-C	5.80	120.62	110.64
1	Y	204	ALA	N-CA-C	5.79	121.39	113.97
1	W	196	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	Q	204	ALA	N-CA-CB	-5.79	103.21	110.90
1	R	198	TYR	N-CA-C	-5.78	99.76	109.07
1	V	205	GLU	CB-CA-C	5.78	120.33	110.56
1	R	277	THR	CA-C-N	5.77	128.34	120.54
1	R	277	THR	C-N-CA	5.77	128.34	120.54
1	Z	50	LYS	N-CA-C	5.77	118.97	109.85
1	P	191	LYS	CB-CA-C	-5.77	102.07	110.96
1	U	44	MET	N-CA-C	-5.76	105.34	112.72
1	Z	324	THR	N-CA-C	5.76	117.64	111.36
1	Q	279	TYR	CA-C-N	5.76	128.32	120.54
1	Q	279	TYR	C-N-CA	5.76	128.32	120.54
1	U	203	THR	N-CA-C	5.76	123.07	110.80
1	X	129	VAL	O-C-N	-5.75	114.55	121.10
1	S	91	TYR	N-CA-C	5.75	118.48	111.82
1	V	331	ALA	N-CA-C	5.74	122.50	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	272	ALA	N-CA-C	5.74	123.02	110.80
1	V	129	VAL	N-CA-C	5.74	121.27	108.88
1	W	106	THR	N-CA-CB	5.73	119.50	110.56
1	O	61	LYS	CB-CA-C	-5.73	100.41	109.80
1	Q	121	GLN	CA-C-N	5.73	129.52	120.47
1	Q	121	GLN	C-N-CA	5.73	129.52	120.47
1	Q	269	MET	CB-CG-SD	5.72	129.87	112.70
1	Y	138	ALA	N-CA-C	5.72	117.19	111.07
1	U	331	ALA	N-CA-C	5.72	122.45	109.81
1	V	255	PHE	N-CA-C	5.72	120.96	113.30
1	R	169	TYR	O-C-N	-5.71	116.25	123.05
1	X	331	ALA	N-CA-C	5.71	122.44	109.81
1	Z	111	ASN	CA-CB-CG	-5.71	106.89	112.60
1	Z	122	ILE	N-CA-C	5.71	117.13	110.62
1	O	338	SER	N-CA-C	5.71	118.27	111.71
1	P	129	VAL	N-CA-C	5.70	121.20	108.88
1	S	129	VAL	N-CA-C	5.70	121.18	108.88
1	U	79	TRP	CA-C-N	5.70	128.17	120.65
1	U	79	TRP	C-N-CA	5.70	128.17	120.65
1	T	17	VAL	N-CA-CB	5.69	118.31	111.31
1	O	329	ILE	N-CA-CB	5.69	117.82	110.99
1	U	185	LEU	N-CA-C	5.69	117.93	111.11
1	P	349	LEU	N-CA-C	5.68	118.89	109.46
1	W	30	VAL	N-CA-C	5.68	116.25	107.78
1	X	48	GLY	CA-C-N	5.68	132.40	121.54
1	X	48	GLY	C-N-CA	5.68	132.40	121.54
1	X	198	TYR	N-CA-C	-5.68	100.45	109.59
1	X	87	HIS	CA-C-N	5.67	128.13	120.65
1	X	87	HIS	C-N-CA	5.67	128.13	120.65
1	R	202	THR	CB-CA-C	5.66	121.69	110.42
1	S	375	PHE	CA-CB-CG	5.66	119.46	113.80
1	T	155	SER	O-C-N	-5.65	117.01	123.40
1	P	62	ARG	N-CA-C	5.65	122.83	110.80
1	S	159	VAL	N-CA-C	5.65	117.55	108.85
1	Z	225	ASN	CA-CB-CG	-5.65	106.95	112.60
1	W	24	ASP	N-CA-C	5.65	118.08	109.95
1	V	202	THR	CA-CB-OG1	5.65	118.07	109.60
1	P	201	VAL	CA-C-O	5.65	127.84	120.78
1	O	276	GLU	CA-CB-CG	-5.64	102.81	114.10
1	V	260	THR	N-CA-C	5.64	118.97	111.75
1	Y	202	THR	CA-CB-CG2	5.64	120.09	110.50
1	R	338	SER	N-CA-C	5.64	119.26	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	266	PHE	CA-CB-CG	-5.64	108.16	113.80
1	T	68	LYS	CB-CA-C	-5.63	102.40	110.62
1	Y	82	MET	CG-SD-CE	-5.63	88.52	100.90
1	O	352	PHE	CA-CB-CG	5.63	119.43	113.80
1	V	347	ALA	N-CA-C	5.63	117.86	111.11
1	Z	261	LEU	CB-CA-C	-5.62	101.45	110.79
1	R	24	ASP	N-CA-C	5.62	118.05	109.95
1	Y	99	GLU	N-CA-C	5.62	117.09	111.07
1	U	95	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	Y	163	VAL	N-CA-C	5.62	113.11	107.55
1	P	329	ILE	N-CA-CB	5.62	116.65	110.53
1	T	343	GLY	CA-C-N	5.61	128.07	120.44
1	T	343	GLY	C-N-CA	5.61	128.07	120.44
1	P	202	THR	CA-C-N	-5.61	113.15	120.44
1	P	202	THR	C-N-CA	-5.61	113.15	120.44
1	P	338	SER	N-CA-C	5.60	118.16	111.71
1	P	95	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	Q	217	CYS	N-CA-C	5.60	118.66	109.76
1	W	114	ALA	N-CA-C	5.59	117.18	111.14
1	V	284	LYS	N-CA-CB	-5.59	104.09	110.35
1	Z	198	TYR	N-CA-C	-5.59	98.10	107.99
1	Q	252	ASN	CB-CG-ND2	5.58	124.77	116.40
1	O	51	ASP	CA-C-N	5.58	131.76	121.94
1	O	51	ASP	C-N-CA	5.58	131.76	121.94
1	V	152	VAL	N-CA-CB	5.58	117.36	111.00
1	V	203	THR	CA-CB-OG1	5.58	117.97	109.60
1	R	159	VAL	CA-C-N	5.57	130.68	123.00
1	R	159	VAL	C-N-CA	5.57	130.68	123.00
1	S	334	GLU	CA-C-N	5.57	132.17	121.54
1	S	334	GLU	C-N-CA	5.57	132.17	121.54
1	Q	196	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	R	167	GLU	CA-CB-CG	5.57	125.23	114.10
1	P	252	ASN	CA-C-N	5.56	127.73	120.28
1	P	252	ASN	C-N-CA	5.56	127.73	120.28
1	T	206	ARG	N-CA-C	5.56	120.56	113.55
1	S	331	ALA	N-CA-C	5.55	122.09	109.81
1	U	350	SER	CA-C-N	5.55	129.15	120.82
1	U	350	SER	C-N-CA	5.55	129.15	120.82
1	T	261	LEU	CB-CA-C	-5.55	101.58	110.79
1	V	338	SER	CA-C-N	5.54	128.66	120.74
1	V	338	SER	C-N-CA	5.54	128.66	120.74
1	Q	128	ASN	CA-C-N	5.54	132.38	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	128	ASN	C-N-CA	5.54	132.38	122.13
1	R	203	THR	O-C-N	-5.54	116.11	122.09
1	P	114	ALA	N-CA-C	5.54	117.00	110.97
1	T	297	ASN	CB-CA-C	-5.53	102.28	111.41
1	V	95	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	X	261	LEU	CB-CA-C	-5.53	101.61	110.79
1	S	223	PHE	CA-CB-CG	-5.51	108.29	113.80
1	T	161	HIS	CA-CB-CG	5.51	119.31	113.80
1	Q	349	LEU	N-CA-C	5.51	118.03	109.60
1	U	40	HIS	CA-CB-CG	5.50	119.30	113.80
1	V	261	LEU	CA-C-N	5.50	128.44	120.79
1	V	261	LEU	C-N-CA	5.50	128.44	120.79
1	V	3	ASP	CA-CB-CG	-5.50	107.10	112.60
1	P	64	ILE	CA-C-N	5.50	132.41	122.02
1	P	64	ILE	C-N-CA	5.50	132.41	122.02
1	Q	151	ILE	N-CA-CB	5.49	117.92	111.66
1	Q	270	GLU	CA-CB-CG	5.49	125.09	114.10
1	Z	256	ARG	CA-C-N	5.49	126.59	119.78
1	Z	256	ARG	C-N-CA	5.49	126.59	119.78
1	Q	132	MET	N-CA-C	5.48	115.78	108.38
1	R	252	ASN	CA-C-N	5.48	127.62	120.28
1	R	252	ASN	C-N-CA	5.48	127.62	120.28
1	X	321	ALA	N-CA-CB	-5.48	103.30	109.49
1	V	179	ASP	N-CA-CB	-5.48	103.00	110.56
1	Z	88	HIS	CA-C-N	5.48	129.03	120.82
1	Z	88	HIS	C-N-CA	5.48	129.03	120.82
1	P	91	TYR	N-CA-C	5.47	119.58	113.01
1	O	103	THR	CB-CA-C	-5.47	100.50	109.80
1	P	137	GLN	CA-C-N	5.47	129.03	120.82
1	P	137	GLN	C-N-CA	5.47	129.03	120.82
1	W	9	VAL	N-CA-C	5.47	116.42	107.24
1	Y	203	THR	N-CA-CB	5.47	119.73	110.49
1	W	217	CYS	N-CA-C	5.46	118.83	110.20
1	W	33	SER	N-CA-C	5.46	118.07	109.39
1	P	45	VAL	CA-C-N	5.46	127.01	120.13
1	P	45	VAL	C-N-CA	5.46	127.01	120.13
1	Z	217	CYS	N-CA-C	5.45	117.93	110.24
1	O	204	ALA	N-CA-CB	-5.45	102.52	110.47
1	S	288	ASP	CB-CG-OD1	5.45	130.92	118.40
1	Q	331	ALA	N-CA-C	5.44	121.83	109.81
1	W	202	THR	N-CA-C	5.44	122.39	110.80
1	O	305	MET	N-CA-C	5.44	117.64	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	31	PHE	O-C-N	-5.44	118.04	121.85
1	S	310	ALA	CA-C-N	5.43	128.11	120.28
1	S	310	ALA	C-N-CA	5.43	128.11	120.28
1	W	332	PRO	N-CA-C	5.43	117.33	110.70
1	X	207	GLU	N-CA-C	5.43	122.36	110.80
1	Y	31	PHE	CA-CB-CG	5.43	119.23	113.80
1	W	201	VAL	CA-C-N	5.42	131.90	121.54
1	W	201	VAL	C-N-CA	5.42	131.90	121.54
1	W	285	CYS	O-C-N	-5.42	118.09	123.46
1	S	275	HIS	CA-CB-CG	5.42	119.22	113.80
1	S	102	PRO	N-CA-C	5.42	119.73	111.34
1	V	65	LEU	N-CA-CB	5.42	117.74	109.94
1	S	269	MET	CG-SD-CE	-5.42	88.99	100.90
1	Z	114	ALA	N-CA-C	5.41	116.98	111.14
1	T	332	PRO	N-CA-C	5.41	117.30	110.70
1	T	192	ILE	N-CA-CB	5.40	117.89	110.54
1	X	66	THR	CA-CB-CG2	5.40	119.69	110.50
1	O	91	TYR	N-CA-C	5.40	119.13	112.54
1	W	286	ASP	CA-CB-CG	5.40	118.00	112.60
1	R	152	VAL	N-CA-C	5.40	115.04	107.37
1	W	37	ARG	O-C-N	-5.40	116.61	121.31
1	U	205	GLU	CA-C-N	5.39	131.84	121.54
1	U	205	GLU	C-N-CA	5.39	131.84	121.54
1	P	106	THR	CA-CB-OG1	5.39	117.69	109.60
1	R	166	TYR	CB-CG-CD1	-5.39	112.72	120.80
1	T	190	MET	N-CA-CB	5.38	117.96	109.94
1	T	284	LYS	CB-CA-C	5.38	120.08	111.73
1	W	55	GLY	N-CA-C	5.38	125.94	113.18
1	T	279	TYR	N-CA-C	5.38	117.00	111.03
1	Z	129	VAL	N-CA-C	5.38	120.50	108.88
1	W	135	ALA	N-CA-C	5.38	118.04	110.14
1	Z	331	ALA	N-CA-C	5.37	121.69	109.81
1	V	274	ILE	N-CA-C	5.37	115.58	110.53
1	W	218	TYR	N-CA-C	-5.37	100.96	108.96
1	T	48	GLY	N-CA-C	5.36	125.88	113.18
1	X	198	TYR	CA-CB-CG	-5.36	104.25	113.90
1	Y	198	TYR	CA-CB-CG	-5.36	104.25	113.90
1	O	198	TYR	CA-CB-CG	-5.36	104.26	113.90
1	P	248	ILE	CA-CB-CG1	5.36	119.50	110.40
1	P	198	TYR	CA-CB-CG	-5.35	104.26	113.90
1	W	198	TYR	CA-CB-CG	-5.35	104.27	113.90
1	P	35	VAL	O-C-N	-5.35	117.30	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	24	ASP	N-CA-C	5.35	117.39	109.69
1	O	48	GLY	N-CA-C	5.35	125.85	113.18
1	U	203	THR	CB-CA-C	-5.35	99.78	110.42
1	X	185	LEU	CA-C-N	5.35	127.76	120.54
1	X	185	LEU	C-N-CA	5.35	127.76	120.54
1	X	269	MET	CG-SD-CE	-5.34	89.14	100.90
1	Z	198	TYR	CA-CB-CG	-5.34	104.28	113.90
1	T	198	TYR	CA-CB-CG	-5.34	104.28	113.90
1	U	198	TYR	CA-CB-CG	-5.34	104.29	113.90
1	V	198	TYR	CA-CB-CG	-5.34	104.29	113.90
1	Q	198	TYR	CA-CB-CG	-5.34	104.29	113.90
1	R	198	TYR	CA-CB-CG	-5.34	104.29	113.90
1	W	331	ALA	N-CA-C	5.34	121.61	109.81
1	P	217	CYS	N-CA-C	5.34	116.83	109.15
1	S	198	TYR	CA-CB-CG	-5.34	104.29	113.90
1	X	187	ASP	CA-CB-CG	-5.33	107.27	112.60
1	T	342	GLY	CA-C-N	5.33	125.90	119.98
1	T	342	GLY	C-N-CA	5.33	125.90	119.98
1	Z	134	VAL	CB-CA-C	5.33	118.70	110.28
1	Y	284	LYS	N-CA-CB	-5.33	104.03	110.53
1	W	205	GLU	CB-CG-CD	5.33	121.65	112.60
1	U	194	THR	CA-C-N	5.32	128.40	120.31
1	U	194	THR	C-N-CA	5.32	128.40	120.31
1	Q	51	ASP	CA-C-N	5.30	131.66	121.54
1	Q	51	ASP	C-N-CA	5.30	131.66	121.54
1	T	329	ILE	CA-CB-CG1	5.30	119.41	110.40
1	O	3	ASP	CA-CB-CG	-5.30	107.30	112.60
1	P	136	ILE	CA-C-N	5.29	128.15	120.79
1	P	136	ILE	C-N-CA	5.29	128.15	120.79
1	V	212	ILE	CB-CA-C	5.29	118.92	111.94
1	S	175	ILE	N-CA-C	5.29	115.73	108.12
1	U	300	SER	N-CA-C	5.28	117.11	108.76
1	X	228	ALA	CA-C-N	5.28	129.06	120.60
1	X	228	ALA	C-N-CA	5.28	129.06	120.60
1	O	255	PHE	CA-C-N	5.28	127.89	120.28
1	O	255	PHE	C-N-CA	5.28	127.89	120.28
1	Z	184	ASP	CA-CB-CG	-5.28	107.32	112.60
1	S	161	HIS	CB-CA-C	-5.28	100.48	109.51
1	Q	202	THR	CB-CA-C	5.28	120.92	110.42
1	W	12	ASN	N-CA-CB	5.28	117.80	109.83
1	U	217	CYS	N-CA-C	5.27	117.31	109.25
1	P	163	VAL	N-CA-C	5.27	113.67	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	210	ARG	CG-CD-NE	-5.27	100.41	112.00
1	R	206	ARG	O-C-N	-5.26	115.59	122.59
1	S	90	PHE	CA-CB-CG	5.26	119.06	113.80
1	R	356	TRP	CB-CA-C	-5.26	101.23	109.70
1	Q	263	GLN	CA-C-N	5.26	126.41	119.84
1	Q	263	GLN	C-N-CA	5.26	126.41	119.84
1	S	65	LEU	CA-C-N	5.26	130.17	122.39
1	S	65	LEU	C-N-CA	5.26	130.17	122.39
1	Q	334	GLU	N-CA-C	-5.25	107.04	113.50
1	O	4	GLU	CA-C-N	5.25	131.57	121.54
1	O	4	GLU	C-N-CA	5.25	131.57	121.54
1	R	286	ASP	CA-C-N	5.25	128.77	120.47
1	R	286	ASP	C-N-CA	5.25	128.77	120.47
1	V	269	MET	CG-SD-CE	-5.25	89.35	100.90
1	Y	44	MET	CA-C-N	5.25	127.38	120.60
1	Y	44	MET	C-N-CA	5.25	127.38	120.60
1	V	334	GLU	CA-C-N	5.25	131.56	121.54
1	V	334	GLU	C-N-CA	5.25	131.56	121.54
1	O	276	GLU	O-C-N	-5.24	114.78	122.43
1	W	284	LYS	N-CA-CB	-5.24	103.49	110.57
1	Q	202	THR	OG1-CB-CG2	-5.24	98.83	109.30
1	W	274	ILE	N-CA-C	5.24	116.01	110.72
1	U	80	ASP	N-CA-C	5.23	116.67	110.97
1	O	209	VAL	CB-CA-C	-5.23	105.19	111.88
1	R	317	ILE	CA-C-N	5.23	128.01	120.38
1	R	317	ILE	C-N-CA	5.23	128.01	120.38
1	S	190	MET	N-CA-CB	5.23	117.77	109.82
1	T	74	GLY	CA-C-N	5.23	127.51	120.50
1	T	74	GLY	C-N-CA	5.23	127.51	120.50
1	V	248	ILE	CA-CB-CG1	5.23	119.29	110.40
1	W	305	MET	N-CA-C	5.23	117.38	111.11
1	Z	319	ALA	N-CA-C	5.22	117.38	111.11
1	Q	250	ILE	N-CA-CB	5.22	117.26	110.99
1	Y	229	THR	CA-C-N	5.22	128.65	120.82
1	Y	229	THR	C-N-CA	5.22	128.65	120.82
1	T	297	ASN	N-CA-C	5.22	117.83	108.17
1	P	306	TYR	CB-CA-C	-5.22	101.52	109.50
1	U	286	ASP	CA-C-N	5.22	131.37	121.97
1	U	286	ASP	C-N-CA	5.22	131.37	121.97
1	U	332	PRO	N-CA-C	5.22	117.07	110.70
1	S	138	ALA	N-CA-C	5.22	116.65	111.07
1	R	161	HIS	N-CA-CB	5.21	119.19	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	49	GLN	N-CA-CB	5.21	119.30	110.49
1	X	205	GLU	CB-CA-C	5.21	119.82	110.81
1	P	128	ASN	CA-C-N	5.21	131.76	122.13
1	P	128	ASN	C-N-CA	5.21	131.76	122.13
1	P	328	LYS	O-C-N	-5.21	117.24	123.28
1	W	267	ILE	N-CA-CB	5.21	116.89	110.64
1	T	370	VAL	N-CA-C	5.20	115.97	110.72
1	Q	328	LYS	O-C-N	-5.20	117.12	123.10
1	R	331	ALA	CA-C-N	5.19	125.73	120.38
1	R	331	ALA	C-N-CA	5.19	125.73	120.38
1	Y	34	ILE	N-CA-C	5.19	115.96	108.48
1	W	334	GLU	CA-C-N	5.19	131.45	121.54
1	W	334	GLU	C-N-CA	5.19	131.45	121.54
1	R	201	VAL	N-CA-CB	5.18	119.78	111.23
1	U	44	MET	CA-C-N	5.18	127.56	120.77
1	U	44	MET	C-N-CA	5.18	127.56	120.77
1	W	162	ASN	CA-C-N	-5.18	118.86	122.59
1	W	162	ASN	C-N-CA	-5.18	118.86	122.59
1	V	347	ALA	CA-C-N	5.18	128.97	120.63
1	V	347	ALA	C-N-CA	5.18	128.97	120.63
1	Y	206	ARG	O-C-N	-5.18	115.70	122.59
1	Q	270	GLU	N-CA-C	5.17	122.03	113.50
1	T	266	PHE	CA-CB-CG	-5.17	108.63	113.80
1	U	297	ASN	CA-CB-CG	-5.17	107.43	112.60
1	X	287	ILE	CA-CB-CG1	5.17	119.19	110.40
1	P	370	VAL	CA-C-N	5.17	127.98	120.79
1	P	370	VAL	C-N-CA	5.17	127.98	120.79
1	V	34	ILE	N-CA-C	5.17	115.56	108.12
1	Z	375	PHE	CA-CB-CG	5.16	118.96	113.80
1	T	195	GLU	CB-CG-CD	5.15	121.35	112.60
1	P	206	ARG	N-CA-C	5.14	119.55	113.12
1	R	340	TRP	CB-CA-C	5.14	119.33	110.79
1	T	306	TYR	N-CA-C	5.14	121.17	109.81
1	R	267	ILE	N-CA-CB	5.14	118.53	110.31
1	S	297	ASN	N-CA-C	5.14	117.07	108.23
1	Q	360	GLN	N-CA-C	5.14	116.57	111.07
1	V	13	GLY	N-CA-C	-5.13	101.02	113.18
1	R	152	VAL	O-C-N	-5.13	116.96	122.45
1	X	24	ASP	N-CA-CB	-5.13	103.12	110.87
1	X	271	SER	CA-C-N	5.13	131.33	121.54
1	X	271	SER	C-N-CA	5.13	131.33	121.54
1	R	166	TYR	CB-CG-CD2	5.13	128.49	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	198	TYR	N-CA-C	-5.13	100.05	108.41
1	Y	202	THR	OG1-CB-CG2	-5.13	99.05	109.30
1	Z	329	ILE	N-CA-CB	5.13	119.06	110.86
1	Z	349	LEU	CA-C-N	5.13	127.92	120.79
1	Z	349	LEU	C-N-CA	5.13	127.92	120.79
1	O	332	PRO	N-CA-C	5.12	116.95	110.70
1	P	296	ASN	CA-C-N	5.12	129.62	121.99
1	P	296	ASN	C-N-CA	5.12	129.62	121.99
1	Q	286	ASP	CA-C-N	5.12	129.02	120.62
1	Q	286	ASP	C-N-CA	5.12	129.02	120.62
1	X	326	LYS	N-CA-C	5.12	117.80	109.24
1	W	125	GLU	CA-C-N	5.12	127.45	120.54
1	W	125	GLU	C-N-CA	5.12	127.45	120.54
1	X	209	VAL	CB-CA-C	-5.12	105.42	111.97
1	U	162	ASN	CA-CB-CG	-5.12	107.48	112.60
1	Y	228	ALA	CA-C-N	5.12	127.13	120.28
1	Y	228	ALA	C-N-CA	5.12	127.13	120.28
1	V	349	LEU	N-CA-C	5.11	117.85	110.28
1	X	207	GLU	CA-CB-CG	5.11	124.32	114.10
1	R	45	VAL	CA-C-N	5.11	126.56	120.13
1	R	45	VAL	C-N-CA	5.11	126.56	120.13
1	Q	98	PRO	CA-C-N	5.10	127.07	120.44
1	Q	98	PRO	C-N-CA	5.10	127.07	120.44
1	R	129	VAL	N-CA-C	5.10	119.89	108.88
1	S	24	ASP	N-CA-C	5.10	117.29	109.95
1	O	331	ALA	N-CA-C	5.09	121.07	109.81
1	S	89	THR	CB-CA-C	-5.09	102.28	110.74
1	Z	348	SER	N-CA-C	5.09	117.49	111.33
1	R	88	HIS	CA-C-N	5.09	127.81	120.38
1	R	88	HIS	C-N-CA	5.09	127.81	120.38
1	U	287	ILE	N-CA-C	5.09	119.93	109.34
1	W	189	LEU	CA-C-N	5.09	127.41	120.54
1	W	189	LEU	C-N-CA	5.09	127.41	120.54
1	U	81	ASP	CA-C-N	5.09	127.10	120.28
1	U	81	ASP	C-N-CA	5.09	127.10	120.28
1	R	23	GLY	N-CA-C	5.09	121.76	114.64
1	O	171	LEU	CB-CA-C	5.08	115.56	109.31
1	U	228	ALA	CA-C-N	5.08	127.09	120.28
1	U	228	ALA	C-N-CA	5.08	127.09	120.28
1	R	205	GLU	CB-CG-CD	5.08	121.24	112.60
1	V	2	GLU	N-CA-C	5.08	117.09	110.43
1	W	126	THR	N-CA-C	5.08	117.21	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	357	ILE	N-CA-CB	5.08	116.90	111.46
1	Q	321	ALA	N-CA-C	5.08	117.37	110.01
1	S	50	LYS	N-CA-C	5.08	118.39	110.32
1	Y	374	CYS	N-CA-C	5.08	117.05	109.59
1	U	35	VAL	N-CA-C	-5.07	101.76	108.96
1	Z	161	HIS	CB-CA-C	-5.07	100.09	109.37
1	Y	248	ILE	N-CA-CB	5.07	116.06	110.53
1	Z	3	ASP	CA-C-N	5.07	128.27	120.82
1	Z	3	ASP	C-N-CA	5.07	128.27	120.82
1	P	122	ILE	N-CA-C	5.07	115.79	110.62
1	R	31	PHE	O-C-N	-5.06	117.88	121.83
1	V	319	ALA	N-CA-C	5.06	117.45	111.33
1	R	375	PHE	CA-CB-CG	5.06	118.86	113.80
1	O	373	LYS	N-CA-C	5.06	116.64	111.03
1	U	184	ASP	CA-C-N	5.06	127.37	120.54
1	U	184	ASP	C-N-CA	5.06	127.37	120.54
1	Z	140	LEU	CA-C-N	5.06	127.47	120.29
1	Z	140	LEU	C-N-CA	5.06	127.47	120.29
1	S	262	PHE	CA-CB-CG	-5.05	108.75	113.80
1	S	232	SER	N-CA-C	-5.05	106.21	112.93
1	W	136	ILE	N-CA-C	5.04	115.35	107.99
1	Z	122	ILE	CA-C-N	5.04	127.30	120.44
1	Z	122	ILE	C-N-CA	5.04	127.30	120.44
1	O	278	THR	CA-C-N	5.04	127.45	120.29
1	O	278	THR	C-N-CA	5.04	127.45	120.29
1	U	51	ASP	N-CA-C	5.04	121.54	110.80
1	O	114	ALA	N-CA-C	5.04	116.58	111.14
1	Q	45	VAL	CA-C-N	5.04	126.48	120.13
1	Q	45	VAL	C-N-CA	5.04	126.48	120.13
1	X	52	SER	N-CA-CB	5.04	119.01	110.49
1	Y	252	ASN	CA-C-N	5.04	127.03	120.28
1	Y	252	ASN	C-N-CA	5.04	127.03	120.28
1	Z	298	VAL	CB-CA-C	-5.04	104.33	111.38
1	T	278	THR	CA-C-N	5.04	127.48	120.63
1	T	278	THR	C-N-CA	5.04	127.48	120.63
1	O	276	GLU	CB-CA-C	5.04	119.97	109.95
1	R	41	GLN	CB-CG-CD	5.04	121.16	112.60
1	Y	365	ALA	N-CA-C	5.04	116.85	111.36
1	P	49	GLN	N-CA-CB	5.03	119.00	110.49
1	T	252	ASN	CB-CG-ND2	5.03	123.95	116.40
1	R	212	ILE	N-CA-C	5.03	115.25	110.42
1	O	41	GLN	CB-CA-C	5.03	120.43	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	248	ILE	N-CA-CB	5.03	116.01	110.53
1	X	134	VAL	CB-CA-C	5.03	119.54	111.29
1	O	276	GLU	CG-CD-OE2	-5.03	106.84	118.40
1	R	369	ILE	N-CA-CB	-5.02	102.66	110.54
1	W	210	ARG	CA-C-N	5.02	127.32	120.54
1	W	210	ARG	C-N-CA	5.02	127.32	120.54
1	U	103	THR	N-CA-C	5.02	116.21	107.93
1	Z	312	ARG	CA-C-N	5.02	127.00	120.28
1	Z	312	ARG	C-N-CA	5.02	127.00	120.28
1	S	348	SER	N-CA-C	5.02	118.50	112.38
1	R	167	GLU	CA-C-N	5.01	130.17	122.20
1	R	167	GLU	C-N-CA	5.01	130.17	122.20
1	O	356	TRP	CB-CA-C	-5.01	100.45	110.42
1	Z	147	ARG	N-CA-C	5.01	117.61	109.24
1	Z	125	GLU	CA-C-N	5.01	126.99	120.28
1	Z	125	GLU	C-N-CA	5.01	126.99	120.28
1	Z	346	LEU	CA-C-N	5.00	127.23	120.38
1	Z	346	LEU	C-N-CA	5.00	127.23	120.38

There are no chirality outliers.

All (243) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	177	ARG	Sidechain
1	O	197	GLY	Peptide
1	O	200	PHE	Peptide
1	O	210	ARG	Sidechain
1	O	218	TYR	Sidechain
1	O	240	TYR	Sidechain
1	O	253	GLU	Peptide
1	O	256	ARG	Sidechain
1	O	266	PHE	Peptide
1	O	279	TYR	Sidechain
1	O	28	ARG	Sidechain
1	O	312	ARG	Sidechain
1	O	331	ALA	Peptide
1	O	38	PRO	Peptide
1	O	50	LYS	Peptide
1	O	69	TYR	Sidechain
1	O	91	TYR	Sidechain
1	O	95	ARG	Sidechain
1	P	116	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	P	161	HIS	Sidechain
1	P	197	GLY	Peptide
1	P	200	PHE	Peptide
1	P	208	ILE	Peptide
1	P	210	ARG	Sidechain
1	P	240	TYR	Sidechain
1	P	256	ARG	Sidechain
1	P	266	PHE	Peptide
1	P	28	ARG	Sidechain
1	P	306	TYR	Sidechain
1	P	312	ARG	Sidechain
1	P	331	ALA	Peptide
1	P	53	TYR	Sidechain
1	P	61	LYS	Mainchain
1	P	69	TYR	Sidechain
1	P	95	ARG	Sidechain
1	Q	116	ARG	Sidechain
1	Q	133	TYR	Sidechain
1	Q	147	ARG	Sidechain
1	Q	171	LEU	Peptide
1	Q	187	ASP	Mainchain
1	Q	188	TYR	Sidechain
1	Q	200	PHE	Sidechain,Peptide
1	Q	210	ARG	Sidechain
1	Q	250	ILE	Peptide
1	Q	253	GLU	Peptide
1	Q	256	ARG	Sidechain
1	Q	266	PHE	Peptide
1	Q	269	MET	Peptide
1	Q	270	GLU	Peptide
1	Q	271	SER	Peptide
1	Q	290	ARG	Sidechain
1	Q	316	GLU	Peptide
1	Q	331	ALA	Peptide
1	Q	334	GLU	Peptide
1	Q	34	ILE	Peptide
1	Q	50	LYS	Peptide
1	Q	58	ALA	Peptide
1	Q	69	TYR	Sidechain
1	Q	95	ARG	Sidechain
1	R	169	TYR	Sidechain
1	R	177	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	R	183	ARG	Sidechain
1	R	196	ARG	Sidechain
1	R	197	GLY	Peptide
1	R	200	PHE	Peptide
1	R	210	ARG	Sidechain
1	R	218	TYR	Sidechain
1	R	28	ARG	Sidechain
1	R	312	ARG	Sidechain
1	R	331	ALA	Peptide
1	R	334	GLU	Peptide
1	R	37	ARG	Sidechain
1	R	90	PHE	Sidechain
1	R	91	TYR	Sidechain
1	R	95	ARG	Sidechain
1	S	116	ARG	Sidechain
1	S	143	TYR	Sidechain
1	S	172	PRO	Peptide
1	S	177	ARG	Sidechain
1	S	197	GLY	Peptide
1	S	200	PHE	Sidechain,Peptide
1	S	210	ARG	Sidechain
1	S	223	PHE	Sidechain
1	S	256	ARG	Sidechain
1	S	266	PHE	Peptide
1	S	271	SER	Peptide
1	S	28	ARG	Sidechain
1	S	290	ARG	Sidechain
1	S	306	TYR	Sidechain
1	S	331	ALA	Peptide
1	S	335	ARG	Sidechain
1	S	372	ARG	Sidechain
1	S	50	LYS	Peptide
1	S	53	TYR	Sidechain
1	S	91	TYR	Sidechain
1	T	116	ARG	Sidechain
1	T	124	PHE	Sidechain
1	T	171	LEU	Peptide
1	T	177	ARG	Sidechain
1	T	196	ARG	Sidechain
1	T	197	GLY	Peptide
1	T	200	PHE	Peptide
1	T	210	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	T	266	PHE	Peptide
1	T	306	TYR	Sidechain
1	T	312	ARG	Sidechain
1	T	331	ALA	Peptide
1	T	334	GLU	Peptide
1	T	335	ARG	Sidechain
1	T	38	PRO	Peptide
1	T	53	TYR	Sidechain
1	T	62	ARG	Sidechain
1	T	69	TYR	Sidechain
1	T	91	TYR	Sidechain
1	U	100	GLU	Peptide
1	U	12	ASN	Peptide
1	U	143	TYR	Sidechain
1	U	147	ARG	Sidechain
1	U	168	GLY	Peptide
1	U	169	TYR	Sidechain
1	U	177	ARG	Sidechain
1	U	197	GLY	Peptide
1	U	200	PHE	Peptide
1	U	210	ARG	Sidechain
1	U	253	GLU	Peptide
1	U	256	ARG	Sidechain
1	U	266	PHE	Peptide
1	U	271	SER	Peptide
1	U	28	ARG	Sidechain
1	U	290	ARG	Sidechain
1	U	294	TYR	Sidechain
1	U	312	ARG	Sidechain
1	U	334	GLU	Peptide
1	U	372	ARG	Sidechain
1	U	373	LYS	Peptide
1	U	38	PRO	Peptide
1	U	40	HIS	Sidechain
1	U	62	ARG	Sidechain
1	U	95	ARG	Sidechain
1	V	133	TYR	Sidechain
1	V	177	ARG	Sidechain
1	V	197	GLY	Peptide
1	V	200	PHE	Peptide
1	V	210	ARG	Sidechain
1	V	254	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	V	258	PRO	Peptide
1	V	266	PHE	Peptide
1	V	28	ARG	Sidechain
1	V	290	ARG	Sidechain
1	V	306	TYR	Sidechain
1	V	312	ARG	Sidechain
1	V	331	ALA	Peptide
1	V	335	ARG	Sidechain
1	V	372	ARG	Sidechain
1	V	373	LYS	Peptide
1	V	38	PRO	Peptide
1	V	62	ARG	Sidechain
1	V	95	ARG	Sidechain
1	W	116	ARG	Sidechain
1	W	133	TYR	Sidechain
1	W	169	TYR	Sidechain
1	W	170	ALA	Peptide
1	W	183	ARG	Sidechain
1	W	188	TYR	Sidechain
1	W	210	ARG	Sidechain
1	W	23	GLY	Peptide
1	W	256	ARG	Sidechain
1	W	262	PHE	Sidechain
1	W	271	SER	Peptide
1	W	28	ARG	Sidechain
1	W	306	TYR	Sidechain
1	W	312	ARG	Sidechain
1	W	331	ALA	Peptide
1	W	362	TYR	Sidechain
1	W	37	ARG	Sidechain
1	W	372	ARG	Sidechain
1	W	373	LYS	Peptide
1	W	50	LYS	Peptide
1	W	51	ASP	Peptide
1	W	62	ARG	Sidechain
1	W	69	TYR	Sidechain
1	W	95	ARG	Sidechain
1	X	124	PHE	Sidechain
1	X	133	TYR	Sidechain
1	X	169	TYR	Sidechain
1	X	197	GLY	Peptide
1	X	200	PHE	Peptide

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Mol	Chain	Res	Type	Group
1	X	210	ARG	Sidechain
1	X	215	LYS	Peptide
1	X	256	ARG	Sidechain
1	X	266	PHE	Peptide
1	X	28	ARG	Sidechain
1	X	290	ARG	Sidechain
1	X	312	ARG	Sidechain
1	X	331	ALA	Peptide
1	X	334	GLU	Peptide
1	Y	124	PHE	Sidechain
1	Y	143	TYR	Sidechain
1	Y	147	ARG	Sidechain
1	Y	169	TYR	Sidechain
1	Y	170	ALA	Peptide
1	Y	171	LEU	Peptide
1	Y	177	ARG	Sidechain
1	Y	197	GLY	Peptide
1	Y	200	PHE	Peptide
1	Y	206	ARG	Sidechain
1	Y	210	ARG	Sidechain
1	Y	240	TYR	Sidechain
1	Y	256	ARG	Sidechain
1	Y	266	PHE	Peptide
1	Y	28	ARG	Sidechain
1	Y	31	PHE	Sidechain
1	Y	312	ARG	Sidechain
1	Y	331	ALA	Peptide
1	Y	334	GLU	Peptide
1	Y	362	TYR	Sidechain
1	Y	62	ARG	Sidechain
1	Y	91	TYR	Sidechain
1	Z	116	ARG	Sidechain,Peptide
1	Z	177	ARG	Sidechain
1	Z	197	GLY	Peptide
1	Z	200	PHE	Peptide
1	Z	206	ARG	Sidechain
1	Z	210	ARG	Sidechain
1	Z	221	LEU	Peptide
1	Z	240	TYR	Sidechain
1	Z	26	ALA	Peptide
1	Z	266	PHE	Sidechain
1	Z	28	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	Z	290	ARG	Sidechain
1	Z	294	TYR	Sidechain
1	Z	312	ARG	Sidechain
1	Z	316	GLU	Peptide
1	Z	331	ALA	Peptide
1	Z	334	GLU	Peptide
1	Z	335	ARG	Sidechain
1	Z	372	ARG	Sidechain
1	Z	38	PRO	Peptide
1	Z	62	ARG	Sidechain
1	Z	95	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2936	0	2897	41	0
1	P	2936	0	2896	41	0
1	Q	2936	0	2896	58	0
1	R	2936	0	2896	41	0
1	S	2936	0	2897	45	0
1	T	2936	0	2897	46	0
1	U	2936	0	2896	42	0
1	V	2936	0	2896	55	0
1	W	2936	0	2896	46	0
1	X	2936	0	2897	42	0
1	Y	2936	0	2896	36	0
1	Z	2936	0	2896	25	0
2	O	27	0	12	1	0
2	P	27	0	12	0	0
2	Q	27	0	12	0	0
2	R	27	0	12	0	0
2	S	27	0	12	0	0
2	T	27	0	12	0	0
2	U	27	0	12	1	0
2	V	27	0	12	0	0
2	W	27	0	12	0	0
2	X	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	27	0	12	0	0
2	Z	27	0	12	0	0
3	O	15	0	0	0	0
3	P	15	0	0	1	0
3	Q	15	0	0	0	0
3	R	15	0	0	1	0
3	S	15	0	0	0	0
3	T	20	0	0	1	0
3	U	15	0	0	0	0
3	V	10	0	0	0	0
3	W	15	0	0	0	0
3	X	15	0	0	0	0
3	Y	15	0	0	2	0
3	Z	15	0	0	0	0
4	O	6	0	0	0	0
4	P	5	0	0	0	0
4	Q	7	0	0	0	0
4	R	6	0	0	0	0
4	S	6	0	0	0	0
4	T	6	0	0	0	0
4	U	6	0	0	0	0
4	V	6	0	0	0	0
4	W	6	0	0	0	0
4	X	6	0	0	0	0
4	Y	6	0	0	0	0
4	Z	6	0	0	0	0
All	All	35808	0	34900	433	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (433) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:61:LYS:CD	1:P:61:LYS:CG	1.89	1.50
1:Q:202:THR:HG23	1:Q:203:THR:H	1.48	0.78
1:P:202:THR:HG23	1:P:203:THR:H	1.50	0.76
1:O:201:VAL:HG13	1:O:202:THR:HG22	1.68	0.74
1:V:275:HIS:CD2	1:V:276:GLU:H	2.05	0.74
1:O:201:VAL:HG13	1:O:202:THR:H	1.53	0.72
1:V:203:THR:OG1	1:W:269:MET:HE1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:204:ALA:HB1	1:U:290:ARG:HH21	1.55	0.71
1:V:202:THR:HG23	1:V:203:THR:H	1.57	0.70
1:R:201:VAL:HG13	1:R:202:THR:HG22	1.73	0.69
1:R:193:LEU:HD23	1:R:196:ARG:HE	1.56	0.69
1:W:201:VAL:HG13	1:W:202:THR:H	1.56	0.69
1:O:305:MET:HE2	1:O:305:MET:HA	1.74	0.68
1:T:193:LEU:HD23	1:T:196:ARG:HE	1.59	0.67
1:S:204:ALA:HB1	1:U:290:ARG:NH2	2.10	0.66
1:R:203:THR:OG1	1:S:269:MET:HE1	1.96	0.66
1:Y:202:THR:HG23	1:Y:203:THR:H	1.60	0.66
1:V:40:HIS:CD2	1:V:43:VAL:H	2.14	0.65
1:S:201:VAL:HG13	1:S:202:THR:H	1.62	0.65
1:O:43:VAL:HG22	1:Q:110:LEU:HD13	1.78	0.64
1:O:276:GLU:O	1:O:276:GLU:HG3	1.96	0.64
1:R:40:HIS:CD2	1:R:43:VAL:H	2.16	0.63
1:Q:185:LEU:HD12	1:Q:257:CYS:SG	2.38	0.63
1:V:204:ALA:HB1	1:X:290:ARG:NH2	2.14	0.63
1:X:262:PHE:HA	1:X:274:ILE:HG22	1.80	0.62
1:O:203:THR:OG1	1:P:269:MET:HE1	2.00	0.62
1:P:34:ILE:HB	1:P:67:LEU:HD11	1.81	0.62
1:Q:40:HIS:CD2	1:Q:43:VAL:H	2.17	0.62
1:T:262:PHE:HA	1:T:274:ILE:HG22	1.82	0.62
1:P:284:LYS:C	1:P:284:LYS:HD2	2.26	0.61
1:R:47:MET:SD	1:T:170:ALA:HB3	2.41	0.60
1:P:202:THR:HG23	1:P:203:THR:N	2.15	0.60
1:U:198:TYR:N	1:U:198:TYR:HD2	1.99	0.60
1:Y:284:LYS:HD2	1:Y:284:LYS:C	2.27	0.60
1:Q:198:TYR:HD2	1:Q:198:TYR:N	2.00	0.59
1:Z:198:TYR:N	1:Z:198:TYR:HD2	2.00	0.59
1:U:217:CYS:HA	1:U:254:ARG:HA	1.85	0.59
1:S:198:TYR:N	1:S:198:TYR:HD2	2.01	0.59
1:U:198:TYR:N	1:U:198:TYR:CD2	2.70	0.59
1:X:202:THR:HG23	1:X:203:THR:H	1.67	0.59
1:R:287:ILE:HG23	1:R:288:ASP:OD2	2.03	0.58
1:P:88:HIS:CE1	1:P:92:ASN:HD21	2.21	0.58
1:U:201:VAL:HG13	1:U:202:THR:H	1.67	0.58
1:W:202:THR:HG23	1:W:203:THR:H	1.67	0.58
1:R:198:TYR:HD2	1:R:198:TYR:N	2.01	0.58
1:S:202:THR:OG1	1:T:269:MET:HE3	2.04	0.58
1:T:21:PHE:CZ	1:T:94:LEU:HD22	2.39	0.58
1:W:47:MET:SD	1:Y:170:ALA:HB3	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:305:MET:HA	1:S:335:ARG:HH21	1.69	0.57
1:X:199:SER:HB3	1:X:201:VAL:HB	1.85	0.57
1:Y:201:VAL:HG13	1:Y:202:THR:H	1.67	0.57
1:Z:198:TYR:N	1:Z:198:TYR:CD2	2.72	0.57
1:S:73:HIC:HD2	1:S:73:HIC:O	2.04	0.57
1:S:198:TYR:N	1:S:198:TYR:CD2	2.72	0.57
1:T:202:THR:OG1	1:U:269:MET:HE3	2.05	0.57
1:P:40:HIS:CD2	1:P:43:VAL:H	2.22	0.57
1:R:198:TYR:N	1:R:198:TYR:CD2	2.73	0.57
1:V:165:ILE:HG12	1:V:170:ALA:HB2	1.85	0.57
1:Z:21:PHE:CZ	1:Z:94:LEU:HD22	2.39	0.57
1:S:103:THR:HG21	1:S:123:MET:HE1	1.87	0.57
1:Y:198:TYR:HD2	1:Y:198:TYR:N	2.01	0.57
1:Q:198:TYR:N	1:Q:198:TYR:CD2	2.72	0.56
1:Q:275:HIS:CD2	1:Q:276:GLU:H	2.23	0.56
1:O:38:PRO:HB3	1:O:65:LEU:HD23	1.87	0.56
1:S:35:VAL:HG12	1:S:36:GLY:H	1.69	0.56
1:W:203:THR:OG1	1:X:269:MET:HE1	2.04	0.56
1:V:204:ALA:HB1	1:X:290:ARG:HH21	1.70	0.56
1:S:203:THR:OG1	1:T:269:MET:HE1	2.05	0.56
1:R:261:LEU:HD11	1:R:303:THR:CG2	2.36	0.56
1:Y:298:VAL:HG12	1:Y:330:ILE:HB	1.88	0.56
1:T:198:TYR:HD2	1:T:198:TYR:N	2.02	0.56
1:U:159:VAL:HG12	1:U:179:ASP:HA	1.88	0.56
1:Y:198:TYR:N	1:Y:198:TYR:CD2	2.74	0.56
1:O:198:TYR:HD2	1:O:198:TYR:N	2.04	0.56
1:P:246:GLN:HE21	1:P:246:GLN:HA	1.71	0.56
1:V:198:TYR:HD2	1:V:198:TYR:N	2.02	0.56
1:O:73:HIC:HD2	1:O:73:HIC:O	2.06	0.55
1:V:172:PRO:HG2	1:V:173:HIS:CE1	2.41	0.55
1:T:198:TYR:N	1:T:198:TYR:CD2	2.74	0.55
1:P:202:THR:HG21	3:R:801:PO4:O2	2.07	0.55
1:Q:202:THR:OG1	1:R:269:MET:HE3	2.07	0.55
1:X:47:MET:SD	1:Z:170:ALA:HB3	2.46	0.55
1:Z:185:LEU:HD22	1:Z:185:LEU:H	1.72	0.55
1:O:153:LEU:CD2	1:O:313:MET:HE2	2.37	0.55
1:P:198:TYR:N	1:P:198:TYR:HD2	2.04	0.55
1:U:193:LEU:HD23	1:U:196:ARG:HE	1.72	0.55
1:Q:269:MET:HE3	1:Q:271:SER:HB3	1.89	0.54
1:S:193:LEU:HD22	1:S:196:ARG:HH11	1.72	0.54
1:O:262:PHE:CZ	1:O:312:ARG:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:201:VAL:HG21	1:R:179:ASP:HB2	1.88	0.54
1:Q:203:THR:OG1	1:R:269:MET:HE1	2.08	0.54
1:S:40:HIS:CD2	1:S:43:VAL:H	2.25	0.54
1:V:198:TYR:N	1:V:198:TYR:CD2	2.76	0.54
1:W:217:CYS:HA	1:W:254:ARG:HA	1.90	0.54
1:T:204:ALA:HB1	1:V:290:ARG:CZ	2.38	0.54
1:S:203:THR:HG21	1:U:173:HIS:CE1	2.42	0.54
1:T:139:VAL:HG22	1:T:165:ILE:HD13	1.90	0.54
1:Y:202:THR:HG23	1:Y:203:THR:N	2.22	0.54
1:P:198:TYR:N	1:P:198:TYR:CD2	2.76	0.54
1:S:262:PHE:HA	1:S:274:ILE:HG22	1.89	0.53
1:T:204:ALA:HB2	1:V:285:CYS:O	2.08	0.53
1:X:185:LEU:HD21	1:X:261:LEU:HD23	1.89	0.53
1:O:35:VAL:HG12	1:O:36:GLY:H	1.74	0.53
1:T:140:LEU:HB3	1:T:342:GLY:HA3	1.90	0.53
1:O:201:VAL:HG13	1:O:202:THR:N	2.24	0.53
1:X:199:SER:OG	1:Y:73:HIC:HD2	2.08	0.53
1:Y:34:ILE:HG23	1:Y:69:TYR:CD2	2.43	0.53
1:W:282:ILE:HD12	1:W:294:TYR:CD1	2.44	0.53
1:P:275:HIS:CD2	1:P:276:GLU:H	2.27	0.53
1:X:203:THR:OG1	1:Y:269:MET:HE1	2.09	0.53
1:W:153:LEU:HB2	1:W:299:MET:HG2	1.89	0.53
1:X:198:TYR:HD2	1:X:198:TYR:N	2.04	0.53
1:Q:151:ILE:HG23	1:Q:297:ASN:HA	1.91	0.52
1:V:252:ASN:C	1:V:254:ARG:H	2.16	0.52
1:Q:185:LEU:HD21	1:Q:261:LEU:HD23	1.90	0.52
1:S:108:ALA:HB1	1:S:109:PRO:HD2	1.92	0.52
1:U:265:SER:HA	1:U:269:MET:H	1.73	0.52
1:R:202:THR:OG1	1:S:269:MET:HE3	2.09	0.52
1:T:73:HIC:HD2	1:T:73:HIC:O	2.10	0.52
1:U:160:THR:HG21	1:U:274:ILE:HD12	1.92	0.52
1:Y:199:SER:HB2	1:Y:201:VAL:HB	1.91	0.52
1:O:201:VAL:CG1	1:O:202:THR:H	2.21	0.52
1:V:219:VAL:HG22	1:V:258:PRO:HB2	1.91	0.52
1:Y:132:MET:SD	1:Y:357:ILE:HD12	2.50	0.52
1:Z:35:VAL:HG12	1:Z:36:GLY:H	1.75	0.52
1:Q:208:ILE:HD12	1:Q:211:ASP:HB3	1.91	0.52
1:P:47:MET:SD	1:R:170:ALA:HB3	2.50	0.52
1:P:53:TYR:HD1	1:P:65:LEU:HD11	1.75	0.52
1:V:275:HIS:CG	1:V:276:GLU:H	2.28	0.52
1:Q:204:ALA:HB1	1:S:290:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:198:TYR:N	1:X:198:TYR:CD2	2.78	0.51
1:V:142:LEU:HD13	1:V:152:VAL:HG23	1.92	0.51
1:T:47:MET:HE3	1:V:170:ALA:HB3	1.91	0.51
1:T:109:PRO:HG3	1:T:163:VAL:HG21	1.92	0.51
1:Y:76:ILE:HD12	1:Y:76:ILE:H	1.75	0.51
1:S:47:MET:SD	1:U:170:ALA:HB3	2.50	0.51
1:O:198:TYR:N	1:O:198:TYR:CD2	2.77	0.51
1:V:199:SER:OG	1:W:73:HIC:HD2	2.11	0.51
1:U:306:TYR:CE2	2:U:800:ADP:H2	2.28	0.51
1:Z:11:ASP:HB3	1:Z:18:LYS:HB2	1.91	0.51
1:Q:166:TYR:CE1	1:Q:289:ILE:HG22	2.46	0.51
1:Q:202:THR:HG23	1:Q:203:THR:N	2.23	0.51
1:W:198:TYR:HD2	1:W:198:TYR:N	2.06	0.51
1:Y:120:THR:HG23	1:Y:132:MET:SD	2.51	0.51
1:Y:217:CYS:HA	1:Y:254:ARG:HA	1.93	0.50
1:O:40:HIS:NE2	1:O:43:VAL:HG23	2.26	0.50
1:P:43:VAL:HG22	1:R:110:LEU:HD22	1.93	0.50
1:Z:201:VAL:HG13	1:Z:202:THR:H	1.75	0.50
1:O:43:VAL:HG22	1:Q:110:LEU:CD1	2.41	0.50
1:T:20:GLY:HA2	1:T:94:LEU:HD21	1.93	0.50
1:V:203:THR:HG21	1:X:173:HIS:CE1	2.47	0.50
1:W:40:HIS:CD2	1:W:43:VAL:H	2.29	0.50
1:Q:178:LEU:HD11	1:Q:180:LEU:HG	1.93	0.50
1:W:262:PHE:HA	1:W:274:ILE:HG22	1.94	0.49
1:Q:199:SER:OG	1:R:73:HIC:HD2	2.12	0.49
1:W:35:VAL:HG11	1:W:84:LYS:HD2	1.94	0.49
1:W:198:TYR:N	1:W:198:TYR:CD2	2.80	0.49
1:O:40:HIS:CD2	1:O:43:VAL:H	2.31	0.49
1:T:199:SER:OG	1:U:73:HIC:HD2	2.12	0.49
1:P:76:ILE:H	1:P:76:ILE:HD12	1.76	0.49
1:S:165:ILE:HG12	1:S:170:ALA:HB2	1.94	0.49
1:W:202:THR:HG23	1:W:203:THR:N	2.27	0.49
1:W:282:ILE:HB	1:W:294:TYR:CE1	2.48	0.49
1:O:123:MET:HG3	1:O:132:MET:HE3	1.95	0.49
1:U:287:ILE:HA	1:U:290:ARG:HD2	1.94	0.49
1:V:64:ILE:HG22	1:X:172:PRO:HG3	1.93	0.49
1:W:284:LYS:C	1:W:284:LYS:HD2	2.36	0.49
1:Z:217:CYS:HA	1:Z:254:ARG:HA	1.95	0.49
1:Z:262:PHE:HA	1:Z:274:ILE:HG22	1.95	0.49
1:O:204:ALA:HB1	1:Q:290:ARG:NH2	2.27	0.48
1:T:152:VAL:HG12	1:T:152:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:193:LEU:CD2	1:U:196:ARG:HE	2.27	0.48
1:O:204:ALA:HB1	1:Q:290:ARG:CZ	2.44	0.48
1:W:208:ILE:HG12	1:W:242:LEU:HD22	1.94	0.48
1:W:321:ALA:HB1	1:W:322:PRO:HD2	1.93	0.48
1:R:82:MET:HE2	1:R:86:TRP:CE2	2.49	0.48
1:P:201:VAL:HG13	1:P:202:THR:H	1.78	0.48
1:Y:193:LEU:HD21	1:Y:253:GLU:HG2	1.94	0.48
1:X:64:ILE:HG22	1:Z:172:PRO:HG3	1.95	0.48
1:Q:43:VAL:HG11	1:S:172:PRO:HA	1.96	0.48
1:Q:217:CYS:HA	1:Q:254:ARG:HA	1.95	0.48
1:S:217:CYS:HA	1:S:254:ARG:HA	1.95	0.48
1:U:260:THR:HG23	1:U:264:PRO:HA	1.95	0.48
1:X:40:HIS:CD2	1:X:43:VAL:H	2.31	0.48
1:V:282:ILE:HA	1:V:285:CYS:HB2	1.94	0.48
1:T:246:GLN:HA	1:T:246:GLN:HE21	1.78	0.48
1:P:217:CYS:HA	1:P:254:ARG:HA	1.96	0.47
1:U:191:LYS:HD2	1:V:175:ILE:HD13	1.95	0.47
1:T:40:HIS:CD2	1:T:43:VAL:H	2.32	0.47
1:O:199:SER:OG	1:P:73:HIC:HD2	2.14	0.47
1:Q:54:VAL:HG11	1:Q:88:HIS:CG	2.49	0.47
1:R:151:ILE:HG23	1:R:297:ASN:HA	1.96	0.47
1:S:201:VAL:HG13	1:S:202:THR:N	2.26	0.47
1:U:284:LYS:HD2	1:U:284:LYS:C	2.40	0.47
1:P:64:ILE:HG22	1:R:172:PRO:HG3	1.97	0.47
1:P:202:THR:O	1:Q:269:MET:HE1	2.15	0.47
1:Q:208:ILE:HG12	1:Q:242:LEU:HD13	1.95	0.47
1:O:237:GLU:HA	1:O:251:GLY:HA2	1.97	0.47
1:V:199:SER:OG	1:W:73:HIC:CD2	2.63	0.47
1:X:40:HIS:CG	1:X:41:GLN:H	2.32	0.47
1:Z:202:THR:HG23	1:Z:203:THR:H	1.79	0.47
1:O:202:THR:HG1	1:P:269:MET:HE3	1.80	0.47
1:Q:43:VAL:HG22	1:S:110:LEU:CD2	2.45	0.46
1:Q:152:VAL:HG22	1:Q:298:VAL:HG23	1.95	0.46
1:W:193:LEU:HD11	1:W:253:GLU:HG2	1.96	0.46
1:Q:284:LYS:HD2	1:Q:284:LYS:C	2.40	0.46
1:S:109:PRO:CD	1:S:161:HIS:CD2	2.99	0.46
1:V:8:LEU:HB2	1:V:103:THR:HG23	1.97	0.46
1:S:208:ILE:HD12	1:S:211:ASP:HB3	1.98	0.46
1:X:137:GLN:OE1	1:X:161:HIS:CE1	2.68	0.46
1:R:265:SER:HA	1:R:269:MET:H	1.80	0.46
1:O:199:SER:HB3	1:O:201:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:202:THR:OG1	1:P:269:MET:HE3	2.15	0.46
1:T:203:THR:OG1	1:U:269:MET:HE1	2.16	0.46
1:V:109:PRO:HG3	1:V:163:VAL:HG21	1.97	0.46
1:X:202:THR:HG23	1:X:203:THR:N	2.29	0.46
1:O:212:ILE:HG12	1:O:250:ILE:HD13	1.97	0.46
1:Q:197:GLY:C	1:Q:198:TYR:CD2	2.94	0.46
1:R:43:VAL:HG11	1:T:172:PRO:HA	1.98	0.46
1:U:165:ILE:HG12	1:U:170:ALA:HB2	1.98	0.46
1:V:208:ILE:HD12	1:V:211:ASP:HB3	1.97	0.46
1:O:43:VAL:HG22	1:Q:110:LEU:HD22	1.97	0.46
1:T:298:VAL:O	1:T:299:MET:HG3	2.16	0.46
1:Z:151:ILE:CD1	1:Z:282:ILE:HD11	2.45	0.46
1:P:67:LEU:HD12	1:P:67:LEU:HA	1.72	0.46
1:U:197:GLY:C	1:U:198:TYR:CD2	2.94	0.46
1:Y:202:THR:HG22	3:Y:801:PO4:O2	2.16	0.46
1:P:203:THR:HG21	1:R:173:HIS:CE1	2.51	0.46
1:Q:161:HIS:HB3	1:Q:163:VAL:HG23	1.97	0.46
1:P:201:VAL:HG13	1:P:202:THR:HG22	1.97	0.45
1:P:208:ILE:HD12	1:P:211:ASP:HB3	1.98	0.45
1:R:202:THR:HG23	1:R:203:THR:H	1.80	0.45
1:W:27:PRO:HG2	1:W:30:VAL:HG11	1.98	0.45
1:X:185:LEU:HD21	1:X:261:LEU:CD2	2.46	0.45
1:Q:40:HIS:CD2	1:Q:43:VAL:HG23	2.52	0.45
1:Q:109:PRO:HG3	1:Q:163:VAL:HG21	1.98	0.45
1:V:39:ARG:HH22	1:W:263:GLN:HG2	1.81	0.45
1:Q:201:VAL:HG13	1:Q:202:THR:H	1.80	0.45
1:U:98:PRO:HB2	1:U:129:VAL:HG22	1.99	0.45
1:P:216:LEU:HG	1:P:250:ILE:HG21	1.98	0.45
1:S:219:VAL:HG21	1:S:309:ILE:HB	1.99	0.45
1:U:193:LEU:HD21	1:U:253:GLU:HG2	1.99	0.45
1:X:73:HIC:CD2	1:X:73:HIC:O	2.64	0.45
1:R:284:LYS:C	1:R:284:LYS:HD2	2.41	0.45
1:T:47:MET:CE	1:V:170:ALA:HB3	2.47	0.45
1:X:275:HIS:CD2	1:X:275:HIS:H	2.34	0.45
1:Y:27:PRO:HA	1:Y:340:TRP:CH2	2.52	0.45
1:Q:199:SER:OG	1:R:73:HIC:CD2	2.65	0.45
1:T:73:HIC:O	1:T:73:HIC:CD2	2.65	0.45
1:W:35:VAL:HG11	1:W:84:LYS:CD	2.46	0.45
1:P:153:LEU:HB2	1:P:299:MET:HG2	1.99	0.45
1:S:292:ASP:HA	1:S:295:ALA:HB3	1.99	0.45
1:T:184:ASP:OD2	1:T:185:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:212:ILE:HG12	1:R:250:ILE:HD13	1.99	0.44
1:V:26:ALA:HB1	1:V:27:PRO:HD2	1.98	0.44
1:W:208:ILE:O	1:W:212:ILE:HG22	2.17	0.44
1:Y:193:LEU:HD22	1:Y:196:ARG:HE	1.81	0.44
1:Z:151:ILE:HA	1:Z:164:PRO:HA	1.99	0.44
1:O:284:LYS:HD2	1:O:284:LYS:C	2.42	0.44
1:R:76:ILE:HD12	1:R:76:ILE:H	1.83	0.44
1:V:48:GLY:O	1:V:49:GLN:HB2	2.18	0.44
1:V:193:LEU:HD23	1:V:196:ARG:HE	1.83	0.44
1:W:43:VAL:HG22	1:Y:110:LEU:HD22	1.99	0.44
1:Q:172:PRO:HG2	1:Q:173:HIS:CE1	2.53	0.44
1:Y:201:VAL:HG13	1:Y:202:THR:N	2.32	0.44
1:Q:49:GLN:HE21	1:Q:49:GLN:C	2.25	0.44
1:U:164:PRO:HB3	1:U:293:LEU:HD22	1.99	0.44
1:P:144:ALA:HB1	1:P:341:ILE:HG22	1.99	0.44
1:T:203:THR:HG21	1:V:173:HIS:CE1	2.53	0.44
1:U:199:SER:OG	1:V:73:HIC:HD2	2.18	0.44
1:W:35:VAL:HG21	1:W:84:LYS:HG3	2.00	0.44
1:W:43:VAL:HG22	1:Y:110:LEU:HD13	1.98	0.44
1:X:102:PRO:HB2	1:X:356:TRP:CZ2	2.53	0.44
1:X:259:GLU:CD	1:X:312:ARG:HH12	2.25	0.44
1:Q:133:TYR:CE1	1:Q:374:CYS:HA	2.52	0.44
1:X:176:MET:HG2	1:X:277:THR:HG23	2.00	0.44
1:O:204:ALA:HB2	1:Q:285:CYS:H	1.83	0.44
1:O:326:LYS:HD3	1:O:327:ILE:H	1.82	0.44
1:R:258:PRO:HB3	1:R:306:TYR:CE1	2.52	0.44
1:X:321:ALA:HB1	1:X:322:PRO:HD2	1.99	0.44
1:O:150:GLY:HA2	1:O:296:ASN:HB3	2.00	0.43
1:T:254:ARG:NH1	3:T:803:PO4:O3	2.51	0.43
1:U:184:ASP:OD2	1:U:185:LEU:HD22	2.18	0.43
1:P:129:VAL:HG11	1:P:132:MET:HB3	2.00	0.43
1:P:199:SER:OG	1:Q:73:HIC:HD2	2.19	0.43
1:R:165:ILE:HA	1:R:170:ALA:HA	2.00	0.43
1:V:202:THR:OG1	1:W:269:MET:HE3	2.18	0.43
1:W:184:ASP:O	1:W:188:TYR:HB3	2.18	0.43
1:P:142:LEU:HD13	1:P:152:VAL:HG23	2.00	0.43
1:P:178:LEU:HG	1:P:180:LEU:H	1.83	0.43
1:W:9:VAL:HG13	1:W:104:LEU:HD23	2.01	0.43
1:X:202:THR:OG1	1:Y:269:MET:HE3	2.18	0.43
1:R:48:GLY:HA2	1:T:169:TYR:CD2	2.53	0.43
1:T:47:MET:SD	1:V:170:ALA:HB3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:108:ALA:HB1	1:V:109:PRO:HD2	2.00	0.43
1:W:73:HIC:HD2	1:W:73:HIC:O	2.18	0.43
1:R:173:HIS:CD2	1:R:173:HIS:N	2.86	0.43
1:S:260:THR:HG21	1:S:267:ILE:HG13	1.99	0.43
1:T:49:GLN:HG3	1:V:375:PHE:CE2	2.54	0.43
1:U:73:HIC:HD2	1:U:73:HIC:O	2.19	0.43
1:V:73:HIC:CD2	1:V:73:HIC:O	2.67	0.43
1:Y:165:ILE:HG12	1:Y:170:ALA:HB2	2.00	0.43
1:Y:193:LEU:CD2	1:Y:196:ARG:HE	2.32	0.43
1:S:73:HIC:O	1:S:73:HIC:CD2	2.67	0.43
1:T:43:VAL:HG11	1:V:172:PRO:HA	2.01	0.43
1:W:124:PHE:CE1	1:W:359:LYS:HG2	2.53	0.43
1:Y:151:ILE:HG23	1:Y:297:ASN:HA	1.99	0.43
1:Y:202:THR:HG22	3:Y:801:PO4:P	2.59	0.43
1:R:73:HIC:HD2	1:R:73:HIC:O	2.17	0.43
1:U:223:PHE:CE2	1:U:266:PHE:CE2	3.07	0.43
1:X:8:LEU:HB2	1:X:103:THR:HG23	2.00	0.43
1:Q:199:SER:HB3	1:Q:201:VAL:HB	2.00	0.43
1:Q:269:MET:HG3	1:Q:270:GLU:H	1.83	0.43
1:U:203:THR:HG21	1:W:173:HIS:CE1	2.54	0.43
1:V:149:THR:HG23	1:V:166:TYR:HA	2.01	0.43
1:X:48:GLY:HA2	1:Z:169:TYR:CD2	2.53	0.43
1:U:202:THR:OG1	1:V:269:MET:HE3	2.19	0.42
1:W:260:THR:HG23	1:W:264:PRO:HA	2.00	0.42
1:U:9:VAL:HG21	1:U:344:SER:HA	2.01	0.42
1:U:203:THR:HG22	1:U:203:THR:O	2.19	0.42
1:Y:253:GLU:O	1:Y:257:CYS:HB3	2.19	0.42
1:X:63:GLY:O	1:Z:173:HIS:CE1	2.72	0.42
1:X:259:GLU:HG3	1:X:266:PHE:CD1	2.55	0.42
1:Y:203:THR:OG1	1:Z:269:MET:HE1	2.19	0.42
1:Q:174:ALA:HB2	1:Q:284:LYS:O	2.19	0.42
1:Q:188:TYR:CD1	1:Q:188:TYR:C	2.98	0.42
1:T:300:SER:HA	1:T:335:ARG:HB2	2.00	0.42
1:X:73:HIC:O	1:X:73:HIC:HD2	2.19	0.42
1:X:76:ILE:HD12	1:X:76:ILE:H	1.84	0.42
1:Q:252:ASN:HA	1:Q:255:PHE:CZ	2.54	0.42
1:R:17:VAL:HB	1:R:31:PHE:CD1	2.54	0.42
1:S:151:ILE:HG23	1:S:297:ASN:HA	2.02	0.42
1:W:153:LEU:HG	1:W:162:ASN:HD22	1.85	0.42
1:T:288:ASP:O	1:T:289:ILE:HG23	2.19	0.42
1:U:292:ASP:HA	1:U:295:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:197:GLY:C	1:X:198:TYR:HD2	2.28	0.42
1:Q:73:HIC:HD2	1:Q:73:HIC:O	2.20	0.42
1:Q:73:HIC:CD2	1:Q:73:HIC:O	2.68	0.42
1:R:189:LEU:HD11	1:R:253:GLU:HB3	2.02	0.42
1:S:9:VAL:HG21	1:S:344:SER:HA	2.01	0.42
1:U:76:ILE:HG12	1:U:82:MET:HE2	2.02	0.42
1:V:199:SER:CB	1:V:201:VAL:HB	2.50	0.42
1:O:35:VAL:HG12	1:O:36:GLY:N	2.34	0.42
1:O:76:ILE:HG12	1:O:82:MET:HE2	2.00	0.42
1:Q:173:HIS:N	1:Q:173:HIS:CD2	2.87	0.42
1:R:49:GLN:HG2	1:T:375:PHE:CE2	2.55	0.42
1:R:260:THR:HG22	1:R:264:PRO:HA	2.02	0.42
1:T:165:ILE:HA	1:T:170:ALA:HA	2.02	0.42
1:U:199:SER:CB	1:U:201:VAL:HB	2.50	0.42
1:V:120:THR:HA	1:V:132:MET:HE3	2.01	0.42
1:T:171:LEU:HA	1:T:172:PRO:HD3	1.95	0.41
1:V:202:THR:HG23	1:V:203:THR:N	2.30	0.41
1:W:197:GLY:C	1:W:198:TYR:HD2	2.27	0.41
1:Y:202:THR:CG2	1:Y:203:THR:N	2.81	0.41
1:Y:259:GLU:HG3	1:Y:266:PHE:CD1	2.55	0.41
1:P:203:THR:HA	1:Q:269:MET:SD	2.61	0.41
1:Q:191:LYS:HD2	1:R:175:ILE:HG21	2.02	0.41
1:T:201:VAL:HG13	1:T:202:THR:H	1.85	0.41
1:Z:165:ILE:HA	1:Z:170:ALA:HA	2.01	0.41
1:Q:292:ASP:HA	1:Q:295:ALA:HB3	2.02	0.41
1:T:139:VAL:HG22	1:T:165:ILE:CD1	2.50	0.41
1:T:178:LEU:HG	1:T:180:LEU:H	1.85	0.41
1:X:199:SER:OG	1:Y:73:HIC:CD2	2.68	0.41
1:Y:155:SER:HB3	1:Y:304:THR:HG23	2.02	0.41
1:Z:268:GLY:O	1:Z:269:MET:HE2	2.20	0.41
1:O:73:HIC:O	1:O:73:HIC:CD2	2.68	0.41
1:O:190:MET:SD	1:O:190:MET:C	3.03	0.41
1:O:214:GLU:HG3	2:O:800:ADP:C6	2.56	0.41
1:O:283:MET:HE3	1:O:283:MET:HB3	1.98	0.41
1:R:111:ASN:HB3	1:R:116:ARG:HG3	2.03	0.41
1:Q:283:MET:HE3	1:Q:283:MET:HB3	1.92	0.41
1:S:109:PRO:HD3	1:S:161:HIS:CD2	2.55	0.41
1:U:163:VAL:HA	1:U:164:PRO:HD2	1.86	0.41
1:Z:151:ILE:O	1:Z:151:ILE:HG12	2.20	0.41
1:Z:185:LEU:H	1:Z:185:LEU:CD2	2.34	0.41
1:Q:185:LEU:HD11	1:Q:261:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:142:LEU:HD22	1:V:165:ILE:HD12	2.01	0.41
1:W:201:VAL:HG13	1:W:202:THR:N	2.27	0.41
1:X:193:LEU:HD21	1:X:253:GLU:HG2	2.02	0.41
1:Z:291:LYS:HB2	1:Z:292:ASP:H	1.64	0.41
1:O:153:LEU:HD22	1:O:313:MET:HE2	2.02	0.41
1:P:76:ILE:H	1:P:76:ILE:CD1	2.33	0.41
1:Q:291:LYS:HB2	1:Q:292:ASP:H	1.67	0.41
1:T:155:SER:HB3	1:T:304:THR:HG23	2.03	0.41
1:V:62:ARG:HH21	1:W:270:GLU:CD	2.28	0.41
1:P:302:GLY:HA2	1:P:336:LYS:HG3	2.02	0.41
1:R:199:SER:HB3	1:R:201:VAL:CG2	2.51	0.41
1:S:119:MET:HA	1:S:122:ILE:HG22	2.03	0.41
1:S:172:PRO:HG2	1:S:173:HIS:CG	2.56	0.41
1:T:256:ARG:HA	1:T:259:GLU:HB3	2.01	0.41
1:V:171:LEU:HG	1:V:285:CYS:SG	2.61	0.41
1:X:43:VAL:HG22	1:Z:110:LEU:HD22	2.03	0.41
1:T:161:HIS:HB3	1:T:163:VAL:HG23	2.01	0.41
1:T:165:ILE:HG12	1:T:170:ALA:HB2	2.03	0.41
1:V:43:VAL:HG11	1:X:172:PRO:HA	2.03	0.41
1:V:176:MET:HG3	1:V:277:THR:HG21	2.03	0.41
1:X:140:LEU:HD22	1:X:346:LEU:HD22	2.03	0.41
1:Z:306:TYR:HA	1:Z:307:PRO:HD2	1.97	0.41
1:O:37:ARG:HG3	1:O:37:ARG:HH11	1.86	0.41
1:O:258:PRO:HB3	1:O:306:TYR:CE1	2.56	0.41
1:S:150:GLY:HA2	1:S:296:ASN:HB3	2.03	0.41
1:U:203:THR:OG1	1:V:269:MET:HE1	2.22	0.41
1:Y:265:SER:HA	1:Y:269:MET:H	1.86	0.41
1:S:64:ILE:HG22	1:U:172:PRO:HG3	2.02	0.40
1:W:199:SER:OG	1:X:73:HIC:HD2	2.21	0.40
1:Q:43:VAL:CG1	1:S:172:PRO:HA	2.51	0.40
1:R:201:VAL:CG1	1:R:202:THR:HG22	2.47	0.40
1:T:62:ARG:HH21	1:U:270:GLU:HG3	1.87	0.40
1:U:138:ALA:HB1	1:U:165:ILE:HD11	2.02	0.40
1:V:73:HIC:HD2	1:V:73:HIC:O	2.21	0.40
1:V:197:GLY:C	1:V:198:TYR:HD2	2.29	0.40
1:W:70:PRO:HG3	1:W:85:ILE:HD12	2.02	0.40
1:W:292:ASP:HA	1:W:295:ALA:HB3	2.02	0.40
1:Q:142:LEU:HD22	1:Q:165:ILE:HD12	2.03	0.40
1:S:260:THR:HG23	1:S:264:PRO:HA	2.02	0.40
1:V:205:GLU:HG3	1:X:290:ARG:HH22	1.86	0.40
1:W:275:HIS:CD2	1:W:276:GLU:H	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:313:MET:HB2	1:W:329:ILE:HG21	2.04	0.40
1:X:224:GLU:HA	1:X:227:MET:HB2	2.04	0.40
1:Z:302:GLY:HA2	1:Z:336:LYS:HG3	2.04	0.40
1:P:105:LEU:HD23	1:P:105:LEU:HA	1.97	0.40
1:P:254:ARG:NH1	3:P:803:PO4:O2	2.51	0.40
1:R:199:SER:OG	1:S:73:HIC:CD2	2.70	0.40
1:S:180:LEU:HD11	1:S:264:PRO:HG3	2.03	0.40
1:W:102:PRO:HB2	1:W:356:TRP:CZ2	2.57	0.40
1:Y:326:LYS:HD3	1:Y:327:ILE:H	1.85	0.40
1:P:152:VAL:HG22	1:P:298:VAL:HG23	2.04	0.40
1:S:14:SER:HA	1:S:71:ILE:HG23	2.04	0.40
1:S:35:VAL:HG13	1:S:54:VAL:HG22	2.04	0.40
1:S:190:MET:SD	1:S:190:MET:C	3.05	0.40
1:V:98:PRO:HB2	1:V:129:VAL:HG22	2.03	0.40
1:V:242:LEU:HB3	1:V:243:PRO:HD2	2.03	0.40
1:W:240:TYR:CG	1:W:241:GLU:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	O	373/376 (99%)	283 (76%)	66 (18%)	24 (6%)	1	12
1	P	373/376 (99%)	298 (80%)	54 (14%)	21 (6%)	1	14
1	Q	373/376 (99%)	281 (75%)	66 (18%)	26 (7%)	1	11
1	R	373/376 (99%)	295 (79%)	52 (14%)	26 (7%)	1	11
1	S	373/376 (99%)	286 (77%)	67 (18%)	20 (5%)	1	14
1	T	373/376 (99%)	275 (74%)	73 (20%)	25 (7%)	1	11
1	U	373/376 (99%)	284 (76%)	66 (18%)	23 (6%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	373/376 (99%)	293 (79%)	56 (15%)	24 (6%)	1	12
1	W	373/376 (99%)	288 (77%)	60 (16%)	25 (7%)	1	11
1	X	373/376 (99%)	292 (78%)	63 (17%)	18 (5%)	2	16
1	Y	373/376 (99%)	292 (78%)	64 (17%)	17 (5%)	2	16
1	Z	373/376 (99%)	289 (78%)	59 (16%)	25 (7%)	1	11
All	All	4476/4512 (99%)	3456 (77%)	746 (17%)	274 (6%)	2	12

All (274) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	42	GLY
1	O	51	ASP
1	O	129	VAL
1	O	254	ARG
1	P	42	GLY
1	P	55	GLY
1	P	129	VAL
1	P	185	LEU
1	Q	6	THR
1	Q	49	GLN
1	Q	51	ASP
1	Q	52	SER
1	Q	70	PRO
1	Q	129	VAL
1	Q	185	LEU
1	Q	254	ARG
1	Q	271	SER
1	Q	272	ALA
1	Q	291	LYS
1	R	51	ASP
1	R	60	SER
1	R	125	GLU
1	R	167	GLU
1	R	291	LYS
1	S	49	GLN
1	S	51	ASP
1	S	55	GLY
1	S	125	GLU
1	S	129	VAL
1	S	291	LYS

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Mol	Chain	Res	Type
1	S	335	ARG
1	T	42	GLY
1	T	51	ASP
1	T	52	SER
1	T	70	PRO
1	T	214	GLU
1	U	55	GLY
1	U	129	VAL
1	U	203	THR
1	U	254	ARG
1	U	287	ILE
1	V	6	THR
1	V	49	GLN
1	V	52	SER
1	V	60	SER
1	V	113	LYS
1	V	125	GLU
1	V	129	VAL
1	W	49	GLN
1	W	51	ASP
1	W	202	THR
1	W	291	LYS
1	W	350	SER
1	X	49	GLN
1	X	51	ASP
1	X	52	SER
1	X	129	VAL
1	X	272	ALA
1	Y	42	GLY
1	Y	70	PRO
1	Y	125	GLU
1	Y	203	THR
1	Z	6	THR
1	Z	51	ASP
1	Z	70	PRO
1	Z	129	VAL
1	Z	291	LYS
1	Z	297	ASN
1	O	55	GLY
1	O	125	GLU
1	O	185	LEU
1	O	199	SER

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Mol	Chain	Res	Type
1	O	247	VAL
1	O	268	GLY
1	O	271	SER
1	P	5	THR
1	P	45	VAL
1	P	49	GLN
1	P	125	GLU
1	P	251	GLY
1	Q	42	GLY
1	R	42	GLY
1	R	49	GLN
1	R	55	GLY
1	R	95	ARG
1	R	185	LEU
1	S	42	GLY
1	S	173	HIS
1	S	185	LEU
1	S	251	GLY
1	S	268	GLY
1	T	55	GLY
1	T	56	ASP
1	T	125	GLU
1	T	272	ALA
1	U	42	GLY
1	U	51	ASP
1	U	56	ASP
1	U	70	PRO
1	U	95	ARG
1	U	125	GLU
1	U	251	GLY
1	U	279	TYR
1	V	42	GLY
1	V	51	ASP
1	V	55	GLY
1	V	173	HIS
1	V	268	GLY
1	V	291	LYS
1	W	55	GLY
1	W	125	GLU
1	W	185	LEU
1	W	199	SER
1	W	335	ARG

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Mol	Chain	Res	Type
1	X	42	GLY
1	X	55	GLY
1	X	70	PRO
1	X	251	GLY
1	Y	51	ASP
1	Y	55	GLY
1	Y	185	LEU
1	Y	201	VAL
1	Y	251	GLY
1	Y	268	GLY
1	Y	291	LYS
1	Z	49	GLN
1	Z	52	SER
1	Z	55	GLY
1	Z	125	GLU
1	Z	174	ALA
1	Z	201	VAL
1	Z	272	ALA
1	O	5	THR
1	O	56	ASP
1	O	62	ARG
1	O	70	PRO
1	P	70	PRO
1	P	209	VAL
1	P	271	SER
1	Q	125	GLU
1	Q	181	ALA
1	Q	268	GLY
1	R	70	PRO
1	R	129	VAL
1	R	181	ALA
1	R	199	SER
1	R	251	GLY
1	R	271	SER
1	S	60	SER
1	S	181	ALA
1	S	271	SER
1	T	95	ARG
1	T	199	SER
1	T	213	LYS
1	T	347	ALA
1	U	173	HIS

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Mol	Chain	Res	Type
1	U	206	ARG
1	V	70	PRO
1	W	48	GLY
1	W	60	SER
1	W	128	ASN
1	W	129	VAL
1	W	254	ARG
1	W	271	SER
1	X	125	GLU
1	X	128	ASN
1	X	199	SER
1	Y	48	GLY
1	Y	129	VAL
1	Z	42	GLY
1	Z	306	TYR
1	O	6	THR
1	O	351	THR
1	P	6	THR
1	P	174	ALA
1	P	181	ALA
1	Q	41	GLN
1	Q	138	ALA
1	Q	206	ARG
1	Q	335	ARG
1	S	62	ARG
1	S	70	PRO
1	T	129	VAL
1	T	153	LEU
1	T	185	LEU
1	T	315	LYS
1	T	372	ARG
1	U	181	ALA
1	U	348	SER
1	V	185	LEU
1	V	230	ALA
1	V	271	SER
1	W	42	GLY
1	W	236	LEU
1	X	60	SER
1	X	185	LEU
1	X	268	GLY
1	Y	56	ASP

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Mol	Chain	Res	Type
1	Y	254	ARG
1	Z	110	LEU
1	Z	112	PRO
1	Z	173	HIS
1	Z	181	ALA
1	Z	185	LEU
1	O	49	GLN
1	O	110	LEU
1	O	201	VAL
1	O	306	TYR
1	P	113	LYS
1	P	155	SER
1	P	291	LYS
1	P	335	ARG
1	Q	5	THR
1	Q	56	ASP
1	Q	62	ARG
1	Q	332	PRO
1	R	56	ASP
1	R	110	LEU
1	R	254	ARG
1	T	110	LEU
1	T	298	VAL
1	U	197	GLY
1	U	268	GLY
1	U	271	SER
1	U	272	ALA
1	V	110	LEU
1	V	181	ALA
1	V	251	GLY
1	V	335	ARG
1	W	110	LEU
1	X	110	LEU
1	X	242	LEU
1	Y	350	SER
1	Z	315	LYS
1	Z	335	ARG
1	P	223	PHE
1	Q	197	GLY
1	Q	207	GLU
1	R	155	SER
1	R	197	GLY

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Mol	Chain	Res	Type
1	R	272	ALA
1	T	197	GLY
1	T	268	GLY
1	T	289	ILE
1	W	7	ALA
1	Y	110	LEU
1	O	45	VAL
1	R	247	VAL
1	R	268	GLY
1	U	46	GLY
1	V	63	GLY
1	V	158	GLY
1	W	98	PRO
1	W	251	GLY
1	X	98	PRO
1	Z	172	PRO
1	O	48	GLY
1	O	331	ALA
1	R	332	PRO
1	W	70	PRO
1	W	268	GLY
1	W	306	TYR
1	V	247	VAL
1	Z	251	GLY
1	P	242	LEU
1	Q	341	ILE
1	R	182	GLY
1	S	197	GLY
1	Z	197	GLY
1	S	201	VAL
1	S	243	PRO
1	T	45	VAL
1	T	109	PRO
1	U	48	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	O	317/317 (100%)	271 (86%)	46 (14%)	3	13
1	P	317/317 (100%)	267 (84%)	50 (16%)	2	12
1	Q	317/317 (100%)	265 (84%)	52 (16%)	2	10
1	R	317/317 (100%)	273 (86%)	44 (14%)	3	14
1	S	317/317 (100%)	259 (82%)	58 (18%)	2	9
1	T	317/317 (100%)	265 (84%)	52 (16%)	2	10
1	U	317/317 (100%)	264 (83%)	53 (17%)	2	10
1	V	317/317 (100%)	267 (84%)	50 (16%)	2	12
1	W	317/317 (100%)	277 (87%)	40 (13%)	4	16
1	X	317/317 (100%)	262 (83%)	55 (17%)	2	9
1	Y	317/317 (100%)	265 (84%)	52 (16%)	2	10
1	Z	317/317 (100%)	258 (81%)	59 (19%)	1	8
All	All	3804/3804 (100%)	3193 (84%)	611 (16%)	4	11

All (611) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	14	SER
1	O	17	VAL
1	O	24	ASP
1	O	28	ARG
1	O	30	VAL
1	O	37	ARG
1	O	43	VAL
1	O	49	GLN
1	O	57	GLU
1	O	64	ILE
1	O	83	GLU
1	O	95	ARG
1	O	111	ASN
1	O	115	ASN
1	O	116	ARG
1	O	118	LYS
1	O	122	ILE
1	O	129	VAL
1	O	140	LEU
1	O	145	SER
1	O	157	ASP
1	O	171	LEU

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Mol	Chain	Res	Type
1	O	173	HIS
1	O	184	ASP
1	O	188	TYR
1	O	190	MET
1	O	191	LYS
1	O	195	GLU
1	O	205	GLU
1	O	209	VAL
1	O	212	ILE
1	O	229	THR
1	O	234	SER
1	O	244	ASP
1	O	248	ILE
1	O	255	PHE
1	O	274	ILE
1	O	283	MET
1	O	313	MET
1	O	326	LYS
1	O	334	GLU
1	O	344	SER
1	O	351	THR
1	O	354	GLN
1	O	359	LYS
1	O	373	LYS
1	P	25	ASP
1	P	30	VAL
1	P	31	PHE
1	P	33	SER
1	P	37	ARG
1	P	43	VAL
1	P	57	GLU
1	P	59	GLN
1	P	61	LYS
1	P	64	ILE
1	P	83	GLU
1	P	85	ILE
1	P	89	THR
1	P	95	ARG
1	P	111	ASN
1	P	115	ASN
1	P	116	ARG
1	P	118	LYS

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Mol	Chain	Res	Type
1	P	122	ILE
1	P	134	VAL
1	P	140	LEU
1	P	145	SER
1	P	159	VAL
1	P	173	HIS
1	P	179	ASP
1	P	184	ASP
1	P	188	TYR
1	P	189	LEU
1	P	190	MET
1	P	191	LYS
1	P	195	GLU
1	P	208	ILE
1	P	224	GLU
1	P	246	GLN
1	P	248	ILE
1	P	255	PHE
1	P	270	GLU
1	P	276	GLU
1	P	281	SER
1	P	283	MET
1	P	288	ASP
1	P	289	ILE
1	P	305	MET
1	P	318	THR
1	P	326	LYS
1	P	327	ILE
1	P	352	PHE
1	P	354	GLN
1	P	372	ARG
1	P	373	LYS
1	Q	1	ASP
1	Q	2	GLU
1	Q	14	SER
1	Q	24	ASP
1	Q	25	ASP
1	Q	30	VAL
1	Q	31	PHE
1	Q	33	SER
1	Q	37	ARG
1	Q	43	VAL

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Mol	Chain	Res	Type
1	Q	49	GLN
1	Q	67	LEU
1	Q	70	PRO
1	Q	83	GLU
1	Q	89	THR
1	Q	95	ARG
1	Q	115	ASN
1	Q	116	ARG
1	Q	118	LYS
1	Q	119	MET
1	Q	120	THR
1	Q	122	ILE
1	Q	134	VAL
1	Q	139	VAL
1	Q	155	SER
1	Q	157	ASP
1	Q	159	VAL
1	Q	165	ILE
1	Q	173	HIS
1	Q	184	ASP
1	Q	186	THR
1	Q	188	TYR
1	Q	189	LEU
1	Q	190	MET
1	Q	191	LYS
1	Q	195	GLU
1	Q	198	TYR
1	Q	205	GLU
1	Q	221	LEU
1	Q	244	ASP
1	Q	247	VAL
1	Q	248	ILE
1	Q	255	PHE
1	Q	270	GLU
1	Q	283	MET
1	Q	284	LYS
1	Q	289	ILE
1	Q	305	MET
1	Q	326	LYS
1	Q	352	PHE
1	Q	354	GLN
1	Q	373	LYS

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Mol	Chain	Res	Type
1	R	24	ASP
1	R	28	ARG
1	R	30	VAL
1	R	31	PHE
1	R	34	ILE
1	R	41	GLN
1	R	49	GLN
1	R	64	ILE
1	R	92	ASN
1	R	95	ARG
1	R	111	ASN
1	R	116	ARG
1	R	118	LYS
1	R	119	MET
1	R	122	ILE
1	R	134	VAL
1	R	140	LEU
1	R	143	TYR
1	R	145	SER
1	R	151	ILE
1	R	167	GLU
1	R	173	HIS
1	R	184	ASP
1	R	188	TYR
1	R	190	MET
1	R	191	LYS
1	R	195	GLU
1	R	198	TYR
1	R	201	VAL
1	R	203	THR
1	R	224	GLU
1	R	229	THR
1	R	244	ASP
1	R	248	ILE
1	R	252	ASN
1	R	260	THR
1	R	270	GLU
1	R	283	MET
1	R	289	ILE
1	R	305	MET
1	R	326	LYS
1	R	334	GLU

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Mol	Chain	Res	Type
1	R	354	GLN
1	R	373	LYS
1	S	18	LYS
1	S	24	ASP
1	S	25	ASP
1	S	28	ARG
1	S	30	VAL
1	S	31	PHE
1	S	34	ILE
1	S	37	ARG
1	S	38	PRO
1	S	40	HIS
1	S	49	GLN
1	S	59	GLN
1	S	64	ILE
1	S	67	LEU
1	S	92	ASN
1	S	95	ARG
1	S	115	ASN
1	S	116	ARG
1	S	118	LYS
1	S	119	MET
1	S	132	MET
1	S	134	VAL
1	S	140	LEU
1	S	145	SER
1	S	148	THR
1	S	151	ILE
1	S	153	LEU
1	S	171	LEU
1	S	184	ASP
1	S	188	TYR
1	S	190	MET
1	S	191	LYS
1	S	195	GLU
1	S	198	TYR
1	S	203	THR
1	S	205	GLU
1	S	207	GLU
1	S	221	LEU
1	S	224	GLU
1	S	229	THR

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Mol	Chain	Res	Type
1	S	244	ASP
1	S	248	ILE
1	S	252	ASN
1	S	283	MET
1	S	284	LYS
1	S	287	ILE
1	S	288	ASP
1	S	303	THR
1	S	305	MET
1	S	323	SER
1	S	326	LYS
1	S	327	ILE
1	S	336	LYS
1	S	352	PHE
1	S	354	GLN
1	S	369	ILE
1	S	373	LYS
1	S	375	PHE
1	T	1	ASP
1	T	5	THR
1	T	25	ASP
1	T	30	VAL
1	T	41	GLN
1	T	49	GLN
1	T	57	GLU
1	T	64	ILE
1	T	67	LEU
1	T	70	PRO
1	T	83	GLU
1	T	85	ILE
1	T	95	ARG
1	T	111	ASN
1	T	115	ASN
1	T	116	ARG
1	T	118	LYS
1	T	119	MET
1	T	122	ILE
1	T	129	VAL
1	T	134	VAL
1	T	136	ILE
1	T	140	LEU
1	T	151	ILE

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Mol	Chain	Res	Type
1	T	153	LEU
1	T	173	HIS
1	T	184	ASP
1	T	188	TYR
1	T	190	MET
1	T	191	LYS
1	T	195	GLU
1	T	198	TYR
1	T	212	ILE
1	T	216	LEU
1	T	221	LEU
1	T	224	GLU
1	T	244	ASP
1	T	246	GLN
1	T	248	ILE
1	T	275	HIS
1	T	276	GLU
1	T	283	MET
1	T	284	LYS
1	T	289	ILE
1	T	292	ASP
1	T	305	MET
1	T	326	LYS
1	T	338	SER
1	T	346	LEU
1	T	354	GLN
1	T	370	VAL
1	T	373	LYS
1	U	2	GLU
1	U	28	ARG
1	U	30	VAL
1	U	31	PHE
1	U	34	ILE
1	U	37	ARG
1	U	43	VAL
1	U	49	GLN
1	U	64	ILE
1	U	67	LEU
1	U	83	GLU
1	U	85	ILE
1	U	95	ARG
1	U	111	ASN

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Mol	Chain	Res	Type
1	U	116	ARG
1	U	118	LYS
1	U	122	ILE
1	U	123	MET
1	U	140	LEU
1	U	151	ILE
1	U	159	VAL
1	U	171	LEU
1	U	173	HIS
1	U	184	ASP
1	U	188	TYR
1	U	189	LEU
1	U	190	MET
1	U	191	LYS
1	U	195	GLU
1	U	198	TYR
1	U	203	THR
1	U	205	GLU
1	U	219	VAL
1	U	234	SER
1	U	248	ILE
1	U	255	PHE
1	U	270	GLU
1	U	283	MET
1	U	284	LYS
1	U	288	ASP
1	U	289	ILE
1	U	291	LYS
1	U	300	SER
1	U	305	MET
1	U	325	MET
1	U	326	LYS
1	U	334	GLU
1	U	336	LYS
1	U	352	PHE
1	U	354	GLN
1	U	356	TRP
1	U	372	ARG
1	U	373	LYS
1	V	1	ASP
1	V	5	THR
1	V	24	ASP

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Mol	Chain	Res	Type
1	V	25	ASP
1	V	30	VAL
1	V	31	PHE
1	V	34	ILE
1	V	37	ARG
1	V	43	VAL
1	V	57	GLU
1	V	64	ILE
1	V	67	LEU
1	V	83	GLU
1	V	95	ARG
1	V	111	ASN
1	V	116	ARG
1	V	118	LYS
1	V	122	ILE
1	V	129	VAL
1	V	132	MET
1	V	140	LEU
1	V	173	HIS
1	V	184	ASP
1	V	188	TYR
1	V	189	LEU
1	V	190	MET
1	V	191	LYS
1	V	192	ILE
1	V	195	GLU
1	V	203	THR
1	V	208	ILE
1	V	212	ILE
1	V	244	ASP
1	V	248	ILE
1	V	283	MET
1	V	284	LYS
1	V	289	ILE
1	V	305	MET
1	V	318	THR
1	V	325	MET
1	V	326	LYS
1	V	327	ILE
1	V	338	SER
1	V	349	LEU
1	V	352	PHE

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Mol	Chain	Res	Type
1	V	354	GLN
1	V	356	TRP
1	V	357	ILE
1	V	373	LYS
1	V	375	PHE
1	W	25	ASP
1	W	28	ARG
1	W	37	ARG
1	W	49	GLN
1	W	64	ILE
1	W	76	ILE
1	W	85	ILE
1	W	95	ARG
1	W	115	ASN
1	W	116	ARG
1	W	119	MET
1	W	120	THR
1	W	122	ILE
1	W	132	MET
1	W	140	LEU
1	W	143	TYR
1	W	151	ILE
1	W	173	HIS
1	W	179	ASP
1	W	185	LEU
1	W	188	TYR
1	W	189	LEU
1	W	190	MET
1	W	195	GLU
1	W	201	VAL
1	W	205	GLU
1	W	219	VAL
1	W	221	LEU
1	W	248	ILE
1	W	252	ASN
1	W	283	MET
1	W	284	LYS
1	W	288	ASP
1	W	305	MET
1	W	318	THR
1	W	326	LYS
1	W	348	SER

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Mol	Chain	Res	Type
1	W	354	GLN
1	W	361	GLU
1	W	373	LYS
1	X	5	THR
1	X	30	VAL
1	X	34	ILE
1	X	37	ARG
1	X	40	HIS
1	X	49	GLN
1	X	89	THR
1	X	95	ARG
1	X	116	ARG
1	X	118	LYS
1	X	122	ILE
1	X	129	VAL
1	X	134	VAL
1	X	139	VAL
1	X	140	LEU
1	X	152	VAL
1	X	153	LEU
1	X	165	ILE
1	X	171	LEU
1	X	173	HIS
1	X	184	ASP
1	X	188	TYR
1	X	190	MET
1	X	191	LYS
1	X	195	GLU
1	X	205	GLU
1	X	206	ARG
1	X	207	GLU
1	X	216	LEU
1	X	224	GLU
1	X	229	THR
1	X	246	GLN
1	X	248	ILE
1	X	255	PHE
1	X	269	MET
1	X	270	GLU
1	X	274	ILE
1	X	275	HIS
1	X	281	SER

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Mol	Chain	Res	Type
1	X	283	MET
1	X	287	ILE
1	X	288	ASP
1	X	289	ILE
1	X	291	LYS
1	X	305	MET
1	X	317	ILE
1	X	326	LYS
1	X	329	ILE
1	X	334	GLU
1	X	335	ARG
1	X	338	SER
1	X	344	SER
1	X	352	PHE
1	X	354	GLN
1	X	373	LYS
1	Y	1	ASP
1	Y	16	LEU
1	Y	28	ARG
1	Y	30	VAL
1	Y	34	ILE
1	Y	37	ARG
1	Y	43	VAL
1	Y	49	GLN
1	Y	64	ILE
1	Y	67	LEU
1	Y	70	PRO
1	Y	82	MET
1	Y	95	ARG
1	Y	115	ASN
1	Y	116	ARG
1	Y	117	GLU
1	Y	118	LYS
1	Y	119	MET
1	Y	122	ILE
1	Y	129	VAL
1	Y	140	LEU
1	Y	151	ILE
1	Y	173	HIS
1	Y	184	ASP
1	Y	188	TYR
1	Y	190	MET

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Mol	Chain	Res	Type
1	Y	191	LYS
1	Y	195	GLU
1	Y	202	THR
1	Y	203	THR
1	Y	216	LEU
1	Y	219	VAL
1	Y	221	LEU
1	Y	227	MET
1	Y	229	THR
1	Y	248	ILE
1	Y	275	HIS
1	Y	277	THR
1	Y	278	THR
1	Y	283	MET
1	Y	284	LYS
1	Y	289	ILE
1	Y	305	MET
1	Y	326	LYS
1	Y	327	ILE
1	Y	329	ILE
1	Y	338	SER
1	Y	344	SER
1	Y	354	GLN
1	Y	369	ILE
1	Y	373	LYS
1	Y	375	PHE
1	Z	17	VAL
1	Z	25	ASP
1	Z	28	ARG
1	Z	30	VAL
1	Z	31	PHE
1	Z	37	ARG
1	Z	40	HIS
1	Z	43	VAL
1	Z	49	GLN
1	Z	64	ILE
1	Z	67	LEU
1	Z	81	ASP
1	Z	82	MET
1	Z	83	GLU
1	Z	85	ILE
1	Z	95	ARG

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Mol	Chain	Res	Type
1	Z	115	ASN
1	Z	116	ARG
1	Z	118	LYS
1	Z	122	ILE
1	Z	140	LEU
1	Z	151	ILE
1	Z	159	VAL
1	Z	163	VAL
1	Z	173	HIS
1	Z	179	ASP
1	Z	184	ASP
1	Z	188	TYR
1	Z	189	LEU
1	Z	190	MET
1	Z	191	LYS
1	Z	195	GLU
1	Z	198	TYR
1	Z	205	GLU
1	Z	206	ARG
1	Z	207	GLU
1	Z	208	ILE
1	Z	211	ASP
1	Z	221	LEU
1	Z	224	GLU
1	Z	244	ASP
1	Z	248	ILE
1	Z	257	CYS
1	Z	260	THR
1	Z	270	GLU
1	Z	277	THR
1	Z	282	ILE
1	Z	283	MET
1	Z	288	ASP
1	Z	289	ILE
1	Z	305	MET
1	Z	313	MET
1	Z	323	SER
1	Z	326	LYS
1	Z	334	GLU
1	Z	351	THR
1	Z	352	PHE
1	Z	354	GLN

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Mol	Chain	Res	Type
1	Z	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	49	GLN
1	O	87	HIS
1	O	115	ASN
1	O	246	GLN
1	O	275	HIS
1	P	41	GLN
1	P	92	ASN
1	P	246	GLN
1	P	275	HIS
1	Q	49	GLN
1	Q	115	ASN
1	Q	275	HIS
1	R	87	HIS
1	R	128	ASN
1	S	40	HIS
1	S	49	GLN
1	S	225	ASN
1	S	246	GLN
1	T	49	GLN
1	T	115	ASN
1	T	173	HIS
1	T	246	GLN
1	U	101	HIS
1	U	115	ASN
1	U	314	GLN
1	V	101	HIS
1	V	115	ASN
1	V	173	HIS
1	V	275	HIS
1	W	87	HIS
1	W	101	HIS
1	W	115	ASN
1	W	162	ASN
1	W	275	HIS
1	X	92	ASN
1	X	101	HIS
1	X	121	GLN

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Mol	Chain	Res	Type
1	X	161	HIS
1	X	275	HIS
1	Y	41	GLN
1	Y	115	ASN
1	Y	162	ASN
1	Y	275	HIS
1	Z	101	HIS
1	Z	115	ASN
1	Z	246	GLN
1	Z	275	HIS
1	Z	280	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	HIC	P	73	1	10,11,12	2.15	1 (10%)	9,14,16	5.95	4 (44%)
1	HIC	O	73	1	10,11,12	1.26	1 (10%)	9,14,16	4.34	5 (55%)
1	HIC	Y	73	1	10,11,12	2.32	1 (10%)	9,14,16	6.51	4 (44%)
1	HIC	S	73	1	10,11,12	2.54	1 (10%)	9,14,16	6.97	4 (44%)
1	HIC	U	73	1	10,11,12	2.21	1 (10%)	9,14,16	4.94	4 (44%)
1	HIC	Z	73	1	10,11,12	2.57	2 (20%)	9,14,16	7.80	5 (55%)
1	HIC	X	73	1	10,11,12	2.49	1 (10%)	9,14,16	5.29	4 (44%)
1	HIC	R	73	1	10,11,12	2.28	1 (10%)	9,14,16	6.52	7 (77%)
1	HIC	W	73	1	10,11,12	2.51	1 (10%)	9,14,16	8.14	4 (44%)
1	HIC	V	73	1	10,11,12	2.41	1 (10%)	9,14,16	6.06	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	T	73	1	10,11,12	2.09	1 (10%)	9,14,16	5.84	5 (55%)
1	HIC	Q	73	1	10,11,12	2.30	2 (20%)	9,14,16	5.95	5 (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
1	HIC	P	73	1	-	0/5/6/8	0/1/1/1
1	HIC	O	73	1	-	0/5/6/8	0/1/1/1
1	HIC	Y	73	1	-	0/5/6/8	0/1/1/1
1	HIC	S	73	1	-	0/5/6/8	0/1/1/1
1	HIC	U	73	1	-	0/5/6/8	0/1/1/1
1	HIC	Z	73	1	-	0/5/6/8	0/1/1/1
1	HIC	X	73	1	-	1/5/6/8	0/1/1/1
1	HIC	R	73	1	-	0/5/6/8	0/1/1/1
1	HIC	W	73	1	-	0/5/6/8	0/1/1/1
1	HIC	V	73	1	-	1/5/6/8	0/1/1/1
1	HIC	T	73	1	-	1/5/6/8	0/1/1/1
1	HIC	Q	73	1	-	0/5/6/8	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	73	HIC	CZ-NE2	-7.68	1.26	1.46
1	Z	73	HIC	CZ-NE2	-7.67	1.27	1.46
1	W	73	HIC	CZ-NE2	-7.59	1.27	1.46
1	X	73	HIC	CZ-NE2	-7.51	1.27	1.46
1	V	73	HIC	CZ-NE2	-7.35	1.27	1.46
1	Y	73	HIC	CZ-NE2	-7.16	1.28	1.46
1	R	73	HIC	CZ-NE2	-6.89	1.29	1.46
1	Q	73	HIC	CZ-NE2	-6.82	1.29	1.46
1	P	73	HIC	CZ-NE2	-6.57	1.29	1.46
1	U	73	HIC	CZ-NE2	-6.56	1.29	1.46
1	T	73	HIC	CZ-NE2	-6.29	1.30	1.46
1	O	73	HIC	CZ-NE2	-3.51	1.37	1.46
1	Z	73	HIC	CA-N	-2.09	1.42	1.48
1	Q	73	HIC	CA-N	-2.02	1.42	1.48

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	73	HIC	CZ-NE2-CD2	19.71	151.91	126.03
1	Z	73	HIC	CZ-NE2-CD2	18.58	150.43	126.03
1	S	73	HIC	CZ-NE2-CD2	16.01	147.05	126.03
1	Y	73	HIC	CZ-NE2-CD2	14.24	144.73	126.03
1	R	73	HIC	CZ-NE2-CD2	13.63	143.93	126.03
1	V	73	HIC	CZ-NE2-CD2	13.02	143.12	126.03
1	P	73	HIC	CZ-NE2-CD2	12.65	142.64	126.03
1	Q	73	HIC	CZ-NE2-CD2	12.52	142.47	126.03
1	O	73	HIC	NE2-CE1-ND1	-11.29	108.34	112.66
1	T	73	HIC	CZ-NE2-CD2	11.18	140.71	126.03
1	W	73	HIC	CZ-NE2-CE1	-11.10	100.52	126.71
1	T	73	HIC	NE2-CE1-ND1	-10.77	108.54	112.66
1	U	73	HIC	NE2-CE1-ND1	-10.71	108.56	112.66
1	Z	73	HIC	CZ-NE2-CE1	-10.56	101.79	126.71
1	R	73	HIC	NE2-CE1-ND1	-10.55	108.62	112.66
1	X	73	HIC	NE2-CE1-ND1	-10.31	108.72	112.66
1	Y	73	HIC	NE2-CE1-ND1	-9.87	108.88	112.66
1	X	73	HIC	CZ-NE2-CD2	9.56	138.59	126.03
1	P	73	HIC	NE2-CE1-ND1	-9.48	109.03	112.66
1	Q	73	HIC	NE2-CE1-ND1	-9.44	109.05	112.66
1	S	73	HIC	CZ-NE2-CE1	-9.23	104.92	126.71
1	V	73	HIC	NE2-CE1-ND1	-9.11	109.17	112.66
1	S	73	HIC	NE2-CE1-ND1	-8.86	109.27	112.66
1	W	73	HIC	NE2-CE1-ND1	-8.62	109.36	112.66
1	Z	73	HIC	NE2-CE1-ND1	-8.60	109.37	112.66
1	Y	73	HIC	CZ-NE2-CE1	-8.30	107.13	126.71
1	R	73	HIC	CZ-NE2-CE1	-8.16	107.45	126.71
1	V	73	HIC	CZ-NE2-CE1	-7.81	108.28	126.71
1	Q	73	HIC	CZ-NE2-CE1	-7.59	108.80	126.71
1	U	73	HIC	CZ-NE2-CD2	7.50	135.88	126.03
1	P	73	HIC	CZ-NE2-CE1	-7.50	109.01	126.71
1	T	73	HIC	CZ-NE2-CE1	-6.79	110.68	126.71
1	X	73	HIC	CZ-NE2-CE1	-5.91	112.76	126.71
1	U	73	HIC	CZ-NE2-CE1	-4.87	115.22	126.71
1	O	73	HIC	CD2-NE2-CE1	4.60	108.53	106.71
1	U	73	HIC	CD2-NE2-CE1	3.67	108.16	106.71
1	X	73	HIC	CD2-NE2-CE1	3.30	108.01	106.71
1	T	73	HIC	CD2-NE2-CE1	3.18	107.97	106.71
1	Z	73	HIC	CB-CG-CD2	-2.88	123.02	129.96
1	O	73	HIC	CZ-NE2-CD2	-2.67	122.53	126.03
1	V	73	HIC	CD2-NE2-CE1	2.55	107.72	106.71
1	P	73	HIC	CD2-NE2-CE1	2.42	107.67	106.71
1	S	73	HIC	CB-CG-CD2	-2.39	124.20	129.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	73	HIC	CD2-NE2-CE1	2.28	107.61	106.71
1	Z	73	HIC	CB-CG-ND1	2.26	128.49	121.74
1	R	73	HIC	CD2-NE2-CE1	2.19	107.57	106.71
1	O	73	HIC	CB-CG-CD2	-2.17	124.72	129.96
1	W	73	HIC	CB-CG-CD2	-2.16	124.75	129.96
1	R	73	HIC	CB-CG-CD2	-2.16	124.75	129.96
1	Q	73	HIC	CD2-NE2-CE1	2.10	107.54	106.71
1	T	73	HIC	CE1-ND1-CG	2.08	109.14	105.80
1	Q	73	HIC	CB-CG-CD2	-2.07	124.98	129.96
1	R	73	HIC	CB-CG-ND1	2.02	127.79	121.74
1	O	73	HIC	CB-CG-ND1	2.02	127.78	121.74
1	R	73	HIC	CE1-ND1-CG	2.01	109.02	105.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	V	73	HIC	O-C-CA-CB
1	X	73	HIC	O-C-CA-CB
1	T	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

11 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	73	HIC	1	0
1	O	73	HIC	2	0
1	Y	73	HIC	2	0
1	S	73	HIC	3	0
1	U	73	HIC	2	0
1	X	73	HIC	3	0
1	R	73	HIC	3	0
1	W	73	HIC	3	0
1	V	73	HIC	3	0
1	T	73	HIC	2	0
1	Q	73	HIC	3	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 120 ligands modelled in this entry, 72 are monoatomic - leaving 48 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
3	PO4	T	802	-	4,4,4	1.87	1 (25%)	6,6,6	2.10	2 (33%)
3	PO4	Z	801	-	4,4,4	1.90	1 (25%)	6,6,6	3.38	2 (33%)
3	PO4	W	801	-	4,4,4	1.75	1 (25%)	6,6,6	3.24	2 (33%)
3	PO4	Y	803	-	4,4,4	1.96	1 (25%)	6,6,6	4.04	4 (66%)
3	PO4	U	801	-	4,4,4	3.24	1 (25%)	6,6,6	5.80	2 (33%)
2	ADP	Q	800	4	28,29,29	2.13	2 (7%)	43,45,45	1.08	4 (9%)
3	PO4	P	801	-	4,4,4	2.00	1 (25%)	6,6,6	3.20	2 (33%)
3	PO4	Q	801	4	4,4,4	1.84	1 (25%)	6,6,6	4.30	2 (33%)
3	PO4	V	803	-	4,4,4	1.87	1 (25%)	6,6,6	3.22	3 (50%)
3	PO4	Q	803	-	4,4,4	1.80	1 (25%)	6,6,6	3.03	2 (33%)
3	PO4	T	803	-	4,4,4	1.91	1 (25%)	6,6,6	4.04	3 (50%)
3	PO4	X	801	-	4,4,4	1.57	1 (25%)	6,6,6	2.05	2 (33%)
2	ADP	Y	800	4	28,29,29	1.52	2 (7%)	43,45,45	0.98	3 (6%)
3	PO4	Z	802	-	4,4,4	1.94	1 (25%)	6,6,6	3.29	4 (66%)
3	PO4	U	802	-	4,4,4	1.42	1 (25%)	6,6,6	2.52	3 (50%)
3	PO4	V	802	-	4,4,4	1.87	1 (25%)	6,6,6	2.62	2 (33%)
2	ADP	O	800	4	28,29,29	2.28	2 (7%)	43,45,45	1.16	5 (11%)
2	ADP	U	800	4	28,29,29	2.11	2 (7%)	43,45,45	1.14	4 (9%)
3	PO4	X	802	-	4,4,4	1.76	1 (25%)	6,6,6	2.49	2 (33%)
3	PO4	Z	803	-	4,4,4	1.80	1 (25%)	6,6,6	2.82	2 (33%)
2	ADP	W	800	4	28,29,29	1.93	2 (7%)	43,45,45	1.02	4 (9%)
2	ADP	X	800	4	28,29,29	2.12	2 (7%)	43,45,45	1.12	5 (11%)
3	PO4	T	376	-	4,4,4	1.72	1 (25%)	6,6,6	3.29	2 (33%)
3	PO4	P	803	-	4,4,4	3.15	2 (50%)	6,6,6	6.91	5 (83%)
3	PO4	Q	802	-	4,4,4	1.85	1 (25%)	6,6,6	2.21	2 (33%)
3	PO4	Y	801	4	4,4,4	2.03	1 (25%)	6,6,6	2.09	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	X	803	-	4,4,4	1.82	1 (25%)	6,6,6	4.36	5 (83%)
2	ADP	T	800	4	28,29,29	1.96	2 (7%)	43,45,45	1.17	5 (11%)
3	PO4	U	803	-	4,4,4	1.82	1 (25%)	6,6,6	2.16	2 (33%)
3	PO4	W	803	-	4,4,4	1.93	1 (25%)	6,6,6	3.44	2 (33%)
3	PO4	O	801	-	4,4,4	1.74	1 (25%)	6,6,6	3.17	2 (33%)
3	PO4	R	801	-	4,4,4	1.94	1 (25%)	6,6,6	2.84	2 (33%)
2	ADP	S	800	4	28,29,29	1.72	2 (7%)	43,45,45	0.98	3 (6%)
3	PO4	Y	802	-	4,4,4	1.91	1 (25%)	6,6,6	1.99	2 (33%)
3	PO4	W	802	-	4,4,4	1.65	1 (25%)	6,6,6	2.14	2 (33%)
3	PO4	S	803	-	4,4,4	1.95	1 (25%)	6,6,6	3.19	3 (50%)
3	PO4	S	802	-	4,4,4	1.90	1 (25%)	6,6,6	2.00	2 (33%)
3	PO4	T	801	4	4,4,4	1.79	1 (25%)	6,6,6	3.31	2 (33%)
2	ADP	Z	800	4	28,29,29	2.02	2 (7%)	43,45,45	1.03	3 (6%)
3	PO4	O	803	-	4,4,4	2.10	1 (25%)	6,6,6	3.15	4 (66%)
3	PO4	O	802	-	4,4,4	1.79	1 (25%)	6,6,6	2.42	2 (33%)
3	PO4	P	802	-	4,4,4	1.56	1 (25%)	6,6,6	1.87	2 (33%)
2	ADP	P	800	4	28,29,29	1.98	2 (7%)	43,45,45	0.97	3 (6%)
3	PO4	R	802	-	4,4,4	1.55	1 (25%)	6,6,6	2.33	1 (16%)
3	PO4	R	803	-	4,4,4	2.08	1 (25%)	6,6,6	5.83	5 (83%)
3	PO4	S	801	-	4,4,4	1.42	1 (25%)	6,6,6	2.21	2 (33%)
2	ADP	V	800	4	28,29,29	1.83	2 (7%)	43,45,45	1.01	3 (6%)
2	ADP	R	800	4	28,29,29	2.14	2 (7%)	43,45,45	1.25	4 (9%)

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
2	ADP	Y	800	4	-	0/16/32/32	0/3/3/3
2	ADP	O	800	4	-	0/16/32/32	0/3/3/3
2	ADP	X	800	4	-	0/16/32/32	0/3/3/3
2	ADP	Z	800	4	-	0/16/32/32	0/3/3/3
2	ADP	T	800	4	-	0/16/32/32	0/3/3/3
2	ADP	Q	800	4	-	2/16/32/32	0/3/3/3
2	ADP	U	800	4	-	0/16/32/32	0/3/3/3
2	ADP	P	800	4	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	W	800	4	-	1/16/32/32	0/3/3/3
2	ADP	V	800	4	-	0/16/32/32	0/3/3/3
2	ADP	R	800	4	-	0/16/32/32	0/3/3/3
2	ADP	S	800	4	-	0/16/32/32	0/3/3/3

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	800	ADP	PA-O3A	-11.42	1.47	1.59
2	X	800	ADP	PA-O3A	-10.71	1.47	1.59
2	R	800	ADP	PA-O3A	-10.70	1.48	1.59
2	Q	800	ADP	PA-O3A	-10.59	1.48	1.59
2	U	800	ADP	PA-O3A	-10.49	1.48	1.59
2	Z	800	ADP	PA-O3A	-10.08	1.48	1.59
2	P	800	ADP	PA-O3A	-9.81	1.48	1.59
2	T	800	ADP	PA-O3A	-9.70	1.49	1.59
2	W	800	ADP	PA-O3A	-9.59	1.49	1.59
2	V	800	ADP	PA-O3A	-8.98	1.49	1.59
2	S	800	ADP	PA-O3A	-8.41	1.50	1.59
2	Y	800	ADP	PA-O3A	-7.32	1.51	1.59
3	U	801	PO4	P-O1	5.85	1.64	1.50
3	P	803	PO4	P-O1	5.68	1.63	1.50
3	O	803	PO4	P-O4	3.60	1.65	1.54
3	Z	802	PO4	P-O4	3.59	1.65	1.54
3	P	801	PO4	P-O4	3.57	1.65	1.54
3	Y	801	PO4	P-O4	3.54	1.65	1.54
3	R	803	PO4	P-O4	3.44	1.64	1.54
3	S	803	PO4	P-O4	3.28	1.64	1.54
3	R	801	PO4	P-O4	3.28	1.64	1.54
3	V	802	PO4	P-O4	3.21	1.64	1.54
3	Z	801	PO4	P-O4	3.19	1.63	1.54
3	Y	802	PO4	P-O4	3.16	1.63	1.54
3	Y	803	PO4	P-O4	3.11	1.63	1.54
3	X	803	PO4	P-O4	3.07	1.63	1.54
3	T	802	PO4	P-O4	3.04	1.63	1.54
3	Q	803	PO4	P-O4	3.01	1.63	1.54
3	T	801	PO4	P-O4	3.01	1.63	1.54
3	T	803	PO4	P-O4	2.96	1.63	1.54
3	W	801	PO4	P-O4	2.95	1.63	1.54
3	S	802	PO4	P-O4	2.95	1.63	1.54
3	O	802	PO4	P-O4	2.94	1.63	1.54
3	T	376	PO4	P-O4	2.93	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	802	PO4	P-O4	2.89	1.63	1.54
3	Q	801	PO4	P-O4	2.88	1.63	1.54
3	Q	802	PO4	P-O4	2.86	1.63	1.54
3	W	803	PO4	P-O4	2.83	1.62	1.54
3	V	803	PO4	P-O4	2.83	1.62	1.54
3	U	803	PO4	P-O4	2.82	1.62	1.54
3	W	802	PO4	P-O4	2.70	1.62	1.54
3	O	801	PO4	P-O4	2.62	1.62	1.54
3	Z	803	PO4	P-O4	2.61	1.62	1.54
3	P	802	PO4	P-O4	2.52	1.62	1.54
3	X	801	PO4	P-O4	2.50	1.61	1.54
3	R	802	PO4	P-O4	2.39	1.61	1.54
3	U	802	PO4	P-O4	2.10	1.60	1.54
3	S	801	PO4	P-O4	2.10	1.60	1.54
3	P	803	PO4	P-O3	-2.08	1.48	1.54
2	W	800	ADP	PB-O2B	-2.06	1.47	1.54
2	Y	800	ADP	PB-O2B	-2.05	1.47	1.54
2	S	800	ADP	PB-O2B	-2.05	1.47	1.54
2	Q	800	ADP	PB-O2B	-2.04	1.47	1.54
2	O	800	ADP	PB-O2B	-2.04	1.47	1.54
2	R	800	ADP	PB-O2B	-2.04	1.47	1.54
2	T	800	ADP	PB-O2B	-2.04	1.47	1.54
2	U	800	ADP	PB-O2B	-2.04	1.47	1.54
2	P	800	ADP	PB-O2B	-2.03	1.47	1.54
2	V	800	ADP	PB-O2B	-2.03	1.47	1.54
2	Z	800	ADP	PB-O2B	-2.02	1.47	1.54
2	X	800	ADP	PB-O2B	-2.02	1.47	1.54

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	803	PO4	O4-P-O1	-13.32	63.84	110.95
3	U	801	PO4	O4-P-O1	-11.70	69.57	110.95
3	R	803	PO4	O4-P-O1	-10.01	75.57	110.95
3	U	801	PO4	O3-P-O2	7.96	132.67	107.91
3	X	803	PO4	O4-P-O1	-7.82	83.28	110.95
3	Q	801	PO4	O4-P-O1	-7.54	84.30	110.95
3	Q	801	PO4	O3-P-O2	7.13	130.09	107.91
3	P	803	PO4	O2-P-O1	-6.37	88.42	110.95
3	T	803	PO4	O4-P-O1	-6.36	88.47	110.95
3	Z	801	PO4	O4-P-O1	-6.34	88.54	110.95
3	W	803	PO4	O3-P-O2	6.32	127.58	107.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	376	PO4	O3-P-O2	6.09	126.86	107.91
3	P	803	PO4	O3-P-O2	5.98	126.51	107.91
3	R	803	PO4	O4-P-O3	-5.97	89.33	107.91
3	R	803	PO4	O4-P-O2	-5.94	89.43	107.91
3	Y	803	PO4	O4-P-O1	-5.94	89.95	110.95
3	Y	803	PO4	O3-P-O2	5.91	126.31	107.91
3	T	803	PO4	O3-P-O2	5.91	126.30	107.91
3	T	801	PO4	O3-P-O2	5.89	126.23	107.91
3	O	803	PO4	O3-P-O2	5.84	126.08	107.91
3	W	801	PO4	O4-P-O1	-5.83	90.35	110.95
3	Z	802	PO4	O3-P-O2	5.81	125.99	107.91
3	P	801	PO4	O3-P-O2	5.80	125.97	107.91
3	Q	803	PO4	O3-P-O2	5.74	125.76	107.91
3	V	803	PO4	O3-P-O2	5.73	125.75	107.91
3	R	801	PO4	O3-P-O2	5.61	125.38	107.91
3	Z	803	PO4	O3-P-O2	5.53	125.13	107.91
3	O	801	PO4	O4-P-O1	-5.49	91.52	110.95
3	S	803	PO4	O3-P-O2	5.45	124.85	107.91
3	O	801	PO4	O3-P-O2	5.41	124.74	107.91
3	W	803	PO4	O4-P-O1	-5.28	92.28	110.95
3	V	802	PO4	O3-P-O2	5.24	124.22	107.91
3	X	803	PO4	O3-P-O2	5.23	124.18	107.91
3	R	803	PO4	O3-P-O2	5.23	124.17	107.91
3	Z	801	PO4	O3-P-O2	5.20	124.09	107.91
3	T	376	PO4	O4-P-O1	-5.15	92.75	110.95
3	R	802	PO4	O3-P-O2	5.09	123.74	107.91
3	W	801	PO4	O3-P-O2	5.01	123.51	107.91
3	P	803	PO4	O3-P-O1	-4.94	93.49	110.95
3	O	802	PO4	O3-P-O2	4.92	123.21	107.91
3	X	802	PO4	O3-P-O2	4.91	123.20	107.91
3	V	803	PO4	O4-P-O1	-4.89	93.66	110.95
3	S	803	PO4	O4-P-O1	-4.84	93.84	110.95
3	P	801	PO4	O4-P-O1	-4.82	93.89	110.95
3	T	801	PO4	O4-P-O1	-4.70	94.35	110.95
3	Q	802	PO4	O3-P-O2	4.48	121.84	107.91
3	W	802	PO4	O3-P-O2	4.41	121.64	107.91
3	U	802	PO4	O3-P-O2	4.40	121.60	107.91
3	U	803	PO4	O3-P-O2	4.35	121.46	107.91
3	T	802	PO4	O3-P-O2	4.33	121.40	107.91
3	T	803	PO4	O4-P-O3	-4.22	94.77	107.91
3	Q	803	PO4	O4-P-O1	-4.20	96.11	110.95
3	S	801	PO4	O3-P-O2	4.17	120.88	107.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	801	PO4	O3-P-O2	4.09	120.64	107.91
3	Z	802	PO4	O4-P-O1	-3.92	97.08	110.95
3	S	802	PO4	O3-P-O2	3.91	120.09	107.91
3	Y	801	PO4	O4-P-O3	-3.68	96.45	107.91
3	O	803	PO4	O4-P-O1	-3.57	98.33	110.95
3	Y	803	PO4	O4-P-O2	-3.47	97.10	107.91
3	X	803	PO4	O4-P-O3	-3.47	97.13	107.91
3	Y	802	PO4	O3-P-O2	3.46	118.69	107.91
3	Y	803	PO4	O4-P-O3	-3.46	97.14	107.91
3	P	802	PO4	O3-P-O2	3.44	118.60	107.91
3	R	801	PO4	O4-P-O1	-3.37	99.04	110.95
2	R	800	ADP	O2A-PA-O3A	3.33	116.28	107.27
2	T	800	ADP	O2A-PA-O3A	3.31	116.23	107.27
3	Z	803	PO4	O4-P-O1	-3.27	99.39	110.95
3	S	801	PO4	O4-P-O1	-3.26	99.42	110.95
2	W	800	ADP	O3B-PB-O2B	3.23	119.92	107.80
2	U	800	ADP	O3B-PB-O2B	3.22	119.89	107.80
2	O	800	ADP	O3B-PB-O2B	3.22	119.89	107.80
2	X	800	ADP	O3B-PB-O2B	3.22	119.89	107.80
2	S	800	ADP	O3B-PB-O2B	3.22	119.89	107.80
2	T	800	ADP	O3B-PB-O2B	3.22	119.88	107.80
2	Q	800	ADP	O3B-PB-O2B	3.22	119.87	107.80
2	P	800	ADP	O3B-PB-O2B	3.22	119.86	107.80
2	Y	800	ADP	O3B-PB-O2B	3.21	119.86	107.80
2	V	800	ADP	O3B-PB-O2B	3.21	119.85	107.80
2	Z	800	ADP	O3B-PB-O2B	3.21	119.85	107.80
2	R	800	ADP	O3B-PB-O2B	3.21	119.85	107.80
3	Z	802	PO4	O4-P-O3	-3.15	98.10	107.91
3	Y	802	PO4	O4-P-O3	-3.13	98.18	107.91
2	Q	800	ADP	O2A-PA-O3A	3.04	115.49	107.27
2	X	800	ADP	O2A-PA-O3A	2.98	115.33	107.27
3	V	802	PO4	O4-P-O1	-2.94	100.56	110.95
2	O	800	ADP	O2A-PA-O3A	2.90	115.12	107.27
3	U	802	PO4	O4-P-O3	-2.86	99.00	107.91
3	X	802	PO4	O4-P-O1	-2.84	100.89	110.95
2	S	800	ADP	O2A-PA-O3A	2.79	114.83	107.27
2	O	800	ADP	O3B-PB-O1B	-2.78	99.99	110.83
2	U	800	ADP	O3B-PB-O1B	-2.78	100.00	110.83
2	R	800	ADP	O3B-PB-O1B	-2.78	100.01	110.83
2	W	800	ADP	O3B-PB-O1B	-2.78	100.02	110.83
2	Y	800	ADP	O3B-PB-O1B	-2.78	100.02	110.83
2	Z	800	ADP	O3B-PB-O1B	-2.78	100.02	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	800	ADP	O3B-PB-O1B	-2.77	100.03	110.83
2	T	800	ADP	O3B-PB-O1B	-2.77	100.03	110.83
2	X	800	ADP	O3B-PB-O1B	-2.77	100.05	110.83
2	V	800	ADP	O3B-PB-O1B	-2.77	100.05	110.83
2	P	800	ADP	O3B-PB-O1B	-2.77	100.06	110.83
2	P	800	ADP	O2A-PA-O3A	2.77	114.75	107.27
2	Q	800	ADP	O3B-PB-O1B	-2.76	100.07	110.83
2	R	800	ADP	O3B-PB-O3A	-2.72	95.52	104.64
2	V	800	ADP	O2A-PA-O3A	2.69	114.55	107.27
2	W	800	ADP	O2A-PA-O3A	2.60	114.31	107.27
3	X	803	PO4	O4-P-O2	-2.54	100.02	107.91
3	U	803	PO4	O4-P-O1	-2.54	101.98	110.95
3	Y	801	PO4	O3-P-O2	2.51	115.73	107.91
3	X	801	PO4	O4-P-O1	-2.49	102.14	110.95
3	U	802	PO4	O4-P-O1	-2.46	102.27	110.95
3	O	803	PO4	O4-P-O2	-2.45	100.29	107.91
3	Q	802	PO4	O4-P-O3	-2.44	100.32	107.91
2	Y	800	ADP	O2A-PA-O3A	2.41	113.78	107.27
3	O	803	PO4	O4-P-O3	-2.37	100.55	107.91
2	Q	800	ADP	O3B-PB-O3A	-2.36	96.73	104.64
3	X	803	PO4	O2-P-O1	2.35	119.27	110.95
3	Y	801	PO4	O4-P-O2	2.34	115.19	107.91
3	S	803	PO4	O4-P-O3	-2.32	100.69	107.91
3	P	803	PO4	O4-P-O3	2.30	115.07	107.91
2	U	800	ADP	N6-C6-N1	-2.30	113.26	118.38
2	U	800	ADP	O2A-PA-O3A	2.27	113.42	107.27
2	T	800	ADP	O3B-PB-O3A	-2.26	97.06	104.64
2	X	800	ADP	O3B-PB-O3A	-2.24	97.12	104.64
3	O	802	PO4	O4-P-O1	-2.23	103.05	110.95
2	W	800	ADP	O3B-PB-O3A	-2.23	97.15	104.64
2	X	800	ADP	O4'-C1'-N9	2.17	112.25	108.09
3	W	802	PO4	O4-P-O3	-2.14	101.26	107.91
3	V	803	PO4	O4-P-O3	-2.13	101.28	107.91
3	R	803	PO4	O2-P-O1	2.12	118.45	110.95
2	O	800	ADP	O3B-PB-O3A	-2.11	97.56	104.64
3	P	802	PO4	O3-P-O1	-2.09	103.56	110.95
2	Z	800	ADP	O3B-PB-O3A	-2.06	97.72	104.64
2	O	800	ADP	PA-O5'-C5'	2.06	133.17	121.35
2	T	800	ADP	N6-C6-N1	-2.06	113.79	118.38
3	T	802	PO4	O4-P-O2	-2.03	101.59	107.91
3	Z	802	PO4	O4-P-O2	-2.02	101.63	107.91
3	S	802	PO4	O4-P-O2	-2.01	101.65	107.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

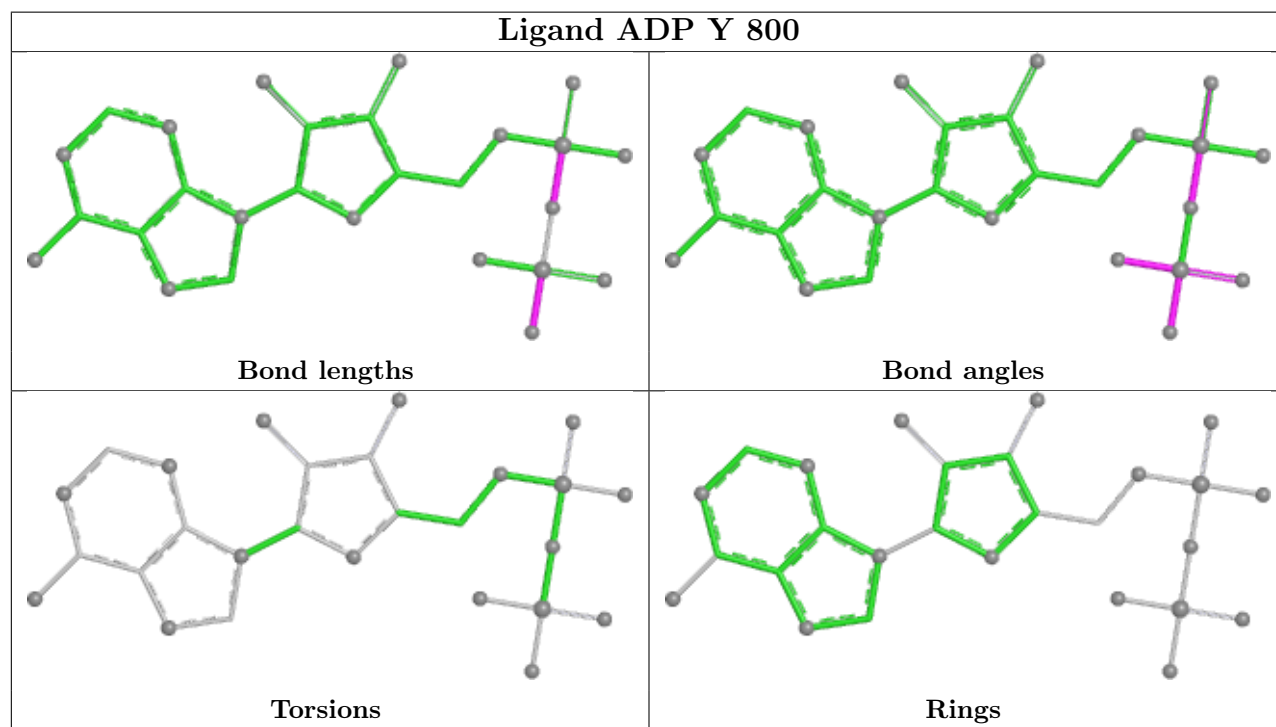
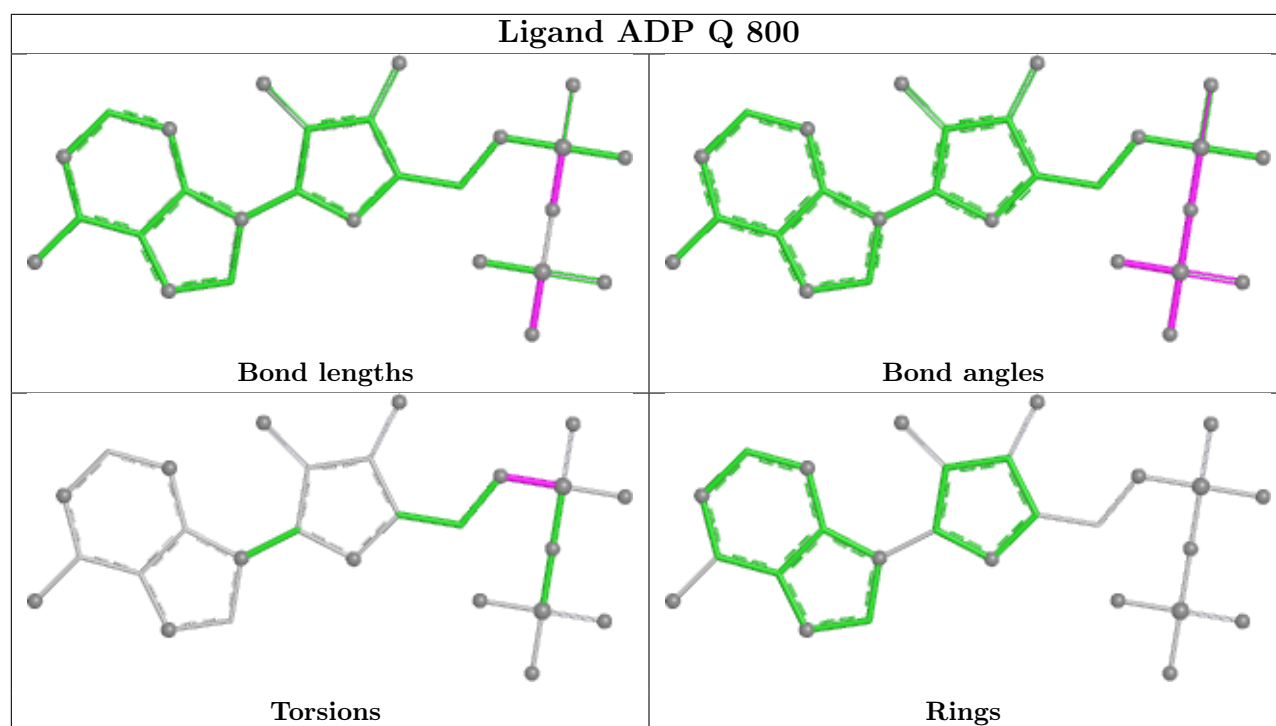
Mol	Chain	Res	Type	Atoms
2	Q	800	ADP	C5'-O5'-PA-O2A
2	W	800	ADP	C3'-C4'-C5'-O5'
2	Q	800	ADP	C5'-O5'-PA-O3A

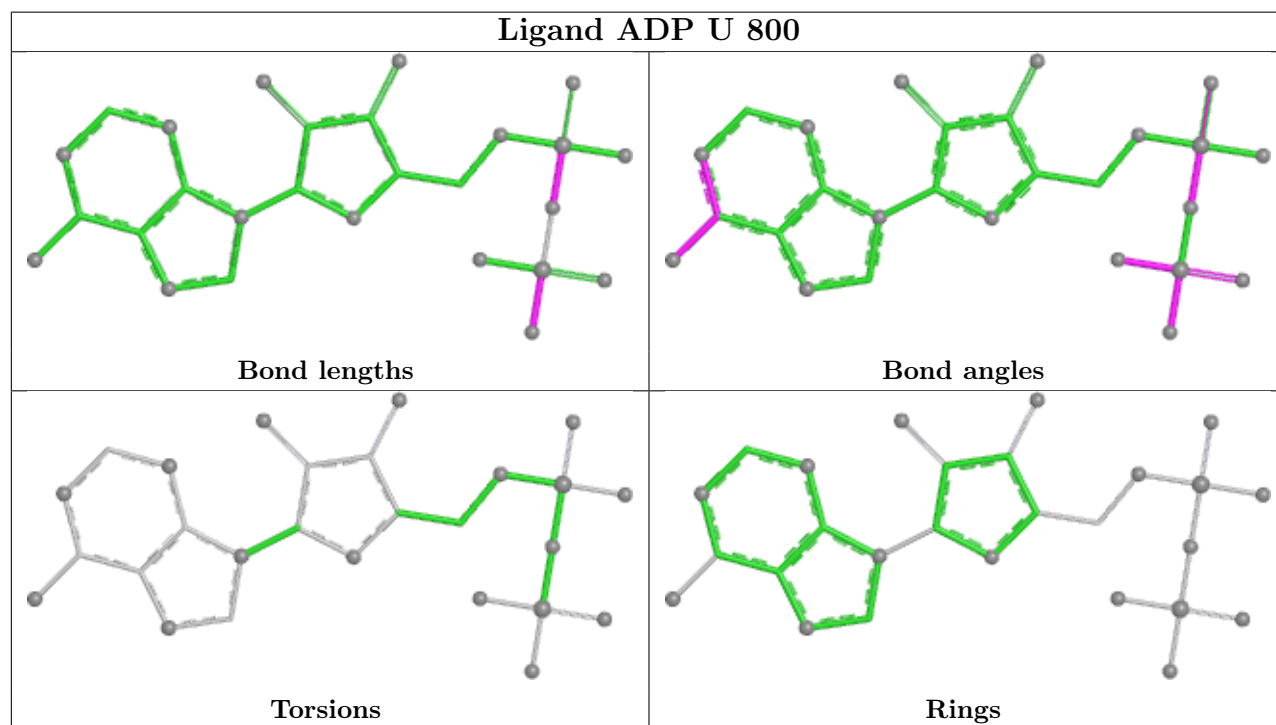
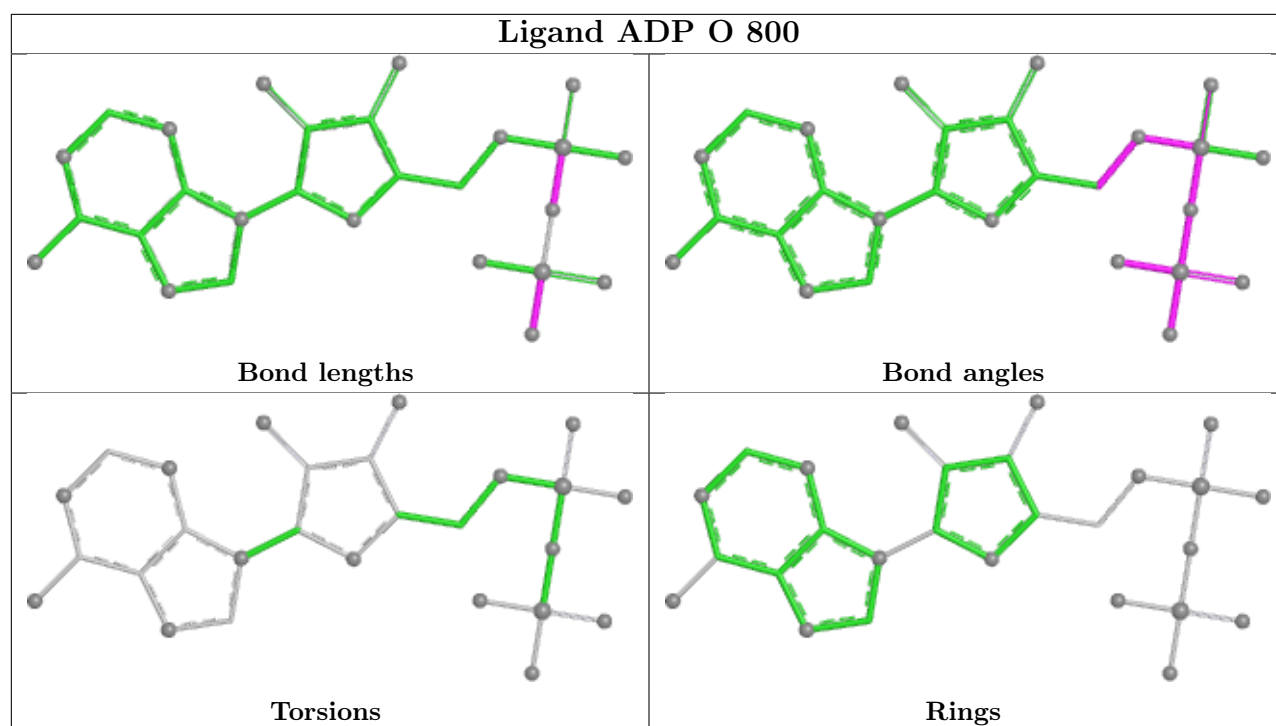
There are no ring outliers.

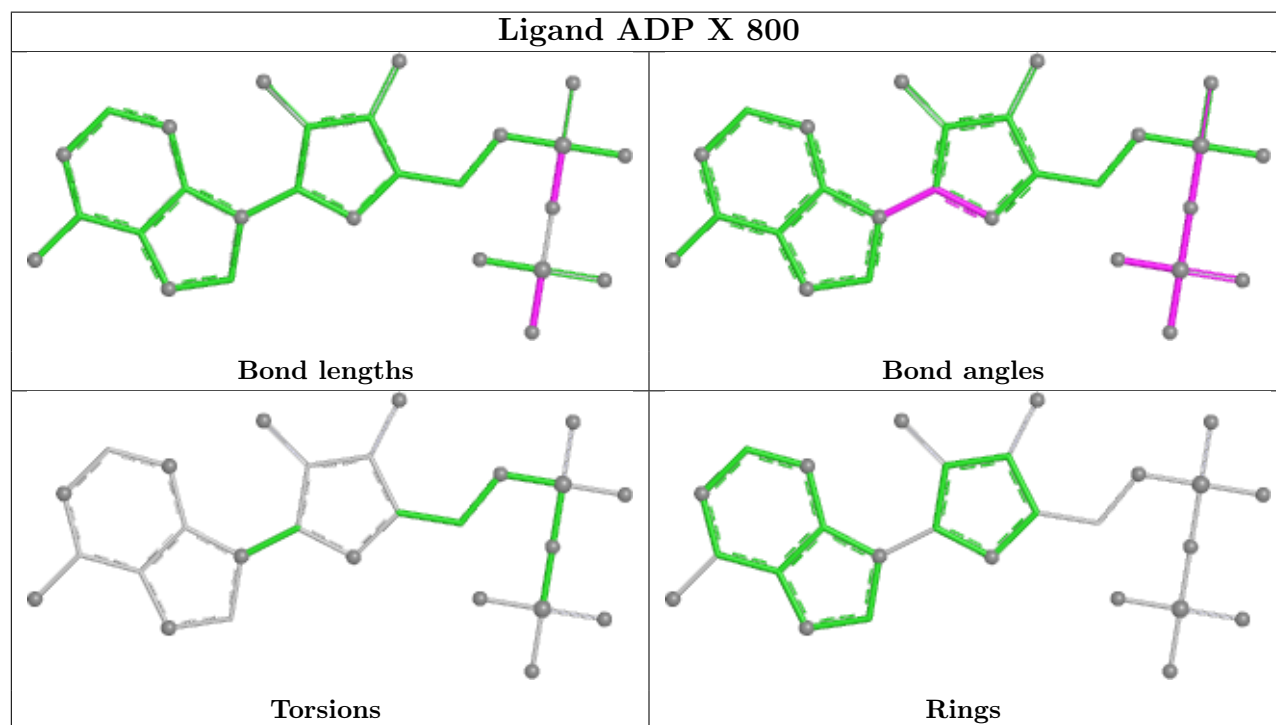
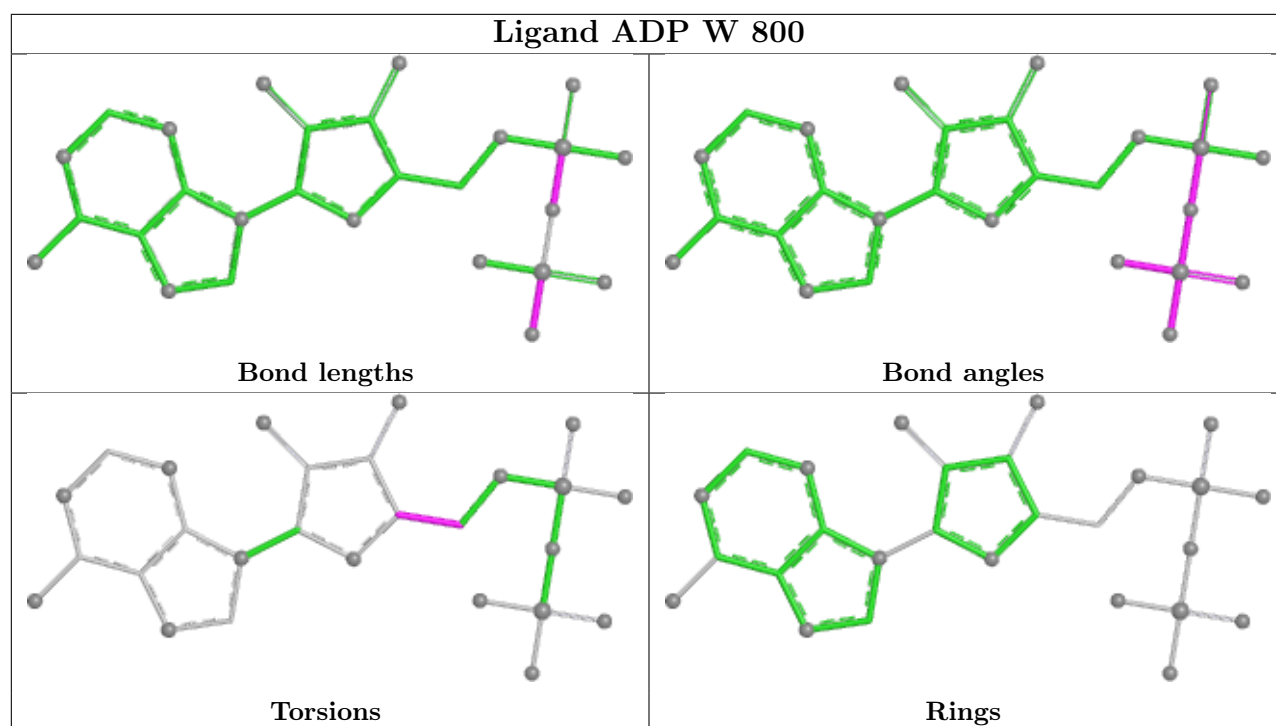
6 monomers are involved in 7 short contacts:

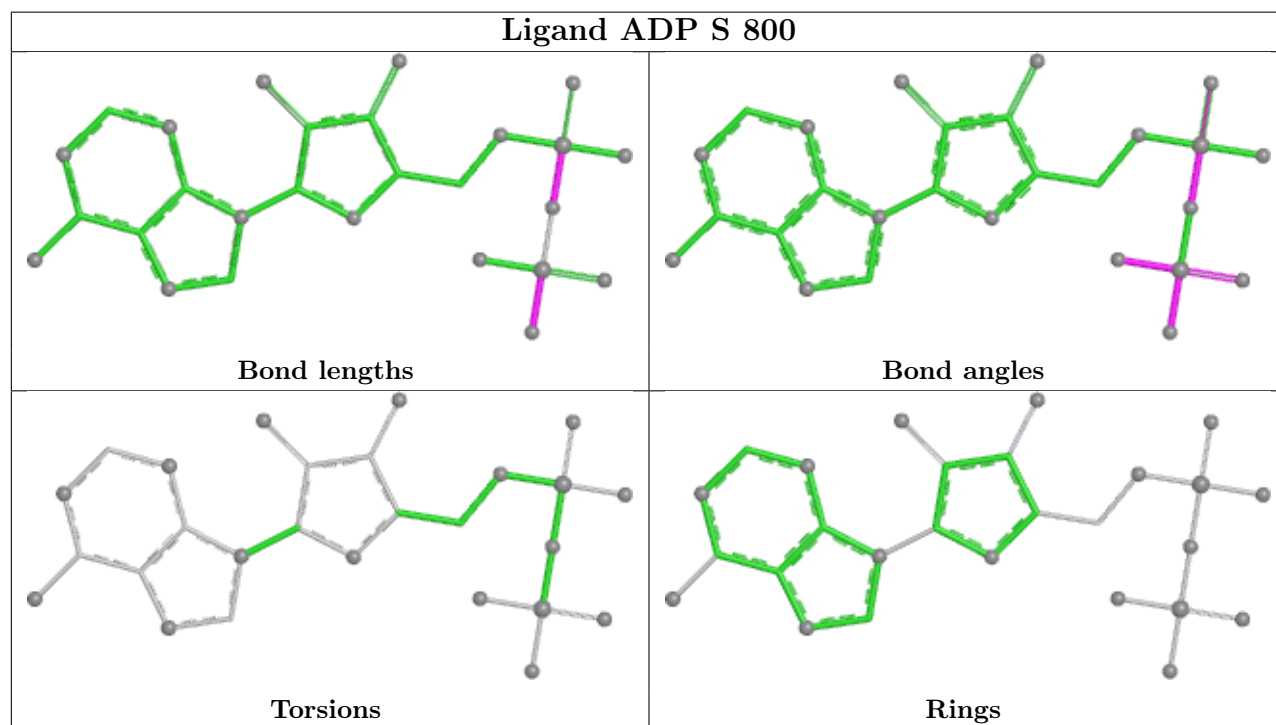
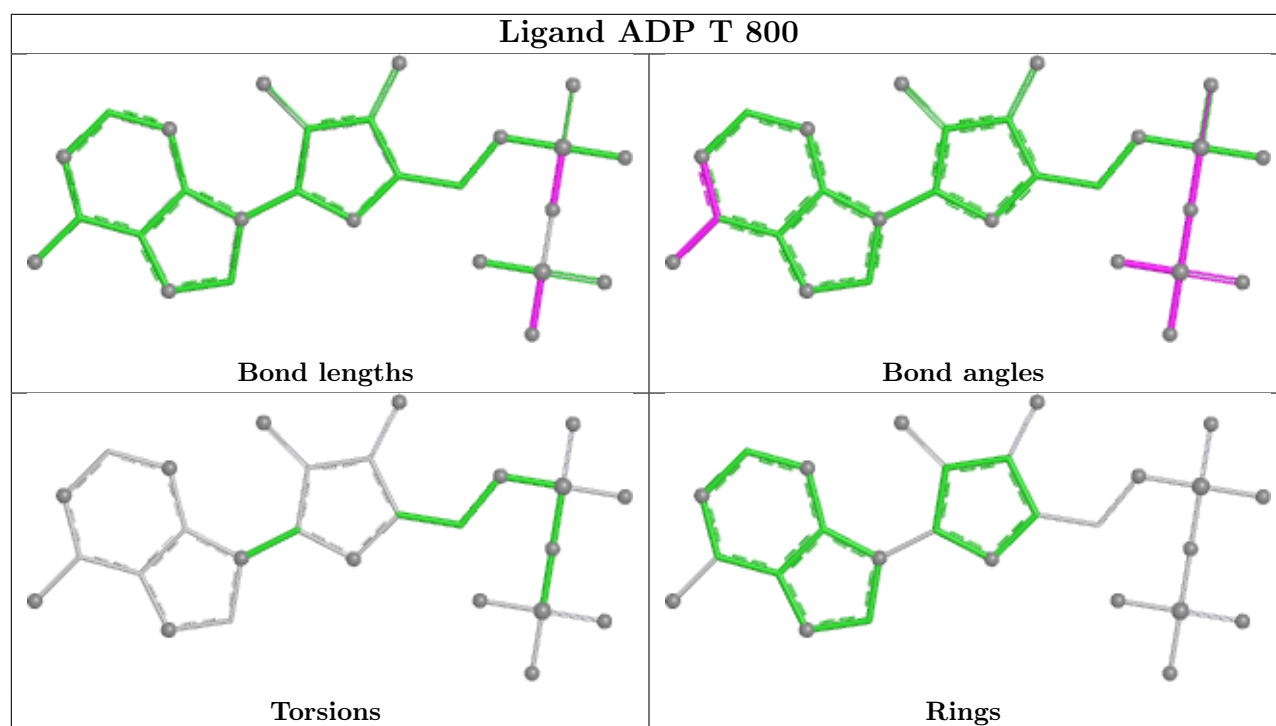
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	803	PO4	1	0
2	O	800	ADP	1	0
2	U	800	ADP	1	0
3	P	803	PO4	1	0
3	Y	801	PO4	2	0
3	R	801	PO4	1	0

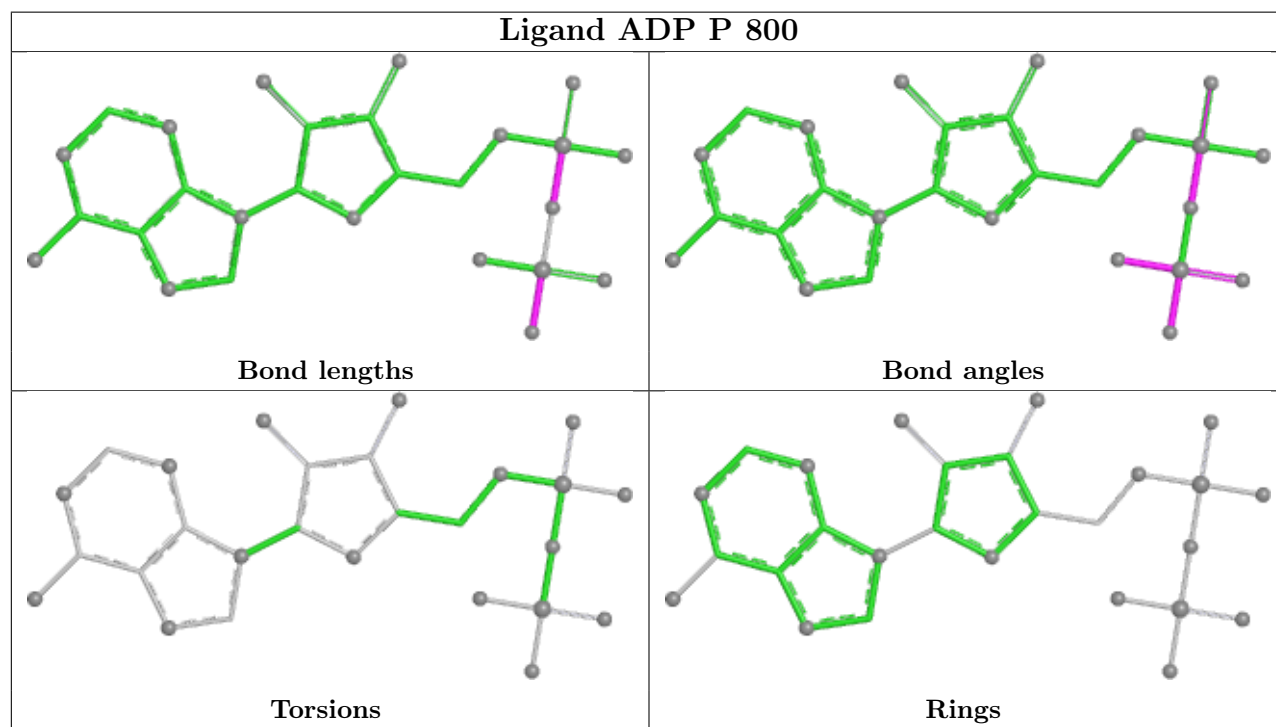
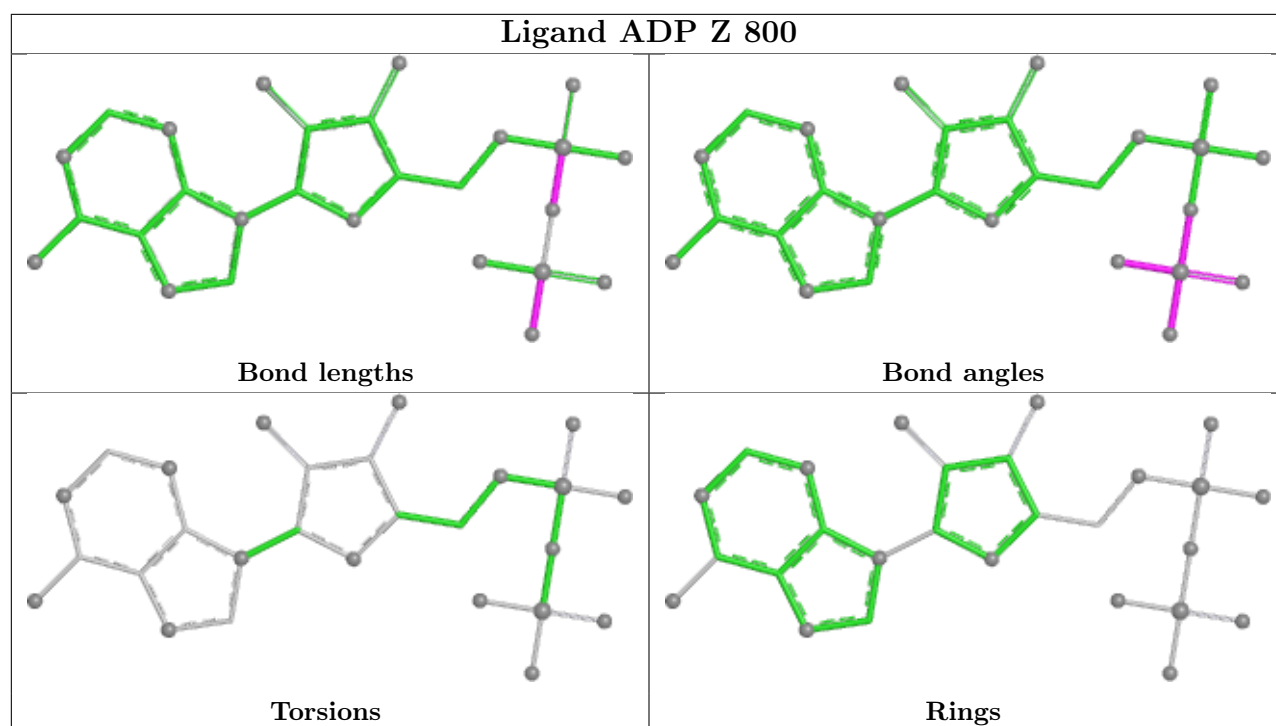
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

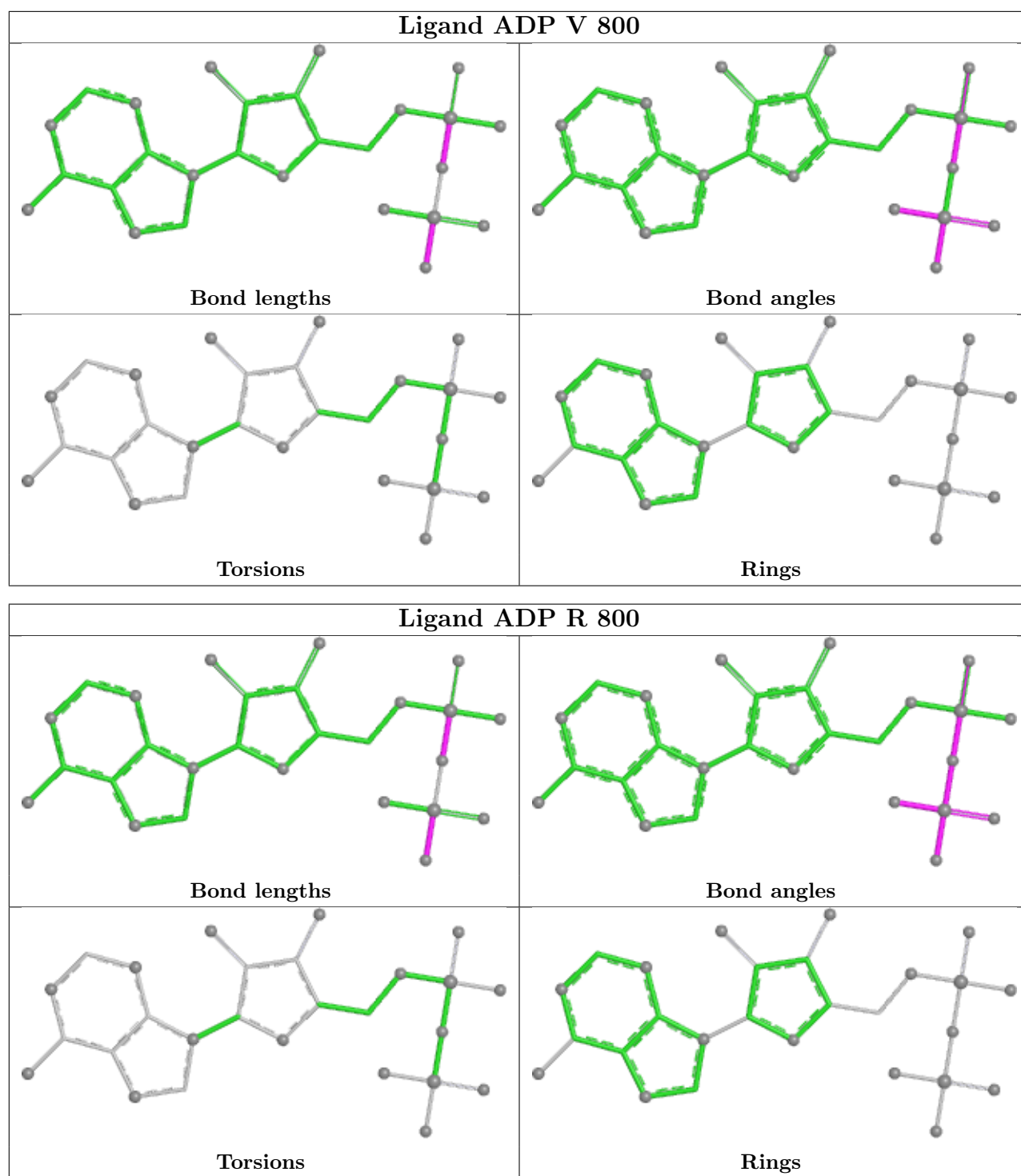












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1674. These allow visual inspection of the internal detail of the map and identification of artifacts.

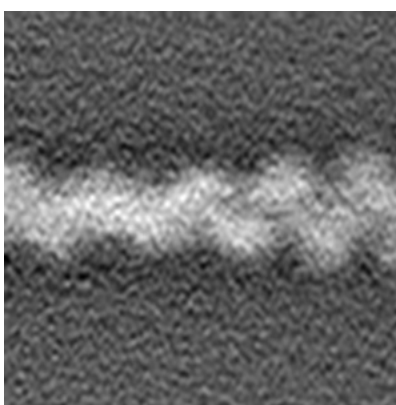
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

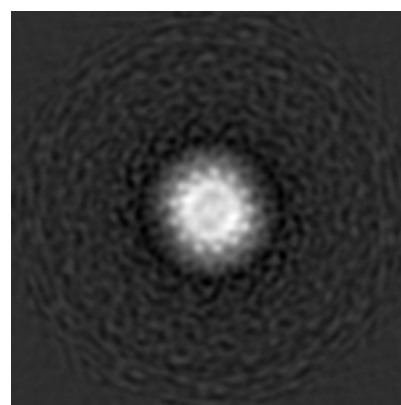
6.1.1 Primary map



X



Y

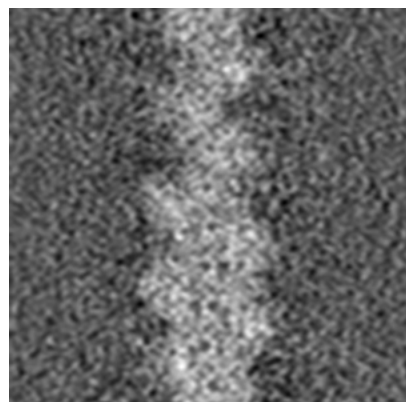


Z

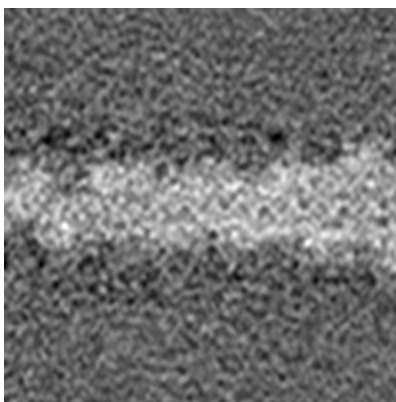
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

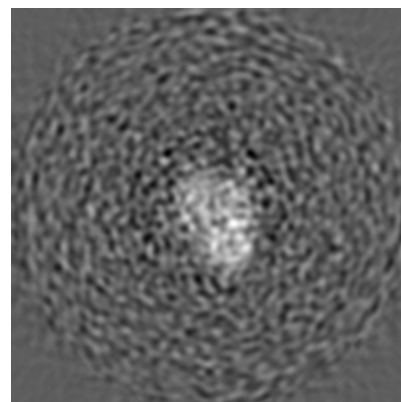
6.2.1 Primary map



X Index: 60



Y Index: 60

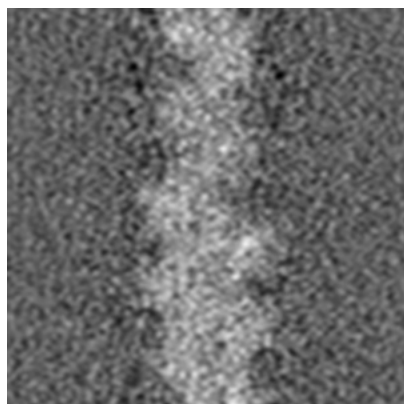


Z Index: 60

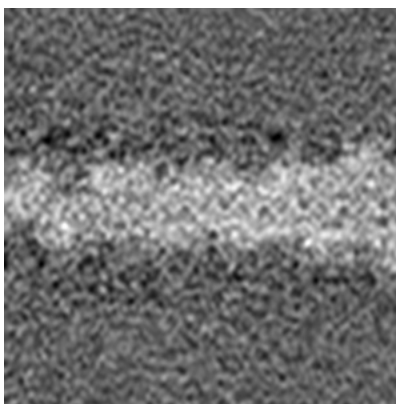
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

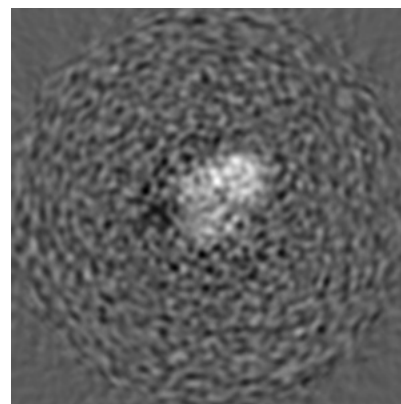
6.3.1 Primary map



X Index: 62



Y Index: 60

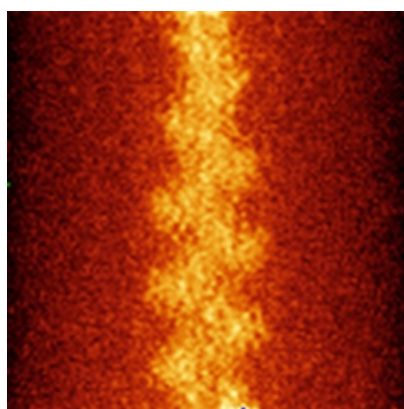


Z Index: 0

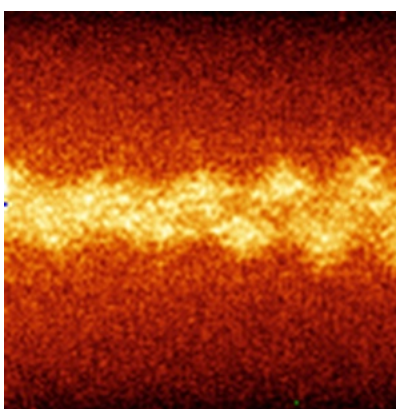
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

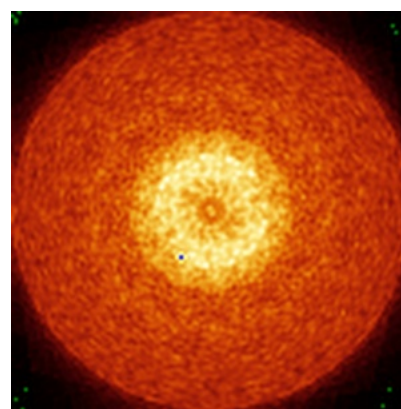
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

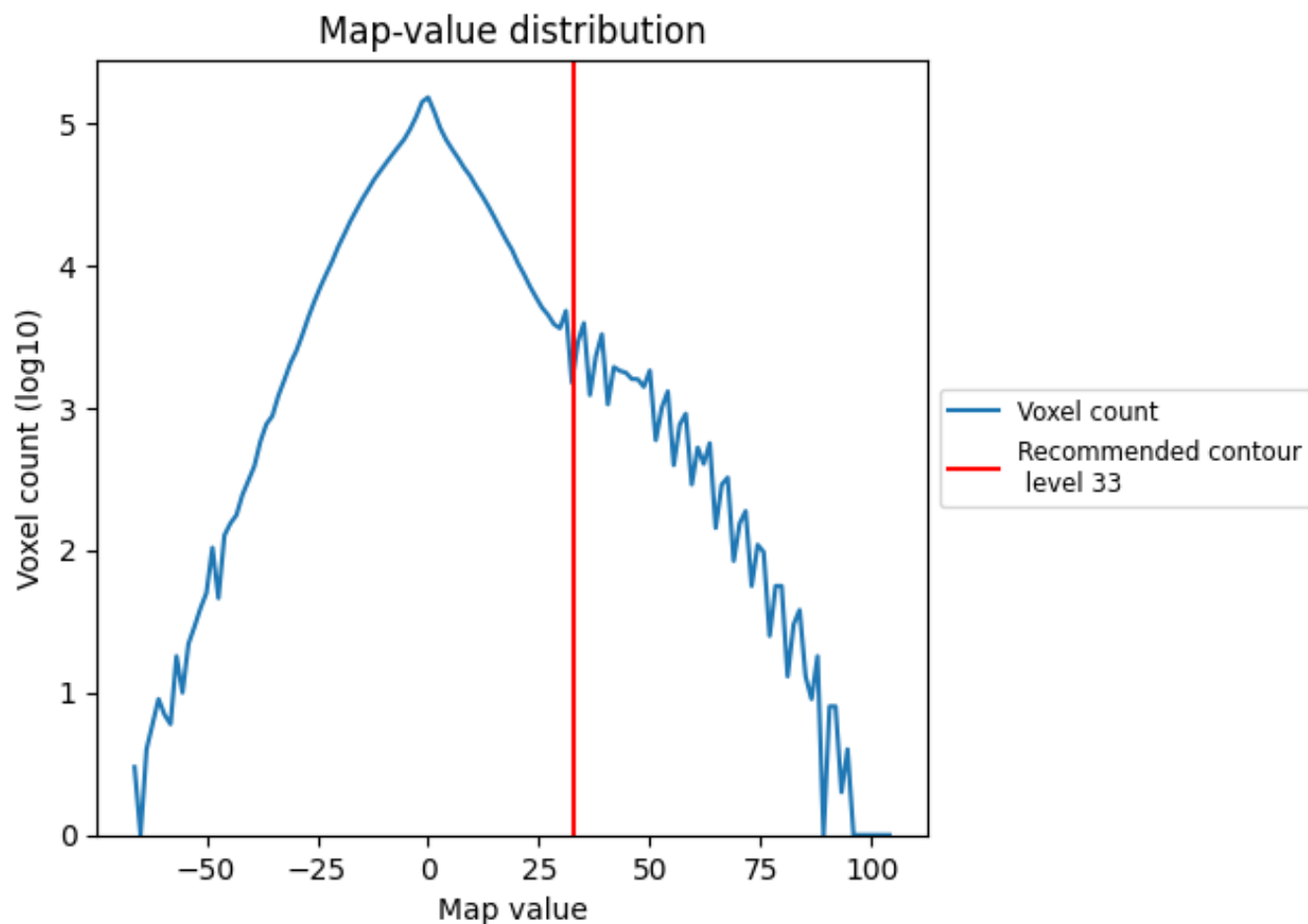
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

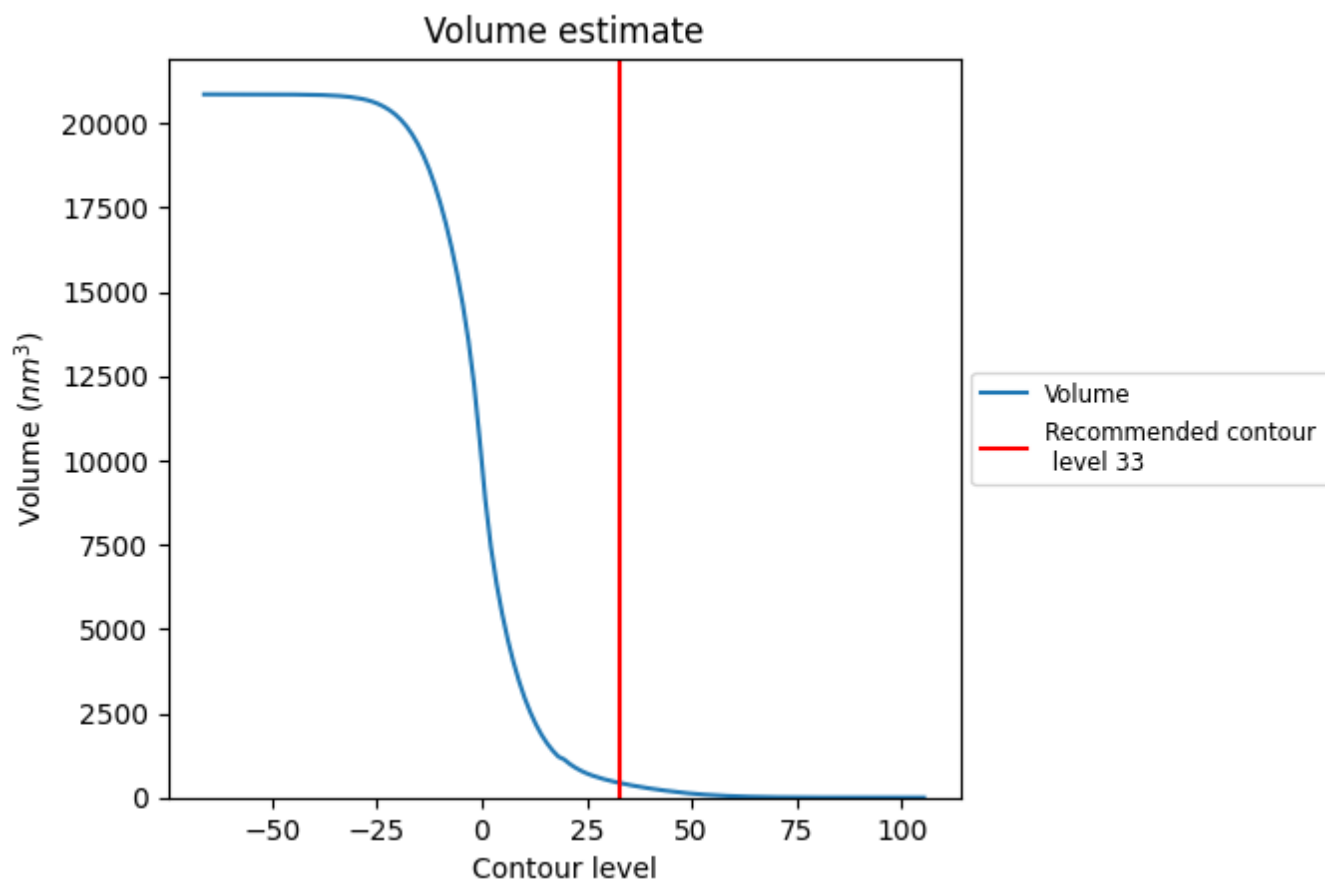
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

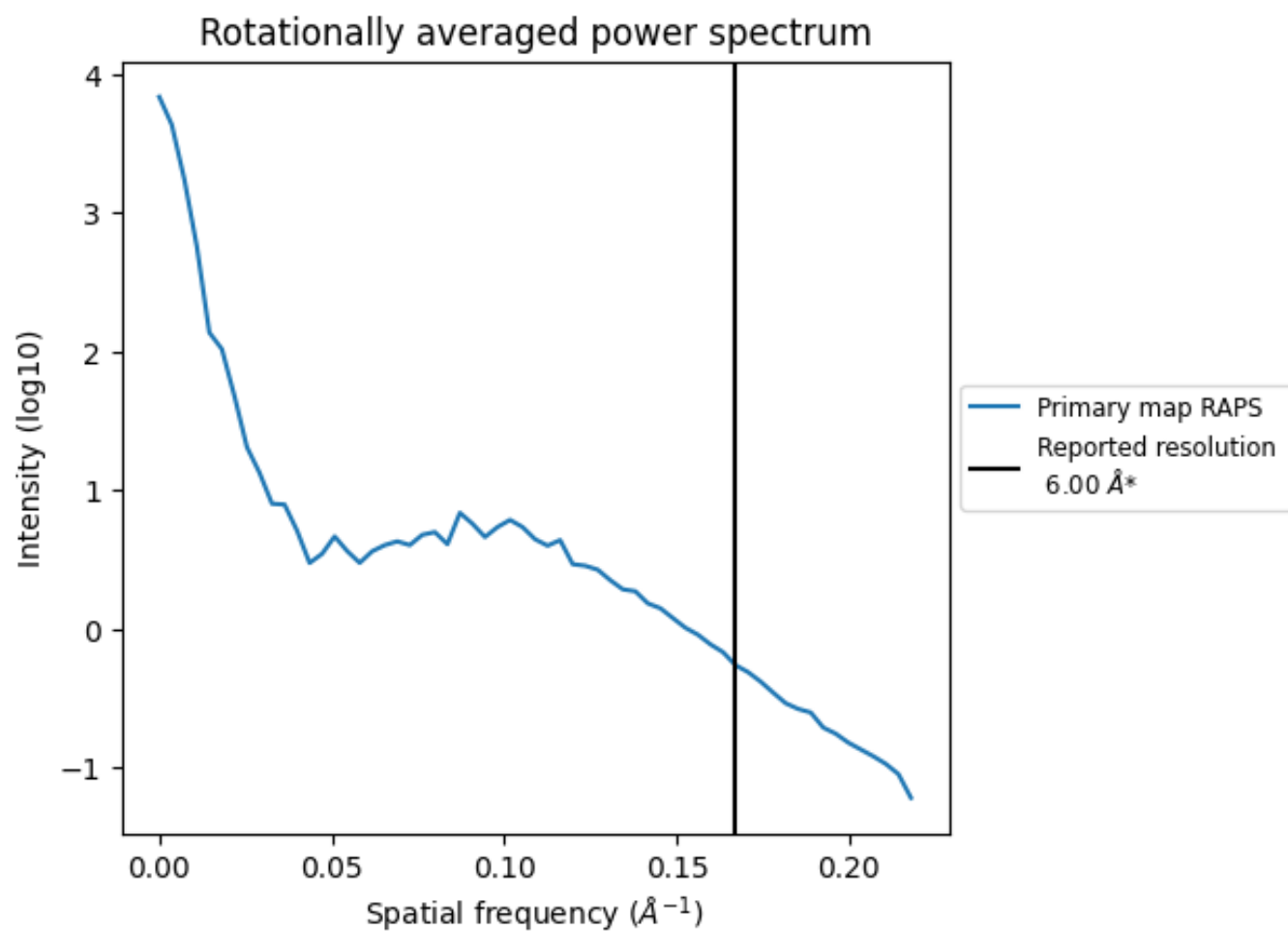
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 430 nm^3 ; this corresponds to an approximate mass of 388 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

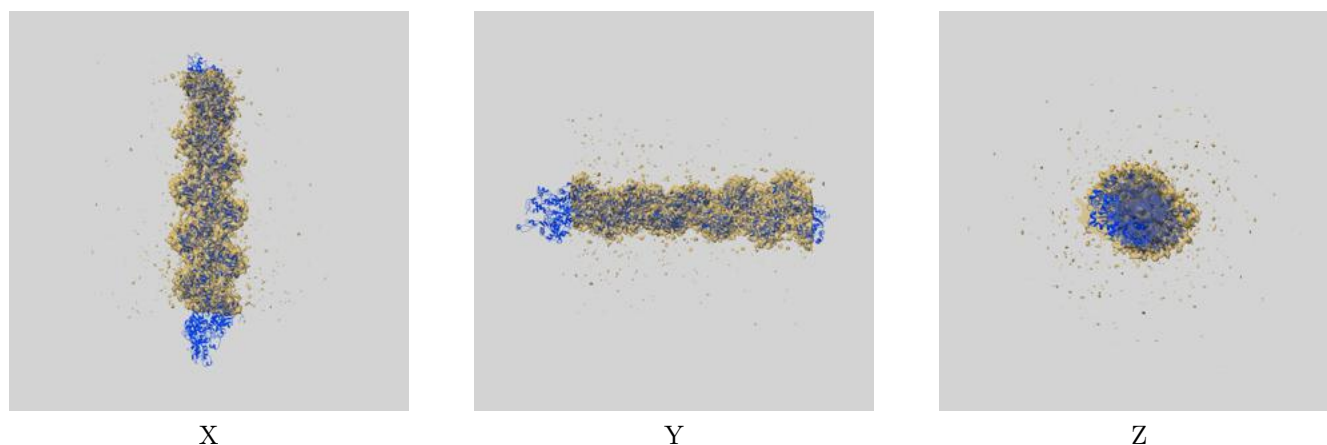
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

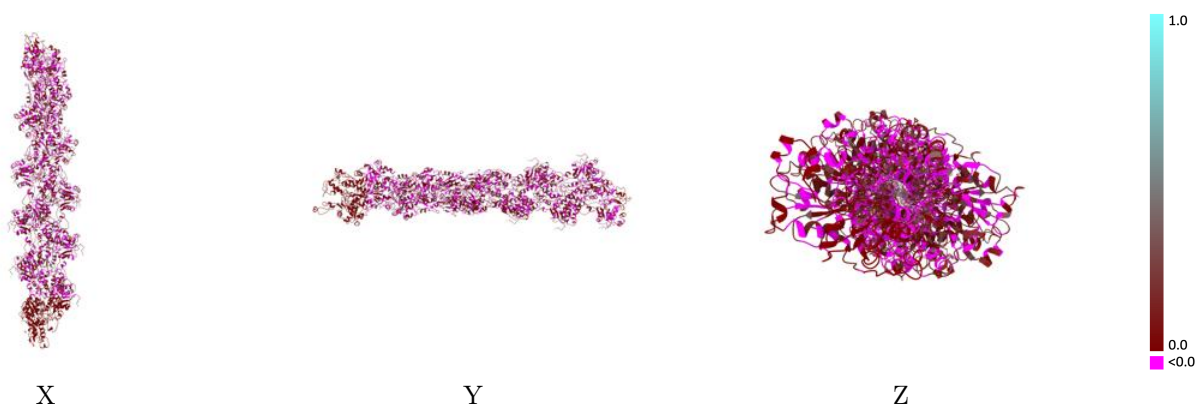
This section contains information regarding the fit between EMDB map EMD-1674 and PDB model 3G37. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



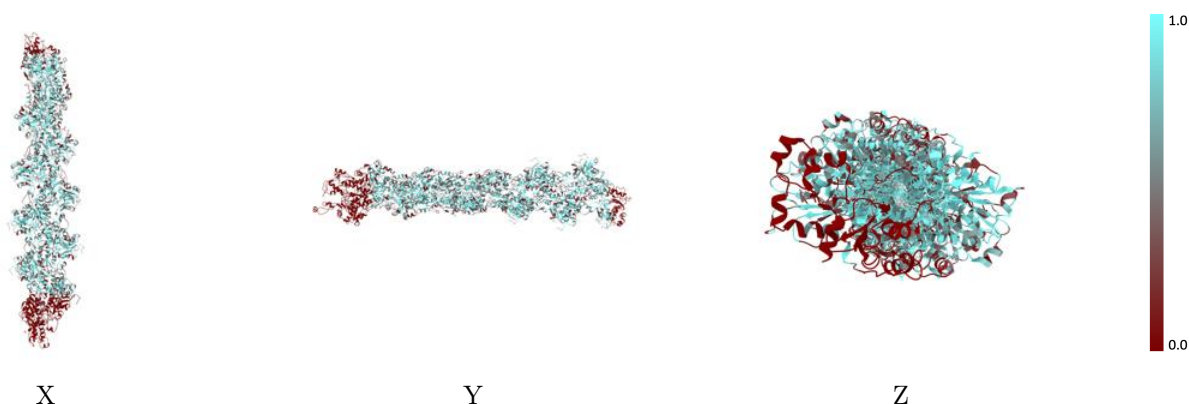
The images above show the 3D surface view of the map at the recommended contour level 33.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



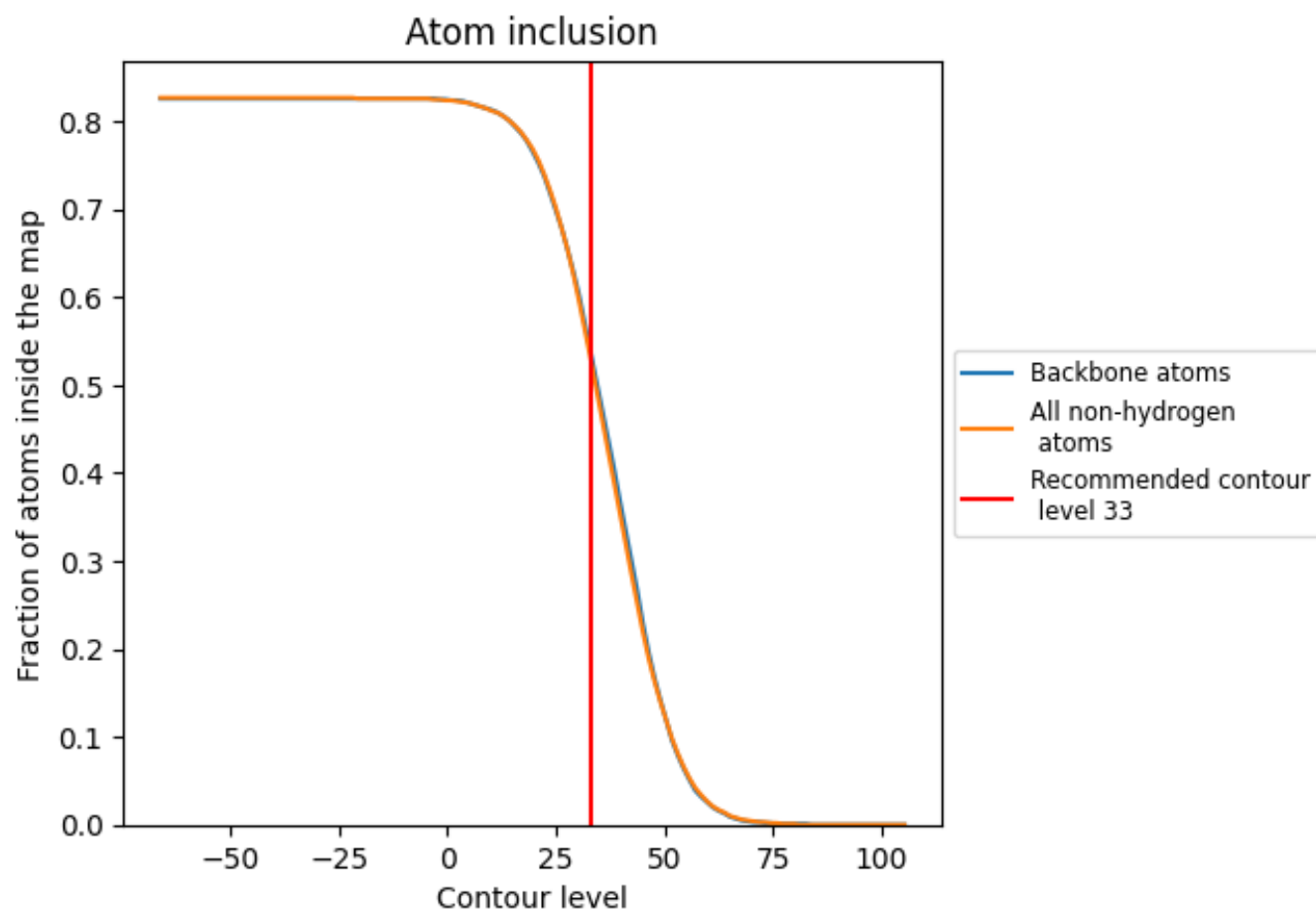
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (33).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5300	0.0660
O	0.3890	0.0510
P	0.6370	0.0790
Q	0.6350	0.0770
R	0.6400	0.0840
S	0.6460	0.0830
T	0.6410	0.0810
U	0.6410	0.0860
V	0.6450	0.0830
W	0.6350	0.0820
X	0.5890	0.0630
Y	0.2590	0.0180
Z	0.0000	-0.0010

