Full wwPDB EM Validation Report ⓘ

Nov 5, 2026 – 12:39 am GMT

PDB ID	:	31ON / pdb_000031on
EMDB ID	:	EMD-58589
Title	:	CryoEM structure of substrate engaged p97 in complex with Ufd1/Npl4 and C-terminal FAF1-State I
Authors	:	Drakonaki, A.; van den Boom, J.; Kroening, A.; Meyer, H.; Gatsogiannis, C.
Deposited on	:	2026-06-16
Resolution	:	3.20 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:

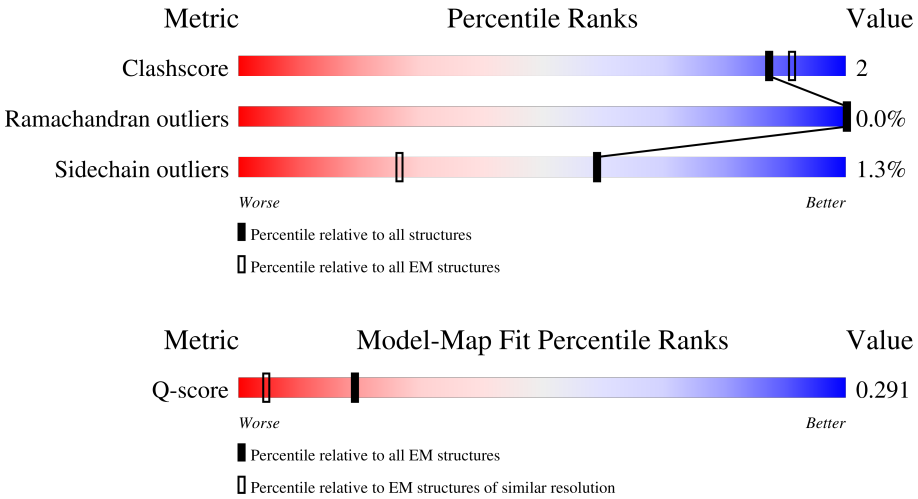
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 3.20 Å.

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



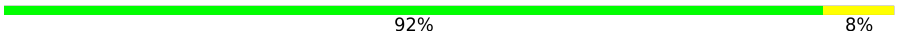
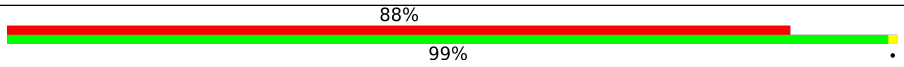
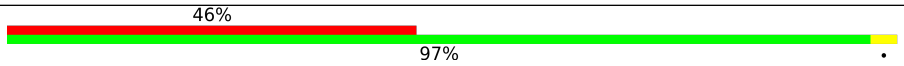
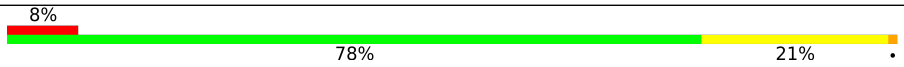
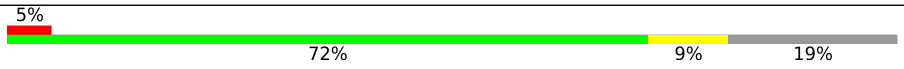
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 <=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	A	826	69% 20% • 10%
1	B	826	69% 22% • 8%
1	C	826	75% 16% 9%
1	D	826	71% 18% • 10%

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Mol	Chain	Length	Quality of chain
1	E	826	
1	F	826	
2	G	608	
3	I	76	
3	J	76	
3	K	76	
3	L	76	
3	M	76	
3	N	76	
4	T	170	
5	H	307	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 46145 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	743	Total	C	N	O	S	0	0
			5803	3651	1030	1092	30		
1	B	759	Total	C	N	O	S	0	0
			5951	3739	1056	1126	30		
1	C	752	Total	C	N	O	S	0	0
			5891	3706	1047	1108	30		
1	D	742	Total	C	N	O	S	0	0
			5789	3643	1025	1091	30		
1	E	732	Total	C	N	O	S	0	0
			5724	3602	1016	1077	29		
1	F	703	Total	C	N	O	S	0	0
			5531	3482	982	1038	29		

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P55072
A	-18	GLY	-	expression tag	UNP P55072
A	-17	SER	-	expression tag	UNP P55072
A	-16	SER	-	expression tag	UNP P55072
A	-15	HIS	-	expression tag	UNP P55072
A	-14	HIS	-	expression tag	UNP P55072
A	-13	HIS	-	expression tag	UNP P55072
A	-12	HIS	-	expression tag	UNP P55072
A	-11	HIS	-	expression tag	UNP P55072
A	-10	HIS	-	expression tag	UNP P55072
A	-9	SER	-	expression tag	UNP P55072
A	-8	SER	-	expression tag	UNP P55072
A	-7	GLY	-	expression tag	UNP P55072
A	-6	LEU	-	expression tag	UNP P55072
A	-5	VAL	-	expression tag	UNP P55072
A	-4	PRO	-	expression tag	UNP P55072
A	-3	ARG	-	expression tag	UNP P55072
A	-2	GLY	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P55072
A	0	HIS	-	expression tag	UNP P55072
A	232	GLU	ALA	variant	UNP P55072
A	578	GLN	GLU	engineered mutation	UNP P55072
B	-19	MET	-	initiating methionine	UNP P55072
B	-18	GLY	-	expression tag	UNP P55072
B	-17	SER	-	expression tag	UNP P55072
B	-16	SER	-	expression tag	UNP P55072
B	-15	HIS	-	expression tag	UNP P55072
B	-14	HIS	-	expression tag	UNP P55072
B	-13	HIS	-	expression tag	UNP P55072
B	-12	HIS	-	expression tag	UNP P55072
B	-11	HIS	-	expression tag	UNP P55072
B	-10	HIS	-	expression tag	UNP P55072
B	-9	SER	-	expression tag	UNP P55072
B	-8	SER	-	expression tag	UNP P55072
B	-7	GLY	-	expression tag	UNP P55072
B	-6	LEU	-	expression tag	UNP P55072
B	-5	VAL	-	expression tag	UNP P55072
B	-4	PRO	-	expression tag	UNP P55072
B	-3	ARG	-	expression tag	UNP P55072
B	-2	GLY	-	expression tag	UNP P55072
B	-1	SER	-	expression tag	UNP P55072
B	0	HIS	-	expression tag	UNP P55072
B	232	GLU	ALA	variant	UNP P55072
B	578	GLN	GLU	engineered mutation	UNP P55072
C	-19	MET	-	initiating methionine	UNP P55072
C	-18	GLY	-	expression tag	UNP P55072
C	-17	SER	-	expression tag	UNP P55072
C	-16	SER	-	expression tag	UNP P55072
C	-15	HIS	-	expression tag	UNP P55072
C	-14	HIS	-	expression tag	UNP P55072
C	-13	HIS	-	expression tag	UNP P55072
C	-12	HIS	-	expression tag	UNP P55072
C	-11	HIS	-	expression tag	UNP P55072
C	-10	HIS	-	expression tag	UNP P55072
C	-9	SER	-	expression tag	UNP P55072
C	-8	SER	-	expression tag	UNP P55072
C	-7	GLY	-	expression tag	UNP P55072
C	-6	LEU	-	expression tag	UNP P55072
C	-5	VAL	-	expression tag	UNP P55072
C	-4	PRO	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP P55072
C	-2	GLY	-	expression tag	UNP P55072
C	-1	SER	-	expression tag	UNP P55072
C	0	HIS	-	expression tag	UNP P55072
C	232	GLU	ALA	variant	UNP P55072
C	578	GLN	GLU	engineered mutation	UNP P55072
D	-19	MET	-	initiating methionine	UNP P55072
D	-18	GLY	-	expression tag	UNP P55072
D	-17	SER	-	expression tag	UNP P55072
D	-16	SER	-	expression tag	UNP P55072
D	-15	HIS	-	expression tag	UNP P55072
D	-14	HIS	-	expression tag	UNP P55072
D	-13	HIS	-	expression tag	UNP P55072
D	-12	HIS	-	expression tag	UNP P55072
D	-11	HIS	-	expression tag	UNP P55072
D	-10	HIS	-	expression tag	UNP P55072
D	-9	SER	-	expression tag	UNP P55072
D	-8	SER	-	expression tag	UNP P55072
D	-7	GLY	-	expression tag	UNP P55072
D	-6	LEU	-	expression tag	UNP P55072
D	-5	VAL	-	expression tag	UNP P55072
D	-4	PRO	-	expression tag	UNP P55072
D	-3	ARG	-	expression tag	UNP P55072
D	-2	GLY	-	expression tag	UNP P55072
D	-1	SER	-	expression tag	UNP P55072
D	0	HIS	-	expression tag	UNP P55072
D	232	GLU	ALA	variant	UNP P55072
D	578	GLN	GLU	engineered mutation	UNP P55072
E	-19	MET	-	initiating methionine	UNP P55072
E	-18	GLY	-	expression tag	UNP P55072
E	-17	SER	-	expression tag	UNP P55072
E	-16	SER	-	expression tag	UNP P55072
E	-15	HIS	-	expression tag	UNP P55072
E	-14	HIS	-	expression tag	UNP P55072
E	-13	HIS	-	expression tag	UNP P55072
E	-12	HIS	-	expression tag	UNP P55072
E	-11	HIS	-	expression tag	UNP P55072
E	-10	HIS	-	expression tag	UNP P55072
E	-9	SER	-	expression tag	UNP P55072
E	-8	SER	-	expression tag	UNP P55072
E	-7	GLY	-	expression tag	UNP P55072
E	-6	LEU	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	VAL	-	expression tag	UNP P55072
E	-4	PRO	-	expression tag	UNP P55072
E	-3	ARG	-	expression tag	UNP P55072
E	-2	GLY	-	expression tag	UNP P55072
E	-1	SER	-	expression tag	UNP P55072
E	0	HIS	-	expression tag	UNP P55072
E	232	GLU	ALA	variant	UNP P55072
E	578	GLN	GLU	engineered mutation	UNP P55072
F	-19	MET	-	initiating methionine	UNP P55072
F	-18	GLY	-	expression tag	UNP P55072
F	-17	SER	-	expression tag	UNP P55072
F	-16	SER	-	expression tag	UNP P55072
F	-15	HIS	-	expression tag	UNP P55072
F	-14	HIS	-	expression tag	UNP P55072
F	-13	HIS	-	expression tag	UNP P55072
F	-12	HIS	-	expression tag	UNP P55072
F	-11	HIS	-	expression tag	UNP P55072
F	-10	HIS	-	expression tag	UNP P55072
F	-9	SER	-	expression tag	UNP P55072
F	-8	SER	-	expression tag	UNP P55072
F	-7	GLY	-	expression tag	UNP P55072
F	-6	LEU	-	expression tag	UNP P55072
F	-5	VAL	-	expression tag	UNP P55072
F	-4	PRO	-	expression tag	UNP P55072
F	-3	ARG	-	expression tag	UNP P55072
F	-2	GLY	-	expression tag	UNP P55072
F	-1	SER	-	expression tag	UNP P55072
F	0	HIS	-	expression tag	UNP P55072
F	232	GLU	ALA	variant	UNP P55072
F	578	GLN	GLU	engineered mutation	UNP P55072

- Molecule 2 is a protein called Nuclear protein localization protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	540	Total	C	N	O	S	0	0
			4305	2731	737	818	19		

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	52	Total	C	N	O	S	0	0
			410	260	67	82	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	76	Total	C	N	O	S	0	0
			594	374	105	114	1		
3	K	76	Total	C	N	O	S	0	0
			594	374	105	114	1		
3	N	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
3	L	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
3	M	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

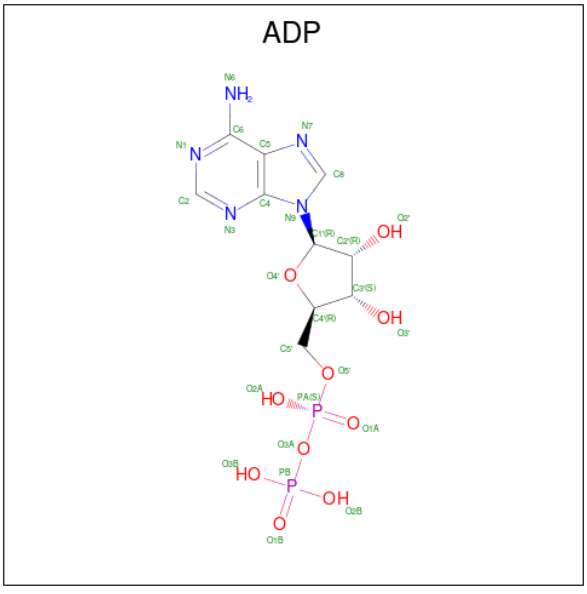
- Molecule 4 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	170	Total	C	N	O	S	0	0
			1422	888	251	280	3		

- Molecule 5 is a protein called Ubiquitin recognition factor in ER-associated degradation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	248	Total	C	N	O	S	0	0
			1954	1242	333	366	13		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

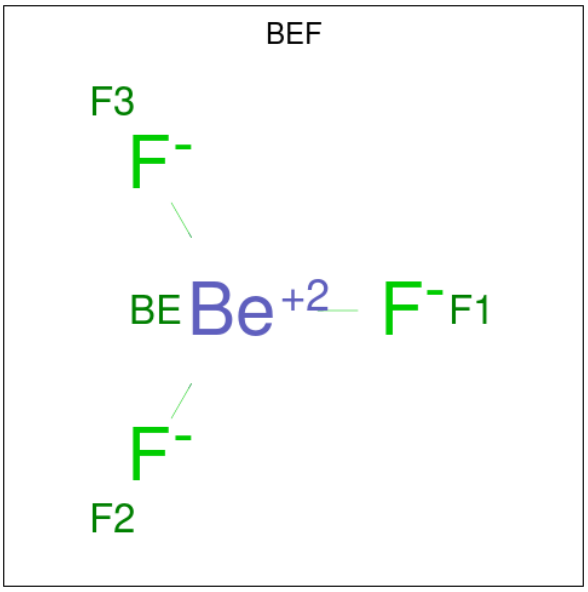


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Mg	0
			2	2	
7	B	1	Total	Mg	0
			1	1	
7	C	2	Total	Mg	0
			2	2	
7	D	3	Total	Mg	0
			3	3	
7	E	2	Total	Mg	0
			2	2	

- Molecule 8 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



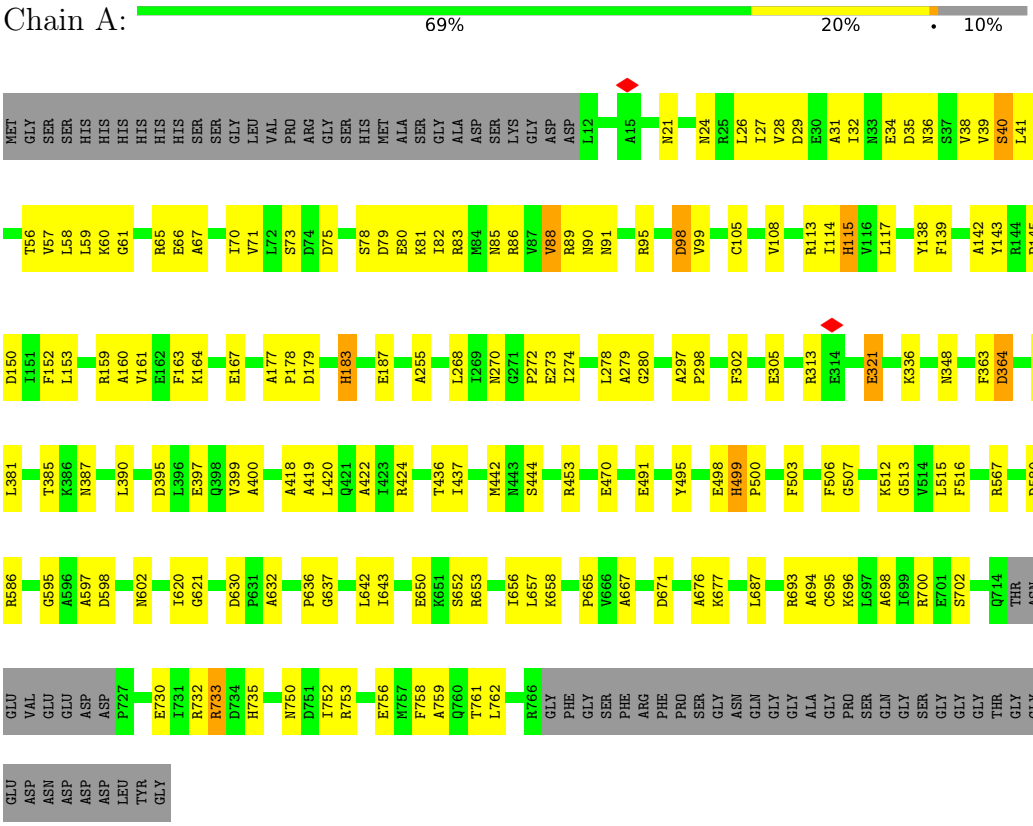
Mol	Chain	Residues	Atoms	AltConf
8	B	1	Total Be F 4 1 3	0
8	B	1	Total Be F 4 1 3	0
8	B	1	Total Be F 4 1 3	0
8	C	1	Total Be F 4 1 3	0
8	D	1	Total Be F 4 1 3	0
8	D	1	Total Be F 4 1 3	0
8	E	1	Total Be F 4 1 3	0
8	E	1	Total Be F 4 1 3	0
8	E	1	Total Be F 4 1 3	0
8	E	1	Total Be F 4 1 3	0

3 Residue-property plots (i)

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.

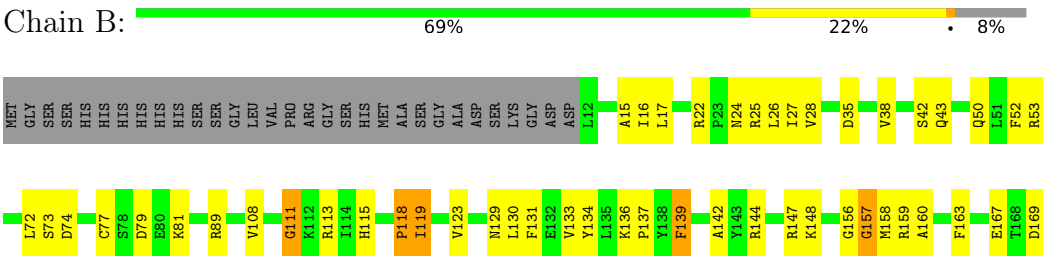
• Molecule 1: Transitional endoplasmic reticulum ATPase

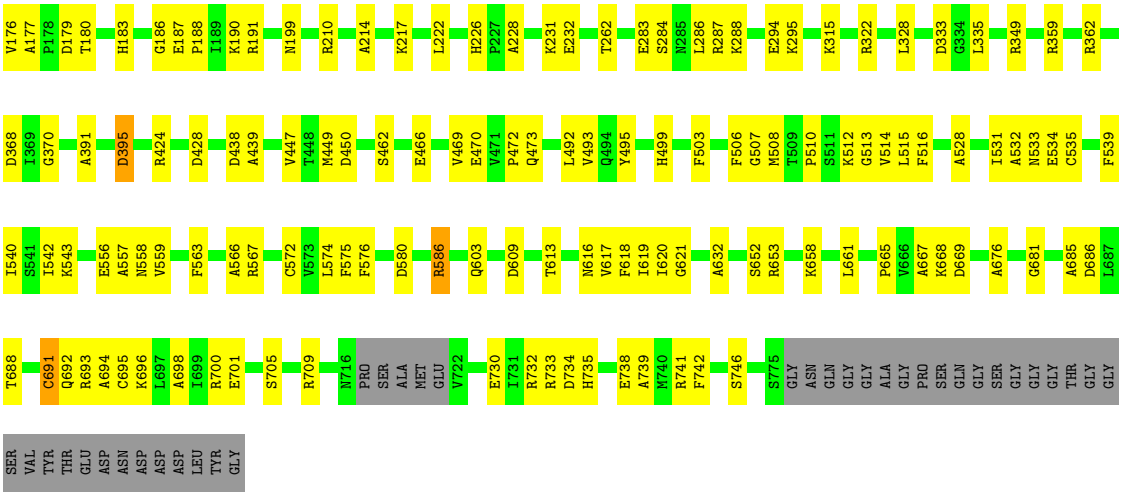
Chain A:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B:

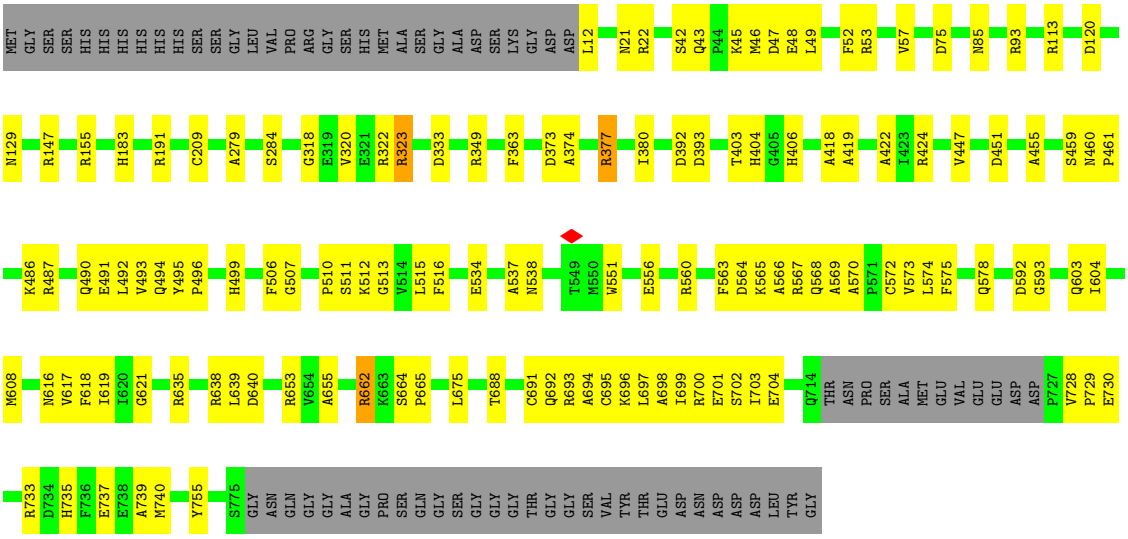




• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain C:

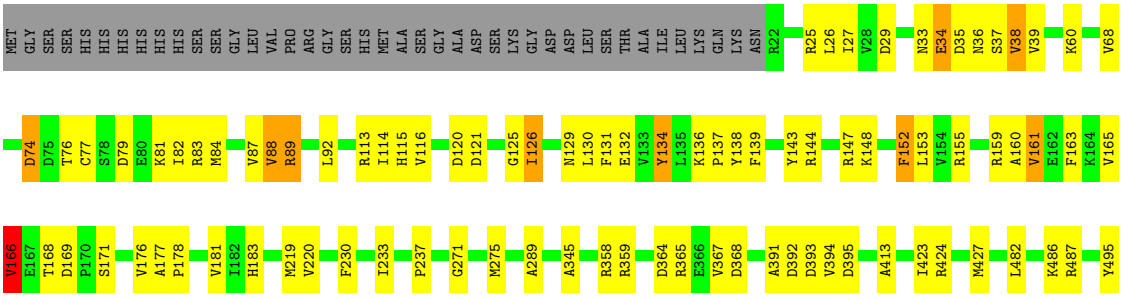


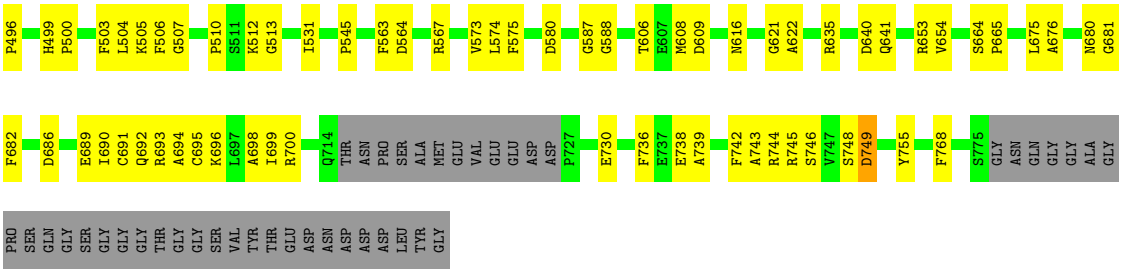


• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain D:



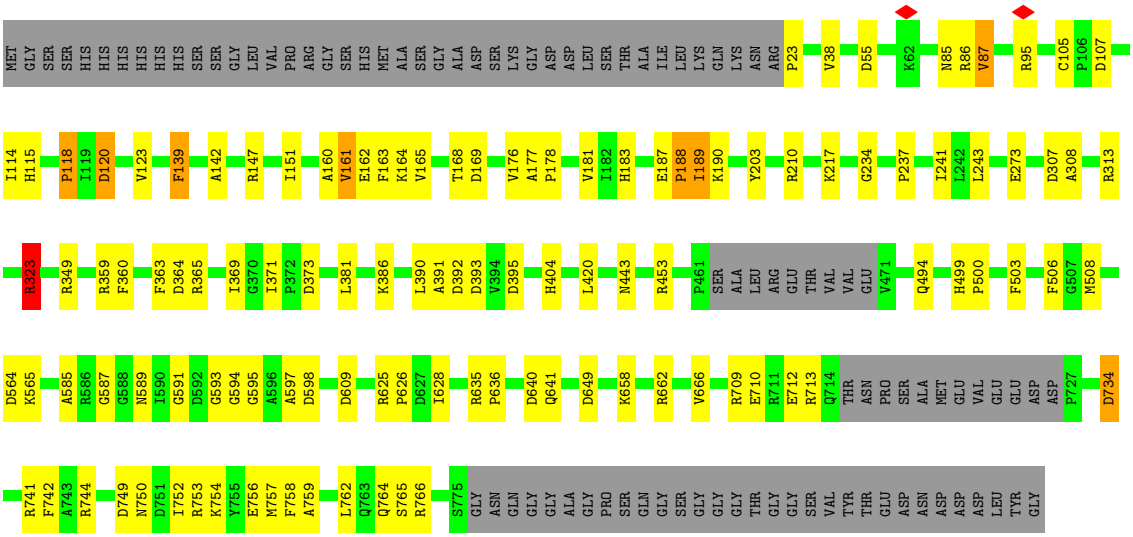




• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain E:

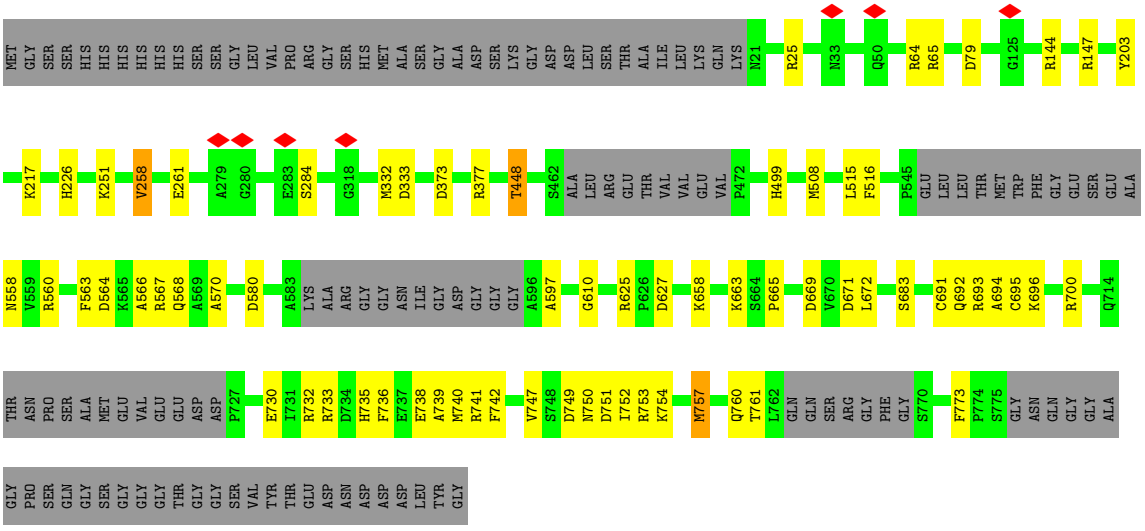




• Molecule 1: Transitional endoplasmic reticulum ATPase

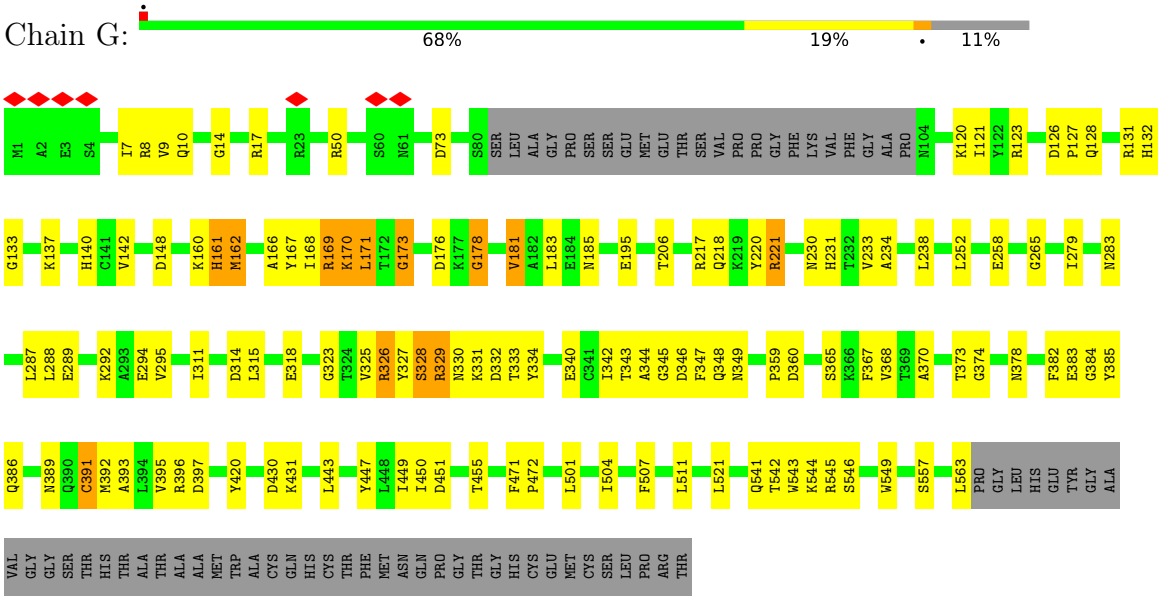
Chain F:





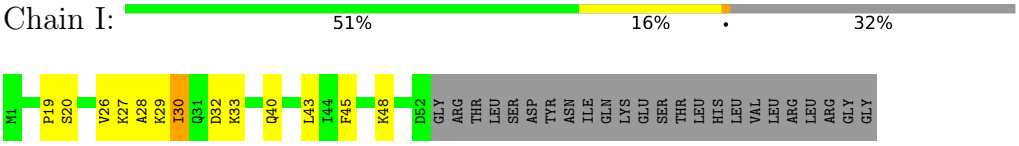
• Molecule 2: Nuclear protein localization protein 4 homolog

Chain G:



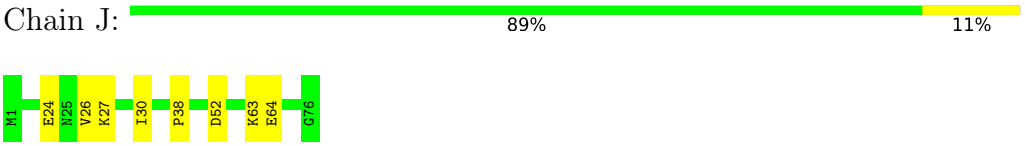
• Molecule 3: Polyubiquitin-B

Chain I:



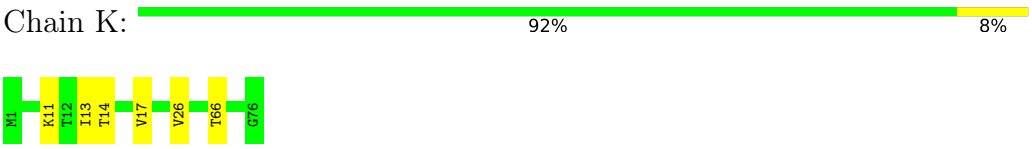
• Molecule 3: Polyubiquitin-B

Chain J:



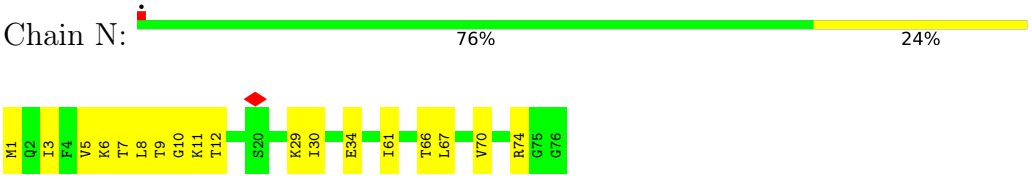
• Molecule 3: Polyubiquitin-B

Chain K:



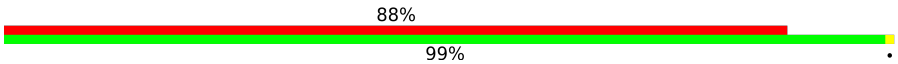
• Molecule 3: Polyubiquitin-B

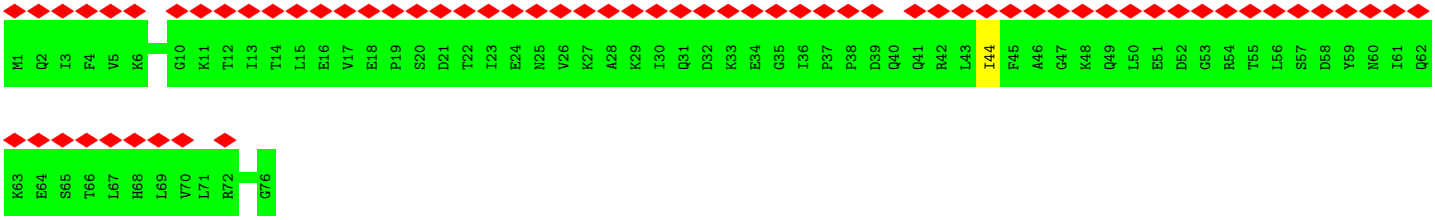
Chain N:



• Molecule 3: Polyubiquitin-B

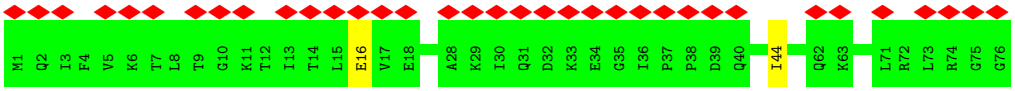
Chain L:



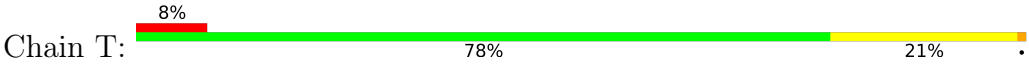


• Molecule 3: Polyubiquitin-B





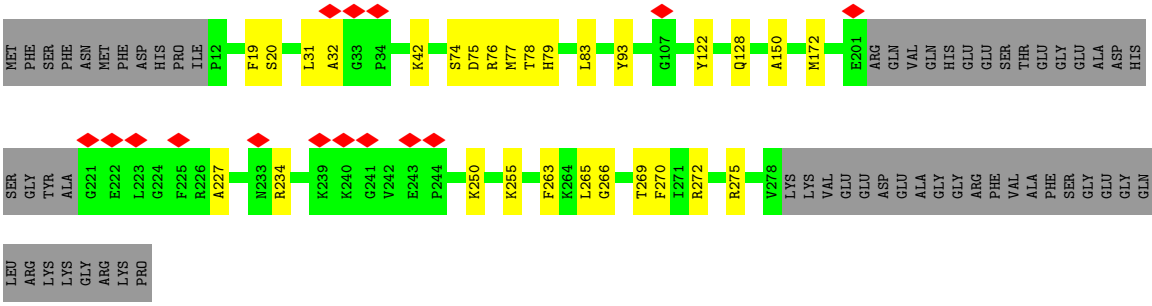
• Molecule 4: FAS-associated factor 1





• Molecule 5: Ubiquitin recognition factor in ER-associated degradation protein 1





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	270000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	60.748	Depositor
Minimum map value	-20.421	Depositor
Average map value	0.027	Depositor
Map value standard deviation	1.260	Depositor
Recommended contour level	2.69	Depositor
Map size (Å)	453.888, 453.888, 453.888	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.788, 0.788, 0.788	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.75	71/5896 (1.2%)	1.88	186/7960 (2.3%)
1	B	1.82	78/6048 (1.3%)	1.95	211/8164 (2.6%)
1	C	1.53	59/5988 (1.0%)	1.77	150/8081 (1.9%)
1	D	1.70	78/5886 (1.3%)	1.86	180/7948 (2.3%)
1	E	1.44	44/5820 (0.8%)	1.74	126/7854 (1.6%)
1	F	1.18	28/5620 (0.5%)	1.58	67/7581 (0.9%)
2	G	1.45	44/4404 (1.0%)	1.45	109/5967 (1.8%)
3	I	1.27	1/414 (0.2%)	1.60	8/557 (1.4%)
3	J	0.18	0/600	0.45	0/806
3	K	0.16	0/600	0.44	0/806
3	L	0.10	0/607	0.57	2/816 (0.2%)
3	M	0.10	0/607	0.67	4/816 (0.5%)
3	N	0.22	0/607	0.54	0/816
4	T	1.63	7/1445 (0.5%)	1.79	52/1939 (2.7%)
5	H	0.85	6/1995 (0.3%)	1.29	39/2694 (1.4%)
All	All	1.50	416/46537 (0.9%)	1.70	1134/62805 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
1	D	0	3
1	E	0	5
1	F	0	2
2	G	0	3
4	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	H	0	1
All	All	0	20

All (416) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	499	HIS	CE1-NE2	-10.90	1.21	1.32
1	C	499	HIS	CD2-NE2	-9.96	1.26	1.37
1	B	226	HIS	CE1-NE2	-9.35	1.23	1.32
1	B	499	HIS	CE1-NE2	-9.06	1.23	1.32
1	B	735	HIS	CE1-NE2	-8.96	1.23	1.32
1	B	115	HIS	ND1-CE1	-8.93	1.23	1.32
1	A	183	HIS	CE1-NE2	-8.91	1.23	1.32
1	D	499	HIS	CE1-NE2	-8.90	1.23	1.32
1	B	115	HIS	CE1-NE2	-8.89	1.23	1.32
1	A	115	HIS	CE1-NE2	-8.88	1.23	1.32
1	A	735	HIS	CE1-NE2	-8.87	1.23	1.32
1	B	177	ALA	CA-CB	-8.87	1.43	1.54
2	G	132	HIS	CE1-NE2	-8.86	1.23	1.32
1	C	404	HIS	ND1-CE1	-8.85	1.23	1.32
1	C	406	HIS	CE1-NE2	-8.84	1.23	1.32
1	C	735	HIS	CE1-NE2	-8.81	1.23	1.32
2	G	161	HIS	CE1-NE2	-8.79	1.23	1.32
1	E	499	HIS	CE1-NE2	-8.76	1.23	1.32
2	G	140	HIS	CE1-NE2	-8.74	1.23	1.32
1	D	115	HIS	ND1-CE1	-8.69	1.23	1.32
1	D	115	HIS	CE1-NE2	-8.68	1.23	1.32
2	G	8	ARG	CZ-NH2	-8.58	1.22	1.33
1	D	183	HIS	ND1-CE1	-8.57	1.24	1.32
1	B	226	HIS	CD2-NE2	-8.54	1.28	1.37
1	D	83	ARG	CZ-NH2	-8.52	1.22	1.33
1	C	487	ARG	CZ-NH2	-8.50	1.22	1.33
1	D	144	ARG	CZ-NH2	-8.48	1.22	1.33
2	G	329	ARG	CZ-NH2	-8.47	1.22	1.33
1	D	89	ARG	CZ-NH2	-8.44	1.22	1.33
1	A	700	ARG	CZ-NH2	-8.44	1.22	1.33
2	G	123	ARG	CZ-NH2	-8.41	1.22	1.33
1	D	653	ARG	CZ-NH2	-8.41	1.22	1.33
1	D	745	ARG	CZ-NH2	-8.39	1.22	1.33
1	E	766	ARG	CZ-NH2	-8.38	1.22	1.33
1	C	560	ARG	CZ-NH2	-8.37	1.22	1.33
1	B	191	ARG	CZ-NH2	-8.37	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	217	ARG	CZ-NH2	-8.36	1.22	1.33
1	C	700	ARG	CZ-NH2	-8.36	1.22	1.33
1	B	53	ARG	CZ-NH2	-8.35	1.22	1.33
1	B	499	HIS	CD2-NE2	-8.35	1.28	1.37
1	A	89	ARG	CZ-NH2	-8.35	1.22	1.33
1	A	147	ARG	CZ-NH2	-8.34	1.22	1.33
1	C	693	ARG	CZ-NH2	-8.34	1.22	1.33
1	B	210	ARG	CZ-NH2	-8.34	1.22	1.33
1	B	653	ARG	CZ-NH2	-8.33	1.22	1.33
1	A	424	ARG	CZ-NH2	-8.33	1.22	1.33
2	G	396	ARG	CZ-NH2	-8.32	1.22	1.33
1	A	95	ARG	CZ-NH2	-8.32	1.22	1.33
1	A	159	ARG	CZ-NH2	-8.32	1.22	1.33
1	D	567	ARG	CZ-NH2	-8.31	1.22	1.33
1	A	86	ARG	CZ-NH2	-8.31	1.22	1.33
1	E	625	ARG	CZ-NH2	-8.31	1.22	1.33
1	D	744	ARG	CZ-NH2	-8.31	1.22	1.33
1	E	349	ARG	CZ-NH2	-8.30	1.22	1.33
1	E	753	ARG	CZ-NH2	-8.30	1.22	1.33
1	A	65	ARG	CZ-NH2	-8.30	1.22	1.33
1	B	700	ARG	CZ-NH2	-8.30	1.22	1.33
1	B	159	ARG	CZ-NH2	-8.29	1.22	1.33
1	C	22	ARG	CZ-NH2	-8.29	1.22	1.33
1	D	487	ARG	CZ-NH2	-8.29	1.22	1.33
1	A	732	ARG	CZ-NH2	-8.28	1.22	1.33
1	C	567	ARG	CZ-NH2	-8.28	1.22	1.33
5	H	272	ARG	CZ-NH2	-8.28	1.22	1.33
1	A	115	HIS	CD2-NE2	-8.27	1.28	1.37
1	F	625	ARG	CZ-NH2	-8.27	1.22	1.33
1	A	653	ARG	CZ-NH2	-8.26	1.22	1.33
2	G	326	ARG	CZ-NH2	-8.26	1.22	1.33
1	B	732	ARG	CZ-NH2	-8.25	1.22	1.33
1	D	365	ARG	CZ-NH2	-8.25	1.22	1.33
1	B	693	ARG	CZ-NH2	-8.25	1.22	1.33
5	H	275	ARG	CZ-NH2	-8.25	1.22	1.33
1	E	86	ARG	CZ-NH2	-8.23	1.22	1.33
1	F	753	ARG	CZ-NH2	-8.23	1.22	1.33
1	C	735	HIS	CD2-NE2	-8.22	1.28	1.37
1	D	113	ARG	CZ-NH2	-8.22	1.22	1.33
1	B	25	ARG	CZ-NH2	-8.20	1.22	1.33
1	F	567	ARG	CZ-NH2	-8.20	1.22	1.33
1	E	713	ARG	CZ-NH2	-8.20	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	693	ARG	CZ-NH2	-8.19	1.22	1.33
1	C	53	ARG	CZ-NH2	-8.19	1.22	1.33
1	D	700	ARG	CZ-NH2	-8.18	1.22	1.33
1	A	753	ARG	CZ-NH2	-8.18	1.22	1.33
2	G	50	ARG	CZ-NH2	-8.18	1.22	1.33
1	C	406	HIS	CD2-NE2	-8.17	1.28	1.37
1	E	662	ARG	CZ-NH2	-8.17	1.22	1.33
1	D	159	ARG	CZ-NH2	-8.15	1.22	1.33
1	F	741	ARG	CZ-NH2	-8.15	1.22	1.33
1	A	586	ARG	CZ-NH2	-8.14	1.22	1.33
1	D	155	ARG	CZ-NH2	-8.13	1.22	1.33
1	B	735	HIS	CD2-NE2	-8.11	1.28	1.37
2	G	161	HIS	CD2-NE2	-8.11	1.28	1.37
1	F	693	ARG	CZ-NH2	-8.11	1.23	1.33
1	D	743	ALA	CA-CB	-8.11	1.39	1.53
1	A	183	HIS	CD2-NE2	-8.09	1.28	1.37
1	E	499	HIS	CD2-NE2	-8.08	1.28	1.37
2	G	140	HIS	CD2-NE2	-8.07	1.28	1.37
1	E	183	HIS	ND1-CE1	-8.06	1.24	1.32
1	B	115	HIS	CD2-NE2	-8.05	1.28	1.37
1	A	735	HIS	CD2-NE2	-8.05	1.28	1.37
1	A	499	HIS	CE1-NE2	-8.05	1.24	1.32
2	G	132	HIS	CD2-NE2	-8.03	1.29	1.37
1	D	115	HIS	CD2-NE2	-7.97	1.29	1.37
1	E	115	HIS	CE1-NE2	-7.95	1.24	1.32
2	G	131	ARG	CZ-NH2	-7.95	1.23	1.33
2	G	169	ARG	CZ-NH2	-7.94	1.23	1.33
1	D	499	HIS	CD2-NE2	-7.94	1.29	1.37
1	F	700	ARG	CZ-NH2	-7.88	1.23	1.33
1	C	570	ALA	CA-CB	-7.85	1.42	1.53
1	A	61	GLY	N-CA	-7.68	1.37	1.44
1	B	183	HIS	CE1-NE2	-7.56	1.25	1.32
1	A	621	GLY	N-CA	-7.51	1.37	1.45
1	C	495	TYR	N-CA	-7.49	1.40	1.46
1	A	499	HIS	CD2-NE2	-7.47	1.29	1.37
1	C	698	ALA	CA-CB	-7.43	1.41	1.53
1	E	115	HIS	CD2-NE2	-7.42	1.29	1.37
4	T	562	PRO	CA-CB	-7.35	1.47	1.53
1	B	566	ALA	CA-CB	-7.31	1.42	1.53
1	B	694	ALA	CA-CB	-7.31	1.42	1.53
1	C	455	ALA	CA-CB	-7.31	1.42	1.53
1	C	418	ALA	CA-CB	-7.31	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	739	ALA	CA-CB	-7.31	1.42	1.53
1	C	419	ALA	CA-CB	-7.30	1.42	1.53
1	C	655	ALA	CA-CB	-7.29	1.42	1.53
1	C	566	ALA	CA-CB	-7.29	1.42	1.53
1	B	676	ALA	CA-CB	-7.29	1.42	1.53
1	C	694	ALA	CA-CB	-7.28	1.42	1.53
1	B	214	ALA	CA-CB	-7.26	1.42	1.53
2	G	393	ALA	CA-CB	-7.25	1.42	1.53
1	B	528	ALA	CA-CB	-7.23	1.42	1.53
1	D	694	ALA	CA-CB	-7.23	1.42	1.53
1	B	557	ALA	CA-CB	-7.22	1.42	1.53
1	A	418	ALA	CA-CB	-7.22	1.42	1.53
1	B	156	GLY	N-CA	-7.21	1.38	1.45
1	B	739	ALA	CA-CB	-7.19	1.42	1.53
1	B	698	ALA	CA-CB	-7.18	1.42	1.53
1	A	694	ALA	CA-CB	-7.17	1.42	1.53
3	I	28	ALA	CA-CB	-7.17	1.42	1.53
1	A	419	ALA	CA-CB	-7.17	1.42	1.53
1	D	676	ALA	CA-CB	-7.17	1.42	1.53
1	A	698	ALA	CA-CB	-7.16	1.42	1.53
1	A	632	ALA	CA-CB	-7.13	1.42	1.53
1	E	759	ALA	CA-CB	-7.13	1.42	1.53
1	D	739	ALA	CA-CB	-7.11	1.42	1.53
2	G	344	ALA	CA-CB	-7.11	1.42	1.53
1	A	676	ALA	CA-CB	-7.10	1.42	1.53
1	A	374	ALA	CA-CB	-7.10	1.42	1.53
1	A	759	ALA	CA-CB	-7.09	1.42	1.53
1	F	694	ALA	CA-CB	-7.09	1.42	1.53
1	F	739	ALA	CA-CB	-7.06	1.42	1.53
1	D	289	ALA	CA-CB	-7.06	1.42	1.53
1	A	667	ALA	CA-CB	-7.06	1.42	1.53
1	C	422	ALA	CA-CB	-7.04	1.42	1.53
1	B	532	ALA	CA-CB	-7.04	1.42	1.53
1	A	513	GLY	N-CA	-7.04	1.38	1.45
4	T	604	ALA	CA-CB	-7.02	1.42	1.53
1	B	667	ALA	CA-CB	-7.02	1.42	1.53
1	A	400	ALA	CA-CB	-6.99	1.42	1.53
1	B	439	ALA	CA-CB	-6.99	1.42	1.53
1	A	585	ALA	CA-CB	-6.97	1.42	1.53
1	B	183	HIS	CD2-NE2	-6.94	1.30	1.37
1	B	391	ALA	CA-CB	-6.93	1.42	1.53
1	E	753	ARG	CZ-NH1	-6.92	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ARG	CZ-NH1	-6.91	1.23	1.32
1	E	308	ALA	CA-CB	-6.90	1.42	1.53
1	E	391	ALA	CA-CB	-6.90	1.42	1.53
1	F	735	HIS	CE1-NE2	-6.86	1.25	1.32
5	H	272	ARG	CZ-NH1	-6.85	1.23	1.32
1	B	700	ARG	CZ-NH1	-6.85	1.23	1.32
2	G	217	ARG	CZ-NH1	-6.85	1.23	1.32
1	D	83	ARG	CZ-NH1	-6.85	1.23	1.32
1	A	732	ARG	CZ-NH1	-6.84	1.23	1.32
1	C	560	ARG	CZ-NH1	-6.84	1.23	1.32
1	F	570	ALA	CA-CB	-6.84	1.42	1.53
1	C	665	PRO	CA-CB	-6.83	1.46	1.54
2	G	8	ARG	CZ-NH1	-6.82	1.23	1.32
1	A	700	ARG	CZ-NH1	-6.80	1.23	1.32
1	B	653	ARG	CZ-NH1	-6.80	1.23	1.32
1	A	89	ARG	CZ-NH1	-6.79	1.23	1.32
1	D	693	ARG	CZ-NH1	-6.78	1.23	1.32
4	T	570	ALA	CA-CB	-6.78	1.42	1.53
2	G	123	ARG	CZ-NH1	-6.78	1.23	1.32
1	D	653	ARG	CZ-NH1	-6.78	1.23	1.32
1	B	621	GLY	N-CA	-6.78	1.38	1.44
1	E	349	ARG	CZ-NH1	-6.78	1.23	1.32
1	B	732	ARG	CZ-NH1	-6.77	1.23	1.32
1	B	191	ARG	CZ-NH1	-6.77	1.23	1.32
1	D	168	THR	C-N	-6.77	1.28	1.33
1	C	700	ARG	CZ-NH1	-6.76	1.23	1.32
2	G	396	ARG	CZ-NH1	-6.75	1.23	1.32
1	A	159	ARG	CZ-NH1	-6.75	1.23	1.32
1	E	713	ARG	CZ-NH1	-6.75	1.23	1.32
1	C	487	ARG	CZ-NH1	-6.74	1.23	1.32
1	D	160	ALA	CA-CB	-6.74	1.42	1.53
1	E	766	ARG	CZ-NH1	-6.74	1.23	1.32
1	A	424	ARG	CZ-NH1	-6.74	1.23	1.32
1	B	693	ARG	CZ-NH1	-6.74	1.23	1.32
1	A	753	ARG	CZ-NH1	-6.74	1.23	1.32
1	C	567	ARG	CZ-NH1	-6.73	1.23	1.32
1	A	653	ARG	CZ-NH1	-6.73	1.23	1.32
1	B	53	ARG	CZ-NH1	-6.72	1.23	1.32
1	F	567	ARG	CZ-NH1	-6.72	1.23	1.32
1	A	160	ALA	CA-CB	-6.72	1.42	1.53
1	C	22	ARG	CZ-NH1	-6.72	1.23	1.32
1	A	86	ARG	CZ-NH1	-6.71	1.23	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	144	ARG	CZ-NH1	-6.71	1.23	1.32
1	D	487	ARG	CZ-NH1	-6.71	1.23	1.32
1	E	625	ARG	CZ-NH1	-6.71	1.23	1.32
1	B	159	ARG	CZ-NH1	-6.71	1.23	1.32
1	D	365	ARG	CZ-NH1	-6.70	1.23	1.32
1	A	147	ARG	CZ-NH1	-6.70	1.23	1.32
1	D	113	ARG	CZ-NH1	-6.70	1.23	1.32
1	B	25	ARG	CZ-NH1	-6.70	1.23	1.32
1	D	744	ARG	CZ-NH1	-6.69	1.23	1.32
1	A	95	ARG	CZ-NH1	-6.69	1.23	1.32
1	C	693	ARG	CZ-NH1	-6.68	1.23	1.32
5	H	275	ARG	CZ-NH1	-6.68	1.23	1.32
1	C	537	ALA	CA-CB	-6.68	1.42	1.53
1	B	210	ARG	CZ-NH1	-6.67	1.23	1.32
1	D	567	ARG	CZ-NH1	-6.67	1.23	1.32
1	D	700	ARG	CZ-NH1	-6.67	1.23	1.32
1	E	86	ARG	CZ-NH1	-6.67	1.23	1.32
2	G	50	ARG	CZ-NH1	-6.67	1.23	1.32
1	D	745	ARG	CZ-NH1	-6.67	1.23	1.32
1	C	53	ARG	CZ-NH1	-6.67	1.23	1.32
1	F	693	ARG	CZ-NH1	-6.66	1.23	1.32
1	D	89	ARG	CZ-NH1	-6.65	1.23	1.32
1	F	753	ARG	CZ-NH1	-6.65	1.23	1.32
1	E	662	ARG	CZ-NH1	-6.65	1.23	1.32
4	T	592	ALA	CA-CB	-6.65	1.42	1.53
1	A	586	ARG	CZ-NH1	-6.64	1.23	1.32
1	F	625	ARG	CZ-NH1	-6.63	1.23	1.32
1	F	741	ARG	CZ-NH1	-6.63	1.23	1.32
2	G	326	ARG	CZ-NH1	-6.63	1.23	1.32
1	B	142	ALA	CA-CB	-6.62	1.42	1.53
2	G	329	ARG	CZ-NH1	-6.62	1.23	1.32
2	G	169	ARG	CZ-NH1	-6.61	1.23	1.32
1	E	585	ALA	CA-CB	-6.61	1.42	1.53
1	B	228	ALA	CA-CB	-6.61	1.43	1.53
1	F	597	ALA	CA-CB	-6.61	1.42	1.53
1	D	159	ARG	CZ-NH1	-6.60	1.23	1.32
1	A	67	ALA	CA-CB	-6.58	1.42	1.53
1	C	569	ALA	CA-CB	-6.58	1.42	1.53
1	D	155	ARG	CZ-NH1	-6.57	1.23	1.32
1	A	280	GLY	N-CA	-6.56	1.37	1.45
1	B	160	ALA	CA-CB	-6.56	1.42	1.53
1	C	374	ALA	CA-CB	-6.52	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	583	ALA	CA-CB	-6.50	1.42	1.53
1	E	595	GLY	N-CA	-6.49	1.37	1.45
2	G	173	GLY	N-CA	-6.46	1.36	1.45
1	B	513	GLY	CA-C	-6.43	1.47	1.52
1	D	345	ALA	CA-CB	-6.41	1.42	1.53
1	B	22	ARG	CZ-NH2	-6.38	1.25	1.33
2	G	345	GLY	N-CA	-6.37	1.37	1.45
2	G	17	ARG	CZ-NH2	-6.37	1.25	1.33
1	D	391	ALA	CA-CB	-6.36	1.42	1.53
2	G	131	ARG	CZ-NH1	-6.35	1.23	1.32
1	F	735	HIS	CD2-NE2	-6.31	1.30	1.37
1	F	700	ARG	CZ-NH1	-6.28	1.24	1.32
2	G	384	GLY	N-CA	-6.24	1.38	1.45
1	B	495	TYR	N-CA	-6.18	1.41	1.46
1	D	622	ALA	CA-CB	-6.04	1.42	1.53
1	B	157	GLY	N-CA	-6.04	1.36	1.45
1	C	495	TYR	CA-CB	-5.99	1.46	1.53
1	C	494	GLN	CD-NE2	-5.96	1.20	1.33
1	D	587	GLY	N-CA	-5.95	1.38	1.45
4	T	560	ALA	CA-CB	-5.93	1.43	1.53
1	D	665	PRO	CA-CB	-5.88	1.46	1.53
1	F	610	GLY	N-CA	-5.88	1.38	1.45
1	D	136	LYS	N-CA	-5.86	1.42	1.46
1	D	653	ARG	CD-NE	-5.84	1.38	1.46
1	B	111	GLY	N-CA	-5.83	1.36	1.45
1	E	142	ALA	CA-CB	-5.82	1.43	1.53
2	G	370	ALA	CA-CB	-5.79	1.42	1.53
1	D	169	ASP	N-CA	-5.78	1.41	1.46
1	D	125	GLY	N-CA	-5.76	1.38	1.45
1	A	424	ARG	CD-NE	-5.72	1.38	1.46
2	G	133	GLY	N-CA	-5.72	1.36	1.44
2	G	332	ASP	CA-CB	-5.72	1.46	1.53
1	B	653	ARG	CD-NE	-5.71	1.38	1.46
1	D	567	ARG	CD-NE	-5.69	1.38	1.46
1	B	118	PRO	CA-CB	-5.65	1.45	1.53
1	D	169	ASP	CA-CB	-5.65	1.47	1.53
2	G	396	ARG	CD-NE	-5.63	1.38	1.46
1	A	147	ARG	CD-NE	-5.63	1.38	1.46
1	C	43	GLN	CA-CB	-5.63	1.47	1.53
1	A	86	ARG	CD-NE	-5.62	1.38	1.46
1	C	729	PRO	CA-CB	-5.61	1.45	1.53
1	B	25	ARG	CD-NE	-5.59	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	ARG	CD-NE	-5.59	1.38	1.46
1	E	765	SER	CA-CB	-5.59	1.44	1.53
1	B	370	GLY	N-CA	-5.58	1.37	1.45
1	D	83	ARG	CD-NE	-5.58	1.38	1.46
1	A	89	ARG	CD-NE	-5.58	1.38	1.46
1	E	591	GLY	N-CA	-5.58	1.37	1.45
1	D	745	ARG	CD-NE	-5.56	1.38	1.46
1	C	487	ARG	CD-NE	-5.56	1.38	1.46
1	D	144	ARG	CD-NE	-5.56	1.38	1.46
1	D	365	ARG	CD-NE	-5.56	1.38	1.46
1	B	210	ARG	CD-NE	-5.55	1.38	1.46
2	G	169	ARG	CD-NE	-5.55	1.38	1.46
1	B	665	PRO	CA-CB	-5.55	1.46	1.53
1	B	732	ARG	CD-NE	-5.55	1.38	1.46
1	B	681	GLY	N-CA	-5.54	1.38	1.45
5	H	275	ARG	CD-NE	-5.53	1.38	1.46
1	B	693	ARG	CD-NE	-5.53	1.38	1.46
1	C	43	GLN	N-CA	-5.53	1.41	1.46
1	C	567	ARG	CD-NE	-5.53	1.38	1.46
1	E	587	GLY	N-CA	-5.52	1.38	1.45
1	A	732	ARG	CD-NE	-5.52	1.38	1.46
1	B	136	LYS	CA-CB	-5.51	1.47	1.53
1	A	753	ARG	CD-NE	-5.50	1.38	1.46
1	B	621	GLY	CA-C	-5.50	1.47	1.52
1	D	507	GLY	N-CA	-5.50	1.38	1.45
1	E	593	GLY	N-CA	-5.49	1.38	1.45
2	G	178	GLY	N-CA	-5.48	1.37	1.45
1	E	766	ARG	CD-NE	-5.48	1.38	1.46
1	C	53	ARG	CD-NE	-5.47	1.38	1.46
1	B	43	GLN	CA-CB	-5.47	1.47	1.53
1	D	271	GLY	N-CA	-5.46	1.37	1.44
1	B	53	ARG	CD-NE	-5.45	1.38	1.46
1	D	237	PRO	CA-CB	-5.45	1.46	1.54
1	F	665	PRO	CA-CB	-5.45	1.46	1.53
1	C	496	PRO	CA-CB	-5.45	1.45	1.53
1	E	753	ARG	CD-NE	-5.44	1.38	1.46
1	B	513	GLY	N-CA	-5.44	1.38	1.45
1	A	637	GLY	N-CA	-5.43	1.38	1.45
1	D	159	ARG	CD-NE	-5.43	1.38	1.46
1	F	753	ARG	CD-NE	-5.43	1.38	1.46
1	B	191	ARG	CD-NE	-5.42	1.38	1.46
2	G	329	ARG	CD-NE	-5.42	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	ALA	CA-CB	-5.42	1.45	1.53
1	D	495	TYR	CA-CB	-5.42	1.47	1.53
1	A	507	GLY	N-CA	-5.42	1.38	1.45
1	F	567	ARG	CD-NE	-5.41	1.38	1.46
1	C	560	ARG	CD-NE	-5.40	1.38	1.46
1	E	636	PRO	CA-CB	-5.40	1.46	1.53
1	D	616	ASN	CA-CB	-5.40	1.46	1.52
1	B	222	LEU	CA-CB	-5.39	1.47	1.53
1	E	86	ARG	CD-NE	-5.39	1.38	1.46
1	E	105	CYS	CA-CB	-5.39	1.47	1.53
2	G	131	ARG	CD-NE	-5.39	1.38	1.46
1	F	741	ARG	CD-NE	-5.39	1.38	1.46
1	A	159	ARG	CD-NE	-5.38	1.38	1.46
1	D	744	ARG	CD-NE	-5.37	1.38	1.46
4	T	608	PHE	CA-CB	-5.37	1.47	1.53
1	E	594	GLY	N-CA	-5.37	1.37	1.45
1	D	113	ARG	CD-NE	-5.37	1.38	1.46
1	B	222	LEU	N-CA	-5.34	1.41	1.46
1	E	349	ARG	CD-NE	-5.34	1.38	1.46
1	A	700	ARG	CD-NE	-5.33	1.38	1.46
1	E	662	ARG	CD-NE	-5.33	1.38	1.46
1	B	368	ASP	CA-CB	-5.33	1.46	1.53
1	C	510	PRO	CA-CB	-5.32	1.46	1.53
1	C	693	ARG	CD-NE	-5.32	1.38	1.46
1	C	22	ARG	CD-NE	-5.32	1.38	1.46
1	B	700	ARG	CD-NE	-5.32	1.38	1.46
1	D	487	ARG	CD-NE	-5.32	1.38	1.46
1	A	595	GLY	N-CA	-5.32	1.37	1.45
1	C	507	GLY	N-CA	-5.32	1.37	1.45
1	A	65	ARG	CD-NE	-5.31	1.38	1.46
1	A	653	ARG	CD-NE	-5.31	1.38	1.46
1	A	495	TYR	N-CA	-5.30	1.41	1.46
5	H	272	ARG	CD-NE	-5.30	1.38	1.46
1	B	543	LYS	CA-CB	-5.29	1.46	1.52
1	E	713	ARG	CD-NE	-5.29	1.38	1.46
1	D	693	ARG	CD-NE	-5.28	1.38	1.46
1	D	746	SER	CA-CB	-5.28	1.47	1.53
1	F	625	ARG	CD-NE	-5.27	1.38	1.46
1	D	588	GLY	N-CA	-5.27	1.38	1.45
2	G	123	ARG	CD-NE	-5.26	1.38	1.46
1	D	700	ARG	CD-NE	-5.26	1.38	1.46
1	B	159	ARG	CD-NE	-5.26	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	499	HIS	ND1-CE1	-5.26	1.27	1.32
2	G	50	ARG	CD-NE	-5.26	1.38	1.46
1	E	234	GLY	N-CA	-5.25	1.37	1.45
1	A	95	ARG	CD-NE	-5.25	1.39	1.46
1	C	499	HIS	CA-CB	-5.23	1.45	1.53
1	A	586	ARG	CD-NE	-5.23	1.39	1.46
1	E	625	ARG	CD-NE	-5.23	1.39	1.46
1	E	160	ALA	CA-CB	-5.22	1.44	1.53
1	D	368	ASP	CA-CB	-5.22	1.46	1.53
2	G	8	ARG	CD-NE	-5.22	1.39	1.46
2	G	326	ARG	CD-NE	-5.22	1.39	1.46
2	G	221	ARG	CZ-NH2	-5.22	1.26	1.33
1	A	36	ASN	CG-ND2	-5.22	1.22	1.33
1	C	461	PRO	CA-CB	-5.20	1.47	1.53
1	F	733	ARG	CZ-NH2	-5.19	1.26	1.33
1	D	155	ARG	CD-NE	-5.18	1.39	1.46
1	C	621	GLY	N-CA	-5.17	1.37	1.45
1	E	118	PRO	CA-CB	-5.17	1.46	1.53
1	F	693	ARG	CD-NE	-5.17	1.39	1.46
1	B	507	GLY	N-CA	-5.16	1.37	1.45
1	A	470	GLU	CA-CB	-5.16	1.46	1.52
1	F	732	ARG	CZ-NH2	-5.15	1.26	1.33
1	C	700	ARG	CD-NE	-5.15	1.39	1.46
1	E	649	ASP	CA-CB	-5.13	1.47	1.53
1	A	636	PRO	CA-CB	-5.12	1.46	1.53
2	G	217	ARG	CD-NE	-5.12	1.39	1.46
1	D	510	PRO	CA-CB	-5.11	1.46	1.53
1	C	491	GLU	CA-CB	-5.10	1.45	1.53
1	D	743	ALA	N-CA	-5.09	1.39	1.46
1	F	700	ARG	CD-NE	-5.08	1.39	1.46
1	B	188	PRO	CA-CB	-5.07	1.46	1.53
1	C	494	GLN	N-CA	-5.07	1.40	1.46
1	D	681	GLY	N-CA	-5.06	1.38	1.45
1	B	73	SER	CA-CB	-5.05	1.46	1.53
1	D	496	PRO	CA-CB	-5.04	1.46	1.53
1	B	137	PRO	CA-CB	-5.04	1.46	1.53
1	C	491	GLU	N-CA	-5.04	1.40	1.46
4	T	563	PRO	CA-CB	-5.03	1.47	1.53
1	E	765	SER	N-CA	-5.03	1.40	1.46
1	D	495	TYR	N-CA	-5.02	1.41	1.46
1	C	603	GLN	CD-NE2	-5.02	1.22	1.33
1	D	621	GLY	N-CA	-5.02	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	472	PRO	CA-CB	-5.01	1.46	1.53
1	A	621	GLY	CA-C	-5.01	1.47	1.51

All (1134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	42	LYS	CA-C-N	10.28	141.55	121.41
5	H	42	LYS	C-N-CA	10.28	141.55	121.41
5	H	128	GLN	CA-C-N	9.85	143.28	122.90
5	H	128	GLN	C-N-CA	9.85	143.28	122.90
5	H	76	ARG	CA-C-N	9.72	137.79	122.62
5	H	76	ARG	C-N-CA	9.72	137.79	122.62
1	F	448	THR	N-CA-C	9.43	121.16	111.07
5	H	172	MET	CA-C-N	9.40	137.80	122.29
5	H	172	MET	C-N-CA	9.40	137.80	122.29
5	H	77	MET	CA-C-N	9.36	137.63	122.10
5	H	77	MET	C-N-CA	9.36	137.63	122.10
3	M	44	ILE	CA-C-N	9.35	138.16	121.89
3	M	44	ILE	C-N-CA	9.35	138.16	121.89
1	B	620	ILE	CA-C-N	9.24	129.53	121.58
1	B	620	ILE	C-N-CA	9.24	129.53	121.58
5	H	79	HIS	CA-C-N	9.00	136.62	121.87
5	H	79	HIS	C-N-CA	9.00	136.62	121.87
3	L	44	ILE	CA-C-N	8.93	136.81	121.64
3	L	44	ILE	C-N-CA	8.93	136.81	121.64
5	H	32	ALA	CA-C-N	8.87	135.80	121.87
5	H	32	ALA	C-N-CA	8.87	135.80	121.87
2	G	383	GLU	CA-C-N	8.63	128.13	122.18
2	G	383	GLU	C-N-CA	8.63	128.13	122.18
5	H	150	ALA	CA-C-N	8.43	136.21	122.29
5	H	150	ALA	C-N-CA	8.43	136.21	122.29
5	H	78	THR	CA-C-N	8.26	136.57	122.37
5	H	78	THR	C-N-CA	8.26	136.57	122.37
1	E	118	PRO	CA-C-N	8.25	129.41	121.65
1	E	118	PRO	C-N-CA	8.25	129.41	121.65
1	A	498	GLU	CA-C-N	8.16	130.61	122.28
1	A	498	GLU	C-N-CA	8.16	130.61	122.28
5	H	19	PHE	CA-C-N	8.16	135.52	121.64
5	H	19	PHE	C-N-CA	8.16	135.52	121.64
5	H	122	TYR	CA-C-N	8.01	136.50	121.69
5	H	122	TYR	C-N-CA	8.01	136.50	121.69
5	H	83	LEU	CA-C-N	8.00	136.13	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	83	LEU	C-N-CA	8.00	136.13	122.37
2	G	161	HIS	CA-CB-CG	7.88	121.68	113.80
1	E	163	PHE	CA-CB-CG	7.79	121.59	113.80
1	E	395	ASP	CA-CB-CG	7.77	120.37	112.60
5	H	20	SER	CA-C-N	7.69	136.15	122.45
5	H	20	SER	C-N-CA	7.69	136.15	122.45
1	A	364	ASP	CA-CB-CG	7.66	120.25	112.60
1	B	131	PHE	CA-CB-CG	7.62	121.42	113.80
1	E	369	ILE	CA-C-N	7.55	127.42	121.61
1	E	369	ILE	C-N-CA	7.55	127.42	121.61
1	C	499	HIS	CA-CB-CG	7.51	121.31	113.80
1	A	620	ILE	CA-C-N	7.49	127.38	121.61
1	A	620	ILE	C-N-CA	7.49	127.38	121.61
1	B	55	ASP	CA-CB-CG	7.49	120.09	112.60
2	G	347	PHE	CA-CB-CG	7.43	121.23	113.80
1	D	748	SER	N-CA-C	7.40	119.99	111.11
1	F	683	SER	N-CA-C	7.39	119.13	111.14
1	D	682	PHE	CA-CB-CG	7.35	121.15	113.80
1	E	503	PHE	CA-CB-CG	7.31	121.11	113.80
1	A	150	ASP	CA-CB-CG	7.28	119.88	112.60
4	T	594	ASN	CA-CB-CG	7.26	119.86	112.60
1	A	115	HIS	CA-CB-CG	7.25	121.05	113.80
1	A	279	ALA	CA-C-N	7.25	127.98	119.94
1	A	279	ALA	C-N-CA	7.25	127.98	119.94
1	A	183	HIS	CA-CB-CG	7.24	121.04	113.80
1	C	563	PHE	CA-CB-CG	7.22	121.02	113.80
1	F	742	PHE	CA-CB-CG	7.21	121.02	113.80
1	D	29	ASP	CA-CB-CG	7.19	119.79	112.60
1	E	750	ASN	CA-CB-CG	7.16	119.75	112.60
1	D	166	VAL	CA-C-N	7.15	135.20	121.54
1	D	166	VAL	C-N-CA	7.15	135.20	121.54
4	T	569	ASN	CA-CB-CG	7.15	119.75	112.60
3	M	16	GLU	CA-C-N	7.15	133.97	122.68
3	M	16	GLU	C-N-CA	7.15	133.97	122.68
4	T	607	GLY	CA-C-N	7.14	130.89	122.89
4	T	607	GLY	C-N-CA	7.14	130.89	122.89
1	C	460	ASN	CA-CB-CG	7.14	119.74	112.60
1	A	139	PHE	CA-CB-CG	7.13	120.93	113.80
1	E	23	PRO	CA-N-CD	-7.11	102.05	112.00
1	A	29	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	163	PHE	CA-CB-CG	7.08	120.89	113.80
4	T	600	PHE	CA-CB-CG	7.06	120.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	ASP	CA-CB-CG	7.05	119.66	112.60
1	B	576	PHE	CA-CB-CG	7.05	120.85	113.80
1	E	393	ASP	CA-CB-CG	7.05	119.65	112.60
1	C	333	ASP	N-CA-C	7.00	121.05	112.23
1	E	139	PHE	CA-CB-CG	6.99	120.79	113.80
1	C	323	ARG	NE-CZ-NH2	6.98	125.48	119.20
2	G	389	ASN	CA-CB-CG	6.94	119.54	112.60
1	C	616	ASN	CA-CB-CG	6.92	119.52	112.60
1	D	115	HIS	CA-CB-CG	6.92	120.72	113.80
1	B	226	HIS	CA-CB-CG	6.91	120.71	113.80
2	G	449	ILE	CA-C-N	6.91	131.63	122.93
2	G	449	ILE	C-N-CA	6.91	131.63	122.93
1	E	742	PHE	CA-CB-CG	6.90	120.70	113.80
1	B	558	ASN	CA-CB-CG	6.90	119.50	112.60
1	A	79	ASP	CA-CB-CG	6.89	119.50	112.60
1	B	79	ASP	CA-CB-CG	6.89	119.49	112.60
2	G	166	ALA	CA-C-N	6.89	129.51	120.28
2	G	166	ALA	C-N-CA	6.89	129.51	120.28
1	B	539	PHE	CA-CB-CG	6.88	120.68	113.80
1	B	533	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	81	LYS	CA-C-N	6.84	132.01	123.12
1	A	81	LYS	C-N-CA	6.84	132.01	123.12
1	C	640	ASP	CA-CB-CG	6.84	119.44	112.60
4	T	623	ASP	CA-CB-CG	6.84	119.44	112.60
1	B	129	ASN	CA-CB-CG	6.83	119.43	112.60
1	B	563	PHE	CA-CB-CG	6.81	120.61	113.80
1	B	616	ASN	CA-CB-CG	6.81	119.41	112.60
1	F	751	ASP	CA-CB-CG	6.80	119.40	112.60
1	D	563	PHE	CA-CB-CG	6.79	120.59	113.80
1	A	602	ASN	CA-CB-CG	6.79	119.39	112.60
1	D	616	ASN	CA-CB-CG	6.78	119.38	112.60
4	T	590	PHE	CA-CB-CG	6.78	120.58	113.80
2	G	126	ASP	CA-CB-CG	6.77	119.37	112.60
1	C	506	PHE	CA-CB-CG	6.76	120.56	113.80
1	C	516	PHE	CA-CB-CG	6.76	120.56	113.80
1	A	735	HIS	CA-CB-CG	6.76	120.56	113.80
1	B	506	PHE	CA-CB-CG	6.75	120.56	113.80
1	E	506	PHE	CA-CB-CG	6.75	120.56	113.80
1	C	392	ASP	CA-C-N	6.75	130.00	120.28
1	C	392	ASP	C-N-CA	6.75	130.00	120.28
1	A	630	ASP	CA-CB-CG	6.75	119.35	112.60
1	E	55	ASP	CA-CB-CG	6.75	119.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	406	HIS	CA-CB-CG	6.74	120.54	113.80
1	E	749	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	21	ASN	CA-CB-CG	6.74	119.33	112.60
1	E	371	ILE	N-CA-C	6.73	114.41	108.63
1	B	438	ASP	CA-CB-CG	6.72	119.32	112.60
1	C	735	HIS	CA-CB-CG	6.71	120.51	113.80
1	B	572	CYS	CA-C-N	6.71	131.51	123.19
1	B	572	CYS	C-N-CA	6.71	131.51	123.19
1	D	139	PHE	CA-CB-CG	6.71	120.51	113.80
1	D	393	ASP	CA-CB-CG	6.70	119.30	112.60
1	E	564	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	91	ASN	CA-CB-CG	6.68	119.28	112.60
1	D	736	PHE	CA-CB-CG	6.65	120.45	113.80
1	C	572	CYS	CA-C-N	6.62	131.81	123.14
1	C	572	CYS	C-N-CA	6.62	131.81	123.14
1	E	598	ASP	CA-CB-CG	6.61	119.21	112.60
1	F	730	GLU	CA-C-N	6.61	130.74	122.48
1	F	730	GLU	C-N-CA	6.61	130.74	122.48
1	B	735	HIS	CA-CB-CG	6.60	120.40	113.80
1	A	516	PHE	CA-CB-CG	6.60	120.40	113.80
1	A	90	ASN	CA-CB-CG	6.60	119.20	112.60
2	G	397	ASP	CA-CB-CG	6.59	119.19	112.60
1	C	47	ASP	CA-CB-CG	6.59	119.19	112.60
1	D	129	ASN	CA-CB-CG	6.58	119.19	112.60
1	A	750	ASN	CA-CB-CG	6.58	119.18	112.60
1	C	512	LYS	CA-C-N	6.57	127.95	121.57
1	C	512	LYS	C-N-CA	6.57	127.95	121.57
1	F	563	PHE	CA-CB-CG	6.57	120.37	113.80
1	A	671	ASP	CA-CB-CG	6.57	119.17	112.60
1	B	742	PHE	CA-CB-CG	6.57	120.37	113.80
1	D	506	PHE	CA-CB-CG	6.56	120.36	113.80
1	C	538	ASN	CA-CB-CG	6.56	119.16	112.60
2	G	360	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	333	ASP	CA-CB-CG	6.56	119.16	112.60
1	D	564	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	506	PHE	CA-CB-CG	6.55	120.35	113.80
1	D	680	ASN	CA-CB-CG	6.54	119.14	112.60
1	C	534	GLU	N-CA-C	6.54	119.74	111.69
1	D	181	VAL	CA-C-N	6.54	131.18	122.93
1	D	181	VAL	C-N-CA	6.54	131.18	122.93
1	D	230	PHE	CA-CB-CG	6.54	120.34	113.80
1	D	81	LYS	CA-C-N	6.54	132.03	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	81	LYS	C-N-CA	6.54	132.03	122.94
1	E	373	ASP	N-CA-C	6.53	118.28	111.03
1	B	24	ASN	CA-CB-CG	6.53	119.13	112.60
1	B	516	PHE	CA-CB-CG	6.53	120.33	113.80
1	E	649	ASP	CA-CB-CG	6.53	119.13	112.60
1	D	79	ASP	CA-CB-CG	6.53	119.13	112.60
4	T	608	PHE	CA-CB-CG	6.53	120.33	113.80
4	T	601	ASP	CA-CB-CG	6.52	119.12	112.60
1	D	131	PHE	CA-CB-CG	6.51	120.31	113.80
1	C	619	ILE	CA-C-N	6.51	131.67	123.14
1	C	619	ILE	C-N-CA	6.51	131.67	123.14
1	A	98	ASP	CA-CB-CG	6.50	119.10	112.60
1	C	21	ASN	CA-CB-CG	6.50	119.10	112.60
1	F	736	PHE	CA-CB-CG	6.50	120.30	113.80
1	B	115	HIS	CA-CB-CG	6.49	120.29	113.80
1	E	758	PHE	CA-CB-CG	6.49	120.29	113.80
1	B	160	ALA	CA-C-N	6.49	131.47	123.10
1	B	160	ALA	C-N-CA	6.49	131.47	123.10
1	A	163	PHE	CA-CB-CG	6.48	120.28	113.80
1	D	74	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	428	ASP	CA-CB-CG	6.47	119.07	112.60
1	E	764	GLN	CA-C-N	6.46	129.23	120.38
1	E	764	GLN	C-N-CA	6.46	129.23	120.38
1	B	395	ASP	CA-CB-CG	6.45	119.05	112.60
1	D	742	PHE	CA-C-N	6.44	129.86	120.71
1	D	742	PHE	C-N-CA	6.44	129.86	120.71
1	C	75	ASP	CA-CB-CG	6.44	119.04	112.60
1	F	558	ASN	CA-CB-CG	6.43	119.03	112.60
1	D	169	ASP	CA-CB-CG	6.42	119.02	112.60
1	C	404	HIS	CA-CB-CG	6.42	120.22	113.80
1	C	575	PHE	CA-CB-CG	6.41	120.21	113.80
1	E	107	ASP	CA-CB-CG	6.41	119.01	112.60
3	I	19	PRO	CA-C-N	6.41	130.42	120.75
3	I	19	PRO	C-N-CA	6.41	130.42	120.75
1	B	368	ASP	CA-CB-CG	6.40	119.00	112.60
1	B	499	HIS	CA-CB-CG	6.40	120.20	113.80
1	C	129	ASN	CA-CB-CG	6.40	119.00	112.60
1	A	598	ASP	CA-CB-CG	6.39	118.99	112.60
2	G	171	LEU	CA-C-N	6.38	128.74	120.44
2	G	171	LEU	C-N-CA	6.38	128.74	120.44
1	D	575	PHE	CA-CB-CG	6.38	120.18	113.80
1	B	503	PHE	CA-CB-CG	6.37	120.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	346	ASP	CA-CB-CG	6.36	118.96	112.60
1	F	333	ASP	CA-C-N	6.35	128.07	120.14
1	F	333	ASP	C-N-CA	6.35	128.07	120.14
1	B	362	ARG	NE-CZ-NH2	6.34	124.91	119.20
2	G	331	LYS	CA-C-N	6.34	132.78	122.39
2	G	331	LYS	C-N-CA	6.34	132.78	122.39
1	B	139	PHE	N-CA-C	6.33	119.16	111.82
1	A	597	ALA	CA-C-N	6.33	128.67	120.44
1	A	597	ALA	C-N-CA	6.33	128.67	120.44
1	D	635	ARG	NE-CZ-NH2	6.33	124.89	119.20
1	E	392	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	556	GLU	CA-C-N	6.32	128.66	120.44
1	B	556	GLU	C-N-CA	6.32	128.66	120.44
1	C	564	ASP	CA-CB-CG	6.31	118.91	112.60
2	G	349	ASN	CA-CB-CG	6.31	118.91	112.60
1	C	49	LEU	CA-C-N	6.29	129.57	120.38
1	C	49	LEU	C-N-CA	6.29	129.57	120.38
4	T	573	VAL	CA-C-N	6.29	131.40	122.72
4	T	573	VAL	C-N-CA	6.29	131.40	122.72
1	B	294	GLU	CA-C-N	6.29	128.62	120.44
1	B	294	GLU	C-N-CA	6.29	128.62	120.44
1	F	750	ASN	CA-CB-CG	6.28	118.88	112.60
1	D	640	ASP	CA-CB-CG	6.28	118.88	112.60
1	D	36	ASN	CA-CB-CG	6.28	118.88	112.60
1	D	503	PHE	CA-CB-CG	6.27	120.07	113.80
1	B	575	PHE	CA-CB-CG	6.27	120.07	113.80
1	A	60	LYS	CA-C-N	6.27	128.75	122.30
1	A	60	LYS	C-N-CA	6.27	128.75	122.30
1	A	26	LEU	CA-C-N	6.26	130.31	122.43
1	A	26	LEU	C-N-CA	6.26	130.31	122.43
1	B	424	ARG	NE-CZ-NH2	6.25	124.83	119.20
2	G	330	ASN	CA-CB-CG	6.25	118.85	112.60
1	C	451	ASP	CA-CB-CG	6.25	118.84	112.60
1	D	220	VAL	N-CA-C	6.24	116.41	110.74
1	E	115	HIS	CA-CB-CG	6.23	120.03	113.80
2	G	185	ASN	CA-CB-CG	6.23	118.83	112.60
1	D	512	LYS	CA-C-N	6.23	128.05	121.45
1	D	512	LYS	C-N-CA	6.23	128.05	121.45
1	A	159	ARG	CD-NE-CZ	6.22	133.11	124.40
1	E	625	ARG	CD-NE-CZ	6.22	133.11	124.40
1	E	609	ASP	CA-CB-CG	6.22	118.82	112.60
1	F	564	ASP	CA-CB-CG	6.21	118.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	LYS	CA-C-O	-6.21	114.13	120.71
1	A	36	ASN	CA-CB-CG	6.20	118.80	112.60
1	B	191	ARG	CD-NE-CZ	6.20	133.07	124.40
1	E	589	ASN	CA-CB-CG	6.19	118.79	112.60
1	B	159	ARG	CD-NE-CZ	6.19	133.06	124.40
1	A	153	LEU	CA-C-N	6.18	128.95	120.35
1	A	153	LEU	C-N-CA	6.18	128.95	120.35
1	D	504	LEU	CA-C-N	6.17	128.47	120.44
1	D	504	LEU	C-N-CA	6.17	128.47	120.44
1	E	120	ASP	CA-CB-CG	6.17	118.77	112.60
5	H	263	PHE	N-CA-CB	6.17	119.15	109.83
2	G	315	LEU	CA-C-N	6.16	131.00	122.93
2	G	315	LEU	C-N-CA	6.16	131.00	122.93
1	E	85	ASN	CA-C-N	6.15	128.85	120.54
1	E	85	ASN	C-N-CA	6.15	128.85	120.54
1	A	453	ARG	NE-CZ-NH2	6.15	124.73	119.20
1	D	395	ASP	CA-CB-CG	6.15	118.75	112.60
1	F	692	GLN	CA-C-N	6.14	128.43	120.44
1	F	692	GLN	C-N-CA	6.14	128.43	120.44
1	F	693	ARG	CD-NE-CZ	6.14	133.00	124.40
4	T	585	PHE	CA-CB-CG	6.14	119.94	113.80
1	C	22	ARG	CD-NE-CZ	6.14	133.00	124.40
1	A	567	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	A	513	GLY	N-CA-C	6.12	120.27	110.90
1	D	25	ARG	NE-CZ-NH2	6.12	124.71	119.20
2	G	140	HIS	CA-CB-CG	6.12	119.92	113.80
1	C	617	VAL	CA-C-N	6.11	130.55	122.30
1	C	617	VAL	C-N-CA	6.11	130.55	122.30
1	C	493	VAL	CA-C-N	6.11	128.38	120.44
1	C	493	VAL	C-N-CA	6.11	128.38	120.44
1	E	164	LYS	CA-C-N	6.10	130.33	121.18
1	E	164	LYS	C-N-CA	6.10	130.33	121.18
1	A	65	ARG	CD-NE-CZ	6.10	132.94	124.40
1	E	243	LEU	N-CA-C	-6.10	99.72	109.96
1	B	686	ASP	CA-CB-CG	6.09	118.69	112.60
1	A	95	ARG	CD-NE-CZ	6.09	132.93	124.40
1	D	368	ASP	CA-CB-CG	6.09	118.69	112.60
2	G	368	VAL	CA-C-N	6.09	131.76	122.93
2	G	368	VAL	C-N-CA	6.09	131.76	122.93
1	C	693	ARG	CD-NE-CZ	6.08	132.91	124.40
1	D	26	LEU	CA-C-N	6.08	130.31	121.80
1	D	26	LEU	C-N-CA	6.08	130.31	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	155	ARG	CD-NE-CZ	6.08	132.91	124.40
1	C	733	ARG	NE-CZ-NH2	6.07	124.66	119.20
1	D	693	ARG	CD-NE-CZ	6.07	132.89	124.40
2	G	50	ARG	CD-NE-CZ	6.06	132.89	124.40
1	C	491	GLU	CA-CB-CG	6.06	126.22	114.10
1	B	534	GLU	N-CA-C	6.06	119.86	112.23
1	A	373	ASP	CA-C-N	6.05	128.71	120.54
1	A	373	ASP	C-N-CA	6.05	128.71	120.54
1	D	686	ASP	CA-CB-CG	6.04	118.64	112.60
1	F	25	ARG	NE-CZ-NH2	6.04	124.64	119.20
1	B	72	LEU	CA-C-N	6.04	130.45	122.30
1	B	72	LEU	C-N-CA	6.04	130.45	122.30
2	G	162	MET	CA-CB-CG	6.04	126.17	114.10
1	C	688	THR	CA-C-N	6.02	128.66	120.54
1	C	688	THR	C-N-CA	6.02	128.66	120.54
2	G	217	ARG	CD-NE-CZ	6.02	132.82	124.40
1	A	387	ASN	CA-CB-CG	6.01	118.61	112.60
1	F	625	ARG	CD-NE-CZ	6.01	132.82	124.40
2	G	283	ASN	CA-CB-CG	6.01	118.61	112.60
1	A	57	VAL	CA-C-N	5.99	130.96	122.09
1	A	57	VAL	C-N-CA	5.99	130.96	122.09
2	G	169	ARG	CD-NE-CZ	5.99	132.79	124.40
1	E	453	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	F	669	ASP	CA-C-N	5.99	129.69	122.26
1	F	669	ASP	C-N-CA	5.99	129.69	122.26
5	H	270	PHE	CA-CB-CG	5.98	119.78	113.80
1	B	741	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	A	24	ASN	CA-CB-CG	5.97	118.57	112.60
1	A	387	ASN	CA-C-N	5.96	130.95	122.72
1	A	387	ASN	C-N-CA	5.96	130.95	122.72
1	C	701	GLU	N-CA-CB	5.96	118.66	110.01
1	D	487	ARG	CD-NE-CZ	5.96	132.75	124.40
1	D	700	ARG	CD-NE-CZ	5.96	132.75	124.40
1	B	428	ASP	CA-C-N	5.96	128.27	120.28
1	B	428	ASP	C-N-CA	5.96	128.27	120.28
1	C	492	LEU	CA-C-N	5.96	129.26	120.74
1	C	492	LEU	C-N-CA	5.96	129.26	120.74
1	C	42	SER	CA-C-N	5.96	129.79	120.97
1	C	42	SER	C-N-CA	5.96	129.79	120.97
1	D	394	VAL	CA-C-N	5.96	130.89	121.72
1	D	394	VAL	C-N-CA	5.96	130.89	121.72
1	F	700	ARG	CD-NE-CZ	5.96	132.74	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	349	ARG	CD-NE-CZ	5.95	132.73	124.40
1	A	503	PHE	CA-CB-CG	5.94	119.74	113.80
2	G	314	ASP	CA-CB-CG	5.94	118.54	112.60
5	H	272	ARG	CD-NE-CZ	5.93	132.71	124.40
2	G	9	VAL	CA-C-N	5.93	129.29	120.87
2	G	9	VAL	C-N-CA	5.93	129.29	120.87
1	C	618	PHE	CA-C-N	5.92	130.48	122.90
1	C	618	PHE	C-N-CA	5.92	130.48	122.90
1	D	482	LEU	CA-C-N	5.92	128.14	120.44
1	D	482	LEU	C-N-CA	5.92	128.14	120.44
2	G	123	ARG	CD-NE-CZ	5.92	132.69	124.40
1	D	160	ALA	CA-C-N	5.92	130.53	123.19
1	D	160	ALA	C-N-CA	5.92	130.53	123.19
1	B	619	ILE	CA-C-N	5.91	131.16	122.94
1	B	619	ILE	C-N-CA	5.91	131.16	122.94
1	E	713	ARG	CD-NE-CZ	5.91	132.68	124.40
1	A	98	ASP	CA-C-N	5.91	129.02	120.98
1	A	98	ASP	C-N-CA	5.91	129.02	120.98
1	D	143	TYR	CA-C-N	5.91	128.59	120.67
1	D	143	TYR	C-N-CA	5.91	128.59	120.67
1	A	586	ARG	CD-NE-CZ	5.90	132.66	124.40
1	B	618	PHE	CA-CB-CG	5.90	119.70	113.80
2	G	8	ARG	CD-NE-CZ	5.89	132.65	124.40
1	B	574	LEU	CA-C-N	5.89	130.85	122.72
1	B	574	LEU	C-N-CA	5.89	130.85	122.72
1	C	593	GLY	CA-C-N	5.89	127.50	120.14
1	C	593	GLY	C-N-CA	5.89	127.50	120.14
1	D	132	GLU	CA-C-N	5.88	127.97	120.56
1	D	132	GLU	C-N-CA	5.88	127.97	120.56
1	B	512	LYS	CA-C-N	5.88	128.06	122.36
1	B	512	LYS	C-N-CA	5.88	128.06	122.36
1	D	168	THR	CA-C-N	5.88	129.34	122.52
1	D	168	THR	C-N-CA	5.88	129.34	122.52
3	I	20	SER	N-CA-C	5.88	118.34	110.35
1	B	24	ASN	CA-C-N	5.88	130.83	122.72
1	B	24	ASN	C-N-CA	5.88	130.83	122.72
1	D	573	VAL	CA-C-N	5.88	131.45	123.11
1	D	573	VAL	C-N-CA	5.88	131.45	123.11
1	B	575	PHE	CA-C-N	5.87	131.45	123.11
1	B	575	PHE	C-N-CA	5.87	131.45	123.11
1	C	618	PHE	CA-CB-CG	5.87	119.67	113.80
1	E	734	ASP	CA-CB-CG	5.87	118.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	773	PHE	CA-CB-CG	5.87	119.67	113.80
1	B	567	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	A	507	GLY	CA-C-N	5.86	130.46	122.84
1	A	507	GLY	C-N-CA	5.86	130.46	122.84
1	E	597	ALA	CA-C-N	5.86	128.06	120.44
1	E	597	ALA	C-N-CA	5.86	128.06	120.44
2	G	169	ARG	CA-C-N	5.85	128.04	120.44
2	G	169	ARG	C-N-CA	5.85	128.04	120.44
1	E	499	HIS	CA-CB-CG	5.85	119.65	113.80
1	A	164	LYS	CA-C-N	5.84	132.49	121.97
1	A	164	LYS	C-N-CA	5.84	132.49	121.97
1	C	52	PHE	CA-CB-CG	5.84	119.64	113.80
1	B	119	ILE	N-CA-CB	5.83	116.89	110.53
1	A	59	LEU	CA-C-N	5.83	131.05	123.00
1	A	59	LEU	C-N-CA	5.83	131.05	123.00
1	B	450	ASP	CA-CB-CG	5.83	118.43	112.60
1	E	307	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	574	LEU	CA-C-N	5.83	131.04	123.00
1	C	574	LEU	C-N-CA	5.83	131.04	123.00
1	F	695	CYS	CA-C-N	5.83	128.01	120.44
1	F	695	CYS	C-N-CA	5.83	128.01	120.44
1	D	640	ASP	CA-C-N	5.82	130.52	122.77
1	D	640	ASP	C-N-CA	5.82	130.52	122.77
1	B	199	ASN	CA-CB-CG	5.82	118.42	112.60
1	E	640	ASP	CA-C-N	5.82	130.16	122.42
1	E	640	ASP	C-N-CA	5.82	130.16	122.42
1	F	740	MET	CA-C-N	5.82	128.00	120.44
1	F	740	MET	C-N-CA	5.82	128.00	120.44
1	C	494	GLN	CA-CB-CG	5.81	125.73	114.10
1	C	616	ASN	CA-C-N	5.81	130.54	122.93
1	C	616	ASN	C-N-CA	5.81	130.54	122.93
1	C	704	GLU	CA-C-N	5.81	128.00	120.44
1	C	704	GLU	C-N-CA	5.81	128.00	120.44
1	B	734	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	494	GLN	N-CA-CB	5.81	118.43	110.01
2	G	326	ARG	CD-NE-CZ	5.81	132.53	124.40
1	C	129	ASN	CA-C-N	5.81	128.34	120.38
1	C	129	ASN	C-N-CA	5.81	128.34	120.38
1	E	759	ALA	CA-C-N	5.80	127.99	120.44
1	E	759	ALA	C-N-CA	5.80	127.99	120.44
1	F	693	ARG	CA-CB-CG	5.80	125.71	114.10
1	D	499	HIS	CA-CB-CG	5.80	119.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	T	609	PRO	CA-C-N	5.79	128.62	120.28
4	T	609	PRO	C-N-CA	5.79	128.62	120.28
1	C	494	GLN	CA-C-N	5.78	127.95	120.44
1	C	494	GLN	C-N-CA	5.78	127.95	120.44
1	C	701	GLU	CA-C-N	5.78	127.95	120.44
1	C	701	GLU	C-N-CA	5.78	127.95	120.44
1	B	147	ARG	NE-CZ-NH2	5.77	124.40	119.20
1	C	492	LEU	N-CA-CB	5.77	119.18	109.78
1	C	702	SER	N-CA-CB	5.76	118.37	110.01
1	B	335	LEU	CA-C-N	5.76	132.98	122.50
1	B	335	LEU	C-N-CA	5.76	132.98	122.50
1	B	539	PHE	CA-C-N	5.74	131.14	122.98
1	B	539	PHE	C-N-CA	5.74	131.14	122.98
4	T	602	PHE	CA-CB-CG	5.74	119.54	113.80
1	E	709	ARG	CA-C-N	5.74	127.90	120.44
1	E	709	ARG	C-N-CA	5.74	127.90	120.44
1	D	616	ASN	CA-C-N	5.74	130.44	122.93
1	D	616	ASN	C-N-CA	5.74	130.44	122.93
1	F	671	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	700	ARG	CA-C-N	5.73	127.89	120.44
1	C	700	ARG	C-N-CA	5.73	127.89	120.44
1	D	153	LEU	CA-C-N	5.73	130.95	122.99
1	D	153	LEU	C-N-CA	5.73	130.95	122.99
1	A	695	CYS	N-CA-CB	5.73	118.31	110.01
1	D	392	ASP	CA-CB-CG	5.73	118.33	112.60
1	E	161	VAL	CA-C-N	5.72	130.38	122.77
1	E	161	VAL	C-N-CA	5.72	130.38	122.77
1	D	609	ASP	N-CA-C	5.72	120.40	112.45
1	B	700	ARG	CD-NE-CZ	5.71	132.40	124.40
1	B	741	ARG	CA-C-N	5.71	131.80	121.92
1	B	741	ARG	C-N-CA	5.71	131.80	121.92
1	B	287	ARG	CA-C-N	5.71	129.39	120.82
1	B	287	ARG	C-N-CA	5.71	129.39	120.82
1	D	171	SER	N-CA-CB	5.71	116.94	110.03
1	A	321	GLU	CA-C-N	5.70	127.85	120.44
1	A	321	GLU	C-N-CA	5.70	127.85	120.44
1	A	665	PRO	CA-C-N	5.70	130.61	123.14
1	A	665	PRO	C-N-CA	5.70	130.61	123.14
1	B	167	GLU	CA-C-N	5.70	130.80	122.77
1	B	167	GLU	C-N-CA	5.70	130.80	122.77
1	B	54	GLY	CA-C-N	5.69	128.95	120.87
1	B	54	GLY	C-N-CA	5.69	128.95	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	616	ASN	CA-C-N	5.69	130.85	123.11
1	B	616	ASN	C-N-CA	5.69	130.85	123.11
1	E	165	VAL	CA-C-N	5.69	130.63	122.72
1	E	165	VAL	C-N-CA	5.69	130.63	122.72
1	A	513	GLY	CA-C-N	5.68	131.72	122.69
1	A	513	GLY	C-N-CA	5.68	131.72	122.69
1	F	560	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	F	566	ALA	CA-C-N	5.67	127.81	120.44
1	F	566	ALA	C-N-CA	5.67	127.81	120.44
1	E	168	THR	CA-C-N	5.67	129.73	122.64
1	E	168	THR	C-N-CA	5.67	129.73	122.64
1	C	515	LEU	CA-C-N	5.67	130.98	123.05
1	C	515	LEU	C-N-CA	5.67	130.98	123.05
1	B	613	THR	CA-C-N	5.66	130.20	122.84
1	B	613	THR	C-N-CA	5.66	130.20	122.84
1	A	700	ARG	CD-NE-CZ	5.66	132.32	124.40
1	C	635	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	G	10	GLN	N-CA-CB	5.65	118.28	109.97
1	C	424	ARG	NE-CZ-NH2	5.64	124.28	119.20
4	T	572	PRO	CA-C-N	5.64	130.84	122.99
4	T	572	PRO	C-N-CA	5.64	130.84	122.99
1	D	505	LYS	N-CA-CB	5.64	118.19	110.01
2	G	148	ASP	CA-CB-CG	5.63	118.23	112.60
1	C	700	ARG	CD-NE-CZ	5.63	132.28	124.40
2	G	127	PRO	CA-C-N	5.63	127.82	120.28
2	G	127	PRO	C-N-CA	5.63	127.82	120.28
4	T	578	ILE	O-C-N	-5.62	115.80	122.77
1	A	56	THR	CA-C-N	5.62	130.90	122.75
1	A	56	THR	C-N-CA	5.62	130.90	122.75
1	E	635	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	B	586	ARG	NE-CZ-NH2	5.62	124.26	119.20
2	G	370	ALA	CA-C-N	5.62	130.96	122.98
2	G	370	ALA	C-N-CA	5.62	130.96	122.98
1	A	752	ILE	CA-C-N	5.62	127.81	120.28
1	A	752	ILE	C-N-CA	5.62	127.81	120.28
1	D	60	LYS	CA-C-N	5.61	126.41	121.58
1	D	60	LYS	C-N-CA	5.61	126.41	121.58
1	D	126	ILE	N-CA-CB	5.61	117.04	110.82
1	D	359	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	C	565	LYS	CA-CB-CG	5.60	125.30	114.10
1	D	113	ARG	CD-NE-CZ	5.60	132.24	124.40
1	A	642	LEU	CA-C-N	5.60	130.54	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	642	LEU	C-N-CA	5.60	130.54	123.10
1	B	77	CYS	CA-C-N	5.58	129.71	120.94
1	B	77	CYS	C-N-CA	5.58	129.71	120.94
1	B	50	GLN	CA-C-N	5.58	130.86	123.05
1	B	50	GLN	C-N-CA	5.58	130.86	123.05
1	E	164	LYS	CA-C-O	-5.58	114.79	120.71
1	B	283	GLU	CA-C-N	5.58	127.76	120.28
1	B	283	GLU	C-N-CA	5.58	127.76	120.28
1	D	698	ALA	CA-C-N	5.58	127.59	120.56
1	D	698	ALA	C-N-CA	5.58	127.59	120.56
1	B	118	PRO	CA-C-N	5.58	129.35	121.66
1	B	118	PRO	C-N-CA	5.58	129.35	121.66
1	B	134	TYR	CA-C-N	5.57	128.21	120.63
1	B	134	TYR	C-N-CA	5.57	128.21	120.63
1	B	492	LEU	CA-C-N	5.57	128.71	120.74
1	B	492	LEU	C-N-CA	5.57	128.71	120.74
1	B	559	VAL	N-CA-CB	5.57	116.47	110.62
1	C	702	SER	CA-C-N	5.57	127.58	120.56
1	C	702	SER	C-N-CA	5.57	127.58	120.56
4	T	577	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	A	115	HIS	CA-C-N	5.57	130.73	122.99
1	A	115	HIS	C-N-CA	5.57	130.73	122.99
1	B	540	ILE	CA-C-N	5.57	130.41	122.72
1	B	540	ILE	C-N-CA	5.57	130.41	122.72
1	D	82	ILE	CA-C-N	5.57	130.17	122.77
1	D	82	ILE	C-N-CA	5.57	130.17	122.77
1	A	113	ARG	CA-C-N	5.56	130.59	122.69
1	A	113	ARG	C-N-CA	5.56	130.59	122.69
1	C	662	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	D	219	MET	CA-C-N	5.56	127.66	120.88
1	D	219	MET	C-N-CA	5.56	127.66	120.88
1	E	741	ARG	CA-C-N	5.56	128.18	120.29
1	E	741	ARG	C-N-CA	5.56	128.18	120.29
2	G	121	ILE	CA-C-N	5.56	128.76	120.87
2	G	121	ILE	C-N-CA	5.56	128.76	120.87
1	B	701	GLU	N-CA-CB	5.56	118.07	110.01
1	E	169	ASP	CA-CB-CG	5.55	118.15	112.60
3	I	28	ALA	CA-C-N	5.55	127.66	120.44
3	I	28	ALA	C-N-CA	5.55	127.66	120.44
1	C	513	GLY	CA-C-N	5.54	130.78	122.58
1	C	513	GLY	C-N-CA	5.54	130.78	122.58
1	E	189	ILE	CA-C-N	5.54	127.64	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	189	ILE	C-N-CA	5.54	127.64	120.44
4	T	600	PHE	CA-C-N	5.54	127.64	120.44
4	T	600	PHE	C-N-CA	5.54	127.64	120.44
2	G	342	ILE	CA-C-N	5.53	127.64	120.44
2	G	342	ILE	C-N-CA	5.53	127.64	120.44
1	A	756	GLU	CA-C-N	5.53	127.63	120.44
1	A	756	GLU	C-N-CA	5.53	127.63	120.44
1	E	162	GLU	CA-C-N	5.53	131.25	122.62
1	E	162	GLU	C-N-CA	5.53	131.25	122.62
1	A	78	SER	CA-C-N	5.53	128.00	120.54
1	A	78	SER	C-N-CA	5.53	128.00	120.54
1	D	574	LEU	CA-C-N	5.53	130.79	123.05
1	D	574	LEU	C-N-CA	5.53	130.79	123.05
1	A	146	ILE	CA-C-N	5.53	130.62	123.00
1	A	146	ILE	C-N-CA	5.53	130.62	123.00
2	G	385	TYR	CA-C-N	5.53	131.45	122.39
2	G	385	TYR	C-N-CA	5.53	131.45	122.39
1	D	38	VAL	CA-C-N	5.52	130.52	122.69
1	D	38	VAL	C-N-CA	5.52	130.52	122.69
2	G	450	ILE	CA-C-N	5.52	130.33	122.72
2	G	450	ILE	C-N-CA	5.52	130.33	122.72
1	A	696	LYS	N-CA-CB	5.51	118.01	110.01
1	B	81	LYS	CA-CB-CG	5.51	125.13	114.10
1	C	491	GLU	CB-CG-CD	5.51	121.97	112.60
1	A	378	LEU	N-CA-CB	5.51	118.00	110.01
2	G	183	LEU	CA-C-N	5.51	130.76	123.05
2	G	183	LEU	C-N-CA	5.51	130.76	123.05
1	F	377	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	650	GLU	N-CA-CB	5.50	117.98	110.01
1	C	560	ARG	CA-C-N	5.50	127.58	120.44
1	C	560	ARG	C-N-CA	5.50	127.58	120.44
1	C	697	LEU	CA-C-N	5.50	127.58	120.44
1	C	697	LEU	C-N-CA	5.50	127.58	120.44
2	G	430	ASP	CA-C-N	5.50	128.19	120.28
2	G	430	ASP	C-N-CA	5.50	128.19	120.28
1	A	114	ILE	CA-C-N	5.49	130.51	122.77
1	A	114	ILE	C-N-CA	5.49	130.51	122.77
1	A	730	GLU	CA-C-N	5.48	129.79	122.01
1	A	730	GLU	C-N-CA	5.48	129.79	122.01
1	B	652	SER	CA-C-N	5.48	127.56	120.44
1	B	652	SER	C-N-CA	5.48	127.56	120.44
1	C	279	ALA	N-CA-C	5.47	118.00	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	381	LEU	CA-C-N	5.47	127.56	120.44
1	E	381	LEU	C-N-CA	5.47	127.56	120.44
1	B	508	MET	CA-C-N	5.47	128.26	120.49
1	B	508	MET	C-N-CA	5.47	128.26	120.49
1	B	515	LEU	CA-C-N	5.47	130.05	122.77
1	B	515	LEU	C-N-CA	5.47	130.05	122.77
1	E	160	ALA	CA-C-N	5.47	130.46	123.13
1	E	160	ALA	C-N-CA	5.47	130.46	123.13
1	A	733	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	658	LYS	CB-CG-CD	5.46	123.86	111.30
1	C	698	ALA	CA-C-N	5.46	127.44	120.56
1	C	698	ALA	C-N-CA	5.46	127.44	120.56
1	A	759	ALA	CA-C-N	5.45	127.53	120.44
1	A	759	ALA	C-N-CA	5.45	127.53	120.44
1	C	730	GLU	CB-CG-CD	5.45	121.87	112.60
1	D	121	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	491	GLU	CA-C-N	5.45	127.90	120.54
1	A	491	GLU	C-N-CA	5.45	127.90	120.54
1	B	514	VAL	CA-C-N	5.45	130.45	122.77
1	B	514	VAL	C-N-CA	5.45	130.45	122.77
1	F	147	ARG	NE-CZ-NH2	5.45	124.10	119.20
4	T	624	VAL	CA-C-N	5.44	127.58	120.28
4	T	624	VAL	C-N-CA	5.44	127.58	120.28
1	A	395	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	147	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	E	641	GLN	CA-C-N	5.43	130.22	122.72
1	E	641	GLN	C-N-CA	5.43	130.22	122.72
1	F	738	GLU	CA-C-N	5.43	127.51	120.44
1	F	738	GLU	C-N-CA	5.43	127.51	120.44
1	A	758	PHE	N-CA-CB	5.43	118.03	109.94
1	E	628	ILE	CA-C-N	5.43	127.78	120.50
1	E	628	ILE	C-N-CA	5.43	127.78	120.50
1	D	730	GLU	CA-C-N	5.43	127.85	120.63
1	D	730	GLU	C-N-CA	5.43	127.85	120.63
1	A	167	GLU	CA-C-N	5.43	130.65	123.00
1	A	167	GLU	C-N-CA	5.43	130.65	123.00
1	A	470	GLU	N-CA-CB	5.42	118.11	110.24
1	C	640	ASP	CA-C-N	5.42	130.65	123.05
1	C	640	ASP	C-N-CA	5.42	130.65	123.05
1	D	690	ILE	N-CA-CB	5.42	116.53	110.51
5	H	227	ALA	CA-C-N	5.42	128.30	120.38
5	H	227	ALA	C-N-CA	5.42	128.30	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	ASP	CA-C-N	5.42	127.55	120.28
1	A	35	ASP	C-N-CA	5.42	127.55	120.28
1	B	349	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	B	542	ILE	CA-C-N	5.41	130.37	122.41
1	B	542	ILE	C-N-CA	5.41	130.37	122.41
1	D	138	TYR	CA-C-N	5.41	129.88	120.68
1	D	138	TYR	C-N-CA	5.41	129.88	120.68
1	F	627	ASP	CA-C-N	5.41	131.71	121.97
1	F	627	ASP	C-N-CA	5.41	131.71	121.97
2	G	7	ILE	CA-C-N	5.40	129.42	120.94
2	G	7	ILE	C-N-CA	5.40	129.42	120.94
4	T	558	GLU	CA-C-N	5.40	127.46	120.44
4	T	558	GLU	C-N-CA	5.40	127.46	120.44
1	D	505	LYS	CG-CD-CE	5.40	123.71	111.30
1	B	513	GLY	CA-C-N	5.39	130.48	122.71
1	B	513	GLY	C-N-CA	5.39	130.48	122.71
1	B	691	CYS	CA-C-N	5.39	127.45	120.44
1	B	691	CYS	C-N-CA	5.39	127.45	120.44
1	D	689	GLU	N-CA-CB	5.39	117.83	110.01
1	D	513	GLY	CA-C-N	5.39	130.72	122.25
1	D	513	GLY	C-N-CA	5.39	130.72	122.25
1	E	187	GLU	N-CA-CB	5.39	118.17	110.03
1	B	603	GLN	CA-C-N	5.39	127.46	120.56
1	B	603	GLN	C-N-CA	5.39	127.46	120.56
1	F	669	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	512	LYS	CA-C-N	5.39	126.58	121.46
1	A	512	LYS	C-N-CA	5.39	126.58	121.46
1	B	693	ARG	N-CA-CB	5.38	117.82	110.01
2	G	359	PRO	CA-C-N	5.38	129.21	120.60
2	G	359	PRO	C-N-CA	5.38	129.21	120.60
1	B	115	HIS	ND1-CG-CD2	-5.38	100.72	106.10
1	A	21	ASN	N-CA-CB	5.38	117.86	109.85
1	C	573	VAL	CA-C-N	5.38	130.92	123.07
1	C	573	VAL	C-N-CA	5.38	130.92	123.07
1	B	157	GLY	CA-C-N	5.38	127.43	120.44
1	B	157	GLY	C-N-CA	5.38	127.43	120.44
1	B	665	PRO	CA-C-N	5.38	130.46	122.99
1	B	665	PRO	C-N-CA	5.38	130.46	122.99
1	B	693	ARG	CD-NE-CZ	5.38	131.93	124.40
1	C	490	GLN	CA-C-N	5.38	127.43	120.44
1	C	490	GLN	C-N-CA	5.38	127.43	120.44
1	D	126	ILE	CA-C-N	5.37	130.16	122.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	126	ILE	C-N-CA	5.37	130.16	122.21
4	T	602	PHE	N-CA-CB	5.37	117.80	110.01
1	B	22	ARG	CA-CB-CG	5.37	124.84	114.10
1	B	322	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	D	77	CYS	N-CA-CB	5.37	117.80	109.48
1	A	758	PHE	CA-CB-CG	5.36	119.16	113.80
1	B	391	ALA	CA-C-N	5.36	127.47	120.28
1	B	391	ALA	C-N-CA	5.36	127.47	120.28
1	B	169	ASP	CA-CB-CG	5.36	117.96	112.60
4	T	633	LEU	CA-C-N	5.36	127.41	120.44
4	T	633	LEU	C-N-CA	5.36	127.41	120.44
1	D	152	PHE	CA-C-N	5.35	131.22	122.81
1	D	152	PHE	C-N-CA	5.35	131.22	122.81
1	C	511	SER	N-CA-CB	5.35	117.84	109.97
1	C	363	PHE	CA-C-N	5.35	128.23	120.79
1	C	363	PHE	C-N-CA	5.35	128.23	120.79
1	C	404	HIS	CE1-NE2-CD2	-5.35	103.65	109.00
1	C	701	GLU	CB-CG-CD	5.34	121.69	112.60
1	D	664	SER	N-CA-CB	5.34	117.50	110.29
2	G	342	ILE	N-CA-CB	5.34	116.44	110.51
1	E	307	ASP	N-CA-CB	5.34	117.76	110.01
1	C	45	LYS	CA-C-N	5.34	127.97	120.28
1	C	45	LYS	C-N-CA	5.34	127.97	120.28
1	D	580	ASP	CA-C-N	5.34	127.70	120.44
1	D	580	ASP	C-N-CA	5.34	127.70	120.44
1	C	603	GLN	N-CA-CB	5.33	117.75	110.01
2	G	340	GLU	CA-C-N	5.33	127.37	120.44
2	G	340	GLU	C-N-CA	5.33	127.37	120.44
1	A	159	ARG	CA-CB-CG	5.33	124.76	114.10
1	D	27	ILE	CA-C-N	5.33	128.32	120.91
1	D	27	ILE	C-N-CA	5.33	128.32	120.91
5	H	269	THR	CA-C-N	5.33	131.18	123.13
5	H	269	THR	C-N-CA	5.33	131.18	123.13
1	B	733	ARG	NE-CZ-NH2	5.33	123.99	119.20
1	D	125	GLY	N-CA-C	5.33	119.12	112.73
1	C	737	GLU	CA-C-N	5.32	127.84	120.29
1	C	737	GLU	C-N-CA	5.32	127.84	120.29
1	D	144	ARG	CB-CG-CD	5.32	123.53	111.30
1	B	119	ILE	CA-C-N	5.31	127.35	120.44
1	B	119	ILE	C-N-CA	5.31	127.35	120.44
1	B	190	LYS	CA-C-N	5.31	127.67	120.65
1	B	190	LYS	C-N-CA	5.31	127.67	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	140	HIS	CA-C-N	5.31	131.69	121.54
2	G	140	HIS	C-N-CA	5.31	131.69	121.54
1	D	424	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	693	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	C	578	GLN	CA-C-N	5.30	127.65	120.38
1	C	578	GLN	C-N-CA	5.30	127.65	120.38
1	D	641	GLN	CA-CB-CG	5.30	124.71	114.10
1	B	115	HIS	CA-C-N	5.30	130.43	122.58
1	B	115	HIS	C-N-CA	5.30	130.43	122.58
1	E	234	GLY	CA-C-N	5.30	130.30	122.94
1	E	234	GLY	C-N-CA	5.30	130.30	122.94
2	G	160	LYS	CA-C-N	5.30	131.22	121.85
2	G	160	LYS	C-N-CA	5.30	131.22	121.85
4	T	597	GLN	CA-C-N	5.29	127.23	120.56
4	T	597	GLN	C-N-CA	5.29	127.23	120.56
1	A	183	HIS	N-CA-CB	5.29	118.32	110.49
1	B	696	LYS	N-CA-CB	5.29	117.68	110.01
1	D	37	SER	CA-C-N	5.29	130.42	123.17
1	D	37	SER	C-N-CA	5.29	130.42	123.17
1	F	693	ARG	CA-C-N	5.29	127.32	120.44
1	F	693	ARG	C-N-CA	5.29	127.32	120.44
5	H	266	GLY	CA-C-N	5.29	131.30	122.73
5	H	266	GLY	C-N-CA	5.29	131.30	122.73
1	F	564	ASP	N-CA-CB	5.29	117.68	110.01
1	A	444	SER	CA-C-N	5.29	128.27	120.82
1	A	444	SER	C-N-CA	5.29	128.27	120.82
1	F	752	ILE	CA-C-N	5.28	127.31	120.44
1	F	752	ILE	C-N-CA	5.28	127.31	120.44
1	A	671	ASP	N-CA-CB	5.28	117.96	110.46
1	D	695	CYS	CA-C-N	5.28	127.31	120.44
1	D	695	CYS	C-N-CA	5.28	127.31	120.44
1	A	90	ASN	CA-C-N	5.28	127.30	120.44
1	A	90	ASN	C-N-CA	5.28	127.30	120.44
1	D	696	LYS	N-CA-CB	5.28	117.66	110.01
1	D	505	LYS	CA-CB-CG	5.27	124.65	114.10
1	D	654	VAL	N-CA-CB	5.27	116.36	110.51
1	C	486	LYS	CA-C-N	5.27	127.30	120.44
1	C	486	LYS	C-N-CA	5.27	127.30	120.44
2	G	170	LYS	CG-CD-CE	5.27	123.43	111.30
1	E	95	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	E	658	LYS	CB-CG-CD	5.27	123.42	111.30
1	A	762	LEU	CA-C-N	5.27	127.29	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	762	LEU	C-N-CA	5.27	127.29	120.44
3	I	33	LYS	CA-CB-CG	5.26	124.63	114.10
1	E	710	GLU	N-CA-CB	5.26	117.64	110.01
1	A	86	ARG	CA-CB-CG	5.26	124.62	114.10
1	B	62	LYS	CB-CA-C	5.26	119.69	109.33
1	B	688	THR	CA-C-N	5.26	127.28	120.44
1	B	688	THR	C-N-CA	5.26	127.28	120.44
1	D	176	VAL	N-CA-CB	5.26	116.65	110.82
1	A	643	ILE	CA-C-N	5.25	129.39	122.30
1	A	643	ILE	C-N-CA	5.25	129.39	122.30
1	C	490	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	F	741	ARG	CA-C-N	5.25	127.32	120.28
1	F	741	ARG	C-N-CA	5.25	127.32	120.28
1	A	138	TYR	CA-CB-CG	5.25	123.35	113.90
4	T	623	ASP	CA-C-N	5.25	128.96	120.82
4	T	623	ASP	C-N-CA	5.25	128.96	120.82
1	F	741	ARG	CD-NE-CZ	5.25	131.75	124.40
1	B	473	GLN	N-CA-CB	5.25	117.72	109.69
1	F	144	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	C	393	ASP	N-CA-CB	-5.24	102.14	110.22
1	C	120	ASP	CA-CB-CG	5.24	117.84	112.60
1	C	664	SER	N-CA-CB	5.24	117.36	110.29
1	D	159	ARG	CA-CB-CG	5.24	124.58	114.10
1	A	753	ARG	CA-C-N	5.24	127.25	120.44
1	A	753	ARG	C-N-CA	5.24	127.25	120.44
1	B	617	VAL	CA-C-N	5.24	130.52	122.77
1	B	617	VAL	C-N-CA	5.24	130.52	122.77
2	G	181	VAL	N-CA-CB	5.24	116.64	110.82
1	A	399	VAL	CA-C-N	5.24	127.30	120.28
1	A	399	VAL	C-N-CA	5.24	127.30	120.28
1	A	499	HIS	CA-CB-CG	5.24	119.04	113.80
1	B	42	SER	N-CA-CB	5.24	117.87	109.28
1	D	134	TYR	CA-C-N	5.23	127.24	120.44
1	D	134	TYR	C-N-CA	5.23	127.24	120.44
1	D	749	ASP	CA-CB-CG	5.23	117.83	112.60
5	H	265	LEU	N-CA-CB	5.23	117.84	110.36
2	G	137	LYS	CA-C-N	5.23	130.92	122.29
2	G	137	LYS	C-N-CA	5.23	130.92	122.29
1	A	27	ILE	CA-C-N	5.23	127.70	120.49
1	A	27	ILE	C-N-CA	5.23	127.70	120.49
1	C	12	LEU	O-C-N	-5.23	114.64	123.00
1	E	753	ARG	CD-NE-CZ	5.23	131.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	53	ARG	CA-CB-CG	5.23	124.55	114.10
1	B	450	ASP	N-CA-CB	5.23	117.73	109.94
1	E	393	ASP	CA-C-N	5.22	128.40	120.77
1	E	393	ASP	C-N-CA	5.22	128.40	120.77
1	A	420	LEU	N-CA-CB	5.22	117.58	110.01
1	B	632	ALA	CA-C-N	5.22	127.84	120.42
1	B	632	ALA	C-N-CA	5.22	127.84	120.42
1	D	738	GLU	CA-C-N	5.22	127.27	120.28
1	D	738	GLU	C-N-CA	5.22	127.27	120.28
1	B	26	LEU	CA-C-N	5.21	129.59	122.34
1	B	26	LEU	C-N-CA	5.21	129.59	122.34
1	A	515	LEU	CA-C-N	5.21	128.17	120.82
1	A	515	LEU	C-N-CA	5.21	128.17	120.82
1	C	52	PHE	CA-C-N	5.21	128.17	120.82
1	C	52	PHE	C-N-CA	5.21	128.17	120.82
1	E	762	LEU	CA-C-N	5.21	127.22	120.44
1	E	762	LEU	C-N-CA	5.21	127.22	120.44
3	I	30	ILE	CA-C-N	5.21	127.21	120.44
3	I	30	ILE	C-N-CA	5.21	127.21	120.44
1	D	367	VAL	CA-C-N	5.21	130.09	122.85
1	D	367	VAL	C-N-CA	5.21	130.09	122.85
4	T	598	ILE	CA-C-N	5.20	127.11	120.56
4	T	598	ILE	C-N-CA	5.20	127.11	120.56
1	A	397	GLU	N-CA-CB	5.20	117.55	110.01
1	B	469	VAL	CA-C-N	5.20	129.96	122.16
1	B	469	VAL	C-N-CA	5.20	129.96	122.16
1	C	691	CYS	CA-C-N	5.20	127.25	120.28
1	C	691	CYS	C-N-CA	5.20	127.25	120.28
2	G	17	ARG	CD-NE-CZ	5.20	131.68	124.40
1	D	393	ASP	CA-C-N	5.20	127.58	120.35
1	D	393	ASP	C-N-CA	5.20	127.58	120.35
1	B	466	GLU	CA-C-N	5.20	130.54	122.49
1	B	466	GLU	C-N-CA	5.20	130.54	122.49
1	D	33	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	145	PRO	CA-C-N	5.19	130.47	122.68
1	A	145	PRO	C-N-CA	5.19	130.47	122.68
1	F	753	ARG	CD-NE-CZ	5.19	131.67	124.40
1	B	232	GLU	N-CA-CB	5.19	117.48	109.91
1	F	696	LYS	CA-CB-CG	5.19	124.48	114.10
1	A	80	GLU	CA-C-N	5.19	130.38	122.65
1	A	80	GLU	C-N-CA	5.19	130.38	122.65
1	D	83	ARG	CB-CG-CD	5.19	123.23	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	531	ILE	N-CA-CB	5.18	116.27	110.62
1	C	560	ARG	CD-NE-CZ	5.18	131.66	124.40
1	A	761	THR	CA-C-N	5.18	127.18	120.44
1	A	761	THR	C-N-CA	5.18	127.18	120.44
1	A	700	ARG	N-CA-CB	5.18	117.66	109.94
1	D	81	LYS	CA-CB-CG	5.18	124.45	114.10
1	A	58	LEU	CA-C-N	5.17	130.70	122.94
1	A	58	LEU	C-N-CA	5.17	130.70	122.94
1	D	183	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
1	C	191	ARG	NE-CZ-NH2	5.17	123.86	119.20
1	E	503	PHE	CA-C-N	5.17	127.17	120.44
1	E	503	PHE	C-N-CA	5.17	127.17	120.44
1	D	115	HIS	ND1-CG-CD2	-5.17	100.93	106.10
1	B	148	LYS	CA-CB-CG	5.17	124.44	114.10
1	F	567	ARG	CA-C-N	5.17	127.16	120.44
1	F	567	ARG	C-N-CA	5.17	127.16	120.44
4	T	603	VAL	CA-C-N	5.17	127.21	120.28
4	T	603	VAL	C-N-CA	5.17	127.21	120.28
1	A	702	SER	CA-C-N	5.17	127.07	120.56
1	A	702	SER	C-N-CA	5.17	127.07	120.56
1	C	491	GLU	CA-C-N	5.17	128.57	120.82
1	C	491	GLU	C-N-CA	5.17	128.57	120.82
1	D	694	ALA	CA-C-N	5.17	127.16	120.44
1	D	694	ALA	C-N-CA	5.17	127.16	120.44
1	A	47	ASP	CA-C-N	5.16	127.20	120.28
1	A	47	ASP	C-N-CA	5.16	127.20	120.28
1	C	592	ASP	N-CA-C	5.16	117.64	111.71
2	G	176	ASP	CA-C-N	5.16	129.45	122.07
2	G	176	ASP	C-N-CA	5.16	129.45	122.07
1	D	486	LYS	CA-C-N	5.15	127.14	120.44
1	D	486	LYS	C-N-CA	5.15	127.14	120.44
1	D	699	ILE	CA-C-N	5.15	127.50	120.54
1	D	699	ILE	C-N-CA	5.15	127.50	120.54
1	E	55	ASP	CA-C-N	5.15	128.19	120.87
1	E	55	ASP	C-N-CA	5.15	128.19	120.87
1	D	692	GLN	CA-C-N	5.15	127.14	120.44
1	D	692	GLN	C-N-CA	5.15	127.14	120.44
1	E	508	MET	CA-C-N	5.15	128.48	120.60
1	E	508	MET	C-N-CA	5.15	128.48	120.60
1	F	757	MET	N-CA-CB	5.15	117.48	110.01
2	G	181	VAL	CA-C-N	5.15	130.95	123.12
2	G	181	VAL	C-N-CA	5.15	130.95	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	404	HIS	ND1-CG-CD2	-5.15	100.95	106.10
1	D	691	CYS	CA-C-N	5.15	127.13	120.44
1	D	691	CYS	C-N-CA	5.15	127.13	120.44
1	B	447	VAL	CA-C-N	5.15	129.02	120.94
1	B	447	VAL	C-N-CA	5.15	129.02	120.94
1	B	700	ARG	N-CA-CB	5.15	117.47	110.01
1	D	120	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	358	ARG	NE-CZ-NH2	5.15	123.83	119.20
1	D	675	LEU	CA-C-N	5.15	127.13	120.44
1	D	675	LEU	C-N-CA	5.15	127.13	120.44
1	B	113	ARG	CA-C-N	5.14	130.14	122.99
1	B	113	ARG	C-N-CA	5.14	130.14	122.99
1	B	685	ALA	CA-C-N	5.14	127.13	120.44
1	B	685	ALA	C-N-CA	5.14	127.13	120.44
1	C	404	HIS	CG-CD2-NE2	5.14	112.34	107.20
2	G	449	ILE	N-CA-CB	5.14	116.63	110.31
4	T	568	GLU	CA-C-N	5.14	130.65	122.94
4	T	568	GLU	C-N-CA	5.14	130.65	122.94
4	T	601	ASP	CA-C-N	5.14	127.12	120.44
4	T	601	ASP	C-N-CA	5.14	127.12	120.44
1	B	179	ASP	CA-C-N	5.14	128.01	120.71
1	B	179	ASP	C-N-CA	5.14	128.01	120.71
1	E	494	GLN	CA-CB-CG	5.14	124.38	114.10
1	D	608	MET	CA-CB-CG	5.14	124.38	114.10
2	G	120	LYS	CA-C-N	5.14	130.29	123.10
2	G	120	LYS	C-N-CA	5.14	130.29	123.10
1	E	744	ARG	NE-CZ-NH2	5.14	123.82	119.20
1	F	691	CYS	N-CA-CB	5.13	117.41	109.91
1	E	626	PRO	CA-C-N	5.13	127.16	120.28
1	E	626	PRO	C-N-CA	5.13	127.16	120.28
1	F	663	LYS	CB-CG-CD	5.13	123.11	111.30
1	F	665	PRO	CA-C-N	5.13	129.97	122.69
1	F	665	PRO	C-N-CA	5.13	129.97	122.69
1	E	392	ASP	CA-C-N	5.13	129.93	122.08
1	E	392	ASP	C-N-CA	5.13	129.93	122.08
2	G	328	SER	CA-C-N	5.13	131.16	122.65
2	G	328	SER	C-N-CA	5.13	131.16	122.65
2	G	386	GLN	CB-CG-CD	5.13	121.31	112.60
1	A	161	VAL	CA-C-N	5.12	128.75	121.42
1	A	161	VAL	C-N-CA	5.12	128.75	121.42
1	C	510	PRO	CA-C-N	5.12	128.14	120.87
1	C	510	PRO	C-N-CA	5.12	128.14	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	147	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	D	87	VAL	N-CA-CB	5.12	116.54	110.55
1	A	88	VAL	N-CA-CB	5.12	116.54	110.55
1	A	148	LYS	CA-CB-CG	5.12	124.34	114.10
2	G	367	PHE	CA-C-N	5.12	129.82	122.45
2	G	367	PHE	C-N-CA	5.12	129.82	122.45
1	C	494	GLN	CB-CG-CD	5.12	121.30	112.60
1	D	183	HIS	ND1-CG-CD2	-5.12	100.98	106.10
1	D	699	ILE	N-CA-CB	5.12	116.53	110.55
1	F	580	ASP	CA-C-N	5.12	127.14	120.28
1	F	580	ASP	C-N-CA	5.12	127.14	120.28
1	B	136	LYS	CB-CG-CD	5.11	123.06	111.30
2	G	343	THR	CA-C-N	5.11	127.40	120.65
2	G	343	THR	C-N-CA	5.11	127.40	120.65
1	B	295	LYS	N-CA-CB	5.11	117.42	110.01
1	E	754	LYS	CG-CD-CE	5.11	123.05	111.30
2	G	170	LYS	N-CA-CB	5.11	117.42	110.01
1	C	639	LEU	CA-C-N	5.11	127.89	120.79
1	C	639	LEU	C-N-CA	5.11	127.89	120.79
2	G	345	GLY	CA-C-N	5.11	127.08	120.44
2	G	345	GLY	C-N-CA	5.11	127.08	120.44
1	C	155	ARG	NE-CZ-NH2	5.11	123.79	119.20
2	G	396	ARG	CD-NE-CZ	5.11	131.55	124.40
1	B	231	LYS	CA-C-N	5.10	127.39	120.65
1	B	231	LYS	C-N-CA	5.10	127.39	120.65
1	D	131	PHE	N-CA-CB	5.10	117.41	110.01
2	G	73	ASP	CA-C-N	5.10	130.88	123.12
2	G	73	ASP	C-N-CA	5.10	130.88	123.12
1	A	667	ALA	CA-C-N	5.10	127.12	120.28
1	A	667	ALA	C-N-CA	5.10	127.12	120.28
1	A	152	PHE	CA-C-N	5.10	131.28	121.54
1	A	152	PHE	C-N-CA	5.10	131.28	121.54
5	H	263	PHE	CA-CB-CG	5.10	118.90	113.80
1	B	172	PRO	CA-C-N	5.10	130.57	122.62
1	B	172	PRO	C-N-CA	5.10	130.57	122.62
1	C	48	GLU	CA-CB-CG	5.10	124.30	114.10
1	C	568	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	D	161	VAL	CA-C-N	5.09	131.07	122.87
1	D	161	VAL	C-N-CA	5.09	131.07	122.87
1	B	438	ASP	N-CA-CB	5.09	117.56	109.51
1	B	658	LYS	CB-CG-CD	5.09	123.01	111.30
2	G	218	GLN	N-CA-CB	5.09	117.48	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	500	PRO	CA-C-N	5.09	127.10	120.28
1	E	500	PRO	C-N-CA	5.09	127.10	120.28
1	E	756	GLU	N-CA-CB	5.09	117.60	110.12
4	T	558	GLU	N-CA-CB	5.09	117.39	110.01
1	A	66	GLU	CA-CB-CG	5.08	124.27	114.10
1	A	758	PHE	CA-C-N	5.08	127.05	120.44
1	A	758	PHE	C-N-CA	5.08	127.05	120.44
1	D	564	ASP	N-CA-CB	5.08	117.38	110.01
1	E	564	ASP	CA-C-N	5.08	127.05	120.44
1	E	564	ASP	C-N-CA	5.08	127.05	120.44
1	B	25	ARG	CA-C-N	5.08	130.49	122.36
1	B	25	ARG	C-N-CA	5.08	130.49	122.36
1	C	459	SER	N-CA-CB	5.08	117.42	109.85
1	D	364	ASP	CA-C-N	5.08	130.15	122.99
1	D	364	ASP	C-N-CA	5.08	130.15	122.99
1	E	386	LYS	CB-CG-CD	5.08	122.98	111.30
1	A	48	GLU	CA-C-N	5.08	130.78	122.65
1	A	48	GLU	C-N-CA	5.08	130.78	122.65
1	A	99	VAL	N-CA-CB	5.08	116.56	110.31
1	A	653	ARG	CA-C-N	5.08	126.96	120.56
1	A	653	ARG	C-N-CA	5.08	126.96	120.56
1	B	676	ALA	CA-C-N	5.08	127.39	120.54
1	B	676	ALA	C-N-CA	5.08	127.39	120.54
1	C	703	ILE	N-CA-CB	5.08	116.49	110.55
1	B	470	GLU	N-CA-CB	5.08	117.42	110.57
1	D	487	ARG	CG-CD-NE	5.08	123.17	112.00
5	H	263	PHE	CA-C-N	5.08	130.16	123.00
5	H	263	PHE	C-N-CA	5.08	130.16	123.00
4	T	634	LEU	CA-C-N	5.08	127.04	120.44
4	T	634	LEU	C-N-CA	5.08	127.04	120.44
1	B	187	GLU	CA-CB-CG	5.07	124.24	114.10
1	E	188	PRO	CA-C-N	5.07	130.57	122.56
1	E	188	PRO	C-N-CA	5.07	130.57	122.56
1	F	696	LYS	CA-C-N	5.07	127.08	120.28
1	F	696	LYS	C-N-CA	5.07	127.08	120.28
1	A	363	PHE	CA-C-N	5.07	128.71	120.60
1	A	363	PHE	C-N-CA	5.07	128.71	120.60
1	A	652	SER	CA-C-N	5.07	127.03	120.44
1	A	652	SER	C-N-CA	5.07	127.03	120.44
1	C	377	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	B	315	LYS	N-CA-C	5.07	118.61	112.23
1	A	756	GLU	CB-CG-CD	5.06	121.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	695	CYS	CA-C-N	5.06	127.02	120.44
1	B	695	CYS	C-N-CA	5.06	127.02	120.44
1	B	510	PRO	CA-C-N	5.06	128.66	121.42
1	B	510	PRO	C-N-CA	5.06	128.66	121.42
1	B	158	MET	CA-C-N	5.06	129.88	122.39
1	B	158	MET	C-N-CA	5.06	129.88	122.39
1	D	137	PRO	CA-C-N	5.06	129.07	120.88
1	D	137	PRO	C-N-CA	5.06	129.07	120.88
1	D	183	HIS	CG-CD2-NE2	5.06	112.26	107.20
1	F	735	HIS	CA-C-N	5.06	127.02	120.44
1	F	735	HIS	C-N-CA	5.06	127.02	120.44
1	A	40	SER	CA-C-N	5.05	130.45	122.36
1	A	40	SER	C-N-CA	5.05	130.45	122.36
1	A	650	GLU	CB-CG-CD	5.05	121.19	112.60
1	E	114	ILE	CA-C-N	5.05	130.26	122.93
1	E	114	ILE	C-N-CA	5.05	130.26	122.93
1	E	190	LYS	CB-CG-CD	5.05	122.92	111.30
1	F	760	GLN	N-CA-CB	5.05	117.55	110.12
1	B	618	PHE	CA-C-N	5.05	127.85	120.98
1	B	618	PHE	C-N-CA	5.05	127.85	120.98
1	C	696	LYS	N-CA-CB	5.05	117.47	109.94
1	D	621	GLY	CA-C-N	5.05	130.52	122.74
1	D	621	GLY	C-N-CA	5.05	130.52	122.74
1	D	114	ILE	CA-C-N	5.05	130.44	123.07
1	D	114	ILE	C-N-CA	5.05	130.44	123.07
1	E	712	GLU	CA-C-N	5.05	127.05	120.28
1	E	712	GLU	C-N-CA	5.05	127.05	120.28
1	E	749	ASP	N-CA-CB	5.05	117.46	109.94
4	T	557	LEU	CA-C-N	5.05	127.00	120.44
4	T	557	LEU	C-N-CA	5.05	127.00	120.44
2	G	396	ARG	CA-CB-CG	5.05	124.20	114.10
1	A	88	VAL	CA-C-N	5.05	127.00	120.44
1	A	88	VAL	C-N-CA	5.05	127.00	120.44
1	A	148	LYS	N-CA-CB	5.05	117.06	109.34
1	B	52	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	692	GLN	CA-C-N	5.04	127.00	120.44
1	B	692	GLN	C-N-CA	5.04	127.00	120.44
4	T	612	GLU	CA-C-N	5.04	130.62	122.29
4	T	612	GLU	C-N-CA	5.04	130.62	122.29
1	B	81	LYS	CG-CD-CE	5.04	122.90	111.30
1	B	148	LYS	N-CA-CB	5.04	117.30	109.48
2	G	431	LYS	CA-CB-CG	5.04	124.19	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	VAL	CA-C-N	5.04	130.65	122.68
1	A	99	VAL	C-N-CA	5.04	130.65	122.68
1	B	746	SER	N-CA-CB	5.04	117.53	110.12
1	E	365	ARG	CB-CA-C	5.04	117.68	111.43
1	A	436	THR	CA-C-N	5.04	127.33	120.63
1	A	436	THR	C-N-CA	5.04	127.33	120.63
1	C	349	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	C	653	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	D	115	HIS	CA-C-N	5.04	130.24	122.68
1	D	115	HIS	C-N-CA	5.04	130.24	122.68
1	A	381	LEU	CA-C-N	5.04	127.03	120.28
1	A	381	LEU	C-N-CA	5.04	127.03	120.28
1	E	766	ARG	CB-CG-CD	5.04	122.89	111.30
4	T	634	LEU	N-CA-CB	5.04	117.31	110.01
1	B	15	ALA	CA-C-N	5.04	126.91	120.56
1	B	15	ALA	C-N-CA	5.04	126.91	120.56
1	E	713	ARG	CG-CD-NE	5.04	123.08	112.00
1	F	567	ARG	N-CA-CB	5.04	117.31	110.01
1	A	67	ALA	CA-C-N	5.03	129.99	122.99
1	A	67	ALA	C-N-CA	5.03	129.99	122.99
1	C	147	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	F	754	LYS	N-CA-CB	5.03	117.52	110.12
1	C	692	GLN	CA-C-N	5.03	126.98	120.44
1	C	692	GLN	C-N-CA	5.03	126.98	120.44
1	E	210	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	B	186	GLY	CA-C-N	5.03	128.32	120.68
1	B	186	GLY	C-N-CA	5.03	128.32	120.68
1	D	27	ILE	N-CA-CB	5.03	116.58	110.95
1	B	74	ASP	CA-C-N	5.03	128.64	120.60
1	B	74	ASP	C-N-CA	5.03	128.64	120.60
1	B	217	LYS	CB-CG-CD	5.03	122.86	111.30
1	B	668	LYS	CB-CG-CD	5.03	122.86	111.30
1	E	139	PHE	CA-C-N	5.03	127.52	120.28
1	E	139	PHE	C-N-CA	5.03	127.52	120.28
2	G	391	CYS	N-CA-CB	5.03	117.43	109.94
1	C	695	CYS	CA-C-N	5.02	127.32	120.54
1	C	695	CYS	C-N-CA	5.02	127.32	120.54
1	A	733	ARG	CA-C-N	5.02	127.01	120.28
1	A	733	ARG	C-N-CA	5.02	127.01	120.28
1	C	699	ILE	N-CA-CB	5.02	116.43	110.55
4	T	611	ASP	CA-C-N	5.02	130.12	122.24
4	T	611	ASP	C-N-CA	5.02	130.12	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	500	PRO	CA-C-N	5.02	127.26	120.38
1	D	500	PRO	C-N-CA	5.02	127.26	120.38
1	D	700	ARG	CA-CB-CG	5.02	124.14	114.10
2	G	169	ARG	CB-CG-CD	5.02	122.85	111.30
1	D	34	GLU	CA-CB-CG	5.02	124.13	114.10
2	G	14	GLY	CA-C-N	5.02	129.41	123.19
2	G	14	GLY	C-N-CA	5.02	129.41	123.19
1	B	55	ASP	CA-C-N	5.02	128.67	121.50
1	B	55	ASP	C-N-CA	5.02	128.67	121.50
1	E	120	ASP	N-CA-CB	5.02	117.94	110.22
1	B	730	GLU	CA-C-N	5.01	128.82	121.80
1	B	730	GLU	C-N-CA	5.01	128.82	121.80
1	E	757	MET	CA-C-N	5.01	126.96	120.44
1	E	757	MET	C-N-CA	5.01	126.96	120.44
1	F	568	GLN	N-CA-CB	5.01	117.28	110.01
1	C	374	ALA	CA-C-N	5.01	127.93	120.31
1	C	374	ALA	C-N-CA	5.01	127.93	120.31
1	D	148	LYS	CB-CG-CD	5.01	122.82	111.30
1	F	658	LYS	CB-CG-CD	5.01	122.83	111.30
2	G	392	MET	CA-C-N	5.01	127.76	120.79
2	G	392	MET	C-N-CA	5.01	127.76	120.79
1	C	700	ARG	N-CA-CB	5.01	117.40	109.94
1	E	565	LYS	N-CA-CB	5.01	117.27	110.01
1	D	88	VAL	CA-C-N	5.01	126.95	120.44
1	D	88	VAL	C-N-CA	5.01	126.95	120.44
1	E	237	PRO	N-CA-CB	5.01	105.99	103.19
2	G	142	VAL	N-CA-CB	5.01	116.49	110.33
1	A	677	LYS	CA-CB-CG	5.01	124.11	114.10
1	B	738	GLU	CA-C-N	5.01	126.95	120.44
1	B	738	GLU	C-N-CA	5.01	126.95	120.44
1	E	359	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	G	128	GLN	CA-C-N	5.01	130.10	122.29
2	G	128	GLN	C-N-CA	5.01	130.10	122.29
2	G	170	LYS	CA-CB-CG	5.01	124.11	114.10
1	B	210	ARG	CA-CB-CG	5.00	124.11	114.10
4	T	596	LEU	CA-C-N	5.00	127.24	120.38
4	T	596	LEU	C-N-CA	5.00	127.24	120.38
1	D	74	ASP	CA-C-N	5.00	127.48	120.28
1	D	74	ASP	C-N-CA	5.00	127.48	120.28
1	C	728	VAL	N-CA-CB	5.00	118.21	111.21
1	D	606	THR	CA-C-N	5.00	126.94	120.44
1	D	606	THR	C-N-CA	5.00	126.94	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	756	GLU	CA-C-N	5.00	126.94	120.44
1	E	756	GLU	C-N-CA	5.00	126.94	120.44
2	G	168	ILE	CA-C-N	5.00	126.98	120.28
2	G	168	ILE	C-N-CA	5.00	126.98	120.28
2	G	451	ASP	CA-C-N	5.00	129.91	122.71
2	G	451	ASP	C-N-CA	5.00	129.91	122.71

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	ARG	Sidechain
1	A	733	ARG	Sidechain
1	B	586	ARG	Sidechain
1	C	323	ARG	Sidechain
1	C	755	TYR	Sidechain
1	D	166	VAL	Peptide
1	D	68	VAL	Peptide
1	D	755	TYR	Sidechain
1	E	313	ARG	Sidechain
1	E	323	ARG	Sidechain
1	E	363	PHE	Peptide
1	E	364	ASP	Peptide
1	E	404	HIS	Peptide
1	F	203	TYR	Sidechain
1	F	65	ARG	Sidechain
2	G	334	TYR	Sidechain
2	G	420	TYR	Sidechain
2	G	447	TYR	Sidechain
5	H	255	LYS	Peptide
4	T	578	ILE	Mainchain

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	A	5803	0	5876	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5951	0	6012	20	0
1	C	5891	0	5965	12	0
1	D	5789	0	5827	20	0
1	E	5724	0	5771	15	0
1	F	5531	0	5604	4	0
2	G	4305	0	4232	64	0
3	I	410	0	429	9	0
3	J	594	0	621	4	0
3	K	594	0	621	4	0
3	L	601	0	629	0	0
3	M	601	0	629	0	0
3	N	601	0	629	34	0
4	T	1422	0	1399	3	0
5	H	1954	0	1958	2	0
6	A	54	0	24	0	0
6	B	54	0	24	0	0
6	C	54	0	24	2	0
6	D	54	0	24	0	0
6	E	54	0	24	0	0
6	F	54	0	24	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
7	D	3	0	0	0	0
7	E	2	0	0	0	0
8	B	12	0	0	0	0
8	C	4	0	0	0	0
8	D	8	0	0	0	0
8	E	16	0	0	0	0
All	All	46145	0	46346	185	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 2.

All (185) 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)
2:G:279:ILE:HG23	2:G:288:LEU:HD11	1.64	0.78
2:G:162:MET:HE1	2:G:170:LYS:HD2	1.67	0.74
2:G:545:ARG:HE	3:N:9:THR:C	1.98	0.71
1:E:123:VAL:HG12	1:E:161:VAL:HG13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:VAL:CG1	1:E:161:VAL:HG13	2.25	0.66
1:C:608:MET:HE3	1:C:638:ARG:HD3	1.78	0.64
2:G:238:LEU:HD11	3:I:45:PHE:HD2	1.65	0.62
3:K:66:THR:HG23	3:K:66:THR:O	2.00	0.61
2:G:231:HIS:CE1	3:I:45:PHE:HE1	2.18	0.60
2:G:252:LEU:HD21	2:G:311:ILE:HB	1.83	0.58
1:A:437:ILE:HG21	1:A:442:MET:HE3	1.85	0.58
2:G:325:VAL:HG23	2:G:374:GLY:CA	2.32	0.58
2:G:231:HIS:ND1	3:I:43:LEU:HD13	2.19	0.57
1:C:113:ARG:HE	1:C:183:HIS:CD2	2.22	0.57
2:G:329:ARG:HG3	2:G:373:THR:HG21	1.85	0.57
1:A:177:ALA:HB3	1:A:179:ASP:OD1	2.04	0.57
1:C:447:VAL:CG2	1:D:233:ILE:HD11	2.35	0.57
2:G:544:LYS:N	3:N:10:GLY:O	2.36	0.57
2:G:545:ARG:HB2	3:N:11:LYS:CB	2.35	0.56
2:G:545:ARG:HD3	3:N:7:THR:N	2.21	0.56
3:N:6:LYS:CG	3:N:11:LYS:H	2.19	0.56
2:G:545:ARG:HE	3:N:10:GLY:N	2.05	0.55
2:G:325:VAL:HG22	2:G:378:ASN:O	2.07	0.55
1:B:118:PRO:HB2	1:B:123:VAL:HG11	1.88	0.55
1:D:116:VAL:HG12	1:D:165:VAL:HG22	1.88	0.54
2:G:542:THR:HA	3:N:10:GLY:HA3	1.90	0.54
2:G:545:ARG:NH2	3:N:6:LYS:HB3	2.23	0.54
2:G:234:ALA:HB1	2:G:382:PHE:HE2	1.73	0.53
2:G:545:ARG:HB2	3:N:11:LYS:CA	2.38	0.53
1:A:34:GLU:HA	1:A:38:VAL:HG23	1.89	0.53
2:G:391:CYS:O	2:G:395:VAL:HG22	2.08	0.53
1:E:177:ALA:HB1	1:E:178:PRO:HD2	1.91	0.53
1:B:493:VAL:HG21	1:B:535:CYS:SG	2.49	0.53
3:K:17:VAL:HG11	3:K:26:VAL:HG22	1.91	0.52
2:G:545:ARG:HG3	3:N:10:GLY:N	2.25	0.52
3:N:61:ILE:HD13	3:N:67:LEU:HD21	1.91	0.52
1:E:120:ASP:HA	1:E:123:VAL:HG22	1.92	0.51
1:F:757:MET:O	1:F:761:THR:HG23	2.10	0.51
2:G:507:PHE:CE2	2:G:511:LEU:HD11	2.45	0.51
2:G:545:ARG:HD2	3:N:11:LYS:N	2.25	0.51
1:E:181:VAL:HG23	1:E:181:VAL:O	2.11	0.51
4:T:529:HIS:O	4:T:533:MET:HG2	2.11	0.51
1:C:447:VAL:HG23	1:D:233:ILE:HD11	1.92	0.51
1:E:189:ILE:HG22	1:E:189:ILE:O	2.11	0.51
1:E:177:ALA:HB1	1:E:178:PRO:CD	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:MET:HE3	1:D:89:ARG:HG2	1.93	0.50
2:G:545:ARG:NE	3:N:10:GLY:HA2	2.27	0.50
3:N:66:THR:HG23	3:N:66:THR:O	2.11	0.50
1:B:119:ILE:O	1:B:123:VAL:HG22	2.12	0.50
2:G:279:ILE:HG23	2:G:288:LEU:CD1	2.40	0.50
3:N:6:LYS:HG3	3:N:11:LYS:H	1.76	0.50
1:B:493:VAL:HG11	1:B:535:CYS:SG	2.52	0.49
1:C:46:MET:HE3	1:C:46:MET:HA	1.94	0.49
2:G:545:ARG:HD3	3:N:8:LEU:N	2.27	0.49
5:H:74:SER:O	5:H:75:ASP:OD1	2.30	0.49
2:G:545:ARG:HD2	3:N:11:LYS:HB2	1.94	0.49
4:T:561:LEU:HD11	4:T:602:PHE:HA	1.94	0.49
1:D:38:VAL:HG22	1:D:39:VAL:N	2.27	0.49
1:A:28:VAL:HG23	1:A:98:ASP:O	2.13	0.49
2:G:543:TRP:HA	3:N:12:THR:HG23	1.95	0.49
1:C:551:TRP:H	1:C:551:TRP:CD1	2.31	0.49
1:A:117:LEU:HD22	1:A:187:GLU:HB3	1.95	0.48
1:A:657:LEU:HD23	1:A:687:LEU:HD21	1.94	0.48
3:N:34:GLU:O	3:N:74:ARG:HG2	2.13	0.48
1:A:32:ILE:HD12	1:A:83:ARG:NH2	2.28	0.48
2:G:542:THR:HA	3:N:10:GLY:CA	2.43	0.48
1:D:177:ALA:HB1	1:D:178:PRO:HD2	1.95	0.48
2:G:234:ALA:HB1	2:G:382:PHE:CE2	2.49	0.48
1:A:85:ASN:OD1	1:A:88:VAL:HG23	2.13	0.48
1:D:126:ILE:HG21	1:D:130:LEU:HD23	1.96	0.47
1:E:139:PHE:HB3	1:E:176:VAL:HG11	1.96	0.47
2:G:328:SER:O	2:G:333:THR:HG23	2.15	0.47
3:N:5:VAL:C	3:N:6:LYS:HD3	2.38	0.47
1:C:380:ILE:CD1	6:C:905:ADP:C2	2.97	0.47
1:D:423:ILE:HG22	1:D:427:MET:HE2	1.96	0.47
1:A:38:VAL:HG12	1:A:70:ILE:HB	1.96	0.47
1:A:40:SER:C	1:A:41:LEU:HD12	2.40	0.47
1:B:108:VAL:HG13	1:B:108:VAL:O	2.15	0.47
1:B:661:LEU:HD21	1:B:691:CYS:SG	2.55	0.47
2:G:318:GLU:H	2:G:325:VAL:HA	1.81	0.46
2:G:544:LYS:O	2:G:549:TRP:HB3	2.15	0.46
1:A:39:VAL:HG22	1:A:70:ILE:O	2.16	0.46
2:G:545:ARG:HH21	3:N:7:THR:N	2.13	0.46
4:T:529:HIS:CE1	4:T:533:MET:HE3	2.50	0.46
1:D:413:ALA:HB2	1:E:360:PHE:CD1	2.51	0.46
1:C:380:ILE:HD13	6:C:905:ADP:C2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:545:ARG:HD3	3:N:7:THR:H	1.80	0.46
1:F:747:VAL:O	1:F:747:VAL:HG13	2.16	0.45
2:G:323:GLY:HA2	3:I:48:LYS:O	2.16	0.45
1:C:318:GLY:HA3	1:C:322:ARG:H	1.81	0.45
2:G:557:SER:N	2:G:563:LEU:HD12	2.31	0.45
1:A:41:LEU:HD11	1:A:82:ILE:HD13	1.97	0.45
1:A:656:ILE:HG22	1:A:687:LEU:HD22	1.98	0.45
2:G:325:VAL:HG23	2:G:374:GLY:HA3	1.95	0.45
1:B:123:VAL:HG12	1:B:130:LEU:HD21	1.99	0.45
1:A:385:THR:HB	1:A:390:LEU:HD11	1.99	0.45
2:G:545:ARG:HH21	3:N:6:LYS:C	2.24	0.45
2:G:348:GLN:HB3	2:G:365:SER:HB3	1.98	0.45
2:G:501:LEU:HA	2:G:504:ILE:HG22	1.98	0.45
1:B:705:SER:O	1:B:709:ARG:HG2	2.17	0.44
3:N:5:VAL:HG21	3:N:30:ILE:HD11	1.99	0.44
1:A:270:ASN:H	1:A:273:GLU:HB3	1.81	0.44
2:G:230:ASN:OD1	2:G:233:VAL:HG23	2.17	0.44
1:A:177:ALA:HB1	1:A:178:PRO:HD2	1.98	0.44
2:G:542:THR:HA	3:N:10:GLY:C	2.42	0.44
2:G:545:ARG:HB2	3:N:11:LYS:HB2	1.97	0.44
1:B:395:ASP:H	1:B:449:MET:CE	2.30	0.44
2:G:287:LEU:HD23	2:G:289:GLU:H	1.83	0.44
3:J:26:VAL:O	3:J:30:ILE:HG12	2.17	0.44
1:B:111:GLY:O	1:B:180:THR:HA	2.17	0.44
1:D:275:MET:SD	1:E:323:ARG:NH2	2.91	0.44
1:D:134:TYR:CZ	1:D:161:VAL:HG21	2.53	0.43
3:I:27:LYS:HA	3:I:30:ILE:HG22	2.00	0.43
3:K:13:ILE:HG22	3:K:14:THR:N	2.33	0.43
2:G:161:HIS:HB3	2:G:221:ARG:HG3	2.00	0.43
2:G:162:MET:O	2:G:220:TYR:HB2	2.18	0.43
1:D:177:ALA:HB1	1:D:178:PRO:CD	2.48	0.43
1:F:672:LEU:HD12	1:F:672:LEU:H	1.84	0.43
1:B:133:VAL:HG12	1:B:157:GLY:HA2	2.01	0.43
1:E:203:TYR:CD2	1:E:217:LYS:HE2	2.52	0.43
1:D:38:VAL:HG22	1:D:39:VAL:H	1.84	0.43
1:E:118:PRO:O	1:E:188:PRO:HA	2.18	0.43
2:G:167:TYR:CE2	2:G:171:LEU:HD11	2.54	0.43
2:G:541:GLN:O	3:N:10:GLY:HA3	2.18	0.43
2:G:545:ARG:O	2:G:546:SER:C	2.60	0.43
1:A:297:ALA:HA	1:A:298:PRO:C	2.44	0.43
1:B:108:VAL:HG23	1:B:173:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:604:ILE:HG22	1:C:608:MET:HE2	2.01	0.43
2:G:546:SER:N	3:N:11:LYS:HG3	2.34	0.43
1:B:27:ILE:HG22	1:B:28:VAL:N	2.34	0.43
1:A:42:SER:HA	1:A:75:ASP:HA	2.01	0.42
1:E:87:VAL:HG13	1:E:151:ILE:O	2.19	0.42
1:A:272:PRO:CD	1:A:305:GLU:HB2	2.49	0.42
1:F:217:LYS:HE2	1:F:258:VAL:HG13	2.01	0.42
3:N:70:VAL:O	3:N:70:VAL:HG13	2.19	0.42
2:G:545:ARG:CD	3:N:8:LEU:N	2.83	0.42
1:E:323:ARG:HH21	1:E:323:ARG:HG2	1.84	0.42
2:G:231:HIS:CE1	3:I:45:PHE:CE1	3.03	0.42
2:G:325:VAL:HG23	2:G:374:GLY:HA2	2.00	0.42
1:A:657:LEU:HG	1:A:687:LEU:HD21	2.01	0.42
1:D:34:GLU:OE2	1:D:35:ASP:O	2.38	0.42
2:G:169:ARG:O	2:G:173:GLY:HA3	2.20	0.42
3:J:24:GLU:CB	3:J:52:ASP:OD1	2.68	0.42
1:C:740:MET:HE3	1:D:768:PHE:CZ	2.54	0.42
1:D:35:ASP:OD1	1:D:38:VAL:HG12	2.20	0.42
2:G:178:GLY:HA2	2:G:181:VAL:HG23	2.01	0.42
1:A:115:HIS:CD2	1:A:183:HIS:O	2.73	0.42
1:D:34:GLU:OE2	1:D:38:VAL:O	2.37	0.42
3:J:27:LYS:HB3	3:J:38:PRO:HB3	2.02	0.42
1:A:46:MET:SD	1:A:73:SER:HA	2.60	0.41
1:E:323:ARG:HH21	1:E:323:ARG:CG	2.33	0.41
2:G:292:LYS:O	2:G:295:VAL:HG12	2.20	0.41
3:K:11:LYS:CE	3:K:13:ILE:HD11	2.49	0.41
1:A:31:ALA:HB1	1:A:34:GLU:HB2	2.03	0.41
2:G:238:LEU:CD1	3:I:45:PHE:HD2	2.31	0.41
2:G:471:PHE:CD1	2:G:472:PRO:HD2	2.55	0.41
3:N:29:LYS:N	3:N:29:LYS:HD3	2.35	0.41
2:G:294:GLU:HG2	2:G:295:VAL:N	2.35	0.41
2:G:455:THR:HB	3:I:40:GLN:HB3	2.01	0.41
1:A:70:ILE:HG22	1:A:71:VAL:N	2.35	0.41
1:B:16:ILE:HG23	1:B:17:LEU:N	2.35	0.41
1:A:31:ALA:HB2	1:A:85:ASN:HA	2.02	0.41
1:A:255:ALA:HB2	1:A:302:PHE:CE1	2.55	0.41
1:B:27:ILE:CG2	1:B:28:VAL:N	2.83	0.41
1:B:284:SER:O	1:B:288:LYS:HG2	2.21	0.41
1:D:84:MET:SD	1:D:88:VAL:HG12	2.60	0.41
2:G:521:LEU:HD12	2:G:521:LEU:N	2.36	0.41
1:A:657:LEU:CD2	1:A:687:LEU:HD21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:GLY:HA3	1:B:180:THR:OG1	2.21	0.41
1:D:74:ASP:CG	1:D:76:THR:HG1	2.29	0.41
1:A:142:ALA:O	1:A:143:TYR:C	2.63	0.41
2:G:258:GLU:HG2	2:G:265:GLY:O	2.21	0.41
5:H:31:LEU:HD13	5:H:93:TYR:CE2	2.56	0.41
3:I:29:LYS:O	3:I:32:ASP:OD1	2.40	0.40
1:B:139:PHE:CG	1:B:176:VAL:HG11	2.55	0.40
1:D:152:PHE:CZ	1:D:163:PHE:HB2	2.57	0.40
2:G:326:ARG:HE	2:G:327:TYR:N	2.20	0.40
1:B:35:ASP:CG	1:B:144:ARG:HH22	2.29	0.40
1:A:105:CYS:SG	1:A:108:VAL:HG22	2.61	0.40
1:A:499:HIS:N	1:A:500:PRO:HD3	2.36	0.40
1:B:28:VAL:CG1	1:B:89:ARG:HD3	2.52	0.40
1:C:373:ASP:O	1:C:377:ARG:CZ	2.69	0.40
2:G:545:ARG:HD3	3:N:8:LEU:H	1.87	0.40
3:J:63:LYS:HG3	3:J:64:GLU:HG2	2.03	0.40
3:N:1:MET:SD	3:N:3:ILE:HG23	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	739/826 (90%)	687 (93%)	52 (7%)	0	100	100
1	B	755/826 (91%)	705 (93%)	50 (7%)	0	100	100
1	C	748/826 (91%)	707 (94%)	41 (6%)	0	100	100
1	D	738/826 (89%)	693 (94%)	44 (6%)	1 (0%)	48	79
1	E	726/826 (88%)	672 (93%)	54 (7%)	0	100	100
1	F	691/826 (84%)	645 (93%)	46 (7%)	0	100	100
2	G	536/608 (88%)	497 (93%)	39 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	50/76 (66%)	48 (96%)	2 (4%)	0	100	100
3	J	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
3	K	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
3	L	74/76 (97%)	74 (100%)	0	0	100	100
3	M	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
3	N	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
4	T	168/170 (99%)	166 (99%)	1 (1%)	1 (1%)	21	56
5	H	244/307 (80%)	233 (96%)	11 (4%)	0	100	100
All	All	5765/6497 (89%)	5407 (94%)	356 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	545	PRO
4	T	620	PRO

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	A	626/696 (90%)	618 (99%)	8 (1%)	61	78
1	B	646/696 (93%)	638 (99%)	8 (1%)	63	79
1	C	638/696 (92%)	628 (98%)	10 (2%)	55	75
1	D	623/696 (90%)	619 (99%)	4 (1%)	78	84
1	E	617/696 (89%)	606 (98%)	11 (2%)	51	74
1	F	603/696 (87%)	588 (98%)	15 (2%)	42	69
2	G	479/531 (90%)	476 (99%)	3 (1%)	78	84
3	I	47/68 (69%)	46 (98%)	1 (2%)	47	71
3	J	66/68 (97%)	66 (100%)	0	100	100
3	K	66/68 (97%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	68/68 (100%)	68 (100%)	0	100 100
3	M	68/68 (100%)	68 (100%)	0	100 100
3	N	68/68 (100%)	68 (100%)	0	100 100
4	T	153/153 (100%)	152 (99%)	1 (1%)	76 83
5	H	219/267 (82%)	217 (99%)	2 (1%)	70 81
All	All	4987/5535 (90%)	4924 (99%)	63 (1%)	59 78

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	LEU
1	A	274	ILE
1	A	278	LEU
1	A	321	GLU
1	A	336	LYS
1	A	348	ASN
1	A	364	ASP
1	A	580	ASP
1	B	38	VAL
1	B	262	THR
1	B	286	LEU
1	B	328	LEU
1	B	359	ARG
1	B	462	SER
1	B	580	ASP
1	B	609	ASP
1	C	57	VAL
1	C	85	ASN
1	C	93	ARG
1	C	209	CYS
1	C	284	SER
1	C	320	VAL
1	C	403	THR
1	C	556	GLU
1	C	662	ARG
1	C	675	LEU
1	D	92	LEU
1	D	166	VAL
1	D	531	ILE
1	D	749	ASP

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Mol	Chain	Res	Type
1	E	38	VAL
1	E	87	VAL
1	E	241	ILE
1	E	273	GLU
1	E	323	ARG
1	E	390	LEU
1	E	420	LEU
1	E	443	ASN
1	E	666	VAL
1	E	734	ASP
1	E	752	ILE
1	F	64	ARG
1	F	79	ASP
1	F	226	HIS
1	F	251	LYS
1	F	258	VAL
1	F	261	GLU
1	F	284	SER
1	F	332	MET
1	F	373	ASP
1	F	448	THR
1	F	499	HIS
1	F	508	MET
1	F	515	LEU
1	F	516	PHE
1	F	749	ASP
2	G	195	GLU
2	G	206	THR
2	G	443	LEU
3	I	26	VAL
4	T	589	ARG
5	H	234	ARG
5	H	250	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	HIS
1	A	387	ASN
1	B	260	ASN
1	B	348	ASN
1	B	404	HIS

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Mol	Chain	Res	Type
1	B	458	GLN
1	B	578	GLN
1	B	624	ASN
1	C	33	ASN
1	C	348	ASN
1	C	578	GLN
1	D	24	ASN
1	D	260	ASN
1	D	340	HIS
1	D	404	HIS
1	D	568	GLN
1	D	602	ASN
1	E	270	ASN
1	E	401	ASN
1	E	538	ASN
1	F	43	GLN
1	F	296	ASN
1	F	421	GLN
1	F	533	ASN
2	G	351	HIS
2	G	362	HIS
2	G	516	ASN
2	G	541	GLN
4	T	630	ASN
5	H	100	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 10 are monoatomic - leaving 22 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	$\#\|Z\| > 2$
6	ADP	B	903	8,7	27,29,29	1.10	2 (7%)	42,45,45	1.46	7 (16%)
6	ADP	D	904	8,7	27,29,29	1.00	0	42,45,45	1.35	7 (16%)
8	BEF	E	904	6	0,3,3	-	-	-		
6	ADP	D	906	8,7	27,29,29	1.04	1 (3%)	42,45,45	1.47	9 (21%)
8	BEF	B	904	6	0,3,3	-	-	-		
6	ADP	A	903	8,7	27,29,29	1.02	1 (3%)	42,45,45	1.23	6 (14%)
8	BEF	E	901	6	0,3,3	-	-	-		
8	BEF	C	901	6	0,3,3	-	-	-		
6	ADP	F	902	-	27,29,29	0.97	0	42,45,45	1.46	8 (19%)
8	BEF	E	907	6	0,3,3	-	-	-		
8	BEF	B	901	6	0,3,3	-	-	-		
8	BEF	E	902	6	0,3,3	-	-	-		
6	ADP	B	906	8,7	27,29,29	1.03	1 (3%)	42,45,45	1.28	6 (14%)
8	BEF	D	901	6	0,3,3	-	-	-		
6	ADP	F	901	-	27,29,29	0.99	0	42,45,45	1.41	8 (19%)
6	ADP	E	903	8,7	27,29,29	1.03	0	42,45,45	1.41	7 (16%)
8	BEF	B	902	6	0,3,3	-	-	-		
6	ADP	C	903	8,7	27,29,29	1.15	3 (11%)	42,45,45	1.27	5 (11%)
6	ADP	C	905	8,7	27,29,29	1.05	1 (3%)	42,45,45	1.39	9 (21%)
6	ADP	E	906	8,7	27,29,29	1.00	1 (3%)	42,45,45	1.34	8 (19%)
6	ADP	A	901	8,7	27,29,29	1.09	2 (7%)	42,45,45	1.47	6 (14%)
8	BEF	D	902	6	0,3,3	-	-	-		

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
6	ADP	F	902	-	-	3/16/32/32	0/3/3/3
6	ADP	B	903	8,7	-	3/16/32/32	0/3/3/3
6	ADP	D	904	8,7	-	4/16/32/32	0/3/3/3
6	ADP	C	903	8,7	-	5/16/32/32	0/3/3/3
6	ADP	C	905	8,7	-	5/16/32/32	0/3/3/3
6	ADP	D	906	8,7	-	3/16/32/32	0/3/3/3
6	ADP	E	906	8,7	-	2/16/32/32	0/3/3/3
6	ADP	A	901	8,7	-	3/16/32/32	0/3/3/3
6	ADP	A	903	8,7	-	3/16/32/32	0/3/3/3
6	ADP	F	901	-	-	7/16/32/32	0/3/3/3
6	ADP	E	903	8,7	-	1/16/32/32	0/3/3/3
6	ADP	B	906	8,7	-	5/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	903	ADP	C5-C4	-2.37	1.34	1.39
6	B	906	ADP	C5-C4	-2.36	1.34	1.39
6	C	905	ADP	C5-C4	-2.31	1.34	1.39
6	B	903	ADP	C5-C4	-2.29	1.34	1.39
6	D	906	ADP	C5-C4	-2.24	1.34	1.39
6	A	901	ADP	C5-C4	-2.20	1.34	1.39
6	C	903	ADP	PB-O2B	-2.13	1.46	1.54
6	A	903	ADP	C5-C4	-2.10	1.35	1.39
6	B	903	ADP	PB-O3B	-2.06	1.46	1.54
6	C	903	ADP	PB-O3B	-2.05	1.47	1.54
6	A	901	ADP	PB-O3B	-2.02	1.47	1.54
6	E	906	ADP	C5-C4	-2.00	1.35	1.39

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	905	ADP	PA-O3A-PB	-4.10	118.75	132.83
6	D	906	ADP	O3B-PB-O3A	3.96	117.90	104.64
6	A	901	ADP	PA-O3A-PB	-3.78	119.86	132.83
6	B	903	ADP	PA-O3A-PB	-3.75	119.95	132.83
6	E	903	ADP	O2B-PB-O3A	3.68	116.99	104.64
6	A	901	ADP	O2B-PB-O3A	3.54	116.50	104.64
6	F	902	ADP	C5-C4-N3	-3.52	122.16	126.75
6	D	904	ADP	O2B-PB-O3A	3.47	116.28	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	906	ADP	PA-O3A-PB	-3.42	121.09	132.83
6	D	906	ADP	C5-C4-N3	-3.19	122.59	126.75
6	F	901	ADP	PA-O3A-PB	-3.18	121.92	132.83
6	F	901	ADP	C5-C4-N3	-3.17	122.62	126.75
6	E	903	ADP	C5-C4-N3	-3.13	122.67	126.75
6	D	904	ADP	C5-C4-N3	-3.11	122.69	126.75
6	C	903	ADP	PA-O3A-PB	-3.10	122.20	132.83
6	C	905	ADP	C5-C4-N3	-3.09	122.72	126.75
6	B	906	ADP	PA-O3A-PB	-3.07	122.30	132.83
6	F	902	ADP	PA-O3A-PB	-3.04	122.40	132.83
6	A	903	ADP	PA-O3A-PB	-3.01	122.50	132.83
6	B	906	ADP	C5-C4-N3	-3.01	122.83	126.75
6	A	901	ADP	C4-C5-N7	3.00	114.27	110.62
6	B	903	ADP	O2B-PB-O3A	2.95	114.52	104.64
6	C	903	ADP	C4-C5-N7	2.93	114.19	110.62
6	B	903	ADP	C4-C5-N7	2.88	114.12	110.62
6	E	903	ADP	PA-O3A-PB	-2.86	123.02	132.83
6	D	904	ADP	C4-C5-N7	2.82	114.06	110.62
6	D	906	ADP	PA-O3A-PB	-2.81	123.20	132.83
6	A	901	ADP	O3B-PB-O3A	2.78	113.96	104.64
6	A	903	ADP	C5-C4-N3	-2.76	123.14	126.75
6	F	902	ADP	C4-C5-N7	2.74	113.95	110.62
6	F	901	ADP	C4-C5-N7	2.70	113.91	110.62
6	A	903	ADP	C4-C5-N7	2.70	113.91	110.62
6	B	903	ADP	C5-C4-N3	-2.69	123.24	126.75
6	B	906	ADP	C4-C5-N7	2.67	113.87	110.62
6	F	902	ADP	N3-C4-N9	2.66	131.46	127.08
6	C	905	ADP	O2B-PB-O3A	2.64	113.49	104.64
6	C	903	ADP	C5-C4-N3	-2.60	123.36	126.75
6	E	906	ADP	O2B-PB-O3A	2.59	113.34	104.64
6	B	903	ADP	O3B-PB-O1B	-2.59	100.55	110.68
6	A	901	ADP	C5-C4-N3	-2.55	123.42	126.75
6	F	902	ADP	C5-C6-N1	2.54	122.85	117.39
6	E	906	ADP	C5-C4-N3	-2.53	123.44	126.75
6	F	901	ADP	O2B-PB-O3A	2.53	113.12	104.64
6	D	904	ADP	PA-O3A-PB	-2.53	124.14	132.83
6	F	901	ADP	O4'-C1'-C2'	-2.53	101.14	106.64
6	E	903	ADP	C4-C5-N7	2.52	113.69	110.62
6	E	906	ADP	C4-C5-N7	2.50	113.67	110.62
6	E	903	ADP	C5-C6-N1	2.49	122.73	117.39
6	D	906	ADP	C5-C6-N1	2.47	122.69	117.39
6	D	904	ADP	C5-C6-N1	2.47	122.69	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	901	ADP	N3-C4-N9	2.46	131.14	127.08
6	F	901	ADP	C5-C6-N1	2.46	122.66	117.39
6	B	906	ADP	C5-C6-N1	2.45	122.64	117.39
6	C	905	ADP	C4-C5-N7	2.43	113.58	110.62
6	C	903	ADP	C5-C6-N1	2.43	122.61	117.39
6	D	906	ADP	O2B-PB-O3A	2.43	112.77	104.64
6	A	903	ADP	O3B-PB-O3A	2.41	112.71	104.64
6	D	906	ADP	C4-C5-N7	2.41	113.55	110.62
6	D	906	ADP	O2B-PB-O1B	-2.40	101.29	110.68
6	B	903	ADP	C5-C6-N1	2.39	122.52	117.39
6	F	902	ADP	O4'-C1'-C2'	-2.39	101.44	106.64
6	E	906	ADP	C5-C6-N1	2.36	122.46	117.39
6	F	902	ADP	C2'-C1'-N9	2.36	119.28	113.30
6	F	902	ADP	C2-N1-C6	-2.34	114.76	118.77
6	D	904	ADP	N3-C4-N9	2.32	130.90	127.08
6	A	903	ADP	C5-C6-N1	2.27	122.27	117.39
6	A	901	ADP	C5-C6-N1	2.26	122.25	117.39
6	E	906	ADP	C2-N1-C6	-2.26	114.89	118.77
6	E	906	ADP	O3B-PB-O1B	-2.25	101.88	110.68
6	C	905	ADP	C5-C6-N1	2.22	122.16	117.39
6	E	903	ADP	C2-N1-C6	-2.22	114.96	118.77
6	C	905	ADP	N6-C6-N1	-2.21	113.50	118.35
6	E	903	ADP	N3-C4-N9	2.20	130.71	127.08
6	A	903	ADP	N3-C4-N9	2.16	130.63	127.08
6	B	906	ADP	C2-N1-C6	-2.15	115.08	118.77
6	D	904	ADP	C2-N1-C6	-2.14	115.10	118.77
6	B	906	ADP	N3-C4-N9	2.14	130.60	127.08
6	C	903	ADP	O2B-PB-O3A	2.12	111.74	104.64
6	C	905	ADP	O2B-PB-O1B	-2.12	102.39	110.68
6	D	906	ADP	N3-C4-N9	2.11	130.56	127.08
6	D	906	ADP	C2-N1-C6	-2.06	115.22	118.77
6	F	901	ADP	O3B-PB-O3A	2.03	111.45	104.64
6	B	903	ADP	C2-N1-C6	-2.02	115.29	118.77
6	C	905	ADP	C2-N1-C6	-2.02	115.30	118.77
6	C	905	ADP	N3-C4-N9	2.02	130.41	127.08
6	E	906	ADP	C3'-C2'-C1'	2.00	105.23	101.43

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	905	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
6	F	901	ADP	C5'-O5'-PA-O3A
6	F	901	ADP	C4'-C5'-O5'-PA
6	F	902	ADP	C2'-C1'-N9-C4
6	A	901	ADP	C3'-C4'-C5'-O5'
6	A	901	ADP	O4'-C4'-C5'-O5'
6	D	904	ADP	C3'-C4'-C5'-O5'
6	F	902	ADP	C4'-C5'-O5'-PA
6	B	903	ADP	O4'-C4'-C5'-O5'
6	D	904	ADP	O4'-C4'-C5'-O5'
6	B	903	ADP	C3'-C4'-C5'-O5'
6	B	906	ADP	O4'-C4'-C5'-O5'
6	C	903	ADP	O4'-C4'-C5'-O5'
6	F	901	ADP	C3'-C4'-C5'-O5'
6	B	906	ADP	C3'-C4'-C5'-O5'
6	C	903	ADP	C3'-C4'-C5'-O5'
6	F	901	ADP	C2'-C1'-N9-C4
6	A	901	ADP	C4'-C5'-O5'-PA
6	B	903	ADP	C4'-C5'-O5'-PA
6	C	903	ADP	C4'-C5'-O5'-PA
6	F	902	ADP	C2'-C1'-N9-C8
6	A	903	ADP	C4'-C5'-O5'-PA
6	D	906	ADP	C4'-C5'-O5'-PA
6	C	903	ADP	PB-O3A-PA-O2A
6	D	904	ADP	PB-O3A-PA-O1A
6	B	906	ADP	C4'-C5'-O5'-PA
6	D	904	ADP	C4'-C5'-O5'-PA
6	F	901	ADP	C5'-O5'-PA-O1A
6	F	901	ADP	C2'-C1'-N9-C8
6	E	903	ADP	C4'-C5'-O5'-PA
6	F	901	ADP	O4'-C4'-C5'-O5'
6	B	906	ADP	PB-O3A-PA-O2A
6	D	906	ADP	PB-O3A-PA-O2A
6	E	906	ADP	PB-O3A-PA-O2A
6	A	903	ADP	O4'-C4'-C5'-O5'
6	B	906	ADP	PB-O3A-PA-O1A
6	D	906	ADP	PB-O3A-PA-O1A
6	C	905	ADP	PA-O3A-PB-O1B
6	A	903	ADP	C3'-C4'-C5'-O5'
6	C	905	ADP	PA-O3A-PB-O3B
6	C	905	ADP	C5'-O5'-PA-O3A
6	C	903	ADP	PB-O3A-PA-O1A
6	C	905	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
6	E	906	ADP	O4'-C4'-C5'-O5'

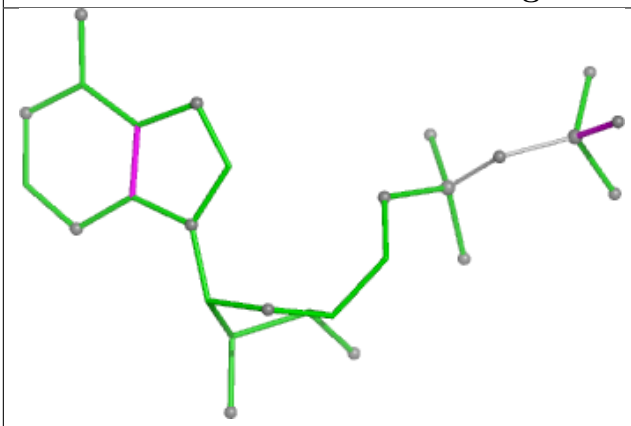
There are no ring outliers.

1 monomer is involved in 2 short contacts:

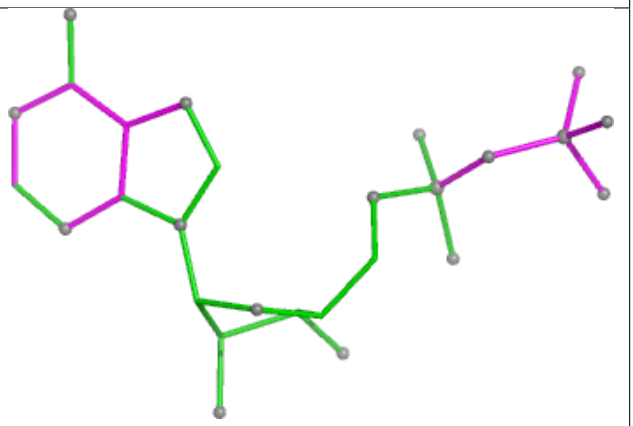
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	905	ADP	2	0

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 then 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.

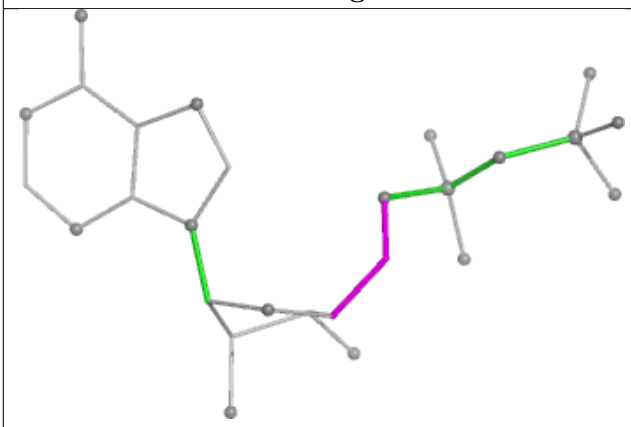
Ligand ADP B 903



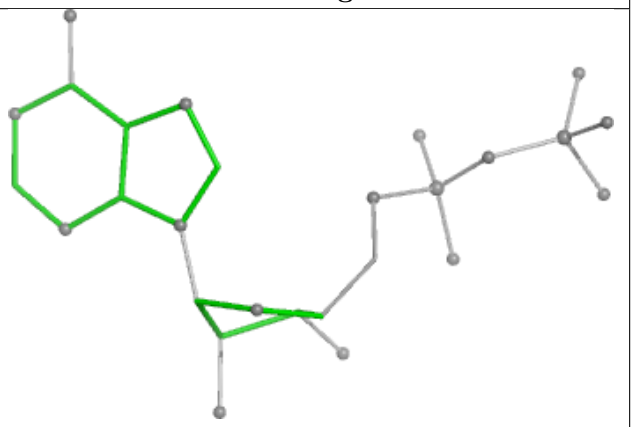
Bond lengths



Bond angles

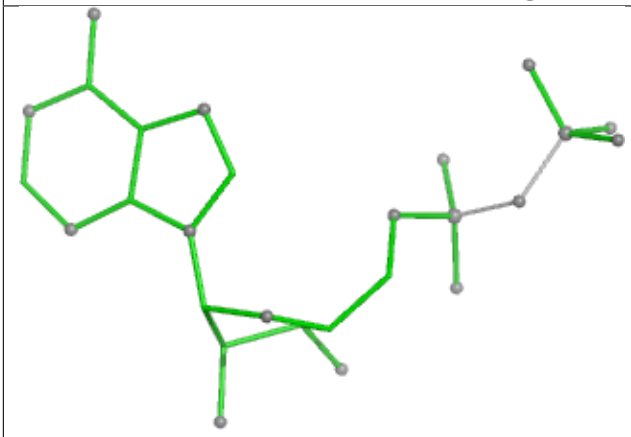


Torsions

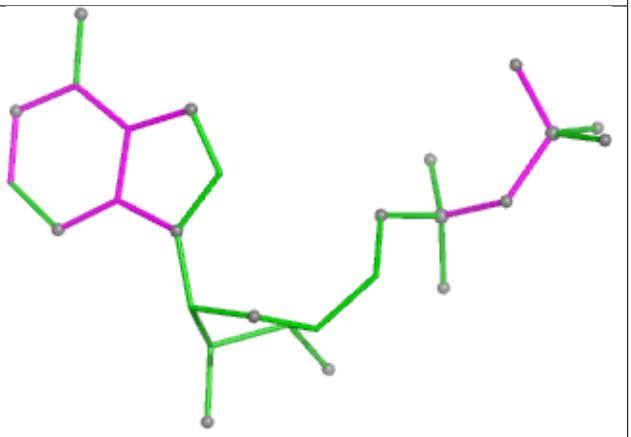


Rings

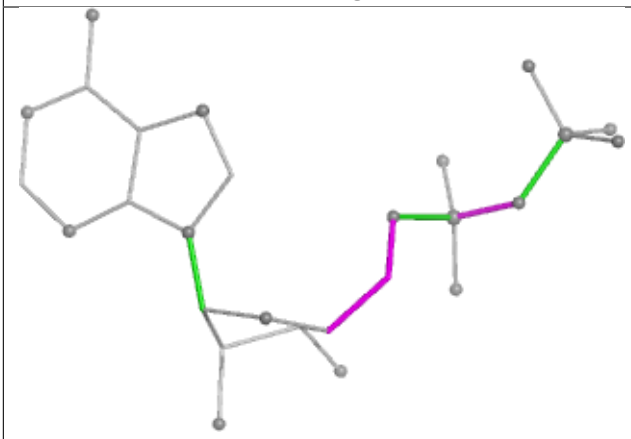
Ligand ADP D 904



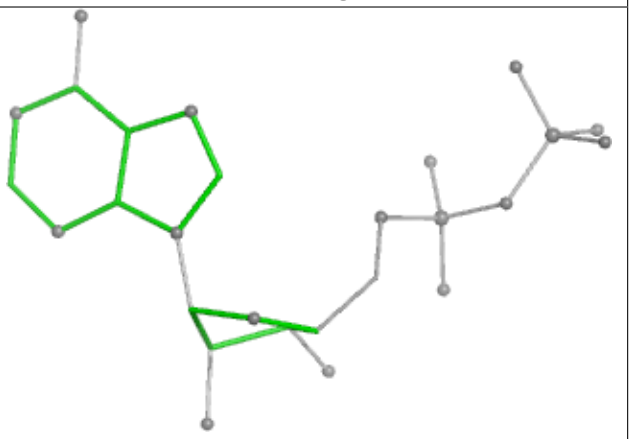
Bond lengths



Bond angles

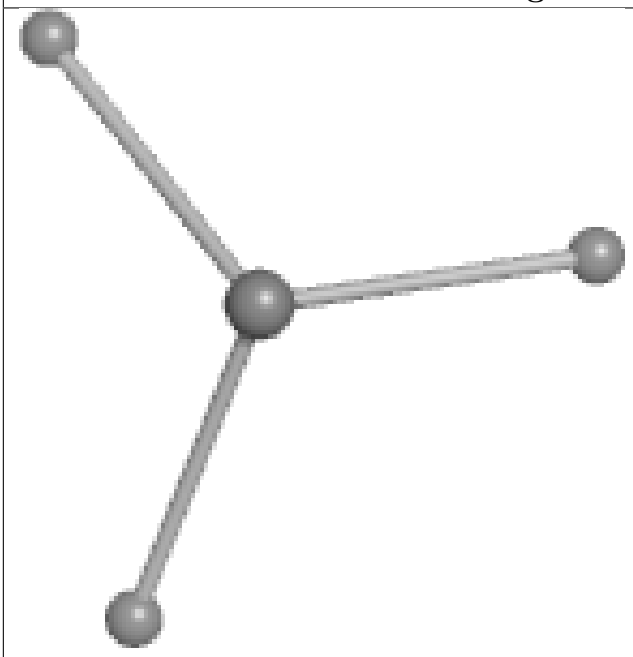


Torsions

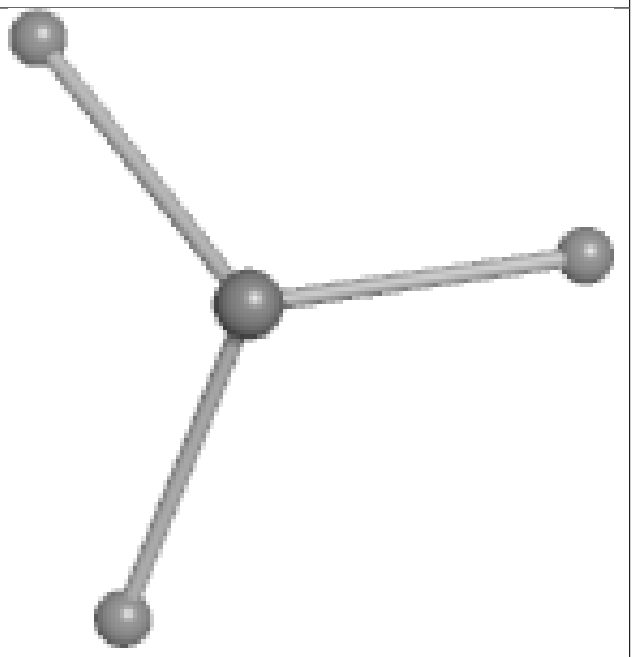


Rings

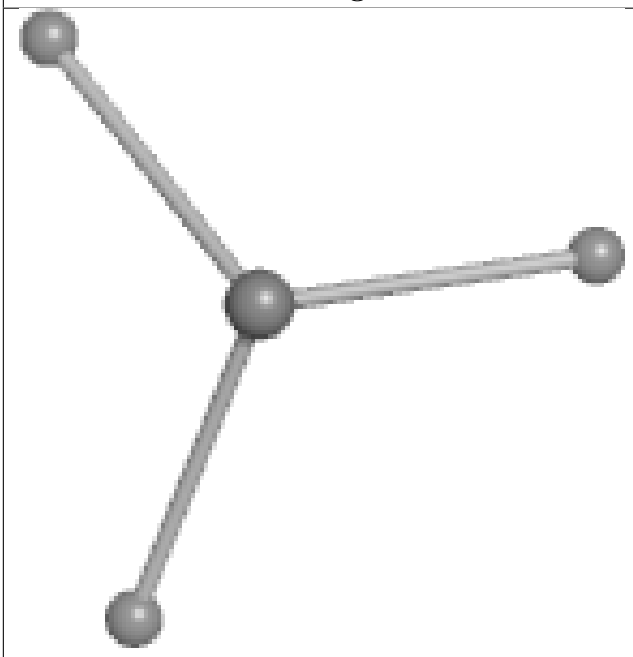
Ligand BEF E 904



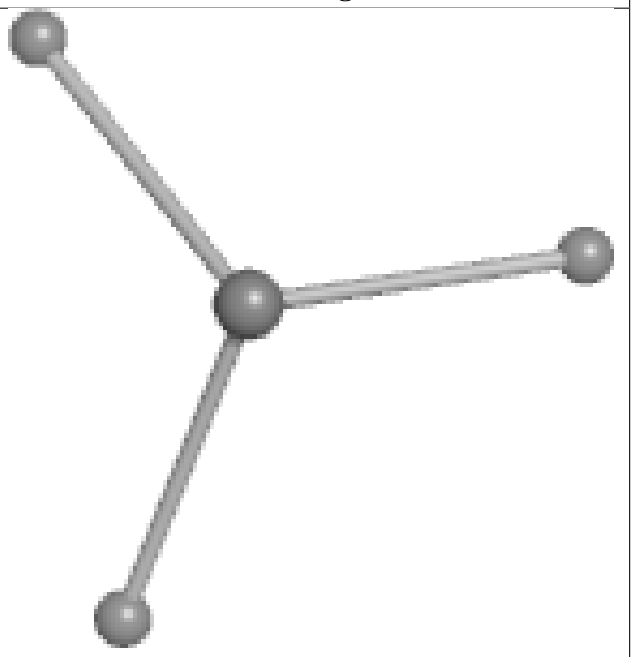
Bond lengths



Bond angles

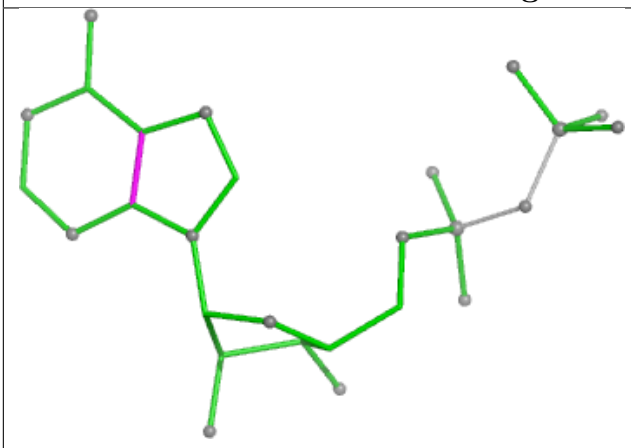


Torsions

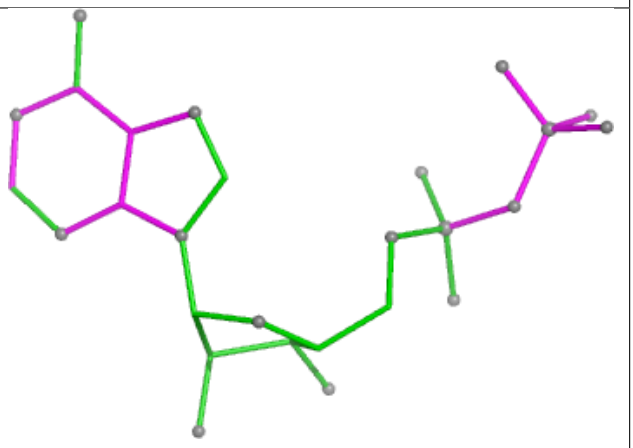


Rings

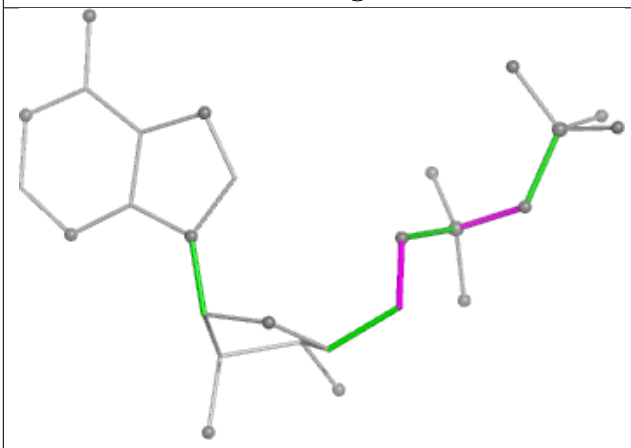
Ligand ADP D 906



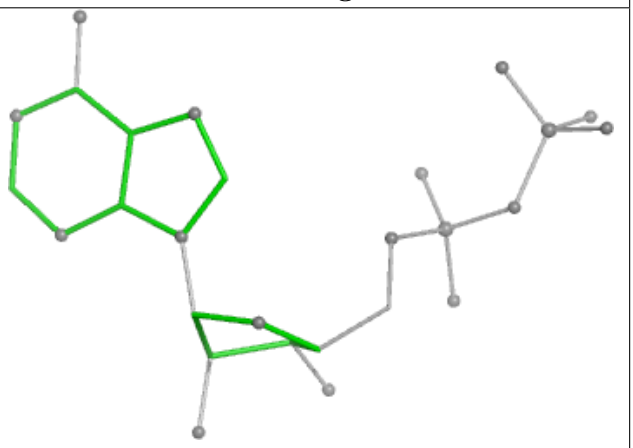
Bond lengths



Bond angles

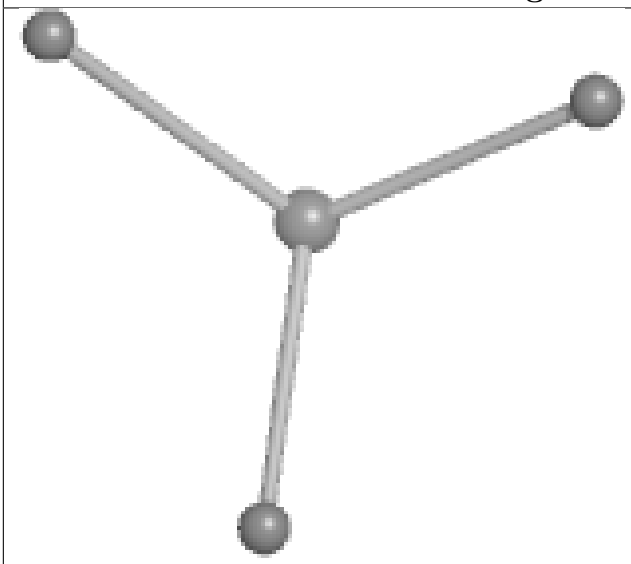


Torsions

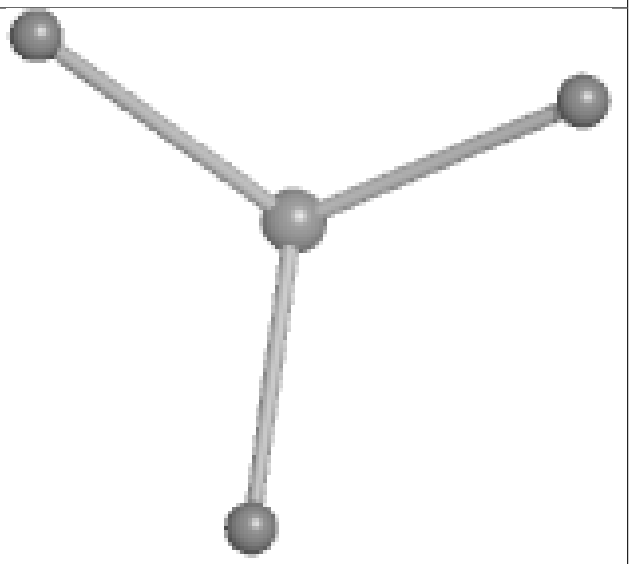


Rings

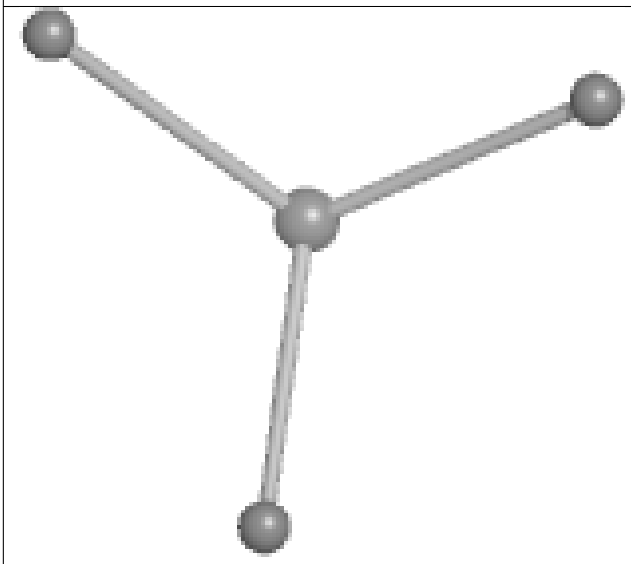
Ligand BEF B 904



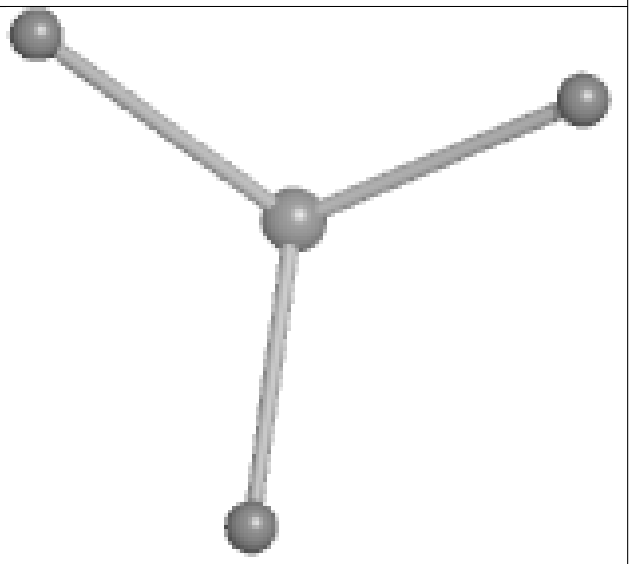
Bond lengths



Bond angles

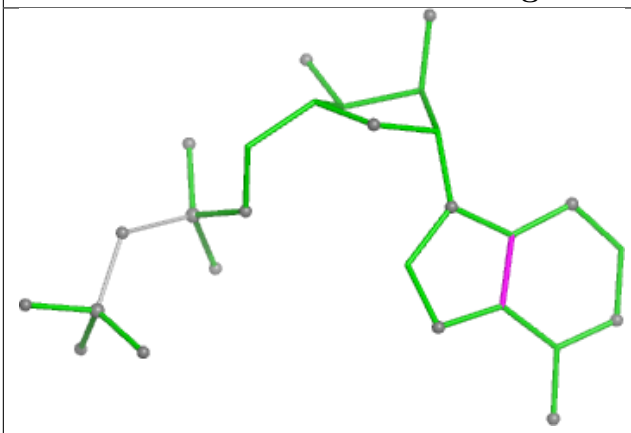


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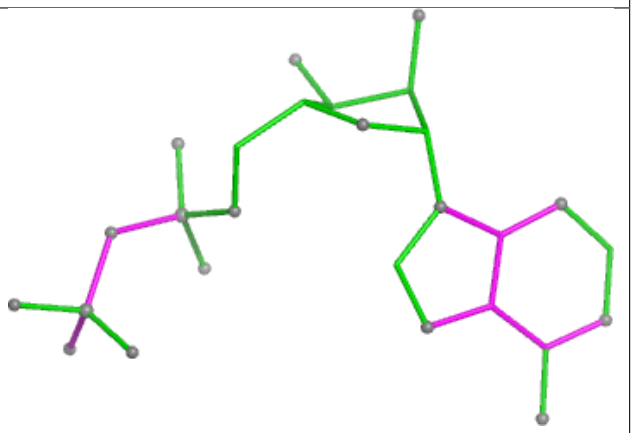


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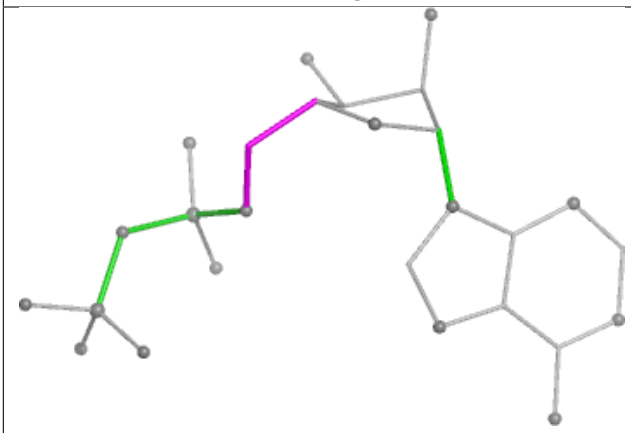
Ligand ADP A 903



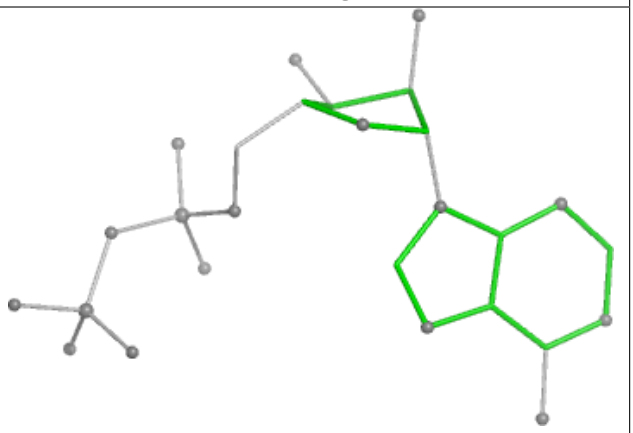
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Bond angles

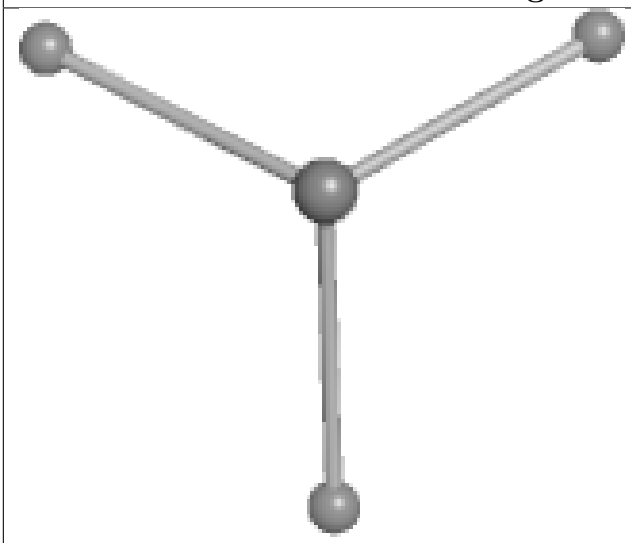


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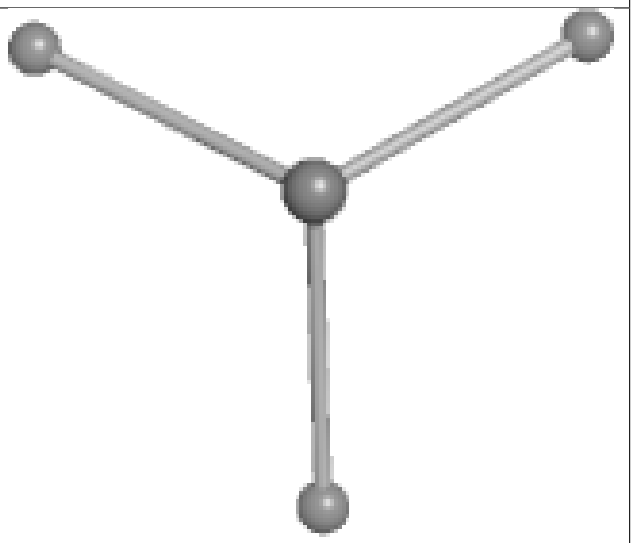


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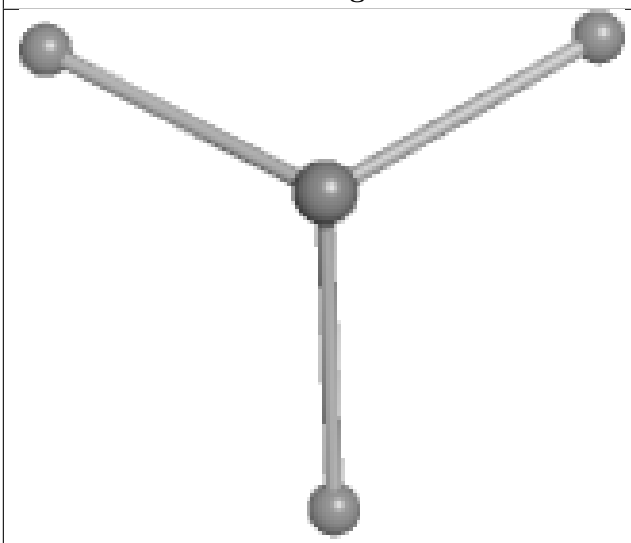
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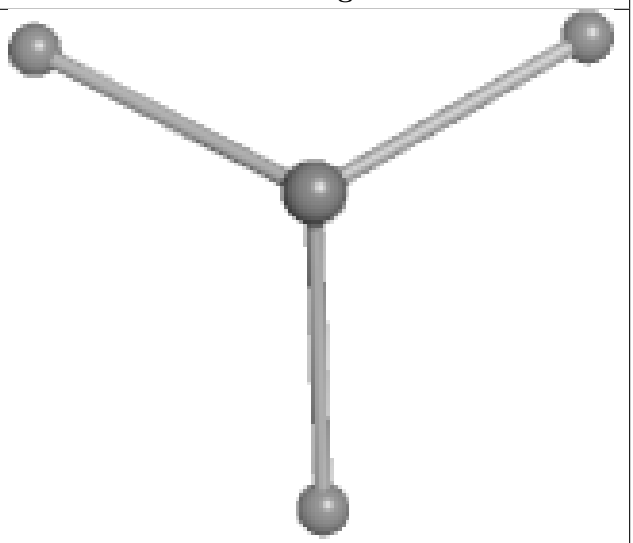
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Bond angles

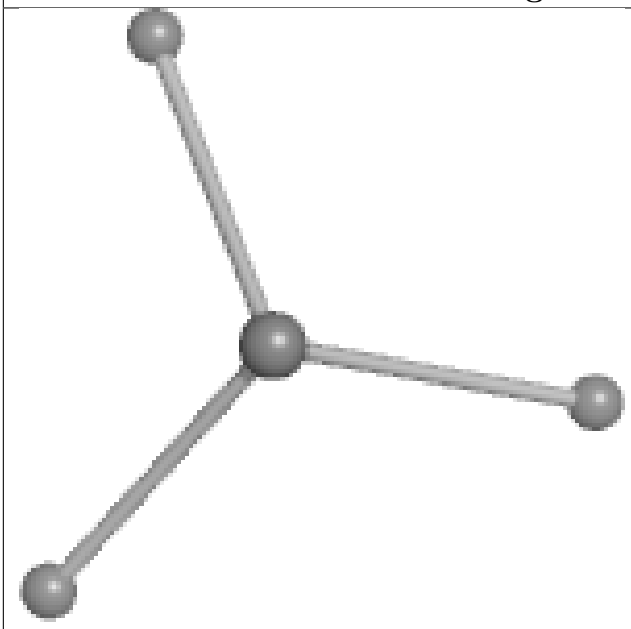


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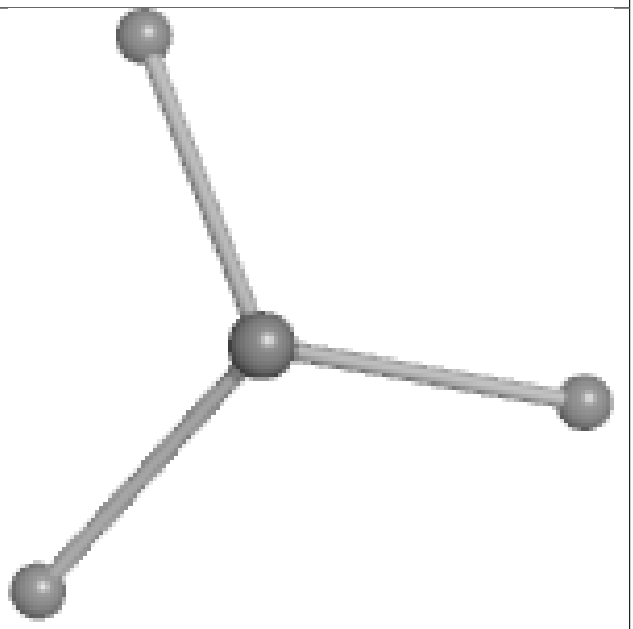


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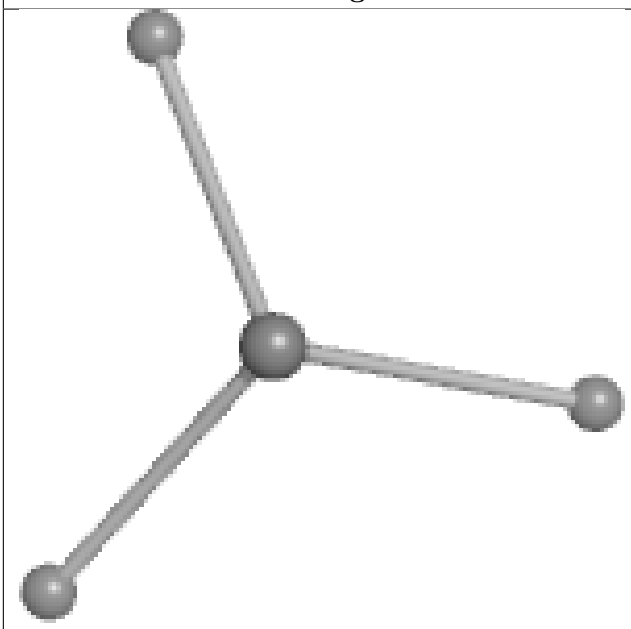
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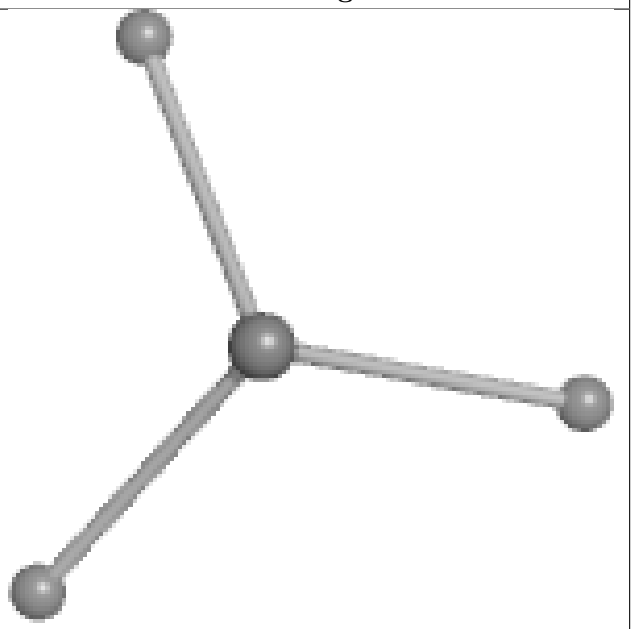
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Bond angles

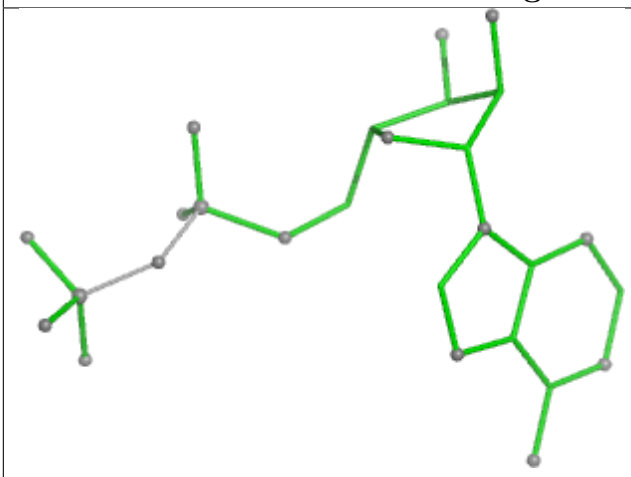


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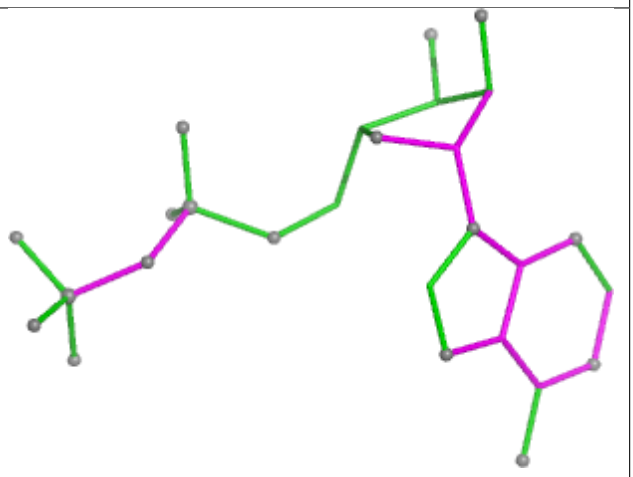


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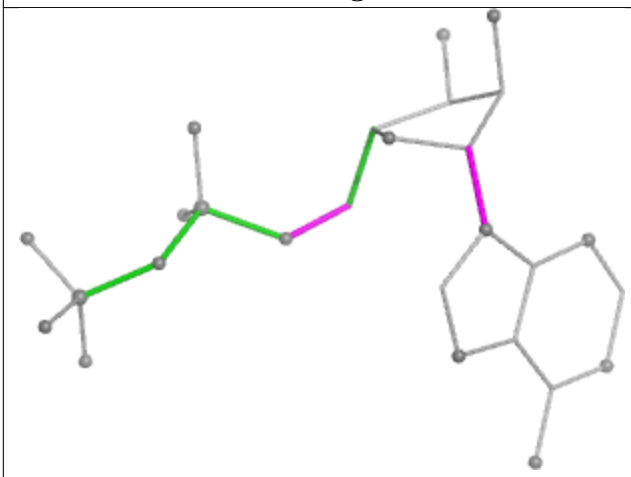
Ligand ADP F 902



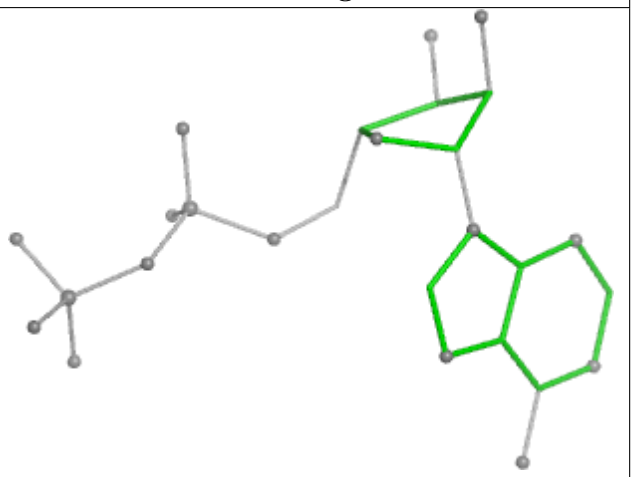
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Bond angles

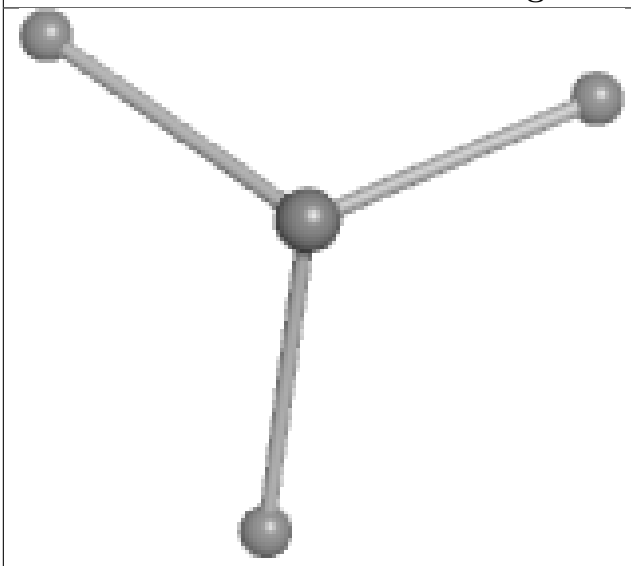


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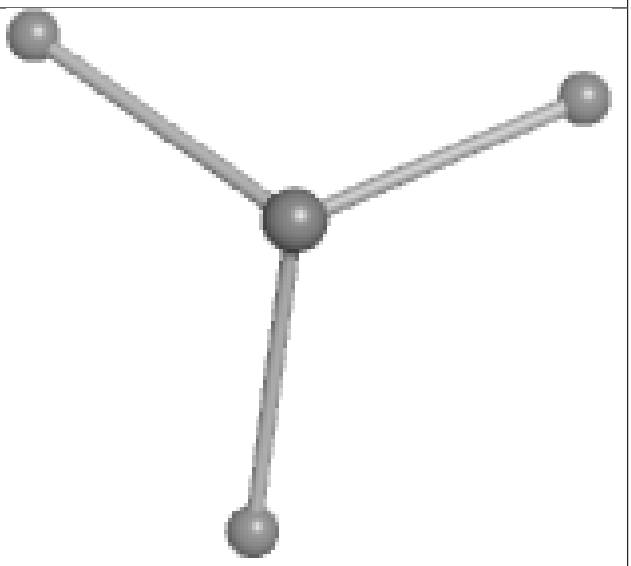


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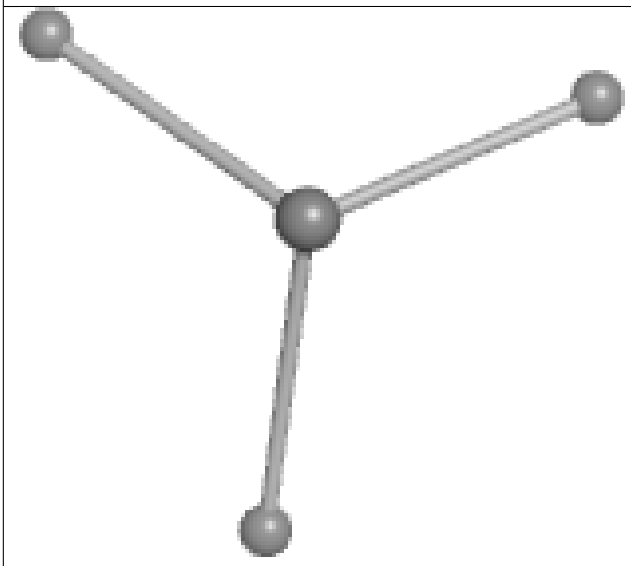
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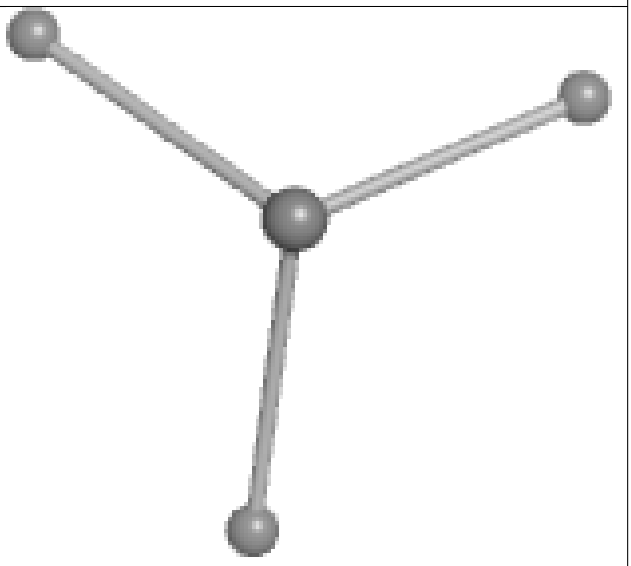
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Bond angles

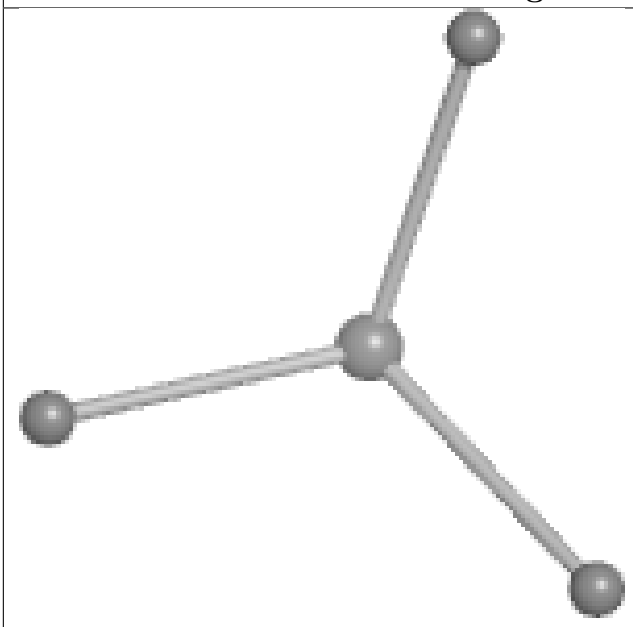


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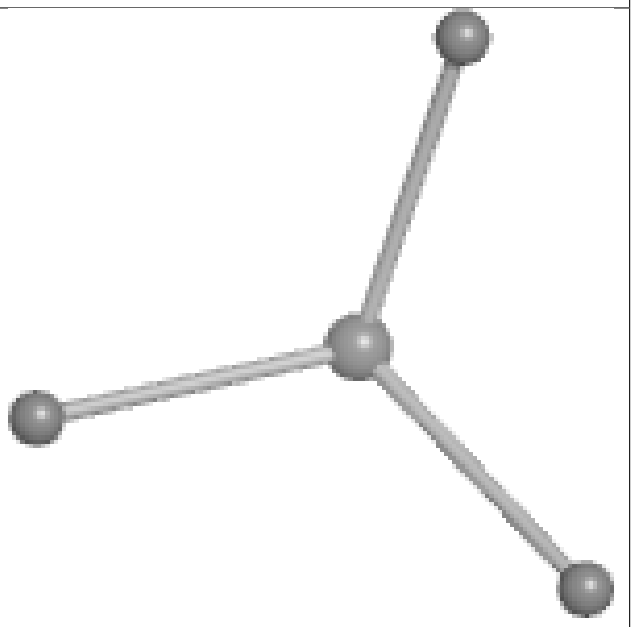


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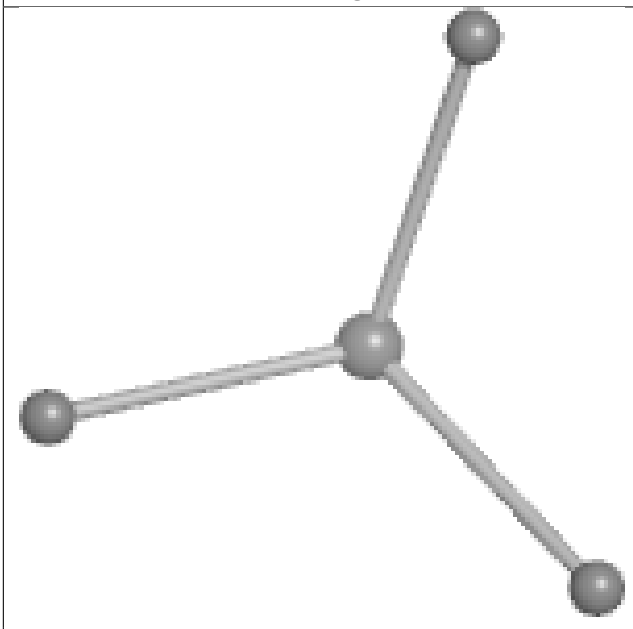
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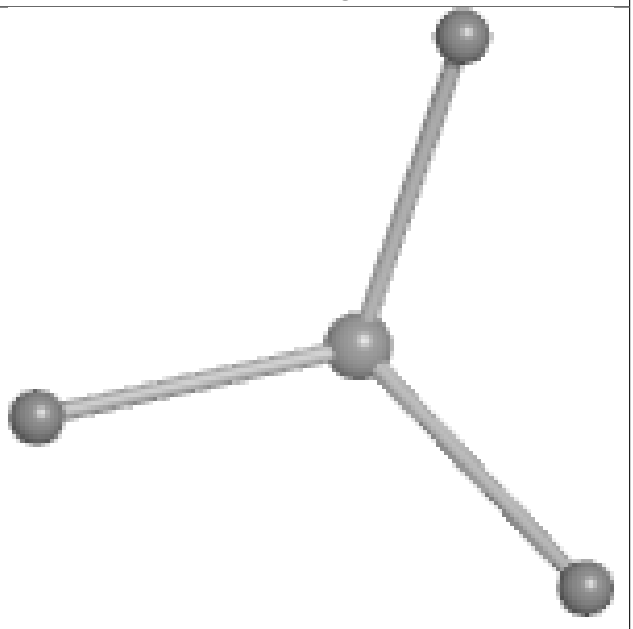
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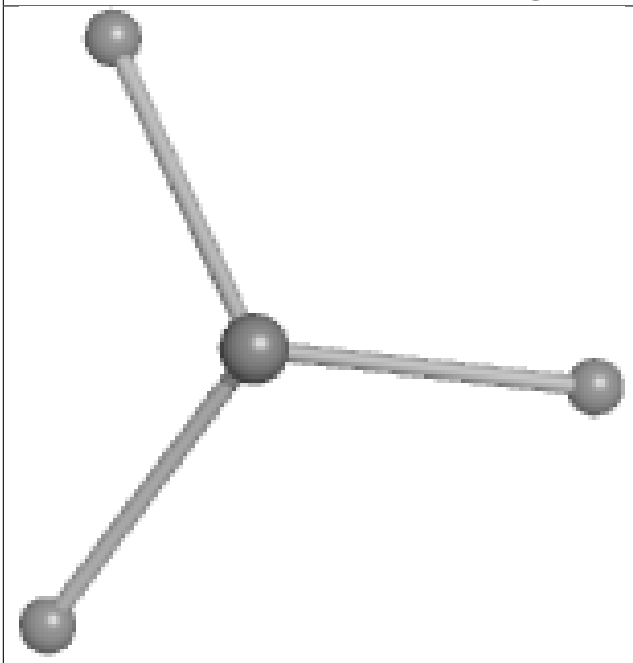


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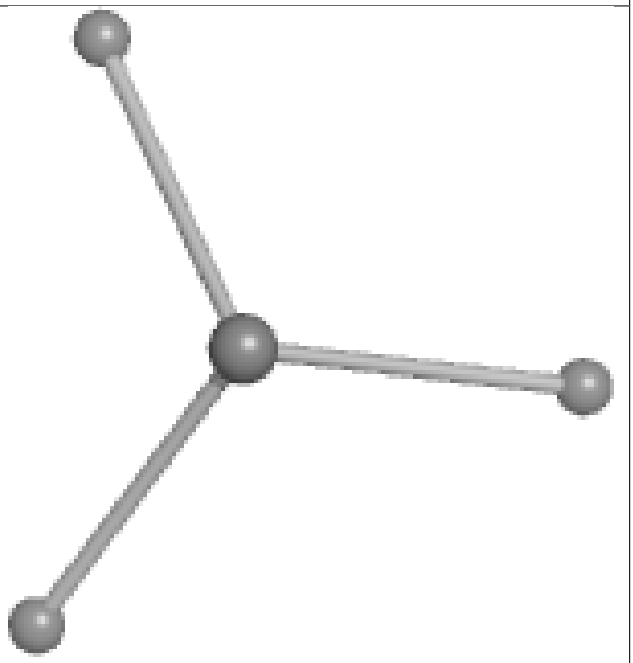


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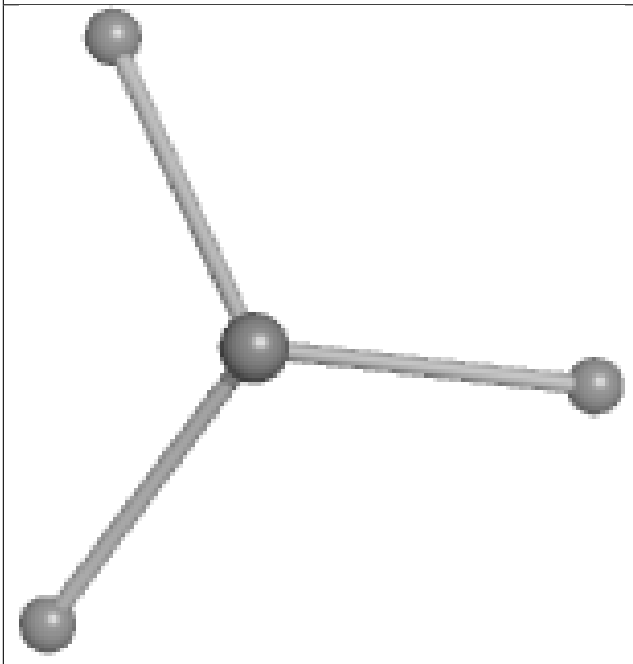
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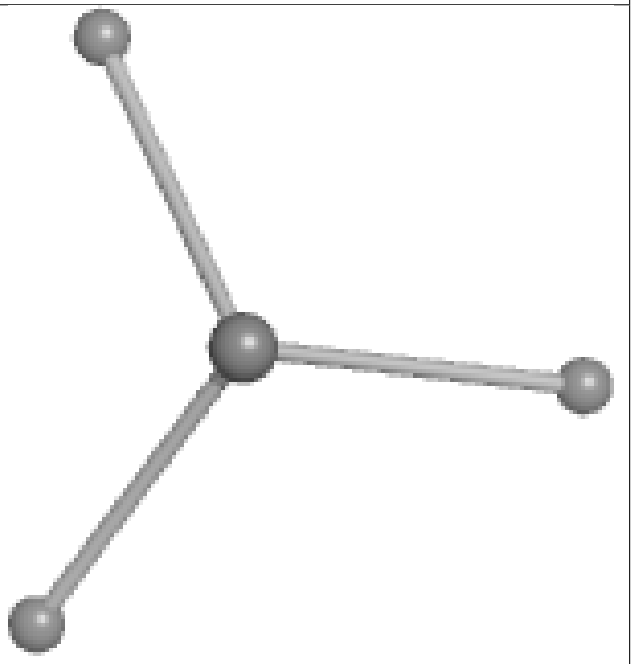
Bond lengths



Bond angles

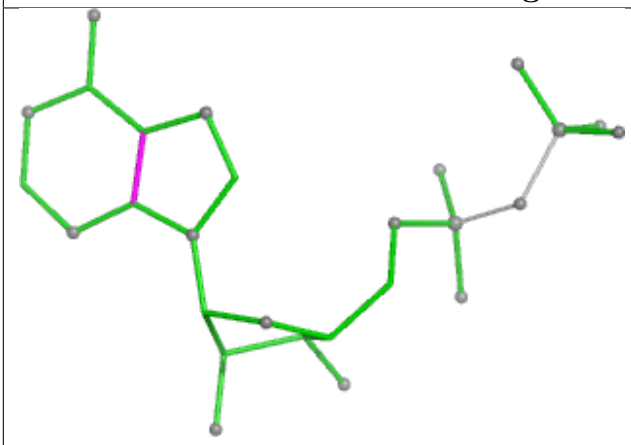


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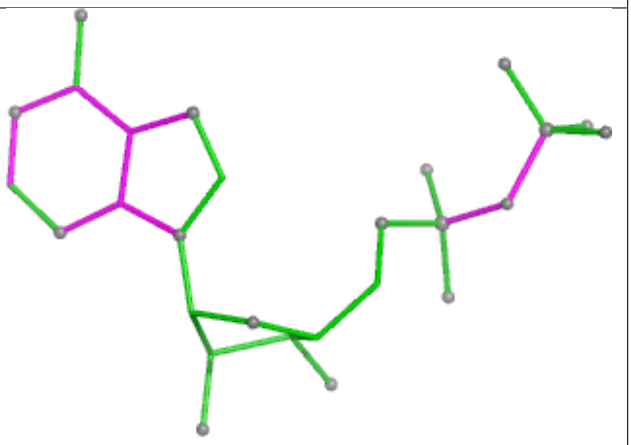


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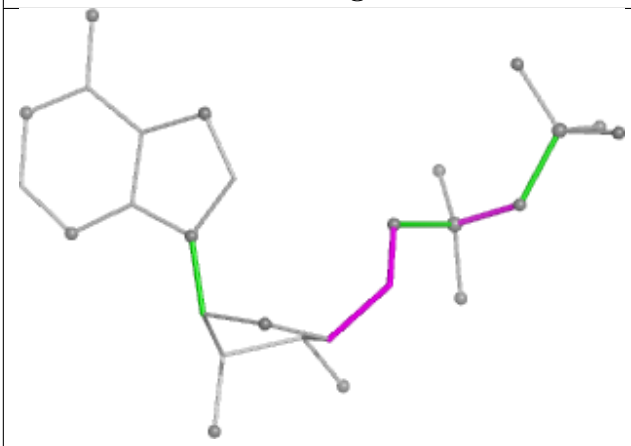
Ligand ADP B 906



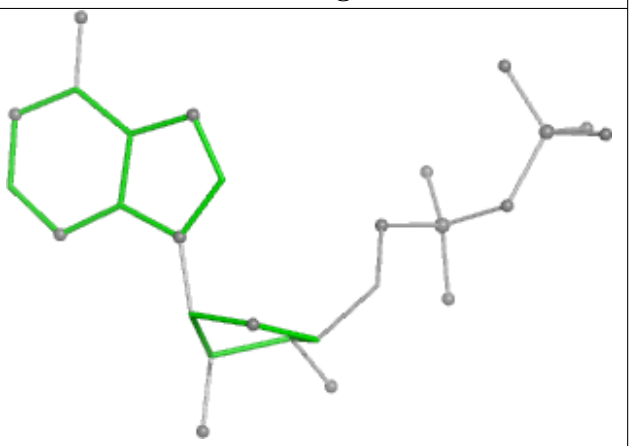
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Bond angles

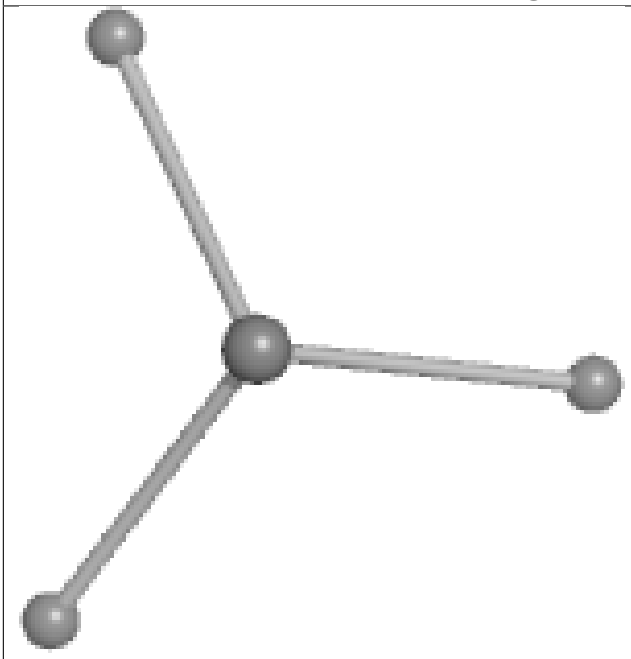


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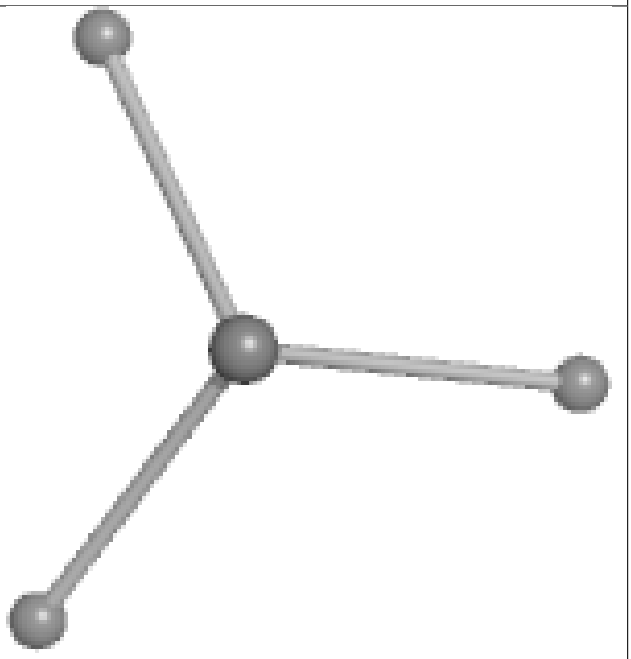


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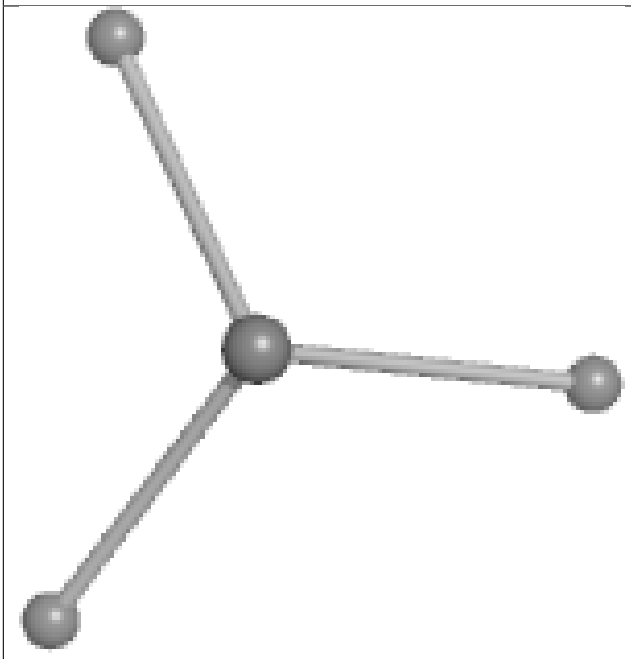
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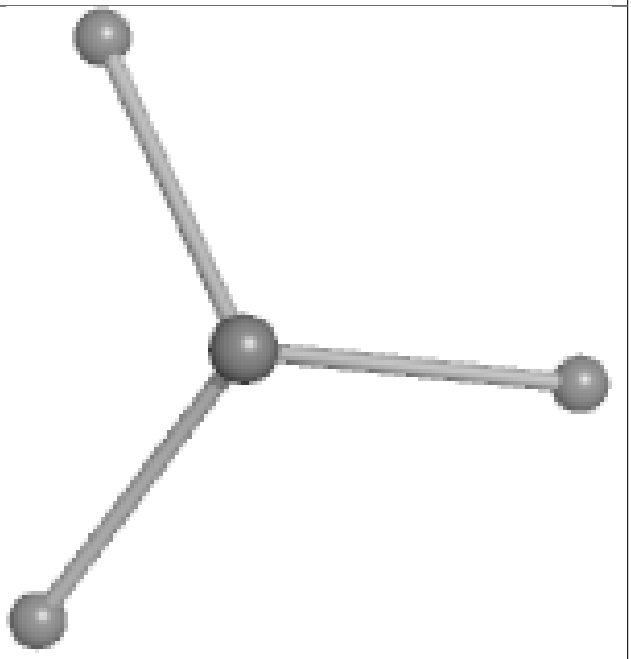
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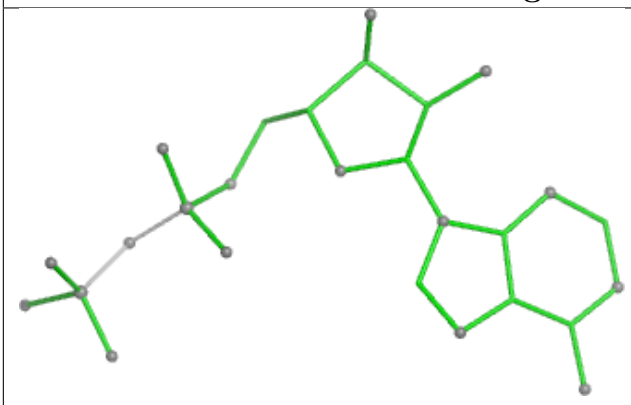


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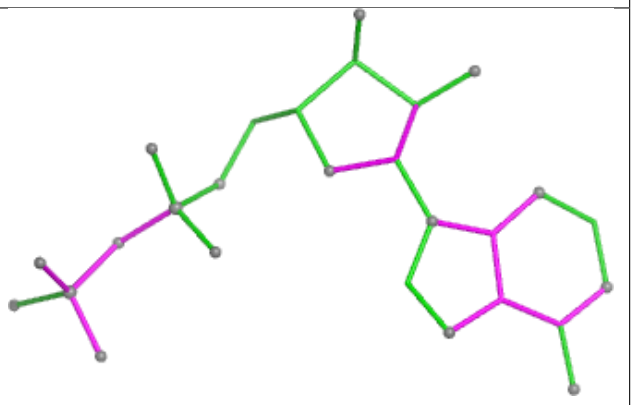


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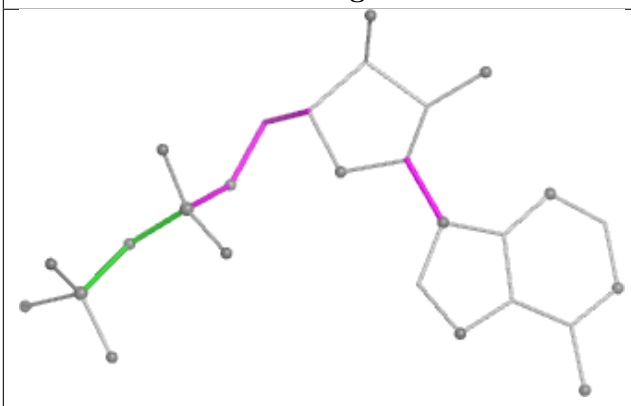
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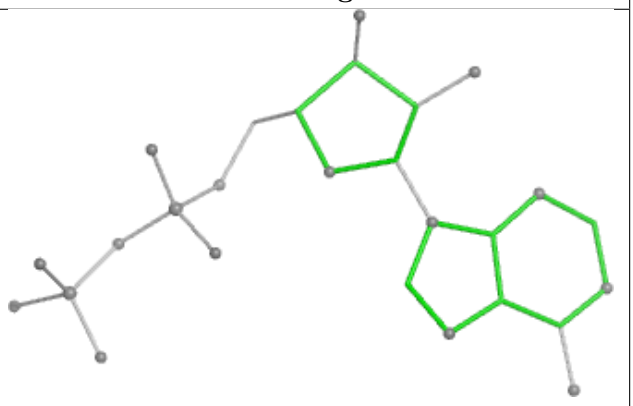
Bond lengths



Bond angles

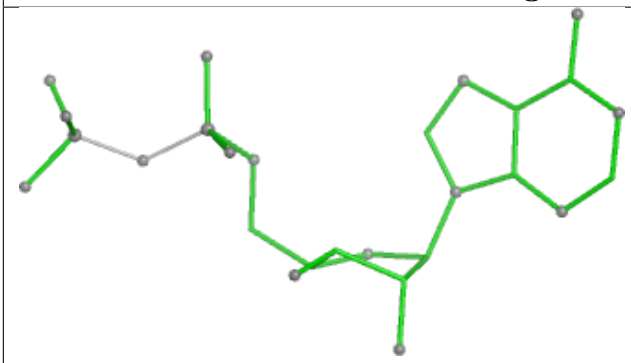


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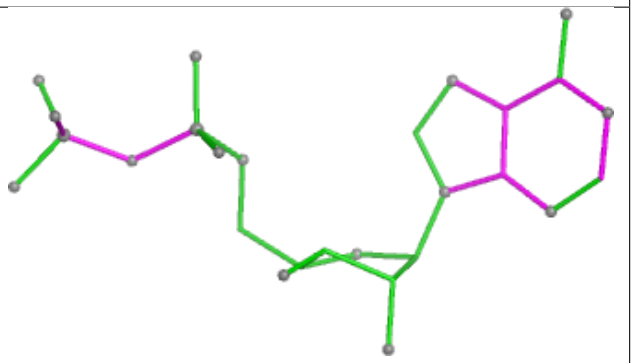


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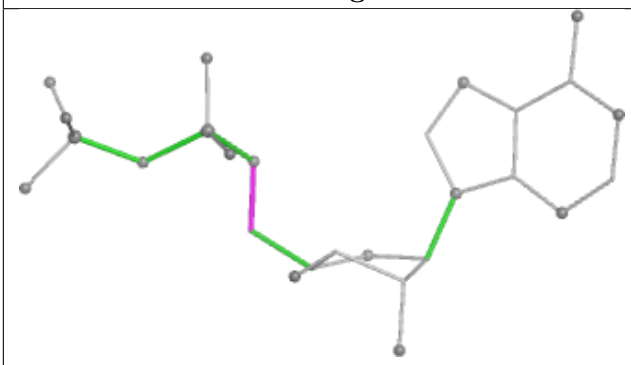
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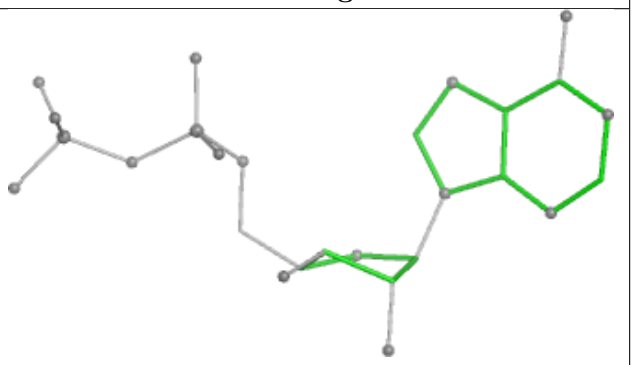
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Bond angles

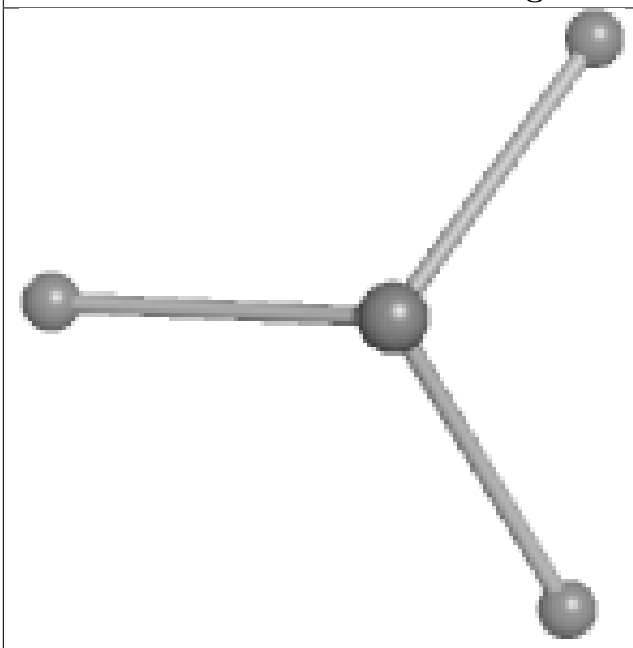


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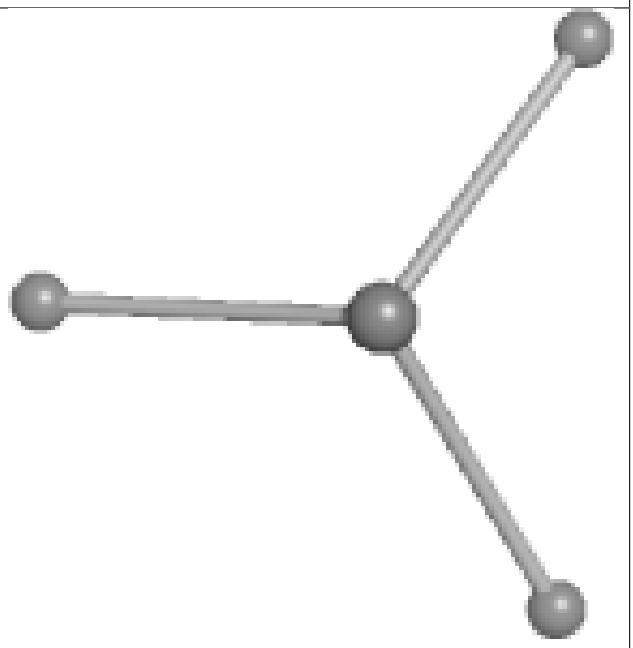


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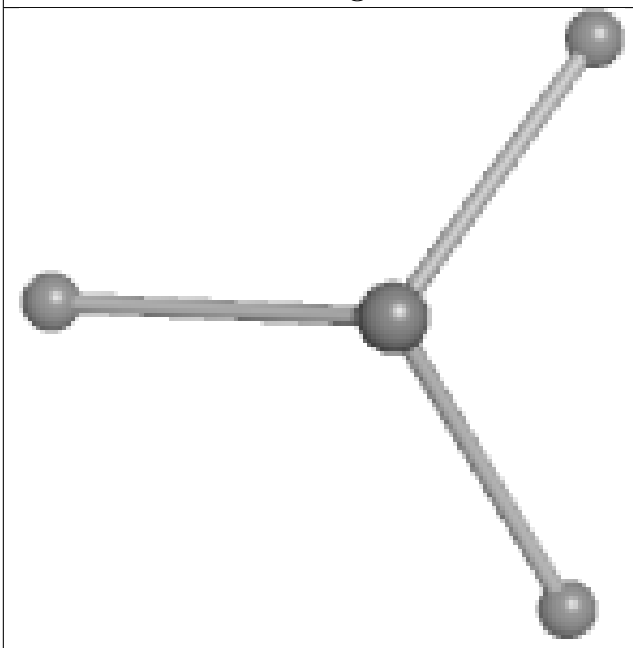
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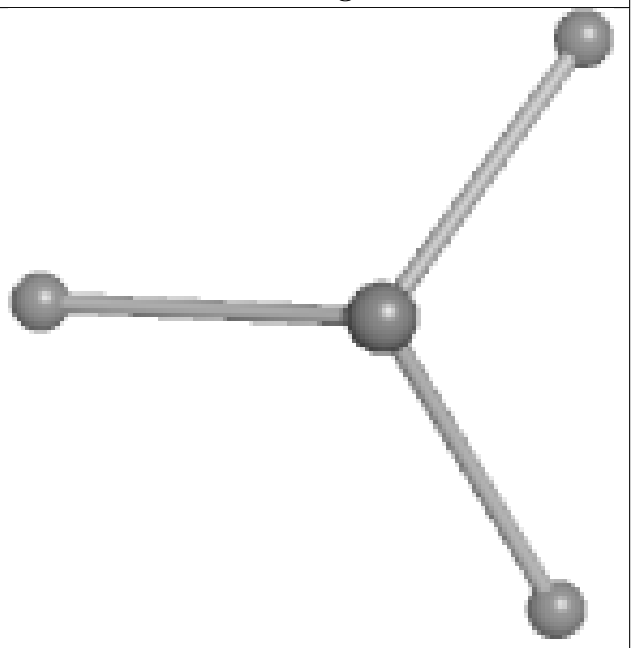
Bond lengths



Bond angles

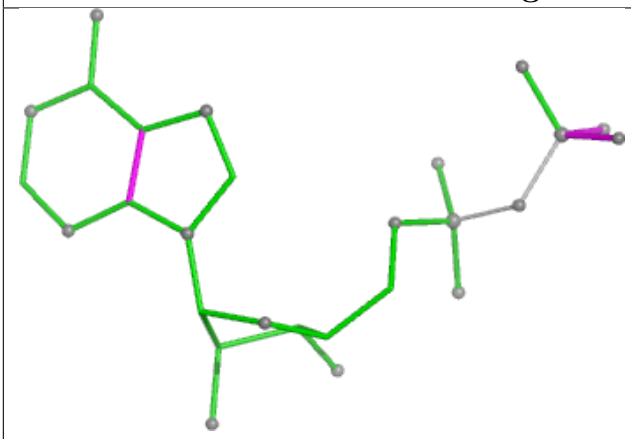


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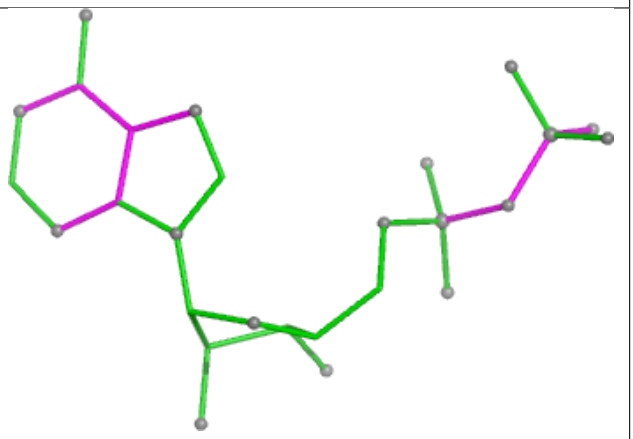


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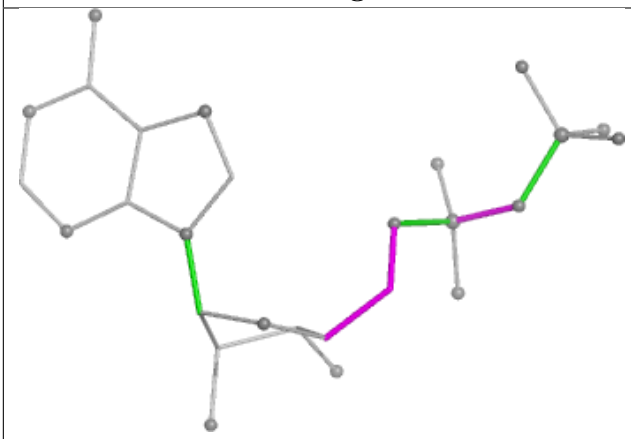
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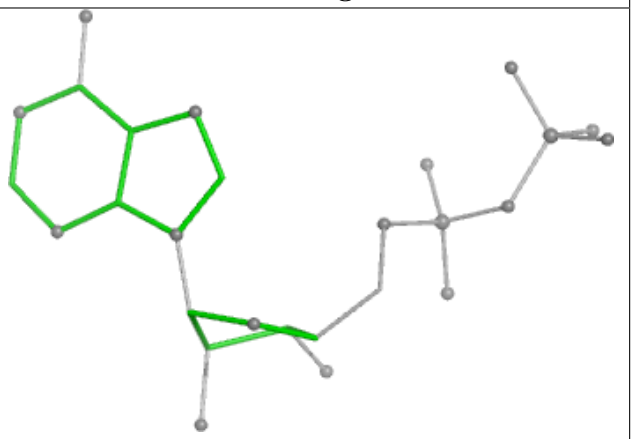
Bond lengths



Bond angles

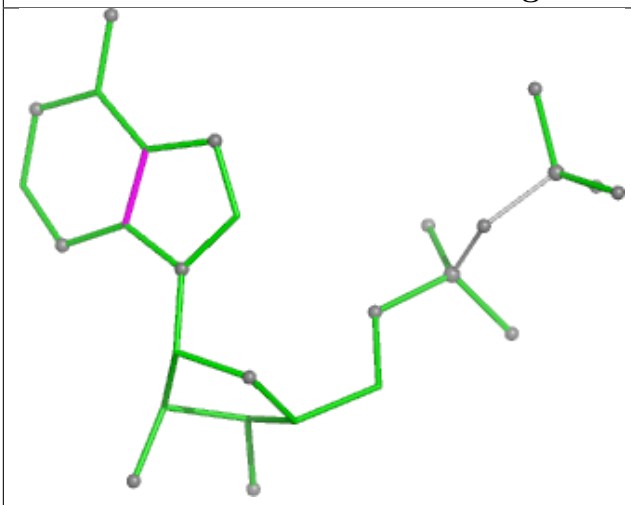


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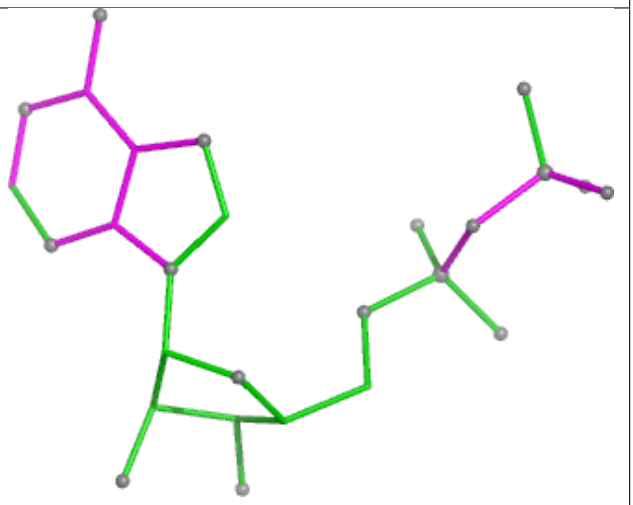


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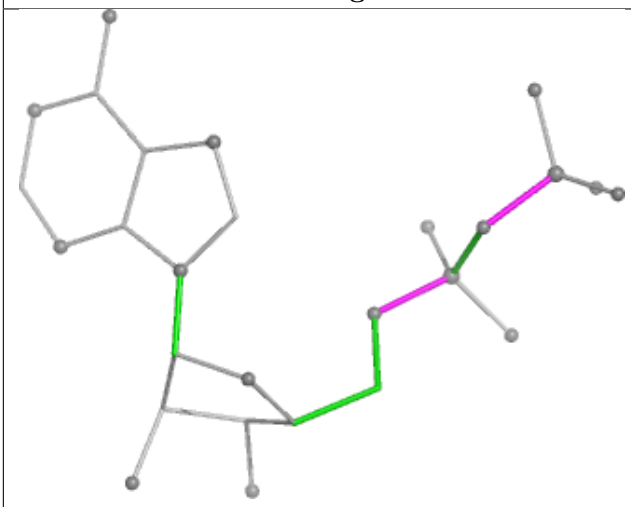
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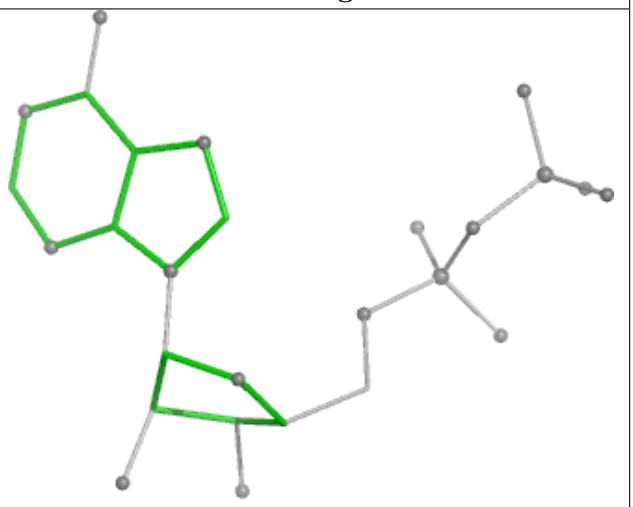
Bond lengths



Bond angles

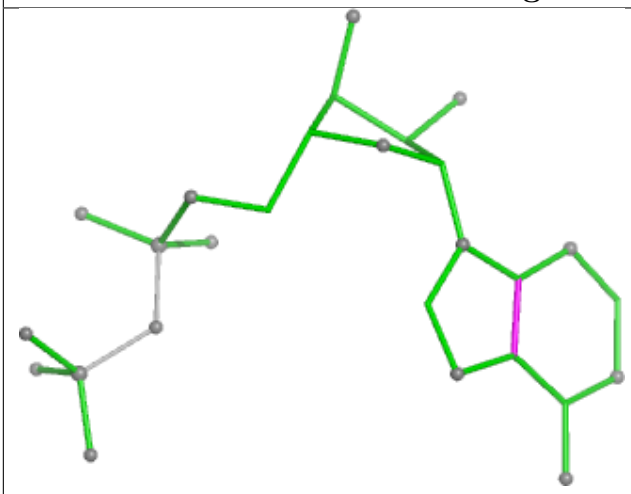


Torsions

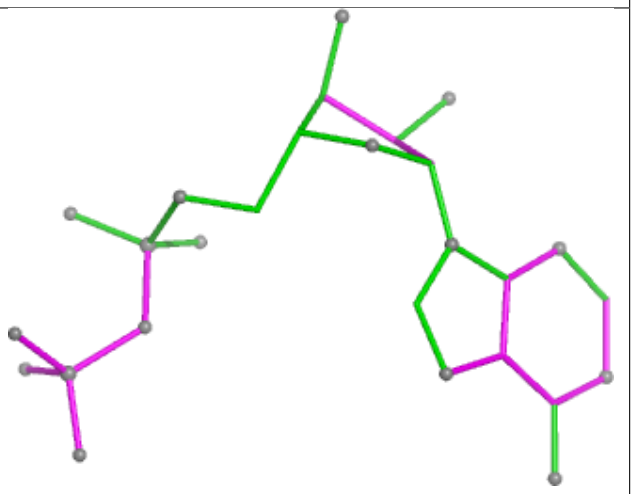


Rings

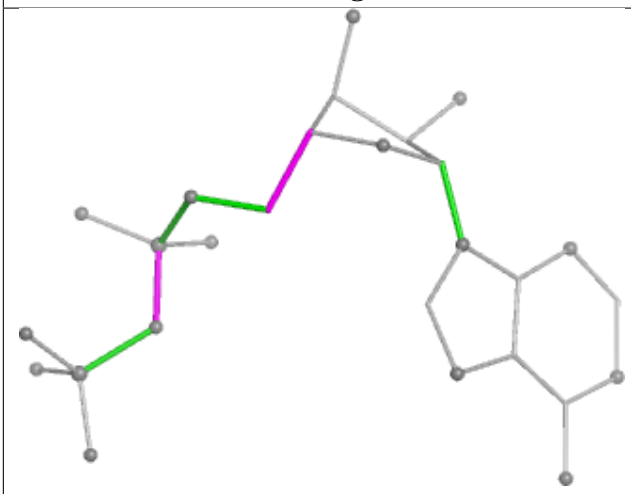
Ligand ADP E 906



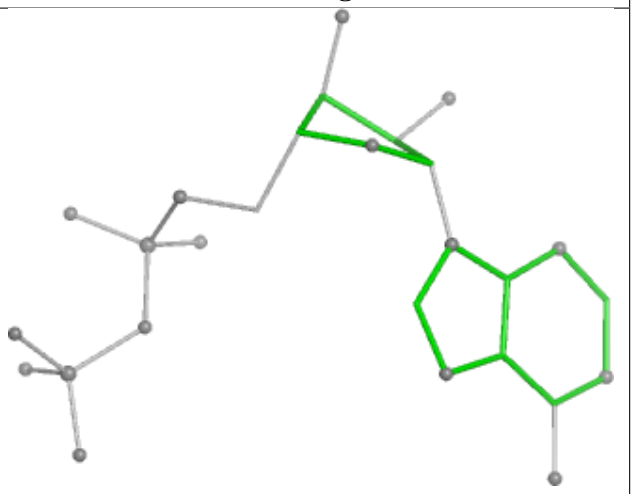
Bond lengths



Bond angles

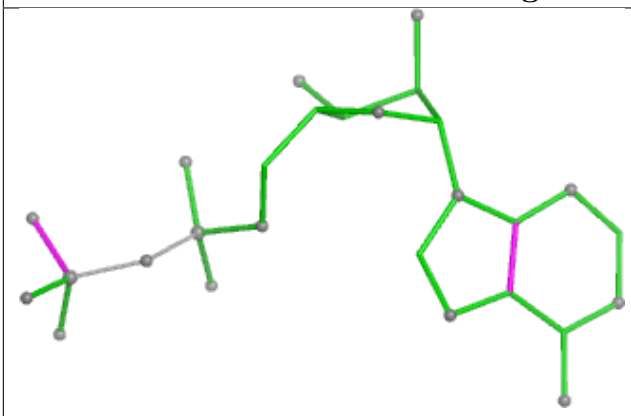


Torsions

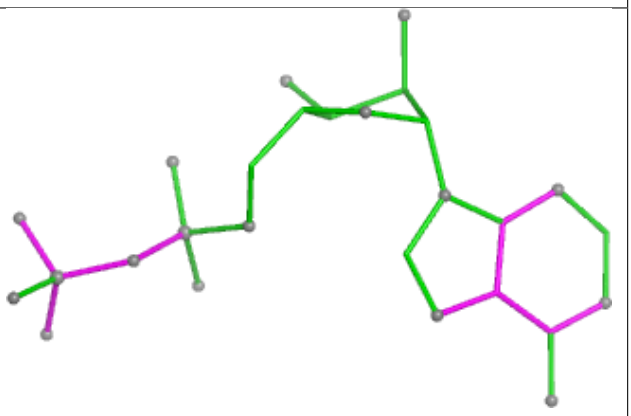


Rings

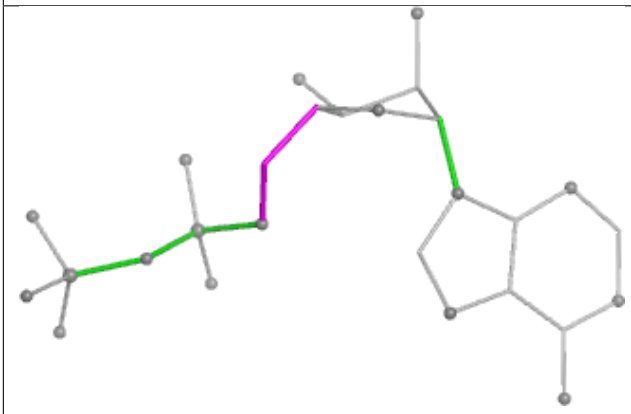
Ligand ADP A 901



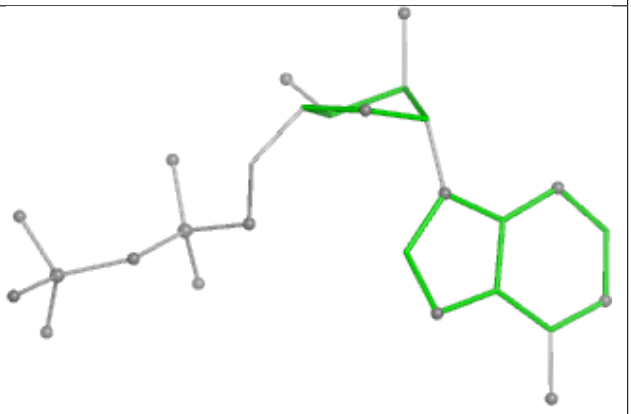
Bond lengths



Bond angles

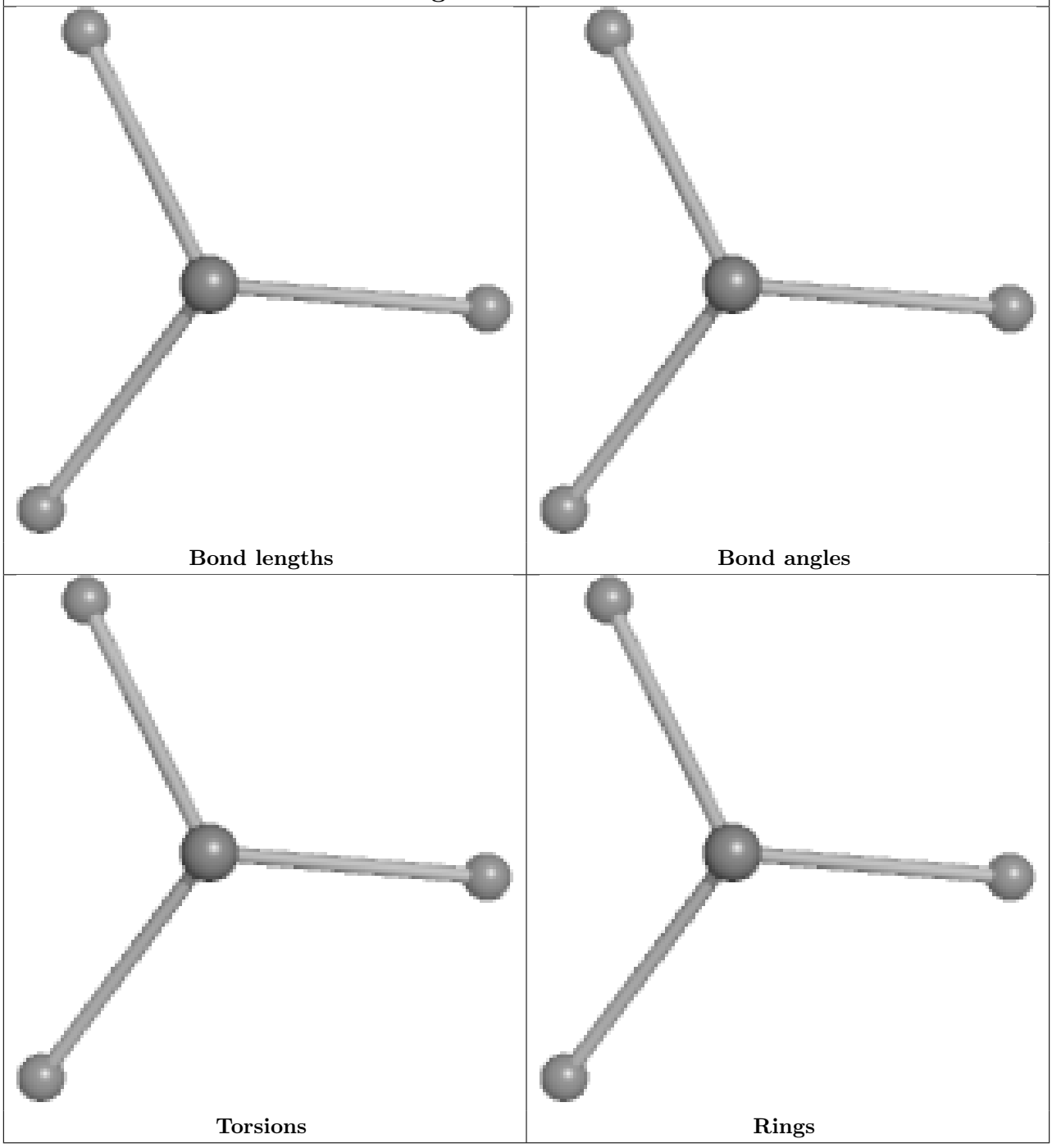


Torsions



Rings

Ligand BEF D 902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

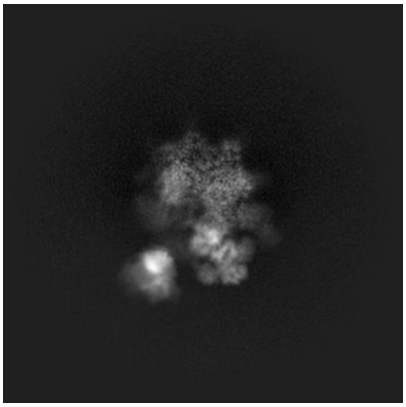
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58589. These allow visual inspection of the internal detail of the map and identification of artifacts.

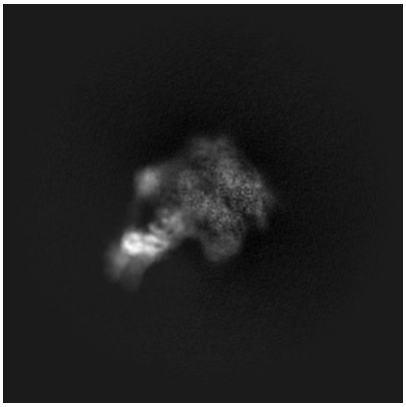
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

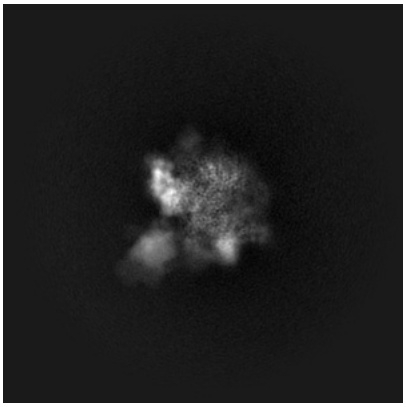
6.1.1 Primary map



X



Y

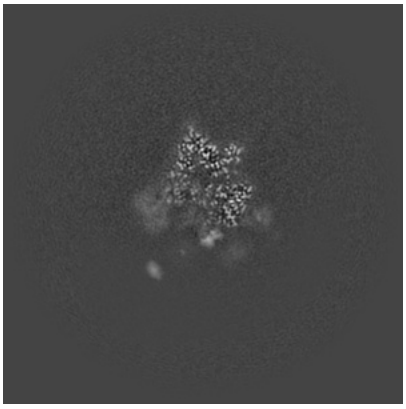


Z

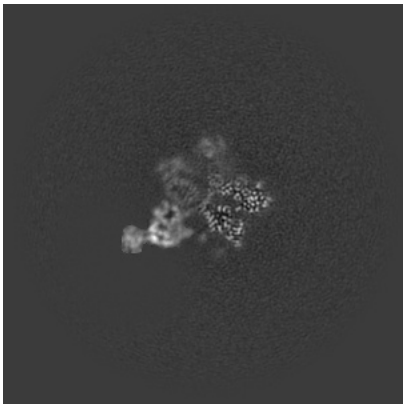
The images above show the map projected in three orthogonal directions.

6.2 Central slices

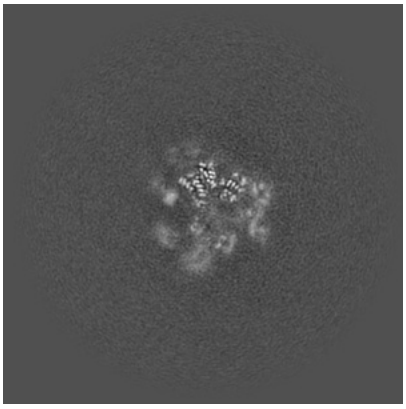
6.2.1 Primary map



X Index: 288



Y Index: 288

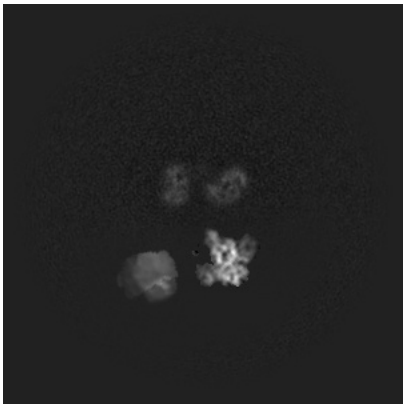


Z Index: 288

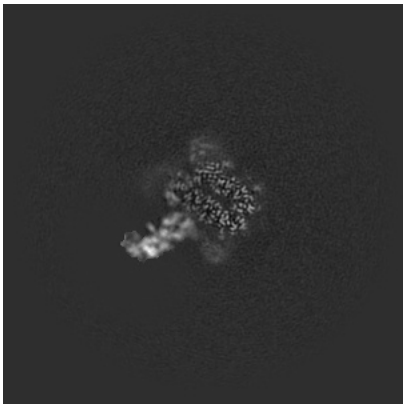
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

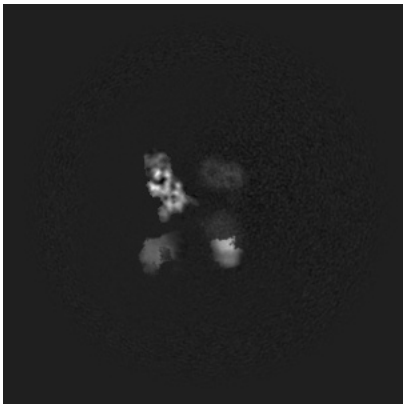
6.3.1 Primary map



X Index: 223



Y Index: 310

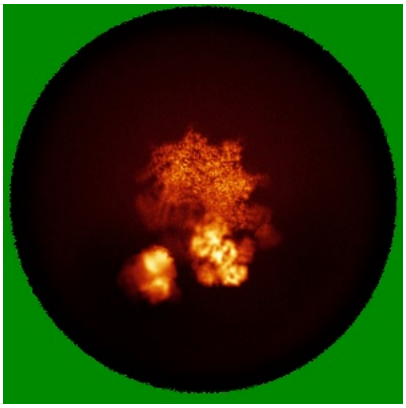


Z Index: 215

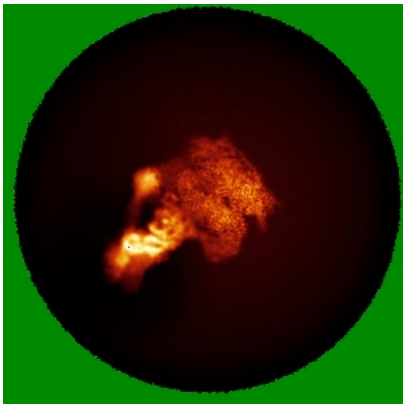
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

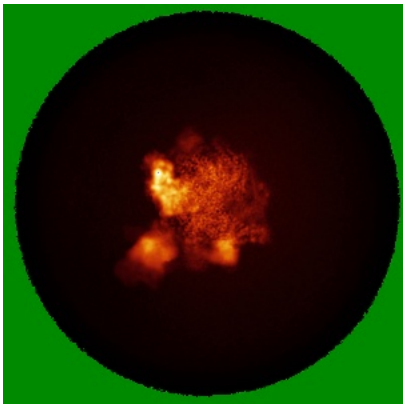
6.4.1 Primary map



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 (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.69. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

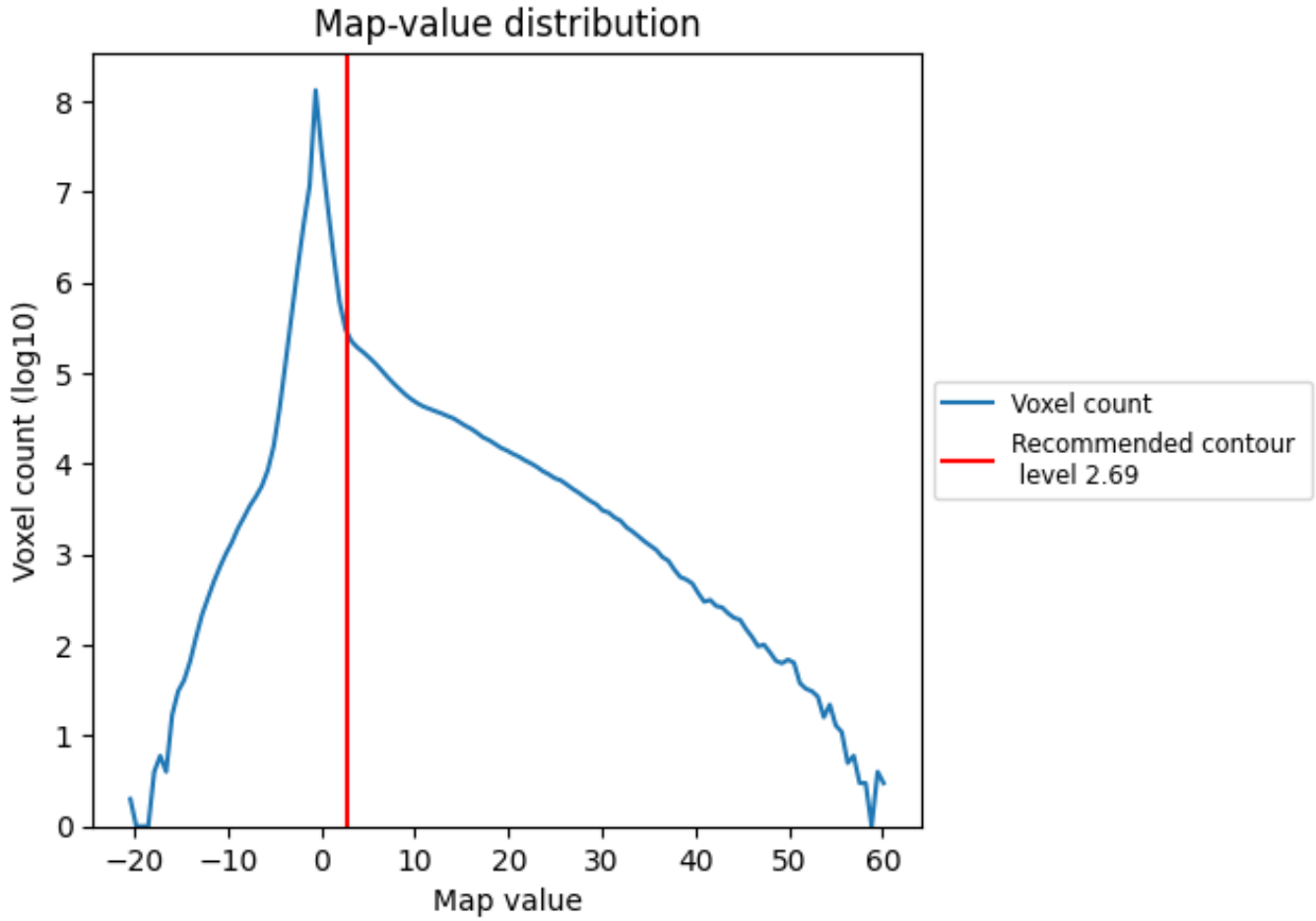
6.6 Mask visualisation (i)

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

7 Map analysis

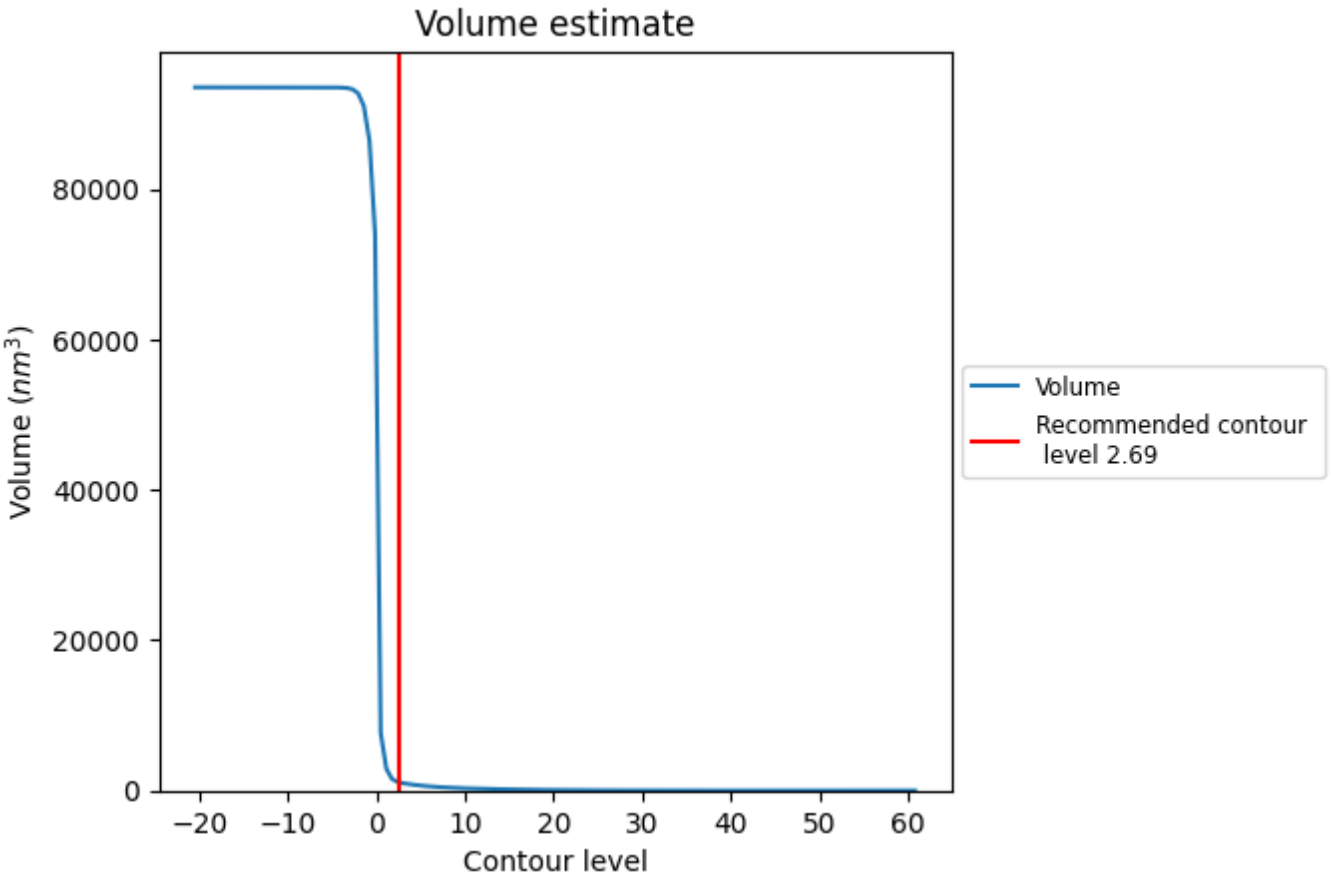
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

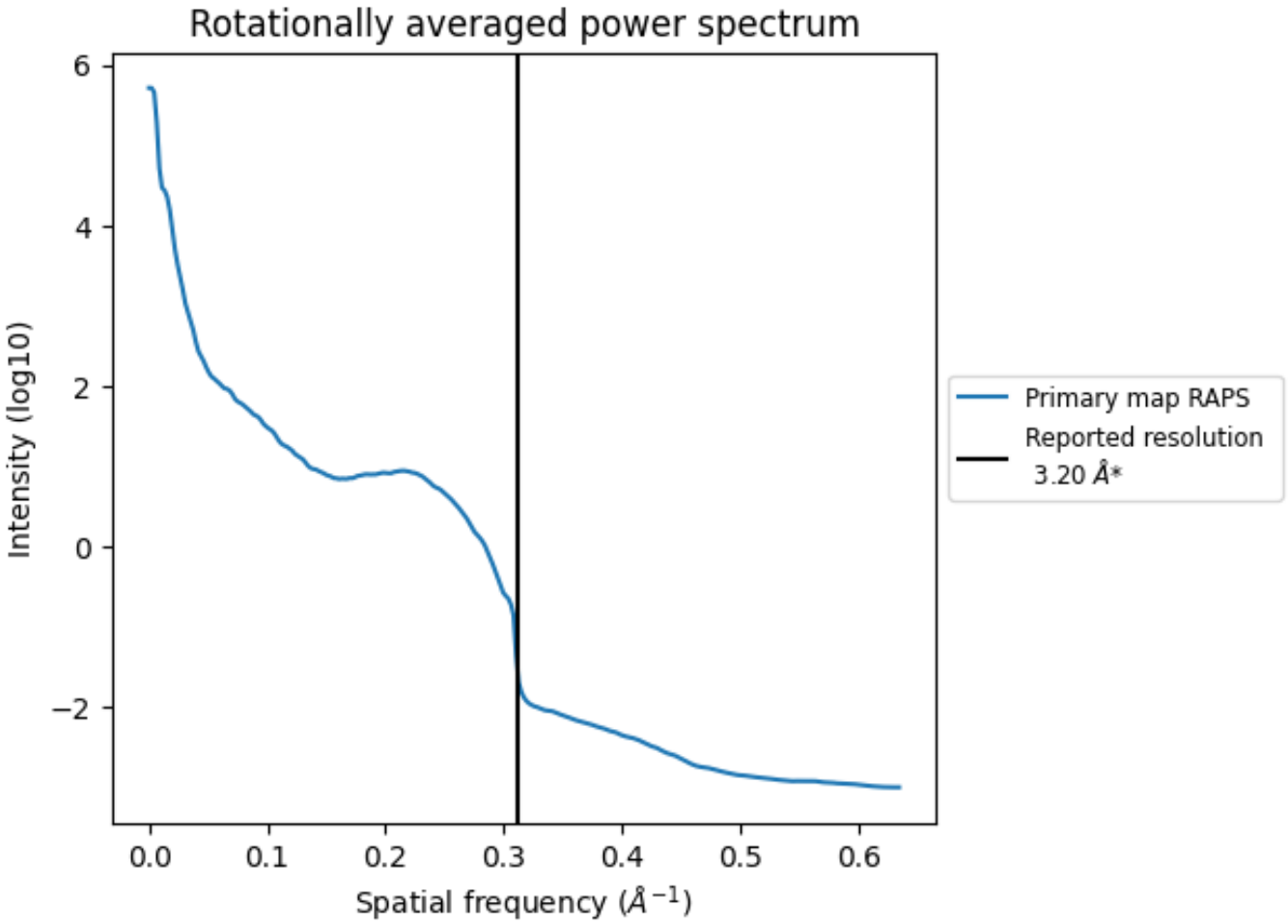
7.2 Volume estimate



The volume at the recommended contour level is 1068 nm^3; this corresponds to an approximate mass of 965 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 (i)



*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

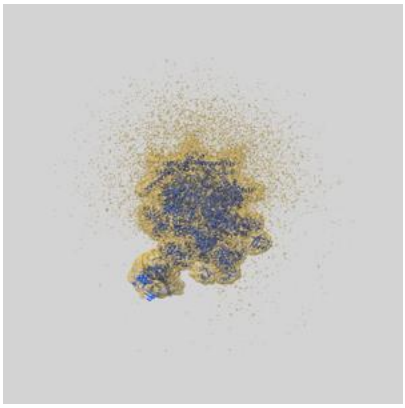
8 Fourier-Shell correlation

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

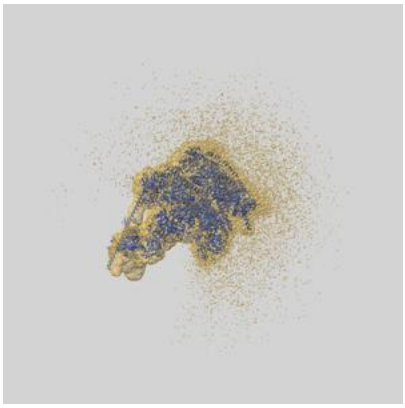
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58589 and PDB model 31ON. Per-residue inclusion information can be found in section 3 on page 11.

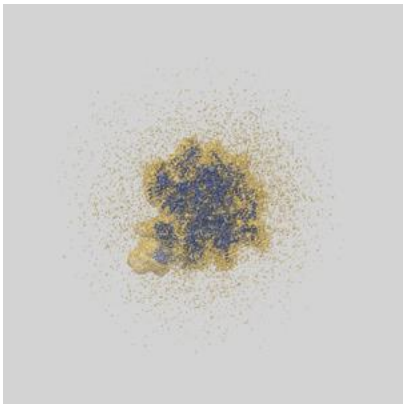
9.1 Map-model overlay



X



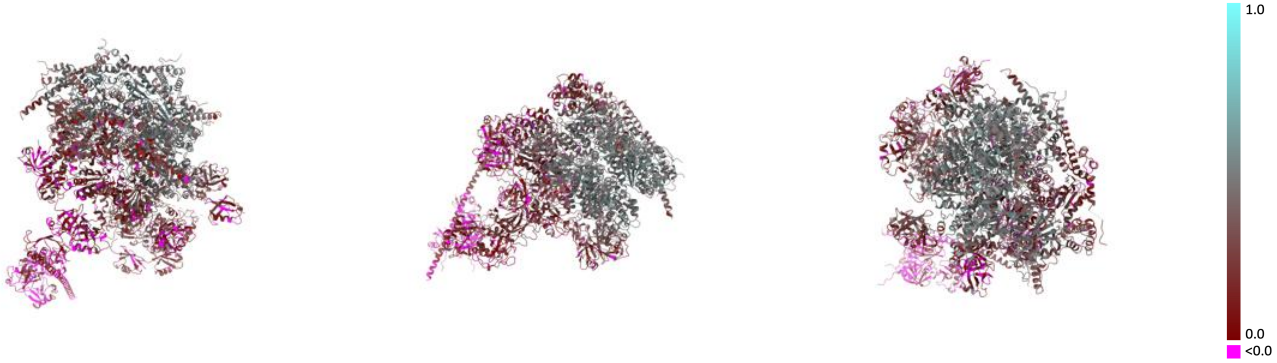
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.69 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.

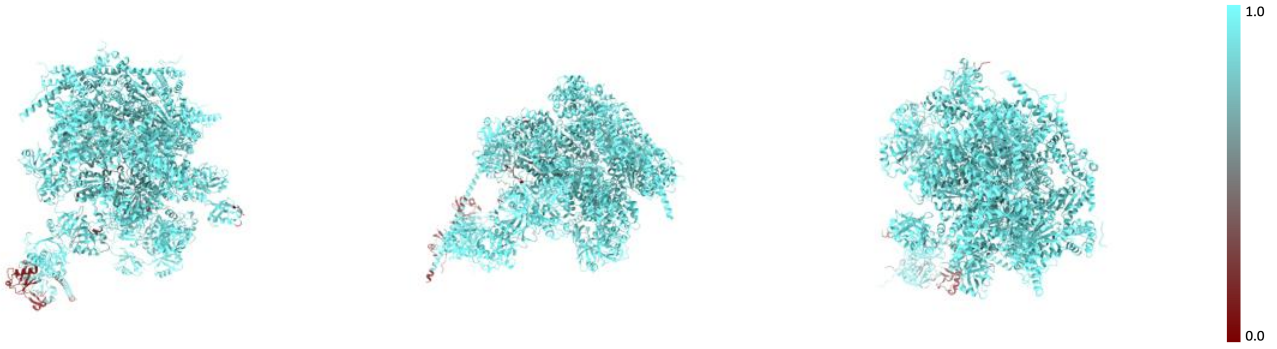
9.2 Q-score mapped to coordinate model



X Y Z

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.

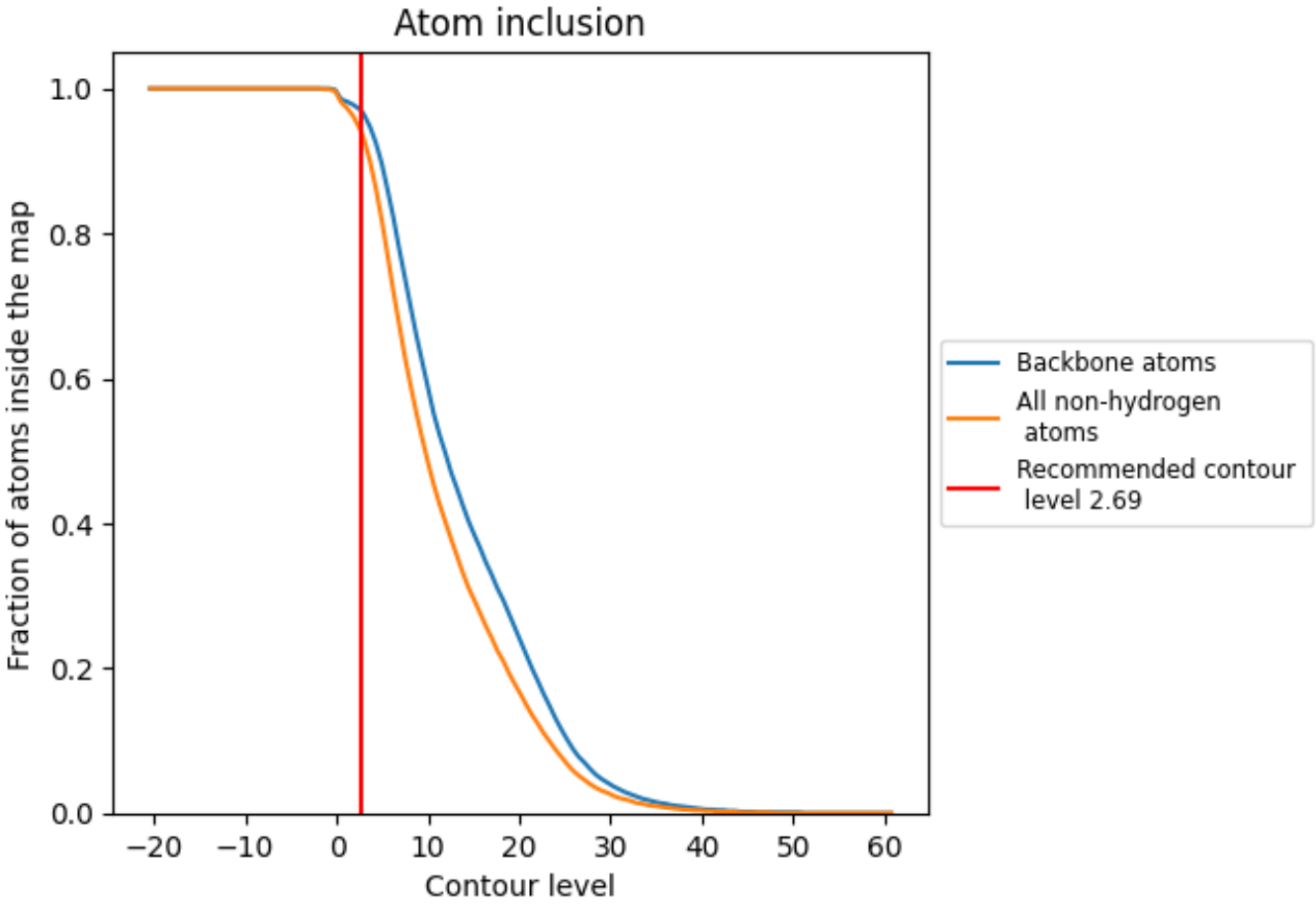
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (2.69).

9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 94% 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 (2.69) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9410	0.2910
A	0.9500	0.3200
B	0.9720	0.4200
C	0.9760	0.4300
D	0.9750	0.4180
E	0.9600	0.2930
F	0.9180	0.1500
G	0.9790	0.2120
H	0.9170	0.0480
I	0.9630	0.2970
J	1.0000	0.1610
K	1.0000	0.1190
L	0.1350	0.0240
M	0.4850	-0.0110
N	0.9490	0.0990
T	0.9100	0.0740

