Full wwPDB EM Validation Report ⓘ

Oct 27, 2026 – 06:35 pm GMT

PDB ID	:	31OR / pdb_000031or
EMDB ID	:	EMD-58599
Title	:	CryoEM structure of substrate engaged p97 in complex with Ufd1/Npl4 and C-terminal FAF1- State IV
Authors	:	Drakonaki, A.; van den Boom, J.; Kroening, A.; Meyer, H.; Gatsogiannis, C.
Deposited on	:	2026-06-16
Resolution	:	8.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

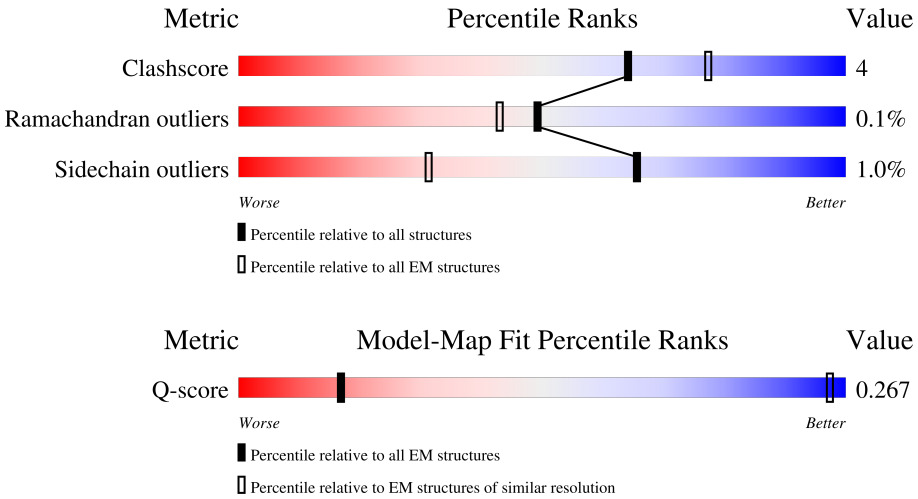
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	361 (7.50 - 8.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	I	76	67% 32%
1	J	76	76% 24%
1	K	76	13% 88% 12%
1	L	76	9% 74% 26%

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Mol	Chain	Length	Quality of chain
1	M	76	9% 78% 21%
1	N	76	43% 74% 26%
2	G	608	10% 84% 5% 11%
3	H	307	9% 57% 23% 20%
4	A	806	86% 8% 6%
4	B	806	86% 7% 7%
4	C	806	79% 11% 9%
4	D	806	8% 75% 14% 11%
4	E	806	77% 12% 11%
4	F	806	84% 8% 8%
5	T	170	11% 81% 19%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 46042 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 Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	76	Total	C	N	O	S	0	0
			594	374	105	114	1		
1	K	76	Total	C	N	O	S	0	0
			594	374	105	114	1		
1	I	52	Total	C	N	O	S	0	0
			410	260	67	82	1		
1	M	76	Total	C	N	O	S	0	0
			602	378	105	118	1		
1	N	76	Total	C	N	O	S	0	0
			602	378	105	118	1		
1	L	76	Total	C	N	O	S	0	0
			602	378	105	118	1		

- 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 Ubiquitin recognition factor in ER-associated degradation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	245	Total	C	N	O	S	0	0
			1928	1224	330	361	13		

- Molecule 4 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	719	Total	C	N	O	S	0	0
			5656	3561	1000	1065	30		
4	B	752	Total	C	N	O	S	0	0
			5878	3696	1044	1108	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	759	Total	C	N	O	S	0	0
			5942	3734	1055	1123	30		
4	F	743	Total	C	N	O	S	0	0
			5807	3653	1031	1093	30		
4	C	731	Total	C	N	O	S	0	0
			5702	3589	1011	1072	30		
4	D	720	Total	C	N	O	S	0	0
			5623	3537	997	1060	29		

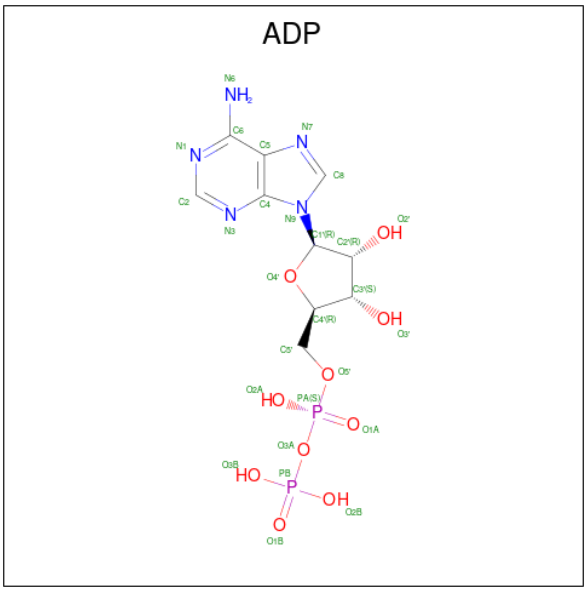
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	232	GLU	ALA	engineered mutation	UNP P55072
E	578	GLN	GLU	engineered mutation	UNP P55072
B	232	GLU	ALA	engineered mutation	UNP P55072
B	578	GLN	GLU	engineered mutation	UNP P55072
A	232	GLU	ALA	engineered mutation	UNP P55072
A	578	GLN	GLU	engineered mutation	UNP P55072
F	232	GLU	ALA	engineered mutation	UNP P55072
F	578	GLN	GLU	engineered mutation	UNP P55072
C	232	GLU	ALA	engineered mutation	UNP P55072
C	578	GLN	GLU	engineered mutation	UNP P55072
D	232	GLU	ALA	engineered mutation	UNP P55072
D	578	GLN	GLU	engineered mutation	UNP P55072

- Molecule 5 is a protein called FAS-associated factor 1.

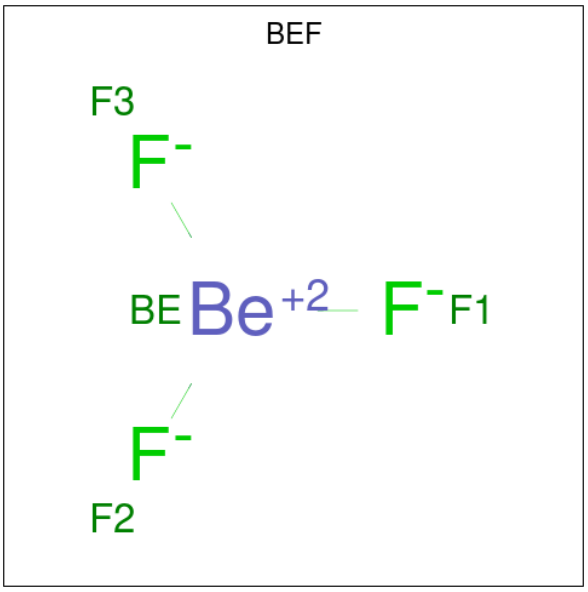
Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	170	Total	C	N	O	S	0	0
			1423	888	251	281	3		

- 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	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	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	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	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	
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	

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	E	1	Total Be F 4 1 3	0
7	B	1	Total Be F 4 1 3	0
7	B	1	Total Be F 4 1 3	0
7	B	1	Total Be F 4 1 3	0
7	A	1	Total Be F 4 1 3	0
7	A	1	Total Be F 4 1 3	0
7	A	1	Total Be F 4 1 3	0
7	F	1	Total Be F 4 1 3	0
7	C	1	Total Be F 4 1 3	0
7	C	1	Total Be F 4 1 3	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
8	E	2	Total Mg 2 2	0

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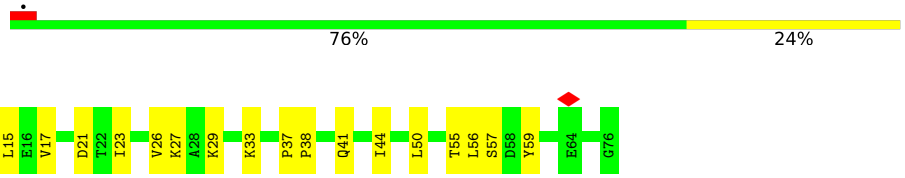
Mol	Chain	Residues	Atoms	AltConf
8	B	2	Total Mg 2 2	0
8	A	2	Total Mg 2 2	0
8	F	2	Total Mg 2 2	0
8	C	2	Total Mg 2 2	0

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.

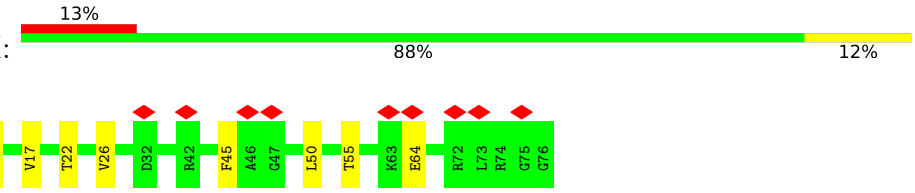
• Molecule 1: Polyubiquitin-B

Chain J:



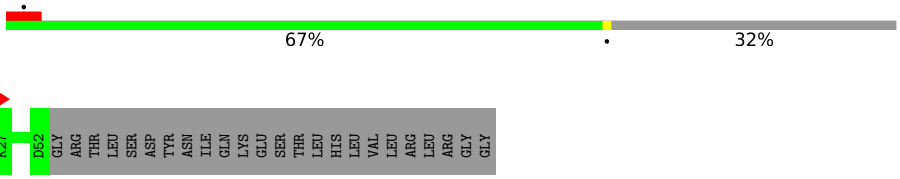
• Molecule 1: Polyubiquitin-B

Chain K:



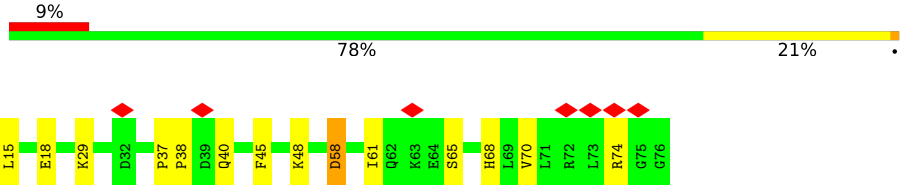
• Molecule 1: Polyubiquitin-B

Chain I:



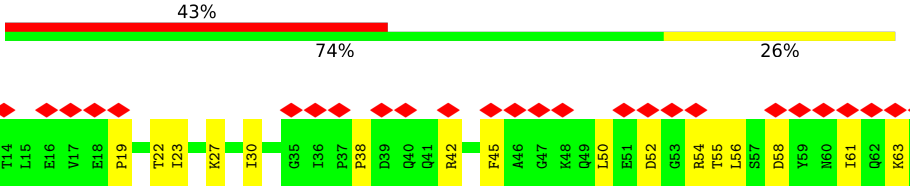
• Molecule 1: Polyubiquitin-B

Chain M:



• Molecule 1: Polyubiquitin-B

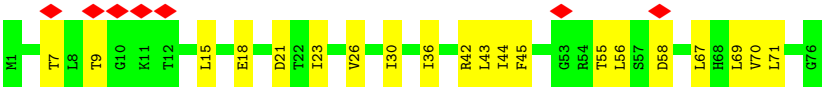
Chain N:



• Molecule 1: Polyubiquitin-B

Chain L:

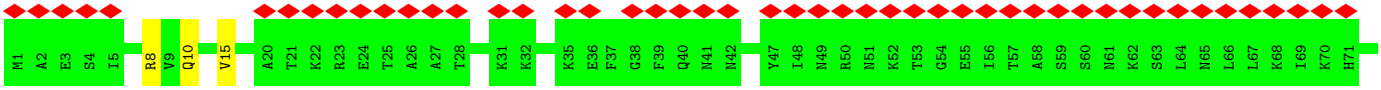




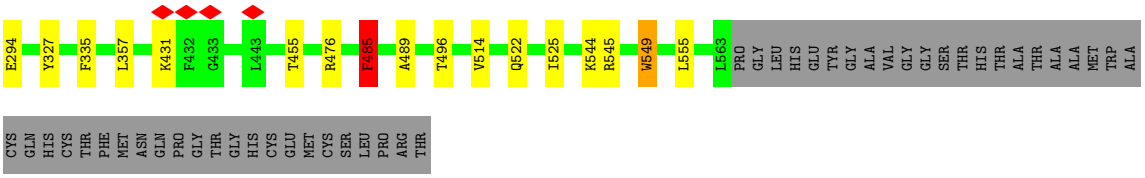
• Molecule 2: Nuclear protein localization protein 4 homolog

Chain G:





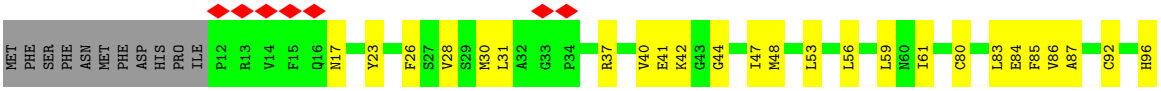


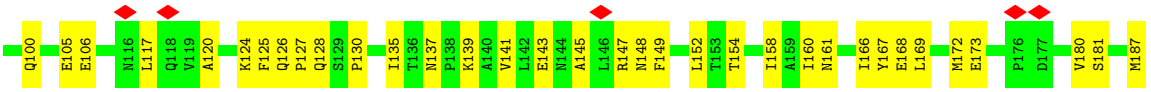


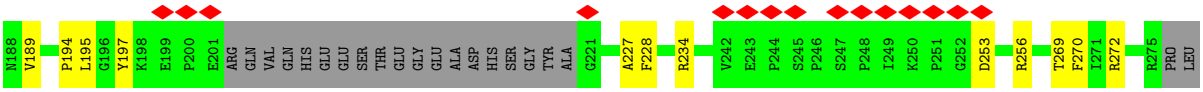
• Molecule 3: Ubiquitin recognition factor in ER-associated degradation protein 1

Chain H:





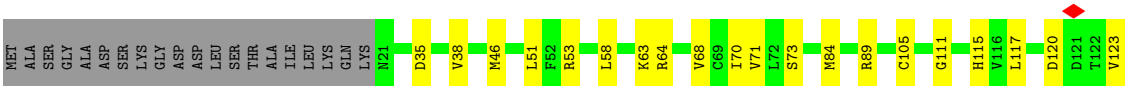


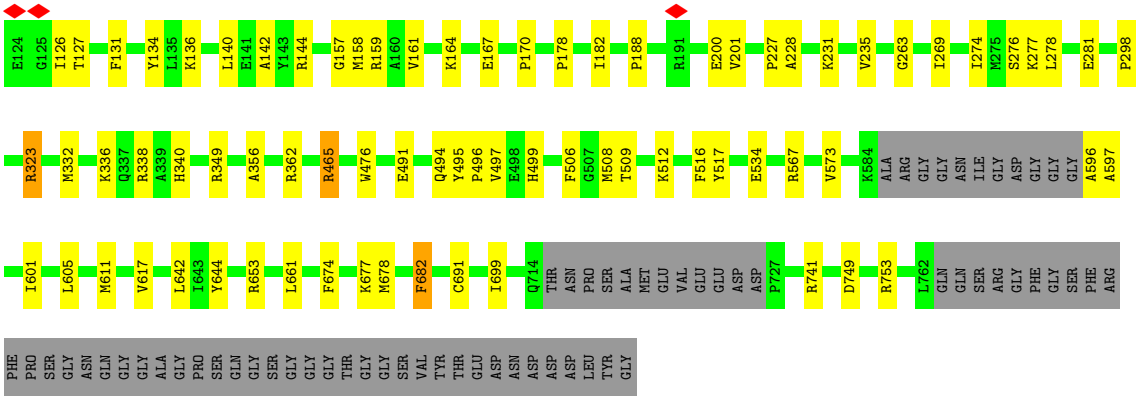


• Molecule 4: Transitional endoplasmic reticulum ATPase

Chain E:



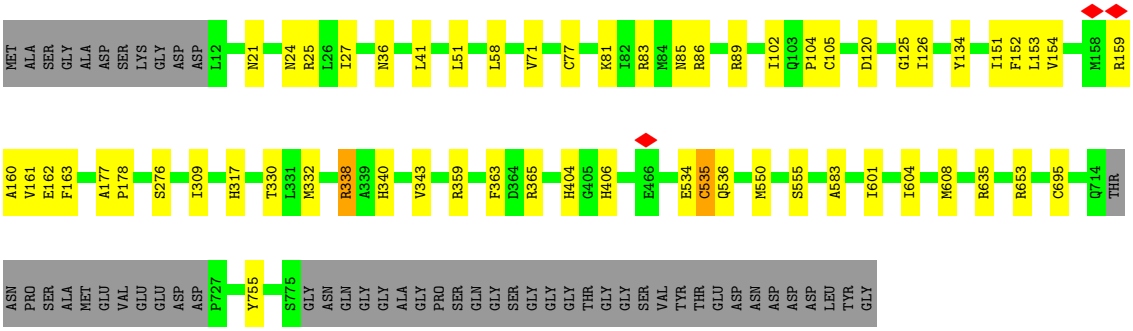




• Molecule 4: Transitional endoplasmic reticulum ATPase

Chain B:

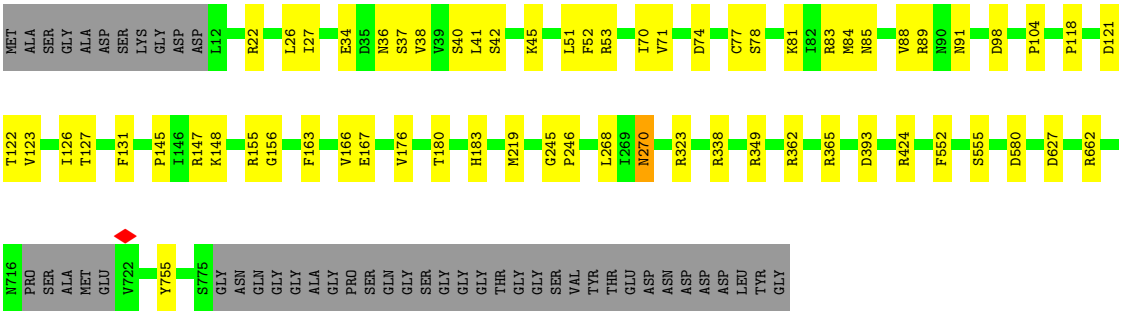




• Molecule 4: Transitional endoplasmic reticulum ATPase

Chain A:

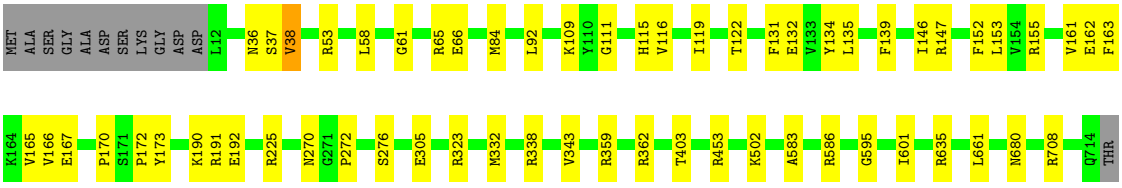




• Molecule 4: Transitional endoplasmic reticulum ATPase

Chain F:



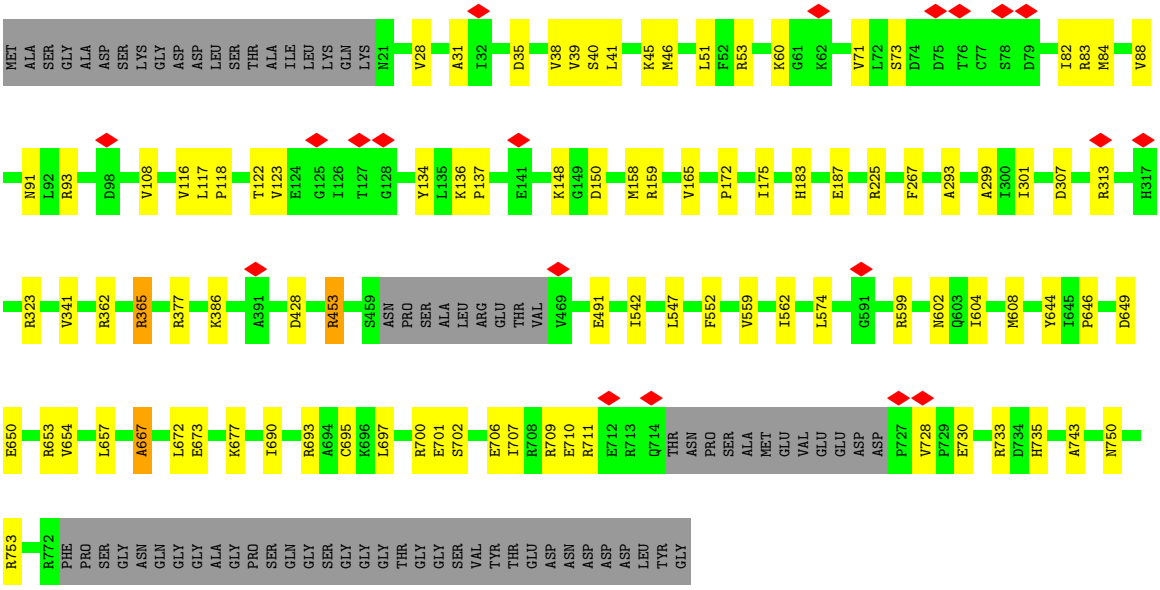




• Molecule 4: Transitional endoplasmic reticulum ATPase

Chain C:

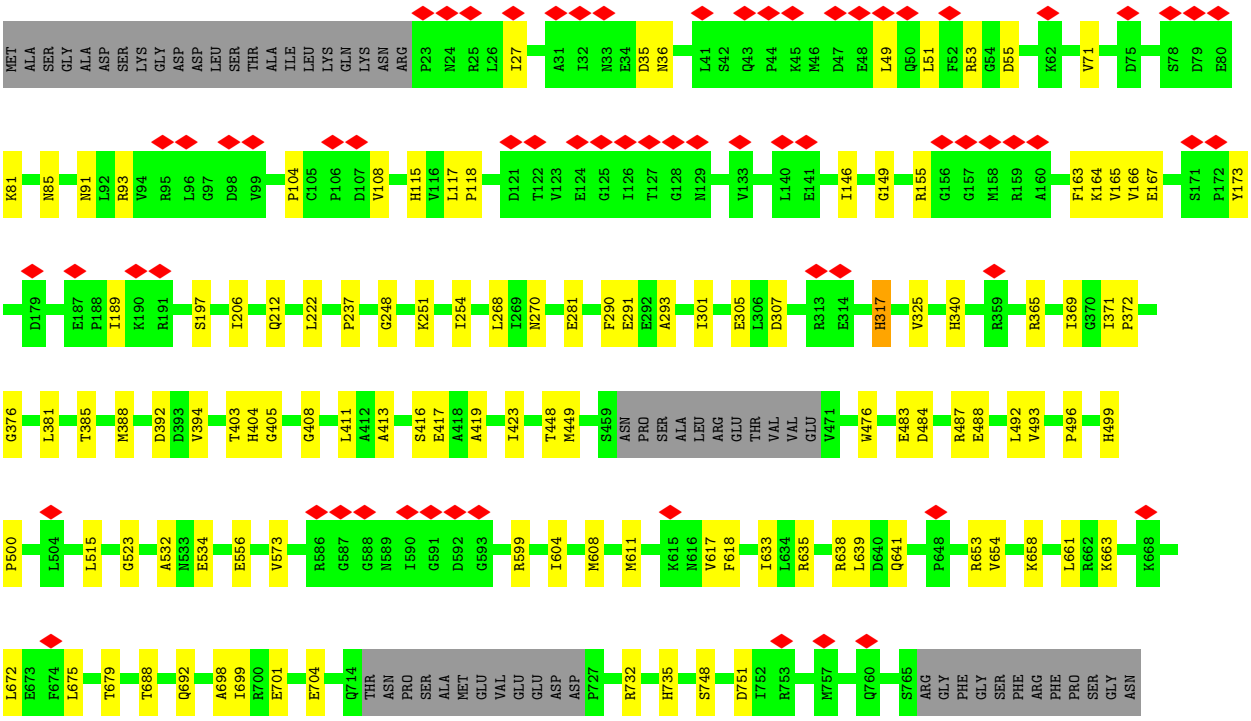


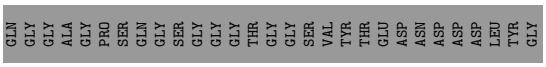


• Molecule 4: Transitional endoplasmic reticulum ATPase

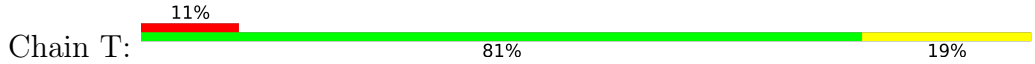
Chain D:







• Molecule 5: FAS-associated factor 1







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39948	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	39.258	Depositor
Minimum map value	-14.817	Depositor
Average map value	0.021	Depositor
Map value standard deviation	1.009	Depositor
Recommended contour level	5.18	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 (i)

5.1 Standard geometry (i)

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

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	I	0.75	0/414	1.34	0/557
1	J	0.43	0/600	0.81	0/806
1	K	0.43	0/600	0.72	0/806
1	L	0.12	0/608	0.36	0/816
1	M	0.45	0/608	0.93	1/816 (0.1%)
1	N	0.43	0/608	0.72	0/816
2	G	0.71	0/4404	1.28	6/5967 (0.1%)
3	H	0.45	0/1968	0.83	7/2655 (0.3%)
4	A	0.67	0/6039	1.27	15/8152 (0.2%)
4	B	0.67	0/5974	1.26	11/8063 (0.1%)
4	C	0.56	0/5795	1.09	10/7820 (0.1%)
4	D	0.44	0/5714	0.88	7/7712 (0.1%)
4	E	0.47	0/5748	0.98	18/7761 (0.2%)
4	F	0.66	0/5900	1.26	19/7965 (0.2%)
5	T	0.42	0/1446	0.80	1/1939 (0.1%)
All	All	0.58	0/46426	1.11	95/62651 (0.2%)

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	M	0	1
2	G	0	3
4	A	0	3
4	B	0	2
4	C	0	2
4	E	0	3
4	F	0	4
All	All	0	18

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	682	PHE	CA-CB-CG	10.89	124.69	113.80
3	H	228	PHE	CA-CB-CG	9.43	123.23	113.80
2	G	485	PHE	CA-CB-CG	-8.54	105.26	113.80
4	E	323	ARG	NE-CZ-NH2	8.15	126.53	119.20
4	A	245	GLY	CA-C-N	6.94	124.72	119.66
4	A	245	GLY	C-N-CA	6.94	124.72	119.66
4	C	552	PHE	CA-CB-CG	6.85	120.65	113.80
1	M	58	ASP	CA-CB-CG	6.85	119.45	112.60
4	F	270	ASN	CA-CB-CG	6.78	119.38	112.60
4	F	270	ASN	CB-CA-C	6.78	122.69	111.31
4	F	362	ARG	NE-CZ-NH2	6.70	125.23	119.20
4	D	237	PRO	N-CA-C	6.67	118.84	110.70
4	A	362	ARG	NE-CZ-NH2	6.67	125.20	119.20
4	E	596	ALA	CA-C-N	6.56	131.10	120.60
4	E	596	ALA	C-N-CA	6.56	131.10	120.60
4	F	359	ARG	NE-CZ-NH2	6.41	124.97	119.20
4	B	359	ARG	NE-CZ-NH2	6.14	124.72	119.20
4	A	424	ARG	NE-CZ-NH2	6.13	124.72	119.20
4	F	586	ARG	NE-CZ-NH2	6.09	124.68	119.20
4	D	317	HIS	N-CA-C	6.08	118.71	111.71
3	H	147	ARG	NE-CZ-NH2	6.01	124.61	119.20
4	B	535	CYS	N-CA-C	5.97	120.25	113.15
4	C	386	LYS	O-C-N	5.96	128.44	122.12
4	E	678	MET	N-CA-C	5.95	118.66	111.40
4	F	53	ARG	NE-CZ-NH2	5.87	124.49	119.20
2	G	242	ARG	NE-CZ-NH2	5.86	124.47	119.20
4	D	305	GLU	N-CA-C	5.86	119.09	109.72
4	E	677	LYS	CA-C-N	5.83	130.44	120.71
4	E	677	LYS	C-N-CA	5.83	130.44	120.71
4	C	225	ARG	NE-CZ-NH2	5.80	124.42	119.20
4	A	662	ARG	NE-CZ-NH2	5.78	124.40	119.20
4	A	323	ARG	NE-CZ-NH2	5.75	124.37	119.20
4	E	674	PHE	CA-C-N	5.75	127.91	120.44
4	E	674	PHE	C-N-CA	5.75	127.91	120.44
5	T	504	ARG	NE-CZ-NH2	5.71	124.34	119.20
4	E	338	ARG	NE-CZ-NH2	5.68	124.31	119.20
4	F	680	ASN	N-CA-C	5.67	117.46	111.28
4	B	338	ARG	NE-CZ-NH2	5.67	124.30	119.20
3	H	272	ARG	NE-CZ-NH2	5.62	124.26	119.20
4	E	323	ARG	CD-NE-CZ	5.58	132.21	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	599	ARG	CD-NE-CZ	5.56	132.19	124.40
4	F	276	SER	CA-C-N	5.56	127.67	120.44
4	F	276	SER	C-N-CA	5.56	127.67	120.44
4	A	365	ARG	NE-CZ-NH2	5.54	124.18	119.20
4	E	349	ARG	NE-CZ-NH2	5.53	124.18	119.20
4	C	602	ASN	CA-CB-CG	5.51	118.11	112.60
4	E	653	ARG	NE-CZ-NH2	5.50	124.15	119.20
4	A	246	PRO	N-CA-CB	5.44	106.24	103.19
4	B	404	HIS	N-CA-C	5.44	117.07	111.03
2	G	522	GLN	N-CA-C	5.43	117.20	111.28
4	E	516	PHE	CA-CB-CG	5.41	119.21	113.80
4	C	453	ARG	NE-CZ-NH2	5.38	124.04	119.20
4	A	22	ARG	NE-CZ-NH2	5.35	124.01	119.20
2	G	335	PHE	CA-CB-CG	5.33	119.13	113.80
4	D	268	LEU	N-CA-C	5.30	120.61	114.04
4	B	276	SER	CA-C-N	5.29	129.66	120.68
4	B	276	SER	C-N-CA	5.29	129.66	120.68
4	F	661	LEU	CA-C-N	5.28	128.74	120.82
4	F	661	LEU	C-N-CA	5.28	128.74	120.82
3	H	256	ARG	NE-CZ-NH2	5.28	123.95	119.20
4	A	627	ASP	CA-CB-CG	5.28	117.88	112.60
4	A	393	ASP	CA-CB-CG	5.27	117.87	112.60
4	B	534	GLU	N-CA-C	5.26	117.81	111.40
4	F	453	ARG	NE-CZ-NH2	5.25	123.92	119.20
4	F	305	GLU	CA-C-N	5.24	131.54	121.54
4	F	305	GLU	C-N-CA	5.24	131.54	121.54
4	D	599	ARG	NE-CZ-NH2	5.24	123.91	119.20
4	B	365	ARG	NE-CZ-NH2	5.23	123.90	119.20
4	C	323	ARG	NE-CZ-NH2	5.23	123.91	119.20
4	F	305	GLU	CB-CA-C	5.23	118.86	111.86
4	E	597	ALA	CA-C-N	5.21	129.02	120.63
4	E	597	ALA	C-N-CA	5.21	129.02	120.63
4	F	595	GLY	CA-C-N	5.21	127.26	120.28
4	F	595	GLY	C-N-CA	5.21	127.26	120.28
4	C	428	ASP	CA-CB-CG	5.20	117.80	112.60
4	C	365	ARG	NE-CZ-NH2	5.17	123.86	119.20
4	B	635	ARG	NE-CZ-NH2	5.17	123.85	119.20
4	E	741	ARG	NE-CZ-NH2	5.16	123.84	119.20
4	F	225	ARG	NE-CZ-NH2	5.16	123.84	119.20
4	A	183	HIS	CB-CG-CD2	-5.14	124.52	131.20
4	A	163	PHE	CA-CB-CG	5.13	118.93	113.80
4	C	93	ARG	NE-CZ-NH2	5.12	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	653	ARG	NE-CZ-NH2	5.11	123.80	119.20
4	B	406	HIS	CB-CG-CD2	-5.11	124.56	131.20
3	H	227	ALA	CA-C-N	5.06	127.06	120.28
3	H	227	ALA	C-N-CA	5.06	127.06	120.28
4	F	745	ARG	NE-CZ-NH2	5.06	123.75	119.20
2	G	476	ARG	NE-CZ-NH2	5.06	123.75	119.20
4	A	349	ARG	NE-CZ-NH2	5.04	123.74	119.20
4	A	552	PHE	N-CA-C	5.04	117.16	111.11
2	G	255	ARG	NE-CZ-NH2	5.03	123.73	119.20
3	H	234	ARG	NE-CZ-NH2	5.03	123.72	119.20
4	D	365	ARG	NE-CZ-NH2	5.02	123.72	119.20
4	E	465	ARG	NE-CZ-NH2	5.00	123.70	119.20
4	C	667	ALA	CB-CA-C	-5.00	110.43	117.23

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	270	ASN	Peptide
4	A	338	ARG	Sidechain
4	A	755	TYR	Sidechain
4	B	338	ARG	Sidechain
4	B	755	TYR	Sidechain
4	C	377	ARG	Sidechain
4	C	599	ARG	Sidechain
4	E	465	ARG	Sidechain
4	E	682	PHE	Sidechain
4	E	89	ARG	Sidechain
4	F	323	ARG	Sidechain
4	F	338	ARG	Sidechain
4	F	708	ARG	Sidechain
4	F	755	TYR	Sidechain
2	G	151	TYR	Sidechain
2	G	220	TYR	Sidechain
2	G	485	PHE	Sidechain
1	M	48	LYS	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	I	410	0	429	0	0
1	J	594	0	621	9	0
1	K	594	0	621	4	0
1	L	602	0	629	14	0
1	M	602	0	629	8	0
1	N	602	0	629	11	0
2	G	4305	0	4232	12	0
3	H	1928	0	1928	41	0
4	A	5942	0	5997	26	0
4	B	5878	0	5942	29	0
4	C	5702	0	5747	49	0
4	D	5623	0	5678	72	0
4	E	5656	0	5734	60	0
4	F	5807	0	5883	33	0
5	T	1423	0	1399	22	0
6	A	54	0	24	0	0
6	B	54	0	24	0	0
6	C	54	0	24	1	0
6	D	54	0	24	3	0
6	E	54	0	24	0	0
6	F	54	0	24	0	0
7	A	12	0	0	0	0
7	B	12	0	0	0	0
7	C	8	0	0	0	0
7	E	4	0	0	0	0
7	F	4	0	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
All	All	46042	0	46242	375	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 4.

All (375) 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)
4:F:36:ASN:ND2	4:F:153:LEU:O	2.03	0.90
4:D:248:GLY:N	6:D:901:ADP:O1B	2.13	0.81
4:D:149:GLY:HA2	4:D:164:LYS:HE2	1.66	0.77
4:D:404:HIS:CD2	4:D:405:GLY:H	2.03	0.76
4:E:123:VAL:HG22	4:E:161:VAL:HG13	1.67	0.76
4:D:115:HIS:H	4:D:167:GLU:HB2	1.52	0.75
4:D:608:MET:HA	4:D:611:MET:HB3	1.70	0.74
4:D:206:ILE:HD13	4:D:254:ILE:HG22	1.69	0.73
4:F:122:THR:HG21	4:F:162:GLU:H	1.54	0.71
5:T:596:LEU:HD21	5:T:636:VAL:HG21	1.71	0.71
4:E:131:PHE:HB2	4:E:182:ILE:HD12	1.71	0.71
4:B:535:CYS:O	4:B:536:GLN:HG2	1.91	0.70
4:E:46:MET:HE1	4:E:73:SER:HA	1.73	0.70
4:D:635:ARG:HE	4:D:638:ARG:HD2	1.55	0.69
5:T:596:LEU:HB2	5:T:629:PRO:HA	1.75	0.69
4:D:385:THR:HA	4:D:388:MET:HG2	1.72	0.69
4:B:41:LEU:HD13	4:B:71:VAL:HG23	1.75	0.69
4:E:136:LYS:O	4:E:140:LEU:HB3	1.92	0.69
4:D:371:ILE:HD12	4:D:372:PRO:HD2	1.75	0.69
4:C:293:ALA:HB2	4:C:301:ILE:HD11	1.75	0.68
4:D:476:TRP:HE1	4:D:534:GLU:HB2	1.57	0.68
4:C:84:MET:SD	4:C:88:VAL:HB	2.34	0.68
4:C:39:VAL:HG23	4:C:84:MET:HB3	1.76	0.67
4:A:36:ASN:HA	4:A:85:ASN:HD21	1.58	0.67
4:C:118:PRO:HB2	4:C:123:VAL:HG21	1.75	0.67
1:N:19:PRO:HA	1:N:56:LEU:HD22	1.75	0.67
4:A:118:PRO:HB2	4:A:123:VAL:HG11	1.77	0.67
4:E:111:GLY:HA2	4:E:170:PRO:HD2	1.76	0.67
1:N:45:PHE:HB3	1:N:50:LEU:HD21	1.78	0.66
3:H:47:ILE:HG22	3:H:87:ALA:HB2	1.78	0.65
4:F:190:LYS:HD3	4:F:192:GLU:H	1.59	0.65
1:J:27:LYS:HB3	1:J:38:PRO:HB3	1.78	0.65
5:T:596:LEU:HD23	5:T:633:LEU:HD23	1.78	0.65
4:D:35:ASP:HA	4:D:85:ASN:HB3	1.78	0.65
4:E:70:ILE:HG13	4:E:144:ARG:HH11	1.60	0.65
3:H:40:VAL:HG21	3:H:83:LEU:HD22	1.80	0.64
4:E:661:LEU:HD21	4:E:691:CYS:SG	2.36	0.64
4:E:567:ARG:HB2	4:E:611:MET:HE1	1.80	0.63
4:E:64:ARG:HH11	4:E:263:GLY:HA2	1.62	0.63
4:F:131:PHE:O	4:F:135:LEU:HB2	1.99	0.63
1:L:42:ARG:HB3	1:L:70:VAL:HB	1.81	0.63
4:F:332:MET:HE3	4:F:343:VAL:HG11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:126:GLN:HE22	3:H:195:LEU:HG	1.65	0.62
4:B:604:ILE:HG22	4:B:608:MET:HE2	1.82	0.62
4:F:146:ILE:HD12	4:F:165:VAL:HG11	1.82	0.61
4:D:93:ARG:HH22	4:D:197:SER:HA	1.64	0.61
4:D:403:THR:HG21	4:D:411:LEU:HD21	1.82	0.61
4:D:419:ALA:O	4:D:423:ILE:HD12	2.01	0.61
1:L:7:THR:HG22	1:L:69:LEU:HD23	1.83	0.60
1:J:15:LEU:HD21	1:J:29:LYS:HB3	1.83	0.60
3:H:23:TYR:HD2	3:H:92:CYS:HB3	1.67	0.60
4:E:508:MET:HA	4:D:663:LYS:HE3	1.84	0.60
4:E:117:LEU:HD11	4:E:164:LYS:HE3	1.84	0.59
5:T:596:LEU:HD11	5:T:636:VAL:HG11	1.84	0.59
4:D:36:ASN:HD22	4:D:155:ARG:HG3	1.67	0.59
4:D:661:LEU:HD13	4:D:672:LEU:HD22	1.83	0.59
1:N:1:MET:HE2	1:N:63:LYS:HA	1.84	0.59
5:T:481:MET:HE2	5:T:484:MET:HE1	1.85	0.59
4:E:749:ASP:HB2	4:E:753:ARG:HH22	1.68	0.59
4:C:657:LEU:HB3	4:C:672:LEU:HD22	1.84	0.59
3:H:56:LEU:HD23	3:H:61:ILE:HD13	1.85	0.58
4:B:21:ASN:HA	4:B:25:ARG:HE	1.66	0.58
4:B:27:ILE:HB	4:B:81:LYS:HG2	1.86	0.58
4:D:251:LYS:HB2	6:D:901:ADP:O2B	2.03	0.58
3:H:42:LYS:HD3	3:H:161:ASN:HB3	1.85	0.58
4:A:34:GLU:HB3	4:A:38:VAL:HG23	1.86	0.57
4:C:41:LEU:HB3	4:C:45:LYS:HE3	1.85	0.57
4:F:65:ARG:HB2	4:F:92:LEU:HA	1.87	0.57
4:A:38:VAL:HG12	4:A:70:ILE:HB	1.85	0.57
4:A:52:PHE:CD2	5:T:641:GLN:HB3	2.39	0.57
1:N:5:VAL:HG21	1:N:30:ILE:HD11	1.86	0.57
4:E:115:HIS:HB2	4:E:167:GLU:HB3	1.87	0.57
4:C:82:ILE:HG12	4:C:84:MET:CE	2.35	0.56
1:M:40:GLN:NE2	1:M:74:ARG:HE	2.04	0.56
4:C:707:ILE:O	4:C:711:ARG:HG2	2.05	0.56
4:E:134:TYR:HE1	4:E:157:GLY:HA3	1.70	0.56
4:B:535:CYS:O	4:B:536:GLN:CG	2.53	0.56
4:D:404:HIS:CG	4:D:405:GLY:H	2.23	0.56
4:A:78:SER:HB2	4:A:81:LYS:HB2	1.88	0.56
4:C:40:SER:O	4:C:41:LEU:HD23	2.06	0.56
4:C:82:ILE:HG12	4:C:84:MET:HE1	1.87	0.56
1:N:23:ILE:HB	1:N:52:ASP:HA	1.87	0.56
4:E:58:LEU:HD13	4:E:105:CYS:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:228:ALA:HA	4:E:231:LYS:HG2	1.87	0.56
4:D:701:GLU:HG2	4:D:735:HIS:CE1	2.40	0.56
1:K:17:VAL:HG11	1:K:26:VAL:HG22	1.88	0.56
4:B:332:MET:HE1	4:B:363:PHE:CZ	2.41	0.55
1:N:27:LYS:HB3	1:N:38:PRO:HB3	1.87	0.55
2:G:8:ARG:HH12	2:G:74:LEU:HB3	1.71	0.55
4:B:535:CYS:C	4:B:536:GLN:HG2	2.33	0.54
4:D:675:LEU:O	4:D:679:THR:HG23	2.08	0.54
4:D:146:ILE:HB	4:D:165:VAL:HG21	1.88	0.54
4:B:134:TYR:HB3	4:B:154:VAL:HG11	1.90	0.54
4:E:126:ILE:HD11	4:E:158:MET:HE3	1.90	0.54
4:A:126:ILE:HG22	4:A:127:THR:H	1.73	0.54
4:F:115:HIS:HB3	4:F:167:GLU:HB2	1.88	0.54
4:E:336:LYS:HA	4:E:336:LYS:HE2	1.90	0.54
1:L:55:THR:HG23	1:L:58:ASP:H	1.72	0.54
4:E:235:VAL:HG11	4:D:416:SER:HA	1.90	0.53
1:L:26:VAL:HG21	1:L:56:LEU:HD21	1.89	0.53
4:E:63:LYS:HD3	4:E:200:GLU:HB2	1.89	0.53
4:F:135:LEU:HD12	4:F:139:PHE:CE2	2.44	0.53
4:A:88:VAL:HA	4:A:91:ASN:HD22	1.73	0.53
4:A:84:MET:SD	4:A:88:VAL:HB	2.49	0.53
4:C:604:ILE:HG22	4:C:608:MET:HE3	1.91	0.53
4:D:493:VAL:O	4:D:496:PRO:HD2	2.09	0.53
4:E:53:ARG:HA	4:E:71:VAL:HG23	1.91	0.52
4:E:227:PRO:C	4:E:231:LYS:HZ2	2.17	0.52
4:F:153:LEU:HG	4:F:155:ARG:H	1.74	0.52
1:N:42:ARG:H	1:N:69:LEU:HD13	1.75	0.52
3:H:30:MET:HE3	3:H:30:MET:O	2.09	0.52
4:E:64:ARG:NH1	4:E:263:GLY:HA2	2.25	0.52
4:B:36:ASN:HA	4:B:85:ASN:HD21	1.74	0.52
4:F:37:SER:OG	4:F:38:VAL:HG13	2.09	0.52
4:D:392:ASP:HB3	4:D:449:MET:HE2	1.92	0.52
3:H:53:LEU:HD13	3:H:85:PHE:CE1	2.45	0.52
4:F:131:PHE:CD2	4:F:132:GLU:HG2	2.45	0.52
2:G:545:ARG:HA	2:G:549:TRP:CD1	2.45	0.52
5:T:510:GLU:O	5:T:513:GLU:HG2	2.11	0.51
4:C:134:TYR:CZ	4:C:158:MET:HE3	2.46	0.51
2:G:15:VAL:HG23	4:C:175:ILE:HG13	1.91	0.51
4:C:267:PHE:HB3	4:C:301:ILE:HD13	1.92	0.51
4:F:135:LEU:HD12	4:F:139:PHE:CZ	2.46	0.51
3:H:139:LYS:HZ3	3:H:189:VAL:N	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:706:GLU:O	4:C:709:ARG:HG3	2.10	0.51
3:H:44:GLY:O	3:H:80:CYS:HB2	2.10	0.51
4:C:702:SER:O	4:C:706:GLU:HG2	2.11	0.51
4:F:58:LEU:HD11	4:F:66:GLU:HB3	1.93	0.50
3:H:143:GLU:HB3	5:T:511:GLN:OE1	2.11	0.50
5:T:600:PHE:HE1	5:T:625:THR:HG22	1.76	0.50
4:E:749:ASP:CG	4:E:753:ARG:HH12	2.19	0.50
4:E:499:HIS:HE1	4:D:699:ILE:HG21	1.75	0.50
4:D:372:PRO:HB2	4:D:376:GLY:HA3	1.93	0.50
3:H:117:LEU:HB2	3:H:181:SER:HB2	1.94	0.50
4:D:290:PHE:HE1	4:D:301:ILE:HG21	1.77	0.50
1:L:23:ILE:HG23	1:L:43:LEU:HD12	1.92	0.50
3:H:137:ASN:ND2	5:T:518:SER:HB2	2.26	0.50
3:H:160:ILE:HG13	3:H:167:TYR:HB2	1.92	0.50
4:D:611:MET:SD	4:D:617:VAL:HB	2.52	0.50
2:G:485:PHE:CG	2:G:555:LEU:HB3	2.47	0.50
3:H:48:MET:HB2	3:H:85:PHE:CD2	2.47	0.50
4:E:508:MET:HG2	4:E:509:THR:N	2.26	0.49
4:B:604:ILE:CG2	4:B:608:MET:HE2	2.42	0.49
4:C:122:THR:HA	4:C:159:ARG:HH11	1.77	0.49
4:C:750:ASN:HA	4:C:753:ARG:HH11	1.77	0.49
4:E:134:TYR:HE2	4:E:161:VAL:HG21	1.76	0.49
5:T:638:LEU:HD22	5:T:642:GLU:HG3	1.94	0.49
4:A:40:SER:HB2	4:A:74:ASP:HB2	1.93	0.49
4:C:84:MET:HG2	4:C:84:MET:O	2.11	0.49
3:H:139:LYS:HZ3	3:H:189:VAL:H	1.59	0.49
4:E:508:MET:HG2	4:E:509:THR:H	1.77	0.49
5:T:596:LEU:HD12	5:T:628:ASP:O	2.12	0.49
4:E:140:LEU:HD11	4:E:178:PRO:HA	1.95	0.49
4:B:36:ASN:HD22	4:B:153:LEU:H	1.61	0.49
5:T:599:VAL:HG21	5:T:633:LEU:HD21	1.95	0.49
4:C:39:VAL:HG12	4:C:71:VAL:HA	1.93	0.49
4:C:116:VAL:HG12	4:C:165:VAL:HG22	1.95	0.49
2:G:485:PHE:CE2	2:G:489:ALA:HB2	2.47	0.49
3:H:28:VAL:HB	3:H:41:GLU:HG2	1.94	0.49
3:H:166:ILE:HG13	1:L:9:THR:HG22	1.95	0.49
4:D:573:VAL:HG23	4:D:618:PHE:HB2	1.93	0.49
2:G:10:GLN:HB2	2:G:15:VAL:HG22	1.95	0.49
4:B:86:ARG:HG2	4:B:89:ARG:HH12	1.78	0.49
4:E:517:TYR:CZ	4:E:644:TYR:HB2	2.47	0.48
4:C:542:ILE:HG12	4:C:547:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:667:ALA:HA	4:C:733:ARG:HG2	1.94	0.48
4:C:693:ARG:HD3	4:C:697:LEU:HD13	1.95	0.48
4:E:269:ILE:HG23	4:E:274:ILE:HD11	1.95	0.48
4:D:515:LEU:HB2	4:D:639:LEU:HD21	1.95	0.48
4:D:635:ARG:NH1	4:D:638:ARG:HH21	2.11	0.48
4:D:166:VAL:HG12	4:D:166:VAL:O	2.14	0.48
4:F:116:VAL:HG22	4:F:165:VAL:HG22	1.96	0.48
3:H:17:ASN:HB3	3:H:59:LEU:HD22	1.96	0.48
4:D:394:VAL:HG22	4:D:449:MET:HE1	1.95	0.48
3:H:105:GLU:HB3	1:L:42:ARG:HH12	1.79	0.48
4:D:49:LEU:HD22	4:D:104:PRO:HD3	1.95	0.48
4:D:293:ALA:HB2	4:D:301:ILE:HD11	1.95	0.48
4:D:654:VAL:O	4:D:658:LYS:HG2	2.14	0.48
5:T:575:LYS:O	5:T:641:GLN:HA	2.14	0.47
4:C:733:ARG:HA	4:C:735:HIS:CE1	2.48	0.47
1:K:45:PHE:HB3	1:K:50:LEU:HD21	1.95	0.47
2:G:259:HIS:CE1	2:G:267:ARG:HH11	2.31	0.47
3:H:96:HIS:CE1	3:H:100:GLN:HE21	2.31	0.47
4:C:35:ASP:H	4:C:38:VAL:HG22	1.79	0.47
3:H:127:PRO:HB2	3:H:194:PRO:HB3	1.96	0.47
4:C:41:LEU:HD21	4:C:82:ILE:HG13	1.94	0.47
4:E:126:ILE:HG22	4:E:127:THR:H	1.80	0.47
4:D:698:ALA:O	4:D:701:GLU:HG3	2.13	0.47
3:H:128:GLN:HB2	3:H:168:GLU:HB2	1.96	0.47
4:C:41:LEU:HB2	4:C:46:MET:SD	2.55	0.47
4:D:493:VAL:HG21	4:D:534:GLU:HG2	1.95	0.47
4:D:653:ARG:HD2	4:D:679:THR:OG1	2.13	0.47
4:E:277:LYS:HG3	4:E:278:LEU:H	1.80	0.47
4:B:332:MET:HE2	4:B:343:VAL:HG11	1.97	0.47
4:A:126:ILE:HG22	4:A:127:THR:N	2.30	0.47
1:N:22:THR:HA	1:N:55:THR:HA	1.97	0.47
3:H:26:PHE:CD2	3:H:30:MET:HG2	2.50	0.47
3:H:125:PHE:HD2	3:H:169:LEU:HB3	1.79	0.47
4:A:41:LEU:HD12	4:A:42:SER:H	1.79	0.47
4:C:299:ALA:HB3	4:C:341:VAL:HG22	1.96	0.47
4:B:177:ALA:HB1	4:B:178:PRO:CD	2.45	0.47
1:M:15:LEU:HD22	1:M:29:LYS:HB3	1.96	0.47
4:C:53:ARG:HG2	4:C:73:SER:HB3	1.97	0.47
4:E:601:ILE:O	4:E:605:LEU:HD23	2.15	0.47
4:E:276:SER:HB3	4:E:281:GLU:OE2	2.14	0.46
4:C:649:ASP:O	4:C:653:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:127:PRO:HA	3:H:169:LEU:HA	1.96	0.46
4:E:46:MET:HB2	4:E:51:LEU:O	2.15	0.46
4:C:695:CYS:HA	4:C:735:HIS:HD2	1.81	0.46
4:B:36:ASN:ND2	4:B:152:PHE:HB2	2.30	0.46
4:D:53:ARG:HH11	4:D:71:VAL:HG13	1.80	0.46
3:H:84:GLU:HB3	1:M:68:HIS:CD2	2.49	0.46
4:B:51:LEU:HD21	4:B:104:PRO:HG3	1.96	0.46
4:B:58:LEU:HB2	4:B:105:CYS:HB2	1.96	0.46
4:D:36:ASN:ND2	4:D:155:ARG:HG3	2.30	0.46
4:E:332:MET:HE2	4:E:332:MET:HB2	1.88	0.46
4:A:51:LEU:HD21	4:A:104:PRO:HB3	1.97	0.46
4:E:158:MET:HE1	4:E:159:ARG:CZ	2.46	0.46
4:A:77:CYS:SG	4:A:83:ARG:HG3	2.56	0.46
4:D:408:GLY:HA2	4:D:411:LEU:HD12	1.97	0.46
1:J:17:VAL:HG11	1:J:26:VAL:HG22	1.98	0.46
4:E:753:ARG:HH21	4:E:753:ARG:HG3	1.80	0.46
4:B:153:LEU:HD13	4:B:162:GLU:OE2	2.16	0.46
1:M:45:PHE:CZ	1:M:61:ILE:HA	2.51	0.46
5:T:591:LEU:O	5:T:633:LEU:HD12	2.16	0.46
5:T:639:PHE:CD1	5:T:640:PRO:HA	2.51	0.46
3:H:145:ALA:HA	3:H:148:ASN:HB2	1.97	0.46
4:E:120:ASP:HB3	4:E:188:PRO:HB3	1.97	0.46
4:E:494:GLN:O	4:E:497:VAL:HG12	2.16	0.45
4:E:506:PHE:O	4:E:506:PHE:CG	2.69	0.45
1:M:45:PHE:HE2	1:M:65:SER:HB3	1.80	0.45
1:L:18:GLU:HG2	1:L:21:ASP:CG	2.41	0.45
2:G:15:VAL:H	4:C:108:VAL:HB	1.81	0.45
3:H:130:PRO:HA	3:H:197:TYR:HB2	1.99	0.45
4:D:556:GLU:CD	4:D:556:GLU:H	2.24	0.45
4:D:732:ARG:H	4:D:732:ARG:HD3	1.81	0.45
4:D:270:ASN:HD21	4:D:307:ASP:CG	2.23	0.45
1:J:23:ILE:HD11	1:J:59:TYR:CE1	2.52	0.45
3:H:106:GLU:HG2	1:L:42:ARG:CZ	2.47	0.45
3:H:124:LYS:HG3	3:H:173:GLU:HB3	1.97	0.45
4:C:673:GLU:O	4:C:677:LYS:HG2	2.17	0.45
4:D:633:ILE:O	4:D:639:LEU:HB3	2.15	0.45
4:B:36:ASN:ND2	4:B:153:LEU:H	2.14	0.45
4:F:115:HIS:H	4:F:167:GLU:HB3	1.81	0.45
4:D:532:ALA:HB2	4:D:573:VAL:HG11	1.99	0.45
2:G:10:GLN:CB	2:G:15:VAL:HG22	2.47	0.45
4:A:40:SER:OG	4:A:83:ARG:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:904:ADP:C8	6:C:904:ADP:H5'1	2.51	0.45
1:N:56:LEU:HD21	1:N:61:ILE:O	2.16	0.45
3:H:149:PHE:CZ	3:H:158:ILE:HB	2.52	0.45
4:E:58:LEU:HA	4:E:68:VAL:HG12	1.98	0.45
4:D:688:THR:HG22	4:D:692:GLN:NE2	2.32	0.45
1:J:21:ASP:O	1:J:56:LEU:HG	2.17	0.44
3:H:28:VAL:HG21	3:H:40:VAL:HG12	1.99	0.44
4:C:728:VAL:HG22	4:C:730:GLU:H	1.83	0.44
4:A:148:LYS:HE2	4:A:166:VAL:O	2.18	0.44
4:C:650:GLU:O	4:C:654:VAL:HG23	2.18	0.44
2:G:549:TRP:CD1	2:G:549:TRP:C	2.94	0.44
4:B:126:ILE:O	4:B:126:ILE:HG22	2.16	0.44
1:K:5:VAL:HG13	1:K:13:ILE:HB	2.00	0.44
4:E:496:PRO:HA	4:E:499:HIS:HB2	1.99	0.44
4:E:699:ILE:HG12	4:F:502:LYS:HB3	2.00	0.44
4:B:125:GLY:HA3	4:B:159:ARG:HG3	1.99	0.44
4:A:27:ILE:HA	4:A:98:ASP:O	2.18	0.44
3:H:135:ILE:HG21	3:H:141:VAL:HG21	1.99	0.44
4:C:46:MET:HB3	4:C:51:LEU:O	2.18	0.44
4:D:413:ALA:O	4:D:417:GLU:HG2	2.17	0.44
4:F:61:GLY:HA3	4:F:92:LEU:HB3	1.99	0.44
4:F:583:ALA:HA	4:F:601:ILE:HD13	2.00	0.44
4:C:690:ILE:HD11	4:C:743:ALA:HB2	1.99	0.44
1:N:54:ARG:NH1	1:N:58:ASP:HB3	2.33	0.44
4:E:63:LYS:HG2	4:E:200:GLU:OE1	2.18	0.44
4:D:484:ASP:O	4:D:488:GLU:HG2	2.17	0.44
4:C:700:ARG:NH2	4:C:701:GLU:HB2	2.33	0.43
2:G:514:VAL:HG22	2:G:525:ILE:HG21	2.00	0.43
3:H:37:ARG:HH21	3:H:83:LEU:HD21	1.82	0.43
4:E:642:LEU:HD12	4:E:642:LEU:HA	1.90	0.43
4:F:66:GLU:HB2	4:F:147:ARG:NE	2.33	0.43
4:C:117:LEU:HD12	4:C:187:GLU:O	2.18	0.43
4:A:37:SER:HB3	4:A:145:PRO:HD2	1.99	0.43
4:F:135:LEU:HD11	4:F:152:PHE:CZ	2.52	0.43
4:D:51:LEU:HD22	4:D:55:ASP:HB3	1.99	0.43
4:D:484:ASP:HA	4:D:487:ARG:HE	1.82	0.43
4:F:116:VAL:HG12	4:F:163:PHE:CD2	2.53	0.43
1:J:55:THR:HG22	1:J:57:SER:H	1.83	0.43
4:B:153:LEU:HD12	4:B:161:VAL:O	2.18	0.43
1:L:45:PHE:HB2	1:L:67:LEU:HD22	2.01	0.43
4:D:27:ILE:HG13	4:D:81:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:212:GLN:HG2	4:D:369:ILE:HA	2.01	0.43
1:L:44:ILE:HD12	1:L:70:VAL:HG21	2.01	0.43
5:T:588:ARG:HG2	5:T:589:ARG:O	2.19	0.43
1:J:50:LEU:HD23	1:J:59:TYR:CZ	2.54	0.43
4:A:155:ARG:HD2	4:A:156:GLY:N	2.34	0.43
5:T:566:LYS:N	5:T:569:ASN:HD21	2.17	0.43
4:D:483:GLU:O	4:D:487:ARG:HG3	2.18	0.43
4:D:404:HIS:CG	4:D:405:GLY:N	2.87	0.42
4:D:523:GLY:HA2	6:D:902:ADP:O2A	2.19	0.42
3:H:161:ASN:ND2	1:L:9:THR:HA	2.33	0.42
4:E:356:ALA:O	4:E:362:ARG:HD2	2.19	0.42
4:E:298:PRO:HA	4:E:340:HIS:O	2.18	0.42
4:F:134:TYR:CE2	4:F:161:VAL:HG21	2.54	0.42
4:E:51:LEU:HD23	4:E:51:LEU:HA	1.89	0.42
4:C:136:LYS:HB2	4:C:137:PRO:HD3	2.02	0.42
1:L:15:LEU:HD11	1:L:30:ILE:HG13	2.00	0.42
4:F:135:LEU:HD11	4:F:152:PHE:HZ	1.83	0.42
4:F:166:VAL:O	4:F:166:VAL:HG13	2.19	0.42
1:M:8:LEU:HD21	1:M:70:VAL:HG22	2.02	0.42
4:C:28:VAL:HA	4:C:82:ILE:O	2.20	0.42
4:C:31:ALA:HA	4:C:83:ARG:HD2	2.02	0.42
4:D:91:ASN:C	4:D:91:ASN:HD22	2.28	0.42
4:D:117:LEU:HB2	4:D:189:ILE:HD11	2.01	0.42
4:B:151:ILE:HD12	4:B:163:PHE:O	2.19	0.42
1:K:22:THR:HA	1:K:55:THR:HA	2.01	0.42
4:E:134:TYR:CE1	4:E:157:GLY:HA3	2.51	0.42
4:B:77:CYS:SG	4:B:83:ARG:HG3	2.59	0.42
4:D:499:HIS:N	4:D:500:PRO:HD2	2.35	0.42
3:H:154:THR:HG23	3:H:172:MET:HA	2.02	0.42
4:F:109:LYS:HB2	4:F:170:PRO:HG3	2.02	0.42
1:M:37:PRO:HA	1:M:38:PRO:HD3	1.97	0.42
2:G:74:LEU:H	2:G:74:LEU:HD23	1.84	0.42
4:B:583:ALA:HA	4:B:601:ILE:CD1	2.49	0.42
4:F:119:ILE:HG21	4:F:191:ARG:HH21	1.84	0.42
5:T:557:LEU:HB3	5:T:601:ASP:OD1	2.20	0.42
5:T:572:PRO:HB3	5:T:639:PHE:CZ	2.55	0.42
1:L:36:ILE:HG21	1:L:71:LEU:HD22	2.01	0.42
4:F:332:MET:HE3	4:F:343:VAL:CG1	2.47	0.41
4:C:91:ASN:OD1	4:C:150:ASP:HB3	2.20	0.41
4:D:381:LEU:HD21	4:D:411:LEU:HD22	2.01	0.41
1:J:13:ILE:HG21	1:J:33:LYS:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:31:LEU:HD21	3:H:86:VAL:HG23	2.01	0.41
3:H:120:ALA:HB2	3:H:180:VAL:HB	2.03	0.41
4:E:512:LYS:HE2	4:E:617:VAL:O	2.19	0.41
4:C:148:LYS:HD3	4:C:172:PRO:HA	2.02	0.41
4:E:70:ILE:HG13	4:E:144:ARG:NH1	2.32	0.41
4:E:499:HIS:CE1	4:D:699:ILE:HG21	2.53	0.41
4:A:147:ARG:HG2	4:A:148:LYS:N	2.35	0.41
1:M:9:THR:HG23	1:M:11:LYS:HE2	2.02	0.41
4:C:574:LEU:HD23	4:C:574:LEU:HA	1.88	0.41
4:D:748:SER:HB3	4:D:751:ASP:CG	2.46	0.41
4:E:277:LYS:HG3	4:E:278:LEU:N	2.36	0.41
4:B:330:THR:HG21	4:A:270:ASN:HB3	2.01	0.41
4:D:492:LEU:HD11	4:D:641:GLN:HG3	2.01	0.41
4:E:38:VAL:HG12	4:E:70:ILE:HB	2.02	0.41
4:E:491:GLU:HG2	4:E:495:TYR:CE2	2.56	0.41
4:A:176:VAL:HG23	4:A:180:THR:HG21	2.02	0.41
4:D:118:PRO:HB3	4:D:163:PHE:CE1	2.56	0.41
4:D:701:GLU:HA	4:D:704:GLU:HG3	2.03	0.41
3:H:152:LEU:HD12	3:H:187:MET:HE1	2.03	0.41
5:T:548:GLU:O	5:T:551:GLU:HG3	2.20	0.41
4:C:559:VAL:O	4:C:562:ILE:HG22	2.21	0.41
3:H:125:PHE:CD2	3:H:169:LEU:HB3	2.56	0.41
4:E:476:TRP:NE1	4:E:534:GLU:HG2	2.36	0.41
4:F:191:ARG:HA	4:F:191:ARG:HD2	1.82	0.41
5:T:533:MET:HE3	5:T:533:MET:HB3	1.92	0.41
4:F:172:PRO:HG2	4:F:173:TYR:CD2	2.56	0.41
4:D:108:VAL:HG13	4:D:173:TYR:HD2	1.86	0.41
4:A:53:ARG:HA	4:A:71:VAL:HG13	2.03	0.40
4:F:116:VAL:HG12	4:F:163:PHE:HD2	1.86	0.40
1:J:37:PRO:O	1:J:41:GLN:HG3	2.22	0.40
4:E:508:MET:CG	4:E:509:THR:H	2.34	0.40
4:B:153:LEU:HD11	4:B:160:ALA:HB1	2.03	0.40
4:A:26:LEU:HD21	4:A:45:LYS:HG2	2.03	0.40
4:A:85:ASN:O	4:A:89:ARG:HG3	2.20	0.40
4:D:392:ASP:HB2	4:D:448:THR:HB	2.03	0.40
1:N:54:ARG:CZ	1:N:58:ASP:HB3	2.52	0.40
4:B:24:ASN:O	4:B:102:ILE:HG22	2.22	0.40
4:A:121:ASP:OD1	4:A:122:THR:HG23	2.22	0.40
4:D:301:ILE:HD13	4:D:301:ILE:HA	1.91	0.40
4:F:111:GLY:HA2	4:F:170:PRO:HD2	2.04	0.40
4:F:601:ILE:HD12	4:F:601:ILE:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:142:ALA:HB1	4:E:144:ARG:NH2	2.37	0.40
4:C:644:TYR:CZ	4:C:646:PRO:HB3	2.56	0.40
4:C:709:ARG:HD2	4:C:710:GLU:N	2.37	0.40
4:D:496:PRO:HA	4:D:499:HIS:HD2	1.86	0.40
4:D:604:ILE:HG22	4:D:608:MET:CE	2.52	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	I	50/76 (66%)	45 (90%)	5 (10%)	0	100	100
1	J	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
1	K	74/76 (97%)	71 (96%)	2 (3%)	1 (1%)	9	40
1	L	74/76 (97%)	74 (100%)	0	0	100	100
1	M	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
1	N	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
2	G	536/608 (88%)	497 (93%)	36 (7%)	3 (1%)	21	59
3	H	241/307 (78%)	228 (95%)	12 (5%)	1 (0%)	30	67
4	A	755/806 (94%)	733 (97%)	22 (3%)	0	100	100
4	B	748/806 (93%)	725 (97%)	23 (3%)	0	100	100
4	C	725/806 (90%)	688 (95%)	37 (5%)	0	100	100
4	D	714/806 (89%)	676 (95%)	37 (5%)	1 (0%)	48	83
4	E	713/806 (88%)	672 (94%)	40 (6%)	1 (0%)	48	83
4	F	739/806 (92%)	703 (95%)	36 (5%)	0	100	100
5	T	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
All	All	5759/6377 (90%)	5492 (95%)	260 (4%)	7 (0%)	49	83

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	199	PRO
4	D	340	HIS
2	G	544	LYS
3	H	253	ASP
1	K	64	GLU
2	G	327	TYR
4	E	201	VAL

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	I	47/68 (69%)	46 (98%)	1 (2%)	47	65
1	J	66/68 (97%)	65 (98%)	1 (2%)	57	72
1	K	66/68 (97%)	66 (100%)	0	100	100
1	L	68/68 (100%)	68 (100%)	0	100	100
1	M	68/68 (100%)	66 (97%)	2 (3%)	37	58
1	N	68/68 (100%)	67 (98%)	1 (2%)	57	72
2	G	479/531 (90%)	470 (98%)	9 (2%)	50	67
3	H	215/267 (80%)	213 (99%)	2 (1%)	70	79
4	A	643/679 (95%)	637 (99%)	6 (1%)	70	79
4	B	635/679 (94%)	628 (99%)	7 (1%)	65	76
4	C	612/679 (90%)	604 (99%)	8 (1%)	61	74
4	D	606/679 (89%)	601 (99%)	5 (1%)	73	80
4	E	616/679 (91%)	612 (99%)	4 (1%)	78	83
4	F	627/679 (92%)	622 (99%)	5 (1%)	73	80
5	T	153/153 (100%)	153 (100%)	0	100	100
All	All	4969/5433 (92%)	4918 (99%)	51 (1%)	65	78

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	44	ILE
2	G	159	VAL
2	G	163	SER
2	G	261	ASP
2	G	294	GLU
2	G	357	LEU
2	G	431	LYS
2	G	455	THR
2	G	496	THR
2	G	549	TRP
3	H	269	THR
3	H	270	PHE
1	I	2	GLN
4	E	35	ASP
4	E	84	MET
4	E	323	ARG
4	E	573	VAL
4	B	120	ASP
4	B	309	ILE
4	B	317	HIS
4	B	340	HIS
4	B	550	MET
4	B	555	SER
4	B	695	CYS
4	A	131	PHE
4	A	167	GLU
4	A	219	MET
4	A	268	LEU
4	A	555	SER
4	A	580	ASP
4	F	38	VAL
4	F	84	MET
4	F	272	PRO
4	F	403	THR
4	F	635	ARG
1	M	18	GLU
1	M	58	ASP
4	C	60	LYS
4	C	183	HIS
4	C	307	ASP
4	C	313	ARG
4	C	362	ARG
4	C	365	ARG

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Mol	Chain	Res	Type
4	C	453	ARG
4	C	491	GLU
4	D	222	LEU
4	D	281	GLU
4	D	291	GLU
4	D	317	HIS
4	D	325	VAL
1	N	8	LEU

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

Mol	Chain	Res	Type
1	J	25	ASN
1	K	40	GLN
2	G	132	HIS
2	G	153	ASN
2	G	197	HIS
2	G	247	GLN
2	G	378	ASN
2	G	469	ASN
2	G	494	GLN
3	H	22	GLN
3	H	100	GLN
3	H	163	ASN
1	I	41	GLN
4	E	270	ASN
4	E	317	HIS
4	E	404	HIS
4	E	406	HIS
4	E	660	ASN
4	B	183	HIS
4	B	215	GLN
4	B	270	ASN
4	B	404	HIS
4	B	536	GLN
4	B	578	GLN
4	A	36	ASN
4	A	260	ASN
4	A	270	ASN
4	A	404	HIS
4	A	760	GLN
4	A	763	GLN

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Mol	Chain	Res	Type
4	A	764	GLN
4	F	270	ASN
4	F	624	ASN
4	F	641	GLN
1	M	40	GLN
1	M	49	GLN
1	M	68	HIS
5	T	541	GLN
5	T	569	ASN
4	C	260	ASN
4	C	494	GLN
4	C	558	ASN
4	C	602	ASN
4	C	603	GLN
4	C	735	HIS
4	D	36	ASN
4	D	692	GLN
1	N	2	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

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	$\#\|Z\| > 2$
7	BEF	E	902	6	0,3,3	-	-	-		
7	BEF	B	906	-	0,3,3	-	-	-		
6	ADP	F	902	8	27,29,29	1.04	0	42,45,45	1.27	6 (14%)
6	ADP	A	903	-	27,29,29	1.03	1 (3%)	42,45,45	1.34	7 (16%)
7	BEF	B	903	-	0,3,3	-	-	-		
7	BEF	C	905	-	0,3,3	-	-	-		
6	ADP	B	902	8	27,29,29	1.05	1 (3%)	42,45,45	1.45	7 (16%)
6	ADP	A	906	8	27,29,29	1.01	1 (3%)	42,45,45	1.28	6 (14%)
6	ADP	F	904	8	27,29,29	1.10	1 (3%)	42,45,45	1.41	7 (16%)
6	ADP	D	902	-	27,29,29	0.97	0	42,45,45	1.20	5 (11%)
6	ADP	D	901	-	27,29,29	0.95	0	42,45,45	1.37	8 (19%)
7	BEF	F	901	-	0,3,3	-	-	-		
7	BEF	C	902	-	0,3,3	-	-	-		
7	BEF	A	901	-	0,3,3	-	-	-		
6	ADP	C	904	8	27,29,29	1.03	1 (3%)	42,45,45	1.39	7 (16%)
6	ADP	C	901	8	27,29,29	1.03	1 (3%)	42,45,45	1.62	8 (19%)
7	BEF	A	902	-	0,3,3	-	-	-		
6	ADP	E	901	8,7	27,29,29	1.05	2 (7%)	42,45,45	1.45	8 (19%)
6	ADP	B	905	-	27,29,29	1.04	1 (3%)	42,45,45	1.30	5 (11%)
7	BEF	B	901	-	0,3,3	-	-	-		
6	ADP	E	904	8	27,29,29	1.02	1 (3%)	42,45,45	1.27	5 (11%)
7	BEF	A	904	-	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	D	902	-	-	3/16/32/32	0/3/3/3
6	ADP	A	906	8	-	2/16/32/32	0/3/3/3
6	ADP	C	904	8	-	6/16/32/32	0/3/3/3
6	ADP	D	901	-	-	0/16/32/32	0/3/3/3
6	ADP	C	901	8	-	3/16/32/32	0/3/3/3
6	ADP	F	902	8	-	4/16/32/32	0/3/3/3
6	ADP	E	901	8,7	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	B	902	8	-	3/16/32/32	0/3/3/3
6	ADP	B	905	-	-	3/16/32/32	0/3/3/3
6	ADP	E	904	8	-	0/16/32/32	0/3/3/3
6	ADP	A	903	-	-	4/16/32/32	0/3/3/3
6	ADP	F	904	8	-	6/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	904	ADP	C5-C4	-2.44	1.34	1.39
6	A	903	ADP	C5-C4	-2.37	1.34	1.39
6	E	901	ADP	C5-C4	-2.36	1.34	1.39
6	E	904	ADP	C5-C4	-2.35	1.34	1.39
6	B	905	ADP	C5-C4	-2.35	1.34	1.39
6	A	906	ADP	C5-C4	-2.25	1.34	1.39
6	B	902	ADP	C5-C4	-2.11	1.35	1.39
6	C	904	ADP	C5-C4	-2.07	1.35	1.39
6	C	901	ADP	C5-C4	-2.04	1.35	1.39
6	E	901	ADP	PB-O2B	-2.01	1.47	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	901	ADP	O3B-PB-O3A	5.12	121.81	104.64
6	F	904	ADP	O2B-PB-O3A	3.82	117.44	104.64
6	B	902	ADP	O3B-PB-O3A	3.75	117.23	104.64
6	F	904	ADP	PA-O3A-PB	-3.73	120.04	132.83
6	E	904	ADP	PA-O3A-PB	-3.69	120.16	132.83
6	D	901	ADP	PA-O3A-PB	-3.60	120.48	132.83
6	A	903	ADP	O2B-PB-O3A	3.56	116.57	104.64
6	E	901	ADP	PA-O3A-PB	-3.52	120.75	132.83
6	A	906	ADP	PA-O3A-PB	-3.47	120.92	132.83
6	C	901	ADP	O2B-PB-O3A	3.47	116.26	104.64
6	E	901	ADP	O2B-PB-O3A	3.42	116.09	104.64
6	F	902	ADP	PA-O3A-PB	-3.27	121.59	132.83
6	C	901	ADP	C5-C4-N3	-3.19	122.59	126.75
6	B	902	ADP	PA-O3A-PB	-3.06	122.32	132.83
6	E	901	ADP	C4-C5-N7	3.04	114.32	110.62
6	C	904	ADP	O3B-PB-O3A	3.00	114.68	104.64
6	F	902	ADP	C4-C5-N7	2.99	114.26	110.62
6	D	901	ADP	C4-C5-N7	2.95	114.21	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	904	ADP	C4-C5-N7	2.95	114.21	110.62
6	B	902	ADP	C5-C4-N3	-2.93	122.93	126.75
6	F	904	ADP	C4-C5-N7	2.89	114.14	110.62
6	F	904	ADP	C5-C4-N3	-2.88	122.99	126.75
6	A	903	ADP	C5-C4-N3	-2.88	122.99	126.75
6	D	902	ADP	PA-O3A-PB	-2.85	123.06	132.83
6	D	902	ADP	C4-C5-N7	2.83	114.06	110.62
6	A	906	ADP	C4-C5-N7	2.82	114.06	110.62
6	D	901	ADP	C5-C4-N3	-2.81	123.08	126.75
6	C	901	ADP	PA-O3A-PB	-2.80	123.22	132.83
6	B	905	ADP	C5-C4-N3	-2.79	123.11	126.75
6	D	902	ADP	C5-C4-N3	-2.79	123.12	126.75
6	A	906	ADP	C5-C4-N3	-2.78	123.13	126.75
6	E	901	ADP	C5-C4-N3	-2.77	123.14	126.75
6	E	904	ADP	C4-C5-N7	2.76	113.98	110.62
6	A	903	ADP	C4-C5-N7	2.75	113.96	110.62
6	C	904	ADP	PA-O3A-PB	-2.74	123.43	132.83
6	C	904	ADP	C5-C4-N3	-2.74	123.18	126.75
6	B	902	ADP	C4-C5-N7	2.69	113.89	110.62
6	B	905	ADP	C4-C5-N7	2.59	113.77	110.62
6	B	905	ADP	PA-O3A-PB	-2.59	123.94	132.83
6	C	901	ADP	C4-C5-N7	2.58	113.76	110.62
6	E	904	ADP	O2B-PB-O3A	2.57	113.24	104.64
6	F	902	ADP	C5-C4-N3	-2.56	123.42	126.75
6	A	903	ADP	PA-O3A-PB	-2.54	124.09	132.83
6	C	904	ADP	O4'-C1'-C2'	-2.53	101.13	106.64
6	E	901	ADP	O3B-PB-O2B	-2.49	98.11	107.64
6	D	902	ADP	C5-C6-N1	2.48	122.72	117.39
6	A	906	ADP	C5-C6-N1	2.48	122.72	117.39
6	E	901	ADP	C5-C6-N1	2.48	122.72	117.39
6	D	901	ADP	C5-C6-N1	2.47	122.70	117.39
6	B	905	ADP	O2B-PB-O3A	2.47	112.92	104.64
6	A	903	ADP	C5-C6-N1	2.46	122.67	117.39
6	D	901	ADP	O3B-PB-O3A	2.45	112.87	104.64
6	B	905	ADP	C5-C6-N1	2.44	122.62	117.39
6	C	901	ADP	C5-C6-N1	2.40	122.54	117.39
6	B	902	ADP	C5-C6-N1	2.40	122.54	117.39
6	F	904	ADP	C5-C6-N1	2.38	122.50	117.39
6	E	904	ADP	C5-C6-N1	2.34	122.42	117.39
6	C	901	ADP	N3-C4-N9	2.34	130.94	127.08
6	F	904	ADP	O3B-PB-O1B	-2.33	101.54	110.68
6	F	902	ADP	C5-C6-N1	2.33	122.39	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	904	ADP	C5-C6-N1	2.30	122.33	117.39
6	E	904	ADP	C5-C4-N3	-2.28	123.78	126.75
6	F	902	ADP	O3B-PB-O2B	-2.28	98.94	107.64
6	E	901	ADP	C2-N1-C6	-2.28	114.86	118.77
6	D	901	ADP	N3-C4-N9	2.27	130.82	127.08
6	B	902	ADP	O2B-PB-O3A	2.22	112.09	104.64
6	D	901	ADP	O2B-PB-O3A	2.17	111.92	104.64
6	D	901	ADP	C2-N1-C6	-2.17	115.05	118.77
6	F	902	ADP	N6-C6-N1	-2.15	113.64	118.35
6	C	901	ADP	C2-N1-C6	-2.14	115.09	118.77
6	A	906	ADP	C2-N1-C6	-2.12	115.12	118.77
6	E	901	ADP	N3-C4-N9	2.10	130.55	127.08
6	F	904	ADP	N3-C4-N9	2.10	130.54	127.08
6	A	903	ADP	C2-N1-C6	-2.09	115.17	118.77
6	B	902	ADP	C2-N1-C6	-2.08	115.19	118.77
6	A	906	ADP	N3-C4-N9	2.07	130.49	127.08
6	C	904	ADP	N3-C4-N9	2.04	130.44	127.08
6	A	903	ADP	N3-C4-N9	2.01	130.40	127.08
6	D	902	ADP	N3-C4-N9	2.00	130.39	127.08

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	905	ADP	C5'-O5'-PA-O3A
6	F	904	ADP	PA-O3A-PB-O2B
6	F	904	ADP	O4'-C4'-C5'-O5'
6	C	904	ADP	C5'-O5'-PA-O1A
6	C	904	ADP	C5'-O5'-PA-O2A
6	C	904	ADP	C4'-C5'-O5'-PA
6	B	902	ADP	C3'-C4'-C5'-O5'
6	F	904	ADP	C3'-C4'-C5'-O5'
6	B	902	ADP	O4'-C4'-C5'-O5'
6	A	903	ADP	O4'-C4'-C5'-O5'
6	A	903	ADP	C3'-C4'-C5'-O5'
6	D	902	ADP	C3'-C4'-C5'-O5'
6	E	901	ADP	O4'-C4'-C5'-O5'
6	C	901	ADP	O4'-C4'-C5'-O5'
6	D	902	ADP	O4'-C4'-C5'-O5'
6	E	901	ADP	C3'-C4'-C5'-O5'
6	F	904	ADP	PA-O3A-PB-O1B
6	F	902	ADP	C4'-C5'-O5'-PA

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

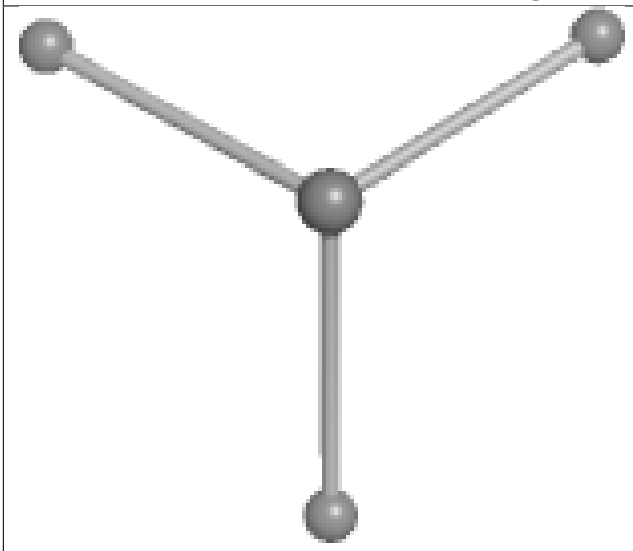
There are no ring outliers.

3 monomers are involved in 4 short contacts:

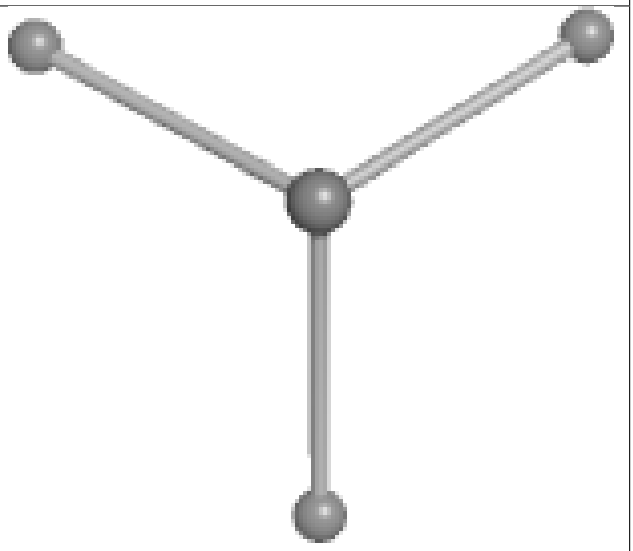
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	902	ADP	1	0
6	D	901	ADP	2	0
6	C	904	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

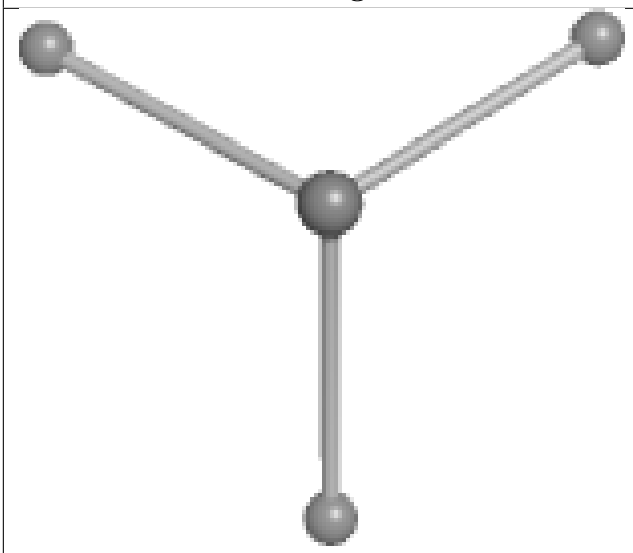
Ligand BEF E 902



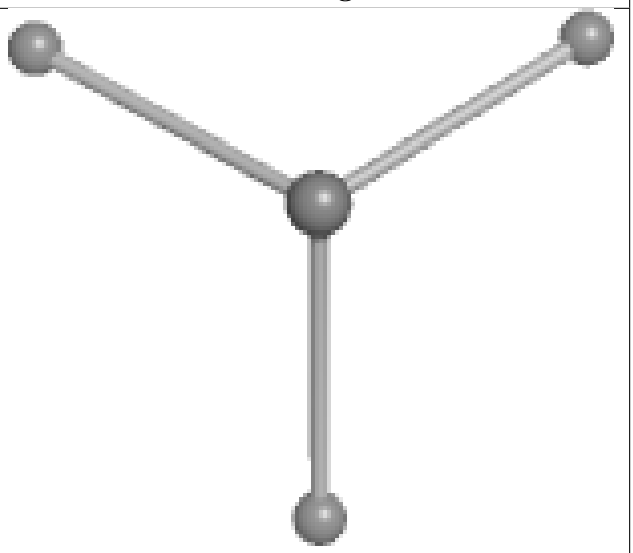
Bond lengths



Bond angles

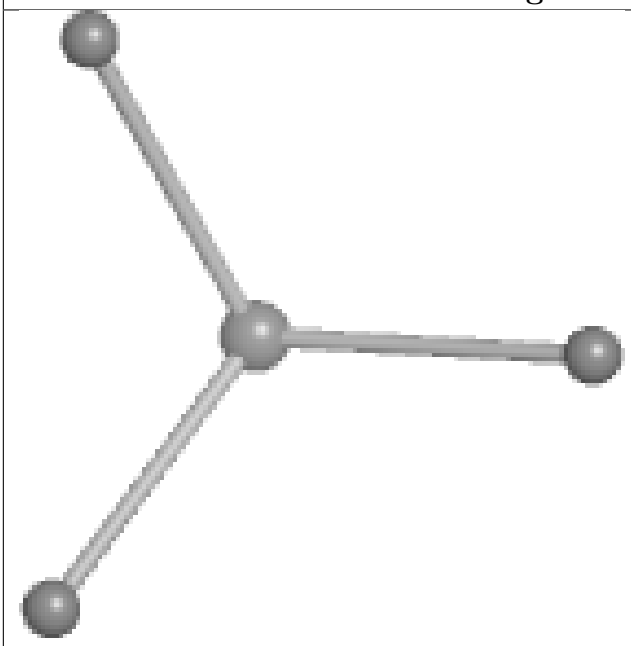


Torsions

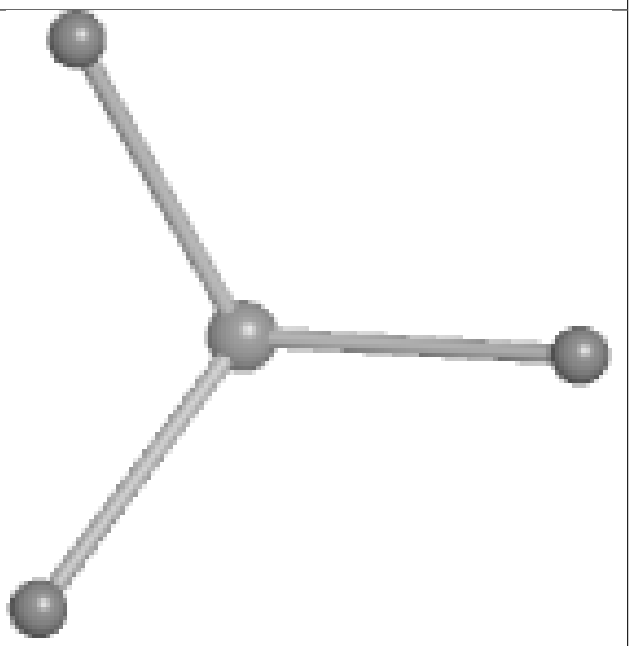


Rings

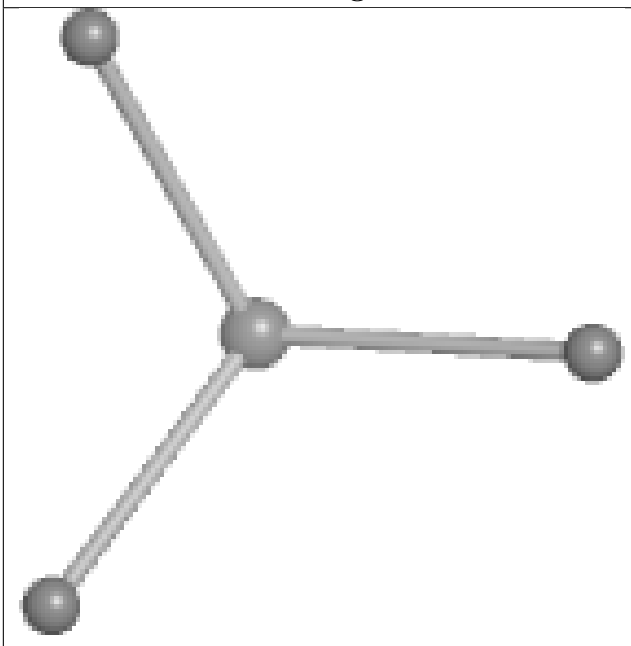
Ligand BEF B 906



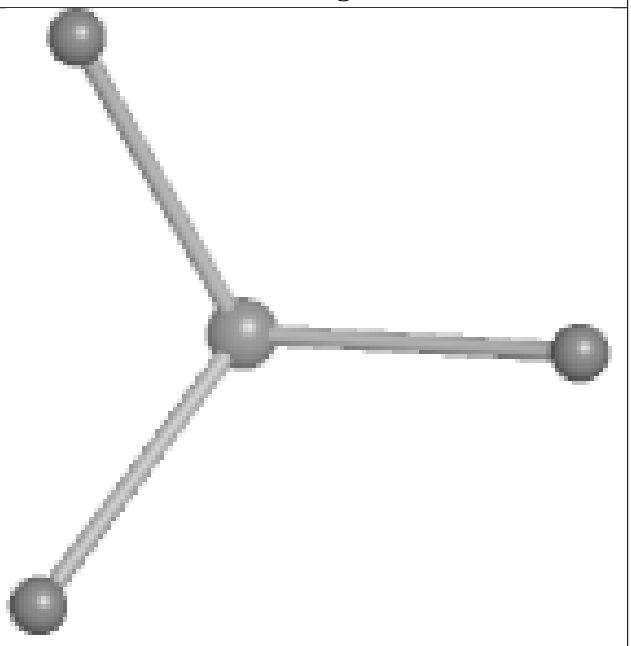
Bond lengths



Bond angles

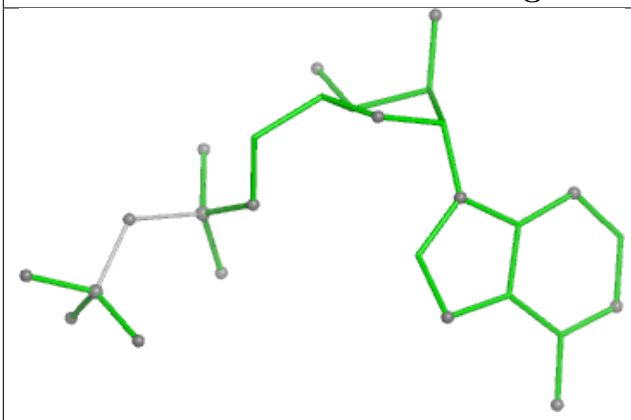


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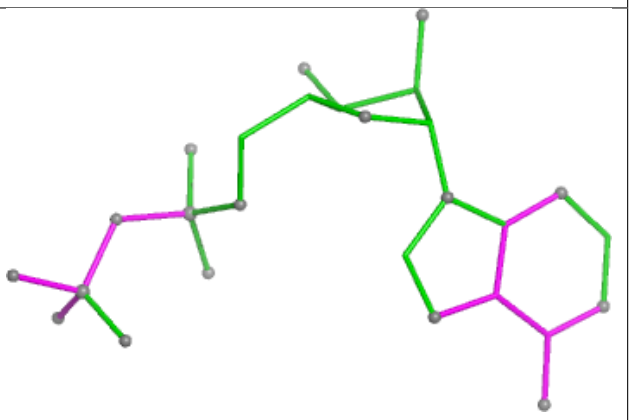


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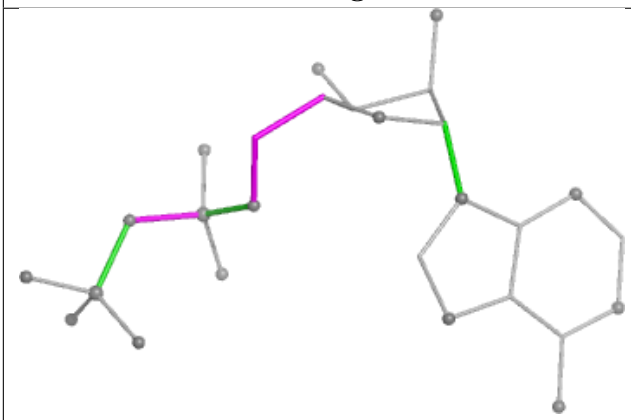
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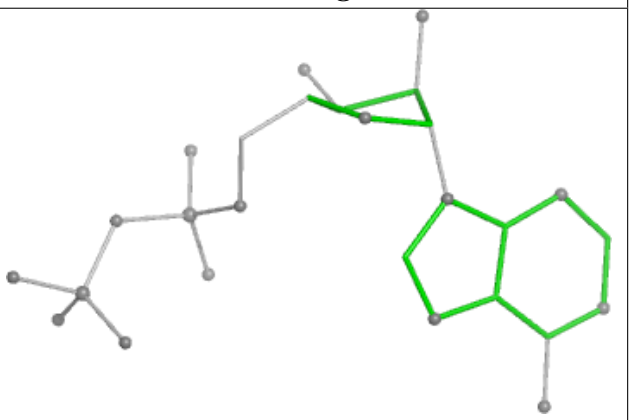
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Bond angles

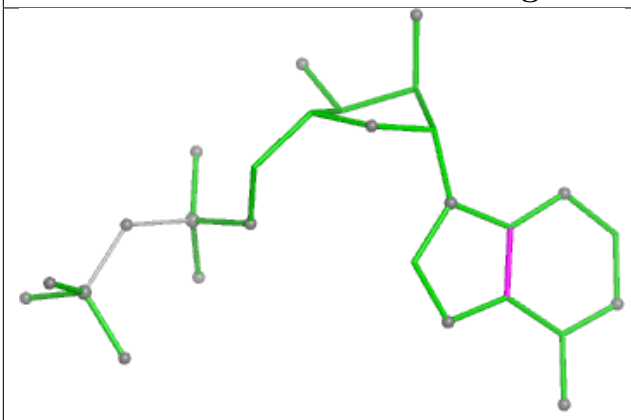


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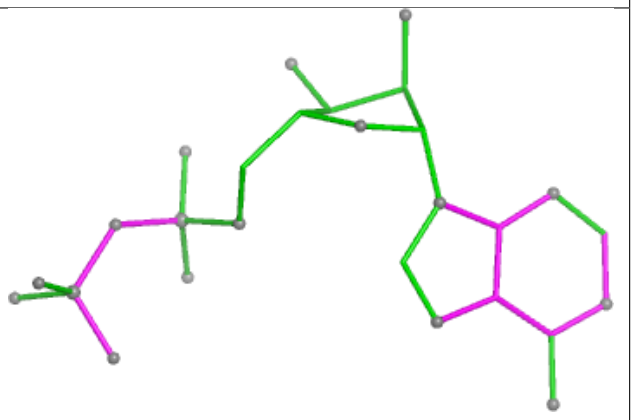


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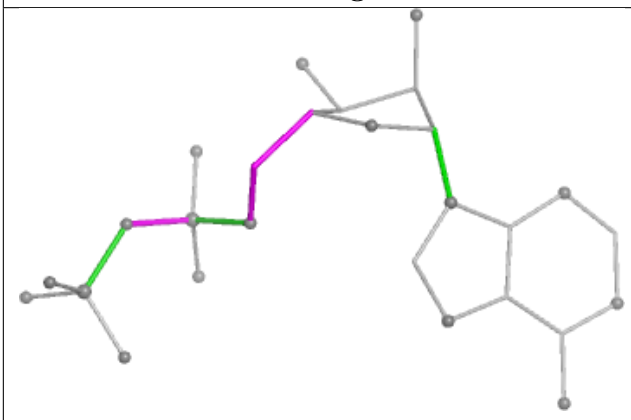
Ligand ADP A 903



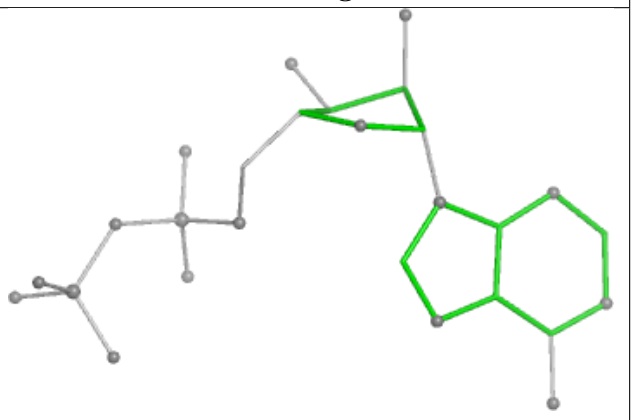
Bond lengths



Bond angles

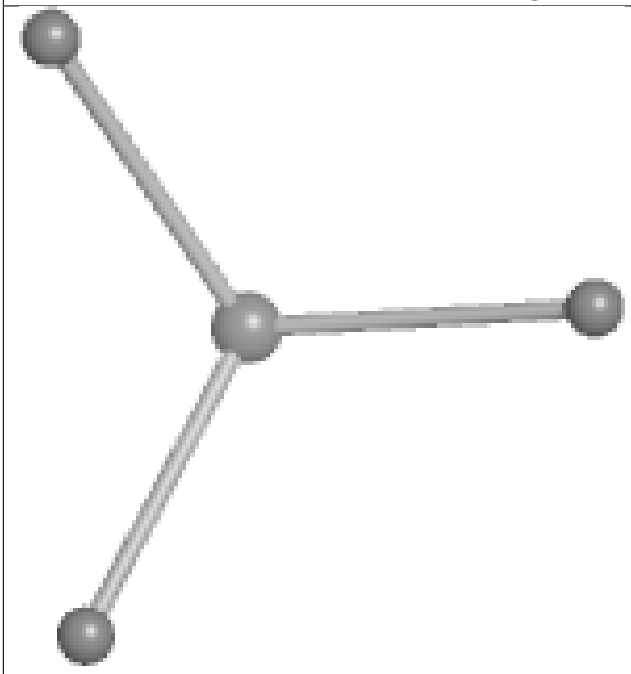


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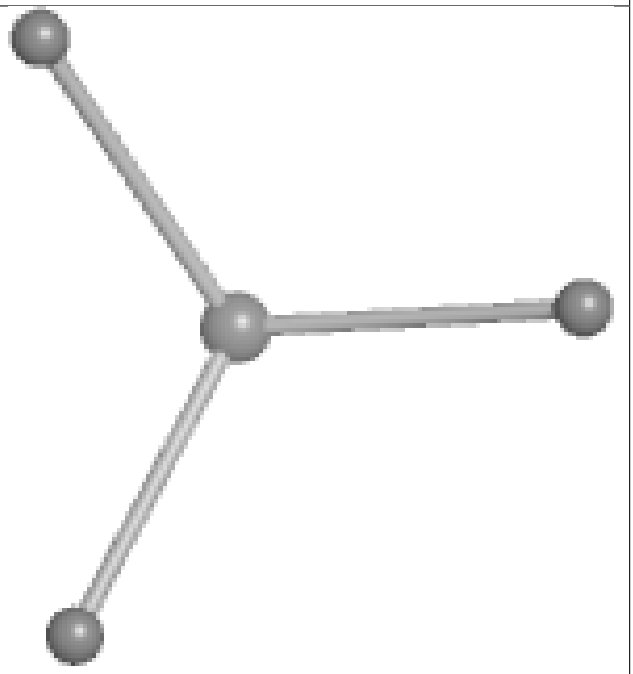


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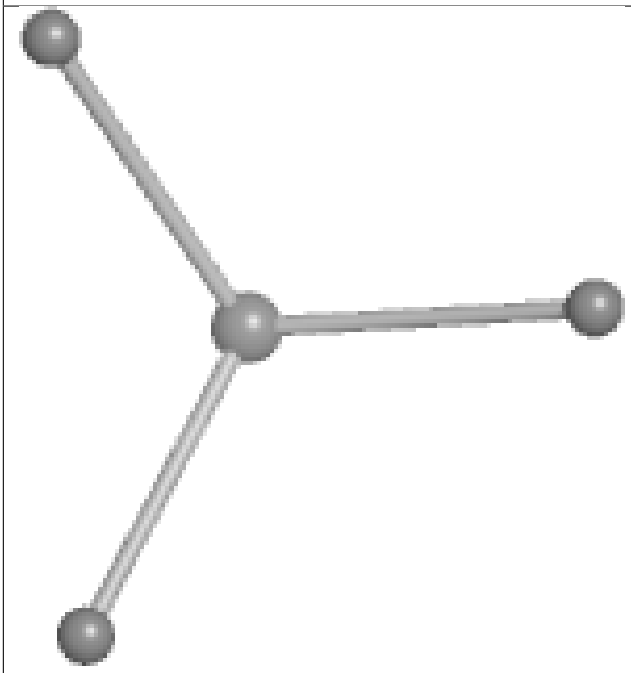
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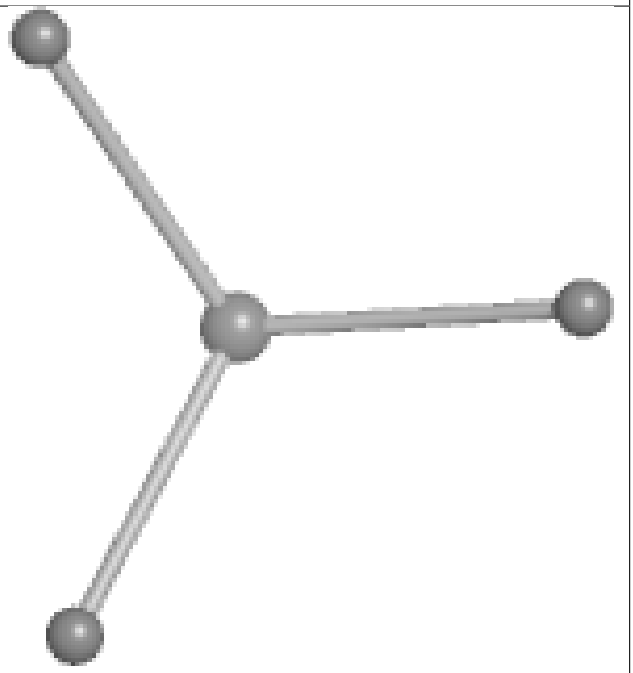
Bond lengths



Bond angles

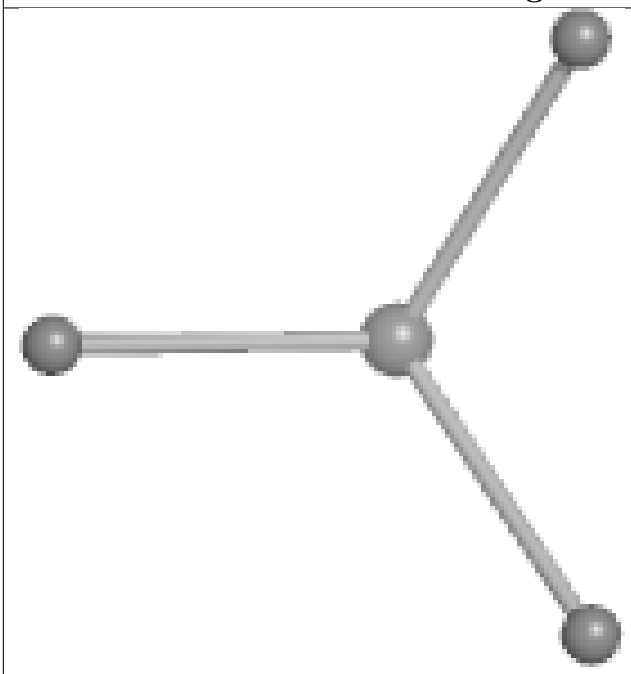


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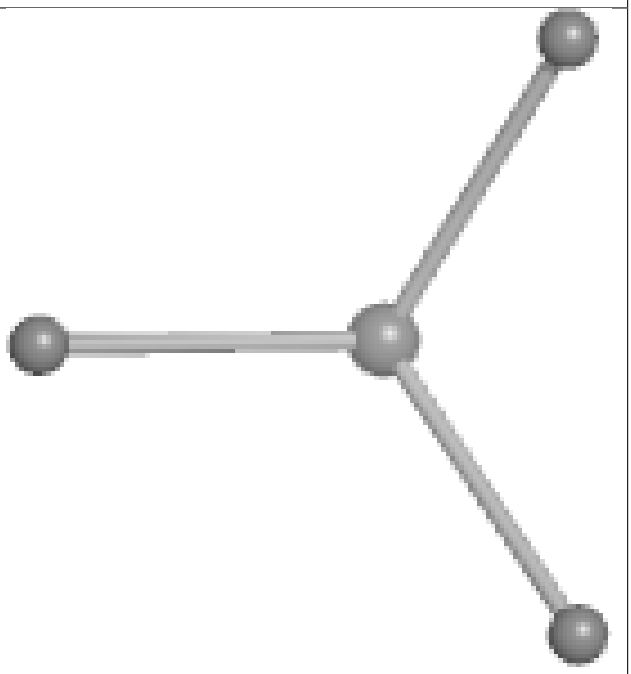


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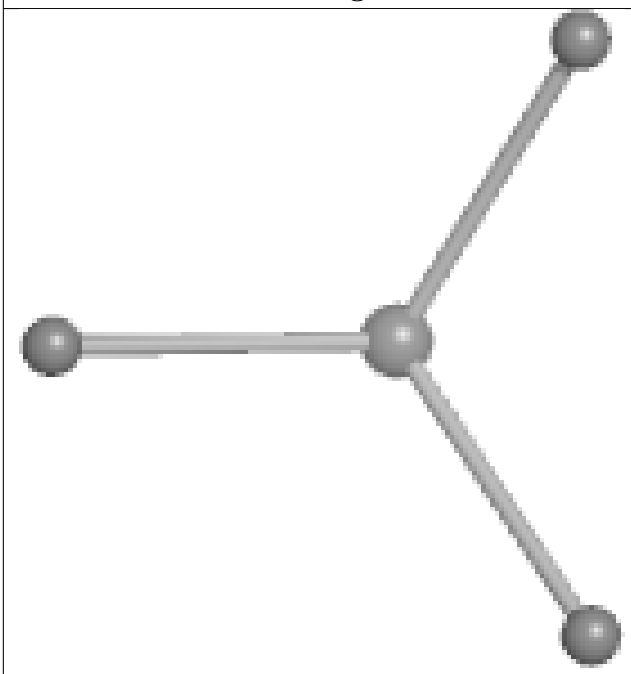
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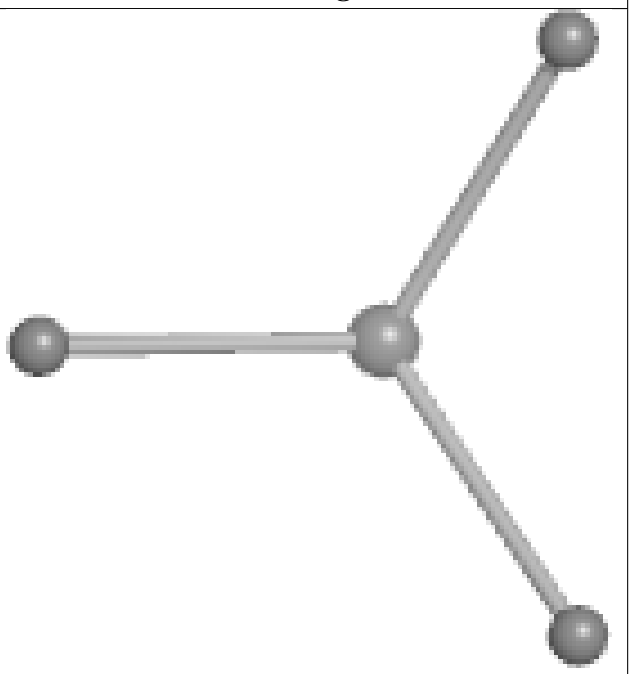
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Bond angles

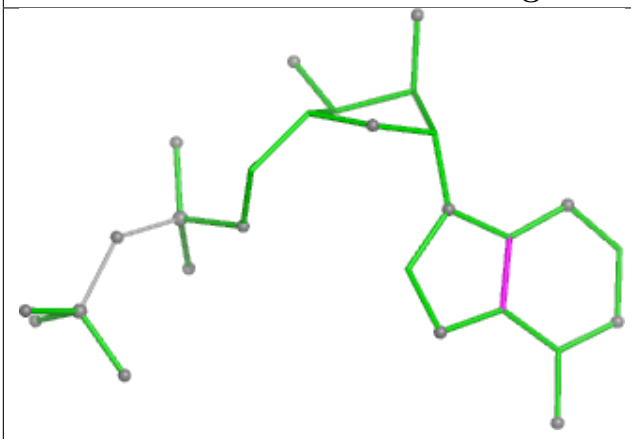


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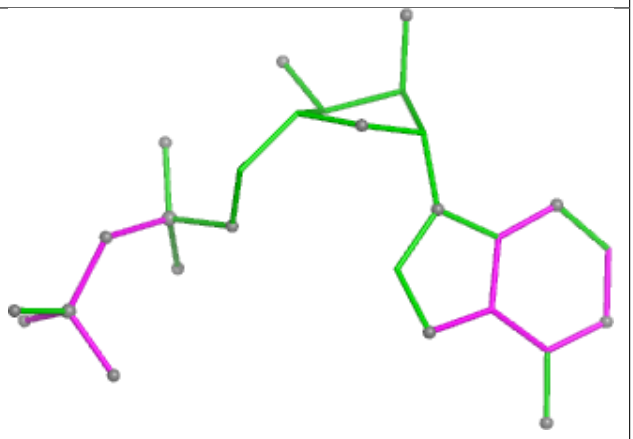


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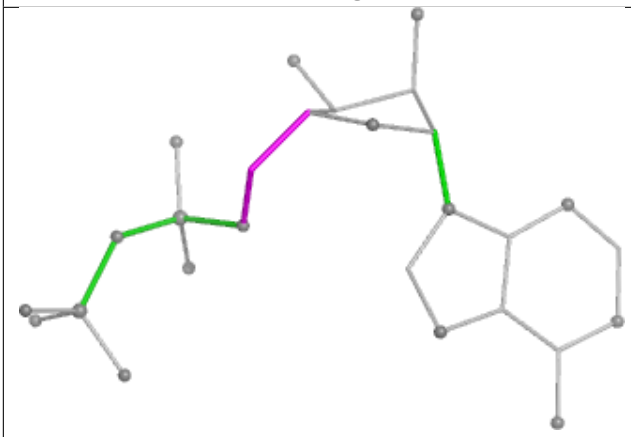
Ligand ADP B 902



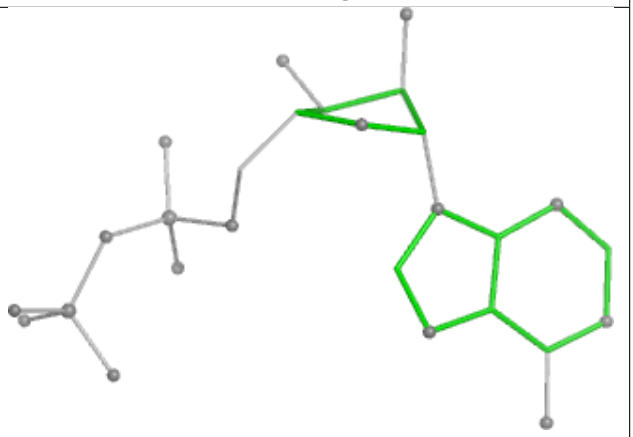
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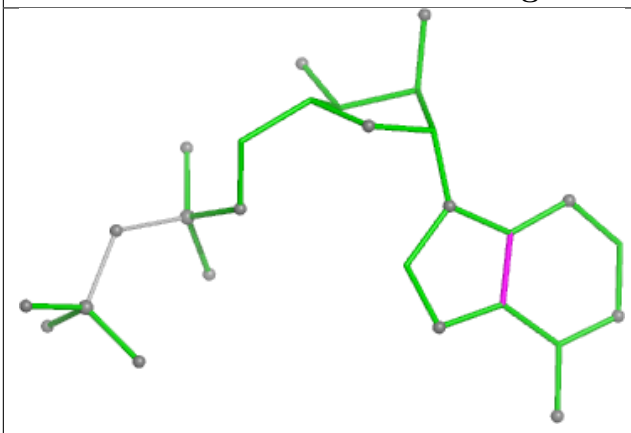


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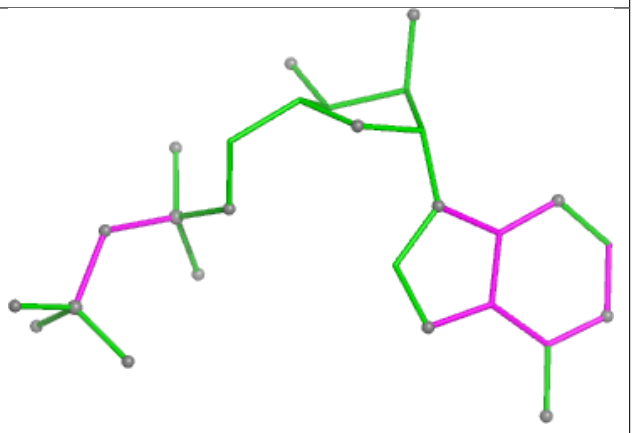


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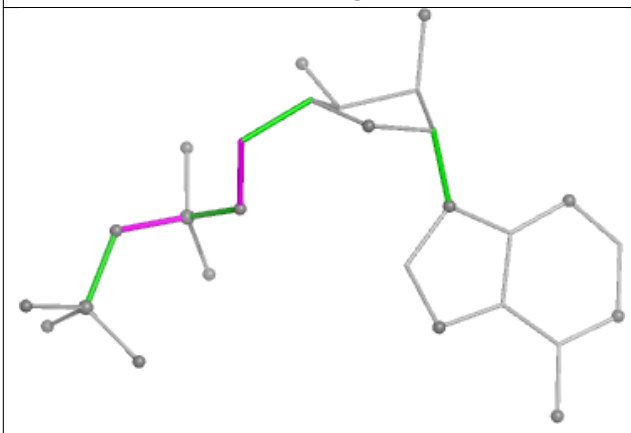
Ligand ADP A 906



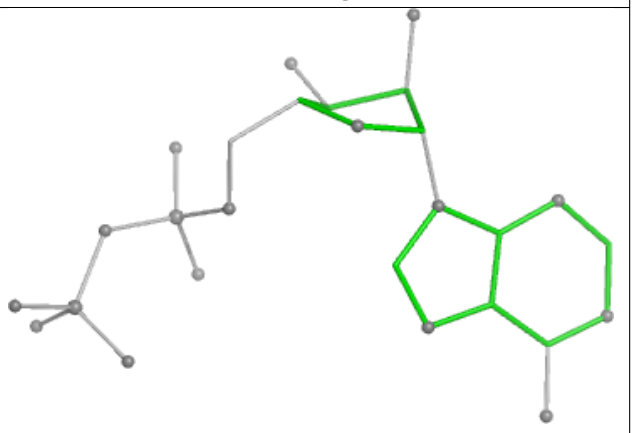
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Bond angles

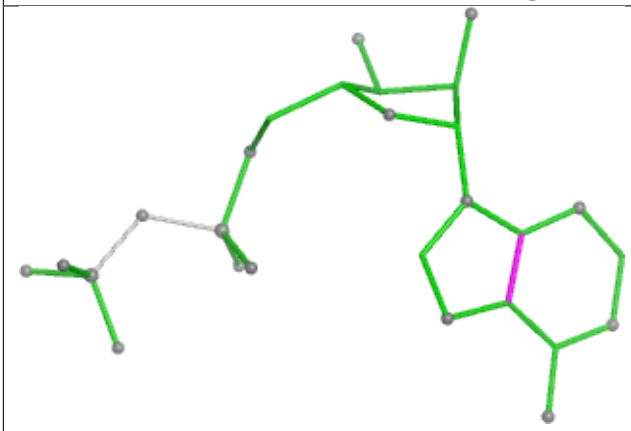


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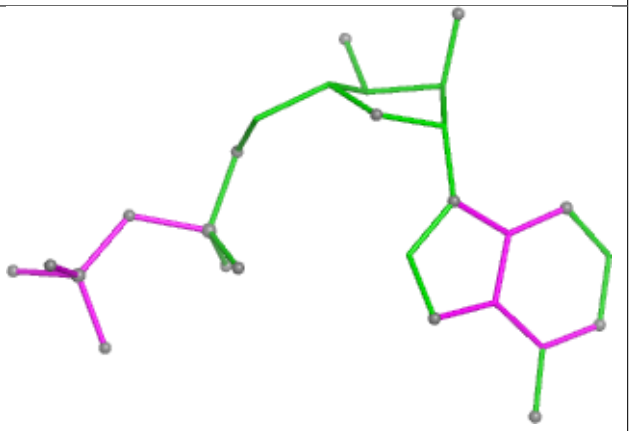


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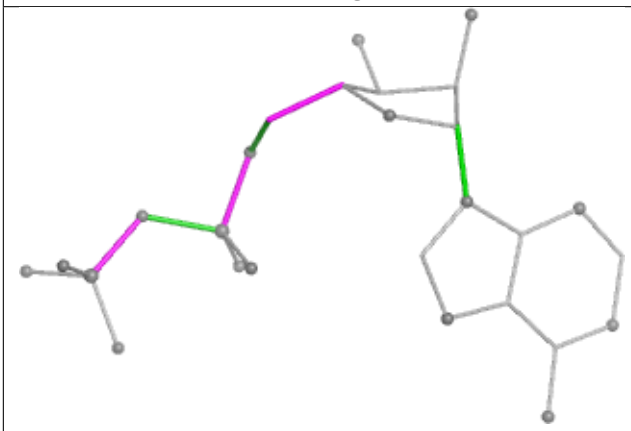
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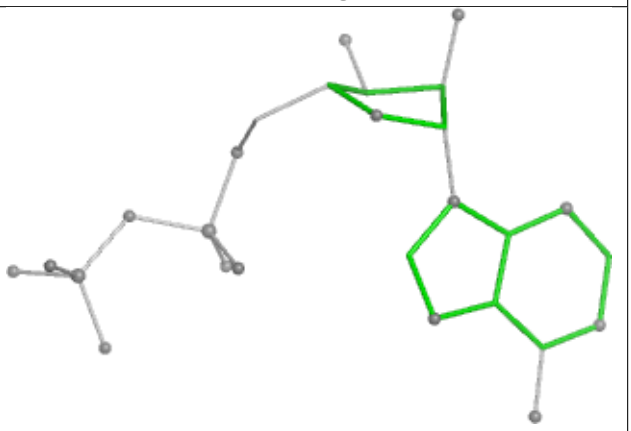
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Bond angles

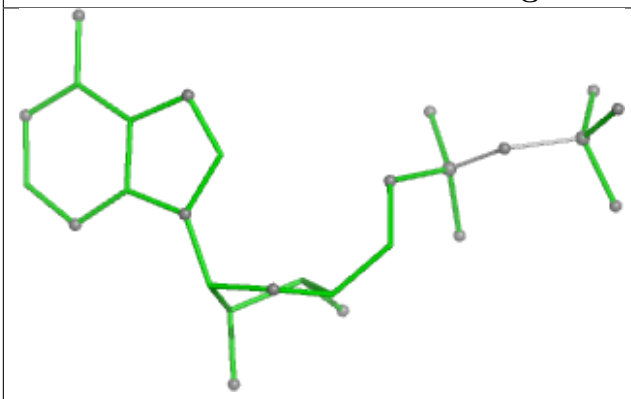


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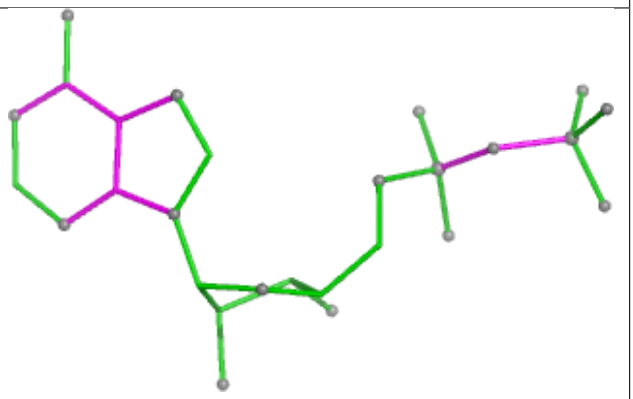


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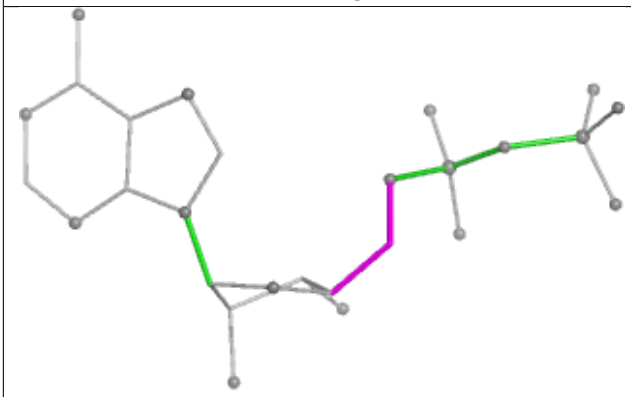
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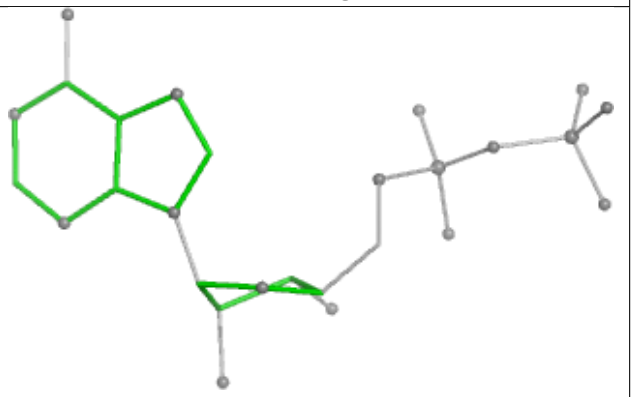
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Bond angles

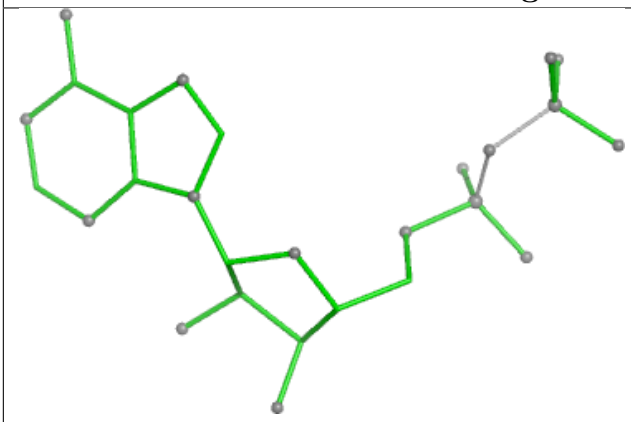


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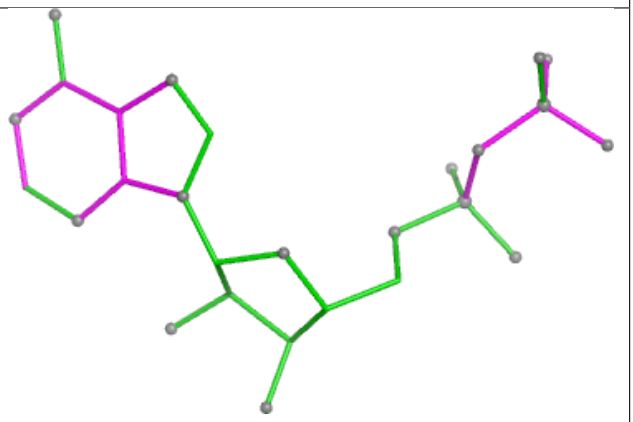


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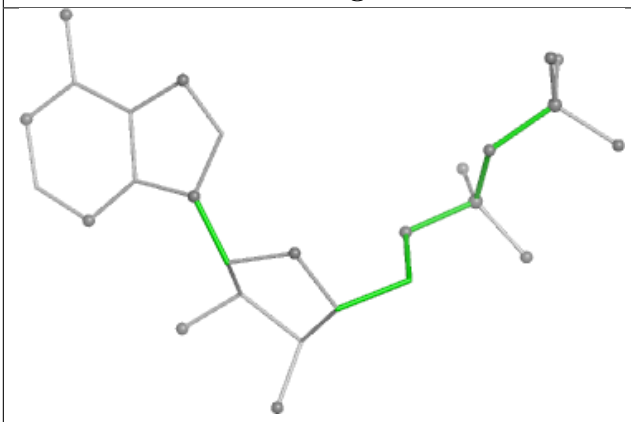
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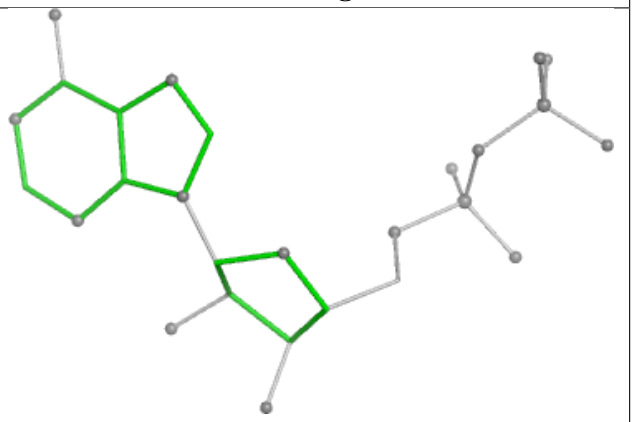
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Bond angles

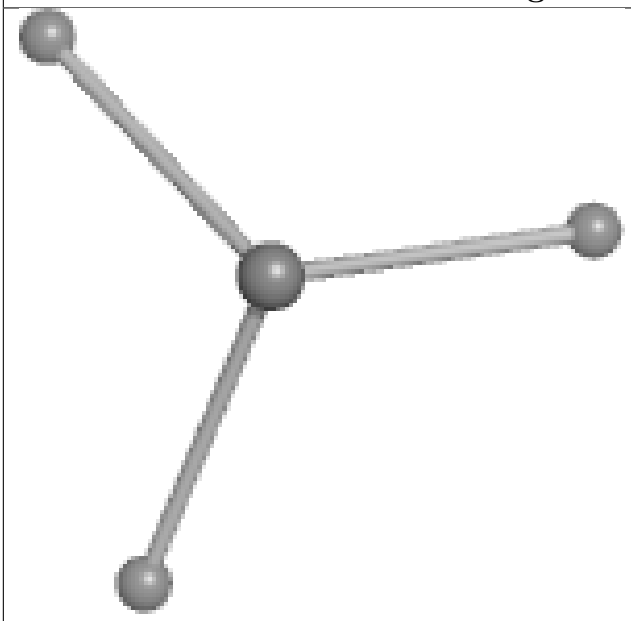


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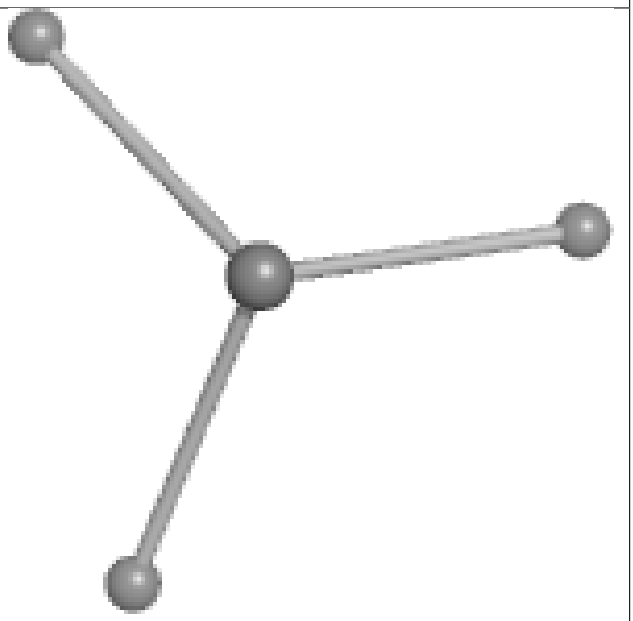


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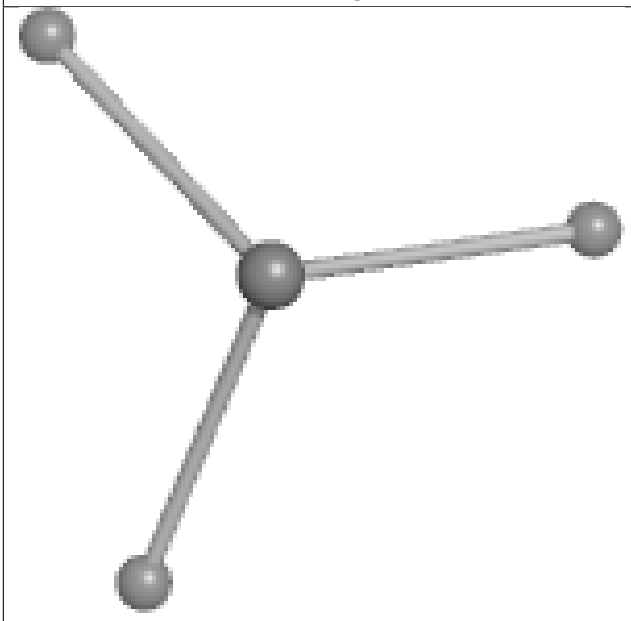
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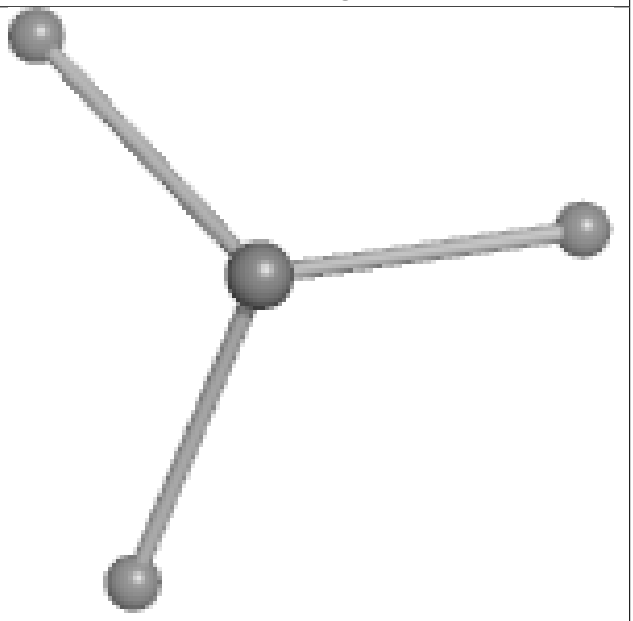
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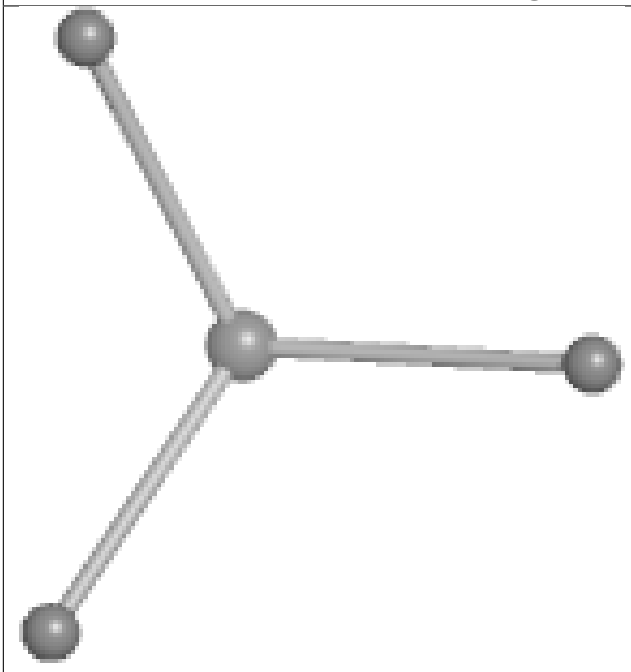


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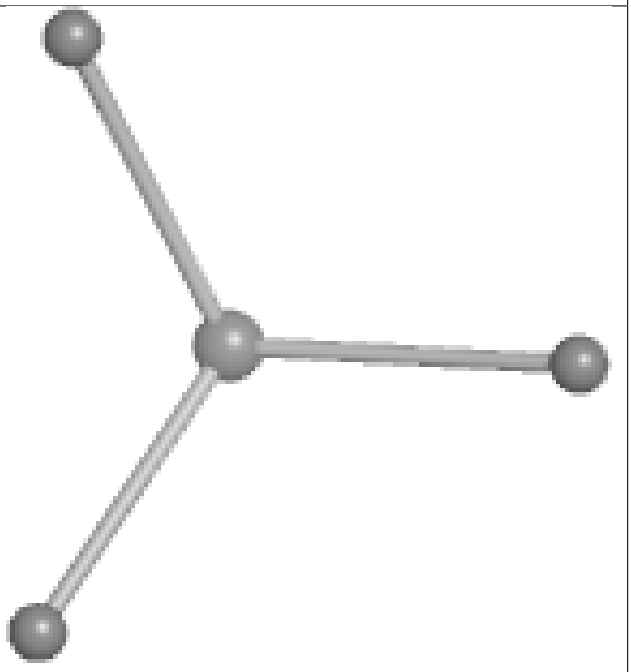


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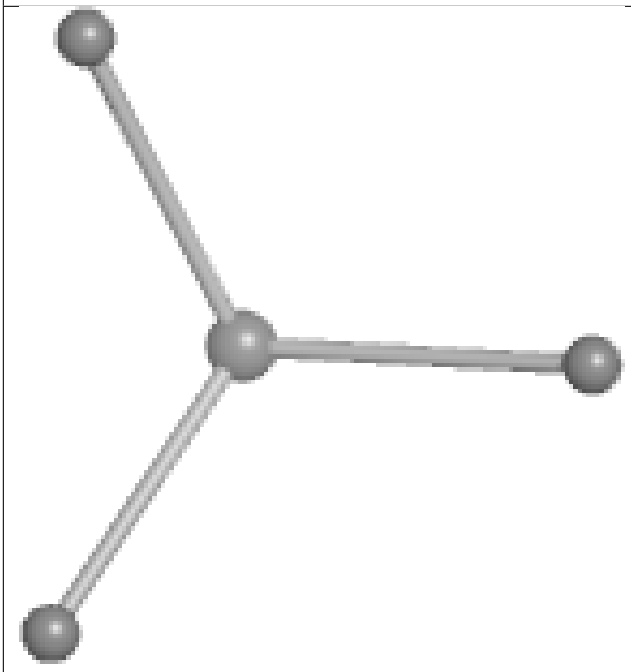
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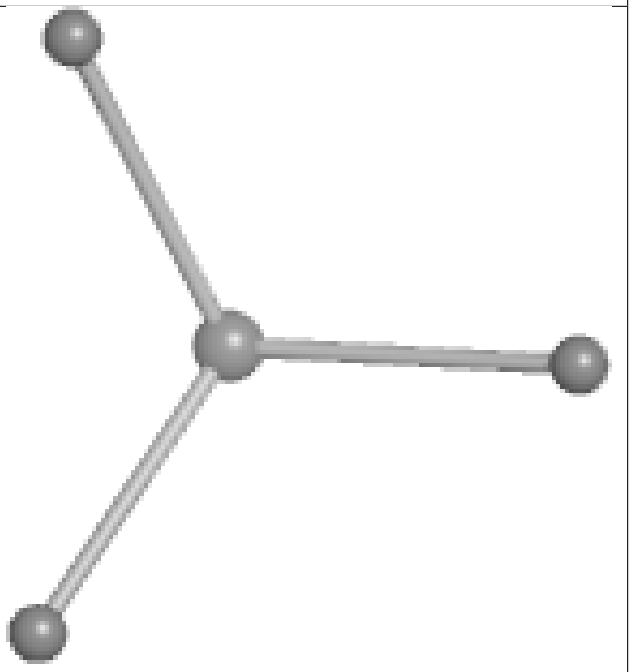
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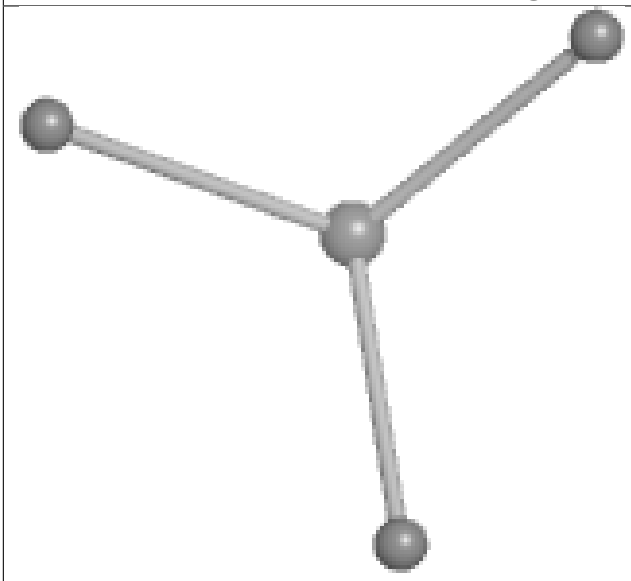


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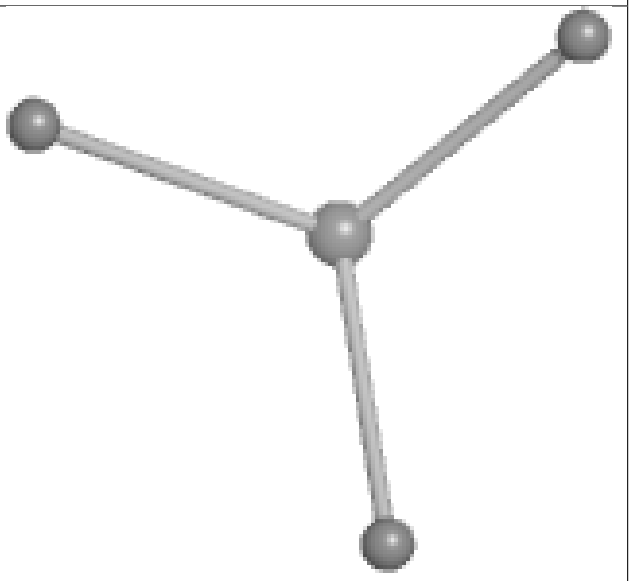


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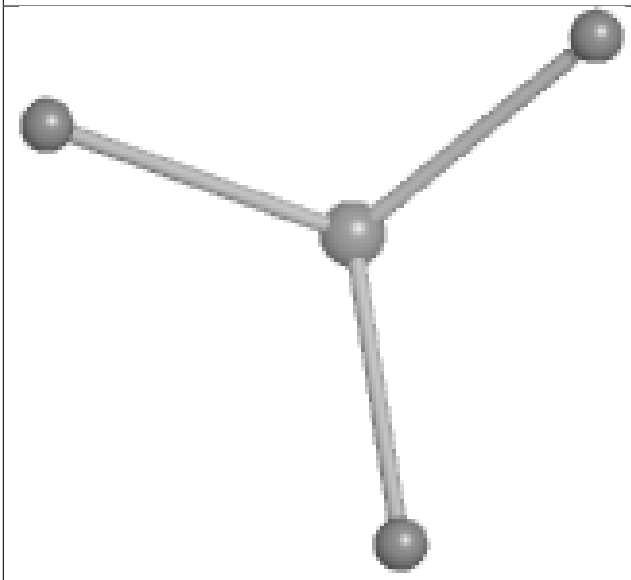
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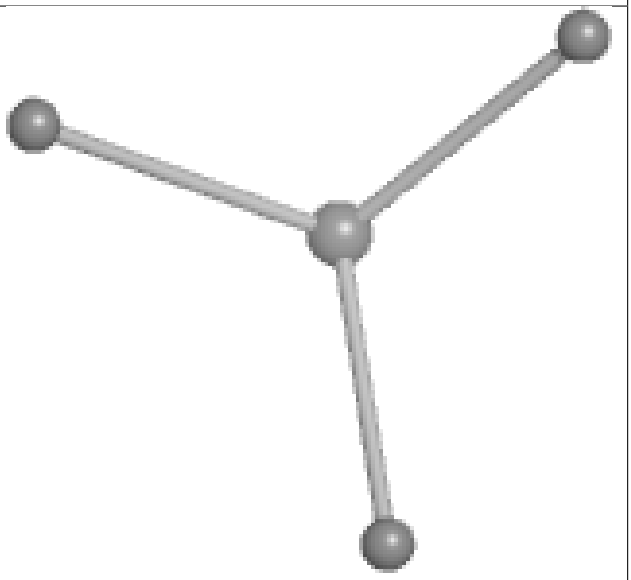
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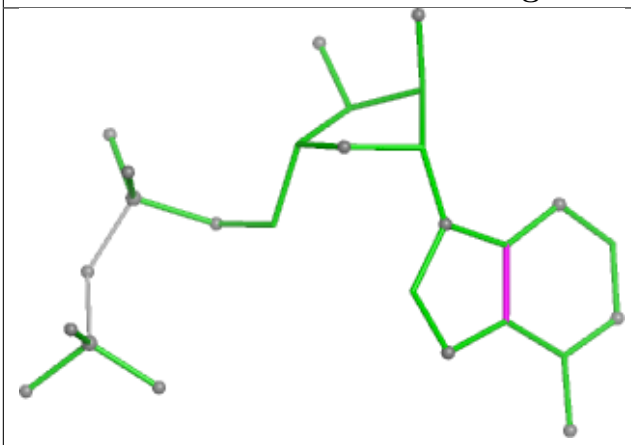


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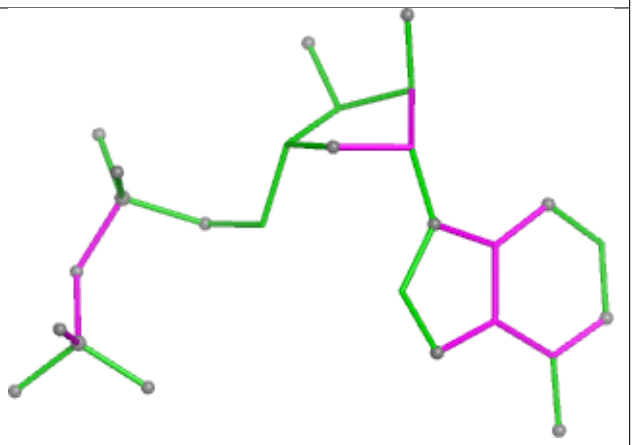


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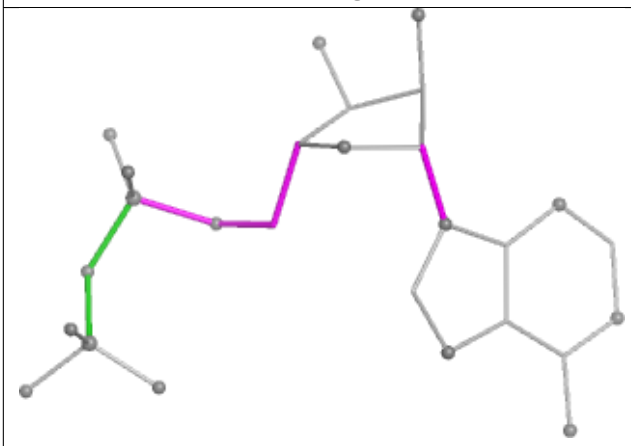
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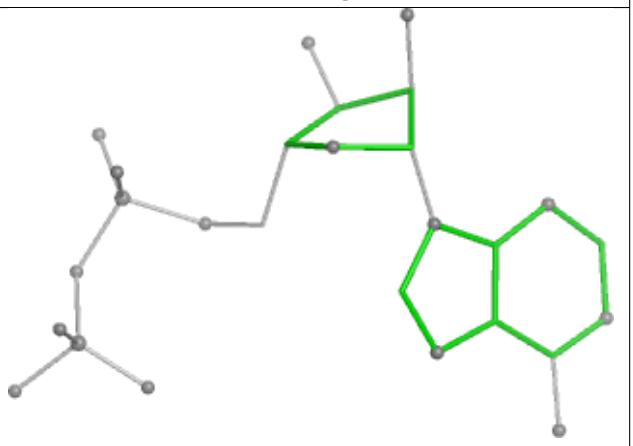
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Bond angles

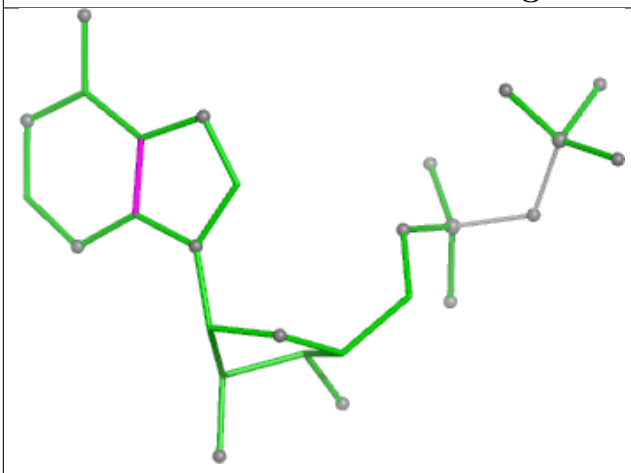


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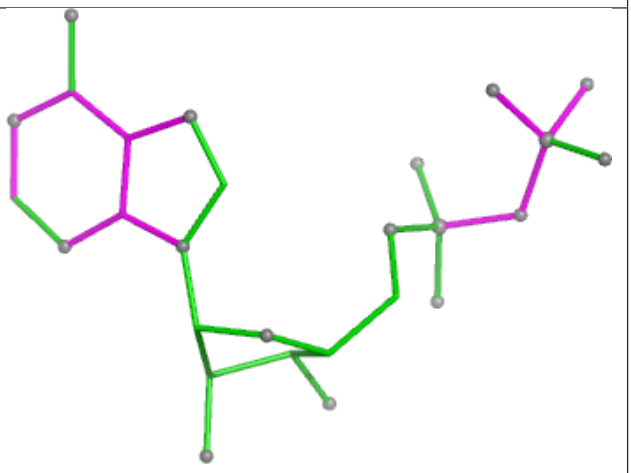


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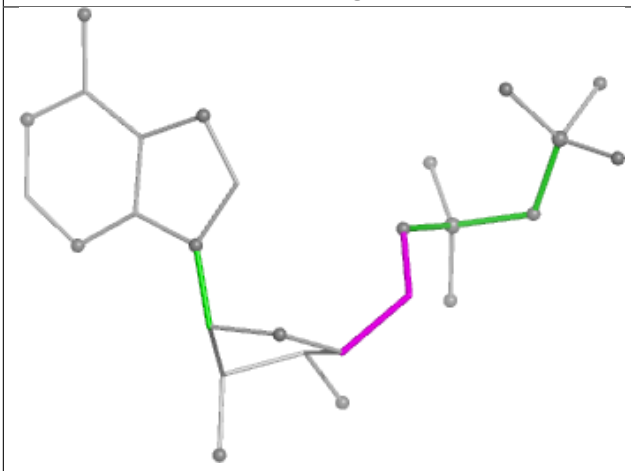
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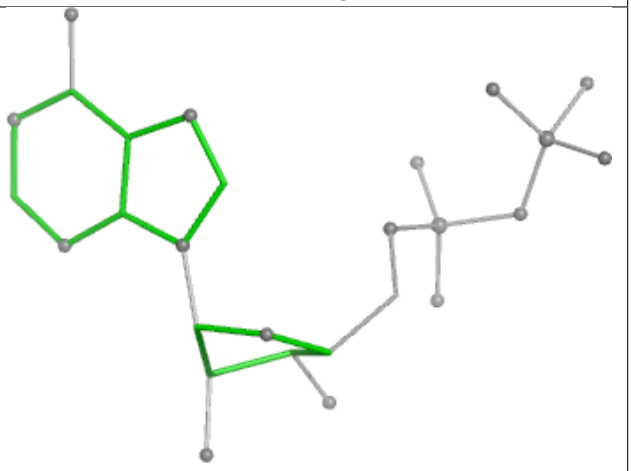
Bond lengths



Bond angles

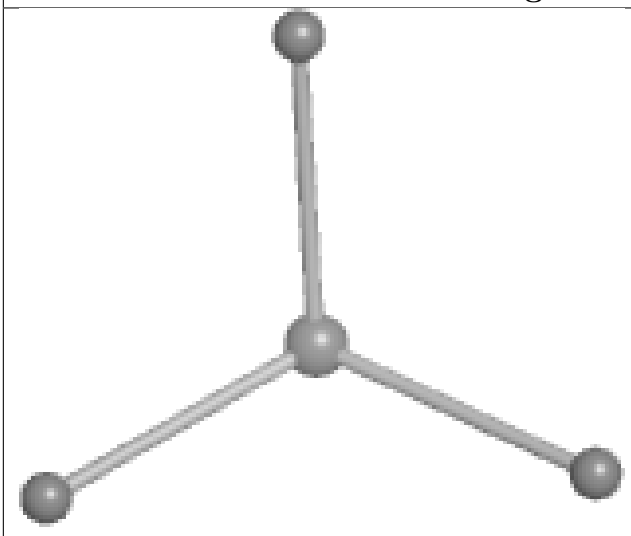


Torsions

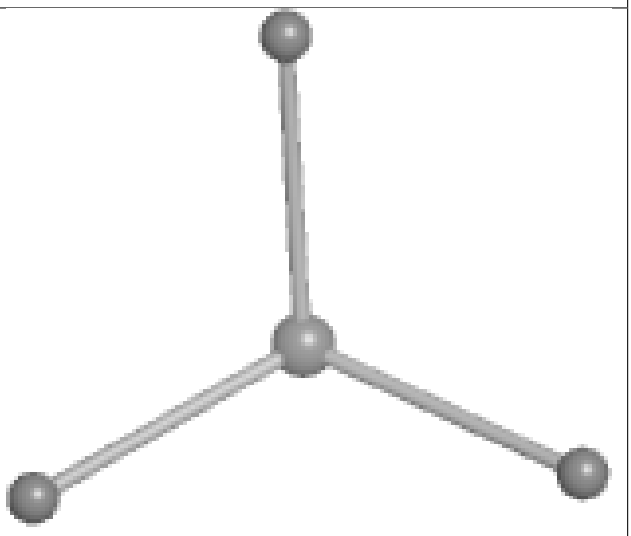


Rings

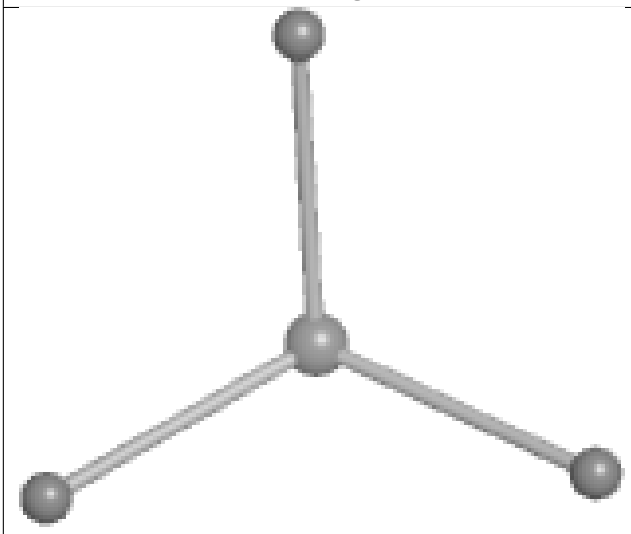
Ligand BEF A 902



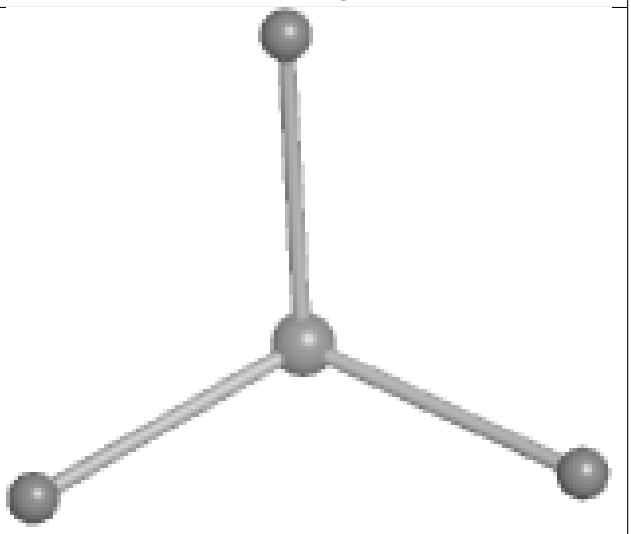
Bond lengths



Bond angles

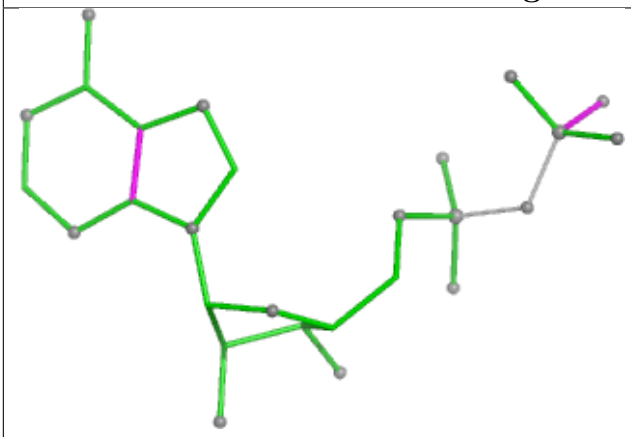


Torsions

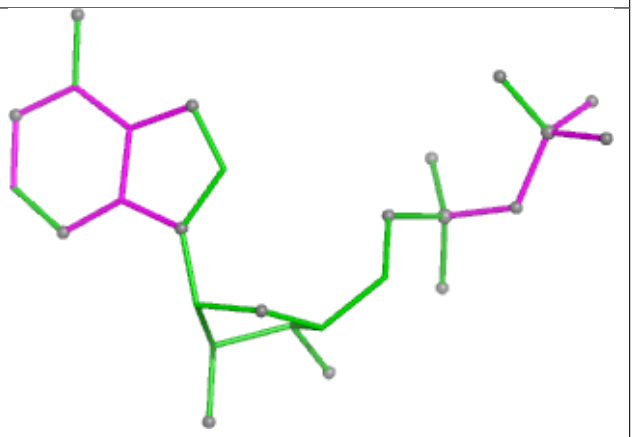


Rings

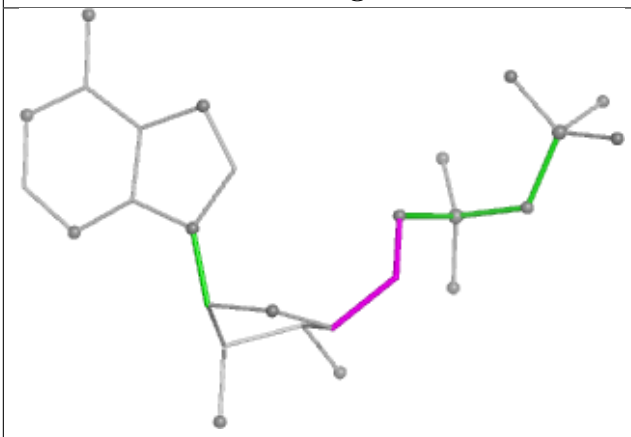
Ligand ADP E 901



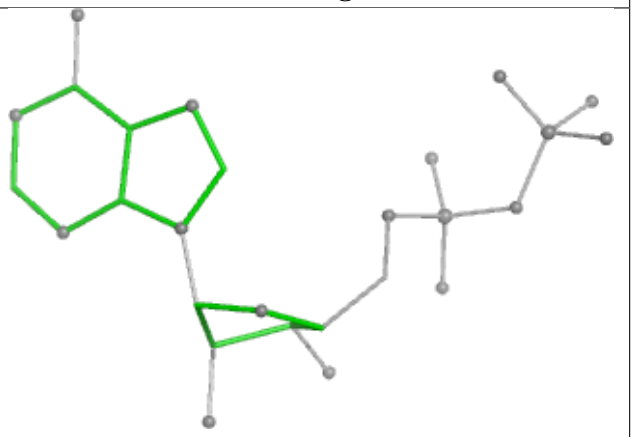
Bond lengths



Bond angles

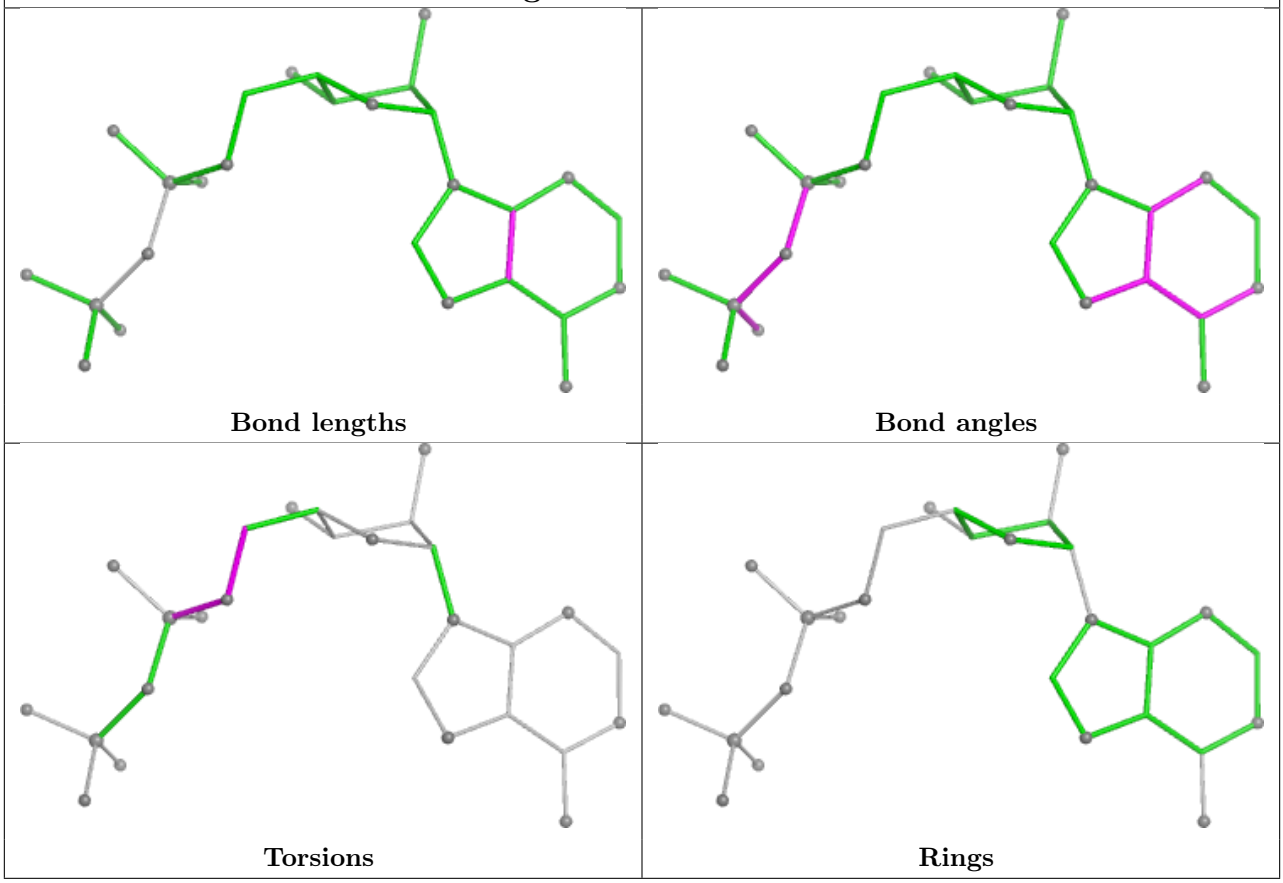


Torsions

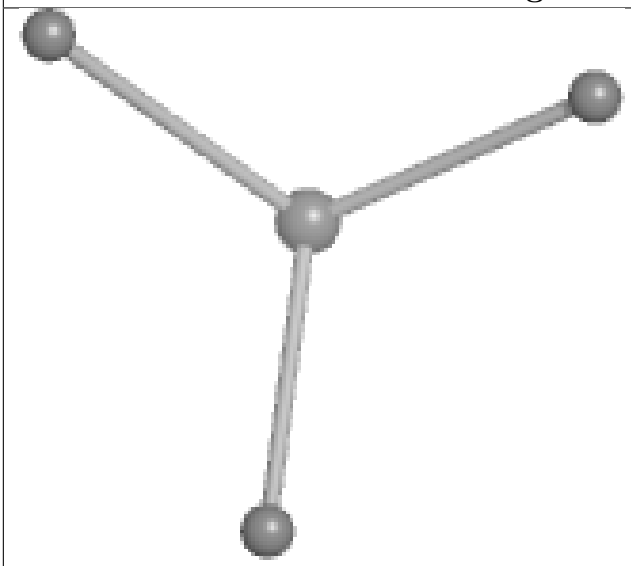


Rings

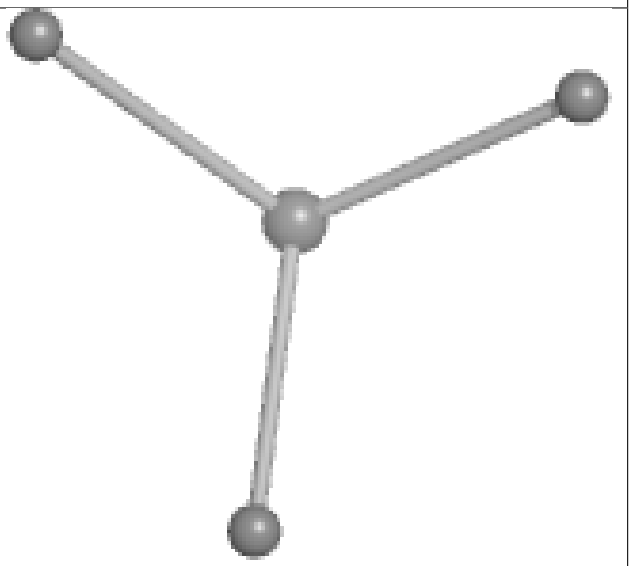
Ligand ADP B 905



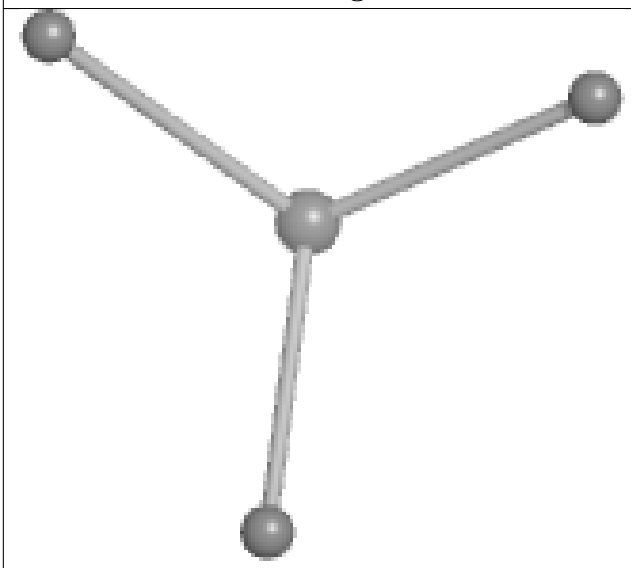
Ligand BEF B 901



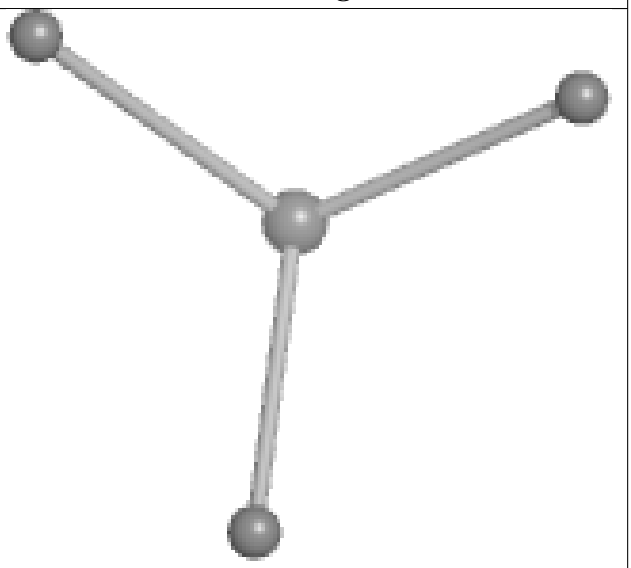
Bond lengths



Bond angles

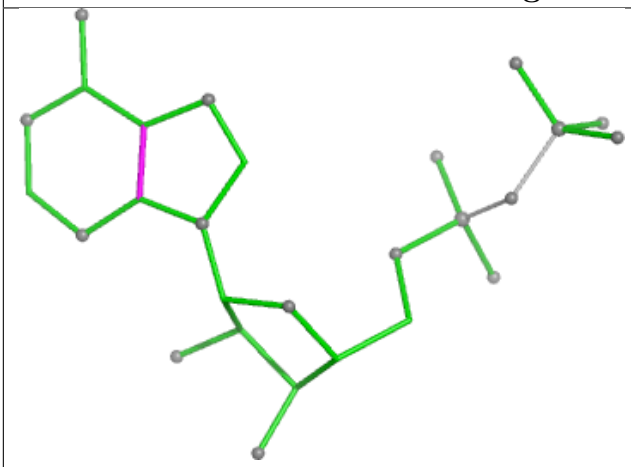


Torsions

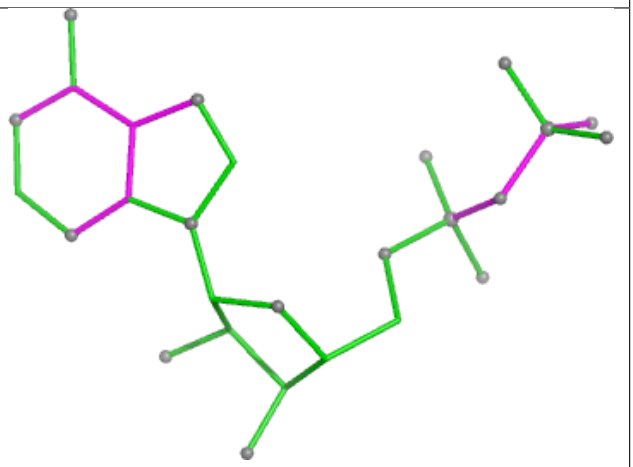


Rings

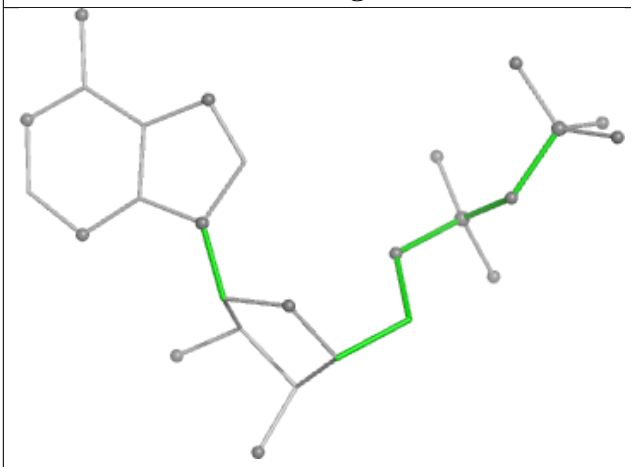
Ligand ADP E 904



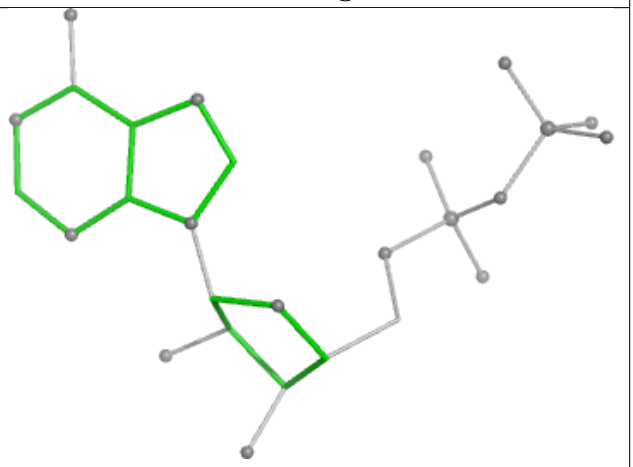
Bond lengths



Bond angles

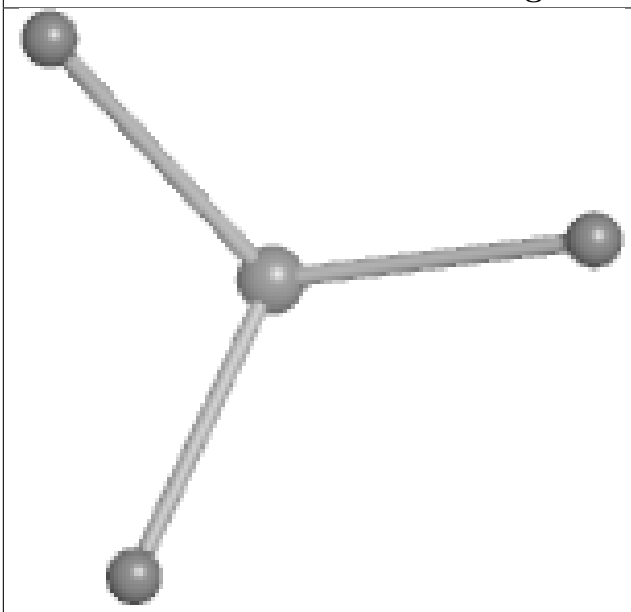


Torsions

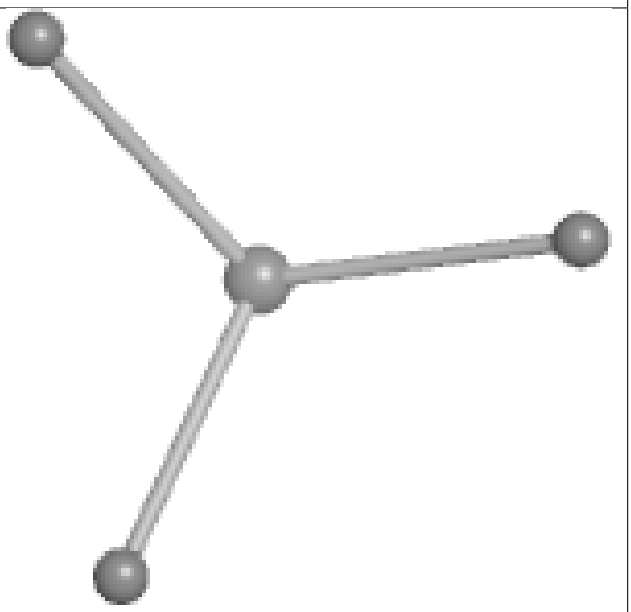


Rings

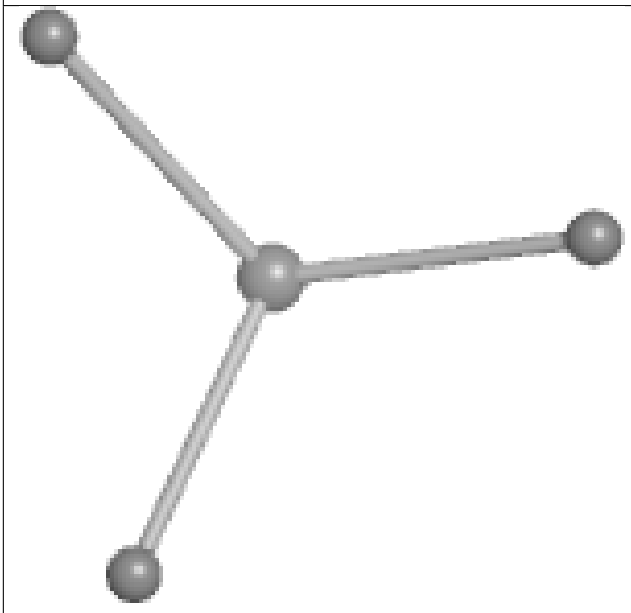
Ligand BEF A 904



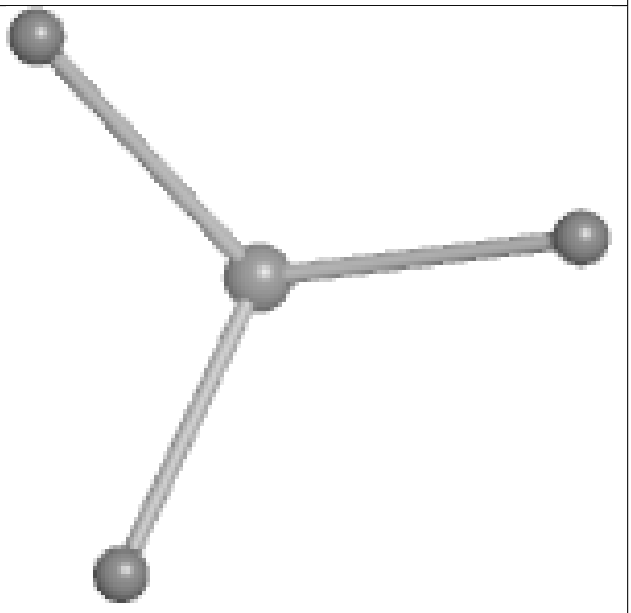
Bond lengths



Bond angles



Torsions



Rings

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.

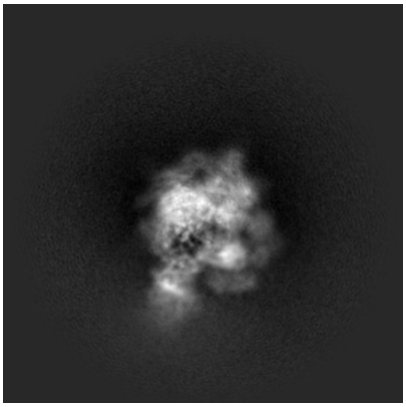
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58599. These allow visual inspection of the internal detail of the map and identification of artifacts.

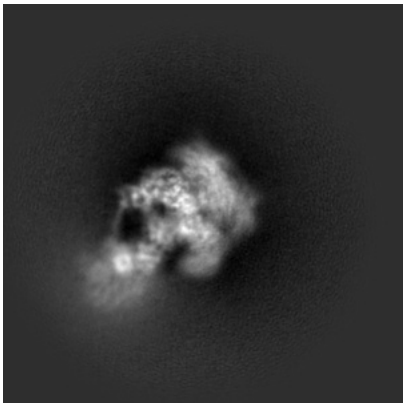
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

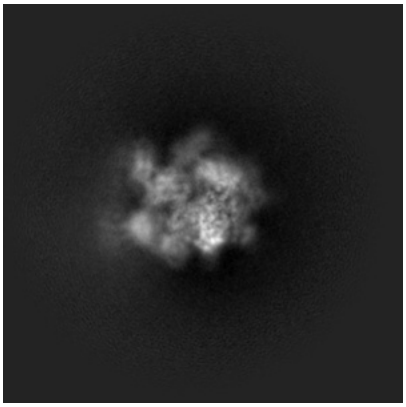
6.1.1 Primary map



X



Y

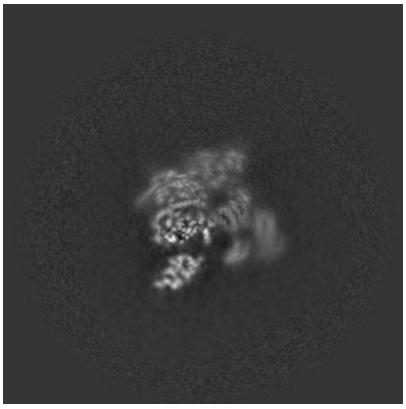


Z

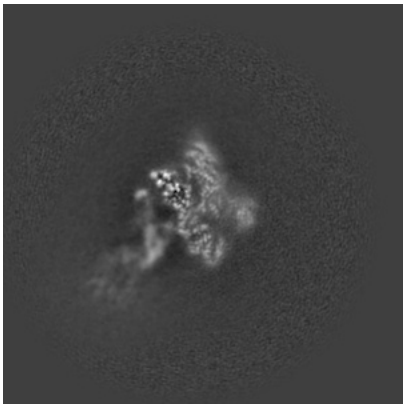
The images above show the map projected in three orthogonal directions.

6.2 Central slices

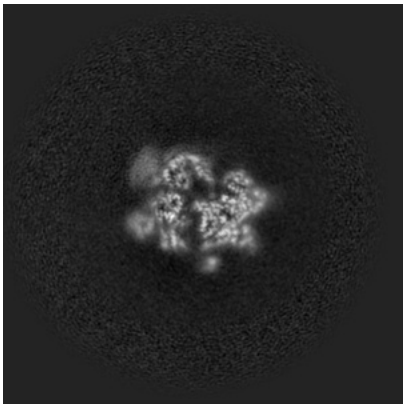
6.2.1 Primary map



X Index: 288



Y Index: 288

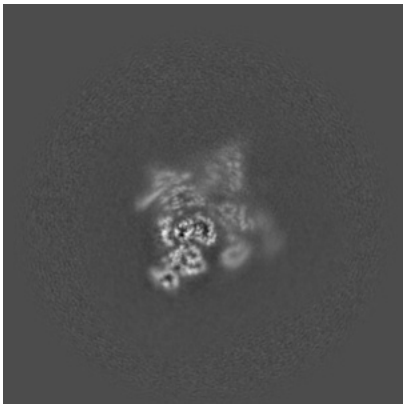


Z Index: 288

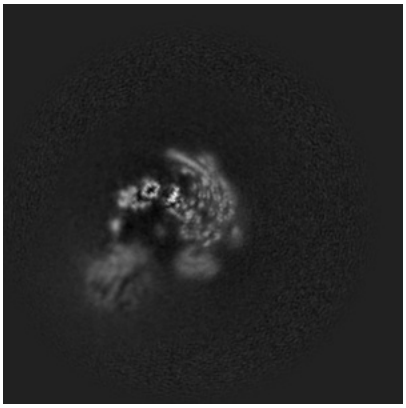
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

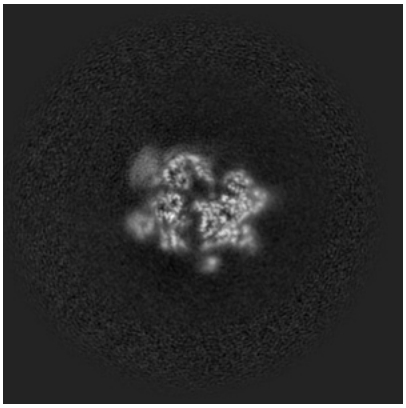
6.3.1 Primary map



X Index: 300



Y Index: 249

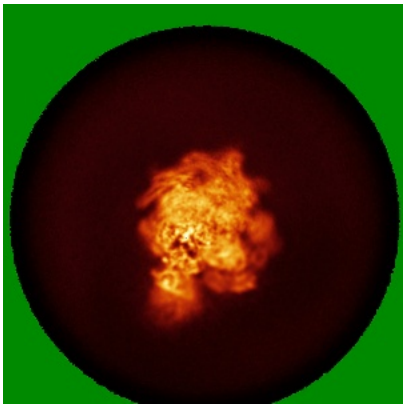


Z Index: 288

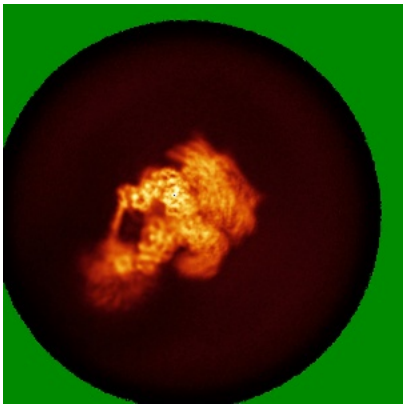
The images above show the largest variance slices of the map in three orthogonal directions.

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

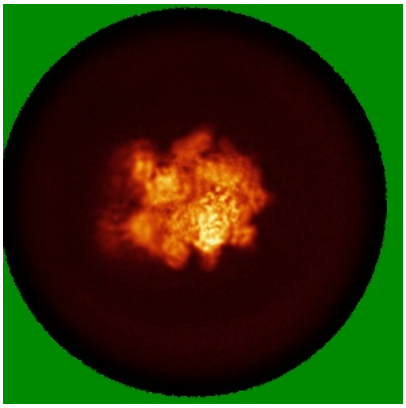
6.4.1 Primary map



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 5.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

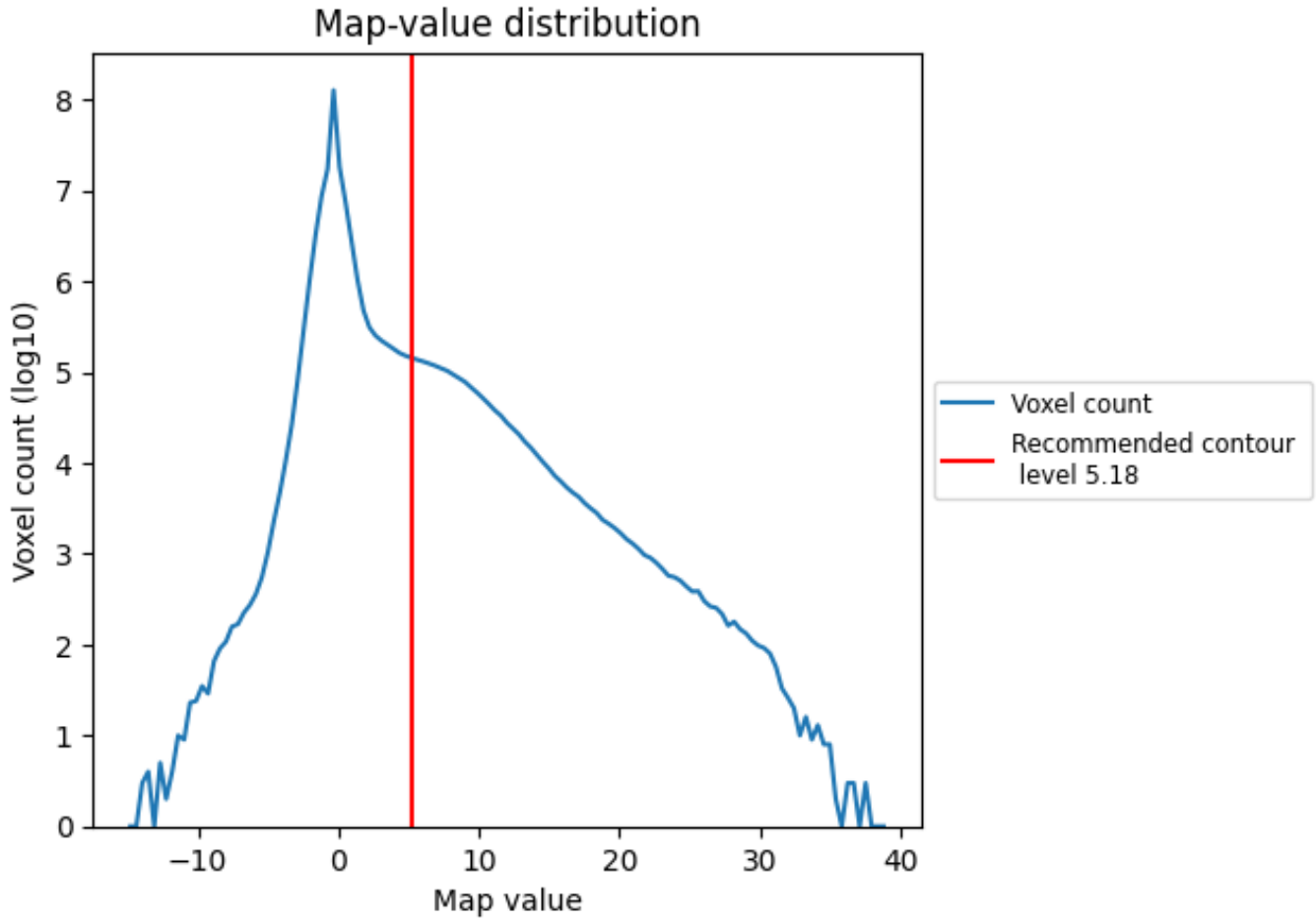
6.6 Mask visualisation (i)

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

7 Map analysis

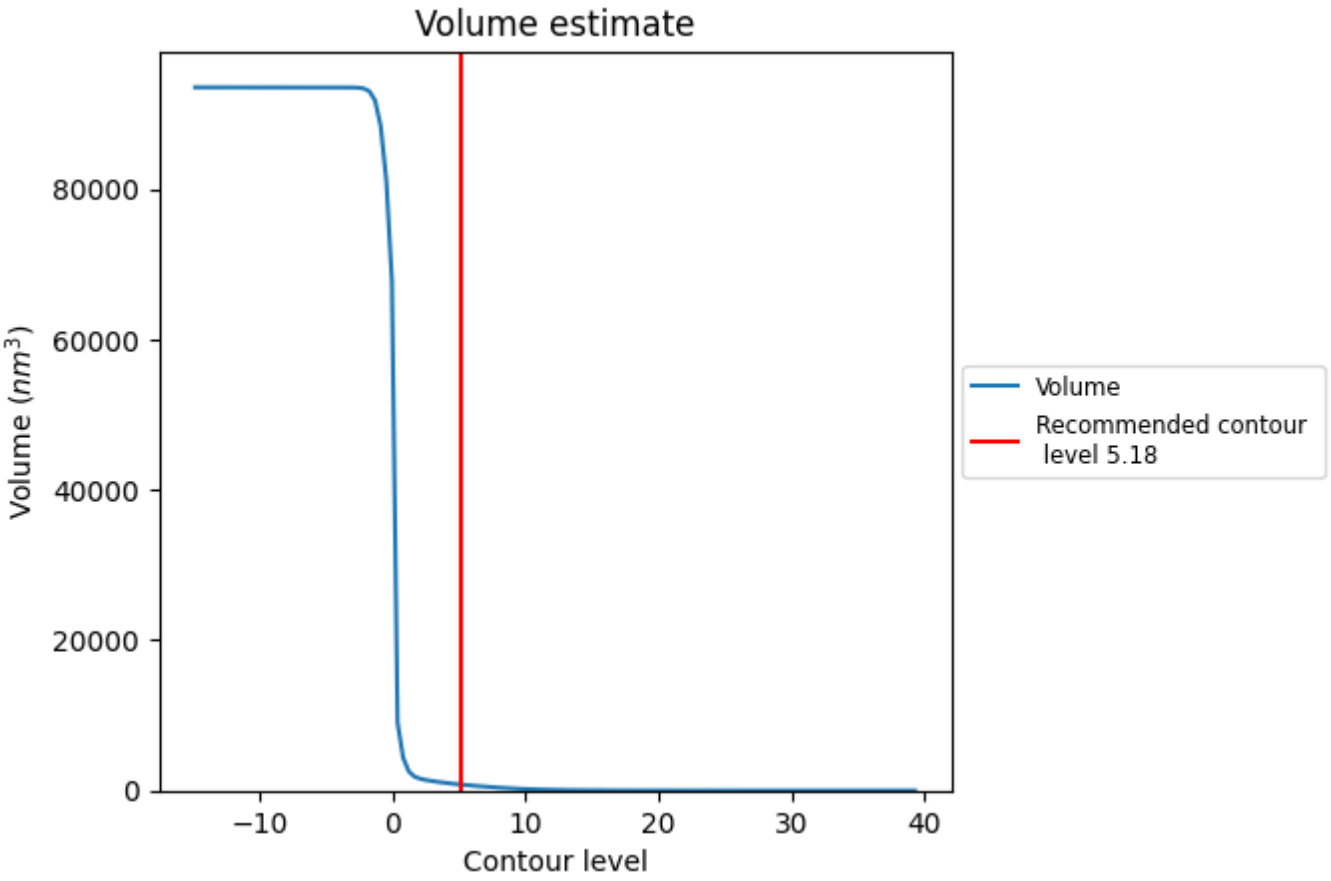
This section contains the results of statistical analysis of the map.

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.

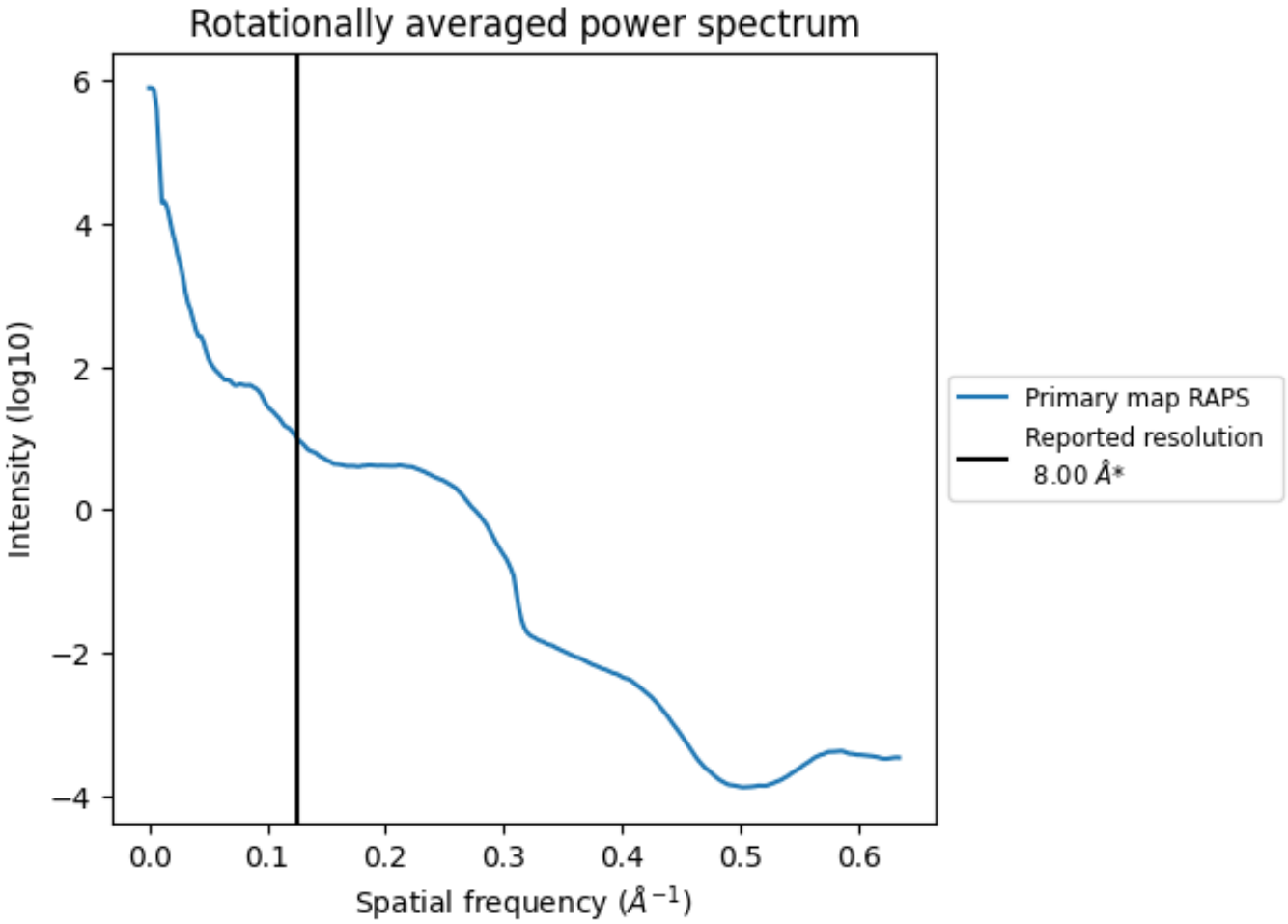
7.2 Volume estimate



The volume at the recommended contour level is 793 nm^3; this corresponds to an approximate mass of 716 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 0.125 Å^{-1}

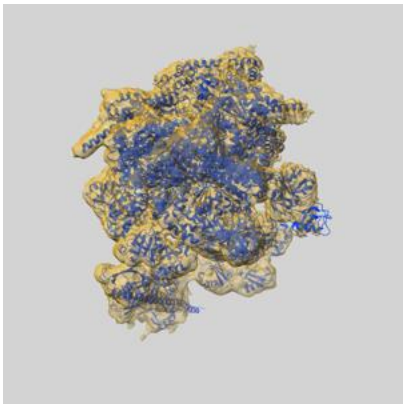
8 Fourier-Shell correlation

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

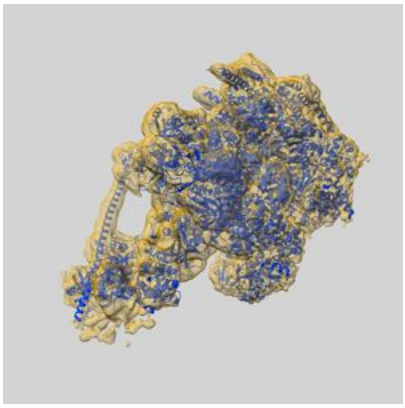
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58599 and PDB model 31OR. Per-residue inclusion information can be found in section 3 on page 9.

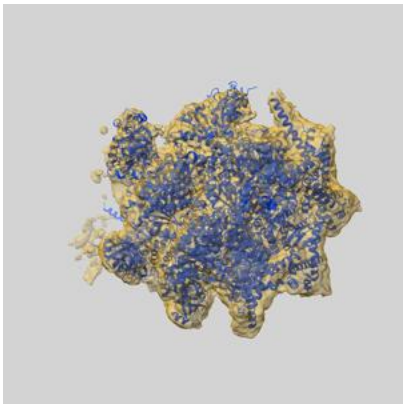
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

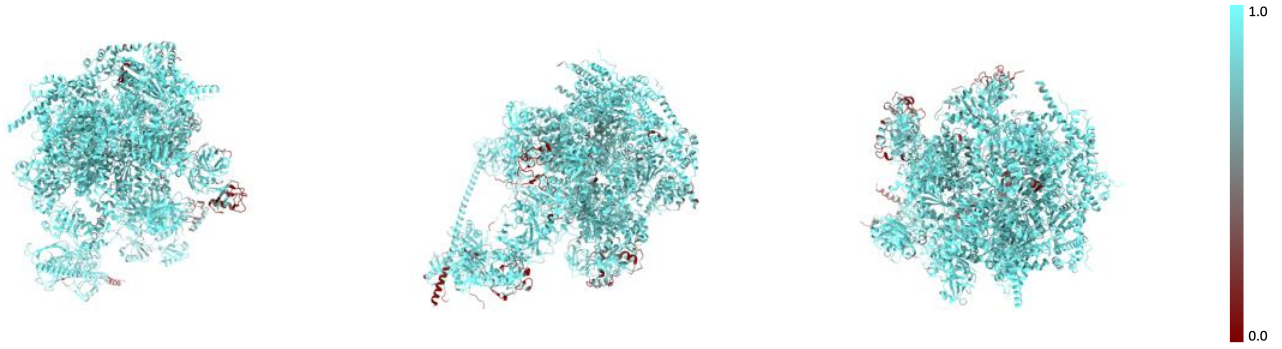
9.2 Q-score mapped to coordinate model (i)



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.

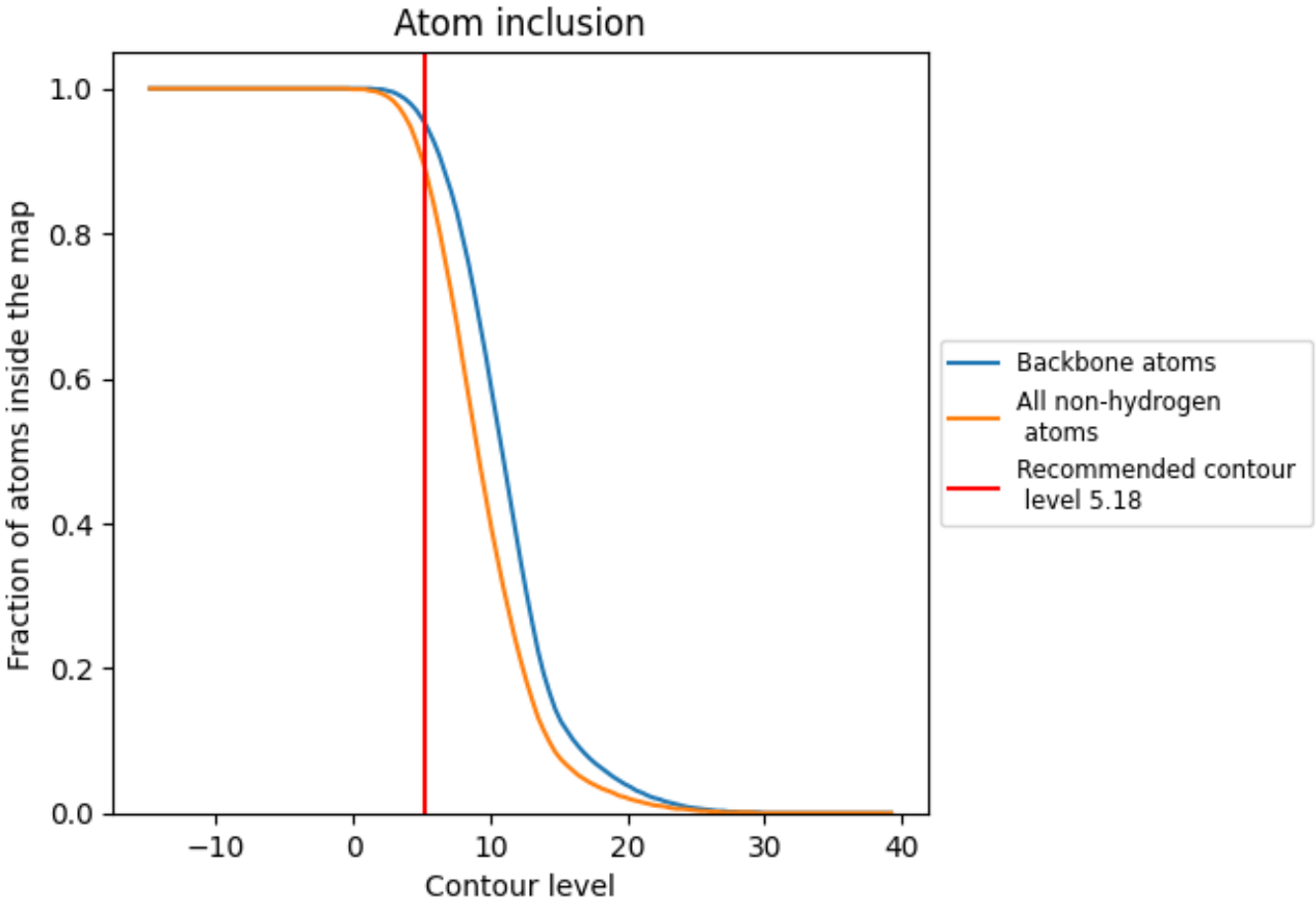
9.3 Atom inclusion mapped to coordinate model (i)



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 (5.18).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (5.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.2670
A	0.9300	0.3370
B	0.9310	0.3390
C	0.8960	0.2900
D	0.8250	0.2450
E	0.9410	0.3300
F	0.9470	0.3120
G	0.8580	0.1620
H	0.8580	0.0860
I	0.8510	0.2400
J	0.9300	0.1480
K	0.8030	0.0710
L	0.8600	0.0440
M	0.8580	0.0600
N	0.4940	0.0880
T	0.8330	0.1860

