Full wwPDB EM Validation Report ⓘ

Oct 27, 2026 – 06:56 pm GMT

PDB ID	:	31OL / pdb_000031ol
EMDB ID	:	EMD-58586
Title	:	CryoEM structure of substrate engaged p97 in complex with Ufd1/Npl4 and Delta-N-FAF1
Authors	:	Drakonaki, A.; van den Boom, J.; Kroening, A.; Meyer, H.; Gatsogiannis, C.
Deposited on	:	2026-06-16
Resolution	:	4.31 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:

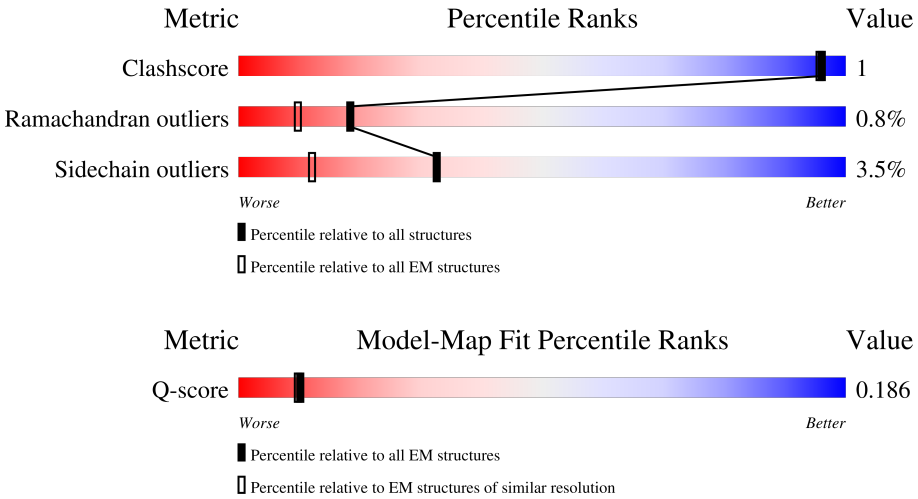
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 4.31 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.



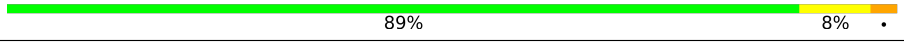
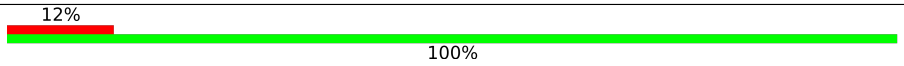
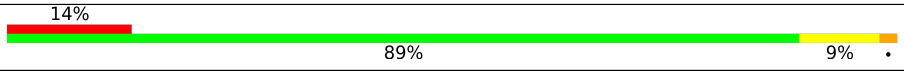
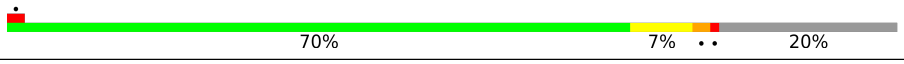
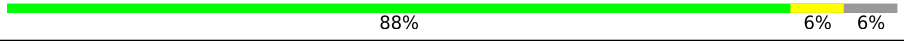
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3904 (3.81 - 4.80)

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	G	608	81% 7% 11%
2	I	76	57% 11% 32%
2	J	76	99%
2	K	76	96%

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Mol	Chain	Length	Quality of chain
2	L	76	
2	M	76	
2	N	76	
3	T	333	
4	H	307	
5	A	806	
5	B	806	
5	C	806	
5	D	806	
5	E	806	
5	F	806	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 47367 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 Nuclear protein localization protein 4 homolog.

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

- Molecule 2 is a protein called Polyubiquitin-B.

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

- Molecule 3 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	333	Total	C	N	O	S	0	0
			2735	1720	477	524	14		

- Molecule 4 is a protein called Ubiquitin recognition factor in ER-associated degradation protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	246	Total	C	N	O	S	0	0
			1941	1235	331	362	13		

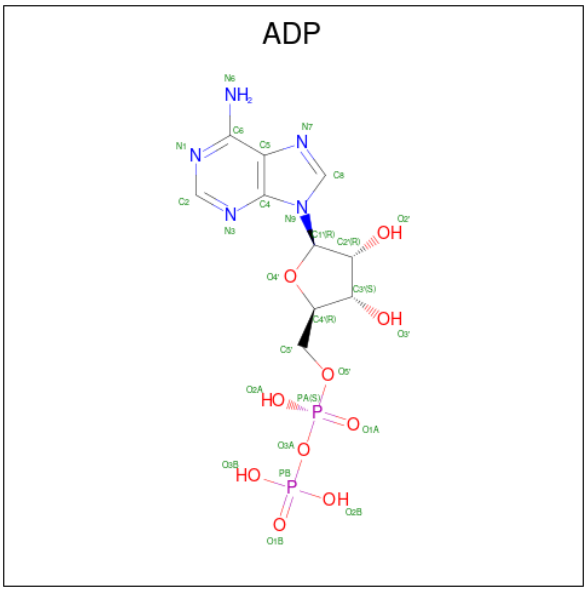
- Molecule 5 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	719	Total	C	N	O	S	0	0
			5656	3561	1000	1065	30		
5	B	752	Total	C	N	O	S	0	0
			5878	3696	1044	1108	30		
5	A	759	Total	C	N	O	S	0	0
			5942	3734	1055	1123	30		
5	F	743	Total	C	N	O	S	0	0
			5807	3653	1031	1093	30		
5	C	731	Total	C	N	O	S	0	0
			5702	3589	1011	1072	30		
5	D	720	Total	C	N	O	S	0	0
			5623	3537	997	1060	29		

There are 12 discrepancies between the modelled and reference sequences:

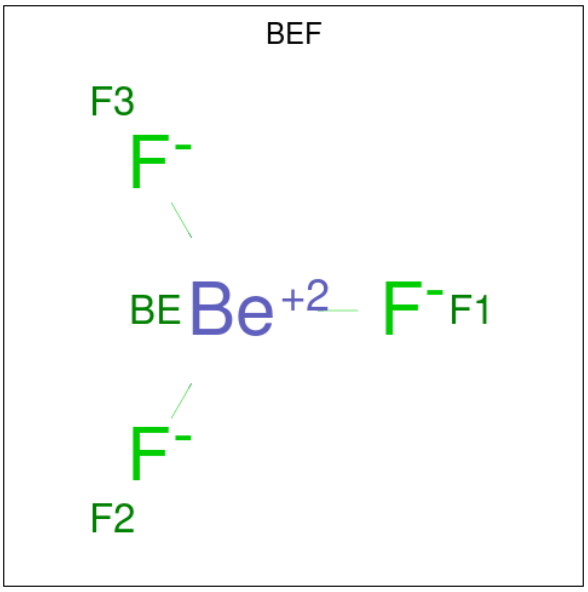
Chain	Residue	Modelled	Actual	Comment	Reference
E	232	GLU	ALA	engineered mutation	UNP P55072
E	578	GLN	GLU	engineered mutation	UNP P55072
B	232	GLU	ALA	engineered mutation	UNP P55072
B	578	GLN	GLU	engineered mutation	UNP P55072
A	232	GLU	ALA	engineered mutation	UNP P55072
A	578	GLN	GLU	engineered mutation	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 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	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	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	1	Total Mg 1 1	0
8	A	3	Total Mg 3 3	0
8	F	1	Total Mg 1 1	0
8	C	3	Total Mg 3 3	0

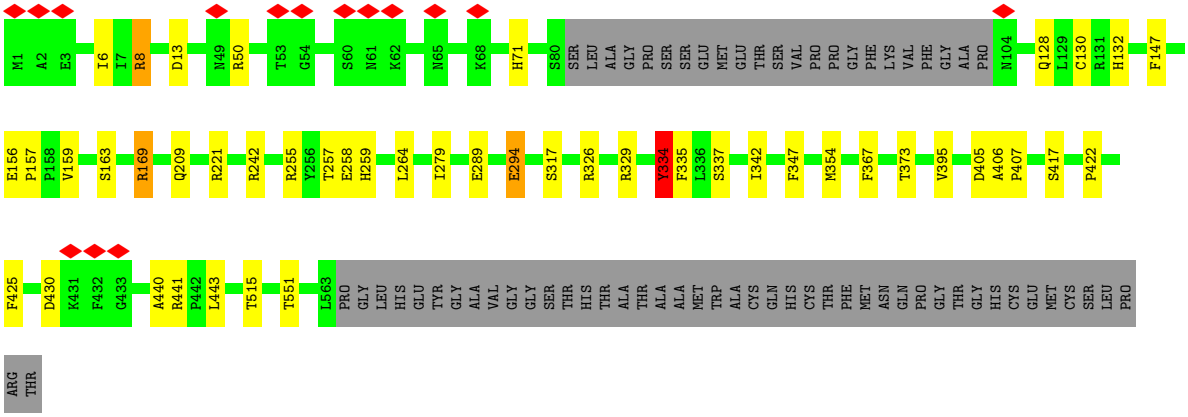
3 Residue-property plots (i)

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: Nuclear protein localization protein 4 homolog

Chain G:

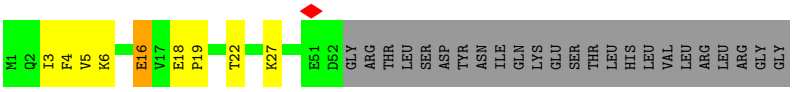




• Molecule 2: Polyubiquitin-B

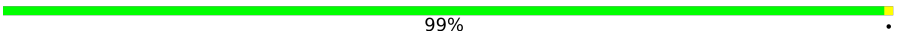
Chain I:





• Molecule 2: Polyubiquitin-B

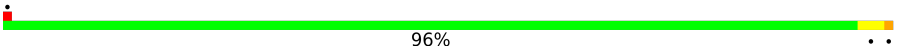
Chain J:

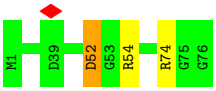




• Molecule 2: Polyubiquitin-B

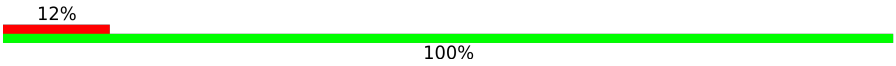
Chain K:

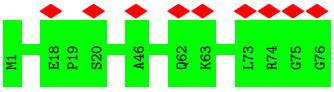




• Molecule 2: Polyubiquitin-B

Chain N:

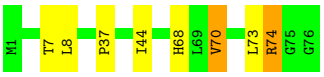




• Molecule 2: Polyubiquitin-B

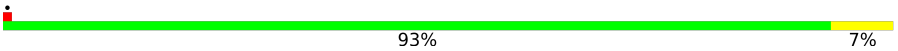
Chain L:

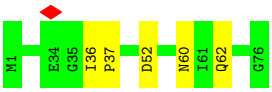




• Molecule 2: Polyubiquitin-B

Chain M:

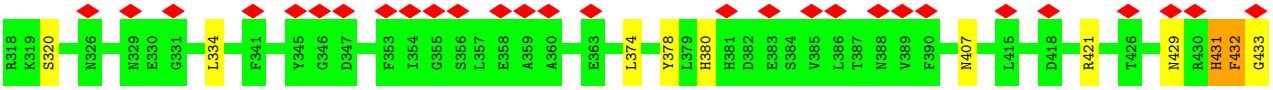


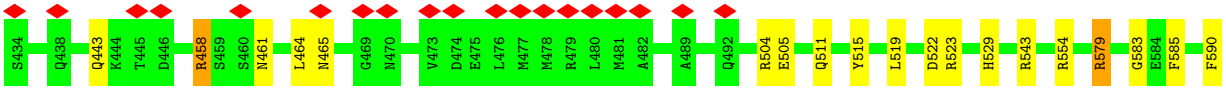


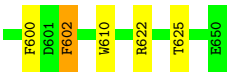
• Molecule 3: FAS-associated factor 1

Chain T:





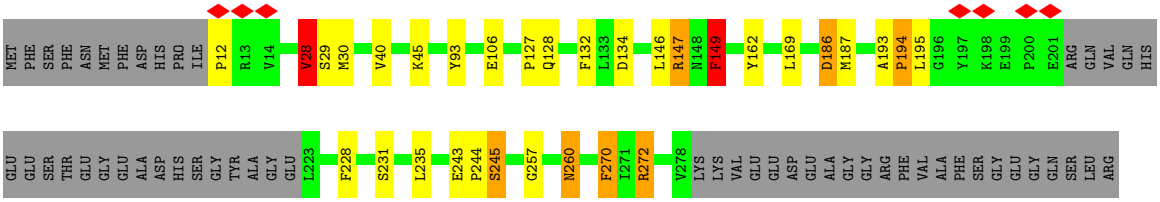




• Molecule 4: Ubiquitin recognition factor in ER-associated degradation protein 1

Chain H:



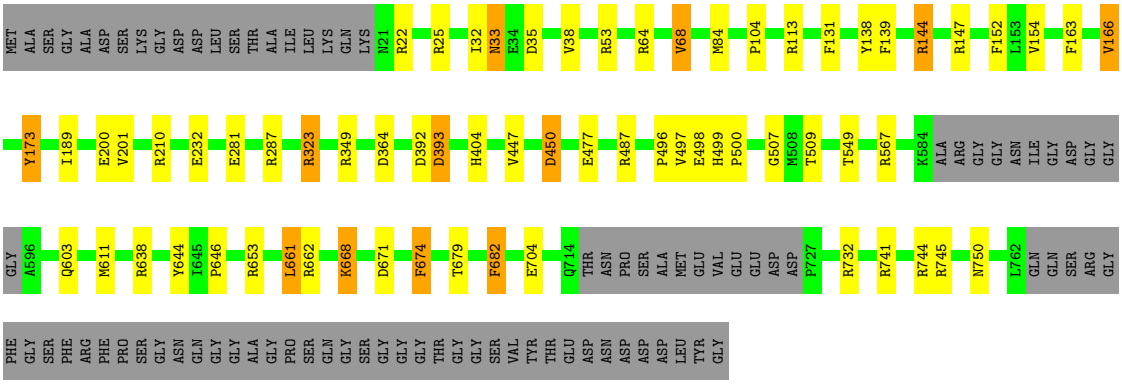




• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain E:

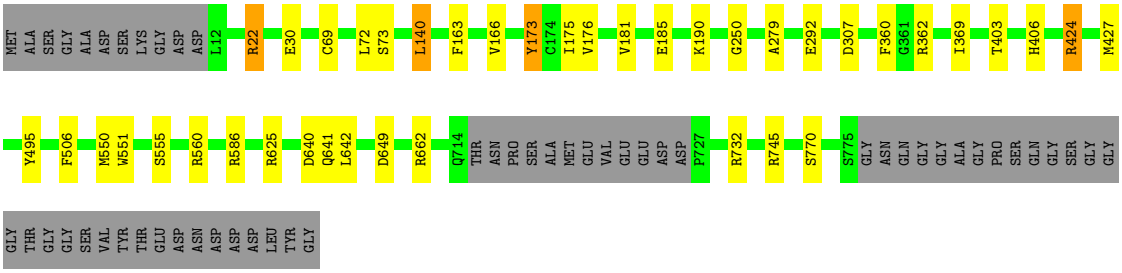




• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain B:

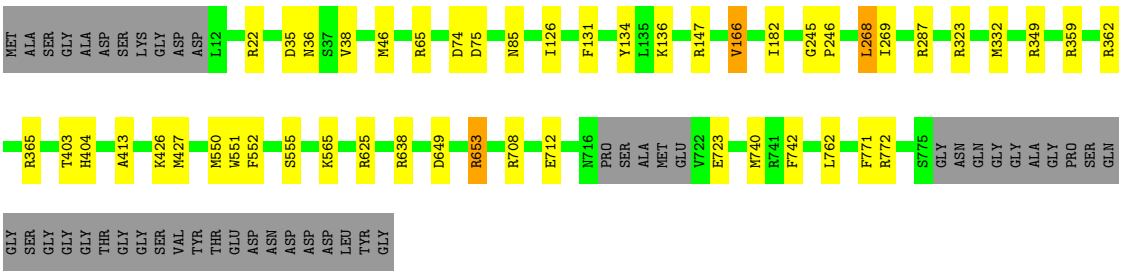




• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain A:



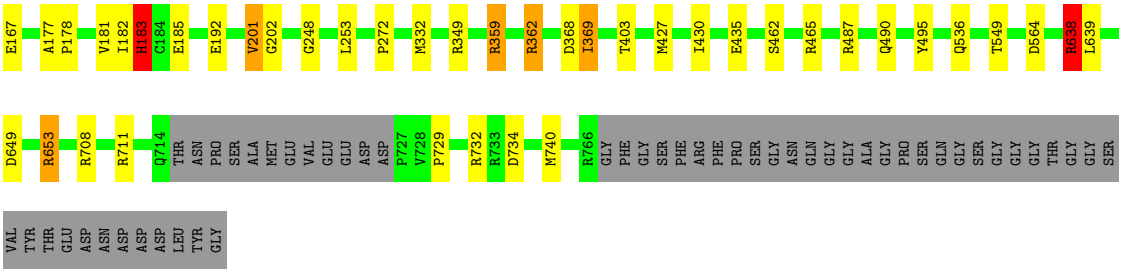


• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain F:



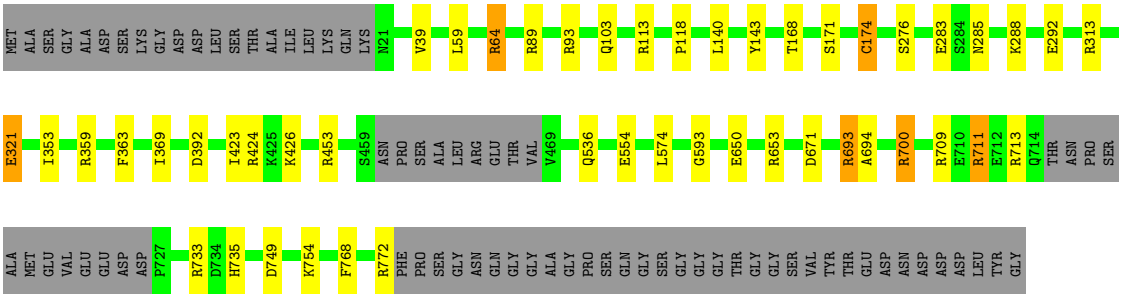




• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain C:

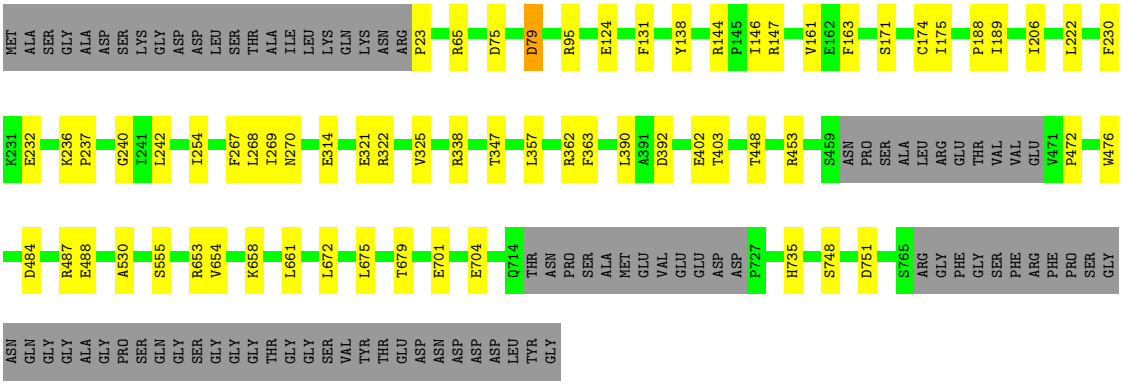




• Molecule 5: Transitional endoplasmic reticulum ATPase

Chain D:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43625	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	0.564	Depositor
Minimum map value	-0.194	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0354	Depositor
Map size (Å)	459.19998, 459.19998, 459.19998	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.05, 2.05, 2.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, 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	G	0.82	0/4404	1.40	16/5967 (0.3%)
2	I	1.11	1/414 (0.2%)	1.80	6/557 (1.1%)
2	J	0.81	0/600	1.34	0/806
2	K	0.89	0/600	1.39	2/806 (0.2%)
2	L	0.88	0/608	1.59	2/816 (0.2%)
2	M	0.86	1/608 (0.2%)	1.45	6/816 (0.7%)
2	N	0.84	0/608	1.31	0/816
3	T	0.80	0/2786	1.39	16/3750 (0.4%)
4	H	0.86	0/1982	1.57	17/2677 (0.6%)
5	A	0.76	1/6039 (0.0%)	1.32	17/8152 (0.2%)
5	B	0.73	0/5974	1.33	15/8063 (0.2%)
5	C	0.76	0/5795	1.40	18/7820 (0.2%)
5	D	0.73	0/5714	1.37	23/7712 (0.3%)
5	E	0.74	0/5748	1.38	29/7761 (0.4%)
5	F	0.74	0/5900	1.34	16/7965 (0.2%)
All	All	0.77	3/47780 (0.0%)	1.38	183/64484 (0.3%)

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	G	0	4
3	T	0	3
4	H	0	2
5	A	0	4
5	B	0	4
5	C	0	4
5	D	0	2
5	E	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	F	0	9
All	All	0	38

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	74	ASP	CG-OD2	-6.26	1.13	1.25
2	M	37	PRO	CA-C	5.96	1.55	1.51
2	I	18	GLU	N-CA	5.49	1.50	1.45

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	149	PHE	CA-CB-CG	10.10	123.89	113.80
3	T	602	PHE	CA-CB-CG	9.54	123.34	113.80
5	F	183	HIS	CA-CB-CG	9.46	123.26	113.80
5	D	448	THR	N-CA-C	7.86	120.55	111.11
5	B	279	ALA	N-CA-C	7.86	120.75	111.71
5	E	392	ASP	CA-C-N	7.83	136.50	121.54
5	E	392	ASP	C-N-CA	7.83	136.50	121.54
5	D	237	PRO	N-CA-C	7.83	120.25	110.70
5	C	772	ARG	NE-CZ-NH2	7.73	126.16	119.20
1	G	329	ARG	NE-CZ-NH2	7.54	125.99	119.20
5	D	268	LEU	N-CA-C	7.53	123.37	114.04
5	E	323	ARG	NE-CZ-NH2	7.40	125.86	119.20
4	H	128	GLN	CA-C-N	7.29	135.42	122.08
4	H	128	GLN	C-N-CA	7.29	135.42	122.08
4	H	270	PHE	CA-CB-CG	7.04	120.84	113.80
5	E	154	VAL	CB-CA-C	6.94	118.79	111.09
4	H	235	LEU	CA-C-N	6.94	134.79	121.54
4	H	235	LEU	C-N-CA	6.94	134.79	121.54
5	E	674	PHE	CA-CB-CG	6.87	120.67	113.80
3	T	458	ARG	NE-CZ-NH2	6.87	125.38	119.20
2	I	16	GLU	N-CA-C	6.84	117.51	108.07
5	F	638	ARG	NE-CZ-NH2	6.79	125.31	119.20
4	H	147	ARG	NE-CZ-NH2	6.73	125.26	119.20
1	G	425	PHE	CA-CB-CG	6.66	120.46	113.80
5	A	742	PHE	CA-CB-CG	-6.64	107.16	113.80
5	C	709	ARG	NE-CZ-NH2	6.62	125.16	119.20
3	T	522	ASP	CA-CB-CG	6.47	119.07	112.60
2	I	18	GLU	N-CA-C	6.41	120.24	109.09
5	C	653	ARG	NE-CZ-NH2	6.41	124.97	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	12	PRO	CA-N-CD	-6.39	103.05	112.00
5	C	313	ARG	NE-CZ-NH2	6.29	124.86	119.20
2	I	22	THR	N-CA-C	6.25	118.57	109.07
3	T	407	ASN	N-CA-C	6.20	117.83	111.14
3	T	585	PHE	CA-CB-CG	6.15	119.95	113.80
3	T	504	ARG	NE-CZ-NH2	6.15	124.73	119.20
1	G	334	TYR	N-CA-C	6.12	118.67	111.02
5	E	131	PHE	CA-CB-CG	6.10	119.90	113.80
5	A	147	ARG	NE-CZ-NH2	6.09	124.68	119.20
2	I	18	GLU	CA-C-N	6.07	127.43	119.84
2	I	18	GLU	C-N-CA	6.07	127.43	119.84
5	F	147	ARG	NE-CZ-NH2	6.07	124.66	119.20
5	F	349	ARG	NE-CZ-NH2	6.05	124.64	119.20
5	F	362	ARG	NE-CZ-NH2	6.03	124.63	119.20
5	E	22	ARG	NE-CZ-NH2	6.00	124.60	119.20
5	D	269	ILE	N-CA-C	5.95	116.93	108.42
5	A	708	ARG	NE-CZ-NH2	5.94	124.55	119.20
5	D	147	ARG	NE-CZ-NH2	5.91	124.52	119.20
2	K	52	ASP	CA-CB-CG	5.90	118.50	112.60
4	H	272	ARG	NE-CZ-NH2	5.89	124.50	119.20
5	D	362	ARG	NE-CZ-NH2	5.86	124.48	119.20
5	B	22	ARG	NE-CZ-NH2	5.85	124.47	119.20
5	B	424	ARG	NE-CZ-NH2	5.83	124.45	119.20
5	E	144	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	M	36	ILE	CA-C-N	5.81	123.90	119.66
2	M	36	ILE	C-N-CA	5.81	123.90	119.66
5	F	490	GLN	OE1-CD-NE2	-5.81	116.79	122.60
5	A	362	ARG	NE-CZ-NH2	5.80	124.42	119.20
5	A	22	ARG	NE-CZ-NH2	5.79	124.41	119.20
5	D	357	LEU	CA-C-N	5.78	129.09	120.31
5	D	357	LEU	C-N-CA	5.78	129.09	120.31
5	D	472	PRO	CA-C-N	5.77	128.59	120.28
5	D	472	PRO	C-N-CA	5.77	128.59	120.28
5	D	79	ASP	CA-CB-CG	5.77	118.37	112.60
5	E	349	ARG	NE-CZ-NH2	5.74	124.37	119.20
1	G	264	LEU	CA-C-N	5.72	125.41	119.92
1	G	264	LEU	C-N-CA	5.72	125.41	119.92
5	C	93	ARG	NE-CZ-NH2	5.70	124.33	119.20
2	I	4	PHE	N-CA-C	5.69	117.83	109.24
3	T	523	ARG	NE-CZ-NH2	5.65	124.29	119.20
4	H	134	ASP	CA-CB-CG	5.64	118.24	112.60
5	F	115	HIS	CB-CG-CD2	-5.62	123.89	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	359	ARG	NE-CZ-NH2	5.61	124.25	119.20
4	H	260	ASN	CA-CB-CG	5.60	118.20	112.60
5	B	406	HIS	CB-CG-CD2	-5.59	123.94	131.20
1	G	430	ASP	CA-CB-CG	5.58	118.18	112.60
5	C	671	ASP	CA-CB-CG	5.58	118.18	112.60
5	F	732	ARG	NE-CZ-NH2	5.57	124.22	119.20
3	T	622	ARG	NE-CZ-NH2	5.56	124.21	119.20
5	B	662	ARG	NE-CZ-NH2	5.56	124.20	119.20
5	E	323	ARG	CD-NE-CZ	5.56	132.18	124.40
1	G	50	ARG	NE-CZ-NH2	5.55	124.20	119.20
5	E	364	ASP	CA-C-N	5.54	129.81	121.40
5	E	364	ASP	C-N-CA	5.54	129.81	121.40
5	A	625	ARG	NE-CZ-NH2	5.53	124.18	119.20
3	T	431	HIS	CA-C-O	5.53	126.60	120.80
5	A	349	ARG	NE-CZ-NH2	5.53	124.17	119.20
5	D	131	PHE	CA-CB-CG	5.52	119.32	113.80
5	E	450	ASP	CA-CB-CG	5.52	118.12	112.60
5	A	75	ASP	CA-CB-CG	5.52	118.12	112.60
5	E	147	ARG	NE-CZ-NH2	5.51	124.16	119.20
5	E	653	ARG	NE-CZ-NH2	5.51	124.16	119.20
5	F	465	ARG	NE-CZ-NH2	5.50	124.15	119.20
5	A	365	ARG	NE-CZ-NH2	5.47	124.12	119.20
5	A	245	GLY	CA-C-N	5.45	123.64	119.66
5	A	245	GLY	C-N-CA	5.45	123.64	119.66
1	G	242	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	G	169	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	G	259	HIS	CB-CG-CD2	-5.40	124.17	131.20
3	T	600	PHE	CA-CB-CG	5.40	119.20	113.80
5	D	453	ARG	NE-CZ-NH2	5.39	124.05	119.20
5	F	653	ARG	NE-CZ-NH2	5.39	124.05	119.20
5	D	95	ARG	NE-CZ-NH2	5.38	124.04	119.20
5	E	662	ARG	NE-CZ-NH2	5.38	124.04	119.20
5	A	653	ARG	NE-CZ-NH2	5.37	124.03	119.20
5	D	403	THR	CA-C-N	5.36	127.72	120.38
5	D	403	THR	C-N-CA	5.36	127.72	120.38
5	C	693	ARG	NE-CZ-NH2	5.35	124.02	119.20
5	C	64	ARG	NE-CZ-NH2	5.35	124.01	119.20
2	L	37	PRO	N-CA-C	5.33	117.20	110.70
3	T	579	ARG	NE-CZ-NH2	5.32	123.99	119.20
5	B	506	PHE	CA-CB-CG	-5.32	108.48	113.80
5	F	564	ASP	CA-CB-CG	-5.32	107.28	112.60
1	G	8	ARG	NE-CZ-NH2	5.31	123.98	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	287	ARG	NE-CZ-NH2	5.30	123.97	119.20
5	E	166	VAL	CA-C-N	5.29	130.64	121.64
5	E	166	VAL	C-N-CA	5.29	130.64	121.64
5	D	338	ARG	NE-CZ-NH2	5.29	123.96	119.20
3	T	432	PHE	CA-C-N	5.28	126.74	120.14
3	T	432	PHE	C-N-CA	5.28	126.74	120.14
5	A	246	PRO	N-CA-CB	5.28	106.14	103.19
4	H	28	VAL	CA-C-N	5.27	128.07	120.38
4	H	28	VAL	C-N-CA	5.27	128.07	120.38
5	B	770	SER	CA-C-N	5.27	128.59	121.05
5	B	770	SER	C-N-CA	5.27	128.59	121.05
5	A	552	PHE	N-CA-C	5.27	117.43	111.11
5	F	487	ARG	NE-CZ-NH2	5.23	123.91	119.20
5	D	144	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	G	255	ARG	NE-CZ-NH2	5.23	123.90	119.20
5	D	270	ASN	CA-CB-CG	5.22	117.82	112.60
2	M	52	ASP	CA-CB-CG	5.22	117.82	112.60
5	B	732	ARG	CA-C-N	5.21	127.57	120.54
5	B	732	ARG	C-N-CA	5.21	127.57	120.54
5	F	120	ASP	N-CA-C	5.20	116.63	111.07
5	C	113	ARG	NE-CZ-NH2	5.20	123.88	119.20
4	H	245	SER	CB-CA-C	5.19	120.39	110.17
1	G	334	TYR	CA-CB-CG	5.19	123.23	113.90
2	M	37	PRO	N-CA-C	5.19	115.45	110.47
5	B	745	ARG	NE-CZ-NH2	5.19	123.87	119.20
5	C	424	ARG	NE-CZ-NH2	5.18	123.86	119.20
5	C	353	ILE	CA-C-N	5.17	127.84	120.49
5	C	353	ILE	C-N-CA	5.17	127.84	120.49
2	K	54	ARG	NE-CZ-NH2	5.17	123.85	119.20
5	E	33	ASN	CA-C-N	5.17	128.66	121.02
5	E	33	ASN	C-N-CA	5.17	128.66	121.02
5	D	65	ARG	NE-CZ-NH2	5.16	123.85	119.20
5	E	638	ARG	NE-CZ-NH2	5.16	123.84	119.20
5	E	404	HIS	CB-CG-CD2	-5.16	124.50	131.20
5	F	94	VAL	N-CA-C	5.16	115.79	108.42
5	D	23	PRO	CA-N-CD	-5.15	104.79	112.00
3	T	421	ARG	NE-CZ-NH2	5.14	123.83	119.20
5	F	144	ARG	NE-CZ-NH2	5.14	123.83	119.20
5	D	555	SER	CA-C-N	5.14	127.59	120.29
5	D	555	SER	C-N-CA	5.14	127.59	120.29
5	E	53	ARG	NE-CZ-NH2	5.12	123.81	119.20
3	T	432	PHE	CA-CB-CG	5.12	118.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	593	GLY	CA-C-N	5.11	126.57	120.13
5	C	593	GLY	C-N-CA	5.11	126.57	120.13
5	E	25	ARG	NE-CZ-NH2	5.11	123.80	119.20
4	H	243	GLU	CB-CA-C	5.10	116.88	109.08
2	M	37	PRO	CA-C-N	5.09	125.13	119.32
2	M	37	PRO	C-N-CA	5.09	125.13	119.32
1	G	515	THR	N-CA-C	5.09	118.65	112.23
5	E	744	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	G	221	ARG	NE-CZ-NH2	5.08	123.78	119.20
5	B	625	ARG	NE-CZ-NH2	5.08	123.78	119.20
5	C	733	ARG	NE-CZ-NH2	5.08	123.78	119.20
5	E	393	ASP	CA-C-N	5.08	127.31	120.50
5	E	393	ASP	C-N-CA	5.08	127.31	120.50
5	E	732	ARG	NE-CZ-NH2	5.07	123.76	119.20
5	A	323	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	H	231	SER	CA-C-N	5.06	124.91	120.10
4	H	231	SER	C-N-CA	5.06	124.91	120.10
5	B	362	ARG	NE-CZ-NH2	5.05	123.74	119.20
5	B	166	VAL	CB-CA-C	5.04	116.06	110.62
2	L	74	ARG	NE-CZ-NH2	5.04	123.74	119.20
5	C	453	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	G	209	GLN	OE1-CD-NE2	-5.03	117.57	122.60
3	T	590	PHE	CA-CB-CG	-5.03	108.77	113.80
5	A	287	ARG	NE-CZ-NH2	5.01	123.71	119.20
5	F	462	SER	N-CA-C	5.01	116.43	111.07
5	C	772	ARG	CD-NE-CZ	5.01	131.41	124.40
5	A	404	HIS	CB-CG-CD2	-5.00	124.69	131.20
5	B	307	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	426	LYS	Peptide
5	A	551	TRP	Peptide
5	A	65	ARG	Sidechain
5	A	653	ARG	Sidechain
5	B	173	TYR	Sidechain
5	B	495	TYR	Sidechain
5	B	560	ARG	Sidechain
5	B	586	ARG	Sidechain
5	C	700	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	C	711	ARG	Sidechain
5	C	713	ARG	Sidechain
5	C	89	ARG	Sidechain
5	D	138	TYR	Sidechain
5	D	267	PHE	Peptide
5	E	113	ARG	Sidechain
5	E	138	TYR	Sidechain
5	E	173	TYR	Sidechain
5	E	447	VAL	Peptide
5	E	682	PHE	Sidechain
5	E	741	ARG	Sidechain
5	F	110	TYR	Sidechain
5	F	143	TYR	Sidechain
5	F	167	GLU	Peptide
5	F	183	HIS	Sidechain
5	F	359	ARG	Sidechain
5	F	495	TYR	Sidechain
5	F	53	ARG	Sidechain
5	F	653	ARG	Sidechain
5	F	708	ARG	Sidechain
1	G	169	ARG	Sidechain
1	G	334	TYR	Sidechain
1	G	441	ARG	Sidechain
1	G	8	ARG	Sidechain
4	H	270	PHE	Sidechain
4	H	272	ARG	Sidechain
3	T	378	TYR	Sidechain
3	T	543	ARG	Sidechain
3	T	554	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	4305	0	4232	9	0
2	I	410	0	429	0	0
2	J	594	0	621	0	0
2	K	594	0	621	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	602	0	629	3	0
2	M	602	0	629	0	0
2	N	602	0	629	0	0
3	T	2735	0	2687	3	0
4	H	1941	0	1949	12	0
5	A	5942	0	5997	7	0
5	B	5878	0	5943	6	0
5	C	5702	0	5745	4	0
5	D	5623	0	5678	16	0
5	E	5656	0	5733	12	0
5	F	5807	0	5884	20	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	0	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	8	0	0	0	0
8	A	3	0	0	0	0
8	B	1	0	0	0	0
8	C	3	0	0	0	0
8	E	2	0	0	0	0
8	F	1	0	0	0	0
All	All	47367	0	47550	84	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 1.

All (84) 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)
5:F:177:ALA:HB1	5:F:178:PRO:CD	2.27	0.64
5:F:177:ALA:HB1	5:F:178:PRO:HD2	1.81	0.61
5:D:661:LEU:HD13	5:D:672:LEU:HD22	1.83	0.60
2:L:8:LEU:HD12	2:L:8:LEU:H	1.66	0.59
4:H:132:PHE:CE1	4:H:169:LEU:HD21	2.39	0.57
5:D:701:GLU:HG2	5:D:735:HIS:CE1	2.40	0.56
5:B:641:GLN:C	5:B:642:LEU:HD12	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:675:LEU:O	5:D:679:THR:HG23	2.07	0.53
4:H:228:PHE:CZ	5:F:115:HIS:CB	2.92	0.53
4:H:228:PHE:CZ	5:F:115:HIS:HB3	2.44	0.53
5:F:143:TYR:HA	5:F:177:ALA:HB2	1.92	0.51
5:F:53:ARG:H	5:F:53:ARG:HD2	1.76	0.51
1:G:342:ILE:HA	1:G:395:VAL:HG11	1.93	0.50
1:G:334:TYR:CD1	1:G:407:PRO:HA	2.47	0.50
5:F:143:TYR:CD2	5:F:177:ALA:CB	2.95	0.49
5:B:640:ASP:OD1	5:B:641:GLN:HG3	2.11	0.49
4:H:228:PHE:CZ	5:F:113:ARG:NH2	2.80	0.48
5:F:115:HIS:CD2	5:F:166:VAL:H	2.32	0.48
5:F:201:VAL:HG13	5:F:202:GLY:H	1.79	0.48
3:T:610:TRP:H	3:T:610:TRP:CD1	2.30	0.48
5:D:654:VAL:O	5:D:658:LYS:HG2	2.14	0.48
5:D:653:ARG:HD2	5:D:679:THR:OG1	2.14	0.48
6:C:902:ADP:C8	6:C:902:ADP:C5'	2.98	0.47
5:D:476:TRP:CE3	5:D:530:ALA:HB1	2.49	0.47
5:B:360:PHE:CG	5:A:413:ALA:HB2	2.49	0.47
5:F:359:ARG:HE	5:F:362:ARG:CZ	2.28	0.46
5:D:206:ILE:HD13	5:D:254:ILE:HG22	1.95	0.46
5:E:68:VAL:HG13	5:E:173:TYR:CE1	2.51	0.46
5:F:369:ILE:N	5:F:369:ILE:HD12	2.31	0.46
5:E:152:PHE:CE1	5:E:163:PHE:HB2	2.51	0.46
5:E:644:TYR:CZ	5:E:646:PRO:HA	2.51	0.46
5:E:679:THR:HB	5:E:682:PHE:CZ	2.51	0.45
4:H:28:VAL:HA	4:H:93:TYR:HB3	1.98	0.45
4:H:146:LEU:HD11	4:H:187:MET:HE2	1.99	0.45
5:D:484:ASP:O	5:D:488:GLU:HG2	2.17	0.45
3:T:511:GLN:HB2	4:H:147:ARG:HH11	1.82	0.45
1:G:130:CYS:HB3	1:G:132:HIS:CE1	2.53	0.44
5:D:484:ASP:HA	5:D:487:ARG:HE	1.82	0.44
5:E:477:GLU:H	5:E:477:GLU:CD	2.26	0.44
5:C:321:GLU:H	5:C:321:GLU:CD	2.26	0.44
5:F:136:LYS:HE3	5:F:182:ILE:HD12	2.00	0.43
1:G:6:ILE:H	1:G:71:HIS:CD2	2.36	0.43
5:F:638:ARG:HH21	5:F:638:ARG:HB2	1.83	0.43
5:C:694:ALA:HB1	5:C:735:HIS:CD2	2.53	0.43
1:G:405:ASP:C	1:G:407:PRO:HD2	2.44	0.43
5:E:496:PRO:HA	5:E:499:HIS:CD2	2.54	0.43
4:H:30:MET:HE3	4:H:106:GLU:OE1	2.18	0.43
5:E:498:GLU:C	5:E:500:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:550:MET:HE1	5:B:551:TRP:CZ2	2.54	0.43
5:A:771:PHE:CG	5:F:740:MET:HG2	2.54	0.43
5:C:168:THR:HG22	5:C:174:CYS:SG	2.58	0.43
5:B:424:ARG:HA	5:B:427:MET:HE2	1.99	0.43
5:A:268:LEU:HD23	5:A:269:ILE:N	2.33	0.42
1:G:156:GLU:HA	1:G:157:PRO:C	2.43	0.42
5:A:359:ARG:HH11	5:F:248:GLY:N	2.17	0.42
2:L:8:LEU:HD11	2:L:70:VAL:HA	2.01	0.42
5:E:668:LYS:HA	5:E:668:LYS:HE2	2.00	0.42
5:D:242:LEU:HD11	5:D:347:THR:HG22	2.00	0.42
4:H:127:PRO:HA	4:H:169:LEU:HA	2.02	0.42
5:D:240:GLY:HA3	5:D:363:PHE:CD1	2.54	0.42
4:H:45:LYS:HE3	4:H:149:PHE:O	2.20	0.41
5:A:131:PHE:CZ	5:A:136:LYS:HE3	2.55	0.41
3:T:429:ASN:HA	3:T:433:GLY:HA3	2.03	0.41
4:H:132:PHE:CZ	4:H:169:LEU:HD21	2.54	0.41
5:D:701:GLU:HA	5:D:704:GLU:HG3	2.03	0.41
5:D:653:ARG:HD2	5:D:679:THR:HG1	1.85	0.41
1:G:337:SER:HB2	1:G:406:ALA:HB1	2.03	0.41
5:A:762:LEU:C	5:A:762:LEU:HD13	2.46	0.41
5:B:72:LEU:HD23	5:B:73:SER:N	2.35	0.41
1:G:294:GLU:H	1:G:294:GLU:CD	2.29	0.41
5:E:682:PHE:CD2	5:E:745:ARG:HG2	2.56	0.41
5:D:748:SER:HB3	5:D:751:ASP:CG	2.46	0.41
5:A:359:ARG:HH11	5:F:248:GLY:H	1.69	0.41
5:F:177:ALA:CB	5:F:178:PRO:CD	2.98	0.41
5:D:189:ILE:HD13	5:D:189:ILE:HA	1.95	0.41
5:E:139:PHE:CD1	5:E:144:ARG:HB2	2.56	0.40
5:F:25:ARG:C	5:F:26:LEU:HD22	2.46	0.40
5:C:285:ASN:HA	5:C:288:LYS:HE2	2.02	0.40
5:F:253:LEU:C	5:F:253:LEU:HD23	2.47	0.40
5:E:567:ARG:HB2	5:E:611:MET:HE1	2.03	0.40
5:D:161:VAL:HG11	5:D:163:PHE:CZ	2.56	0.40
5:E:661:LEU:HD13	5:E:661:LEU:HA	1.96	0.40
1:G:347:PHE:HB3	1:G:367:PHE:CE2	2.57	0.40
2:L:68:HIS:CG	4:H:29:SER:HB3	2.57	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	G	536/608 (88%)	489 (91%)	41 (8%)	6 (1%)	11 45
2	I	50/76 (66%)	43 (86%)	5 (10%)	2 (4%)	2 18
2	J	74/76 (97%)	73 (99%)	1 (1%)	0	100 100
2	K	74/76 (97%)	69 (93%)	5 (7%)	0	100 100
2	L	74/76 (97%)	69 (93%)	5 (7%)	0	100 100
2	M	74/76 (97%)	73 (99%)	1 (1%)	0	100 100
2	N	74/76 (97%)	72 (97%)	2 (3%)	0	100 100
3	T	331/333 (99%)	313 (95%)	16 (5%)	2 (1%)	21 58
4	H	242/307 (79%)	220 (91%)	16 (7%)	6 (2%)	4 26
5	A	755/806 (94%)	710 (94%)	43 (6%)	2 (0%)	36 71
5	B	748/806 (93%)	701 (94%)	43 (6%)	4 (0%)	24 62
5	C	725/806 (90%)	659 (91%)	61 (8%)	5 (1%)	18 55
5	D	714/806 (89%)	660 (92%)	51 (7%)	3 (0%)	30 66
5	E	713/806 (88%)	654 (92%)	48 (7%)	11 (2%)	8 38
5	F	739/806 (92%)	684 (93%)	49 (7%)	6 (1%)	16 52
All	All	5923/6540 (91%)	5489 (93%)	387 (6%)	47 (1%)	18 52

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	245	SER
5	E	393	ASP
5	B	181	VAL
5	B	250	GLY
5	C	276	SER
1	G	13	ASP
1	G	289	GLU
1	G	317	SER

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Mol	Chain	Res	Type
1	G	440	ALA
4	H	194	PRO
5	E	507	GLY
4	H	186	ASP
4	H	260	ASN
5	E	64	ARG
5	E	668	LYS
5	B	140	LEU
5	F	62	LYS
5	D	75	ASP
1	G	147	PHE
4	H	257	GLY
5	E	166	VAL
5	E	200	GLU
5	E	201	VAL
5	E	671	ASP
5	A	638	ARG
5	F	143	TYR
5	C	363	PHE
3	T	583	GLY
5	F	201	VAL
5	F	639	LEU
5	C	140	LEU
2	I	6	LYS
3	T	458	ARG
5	F	729	PRO
5	C	392	ASP
5	C	118	PRO
5	D	188	PRO
1	G	422	PRO
4	H	193	ALA
2	I	19	PRO
5	E	32	ILE
5	E	104	PRO
5	D	236	LYS
5	E	189	ILE
5	B	369	ILE
5	A	166	VAL
5	F	145	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	G	479/531 (90%)	465 (97%)	14 (3%)	37	58
2	I	47/68 (69%)	43 (92%)	4 (8%)	10	30
2	J	66/68 (97%)	65 (98%)	1 (2%)	57	70
2	K	66/68 (97%)	64 (97%)	2 (3%)	36	57
2	L	68/68 (100%)	63 (93%)	5 (7%)	13	34
2	M	68/68 (100%)	66 (97%)	2 (3%)	37	58
2	N	68/68 (100%)	68 (100%)	0	100	100
3	T	298/298 (100%)	281 (94%)	17 (6%)	18	41
4	H	218/267 (82%)	210 (96%)	8 (4%)	30	51
5	A	643/679 (95%)	622 (97%)	21 (3%)	33	55
5	B	635/679 (94%)	621 (98%)	14 (2%)	45	64
5	C	612/679 (90%)	589 (96%)	23 (4%)	29	51
5	D	606/679 (89%)	590 (97%)	16 (3%)	40	60
5	E	616/679 (91%)	597 (97%)	19 (3%)	35	56
5	F	627/679 (92%)	595 (95%)	32 (5%)	21	44
All	All	5117/5578 (92%)	4939 (96%)	178 (4%)	32	54

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	128	GLN
1	G	159	VAL
1	G	163	SER
1	G	257	THR
1	G	258	GLU
1	G	279	ILE
1	G	294	GLU
1	G	326	ARG
1	G	335	PHE
1	G	354	MET

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Mol	Chain	Res	Type
1	G	373	THR
1	G	417	SER
1	G	443	LEU
1	G	551	THR
2	I	3	ILE
2	I	5	VAL
2	I	16	GLU
2	I	27	LYS
2	J	55	THR
2	K	52	ASP
2	K	74	ARG
2	L	7	THR
2	L	44	ILE
2	L	70	VAL
2	L	73	LEU
2	L	74	ARG
2	M	60	ASN
2	M	62	GLN
3	T	320	SER
3	T	334	LEU
3	T	374	LEU
3	T	380	HIS
3	T	431	HIS
3	T	432	PHE
3	T	443	GLN
3	T	461	ASN
3	T	464	LEU
3	T	465	ASN
3	T	505	GLU
3	T	515	TYR
3	T	519	LEU
3	T	529	HIS
3	T	579	ARG
3	T	602	PHE
3	T	625	THR
4	H	28	VAL
4	H	40	VAL
4	H	149	PHE
4	H	162	TYR
4	H	186	ASP
4	H	194	PRO
4	H	195	LEU

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Mol	Chain	Res	Type
4	H	244	PRO
5	E	33	ASN
5	E	35	ASP
5	E	38	VAL
5	E	68	VAL
5	E	84	MET
5	E	210	ARG
5	E	232	GLU
5	E	281	GLU
5	E	323	ARG
5	E	450	ASP
5	E	487	ARG
5	E	497	VAL
5	E	509	THR
5	E	549	THR
5	E	603	GLN
5	E	661	LEU
5	E	674	PHE
5	E	704	GLU
5	E	750	ASN
5	B	22	ARG
5	B	30	GLU
5	B	69	CYS
5	B	140	LEU
5	B	163	PHE
5	B	173	TYR
5	B	175	ILE
5	B	176	VAL
5	B	185	GLU
5	B	190	LYS
5	B	292	GLU
5	B	403	THR
5	B	555	SER
5	B	649	ASP
5	A	35	ASP
5	A	36	ASN
5	A	38	VAL
5	A	46	MET
5	A	85	ASN
5	A	126	ILE
5	A	134	TYR
5	A	166	VAL

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Mol	Chain	Res	Type
5	A	182	ILE
5	A	268	LEU
5	A	332	MET
5	A	403	THR
5	A	427	MET
5	A	550	MET
5	A	555	SER
5	A	565	LYS
5	A	649	ASP
5	A	712	GLU
5	A	723	GLU
5	A	740	MET
5	A	772	ARG
5	F	14	THR
5	F	35	ASP
5	F	38	VAL
5	F	58	LEU
5	F	69	CYS
5	F	95	ARG
5	F	103	GLN
5	F	112	LYS
5	F	113	ARG
5	F	115	HIS
5	F	137	PRO
5	F	141	GLU
5	F	155	ARG
5	F	161	VAL
5	F	181	VAL
5	F	183	HIS
5	F	185	GLU
5	F	192	GLU
5	F	272	PRO
5	F	332	MET
5	F	368	ASP
5	F	369	ILE
5	F	403	THR
5	F	427	MET
5	F	430	ILE
5	F	435	GLU
5	F	536	GLN
5	F	549	THR
5	F	638	ARG

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Mol	Chain	Res	Type
5	F	649	ASP
5	F	711	ARG
5	F	734	ASP
5	C	39	VAL
5	C	59	LEU
5	C	64	ARG
5	C	103	GLN
5	C	143	TYR
5	C	171	SER
5	C	174	CYS
5	C	283	GLU
5	C	292	GLU
5	C	321	GLU
5	C	369	ILE
5	C	423	ILE
5	C	426	LYS
5	C	536	GLN
5	C	554	GLU
5	C	574	LEU
5	C	650	GLU
5	C	693	ARG
5	C	700	ARG
5	C	711	ARG
5	C	749	ASP
5	C	754	LYS
5	C	768	PHE
5	D	79	ASP
5	D	124	GLU
5	D	146	ILE
5	D	171	SER
5	D	174	CYS
5	D	175	ILE
5	D	222	LEU
5	D	230	PHE
5	D	232	GLU
5	D	314	GLU
5	D	321	GLU
5	D	322	ARG
5	D	325	VAL
5	D	390	LEU
5	D	392	ASP
5	D	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	10	GLN
1	G	49	ASN
1	G	71	HIS
1	G	132	HIS
1	G	153	ASN
1	G	330	ASN
1	G	469	ASN
1	G	494	GLN
1	G	541	GLN
2	I	25	ASN
2	K	40	GLN
2	N	40	GLN
2	M	41	GLN
3	T	326	ASN
3	T	461	ASN
3	T	465	ASN
3	T	597	GLN
4	H	144	ASN
5	E	285	ASN
5	E	340	HIS
5	E	406	HIS
5	E	499	HIS
5	E	533	ASN
5	E	603	GLN
5	B	226	HIS
5	B	270	ASN
5	B	317	HIS
5	B	348	ASN
5	B	538	ASN
5	B	763	GLN
5	B	764	GLN
5	A	398	GLN
5	A	458	GLN
5	A	460	ASN
5	F	90	ASN
5	F	212	GLN
5	F	602	ASN
5	C	337	GLN
5	C	494	GLN
5	C	578	GLN
5	C	603	GLN

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Mol	Chain	Res	Type
5	C	624	ASN
5	D	129	ASN
5	D	317	HIS
5	D	401	ASN
5	D	443	ASN
5	D	499	HIS
5	D	533	ASN
5	D	602	ASN
5	D	692	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	902	7,8	27,29,29	1.07	1 (3%)	42,45,45	1.39	6 (14%)
6	ADP	A	904	7	27,29,29	1.08	2 (7%)	42,45,45	1.36	6 (14%)
6	ADP	F	901	7,8	27,29,29	1.17	3 (11%)	42,45,45	1.49	8 (19%)
6	ADP	D	901	-	27,29,29	0.95	1 (3%)	42,45,45	1.41	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	ADP	F	902	7,8	27,29,29	1.11	1 (3%)	42,45,45	1.66	7 (16%)
6	ADP	B	904	7,8	27,29,29	1.03	1 (3%)	42,45,45	1.50	9 (21%)
6	ADP	E	904	7,8	27,29,29	1.12	3 (11%)	42,45,45	1.44	8 (19%)
7	BEF	E	905	6	0,3,3	-	-	-		
6	ADP	A	907	7,8	27,29,29	1.04	1 (3%)	42,45,45	1.39	7 (16%)
6	ADP	C	905	7,8	27,29,29	0.97	0	42,45,45	1.37	7 (16%)
7	BEF	A	905	6	0,3,3	-	-	-		
7	BEF	E	902	6	0,3,3	-	-	-		
6	ADP	E	901	7,8	27,29,29	1.04	2 (7%)	42,45,45	1.64	10 (23%)
7	BEF	A	903	6	0,3,3	-	-	-		
7	BEF	B	905	6	0,3,3	-	-	-		
7	BEF	B	903	6	0,3,3	-	-	-		
6	ADP	D	902	-	27,29,29	0.93	0	42,45,45	1.23	5 (11%)
7	BEF	A	901	6	0,3,3	-	-	-		
6	ADP	C	902	7,8	27,29,29	0.98	0	42,45,45	1.43	9 (21%)
7	BEF	B	901	6	0,3,3	-	-	-		
7	BEF	C	903	6	0,3,3	-	-	-		
7	BEF	C	906	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	B	902	7,8	-	4/16/32/32	0/3/3/3
6	ADP	F	902	7,8	-	4/16/32/32	0/3/3/3
6	ADP	B	904	7,8	-	0/16/32/32	0/3/3/3
6	ADP	A	907	7,8	-	3/16/32/32	0/3/3/3
6	ADP	A	904	7	-	3/16/32/32	0/3/3/3
6	ADP	C	905	7,8	-	5/16/32/32	0/3/3/3
6	ADP	E	904	7,8	-	3/16/32/32	0/3/3/3
6	ADP	D	902	-	-	3/16/32/32	0/3/3/3
6	ADP	C	902	7,8	-	4/16/32/32	0/3/3/3
6	ADP	E	901	7,8	-	4/16/32/32	0/3/3/3
6	ADP	F	901	7,8	-	4/16/32/32	0/3/3/3
6	ADP	D	901	-	-	0/16/32/32	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	901	ADP	C5-C4	-2.52	1.34	1.39
6	E	901	ADP	C5-C4	-2.46	1.34	1.39
6	E	904	ADP	C5-C4	-2.44	1.34	1.39
6	F	902	ADP	C5-C4	-2.41	1.34	1.39
6	B	902	ADP	C5-C4	-2.37	1.34	1.39
6	A	904	ADP	C5-C4	-2.37	1.34	1.39
6	A	907	ADP	C5-C4	-2.36	1.34	1.39
6	F	901	ADP	PB-O2B	-2.28	1.46	1.54
6	E	904	ADP	PB-O3B	-2.18	1.46	1.54
6	E	901	ADP	PB-O2B	-2.15	1.46	1.54
6	B	904	ADP	C5-C4	-2.13	1.35	1.39
6	D	901	ADP	C5-C4	-2.11	1.35	1.39
6	F	901	ADP	C4-N9	-2.05	1.33	1.37
6	E	904	ADP	PB-O2B	-2.05	1.47	1.54
6	A	904	ADP	PB-O3B	-2.01	1.47	1.54

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	902	ADP	PA-O3A-PB	-5.47	114.05	132.83
6	F	902	ADP	O2B-PB-O3A	5.03	121.50	104.64
6	E	901	ADP	PA-O3A-PB	-4.58	117.11	132.83
6	B	904	ADP	PA-O3A-PB	-4.55	117.21	132.83
6	F	901	ADP	PA-O3A-PB	-4.44	117.58	132.83
6	A	907	ADP	PA-O3A-PB	-4.01	119.08	132.83
6	B	902	ADP	PA-O3A-PB	-3.99	119.13	132.83
6	E	901	ADP	O2B-PB-O3A	3.89	117.67	104.64
6	A	904	ADP	O2B-PB-O3A	3.73	117.14	104.64
6	E	904	ADP	PA-O3A-PB	-3.64	120.34	132.83
6	D	901	ADP	PA-O3A-PB	-3.36	121.28	132.83
6	C	905	ADP	O2B-PB-O3A	3.36	115.91	104.64
6	E	904	ADP	C4-C5-N7	3.32	114.66	110.62
6	A	904	ADP	PA-O3A-PB	-3.28	121.57	132.83
6	F	901	ADP	O3B-PB-O2B	-3.24	95.26	107.64
6	C	902	ADP	PA-O3A-PB	-3.17	121.94	132.83
6	D	901	ADP	C5-C4-N3	-3.16	122.63	126.75
6	C	902	ADP	C5-C4-N3	-3.12	122.68	126.75
6	C	905	ADP	C5-C4-N3	-3.12	122.68	126.75
6	D	902	ADP	PA-O3A-PB	-3.09	122.23	132.83
6	B	902	ADP	O3B-PB-O1B	-3.01	98.90	110.68
6	B	904	ADP	C5-C4-N3	-2.94	122.92	126.75
6	F	901	ADP	O2B-PB-O3A	2.93	114.45	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	901	ADP	C4-C5-N7	2.92	114.17	110.62
6	B	904	ADP	O3B-PB-O3A	2.91	114.40	104.64
6	C	905	ADP	PA-O3A-PB	-2.91	122.85	132.83
6	D	901	ADP	O2B-PB-O3A	2.90	114.37	104.64
6	A	904	ADP	C5-C4-N3	-2.83	123.06	126.75
6	A	907	ADP	C5-C4-N3	-2.82	123.06	126.75
6	C	902	ADP	C4-C5-N7	2.81	114.04	110.62
6	F	902	ADP	C4-C5-N7	2.77	114.00	110.62
6	D	902	ADP	C5-C4-N3	-2.76	123.15	126.75
6	D	902	ADP	C4-C5-N7	2.74	113.95	110.62
6	A	907	ADP	C4-C5-N7	2.72	113.93	110.62
6	F	901	ADP	C4-C5-N7	2.70	113.91	110.62
6	D	901	ADP	C4-C5-N7	2.70	113.91	110.62
6	A	907	ADP	O2B-PB-O3A	2.69	113.67	104.64
6	E	901	ADP	O3B-PB-O2B	-2.69	97.34	107.64
6	B	902	ADP	C5-C4-N3	-2.67	123.27	126.75
6	D	901	ADP	C5-C6-N1	2.63	123.04	117.39
6	B	902	ADP	C4-C5-N7	2.60	113.78	110.62
6	D	901	ADP	N3-C4-N9	2.59	131.35	127.08
6	B	904	ADP	C5-C6-N1	2.58	122.93	117.39
6	C	905	ADP	C4-C5-N7	2.57	113.75	110.62
6	A	904	ADP	C5-C6-N1	2.57	122.91	117.39
6	E	901	ADP	O3B-PB-O3A	2.56	113.24	104.64
6	B	902	ADP	C5-C6-N1	2.53	122.82	117.39
6	E	904	ADP	C5-C6-N1	2.53	122.81	117.39
6	E	901	ADP	C5-C6-N1	2.52	122.80	117.39
6	B	904	ADP	C4-C5-N7	2.51	113.67	110.62
6	A	907	ADP	C5-C6-N1	2.51	122.78	117.39
6	F	902	ADP	C5-C4-N3	-2.50	123.49	126.75
6	E	901	ADP	C5-C4-N3	-2.46	123.53	126.75
6	A	904	ADP	C4-C5-N7	2.45	113.60	110.62
6	D	902	ADP	C5-C6-N1	2.43	122.61	117.39
6	E	901	ADP	O3B-PB-O1B	-2.43	101.17	110.68
6	F	901	ADP	C5-C6-N1	2.43	122.60	117.39
6	C	902	ADP	O4'-C1'-C2'	-2.36	101.49	106.64
6	C	905	ADP	C5-C6-N1	2.36	122.45	117.39
6	C	902	ADP	C5-C6-N1	2.35	122.44	117.39
6	C	902	ADP	N3-C4-N9	2.35	130.95	127.08
6	C	905	ADP	N3-C4-N9	2.29	130.86	127.08
6	F	901	ADP	N6-C6-N1	-2.28	113.36	118.35
6	A	904	ADP	C2-N1-C6	-2.28	114.86	118.77
6	F	902	ADP	C5-C6-N1	2.27	122.26	117.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	904	ADP	N6-C6-N1	-2.27	113.39	118.35
6	D	901	ADP	C2-N1-C6	-2.27	114.88	118.77
6	E	904	ADP	C5-C4-N3	-2.26	123.81	126.75
6	C	902	ADP	C2'-C1'-N9	2.25	119.00	113.30
6	E	904	ADP	O2B-PB-O3A	2.23	112.11	104.64
6	F	902	ADP	O2B-PB-O1B	-2.23	101.96	110.68
6	E	904	ADP	O3B-PB-O1B	-2.22	101.98	110.68
6	A	907	ADP	N3-C4-N9	2.22	130.74	127.08
6	C	905	ADP	O3B-PB-O1B	-2.22	102.00	110.68
6	C	902	ADP	C2-N1-C6	-2.17	115.04	118.77
6	A	907	ADP	C2-N1-C6	-2.17	115.05	118.77
6	B	904	ADP	C2-N1-C6	-2.13	115.12	118.77
6	F	901	ADP	C5-C4-N3	-2.12	123.98	126.75
6	B	904	ADP	O2B-PB-O3A	2.11	111.70	104.64
6	E	901	ADP	C2-N1-C6	-2.11	115.15	118.77
6	F	902	ADP	N3-C4-N9	2.09	130.52	127.08
6	B	904	ADP	N3-C4-N9	2.08	130.51	127.08
6	D	902	ADP	N3-C4-N9	2.07	130.49	127.08
6	D	901	ADP	O3B-PB-O3A	2.06	111.56	104.64
6	E	904	ADP	O3B-PB-O3A	2.06	111.56	104.64
6	B	902	ADP	C2-N1-C6	-2.05	115.24	118.77
6	F	901	ADP	C1'-N9-C8	2.05	131.76	127.14
6	E	901	ADP	N3-C4-N9	2.05	130.46	127.08
6	E	904	ADP	C1'-N9-C8	2.01	131.68	127.14
6	C	902	ADP	C6-C5-N7	-2.01	128.27	132.02

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	907	ADP	C5'-O5'-PA-O1A
6	F	901	ADP	PA-O3A-PB-O2B
6	C	905	ADP	C5'-O5'-PA-O2A
6	C	905	ADP	C4'-C5'-O5'-PA
6	E	904	ADP	O4'-C4'-C5'-O5'
6	E	904	ADP	C3'-C4'-C5'-O5'
6	A	904	ADP	O4'-C4'-C5'-O5'
6	A	904	ADP	C3'-C4'-C5'-O5'
6	D	902	ADP	C3'-C4'-C5'-O5'
6	D	902	ADP	O4'-C4'-C5'-O5'
6	E	901	ADP	O4'-C4'-C5'-O5'
6	E	901	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	B	902	ADP	O4'-C4'-C5'-O5'
6	F	901	ADP	O4'-C4'-C5'-O5'
6	F	901	ADP	C3'-C4'-C5'-O5'
6	F	902	ADP	O4'-C4'-C5'-O5'
6	B	902	ADP	C3'-C4'-C5'-O5'
6	C	902	ADP	C4'-C5'-O5'-PA
6	F	902	ADP	C3'-C4'-C5'-O5'
6	D	902	ADP	C4'-C5'-O5'-PA
6	C	902	ADP	O4'-C4'-C5'-O5'
6	C	905	ADP	O4'-C4'-C5'-O5'
6	E	901	ADP	C4'-C5'-O5'-PA
6	A	907	ADP	C5'-O5'-PA-O3A
6	C	905	ADP	C5'-O5'-PA-O3A
6	E	904	ADP	C4'-C5'-O5'-PA
6	A	904	ADP	C4'-C5'-O5'-PA
6	A	907	ADP	C5'-O5'-PA-O2A
6	C	905	ADP	C5'-O5'-PA-O1A
6	C	902	ADP	C3'-C4'-C5'-O5'
6	E	901	ADP	PB-O3A-PA-O1A
6	F	901	ADP	PA-O3A-PB-O1B
6	B	902	ADP	PA-O3A-PB-O2B
6	B	902	ADP	PA-O3A-PB-O3B
6	F	902	ADP	C5'-O5'-PA-O3A
6	C	902	ADP	PB-O3A-PA-O2A
6	F	902	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

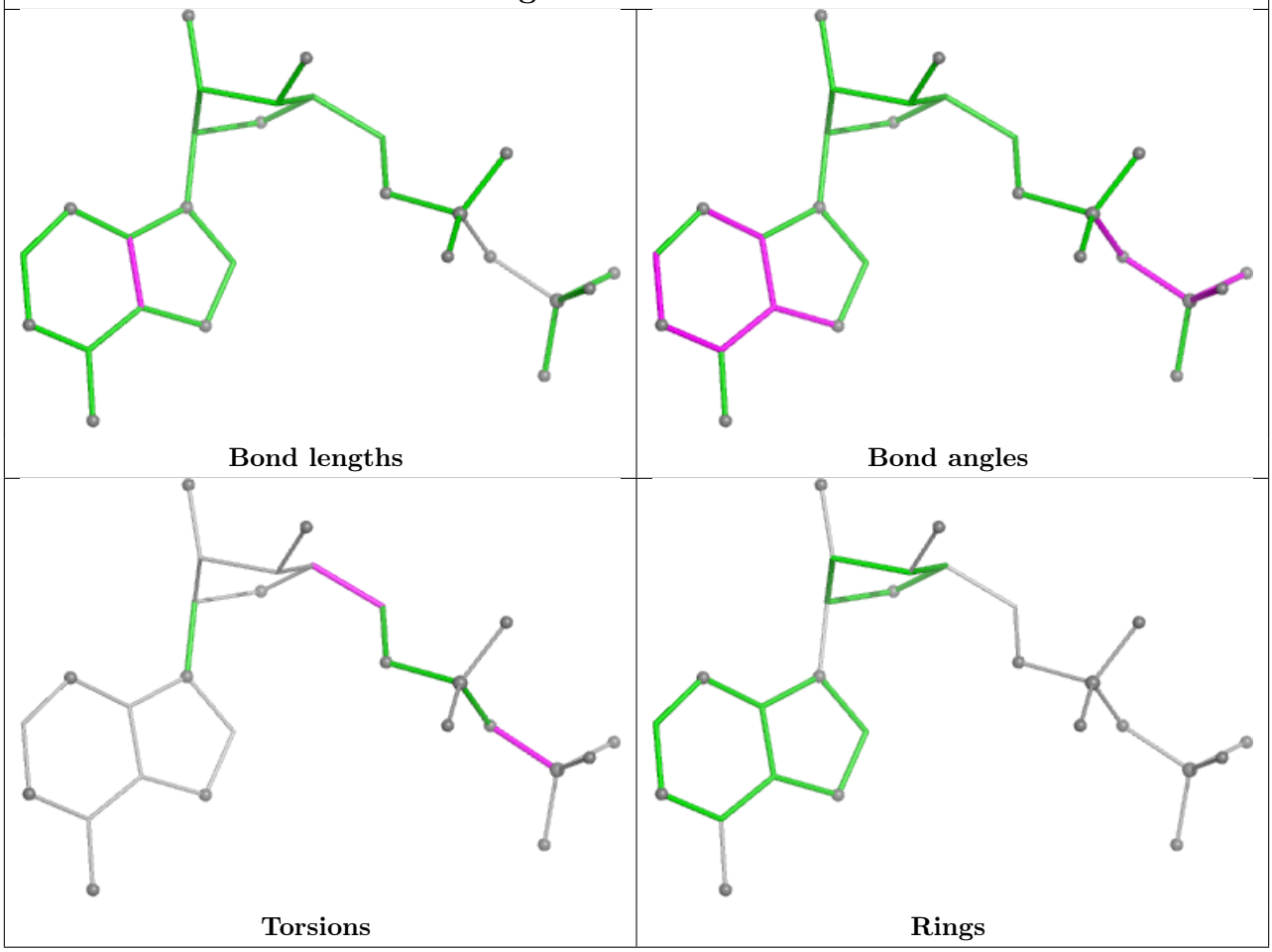
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	902	ADP	1	0

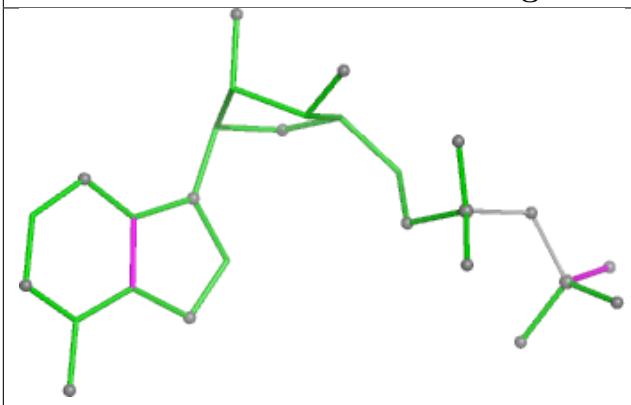
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

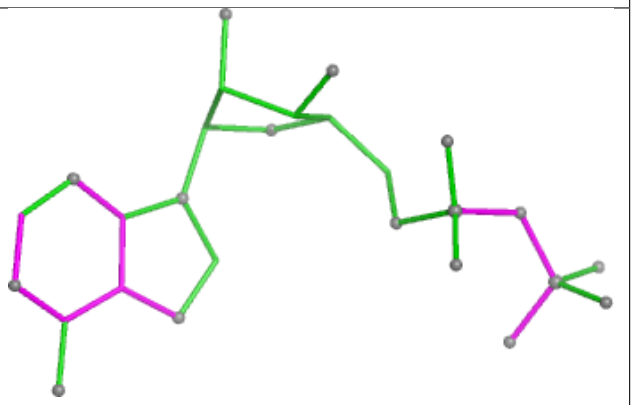
Ligand ADP B 902



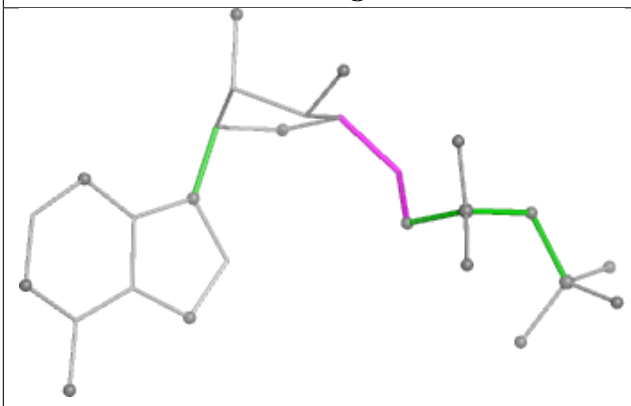
Ligand ADP A 904



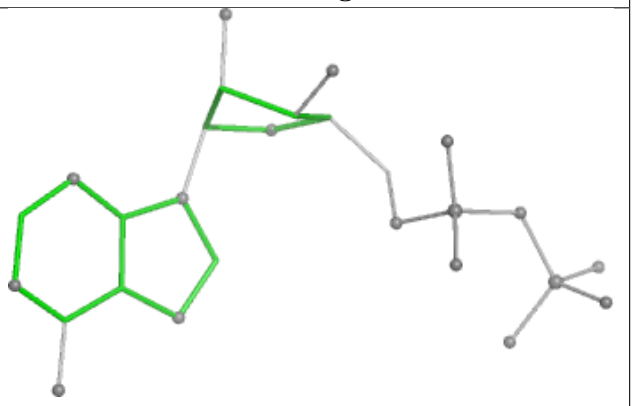
Bond lengths



Bond angles

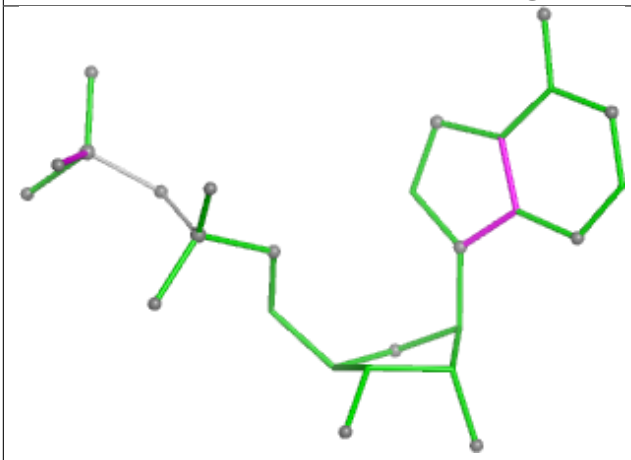


Torsions

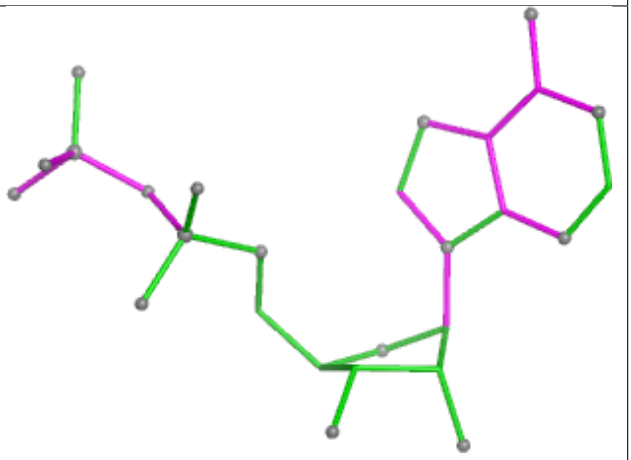


Rings

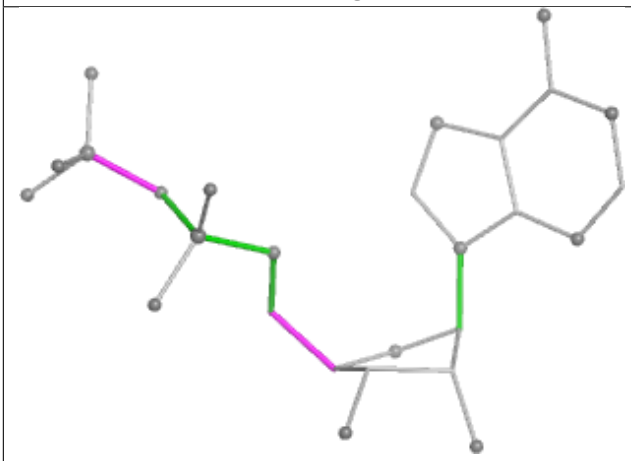
Ligand ADP F 901



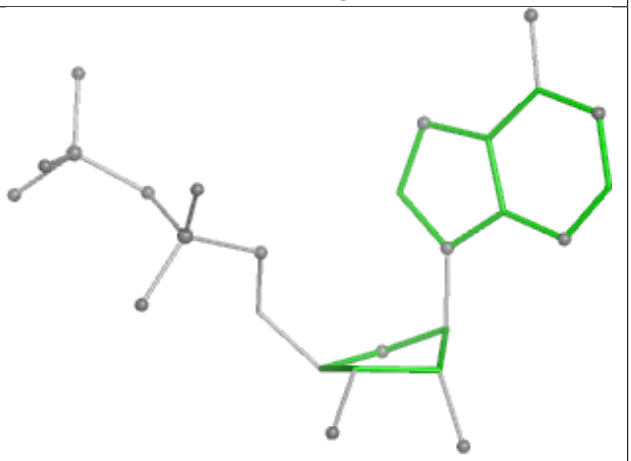
Bond lengths



Bond angles

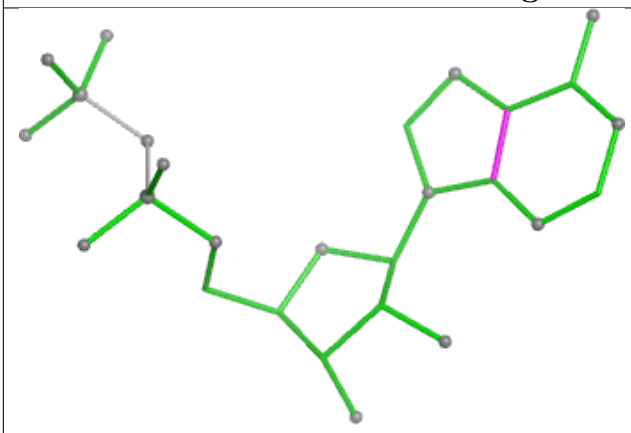


Torsions

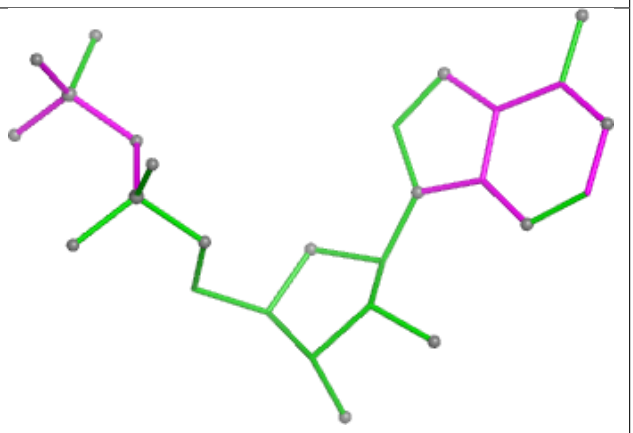


Rings

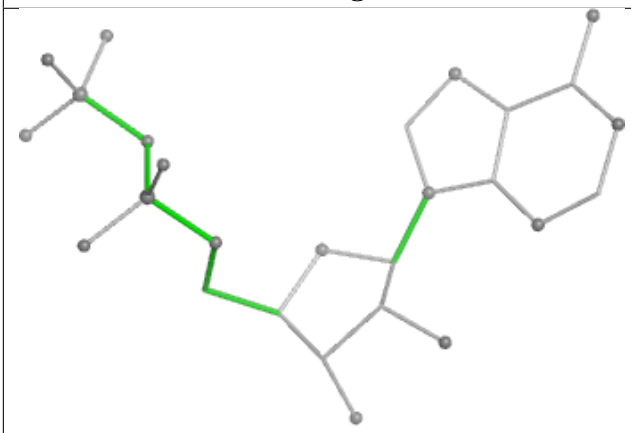
Ligand ADP D 901



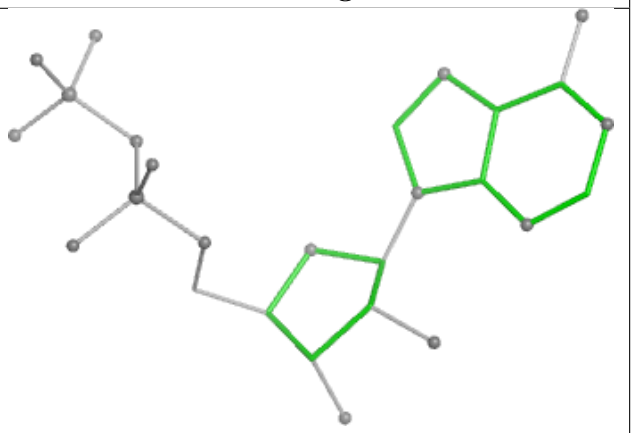
Bond lengths



Bond angles

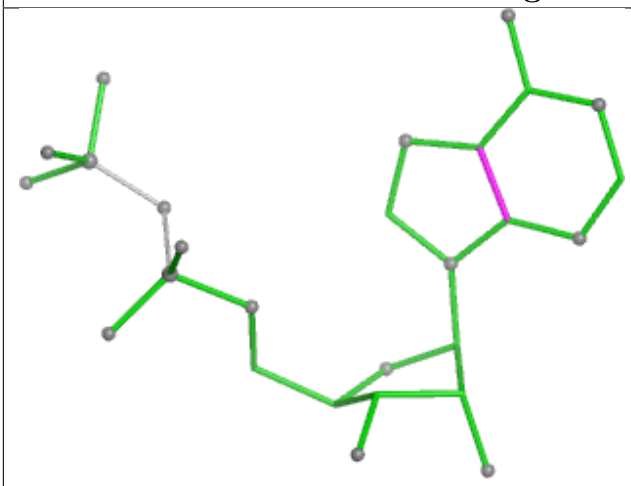


Torsions

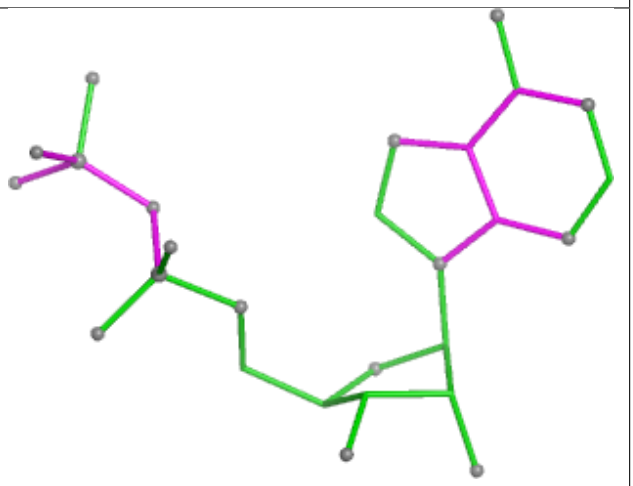


Rings

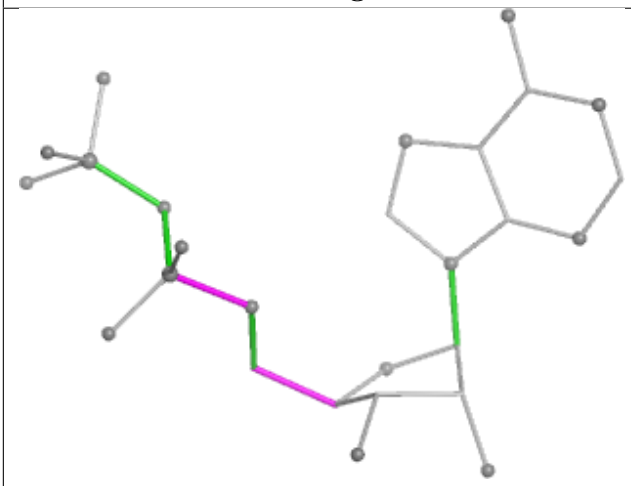
Ligand ADP F 902



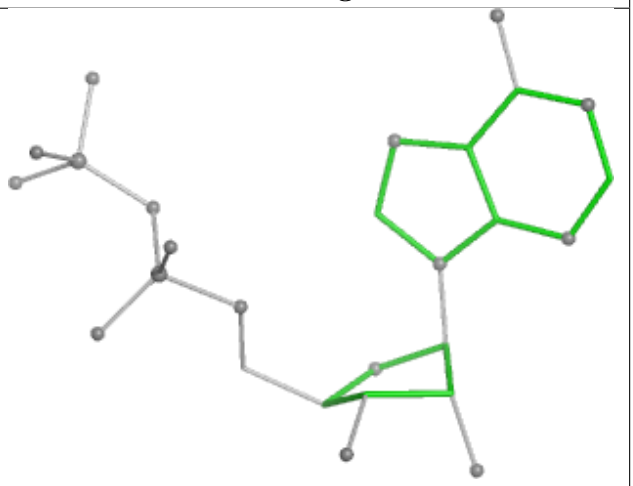
Bond lengths



Bond angles

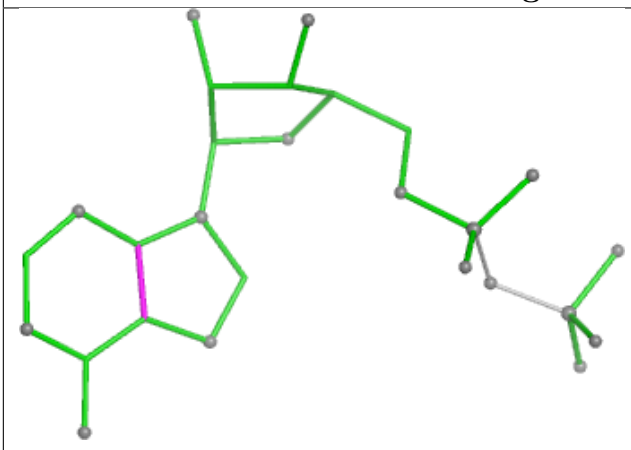


Torsions

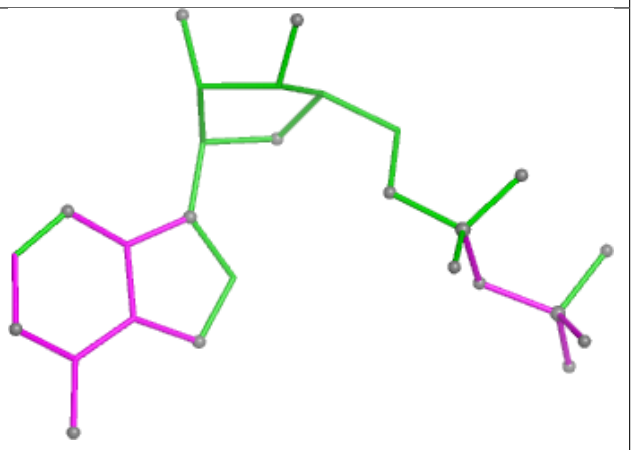


Rings

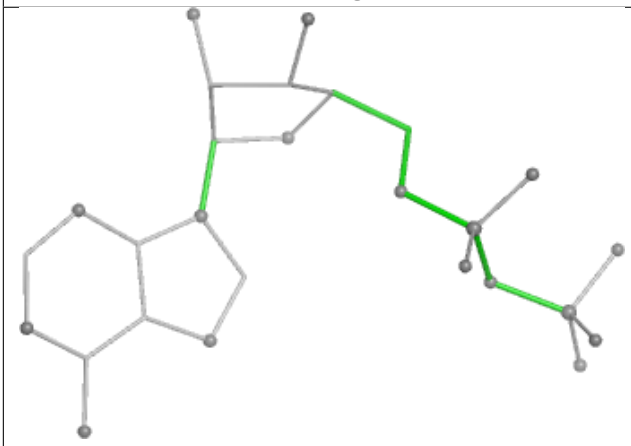
Ligand ADP B 904



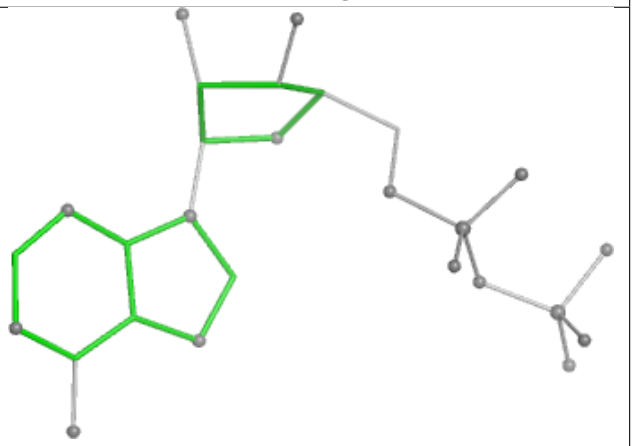
Bond lengths



Bond angles

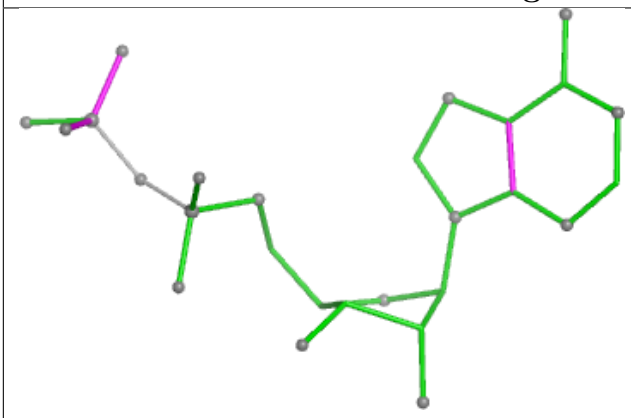


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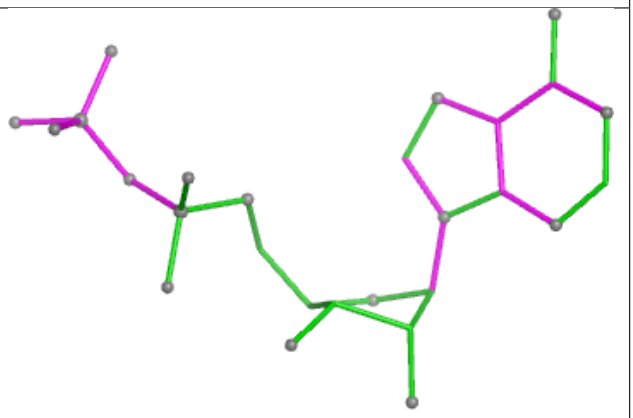


Rings

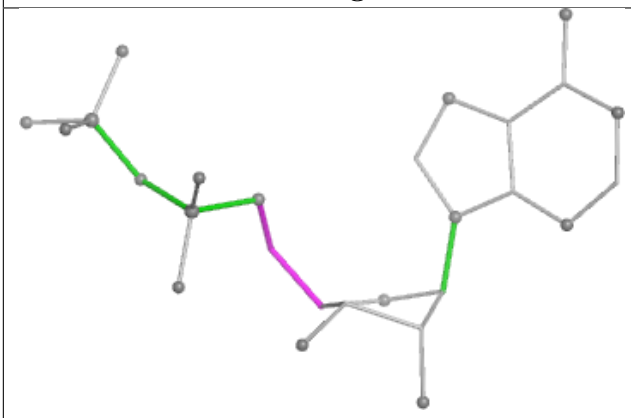
Ligand ADP E 904



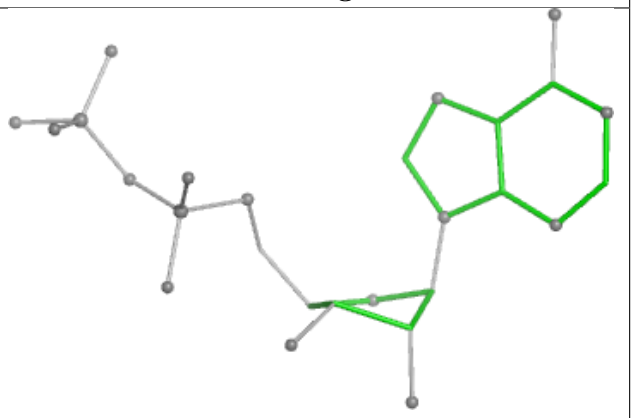
Bond lengths



Bond angles

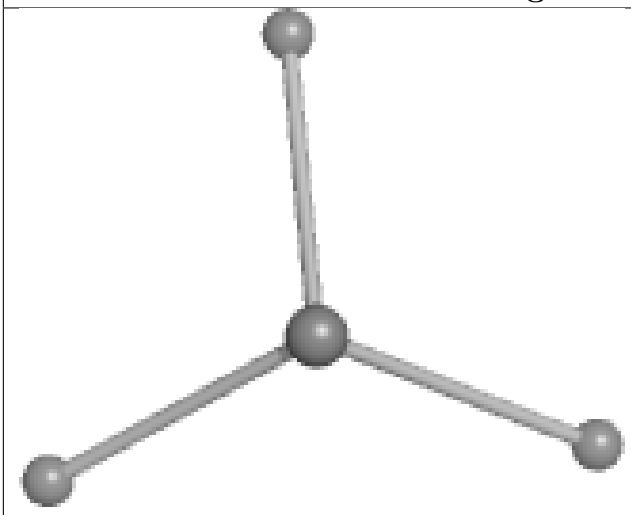


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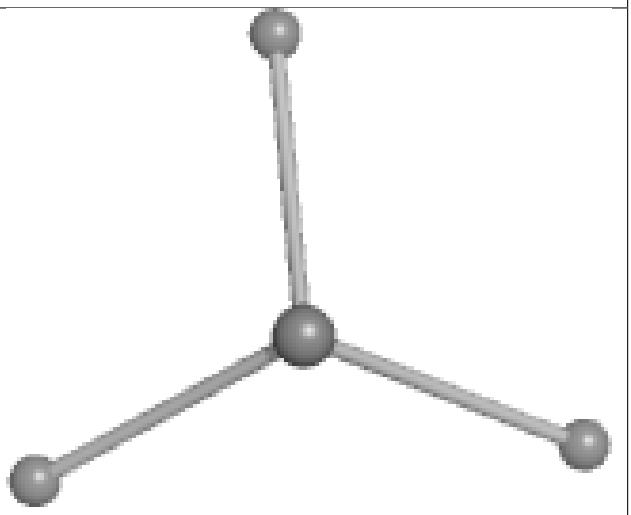


Rings

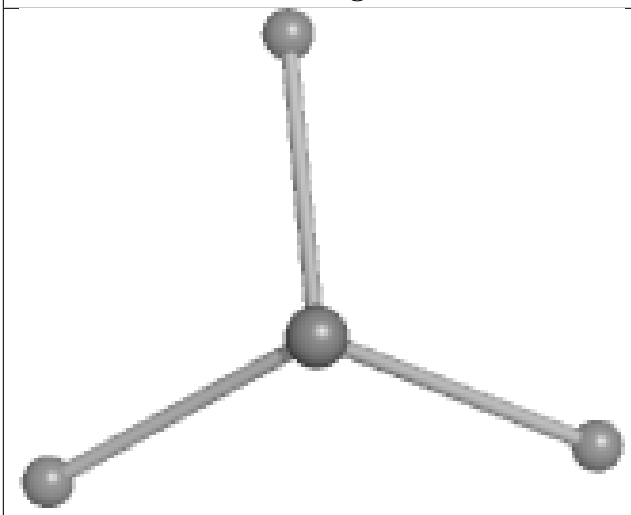
Ligand BEF E 905



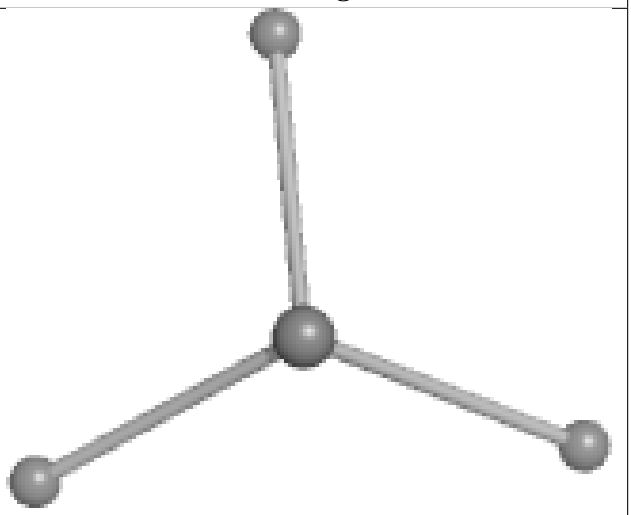
Bond lengths



Bond angles

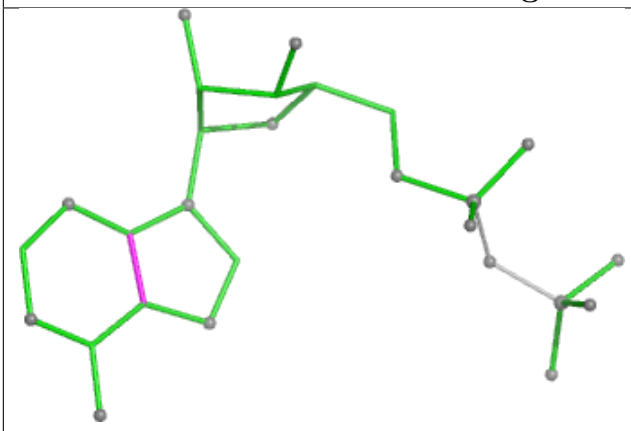


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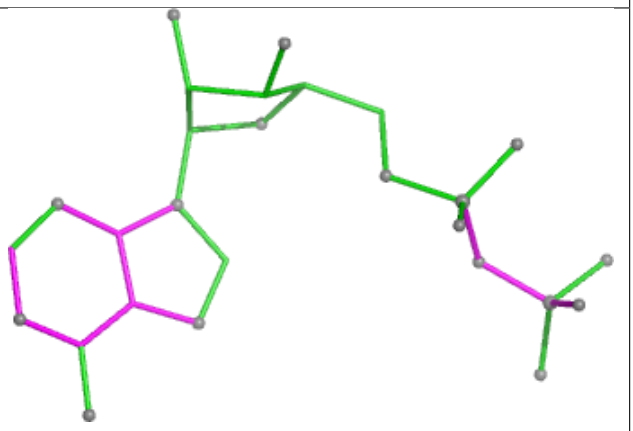


Rings

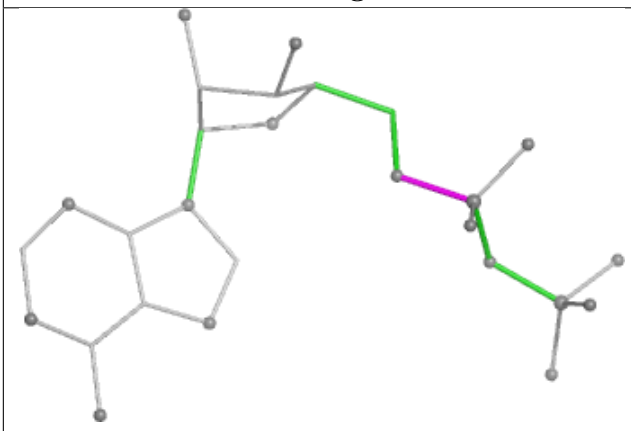
Ligand ADP A 907



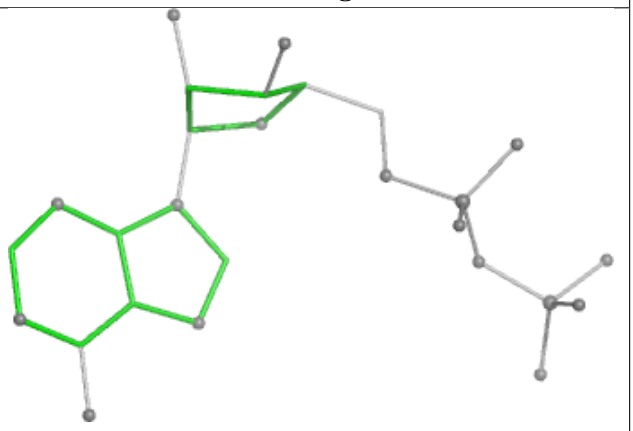
Bond lengths



Bond angles

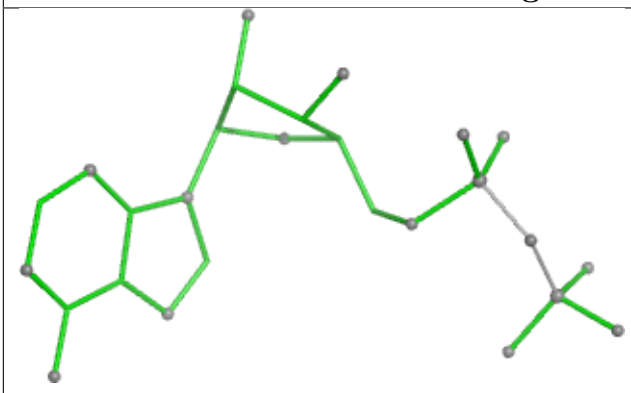


Torsions

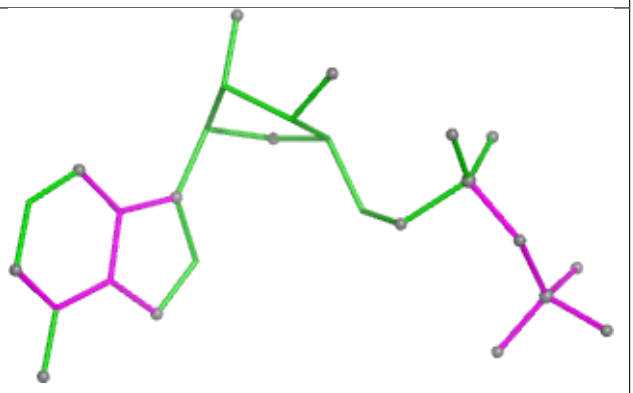


Rings

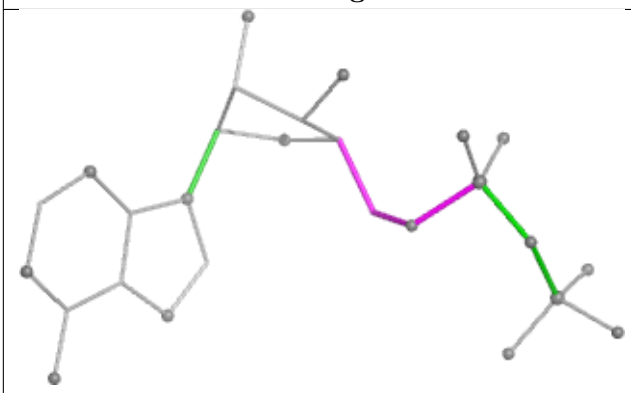
Ligand ADP C 905



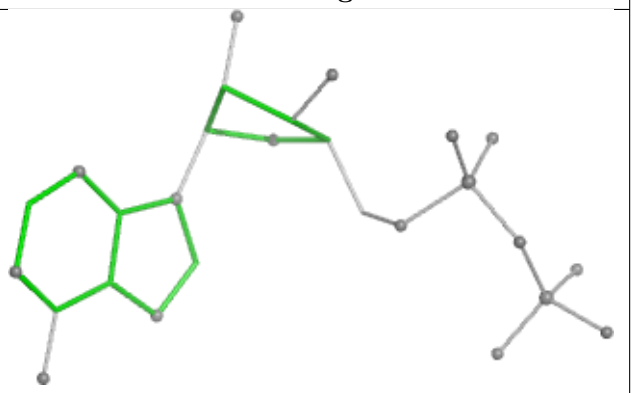
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Bond angles

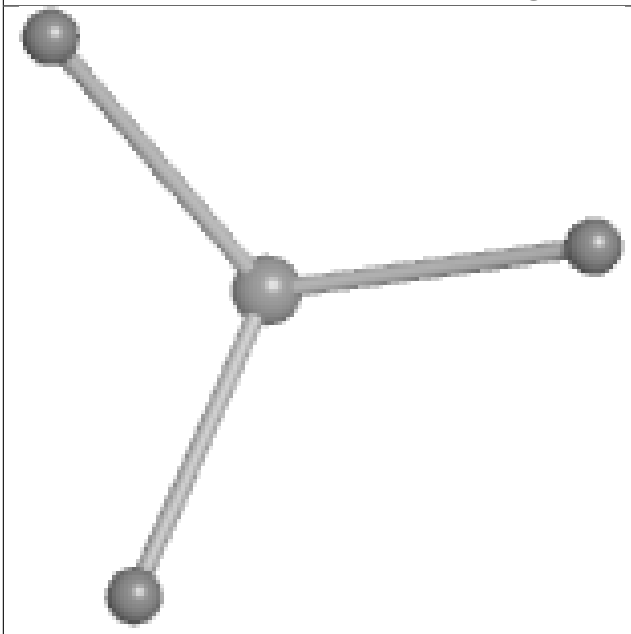


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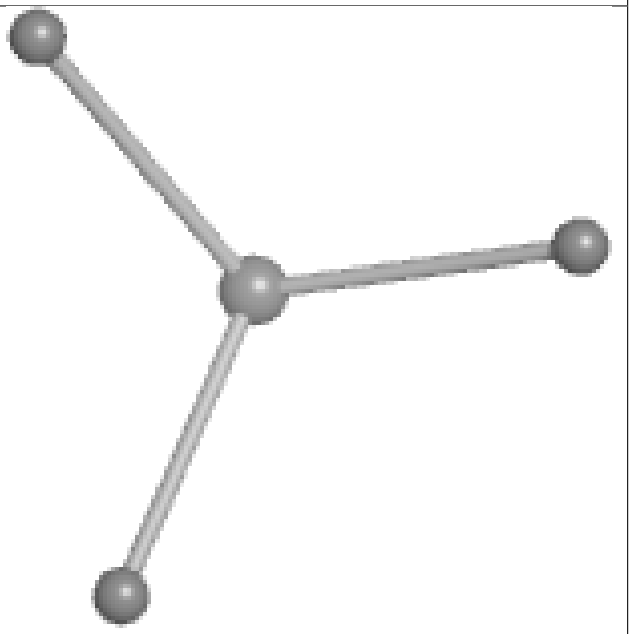


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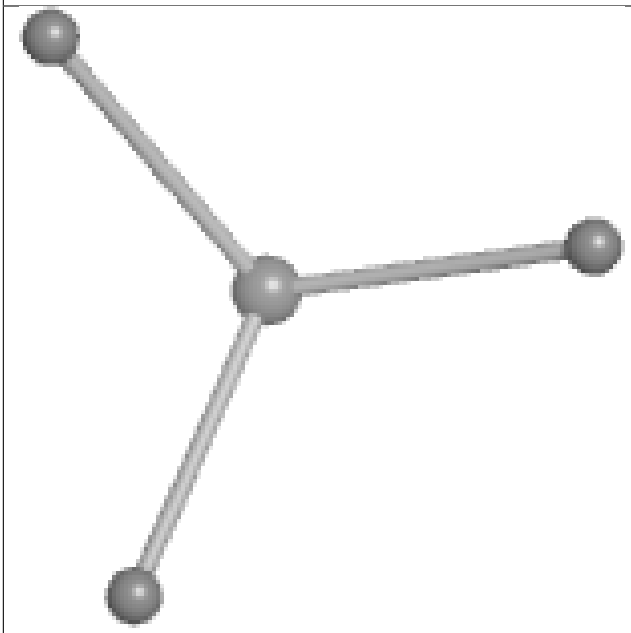
Ligand BEF A 905



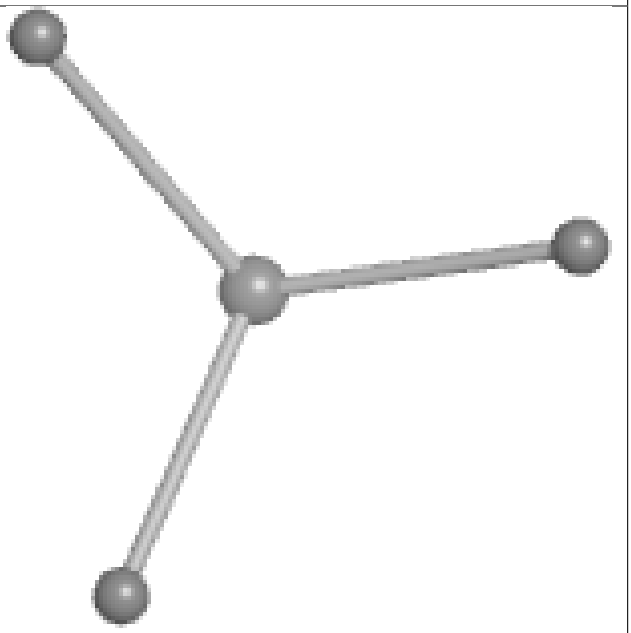
Bond lengths



Bond angles

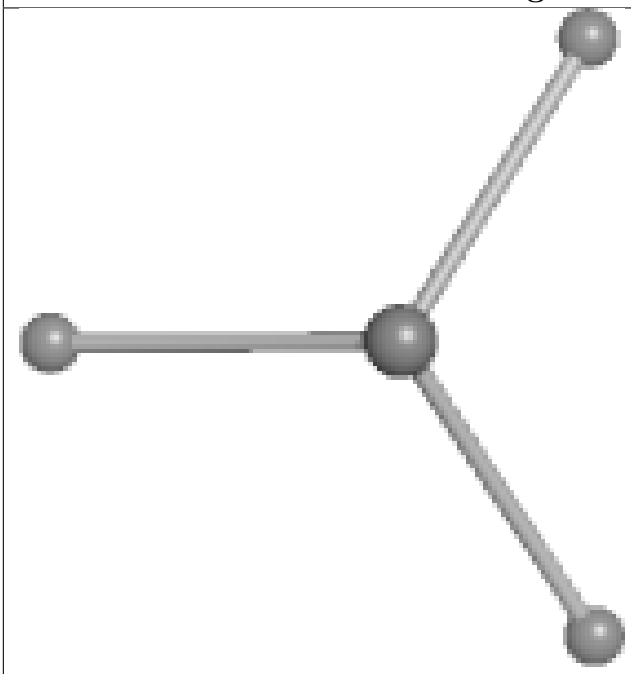


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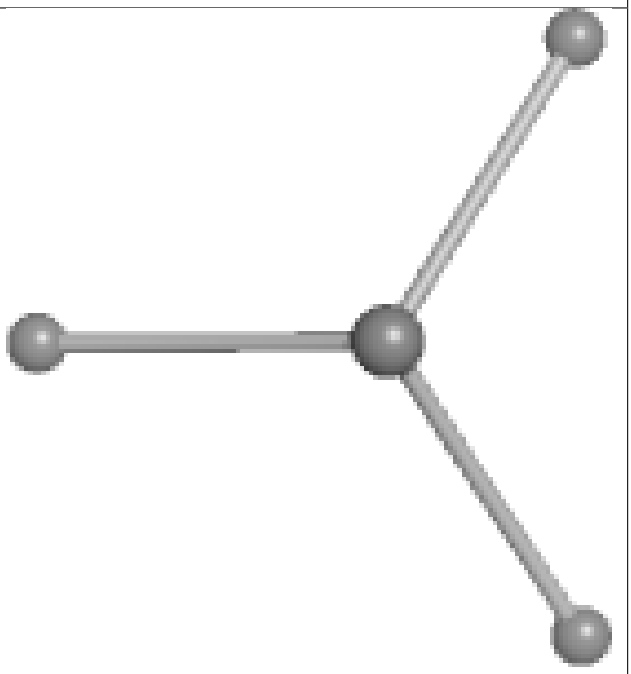


Rings

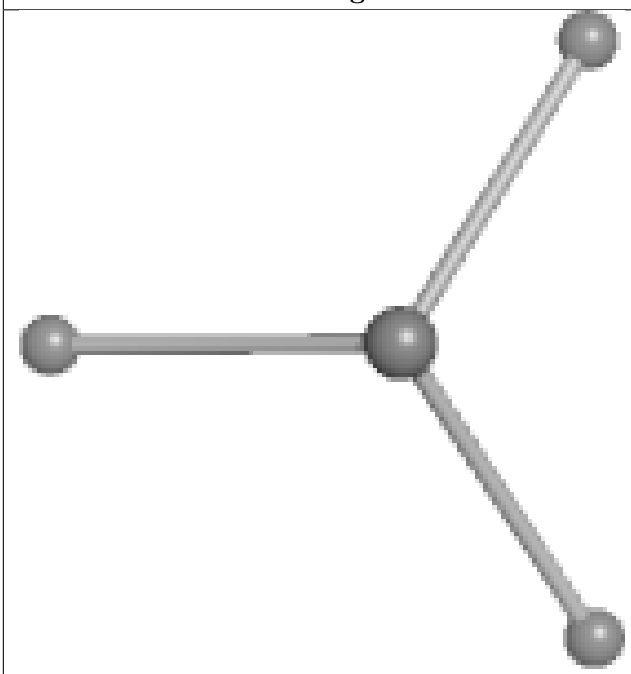
Ligand BEF E 902



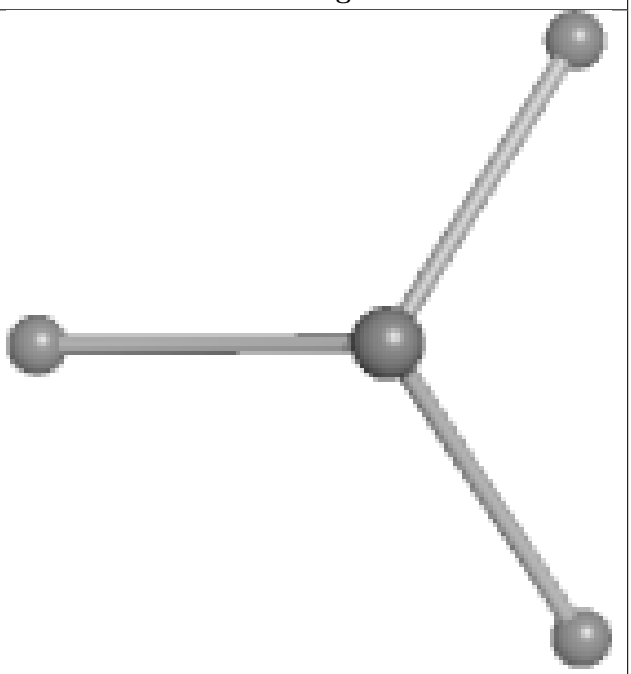
Bond lengths



Bond angles

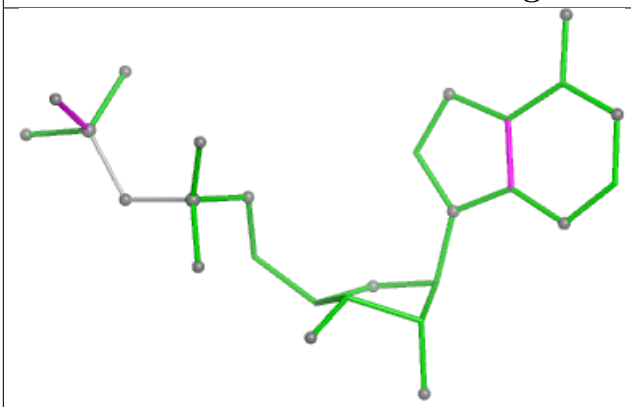


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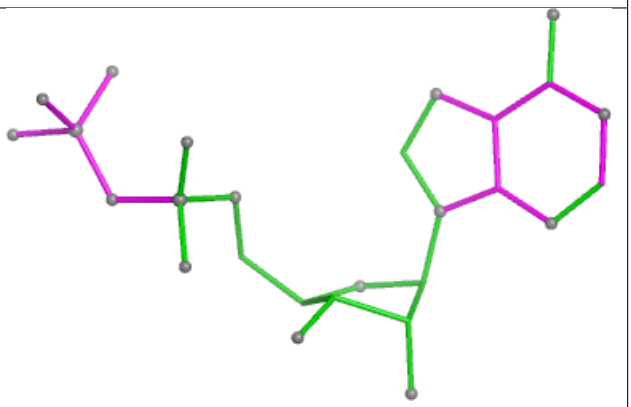


Rings

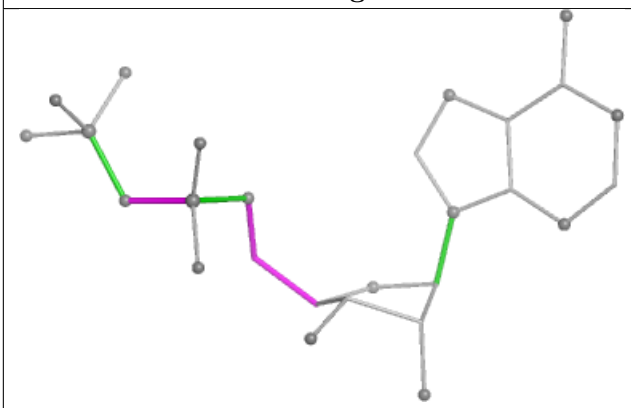
Ligand ADP E 901



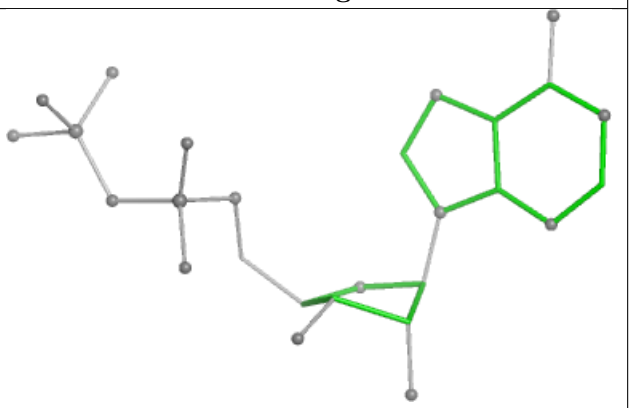
Bond lengths



Bond angles

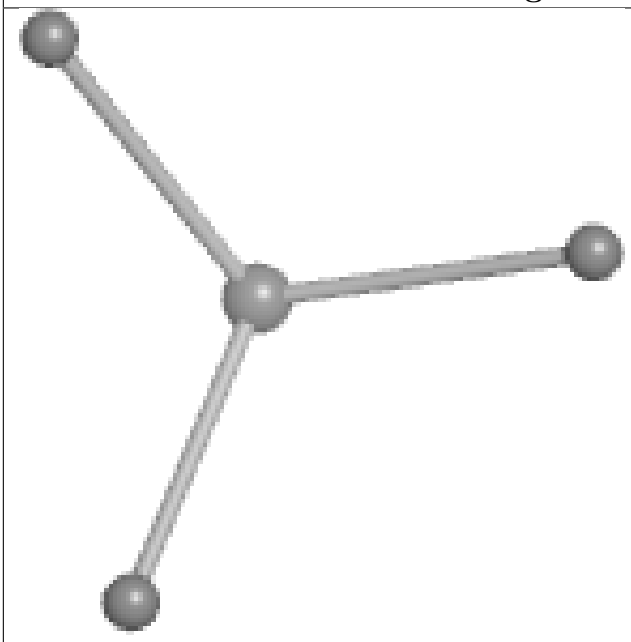


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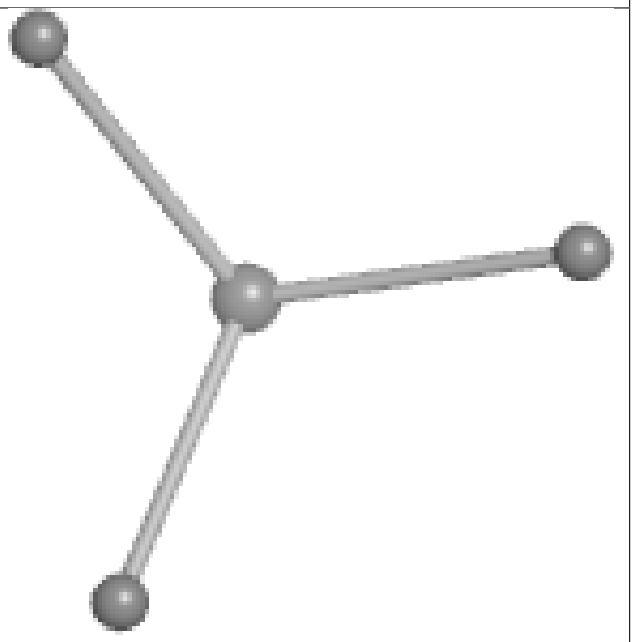


Rings

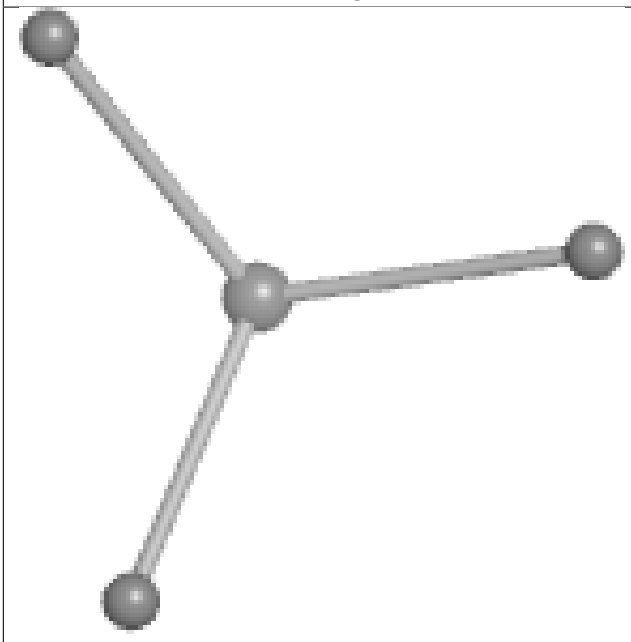
Ligand BEF A 903



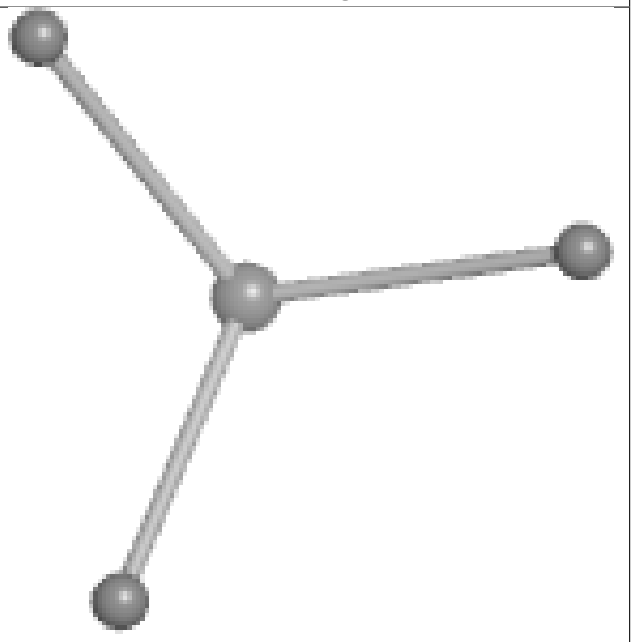
Bond lengths



Bond angles

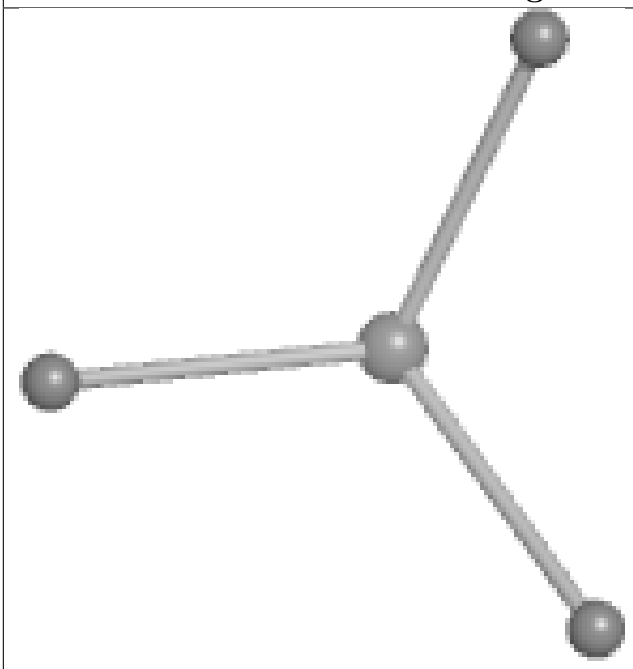


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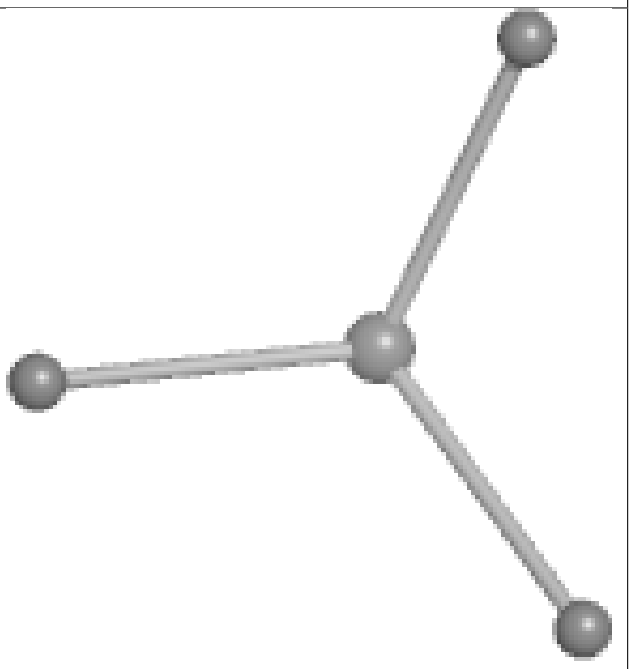


Rings

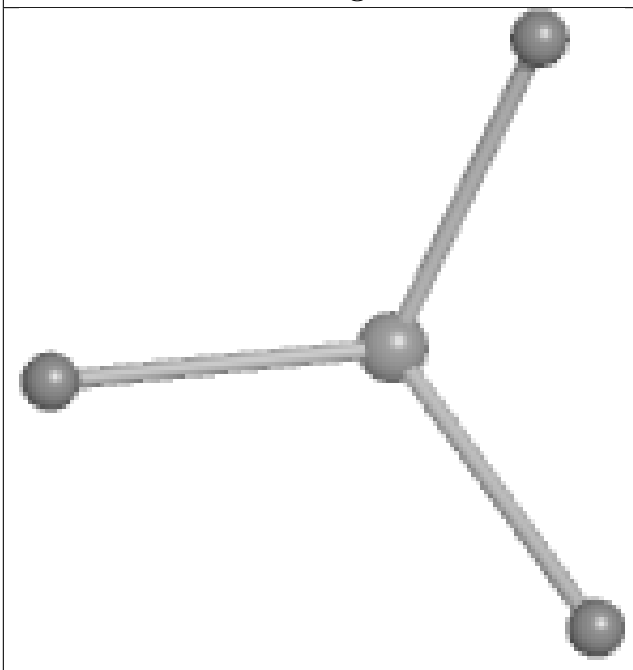
Ligand BEF B 905



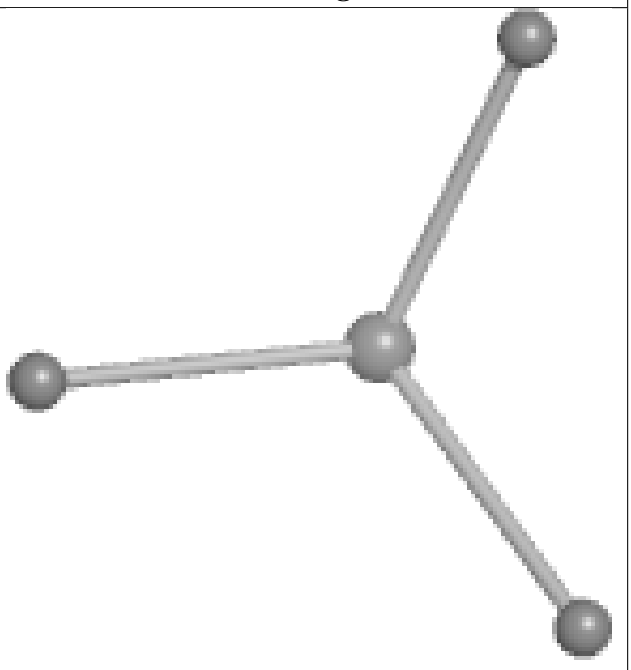
Bond lengths



Bond angles

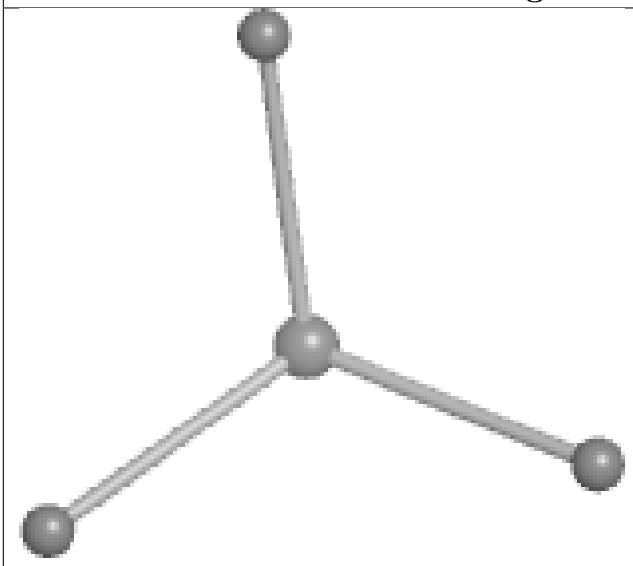


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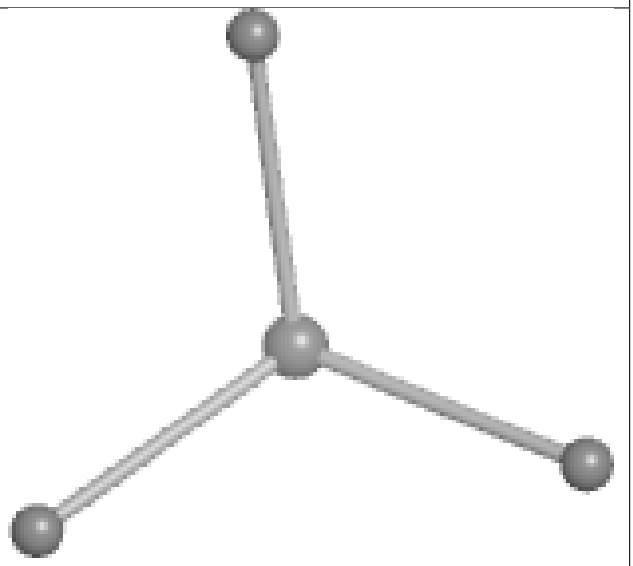


Rings

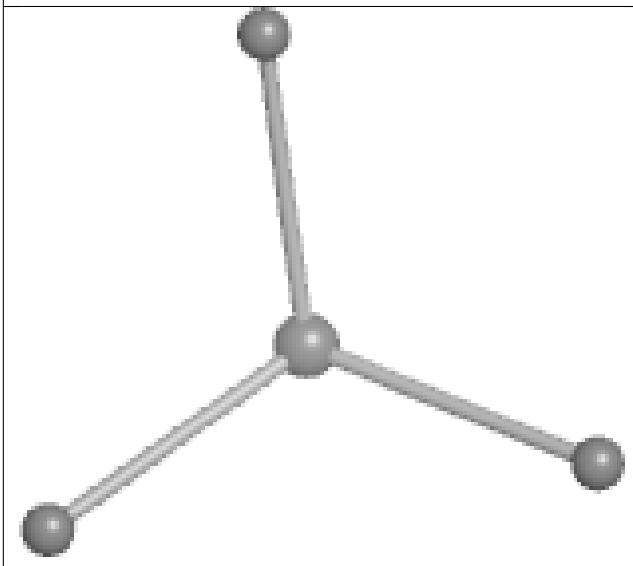
Ligand BEF B 903



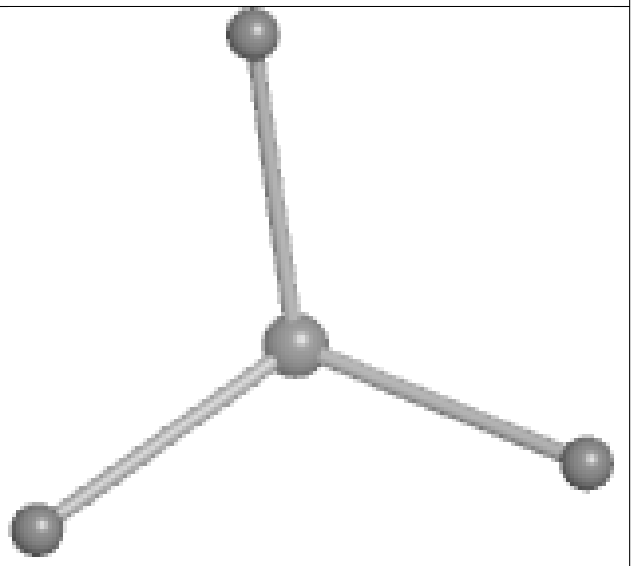
Bond lengths



Bond angles

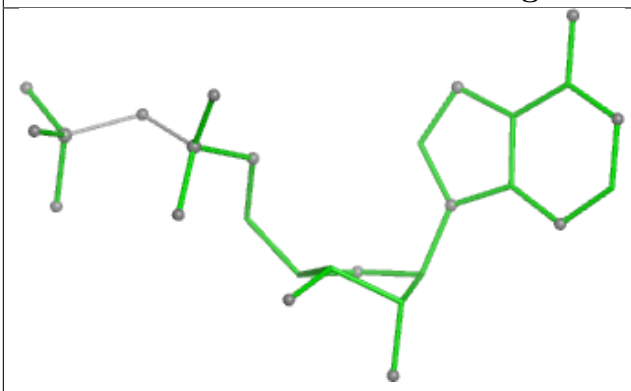


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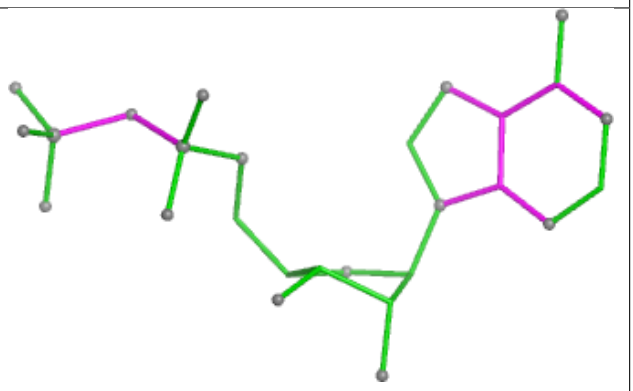


Rings

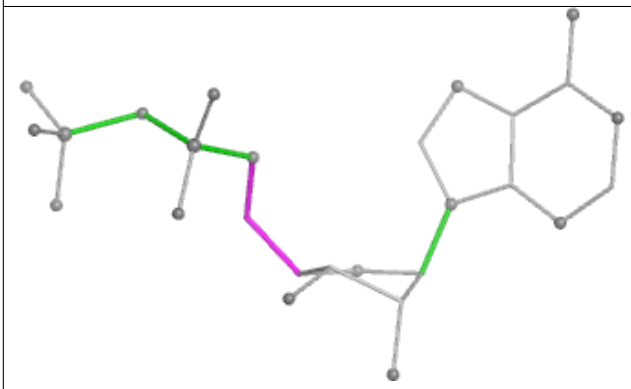
Ligand ADP D 902



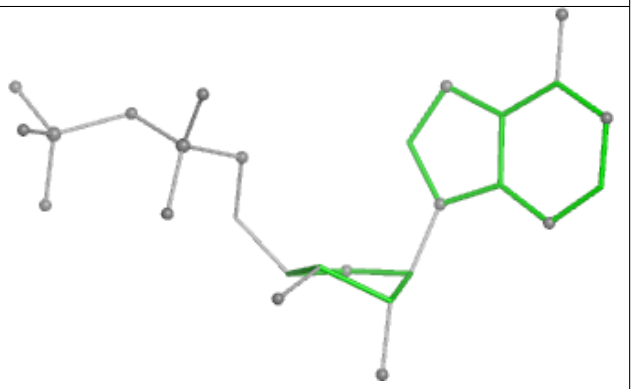
Bond lengths



Bond angles

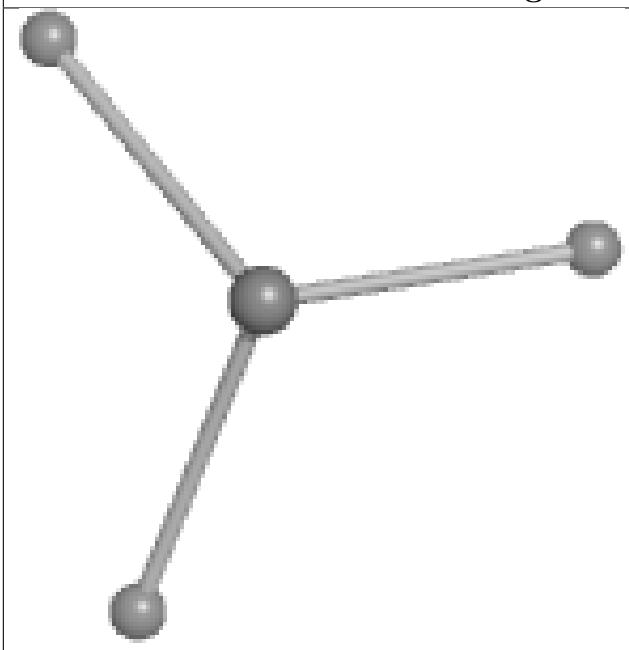


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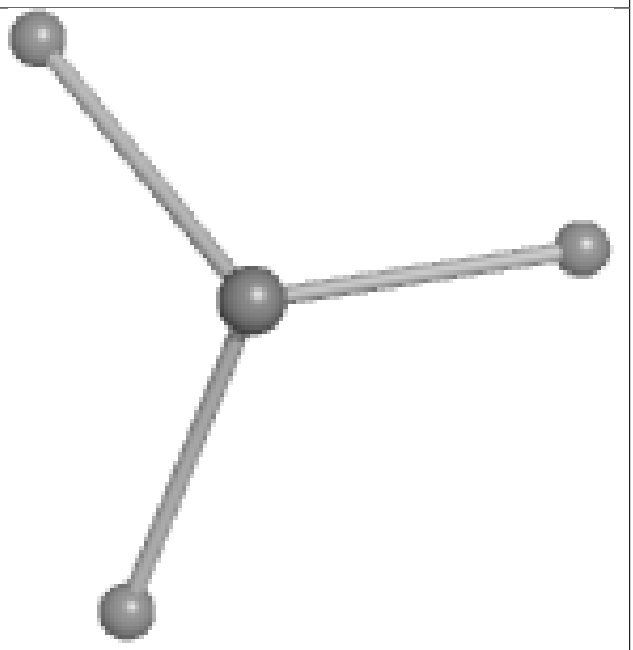


Rings

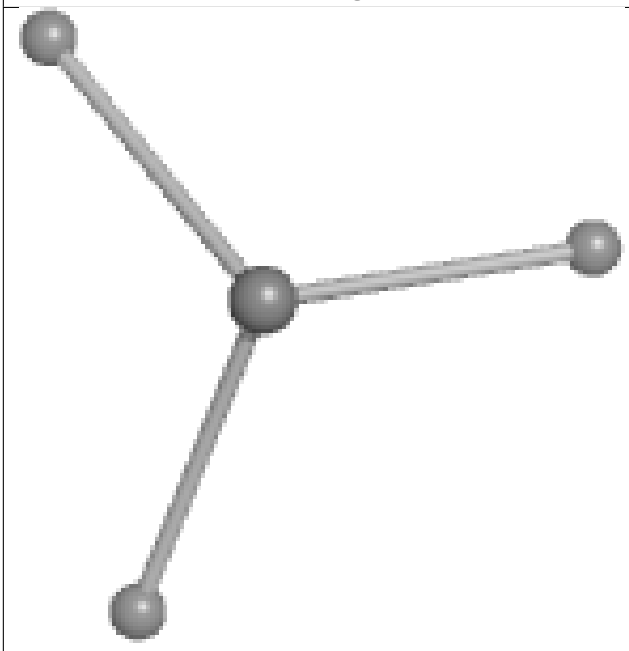
Ligand BEF A 901



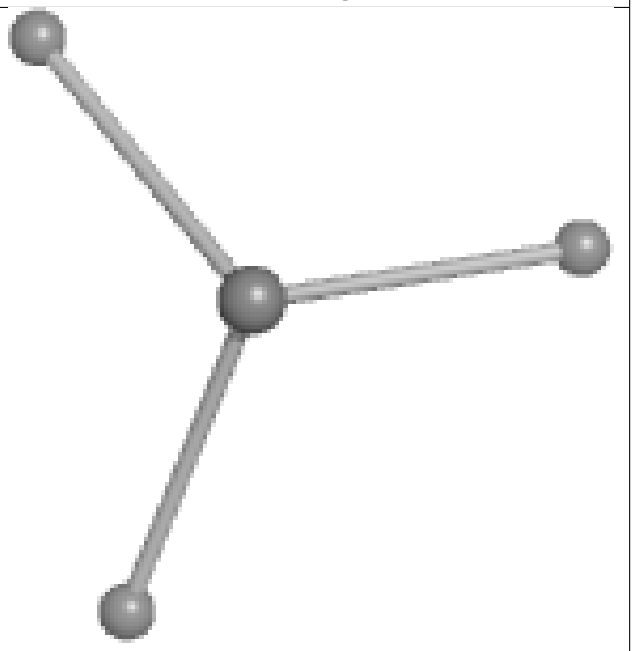
Bond lengths



Bond angles

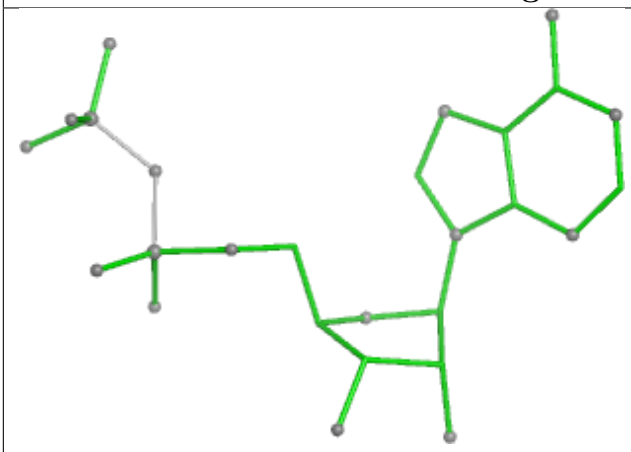


Torsions



Rings

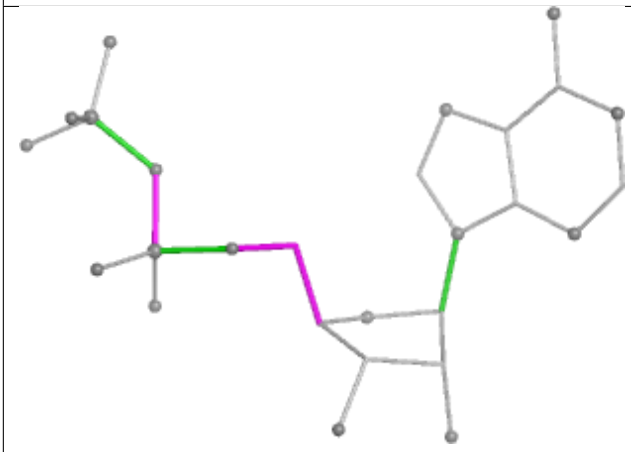
Ligand ADP C 902



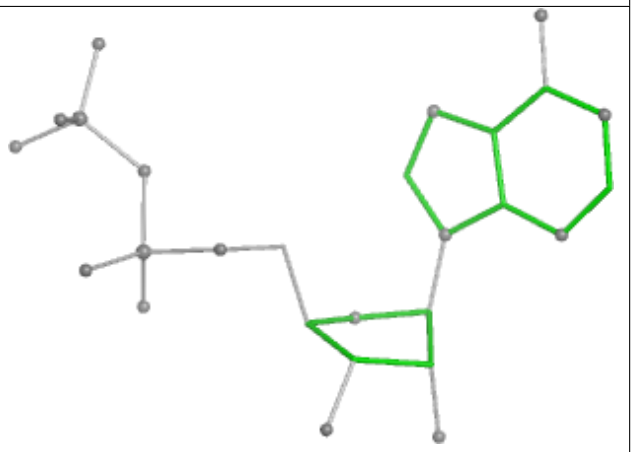
Bond lengths



Bond angles

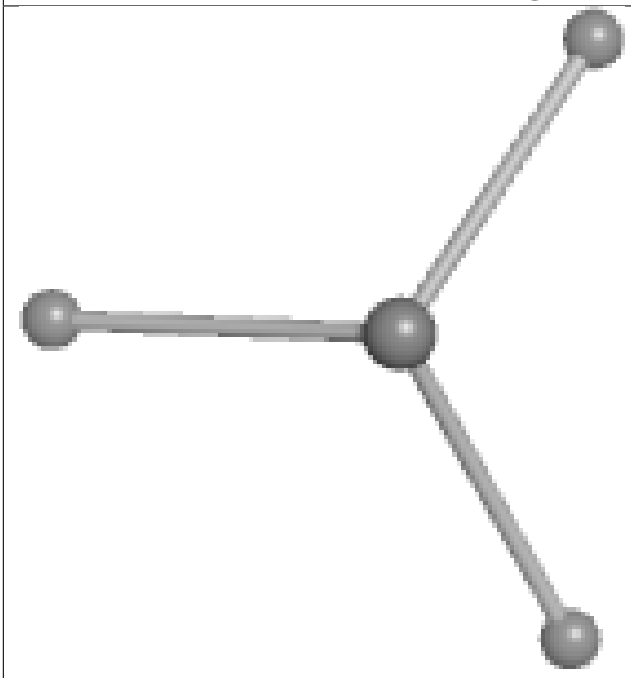


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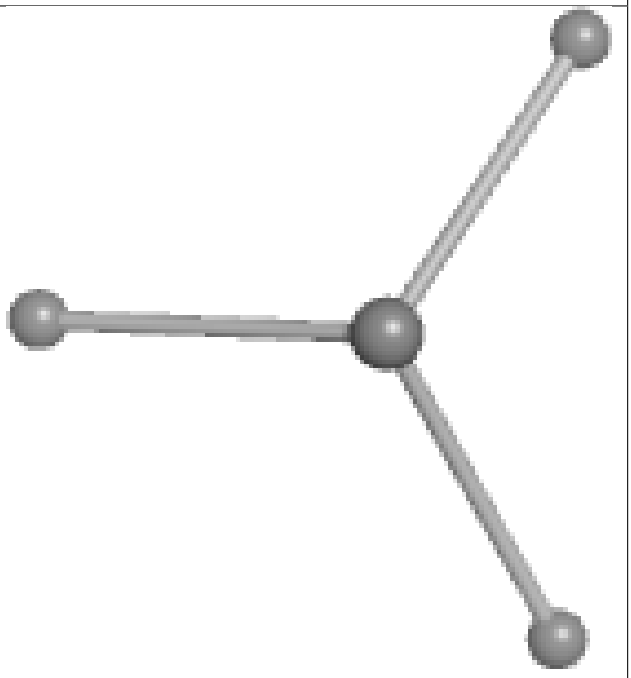


Rings

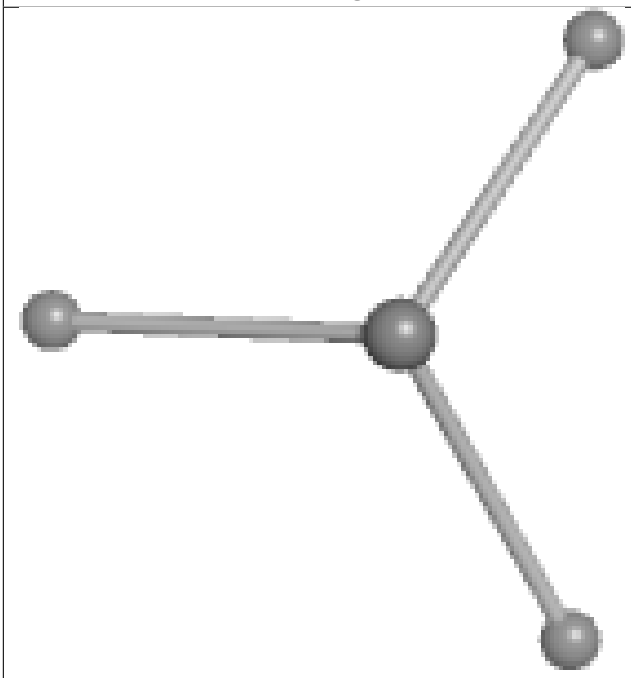
Ligand BEF B 901



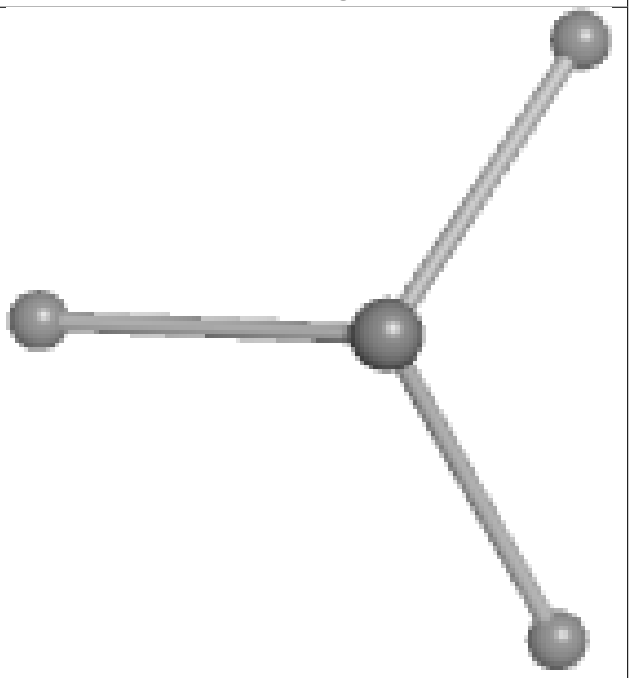
Bond lengths



Bond angles

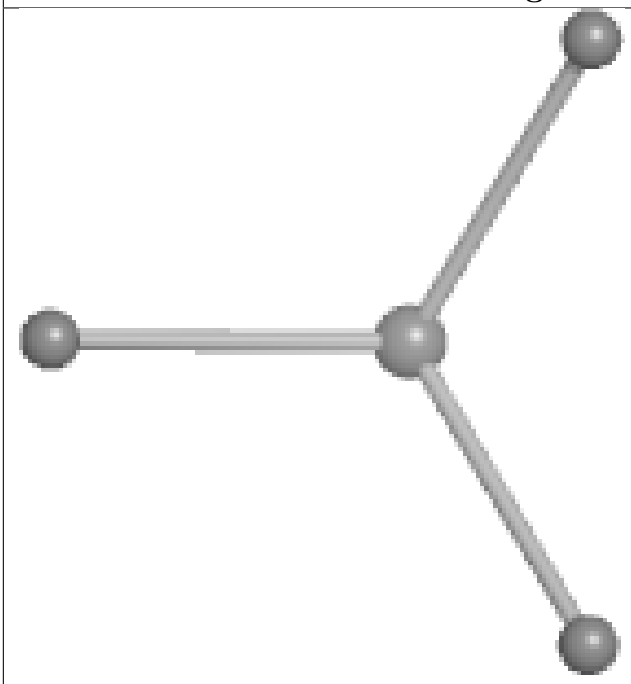


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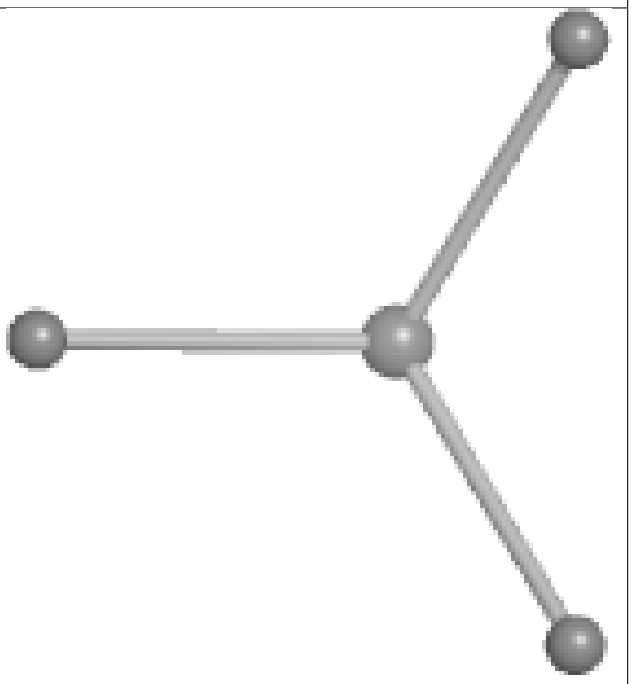


Rings

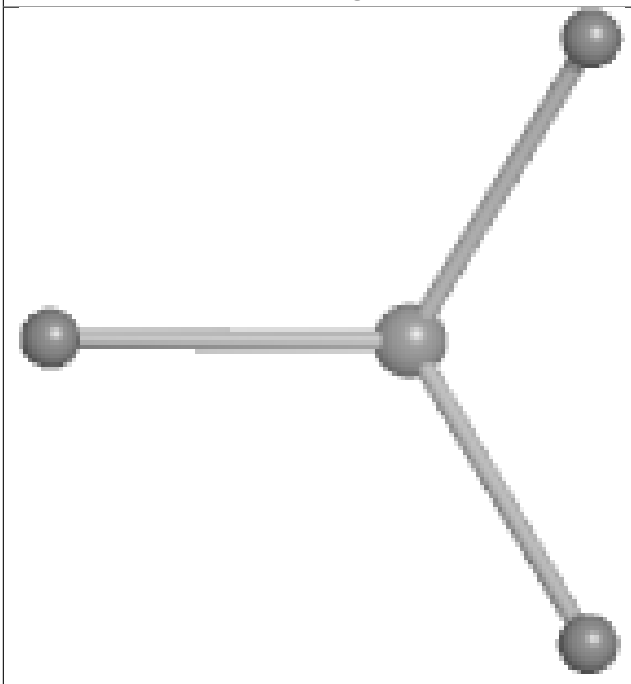
Ligand BEF C 903



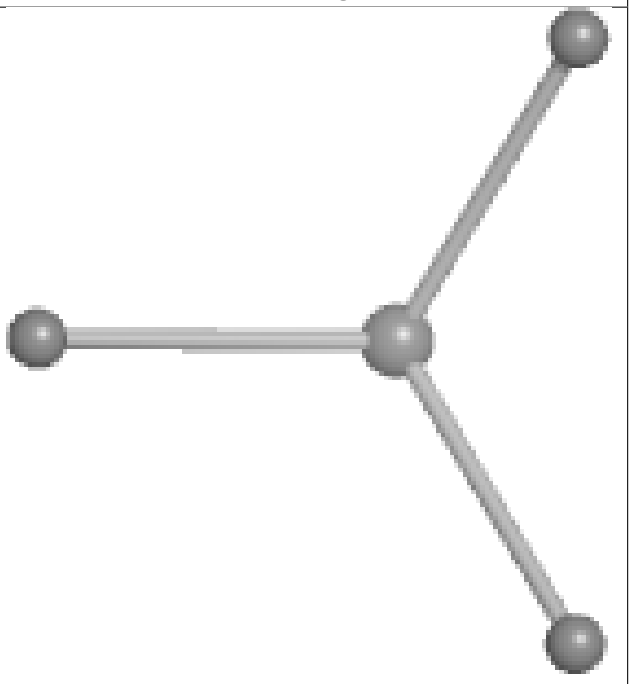
Bond lengths



Bond angles

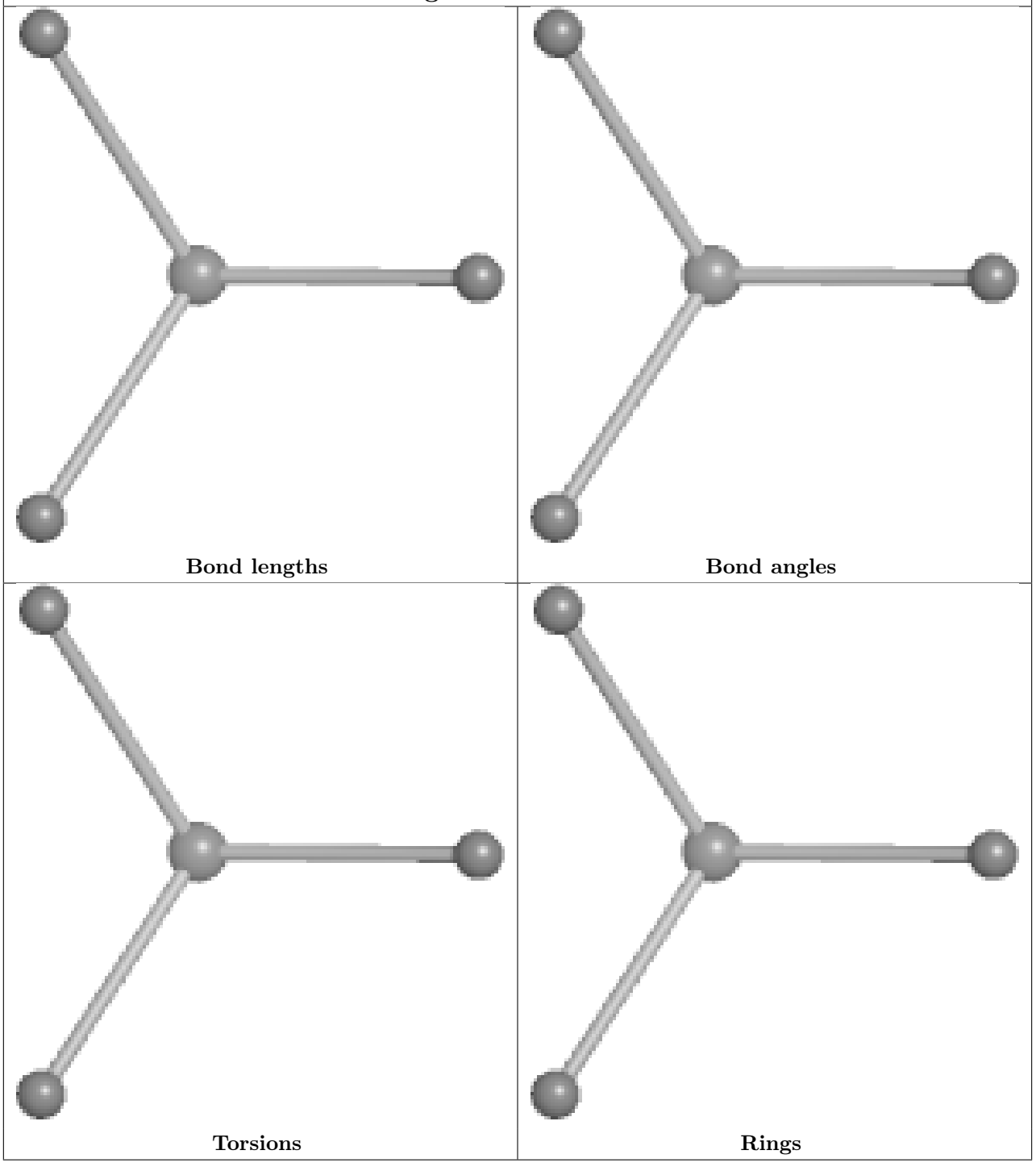


Torsions



Rings

Ligand BEF C 906



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.

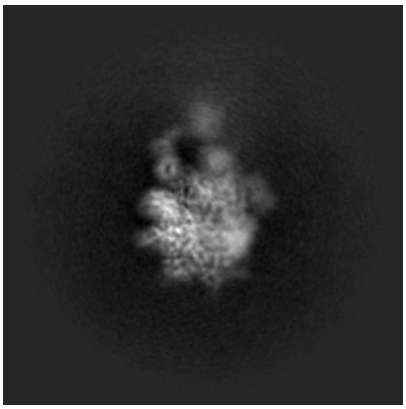
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58586. These allow visual inspection of the internal detail of the map and identification of artifacts.

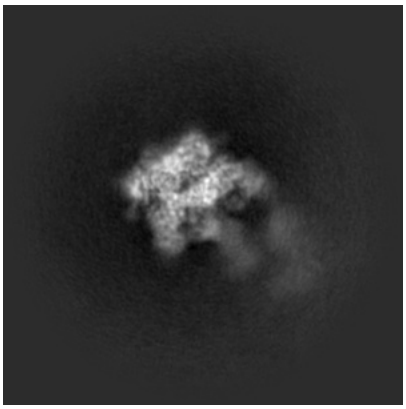
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

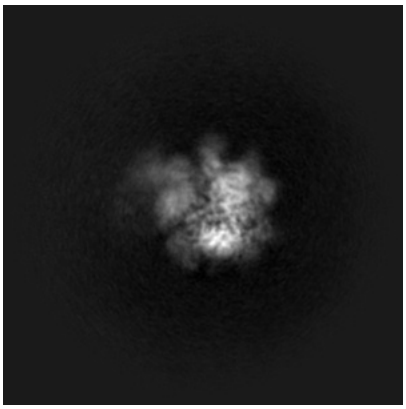
6.1.1 Primary map



X

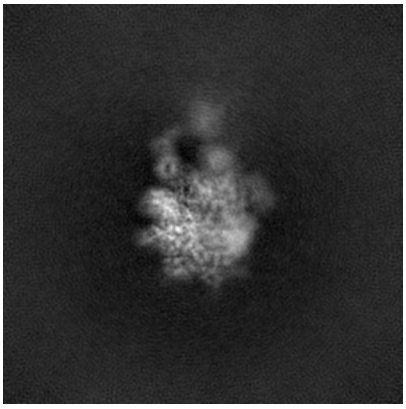


Y

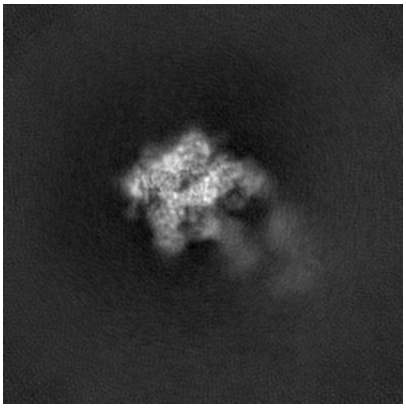


Z

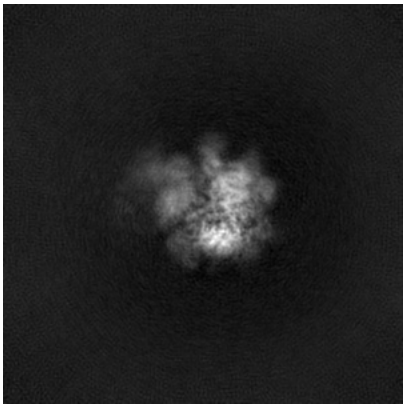
6.1.2 Raw map



X



Y

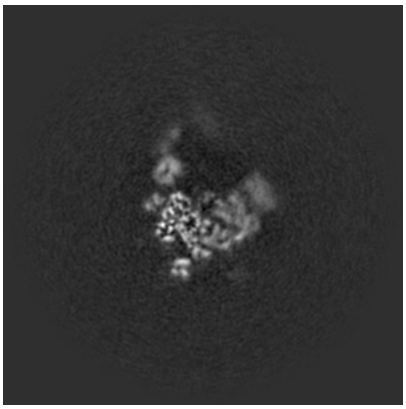


Z

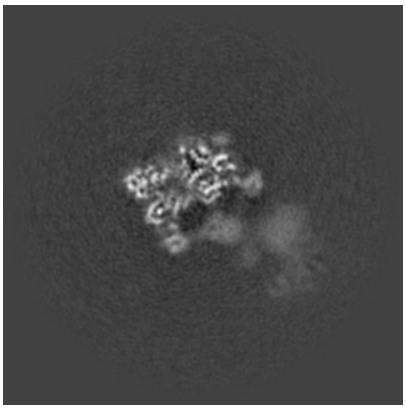
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

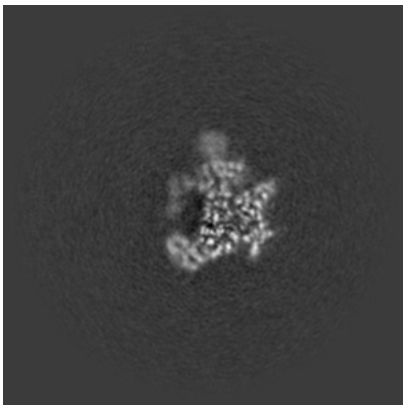
6.2.1 Primary map



X Index: 112

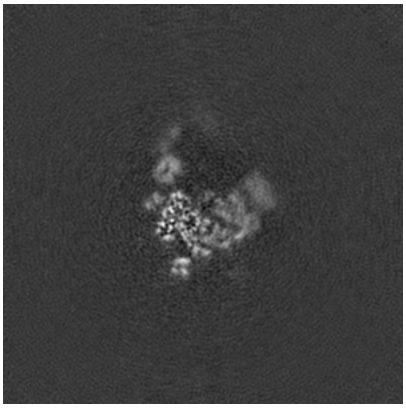


Y Index: 112

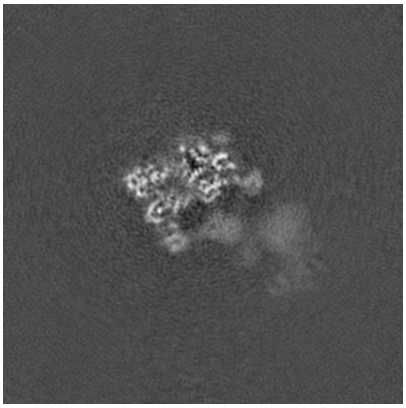


Z Index: 112

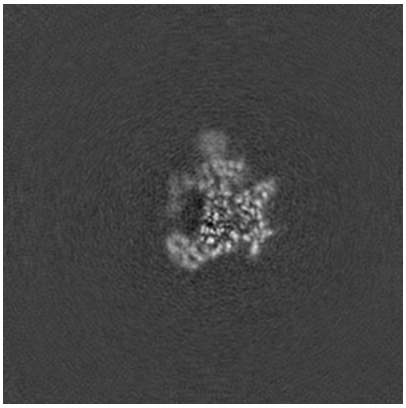
6.2.2 Raw map



X Index: 112



Y Index: 112

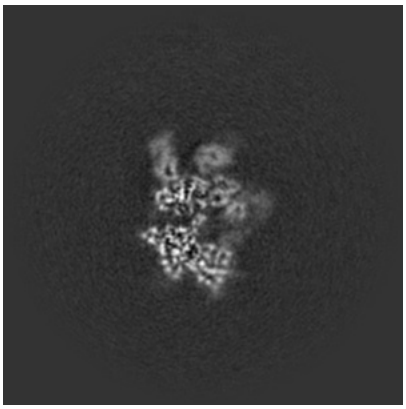


Z Index: 112

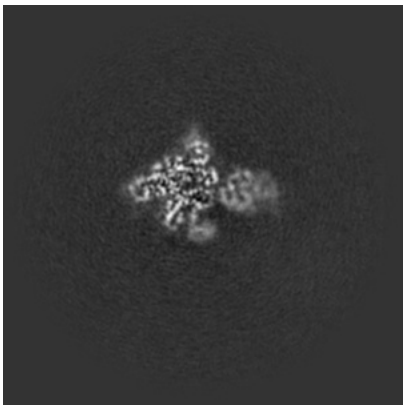
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

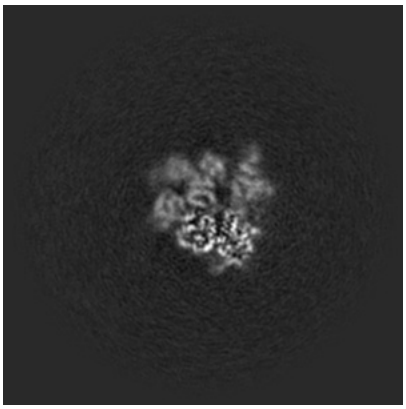
6.3.1 Primary map



X Index: 124

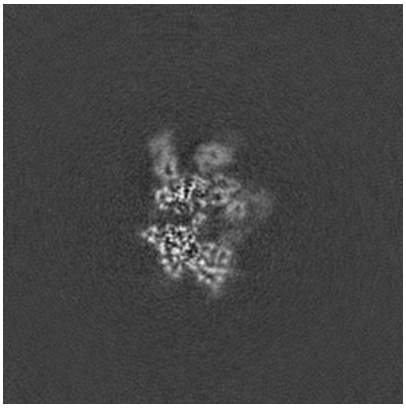


Y Index: 93

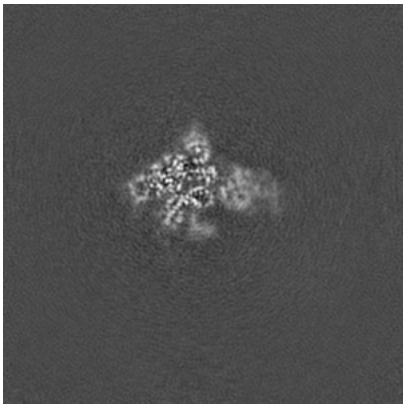


Z Index: 96

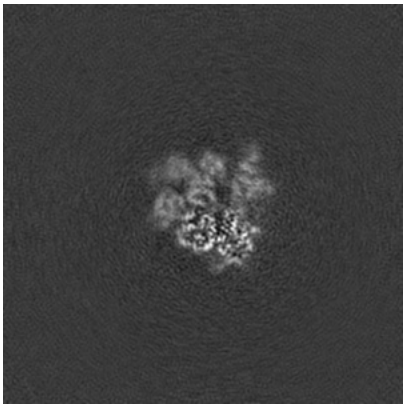
6.3.2 Raw map



X Index: 124



Y Index: 94

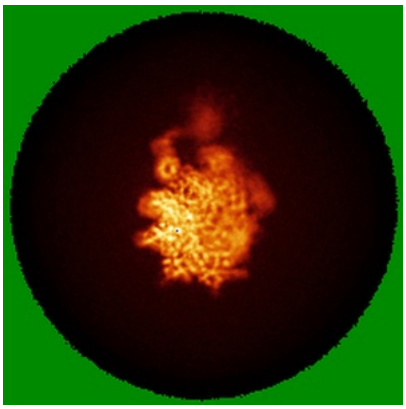


Z Index: 96

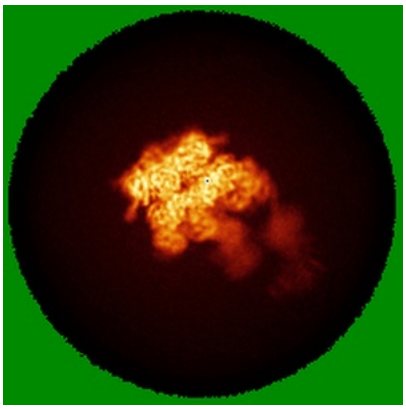
The images above show the largest variance slices of the map in three orthogonal directions.

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

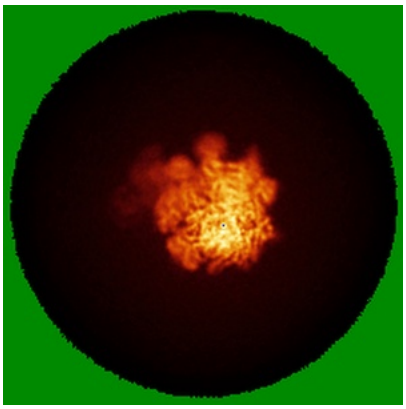
6.4.1 Primary map



X

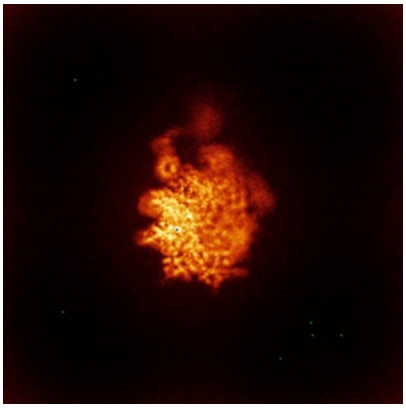


Y

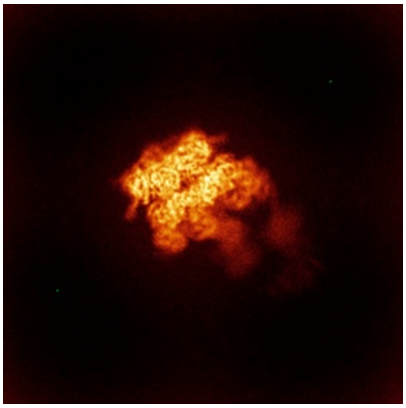


Z

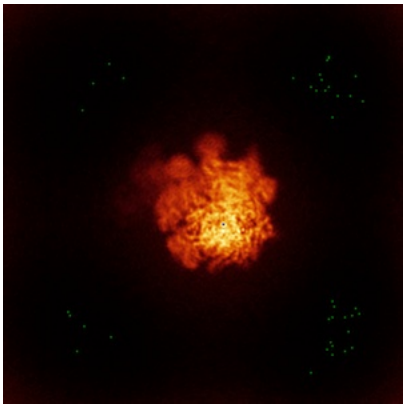
6.4.2 Raw map



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 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

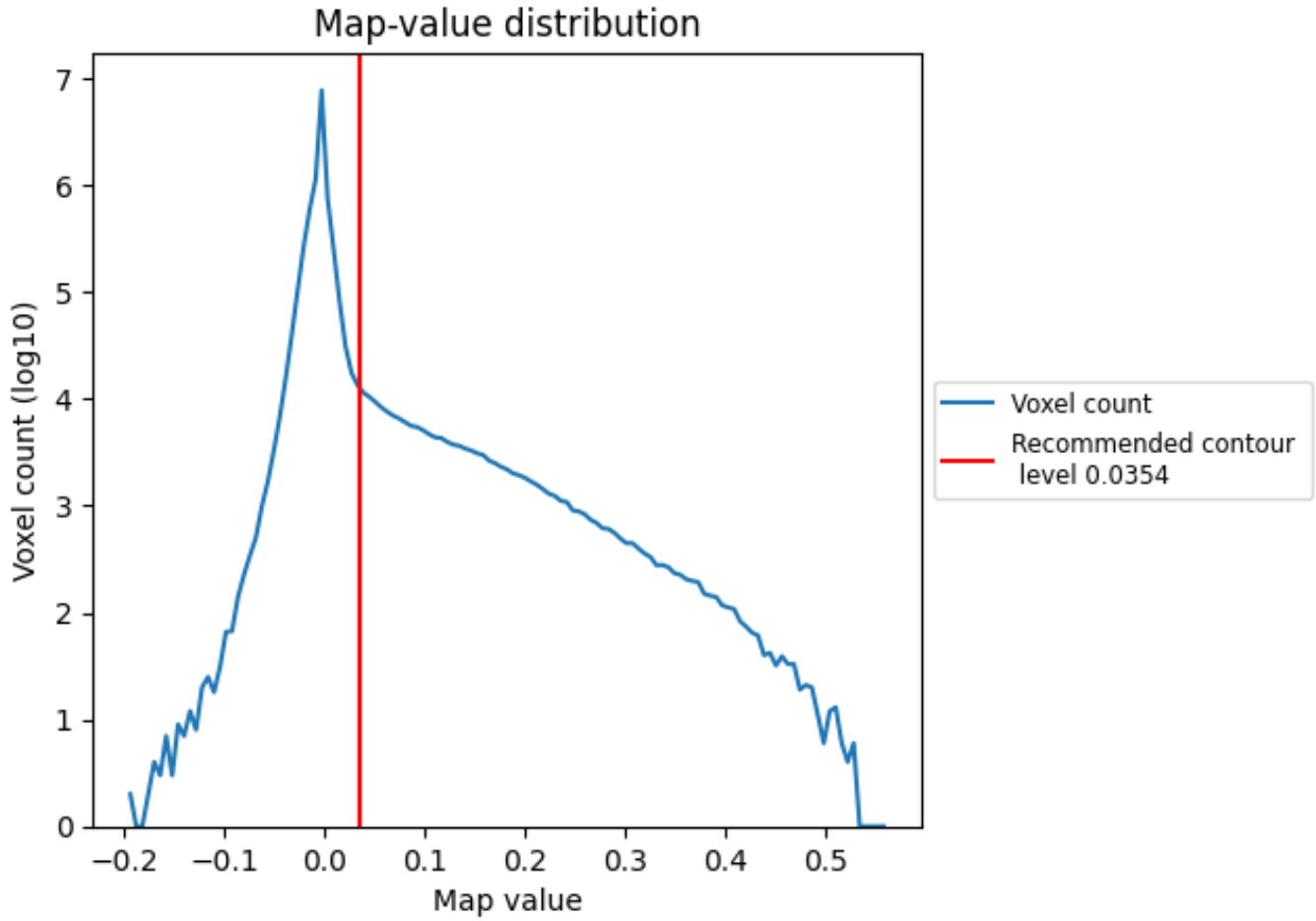
6.6 Mask visualisation (i)

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

7 Map analysis

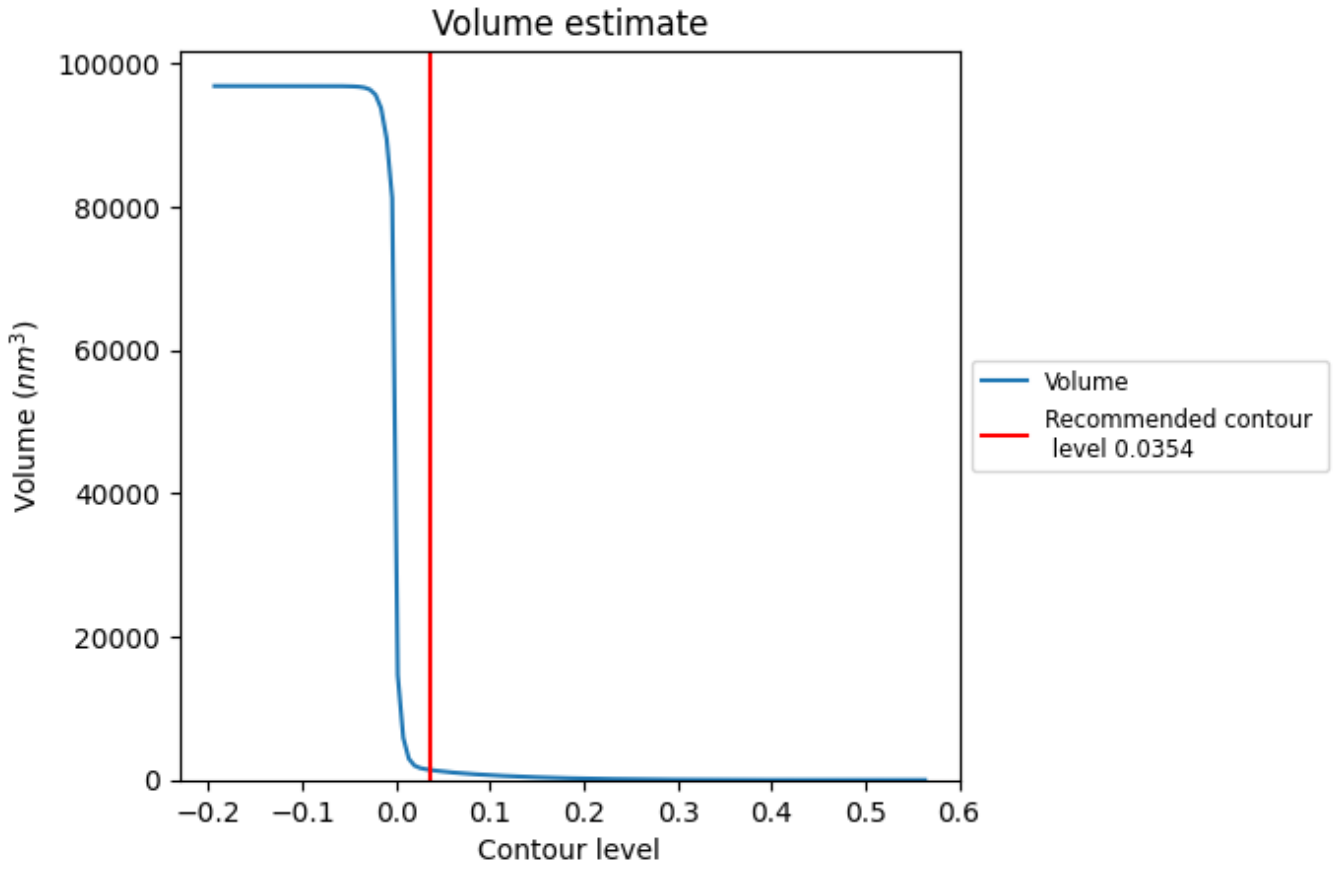
This section contains the results of statistical analysis of the map.

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.

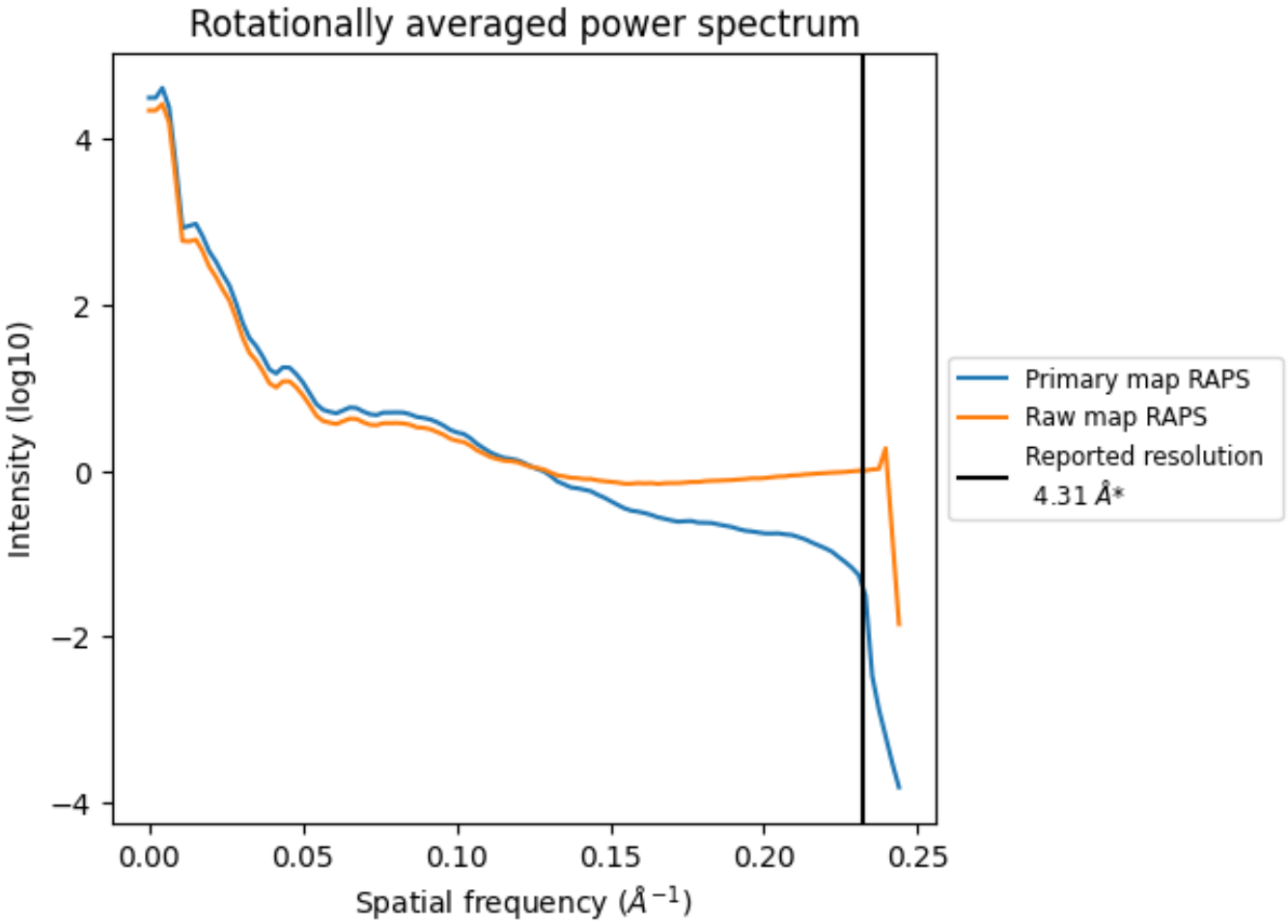
7.2 Volume estimate



The volume at the recommended contour level is 1420 nm^3; this corresponds to an approximate mass of 1282 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)

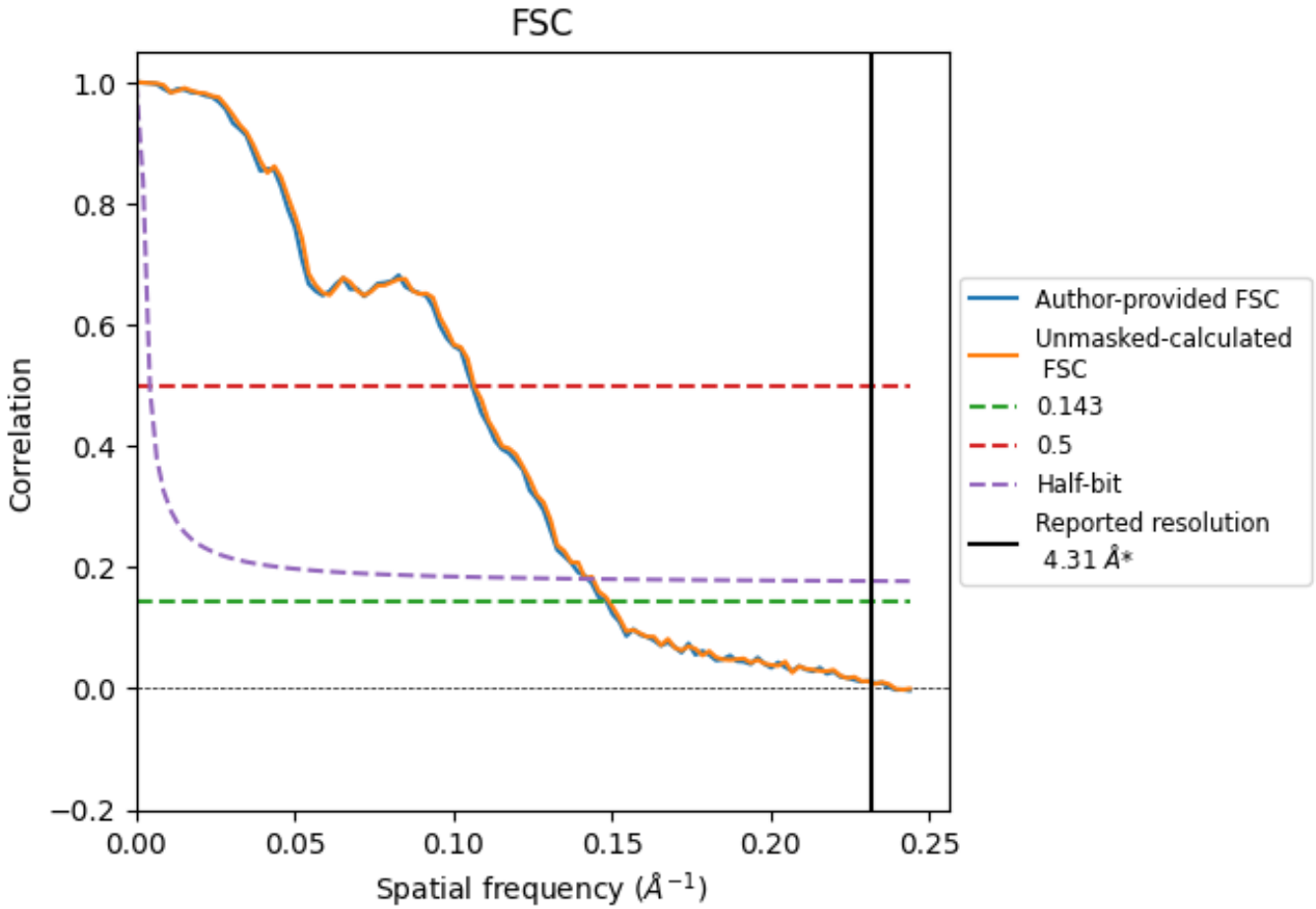


*Reported resolution corresponds to spatial frequency of 0.232 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.232 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.31	-	-
Author-provided FSC curve	6.74	9.44	7.02
Unmasked-calculated*	6.71	9.38	6.94

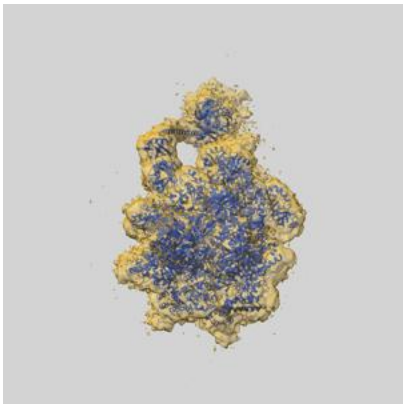
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 6.74 differs from the reported value 4.31 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.71 differs from the reported value 4.31 by more than 10 %

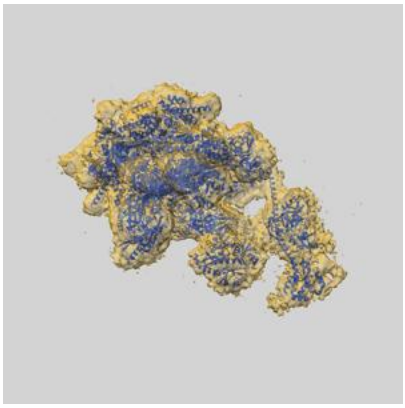
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58586 and PDB model 31OL. Per-residue inclusion information can be found in section 3 on page 9.

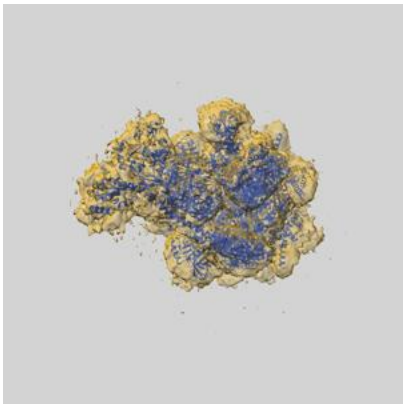
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0354 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.

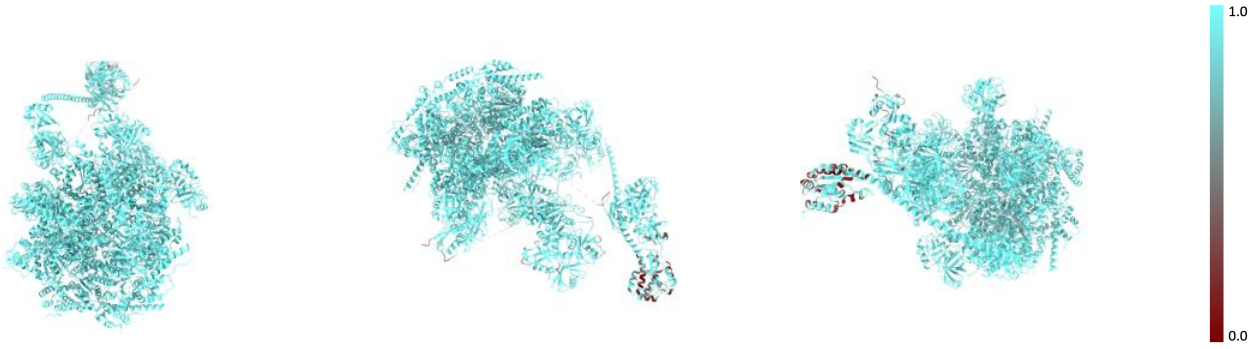
9.2 Q-score mapped to coordinate model (i)



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.

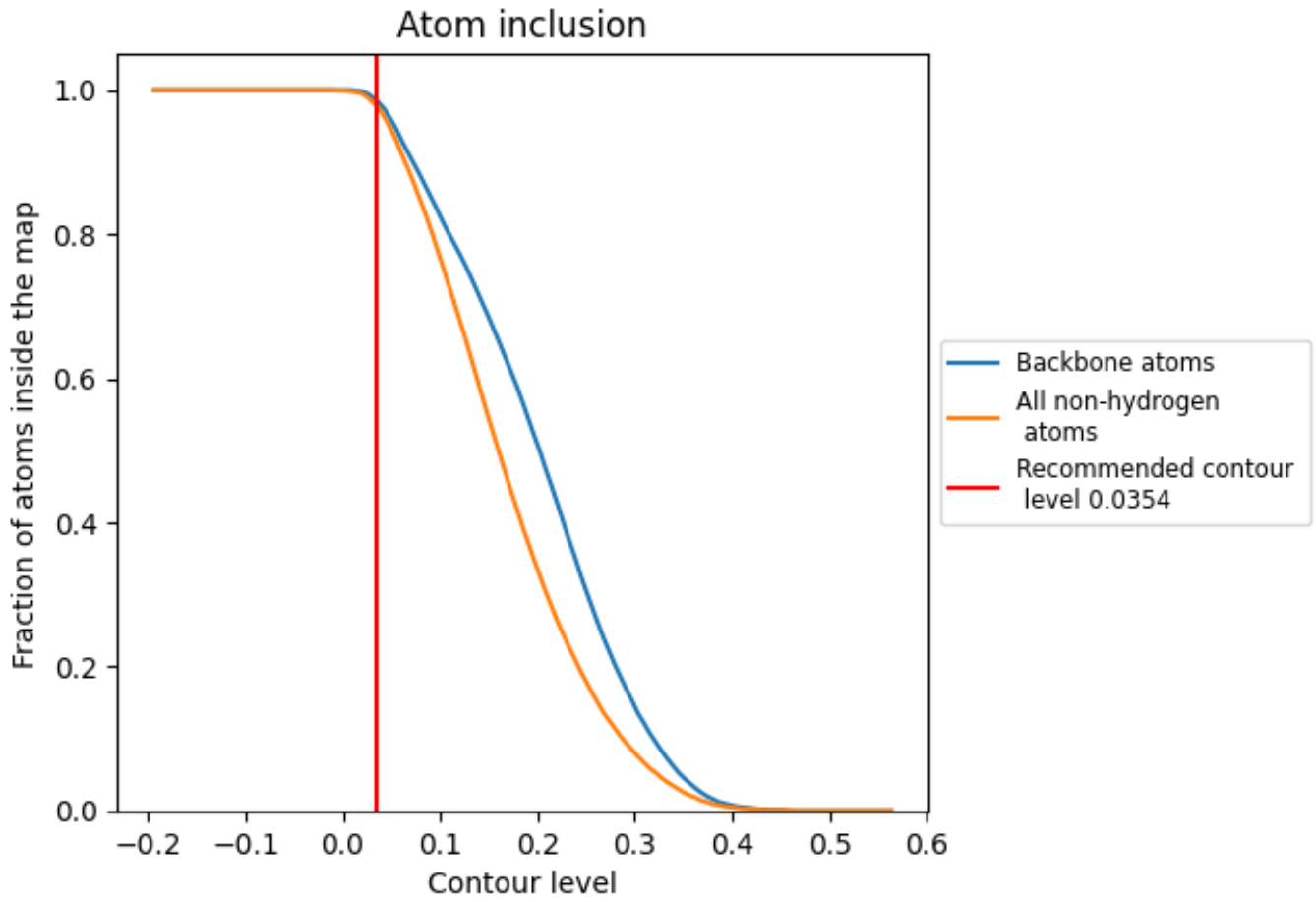
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0354).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9770	0.1860
A	0.9950	0.2550
B	0.9930	0.2430
C	0.9970	0.1930
D	0.9990	0.1570
E	0.9930	0.2170
F	0.9930	0.2490
G	0.9640	0.1070
H	0.9490	0.0800
I	0.9710	0.1560
J	0.9860	0.0740
K	0.9280	0.0130
L	0.9920	0.0620
M	0.9440	0.0630
N	0.8300	0.0930
T	0.8380	0.0910

