Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 11:34 AM JST

PDB ID	:	9UMT / pdb_00009umt
EMDB ID	:	EMD-64312
Title	:	TRiC_HDAC1_close_state
Authors	:	Li, Z.L.; Cong, Y.C.
Deposited on	:	2025-04-23
Resolution	:	3.64 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:

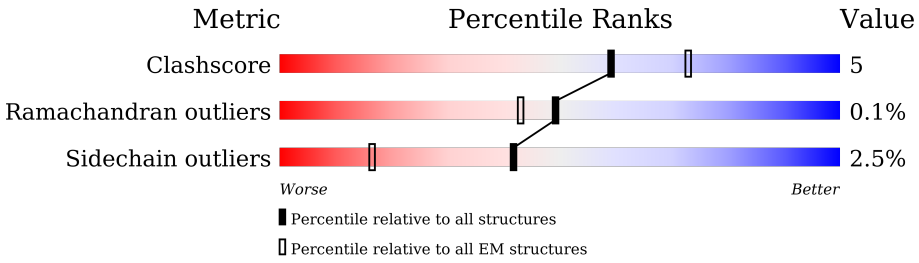
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

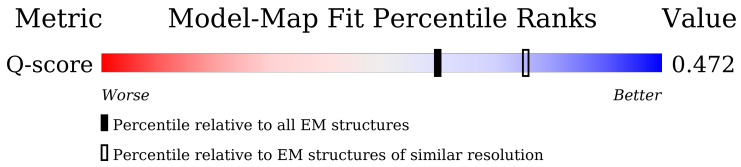
1 Overall quality at a glance

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

The reported resolution of this entry is 3.64 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	11633 (3.14 - 4.14)

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	F	532	87% 12%
2	A	526	87% 12%
3	C	525	83% 15%
4	B	517	85% 15%

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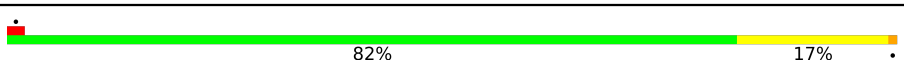
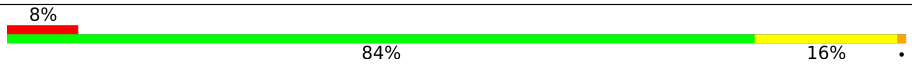
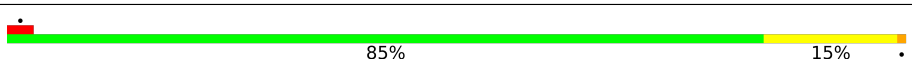
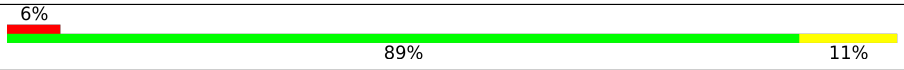
Mol	Chain	Length	Quality of chain
5	G	531	
6	H	525	
7	D	523	
8	E	529	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 32411 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 T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	F	532	4041	2533	707	778	23	0	0

- Molecule 2 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	526	3952	2473	696	764	19	0	0

- Molecule 3 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	525	4085	2546	724	785	30	0	0

- Molecule 4 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	517	3907	2443	679	762	23	0	0

- Molecule 5 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	531	4095	2566	714	785	30	0	0

- Molecule 6 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	525	4023	2528	704	770	21	0	0

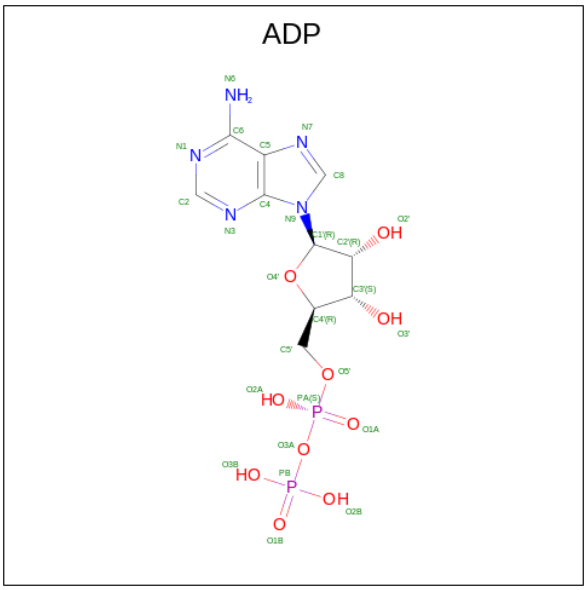
- Molecule 7 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	523	Total	C	N	O	S	0	0
			4014	2535	694	762	23		

- Molecule 8 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	529	Total	C	N	O	S	0	0
			4030	2543	685	775	27		

- Molecule 9 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
9	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	H	1	Total	C	N	O	P	0
			27	10	5	10	2	

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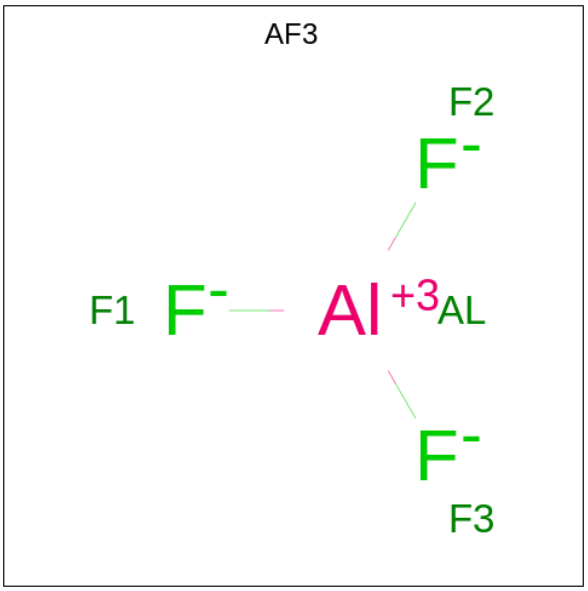
Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	F	1	Total	Mg	0
			1	1	
10	A	1	Total	Mg	0
			1	1	
10	C	1	Total	Mg	0
			1	1	
10	B	1	Total	Mg	0
			1	1	
10	G	1	Total	Mg	0
			1	1	
10	H	1	Total	Mg	0
			1	1	
10	D	1	Total	Mg	0
			1	1	
10	E	1	Total	Mg	0
			1	1	

- Molecule 11 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
11	F	1	Total Al F 4 1 3	0
11	A	1	Total Al F 4 1 3	0
11	C	1	Total Al F 4 1 3	0
11	B	1	Total Al F 4 1 3	0
11	G	1	Total Al F 4 1 3	0
11	H	1	Total Al F 4 1 3	0
11	D	1	Total Al F 4 1 3	0
11	E	1	Total Al F 4 1 3	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	AltConf
12	F	1	Total O 1 1	0
12	A	1	Total O 1 1	0
12	C	1	Total O 1 1	0
12	B	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
12	G	1	Total O 1 1	0
12	H	1	Total O 1 1	0
12	D	1	Total O 1 1	0
12	E	1	Total O 1 1	0

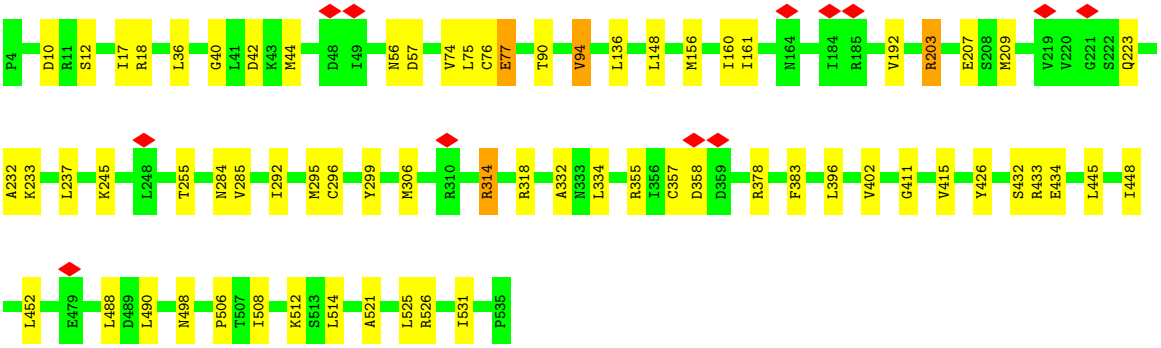
3 Residue-property plots (i)

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: T-complex protein 1 subunit alpha

Chain F:

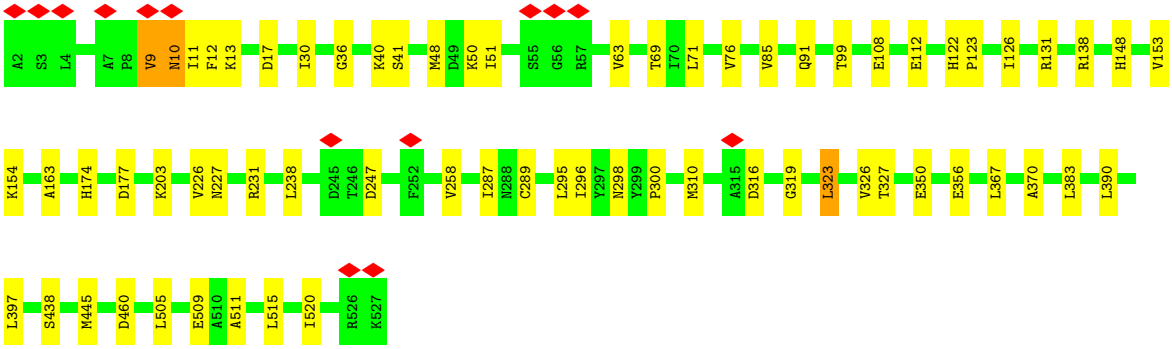




• Molecule 2: T-complex protein 1 subunit beta

Chain A:

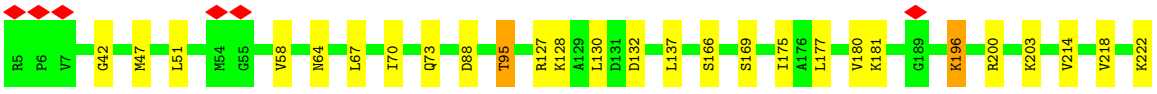


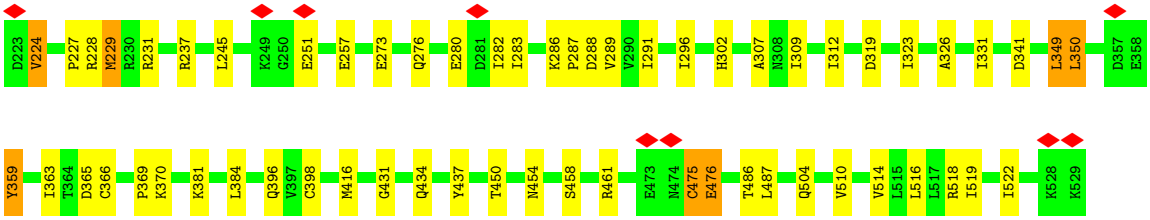


• Molecule 3: T-complex protein 1 subunit gamma

Chain C:



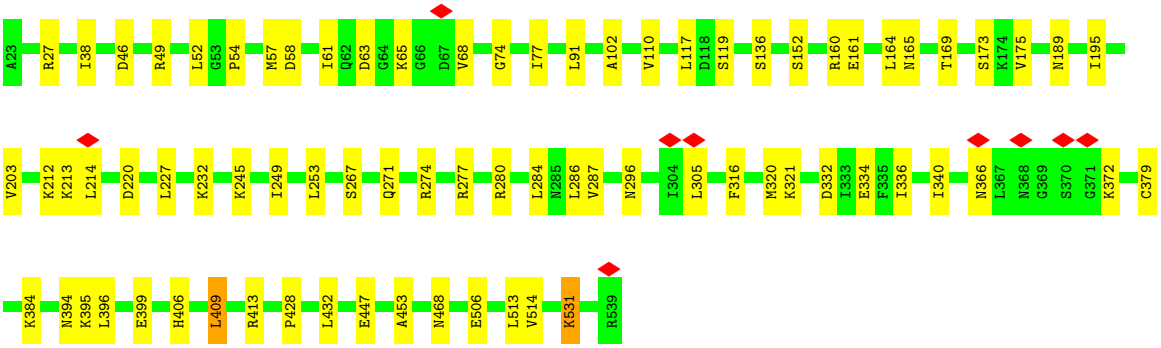




• Molecule 4: T-complex protein 1 subunit delta

Chain B:

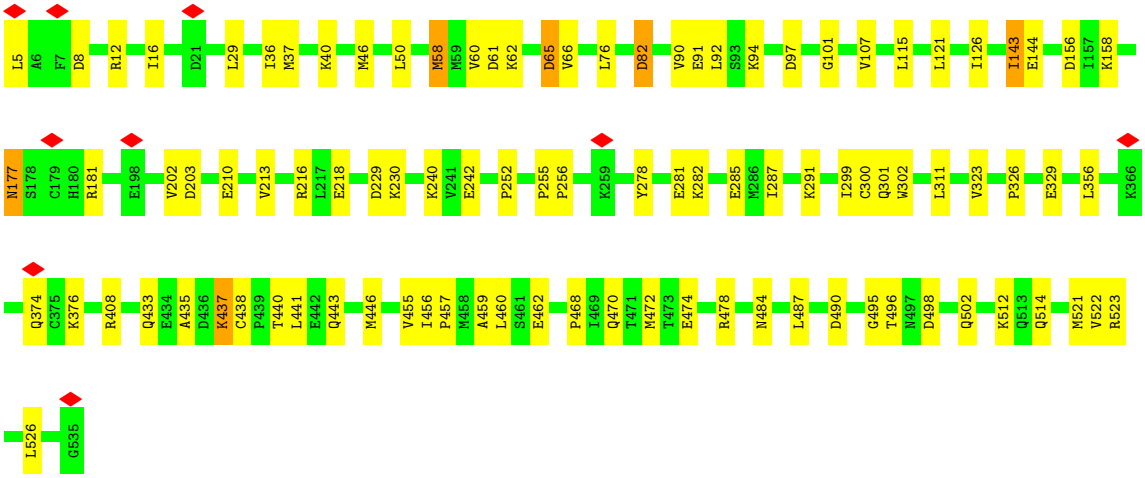




• Molecule 5: T-complex protein 1 subunit epsilon

Chain G:

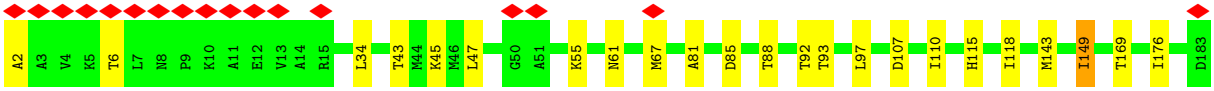


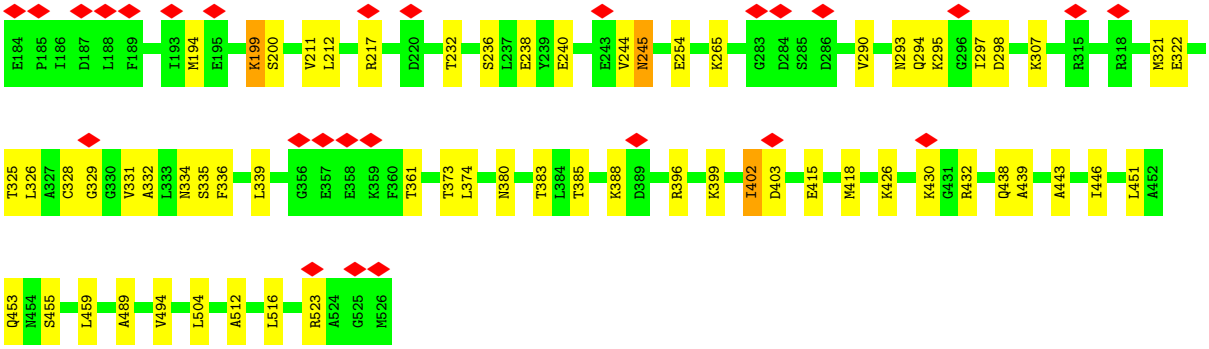


• Molecule 6: T-complex protein 1 subunit zeta

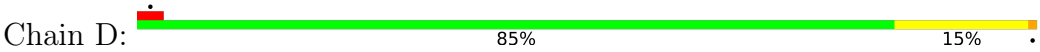
Chain H:

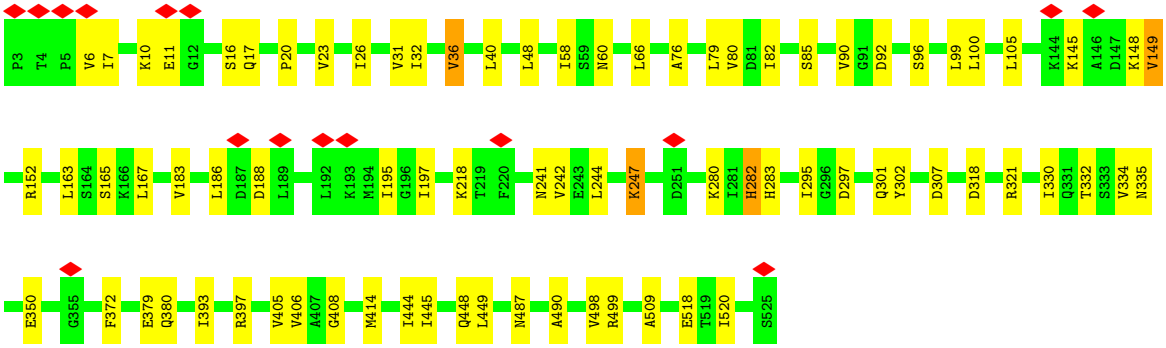




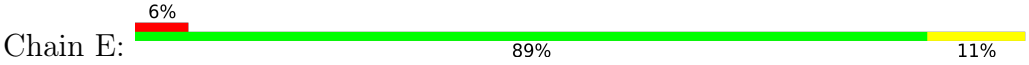


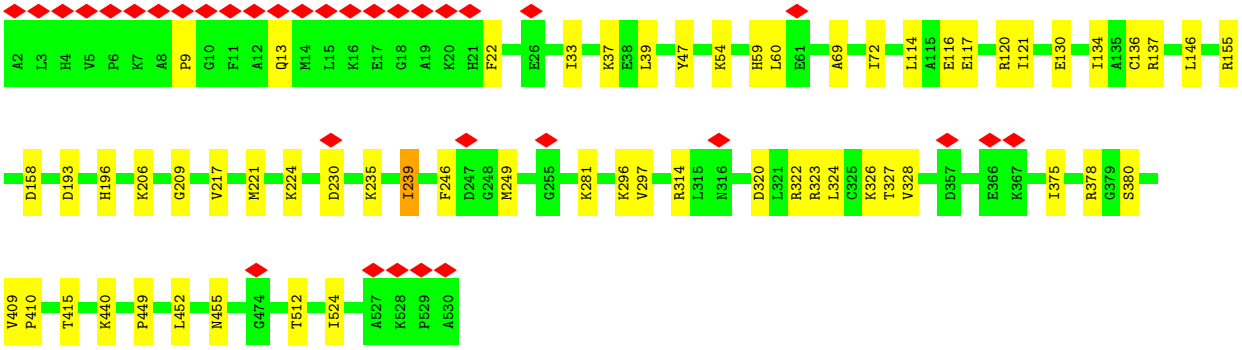
• Molecule 7: T-complex protein 1 subunit eta





• Molecule 8: T-complex protein 1 subunit theta





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	15.578	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.588	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	348.0, 348.0, 348.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	F	0.28	0/4081	0.67	5/5510 (0.1%)
2	A	0.30	0/3995	0.70	7/5386 (0.1%)
3	C	0.32	0/4131	0.74	10/5570 (0.2%)
4	B	0.34	0/3939	0.76	11/5317 (0.2%)
5	G	0.31	0/4145	0.71	5/5584 (0.1%)
6	H	0.35	0/4070	0.82	9/5486 (0.2%)
7	D	0.30	0/4071	0.69	11/5495 (0.2%)
8	E	0.31	0/4088	0.71	4/5525 (0.1%)
All	All	0.31	0/32520	0.73	62/43873 (0.1%)

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	F	0	1
7	D	0	1
All	All	0	2

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	384	LYS	CB-CG-CD	6.95	127.28	111.30
6	H	265	LYS	CB-CG-CD	6.92	127.22	111.30
4	B	321	LYS	CA-CB-CG	6.92	127.94	114.10
7	D	282	HIS	CA-C-N	6.91	132.20	122.46
7	D	282	HIS	C-N-CA	6.91	132.20	122.46
1	F	77	GLU	CA-CB-CG	6.78	127.65	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	437	LYS	CA-CB-CG	6.66	127.42	114.10
2	A	367	LEU	CA-CB-CG	6.58	139.35	116.30
4	B	506	GLU	CA-CB-CG	6.28	126.65	114.10
4	B	65	LYS	CB-CG-CD	6.17	125.48	111.30
5	G	94	LYS	CB-CG-CD	6.15	125.45	111.30
7	D	36	VAL	N-CA-C	-6.11	107.30	113.47
5	G	376	LYS	CB-CG-CD	6.08	125.29	111.30
3	C	381	LYS	CB-CG-CD	6.03	125.16	111.30
6	H	97	LEU	CA-CB-CG	5.88	136.88	116.30
7	D	330	ILE	CA-CB-CG1	5.87	120.37	110.40
7	D	330	ILE	CB-CG1-CD1	5.83	126.04	113.80
3	C	73	GLN	CB-CG-CD	5.81	122.47	112.60
3	C	196	LYS	CB-CG-CD	5.79	124.61	111.30
8	E	326	LYS	CB-CG-CD	5.74	124.50	111.30
8	E	130	GLU	CA-CB-CG	5.61	125.31	114.10
1	F	77	GLU	CB-CG-CD	5.54	122.01	112.60
7	D	302	TYR	CA-CB-CG	5.51	123.81	113.90
6	H	240	GLU	CA-CB-CG	5.50	125.11	114.10
3	C	196	LYS	CA-CB-CG	5.43	124.95	114.10
7	D	6	VAL	CA-C-N	5.39	131.67	121.97
7	D	6	VAL	C-N-CA	5.39	131.67	121.97
2	A	10	ASN	CA-C-N	5.39	131.67	121.97
2	A	10	ASN	C-N-CA	5.39	131.67	121.97
3	C	200	ARG	CA-CB-CG	5.39	124.87	114.10
8	E	249	MET	CA-CB-CG	5.36	124.81	114.10
4	B	395	LYS	CB-CG-CD	5.33	123.56	111.30
8	E	281	LYS	CB-CG-CD	5.31	123.52	111.30
2	A	227	ASN	N-CA-C	-5.29	102.30	109.54
4	B	409	LEU	CA-CB-CG	5.27	134.73	116.30
7	D	307	ASP	CA-CB-CG	5.27	117.87	112.60
3	C	307	ALA	CA-C-N	5.25	130.27	122.82
3	C	307	ALA	C-N-CA	5.25	130.27	122.82
5	G	82	ASP	CA-CB-CG	5.24	117.84	112.60
4	B	27	ARG	CA-C-N	5.24	130.78	122.61
4	B	27	ARG	C-N-CA	5.24	130.78	122.61
6	H	67	MET	CA-CB-CG	5.23	124.57	114.10
3	C	476	GLU	CA-CB-CG	5.22	124.54	114.10
6	H	388	LYS	CB-CG-CD	5.21	123.28	111.30
2	A	247	ASP	CA-CB-CG	5.20	117.80	112.60
4	B	65	LYS	CA-CB-CG	5.20	124.50	114.10
1	F	76	CYS	CA-C-N	-5.18	113.01	122.38
1	F	76	CYS	C-N-CA	-5.18	113.01	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	232	LYS	CB-CG-CD	5.17	123.20	111.30
6	H	143	MET	CB-CG-SD	5.17	128.22	112.70
6	H	446	ILE	CA-C-N	5.16	124.46	120.33
6	H	446	ILE	C-N-CA	5.16	124.46	120.33
6	H	254	GLU	CA-CB-CG	5.16	124.41	114.10
1	F	223	GLN	CB-CG-CD	5.14	121.34	112.60
2	A	9	VAL	CA-C-N	5.13	130.61	122.61
2	A	9	VAL	C-N-CA	5.13	130.61	122.61
5	G	210	GLU	CA-CB-CG	5.09	124.29	114.10
7	D	17	GLN	CB-CG-CD	5.06	121.20	112.60
3	C	475	CYS	CA-C-N	5.04	129.71	122.40
3	C	475	CYS	C-N-CA	5.04	129.71	122.40
7	D	148	LYS	CB-CG-CD	5.04	122.90	111.30
4	B	395	LYS	CA-CB-CG	5.03	124.16	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	D	247	LYS	Peptide
1	F	314	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	F	4041	0	4205	40	0
2	A	3952	0	4070	32	0
3	C	4085	0	4227	52	0
4	B	3907	0	4112	38	0
5	G	4095	0	4212	53	0
6	H	4023	0	4161	45	0
7	D	4014	0	4114	43	0
8	E	4030	0	4099	29	0
9	A	27	0	12	0	0
9	B	27	0	12	0	0
9	C	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	27	0	12	1	0
9	E	27	0	12	0	0
9	F	27	0	12	0	0
9	G	27	0	12	0	0
9	H	27	0	12	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
11	A	4	0	0	0	0
11	B	4	0	0	0	0
11	C	4	0	0	0	0
11	D	4	0	0	0	0
11	E	4	0	0	0	0
11	F	4	0	0	0	0
11	G	4	0	0	0	0
11	H	4	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
12	E	1	0	0	0	0
12	F	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
All	All	32411	0	33296	299	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 5.

All (299) 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)
7:D:445:ILE:O	7:D:449:LEU:HB2	1.91	0.71
5:G:468:PRO:O	5:G:472:MET:HB2	1.94	0.67
2:A:13:LYS:HG2	5:G:82:ASP:HB2	1.82	0.62
1:F:521:ALA:O	1:F:525:LEU:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:136:SER:HB3	4:B:447:GLU:HG2	1.85	0.58
2:A:511:ALA:O	2:A:515:LEU:HB2	2.04	0.58
4:B:428:PRO:O	4:B:432:LEU:HB2	2.03	0.58
2:A:36:GLY:O	2:A:40:LYS:HB2	2.04	0.57
7:D:26:ILE:HG12	7:D:105:LEU:HB3	1.86	0.57
6:H:236:SER:HB3	6:H:295:LYS:HE2	1.87	0.57
1:F:44:MET:HB2	3:C:522:ILE:HA	1.86	0.56
1:F:233:LYS:H	1:F:284:ASN:HB2	1.70	0.56
5:G:107:VAL:HB	5:G:514:GLN:HG2	1.87	0.56
6:H:415:GLU:HA	6:H:418:MET:HG2	1.87	0.56
6:H:194:MET:HE2	6:H:211:VAL:HB	1.88	0.56
3:C:326:ALA:HA	3:C:370:LYS:H	1.70	0.56
7:D:99:LEU:HB3	7:D:444:ILE:HD13	1.88	0.56
6:H:81:ALA:HB1	6:H:92:THR:HG23	1.88	0.56
7:D:518:GLU:HB3	8:E:54:LYS:HD2	1.89	0.55
3:C:237:ARG:H	3:C:288:ASP:HB2	1.72	0.55
3:C:218:VAL:HG11	3:C:323:ILE:HA	1.89	0.54
6:H:325:THR:HG21	6:H:332:ALA:HB2	1.90	0.54
2:A:112:GLU:HB3	2:A:438:SER:HB3	1.88	0.53
3:C:276:GLN:O	3:C:280:GLU:HB2	2.08	0.53
3:C:302:HIS:HB2	6:H:334:ASN:HB2	1.91	0.53
6:H:118:ILE:HG21	6:H:432:ARG:HB3	1.91	0.53
6:H:238:GLU:HA	6:H:298:ASP:HB2	1.90	0.53
7:D:90:VAL:HG11	7:D:498:VAL:HG13	1.91	0.53
4:B:366:ASN:OD1	4:B:372:LYS:NZ	2.42	0.53
3:C:273:GLU:HA	3:C:276:GLN:HB3	1.90	0.53
4:B:54:PRO:HA	4:B:173:SER:HA	1.91	0.52
5:G:438:CYS:HB3	5:G:443:GLN:HB3	1.91	0.52
8:E:209:GLY:HA3	8:E:378:ARG:HH21	1.75	0.52
6:H:194:MET:SD	6:H:194:MET:N	2.83	0.52
3:C:203:LYS:HB3	3:C:384:LEU:HD13	1.92	0.51
4:B:267:SER:H	4:B:271:GLN:HG3	1.75	0.51
1:F:160:ILE:O	3:C:127:ARG:NH2	2.44	0.51
2:A:71:LEU:HB3	2:A:85:VAL:HG22	1.92	0.51
8:E:33:ILE:O	8:E:37:LYS:HB2	2.11	0.51
5:G:8:ASP:N	5:G:8:ASP:OD2	2.44	0.51
5:G:76:LEU:HB3	5:G:90:VAL:HG22	1.93	0.51
7:D:92:ASP:OD1	7:D:92:ASP:N	2.42	0.51
3:C:177:LEU:O	3:C:181:LYS:HB2	2.11	0.51
3:C:291:ILE:HG23	3:C:312:ILE:HB	1.91	0.51
2:A:108:GLU:HG3	2:A:445:MET:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:ARG:HH12	1:F:434:GLU:HG2	1.76	0.51
4:B:332:ASP:OD2	4:B:332:ASP:N	2.40	0.50
8:E:221:MET:HE1	8:E:323:ARG:HB3	1.93	0.50
1:F:136:LEU:HD13	1:F:415:VAL:HG23	1.94	0.50
2:A:41:SER:OG	2:A:50:LYS:NZ	2.44	0.50
2:A:316:ASP:HB3	2:A:319:GLY:H	1.76	0.50
6:H:453:GLN:HG3	6:H:459:LEU:HD11	1.92	0.50
7:D:32:ILE:HD12	7:D:76:ALA:HB1	1.94	0.50
6:H:328:CYS:SG	6:H:329:GLY:N	2.84	0.50
2:A:48:MET:HB2	4:B:531:LYS:HG2	1.94	0.50
5:G:202:VAL:HB	5:G:408:ARG:HG3	1.93	0.50
8:E:9:PRO:HA	8:E:13:GLN:HB2	1.93	0.50
1:F:18:ARG:HH22	4:B:57:MET:HE2	1.76	0.50
3:C:180:VAL:HG21	3:C:398:CYS:HB3	1.94	0.50
5:G:65:ASP:OD1	5:G:65:ASP:N	2.45	0.50
1:F:295:MET:O	1:F:299:TYR:HB2	2.12	0.49
4:B:212:LYS:NZ	4:B:399:GLU:OE1	2.45	0.49
4:B:227:LEU:HD11	4:B:336:ILE:HG13	1.93	0.49
1:F:245:LYS:HD2	3:C:251:GLU:HB2	1.93	0.49
1:F:452:LEU:HD13	1:F:490:LEU:HD21	1.93	0.49
2:A:520:ILE:HG12	5:G:58:MET:HG2	1.94	0.49
2:A:177:ASP:OD2	2:A:177:ASP:N	2.46	0.49
2:A:356:GLU:OE2	4:B:413:ARG:NH1	2.46	0.49
5:G:252:PRO:HB3	5:G:302:TRP:HB2	1.95	0.49
6:H:335:SER:OG	6:H:336:PHE:N	2.46	0.49
7:D:82:ILE:HG22	8:E:380:SER:HB3	1.95	0.49
1:F:40:GLY:O	3:C:518:ARG:NH2	2.45	0.49
2:A:238:LEU:HD22	2:A:287:ILE:HG21	1.94	0.49
4:B:52:LEU:O	4:B:468:ASN:ND2	2.46	0.48
7:D:393:ILE:O	7:D:397:ARG:HB2	2.13	0.48
1:F:332:ALA:HB2	4:B:280:ARG:HH11	1.78	0.48
5:G:457:PRO:HA	5:G:460:LEU:HB2	1.94	0.48
6:H:245:ASN:OD1	6:H:245:ASN:N	2.46	0.48
6:H:399:LYS:NZ	6:H:403:ASP:OD2	2.44	0.48
5:G:229:ASP:OD2	5:G:230:LYS:NZ	2.45	0.48
5:G:484:ASN:ND2	5:G:498:ASP:OD1	2.47	0.48
3:C:128:LYS:HD2	3:C:437:TYR:HE1	1.78	0.48
7:D:60:ASN:ND2	7:D:165:SER:O	2.46	0.48
8:E:47:TYR:O	8:E:455:ASN:ND2	2.47	0.48
1:F:10:ASP:N	1:F:10:ASP:OD1	2.46	0.48
1:F:74:VAL:HG13	4:B:394:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:116:GLU:OE1	8:E:120:ARG:NH1	2.46	0.48
1:F:411:GLY:O	1:F:498:ASN:ND2	2.47	0.48
2:A:323:LEU:O	2:A:327:THR:HB	2.14	0.48
4:B:160:ARG:NH1	4:B:189:ASN:OD1	2.46	0.48
6:H:107:ASP:HA	6:H:110:ILE:HB	1.96	0.48
4:B:91:LEU:HD22	4:B:110:VAL:HG12	1.96	0.47
5:G:459:ALA:HA	5:G:462:GLU:HG2	1.95	0.47
8:E:449:PRO:HA	8:E:452:LEU:HB2	1.97	0.47
2:A:296:ILE:HG23	2:A:300:PRO:HG2	1.96	0.47
3:C:349:LEU:H	3:C:365:ASP:HB2	1.78	0.47
6:H:61:ASN:ND2	6:H:85:ASP:OD2	2.47	0.47
6:H:85:ASP:O	6:H:396:ARG:NH2	2.45	0.47
7:D:280:LYS:HE3	7:D:335:ASN:HB3	1.96	0.47
3:C:231:ARG:NH1	3:C:359:TYR:OH	2.47	0.47
4:B:38:ILE:HG12	4:B:117:LEU:HB3	1.95	0.47
1:F:255:THR:HA	3:C:257:GLU:HB2	1.96	0.47
1:F:334:LEU:HD13	4:B:284:LEU:HD11	1.97	0.47
3:C:175:ILE:HG12	3:C:214:VAL:HG23	1.97	0.47
3:C:366:CYS:HB2	3:C:369:PRO:HG3	1.97	0.47
4:B:46:ASP:OD1	4:B:49:ARG:NH2	2.48	0.47
6:H:212:LEU:HB2	6:H:361:THR:HB	1.97	0.47
8:E:155:ARG:NH2	8:E:193:ASP:OD1	2.47	0.47
1:F:357:CYS:SG	1:F:378:ARG:NH2	2.82	0.47
7:D:58:ILE:HG12	7:D:380:GLN:HB3	1.97	0.47
8:E:239:ILE:HD13	8:E:328:VAL:HG21	1.97	0.47
1:F:432:SER:OG	1:F:433:ARG:N	2.47	0.47
3:C:51:LEU:HD12	6:H:523:ARG:HD3	1.96	0.47
4:B:195:ILE:HG12	4:B:203:VAL:HG22	1.97	0.46
5:G:61:ASP:OD1	5:G:61:ASP:N	2.48	0.46
5:G:156:ASP:N	5:G:156:ASP:OD1	2.47	0.46
5:G:281:GLU:O	5:G:285:GLU:HB2	2.15	0.46
1:F:36:LEU:HD21	1:F:448:ILE:HG23	1.97	0.46
3:C:67:LEU:HD23	3:C:70:ILE:HD12	1.96	0.46
4:B:213:LYS:NZ	4:B:214:LEU:O	2.45	0.46
4:B:220:ASP:OD2	4:B:220:ASP:N	2.40	0.46
6:H:149:ILE:HD13	6:H:169:THR:HG22	1.98	0.46
1:F:203:ARG:HE	1:F:207:GLU:HG3	1.80	0.46
5:G:181:ARG:H	5:G:181:ARG:HG2	1.62	0.46
8:E:440:LYS:HA	8:E:440:LYS:HD3	1.76	0.46
1:F:508:ILE:HG23	1:F:512:LYS:HD2	1.98	0.46
7:D:186:LEU:HD11	7:D:195:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:ILE:HG23	1:F:296:CYS:HB2	1.98	0.46
3:C:64:ASN:HB2	3:C:95:THR:HG21	1.98	0.46
5:G:97:ASP:HA	5:G:101:GLY:HA2	1.98	0.46
2:A:460:ASP:OD2	2:A:460:ASP:N	2.49	0.46
3:C:350:LEU:HD23	3:C:363:ILE:HG23	1.98	0.46
6:H:489:ALA:HB1	6:H:494:VAL:HB	1.98	0.46
7:D:85:SER:OG	8:E:380:SER:O	2.33	0.46
3:C:228:ARG:HH12	6:H:331:VAL:HG22	1.81	0.45
8:E:410:PRO:O	8:E:415:THR:OG1	2.34	0.45
6:H:43:THR:OG1	6:H:45:LYS:NZ	2.50	0.45
2:A:505:LEU:HD13	5:G:216:ARG:HG2	1.98	0.45
5:G:203:ASP:N	5:G:203:ASP:OD2	2.48	0.45
8:E:217:VAL:HG23	8:E:375:ILE:HG12	1.99	0.45
2:A:17:ASP:N	2:A:17:ASP:OD1	2.50	0.45
2:A:51:ILE:HG12	2:A:63:VAL:HG22	1.98	0.45
5:G:143:ILE:HD12	5:G:512:LYS:HG2	1.98	0.45
5:G:278:TYR:O	5:G:282:LYS:HB2	2.17	0.45
4:B:287:VAL:HG11	4:B:316:PHE:HB3	1.98	0.45
6:H:426:LYS:HD2	6:H:438:GLN:HB2	1.99	0.45
7:D:282:HIS:O	7:D:283:HIS:ND1	2.50	0.45
4:B:102:ALA:HB1	4:B:514:VAL:HG22	1.98	0.45
5:G:60:VAL:HG12	5:G:66:VAL:HG22	1.99	0.45
3:C:130:LEU:HB2	3:C:510:VAL:HG11	1.98	0.45
7:D:48:LEU:HD13	7:D:58:ILE:HG22	1.99	0.45
7:D:414:MET:HE3	7:D:414:MET:HB3	1.83	0.45
8:E:322:ARG:HA	8:E:322:ARG:HD2	1.81	0.45
6:H:47:LEU:HB2	6:H:55:LYS:HB3	1.99	0.45
7:D:318:ASP:OD1	7:D:321:ARG:NH1	2.50	0.45
5:G:440:THR:OG1	5:G:441:LEU:N	2.49	0.45
5:G:522:VAL:O	5:G:526:LEU:HB2	2.17	0.45
7:D:197:ILE:HG12	7:D:372:PHE:HB2	1.98	0.45
1:F:156:MET:SD	1:F:156:MET:N	2.90	0.44
4:B:274:ARG:HA	4:B:277:ARG:HB2	1.99	0.44
7:D:96:SER:O	7:D:100:LEU:HB2	2.17	0.44
2:A:226:VAL:HA	4:B:334:GLU:HG2	1.99	0.44
5:G:287:ILE:HG13	5:G:311:LEU:HB3	1.99	0.44
6:H:451:LEU:O	6:H:455:SER:HB2	2.17	0.44
6:H:512:ALA:O	6:H:516:LEU:HB2	2.17	0.44
7:D:40:LEU:HD23	7:D:448:GLN:HB3	1.99	0.44
1:F:285:VAL:HA	1:F:306:MET:HB2	1.99	0.44
5:G:523:ARG:NH1	7:D:167:LEU:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:531:ILE:HB	4:B:61:ILE:HG23	1.99	0.44
6:H:176:ILE:HD12	6:H:176:ILE:HA	1.90	0.44
7:D:79:LEU:HA	7:D:82:ILE:HG12	1.99	0.44
2:A:163:ALA:HB2	2:A:397:LEU:HD11	2.00	0.44
4:B:340:ILE:HG23	4:B:379:CYS:HB3	2.00	0.44
6:H:294:GLN:NE2	6:H:321:MET:SD	2.90	0.44
7:D:188:ASP:OD1	7:D:188:ASP:N	2.50	0.44
8:E:136:CYS:HB2	8:E:512:THR:HG21	1.99	0.44
3:C:42:GLY:H	3:C:454:ASN:HD22	1.64	0.44
3:C:64:ASN:ND2	3:C:88:ASP:OD2	2.51	0.44
3:C:416:MET:HE3	3:C:416:MET:HB3	1.91	0.44
5:G:435:ALA:HB2	5:G:446:MET:HB2	1.99	0.44
6:H:426:LYS:HZ3	6:H:438:GLN:HB2	1.83	0.44
8:E:246:PHE:HB3	8:E:297:VAL:HG13	1.98	0.44
2:A:138:ARG:NH1	5:G:218:GLU:OE1	2.51	0.44
3:C:282:ILE:HG22	3:C:287:PRO:HG3	1.99	0.44
3:C:431:GLY:O	3:C:434:GLN:NE2	2.51	0.44
4:B:161:GLU:HA	4:B:164:LEU:HB2	2.00	0.44
5:G:300:CYS:SG	5:G:301:GLN:N	2.90	0.44
8:E:69:ALA:HA	8:E:72:ILE:HD12	2.00	0.44
2:A:10:ASN:ND2	2:A:12:PHE:O	2.50	0.44
5:G:12:ARG:HH21	7:D:16:SER:HG	1.62	0.44
5:G:46:MET:HE2	5:G:46:MET:HB2	1.87	0.44
5:G:62:LYS:H	5:G:62:LYS:HG2	1.64	0.44
4:B:253:LEU:HD23	4:B:286:LEU:HD13	1.99	0.43
7:D:82:ILE:HG21	7:D:509:ALA:HB2	1.99	0.43
8:E:324:LEU:HA	8:E:327:THR:HG22	2.00	0.43
6:H:307:LYS:HE2	6:H:307:LYS:HB2	1.81	0.43
8:E:114:LEU:HA	8:E:117:GLU:HG3	1.98	0.43
8:E:158:ASP:N	8:E:158:ASP:OD1	2.45	0.43
5:G:356:LEU:H	5:G:374:GLN:HB2	1.83	0.43
6:H:217:ARG:HD2	6:H:217:ARG:HA	1.79	0.43
7:D:408:GLY:O	7:D:487:ASN:ND2	2.45	0.43
7:D:487:ASN:HA	7:D:490:ALA:HB3	2.01	0.43
1:F:445:LEU:HD21	1:F:514:LEU:HD21	2.00	0.43
1:F:12:SER:HB2	1:F:17:ILE:HD11	2.01	0.43
3:C:458:SER:HB3	3:C:461:ARG:HH22	1.83	0.43
5:G:92:LEU:HD22	5:G:521:MET:HG2	2.01	0.43
2:A:289:CYS:HA	2:A:310:MET:HB3	2.01	0.43
7:D:241:ASN:HB3	7:D:332:THR:HB	2.01	0.43
3:C:283:ILE:O	3:C:286:LYS:NZ	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:149:VAL:HA	7:D:152:ARG:HB2	2.01	0.43
8:E:134:ILE:HA	8:E:137:ARG:HG2	2.01	0.43
5:G:490:ASP:OD2	5:G:495:GLY:N	2.52	0.43
7:D:218:LYS:NZ	7:D:350:GLU:OE2	2.48	0.43
7:D:297:ASP:O	7:D:301:GLN:NE2	2.52	0.43
8:E:22:PHE:HB2	8:E:524:ILE:HB	2.01	0.43
4:B:165:ASN:O	4:B:169:THR:OG1	2.32	0.42
5:G:240:LYS:NZ	5:G:242:GLU:OE2	2.52	0.42
6:H:199:LYS:HB2	6:H:200:SER:H	1.60	0.42
3:C:227:PRO:HG3	6:H:322:GLU:HA	2.00	0.42
3:C:287:PRO:HG2	3:C:309:ILE:HD13	2.01	0.42
5:G:291:LYS:HD2	5:G:291:LYS:HA	1.88	0.42
5:G:299:ILE:HG23	5:G:323:VAL:HG21	2.01	0.42
2:A:131:ARG:NH2	5:G:177:ASN:OD1	2.52	0.42
2:A:231:ARG:HG3	2:A:350:GLU:HB3	2.02	0.42
2:A:326:VAL:HB	2:A:370:ALA:HB3	1.99	0.42
5:G:91:GLU:OE2	7:D:379:GLU:N	2.52	0.42
6:H:34:LEU:HD13	6:H:93:THR:HG23	2.01	0.42
6:H:418:MET:HE3	6:H:418:MET:HB2	1.76	0.42
2:A:91:GLN:HB3	2:A:99:THR:HG22	2.00	0.42
2:A:123:PRO:HA	2:A:126:ILE:HD12	2.00	0.42
6:H:430:LYS:HA	6:H:430:LYS:HD3	1.80	0.42
2:A:203:LYS:HB3	2:A:383:LEU:HD13	2.00	0.42
4:B:74:GLY:HA2	4:B:77:ILE:HD12	2.02	0.42
7:D:66:LEU:HB3	7:D:80:VAL:HG22	2.01	0.42
8:E:206:LYS:O	8:E:224:LYS:NZ	2.46	0.42
1:F:42:ASP:OD1	1:F:56:ASN:ND2	2.51	0.42
4:B:119:SER:HB3	4:B:453:ALA:HB1	2.01	0.42
7:D:499:ARG:NH2	9:D:603:ADP:O3'	2.52	0.42
5:G:12:ARG:NH2	7:D:16:SER:OG	2.42	0.42
2:A:154:LYS:HB3	2:A:154:LYS:HE3	1.88	0.42
5:G:50:LEU:HD21	5:G:456:ILE:HG23	2.00	0.42
5:G:496:THR:O	5:G:502:GLN:NE2	2.52	0.42
6:H:211:VAL:HG23	6:H:373:THR:HG21	2.01	0.42
7:D:244:LEU:HB2	7:D:295:ILE:HA	2.01	0.42
3:C:137:LEU:HD23	3:C:137:LEU:HA	1.94	0.42
3:C:458:SER:HB3	3:C:461:ARG:HH12	1.85	0.42
4:B:249:ILE:HD13	4:B:249:ILE:HA	1.90	0.42
5:G:36:ILE:HG12	5:G:115:LEU:HB3	2.01	0.42
6:H:402:ILE:HD13	6:H:402:ILE:HA	1.94	0.42
8:E:296:LYS:HA	8:E:314:ARG:HE	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:475:CYS:HB3	3:C:476:GLU:H	1.69	0.41
7:D:20:PRO:HA	7:D:23:VAL:HG22	2.02	0.41
3:C:203:LYS:HD2	3:C:384:LEU:HB3	2.02	0.41
7:D:244:LEU:HD12	7:D:295:ILE:HG12	2.02	0.41
1:F:306:MET:HE2	1:F:306:MET:HB3	1.95	0.41
1:F:314:ARG:HH11	1:F:318:ARG:HH22	1.67	0.41
1:F:402:VAL:HG23	1:F:506:PRO:HG3	2.03	0.41
2:A:390:LEU:HD12	2:A:390:LEU:HA	1.95	0.41
3:C:196:LYS:NZ	3:C:396:GLN:OE1	2.50	0.41
5:G:16:ILE:HG13	7:D:31:VAL:HG11	2.03	0.41
7:D:10:LYS:HB3	7:D:11:GLU:H	1.76	0.41
1:F:192:VAL:HB	1:F:396:LEU:HB3	2.02	0.41
3:C:245:LEU:HD12	3:C:296:ILE:HG12	2.03	0.41
5:G:478:ARG:HB3	5:G:487:LEU:HD13	2.03	0.41
8:E:320:ASP:OD1	8:E:323:ARG:NH2	2.45	0.41
1:F:203:ARG:HG3	3:C:504:GLN:HE22	1.86	0.41
1:F:355:ARG:HH22	1:F:358:ASP:H	1.67	0.41
3:C:47:MET:HE2	3:C:47:MET:HB2	1.93	0.41
3:C:224:VAL:HG22	3:C:229:MET:HE3	2.03	0.41
3:C:229:MET:H	3:C:229:MET:HG2	1.74	0.41
5:G:326:PRO:HA	5:G:329:GLU:HB2	2.03	0.41
5:G:433:GLN:O	5:G:437:LYS:NZ	2.46	0.41
7:D:145:LYS:HD3	7:D:145:LYS:HA	1.90	0.41
4:B:245:LYS:H	4:B:296:ASN:HB2	1.86	0.41
3:C:51:LEU:HB2	6:H:523:ARG:HH11	1.86	0.41
3:C:132:ASP:OD2	3:C:437:TYR:OH	2.39	0.41
7:D:218:LYS:HA	7:D:218:LYS:HD3	1.91	0.41
1:F:75:LEU:HD22	1:F:94:VAL:HG12	2.03	0.41
1:F:232:ALA:HA	1:F:284:ASN:HD22	1.86	0.41
1:F:245:LYS:HA	1:F:245:LYS:HD3	1.85	0.41
3:C:516:LEU:HA	3:C:519:ILE:HD12	2.01	0.41
5:G:37:MET:HA	5:G:40:LYS:HB2	2.03	0.41
5:G:121:LEU:HB3	5:G:126:ILE:HD12	2.02	0.41
8:E:230:ASP:OD1	8:E:230:ASP:N	2.54	0.41
3:C:486:THR:OG1	3:C:487:LEU:N	2.54	0.40
4:B:63:ASP:OD1	4:B:63:ASP:N	2.49	0.40
4:B:117:LEU:HD23	4:B:117:LEU:HA	1.93	0.40
1:F:57:ASP:OD1	1:F:90:THR:OG1	2.36	0.40
3:C:222:LYS:HD3	3:C:222:LYS:HA	1.96	0.40
5:G:255:PRO:HA	5:G:256:PRO:HD3	1.91	0.40
6:H:293:ASN:HB3	6:H:297:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:336:PHE:HD2	6:H:339:LEU:HD21	1.86	0.40
6:H:2:ALA:O	6:H:6:THR:OG1	2.39	0.40
3:C:341:ASP:OD1	3:C:341:ASP:N	2.54	0.40
6:H:380:ASN:O	6:H:383:THR:OG1	2.36	0.40
8:E:235:LYS:HE2	8:E:235:LYS:HB2	1.90	0.40
1:F:526:ARG:HG3	4:B:175:VAL:HG13	2.03	0.40
3:C:166:SER:HA	3:C:169:SER:HB3	2.03	0.40
6:H:439:ALA:O	6:H:443:ALA:CB	2.70	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	F	530/532 (100%)	506 (96%)	24 (4%)	0	100	100
2	A	524/526 (100%)	498 (95%)	25 (5%)	1 (0%)	43	71
3	C	523/525 (100%)	510 (98%)	13 (2%)	0	100	100
4	B	515/517 (100%)	493 (96%)	22 (4%)	0	100	100
5	G	529/531 (100%)	514 (97%)	15 (3%)	0	100	100
6	H	523/525 (100%)	498 (95%)	24 (5%)	1 (0%)	43	71
7	D	521/523 (100%)	499 (96%)	20 (4%)	2 (0%)	30	59
8	E	527/529 (100%)	503 (95%)	24 (5%)	0	100	100
All	All	4192/4208 (100%)	4021 (96%)	167 (4%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	11	ILE
6	H	199	LYS

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Mol	Chain	Res	Type
7	D	7	ILE
7	D	247	LYS

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	F	444/444 (100%)	434 (98%)	10 (2%)	44	61
2	A	418/418 (100%)	405 (97%)	13 (3%)	35	55
3	C	456/456 (100%)	444 (97%)	12 (3%)	40	58
4	B	441/441 (100%)	431 (98%)	10 (2%)	44	61
5	G	448/448 (100%)	436 (97%)	12 (3%)	39	57
6	H	437/437 (100%)	425 (97%)	12 (3%)	39	57
7	D	430/430 (100%)	421 (98%)	9 (2%)	47	62
8	E	436/436 (100%)	428 (98%)	8 (2%)	51	64
All	All	3510/3510 (100%)	3424 (98%)	86 (2%)	42	59

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	77	GLU
1	F	94	VAL
1	F	148	LEU
1	F	161	ILE
1	F	203	ARG
1	F	209	MET
1	F	237	LEU
1	F	383	PHE
1	F	426	TYR
1	F	488	LEU
2	A	9	VAL
2	A	30	ILE
2	A	69	THR

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Mol	Chain	Res	Type
2	A	76	VAL
2	A	122	HIS
2	A	148	HIS
2	A	153	VAL
2	A	174	HIS
2	A	258	VAL
2	A	295	LEU
2	A	298	ASN
2	A	323	LEU
2	A	509	GLU
3	C	58	VAL
3	C	95	THR
3	C	224	VAL
3	C	229	MET
3	C	289	VAL
3	C	319	ASP
3	C	331	ILE
3	C	349	LEU
3	C	350	LEU
3	C	359	TYR
3	C	450	THR
3	C	514	VAL
4	B	58	ASP
4	B	68	VAL
4	B	152	SER
4	B	305	LEU
4	B	320	MET
4	B	396	LEU
4	B	406	HIS
4	B	409	LEU
4	B	513	LEU
4	B	531	LYS
5	G	5	LEU
5	G	29	LEU
5	G	58	MET
5	G	65	ASP
5	G	143	ILE
5	G	144	GLU
5	G	158	LYS
5	G	177	ASN
5	G	213	VAL
5	G	455	VAL

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Mol	Chain	Res	Type
5	G	470	GLN
5	G	474	GLU
6	H	88	THR
6	H	115	HIS
6	H	149	ILE
6	H	232	THR
6	H	244	VAL
6	H	245	ASN
6	H	290	VAL
6	H	326	LEU
6	H	374	LEU
6	H	385	THR
6	H	402	ILE
6	H	504	LEU
7	D	36	VAL
7	D	149	VAL
7	D	163	LEU
7	D	183	VAL
7	D	242	VAL
7	D	334	VAL
7	D	405	VAL
7	D	406	VAL
7	D	520	ILE
8	E	39	LEU
8	E	59	HIS
8	E	60	LEU
8	E	121	ILE
8	E	146	LEU
8	E	196	HIS
8	E	239	ILE
8	E	409	VAL

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

Mol	Chain	Res	Type
1	F	133	ASN
1	F	262	GLN
2	A	73	ASN
2	A	91	GLN
2	A	122	HIS
2	A	124	GLN
2	A	498	GLN

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Mol	Chain	Res	Type
2	A	519	ASN
3	C	23	GLN
3	C	61	ASN
3	C	64	ASN
3	C	118	HIS
3	C	154	ASN
3	C	188	ASN
3	C	269	GLN
3	C	277	GLN
3	C	390	ASN
3	C	406	GLN
3	C	481	ASN
4	B	25	GLN
4	B	72	ASN
4	B	231	GLN
4	B	262	ASN
4	B	394	ASN
4	B	484	HIS
5	G	145	HIS
5	G	467	ASN
5	G	484	ASN
5	G	497	ASN
5	G	502	GLN
6	H	334	ASN
6	H	514	ASN
7	D	30	GLN
7	D	117	HIS
7	D	301	GLN
8	E	13	GLN
8	E	41	GLN
8	E	91	HIS
8	E	102	ASN
8	E	140	HIS
8	E	219	HIS
8	E	279	GLN

5.3.3 RNA

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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
11	AF3	D	602	9	0,3,3	-	-	-		
11	AF3	B	603	9	0,3,3	-	-	-		
9	ADP	D	603	10,11	27,29,29	1.37	4 (14%)	42,45,45	1.94	12 (28%)
11	AF3	H	603	-	0,3,3	-	-	-		
11	AF3	E	603	9	0,3,3	-	-	-		
9	ADP	C	601	10,11	27,29,29	1.37	4 (14%)	42,45,45	1.92	10 (23%)
11	AF3	G	603	9	0,3,3	-	-	-		
9	ADP	A	601	10,11	27,29,29	1.37	4 (14%)	42,45,45	1.94	10 (23%)
11	AF3	A	603	9,2	0,3,3	-	-	-		
11	AF3	F	603	9	0,3,3	-	-	-		
9	ADP	B	601	10,11	27,29,29	1.37	4 (14%)	42,45,45	1.95	11 (26%)
9	ADP	H	601	10	27,29,29	1.37	4 (14%)	42,45,45	1.94	10 (23%)
9	ADP	E	601	10,11	27,29,29	1.38	4 (14%)	42,45,45	1.93	10 (23%)
9	ADP	F	601	10,11	27,29,29	1.38	4 (14%)	42,45,45	1.91	11 (26%)
9	ADP	G	601	10,11	27,29,29	1.37	4 (14%)	42,45,45	1.93	11 (26%)
11	AF3	C	603	3,9	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
9	ADP	D	603	10,11	-	3/16/32/32	0/3/3/3
9	ADP	C	601	10,11	-	4/16/32/32	0/3/3/3
9	ADP	A	601	10,11	-	1/16/32/32	0/3/3/3
9	ADP	B	601	10,11	-	1/16/32/32	0/3/3/3
9	ADP	H	601	10	-	5/16/32/32	0/3/3/3
9	ADP	E	601	10,11	-	5/16/32/32	0/3/3/3
9	ADP	F	601	10,11	-	2/16/32/32	0/3/3/3
9	ADP	G	601	10,11	-	2/16/32/32	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	601	ADP	C5-C4	4.61	1.47	1.39
9	H	601	ADP	C5-C4	4.61	1.47	1.39
9	G	601	ADP	C5-C4	4.60	1.47	1.39
9	E	601	ADP	C5-C4	4.58	1.47	1.39
9	A	601	ADP	C5-C4	4.57	1.47	1.39
9	B	601	ADP	C5-C4	4.56	1.47	1.39
9	D	603	ADP	C5-C4	4.55	1.47	1.39
9	C	601	ADP	C5-C4	4.52	1.47	1.39
9	E	601	ADP	C5-C6	2.78	1.48	1.41
9	A	601	ADP	C5-C6	2.76	1.48	1.41
9	C	601	ADP	C5-C6	2.76	1.48	1.41
9	G	601	ADP	C5-C6	2.74	1.48	1.41
9	F	601	ADP	C5-C6	2.74	1.48	1.41
9	D	603	ADP	C5-C6	2.73	1.48	1.41
9	B	601	ADP	C5-C6	2.73	1.48	1.41
9	H	601	ADP	C5-C6	2.70	1.48	1.41
9	D	603	ADP	C8-N7	2.49	1.36	1.31
9	A	601	ADP	C8-N7	2.48	1.36	1.31
9	B	601	ADP	C8-N7	2.47	1.36	1.31
9	F	601	ADP	C8-N7	2.45	1.36	1.31
9	G	601	ADP	C8-N7	2.45	1.36	1.31
9	E	601	ADP	C8-N7	2.44	1.36	1.31
9	C	601	ADP	C8-N7	2.43	1.36	1.31
9	H	601	ADP	C8-N7	2.39	1.36	1.31
9	F	601	ADP	C5-N7	-2.16	1.34	1.39
9	A	601	ADP	C5-N7	-2.15	1.35	1.39
9	E	601	ADP	C5-N7	-2.13	1.35	1.39
9	H	601	ADP	C5-N7	-2.13	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	601	ADP	C5-N7	-2.13	1.35	1.39
9	C	601	ADP	C5-N7	-2.12	1.35	1.39
9	G	601	ADP	C5-N7	-2.12	1.35	1.39
9	D	603	ADP	C5-N7	-2.10	1.35	1.39

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	601	ADP	C5-C4-N3	-6.11	118.77	126.75
9	E	601	ADP	C5-C4-N3	-6.11	118.78	126.75
9	A	601	ADP	C5-C4-N3	-6.10	118.79	126.75
9	H	601	ADP	C5-C4-N3	-6.09	118.81	126.75
9	C	601	ADP	C5-C4-N3	-6.08	118.81	126.75
9	D	603	ADP	C5-C4-N3	-6.08	118.82	126.75
9	G	601	ADP	C5-C4-N3	-6.06	118.84	126.75
9	B	601	ADP	C5-C4-N3	-6.02	118.90	126.75
9	H	601	ADP	N3-C4-N9	4.81	135.00	127.08
9	F	601	ADP	N3-C4-N9	4.79	134.98	127.08
9	G	601	ADP	N3-C4-N9	4.78	134.97	127.08
9	E	601	ADP	N3-C4-N9	4.78	134.95	127.08
9	A	601	ADP	N3-C4-N9	4.77	134.94	127.08
9	C	601	ADP	N3-C4-N9	4.74	134.90	127.08
9	B	601	ADP	N3-C4-N9	4.74	134.90	127.08
9	D	603	ADP	N3-C4-N9	4.72	134.86	127.08
9	D	603	ADP	C2-N3-C4	3.96	121.12	111.75
9	C	601	ADP	C2-N3-C4	3.96	121.10	111.75
9	F	601	ADP	C2-N3-C4	3.96	121.09	111.75
9	A	601	ADP	C2-N3-C4	3.95	121.07	111.75
9	E	601	ADP	C2-N3-C4	3.94	121.07	111.75
9	G	601	ADP	C2-N3-C4	3.92	121.02	111.75
9	B	601	ADP	C2-N3-C4	3.92	121.01	111.75
9	H	601	ADP	C2-N3-C4	3.92	121.01	111.75
9	D	603	ADP	N3-C2-N1	-3.39	123.30	128.60
9	C	601	ADP	N3-C2-N1	-3.38	123.32	128.60
9	F	601	ADP	N3-C2-N1	-3.36	123.34	128.60
9	B	601	ADP	N3-C2-N1	-3.36	123.35	128.60
9	G	601	ADP	N3-C2-N1	-3.35	123.36	128.60
9	E	601	ADP	N3-C2-N1	-3.34	123.38	128.60
9	H	601	ADP	N3-C2-N1	-3.34	123.38	128.60
9	A	601	ADP	N3-C2-N1	-3.32	123.41	128.60
9	B	601	ADP	PA-O3A-PB	-3.30	121.50	132.83
9	D	603	ADP	C4-C5-N7	-3.30	106.60	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	601	ADP	C4-C5-N7	-3.26	106.65	110.62
9	F	601	ADP	C4-C5-N7	-3.25	106.66	110.62
9	E	601	ADP	C4-C5-N7	-3.24	106.67	110.62
9	G	601	ADP	C4-C5-N7	-3.24	106.67	110.62
9	H	601	ADP	C4-C5-N7	-3.23	106.69	110.62
9	A	601	ADP	C4-C5-N7	-3.22	106.70	110.62
9	B	601	ADP	C4-C5-N7	-3.21	106.71	110.62
9	H	601	ADP	PA-O3A-PB	-2.93	122.78	132.83
9	A	601	ADP	PA-O3A-PB	-2.90	122.87	132.83
9	E	601	ADP	PA-O3A-PB	-2.82	123.16	132.83
9	D	603	ADP	C5-N7-C8	2.76	107.44	103.51
9	F	601	ADP	C5-N7-C8	2.76	107.43	103.51
9	G	601	ADP	C5-N7-C8	2.75	107.42	103.51
9	B	601	ADP	C5-N7-C8	2.72	107.37	103.51
9	H	601	ADP	C5-N7-C8	2.72	107.37	103.51
9	C	601	ADP	C5-N7-C8	2.72	107.37	103.51
9	A	601	ADP	C5-N7-C8	2.71	107.36	103.51
9	G	601	ADP	PA-O3A-PB	-2.67	123.66	132.83
9	E	601	ADP	C5-N7-C8	2.67	107.30	103.51
9	B	601	ADP	C4-N9-C8	2.63	108.58	105.73
9	G	601	ADP	C4-N9-C8	2.62	108.57	105.73
9	H	601	ADP	C4-N9-C8	2.61	108.56	105.73
9	D	603	ADP	C4-N9-C8	2.57	108.52	105.73
9	F	601	ADP	C4-N9-C8	2.55	108.49	105.73
9	A	601	ADP	C4-N9-C8	2.53	108.47	105.73
9	C	601	ADP	C4-N9-C8	2.52	108.46	105.73
9	E	601	ADP	C4-N9-C8	2.51	108.44	105.73
9	D	603	ADP	PA-O3A-PB	-2.41	124.56	132.83
9	D	603	ADP	C6-C5-N7	2.36	136.42	132.02
9	C	601	ADP	C6-C5-N7	2.33	136.36	132.02
9	G	601	ADP	C6-C5-N7	2.32	136.34	132.02
9	C	601	ADP	PA-O3A-PB	-2.31	124.88	132.83
9	F	601	ADP	C6-C5-N7	2.31	136.33	132.02
9	B	601	ADP	C6-C5-N7	2.31	136.33	132.02
9	H	601	ADP	C3'-C2'-C1'	2.31	105.81	101.43
9	A	601	ADP	C6-C5-N7	2.29	136.29	132.02
9	E	601	ADP	C6-C5-N7	2.29	136.29	132.02
9	F	601	ADP	C3'-C2'-C1'	2.29	105.78	101.43
9	G	601	ADP	C3'-C2'-C1'	2.29	105.77	101.43
9	H	601	ADP	C6-C5-N7	2.27	136.25	132.02
9	A	601	ADP	C3'-C2'-C1'	2.24	105.68	101.43
9	C	601	ADP	C3'-C2'-C1'	2.21	105.62	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	601	ADP	C3'-C2'-C1'	2.19	105.59	101.43
9	F	601	ADP	PA-O3A-PB	-2.17	125.37	132.83
9	D	603	ADP	O4'-C1'-N9	2.09	112.17	108.06
9	E	601	ADP	C3'-C2'-C1'	2.08	105.37	101.43
9	D	603	ADP	C3'-C2'-C1'	2.06	105.33	101.43
9	D	603	ADP	N9-C8-N7	-2.04	111.13	113.91
9	B	601	ADP	N9-C8-N7	-2.03	111.14	113.91
9	G	601	ADP	N9-C8-N7	-2.02	111.15	113.91
9	F	601	ADP	N9-C8-N7	-2.00	111.17	113.91

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	601	ADP	C5'-O5'-PA-O2A
9	H	601	ADP	C5'-O5'-PA-O3A
9	E	601	ADP	C5'-O5'-PA-O1A
9	E	601	ADP	C5'-O5'-PA-O2A
9	E	601	ADP	C5'-O5'-PA-O3A
9	E	601	ADP	O4'-C4'-C5'-O5'
9	E	601	ADP	C3'-C4'-C5'-O5'
9	D	603	ADP	O4'-C4'-C5'-O5'
9	D	603	ADP	C3'-C4'-C5'-O5'
9	F	601	ADP	PB-O3A-PA-O5'
9	A	601	ADP	PB-O3A-PA-O5'
9	C	601	ADP	PB-O3A-PA-O5'
9	G	601	ADP	PB-O3A-PA-O5'
9	D	603	ADP	PB-O3A-PA-O5'
9	C	601	ADP	C5'-O5'-PA-O3A
9	B	601	ADP	C5'-O5'-PA-O3A
9	C	601	ADP	C5'-O5'-PA-O1A
9	H	601	ADP	C5'-O5'-PA-O1A
9	H	601	ADP	C5'-O5'-PA-O2A
9	H	601	ADP	PB-O3A-PA-O1A
9	G	601	ADP	O4'-C4'-C5'-O5'
9	F	601	ADP	PB-O3A-PA-O2A
9	H	601	ADP	PB-O3A-PA-O2A

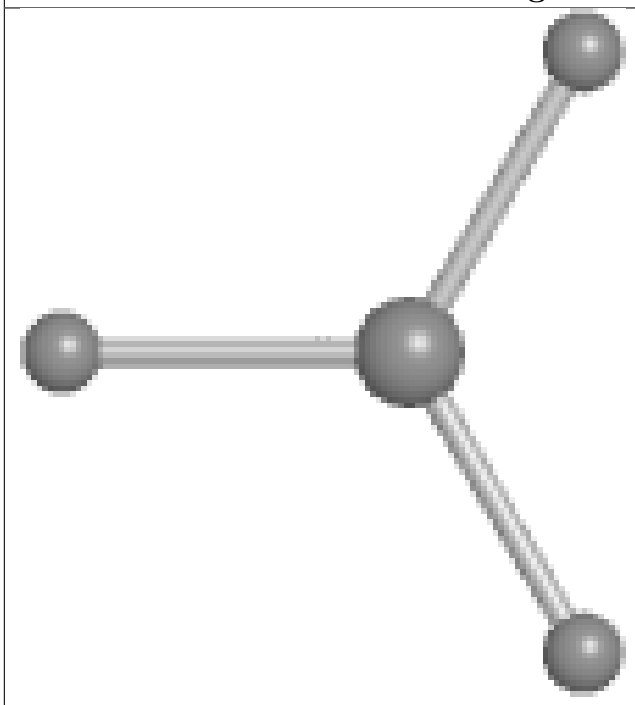
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	603	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 AF3 D 602



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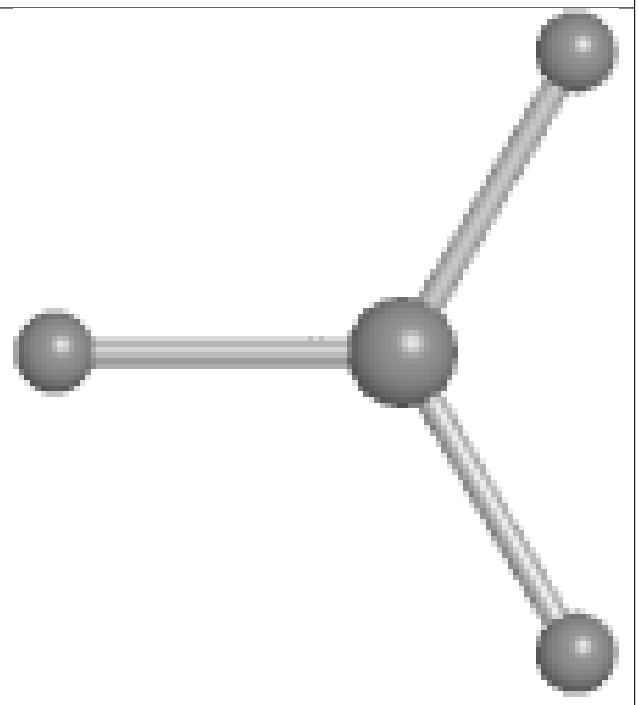

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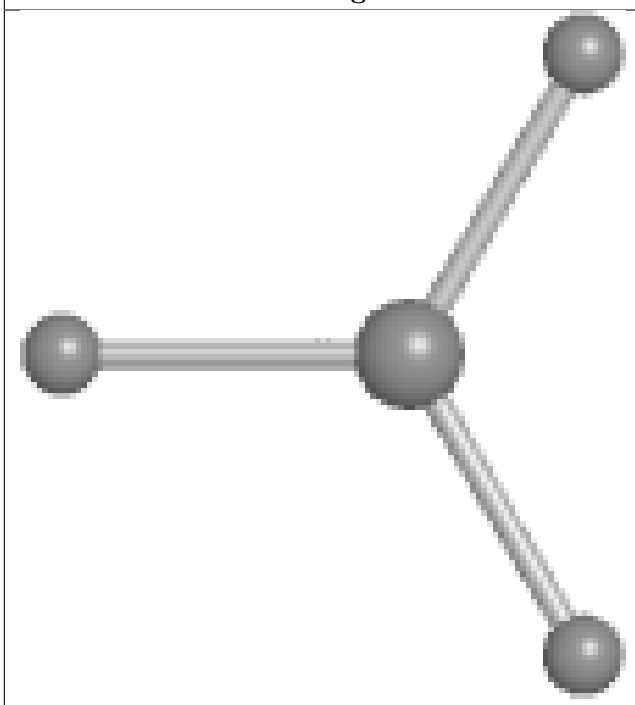

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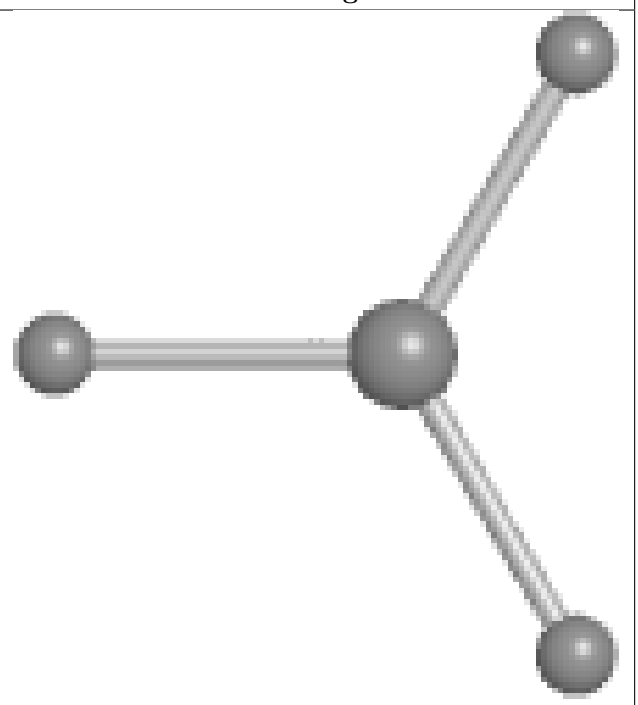
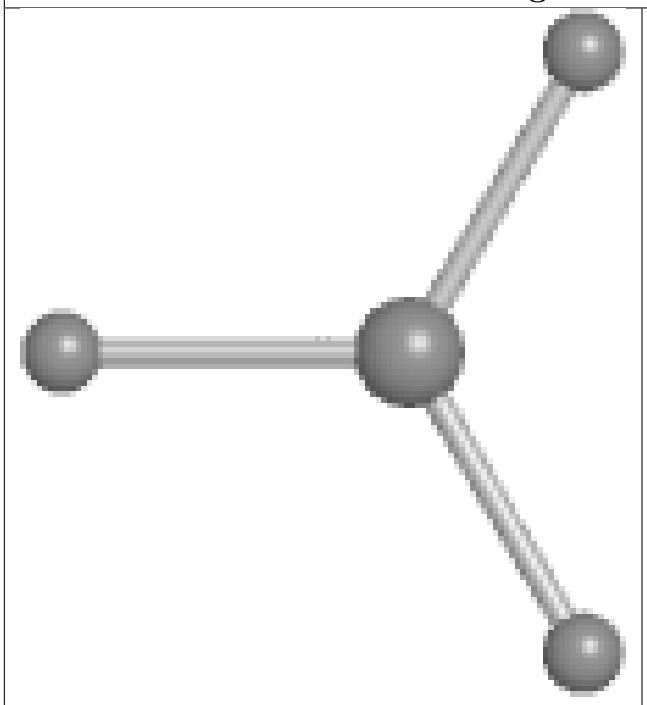


Rings

Ligand AF3 B 603



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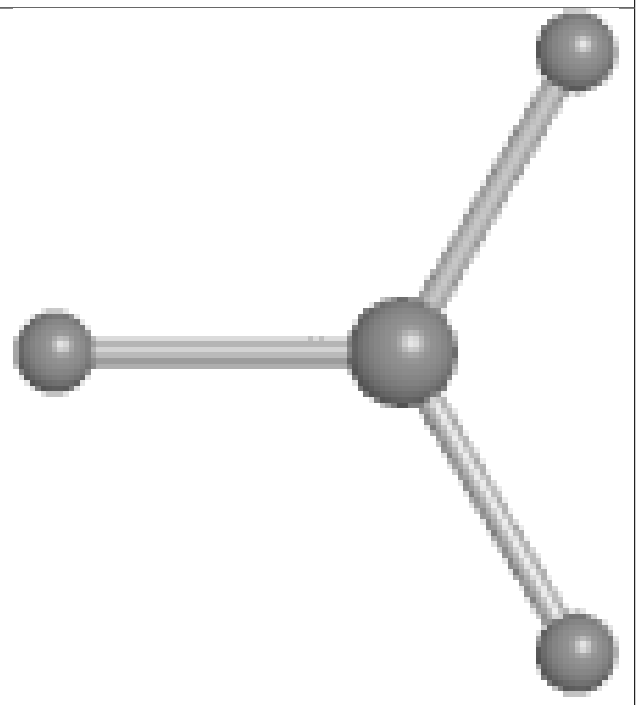

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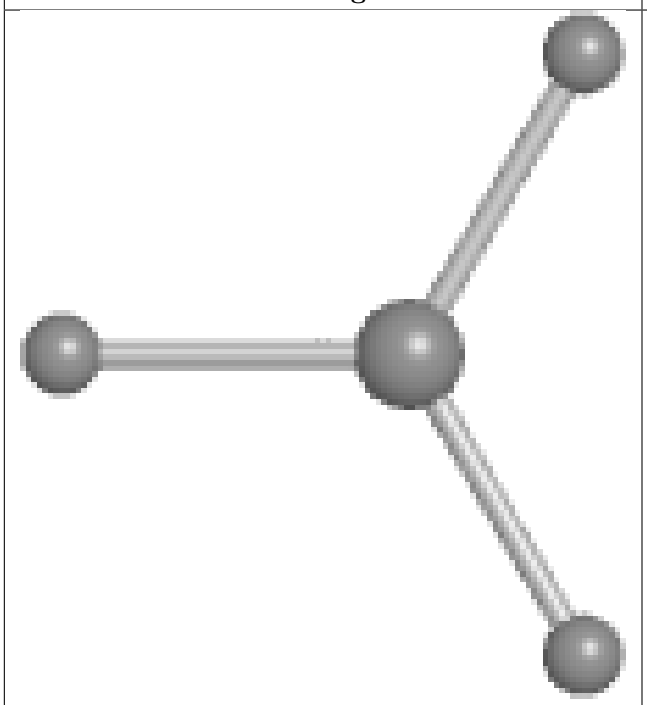

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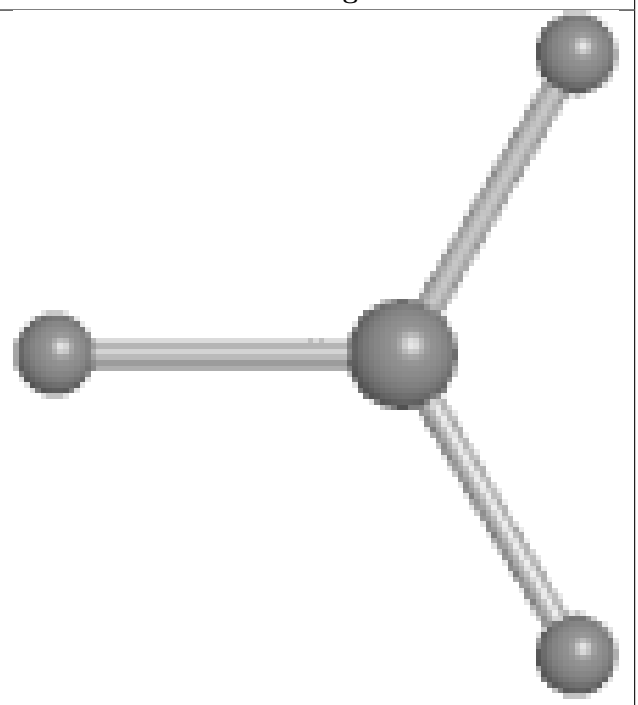
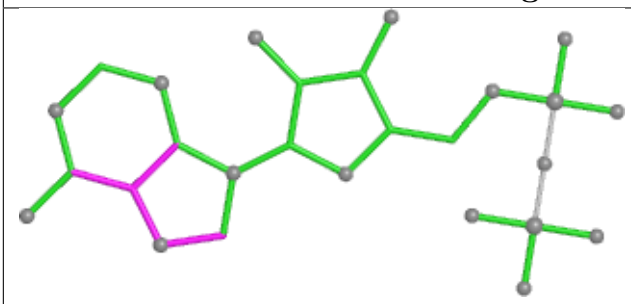


Rings

Ligand ADP D 603



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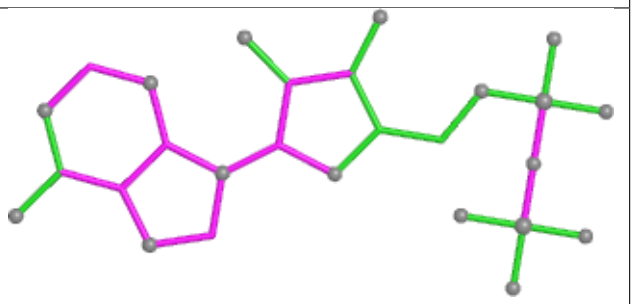

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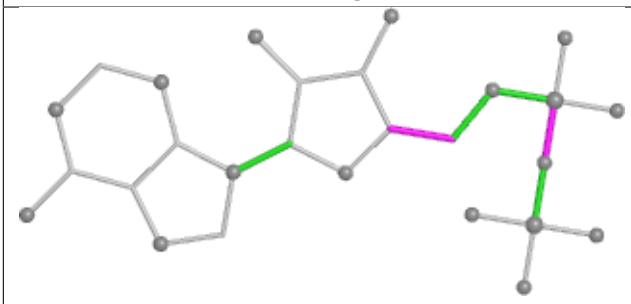

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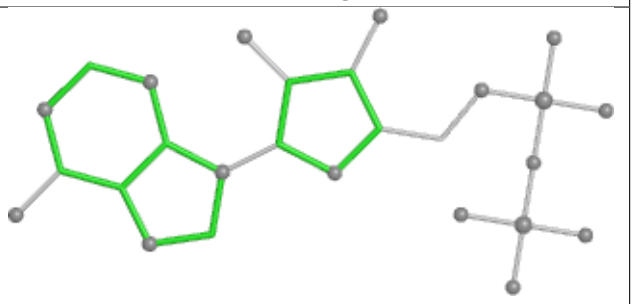
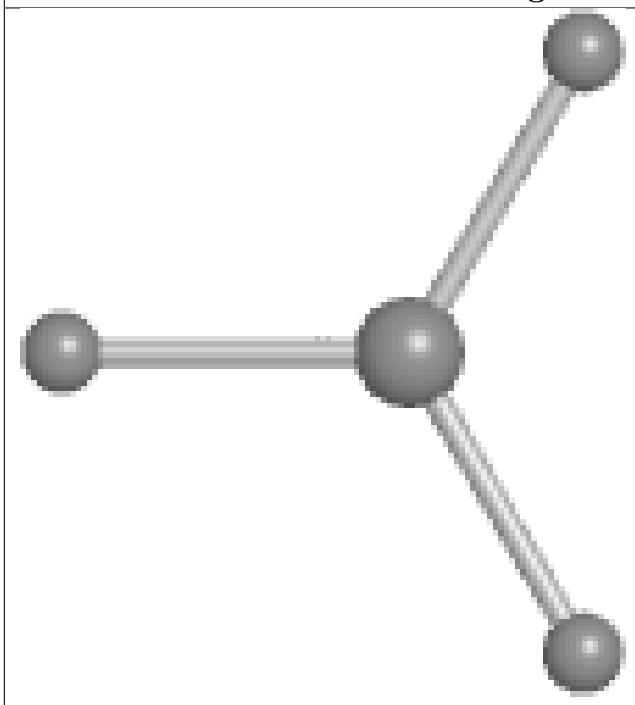


Rings

Ligand AF3 H 603



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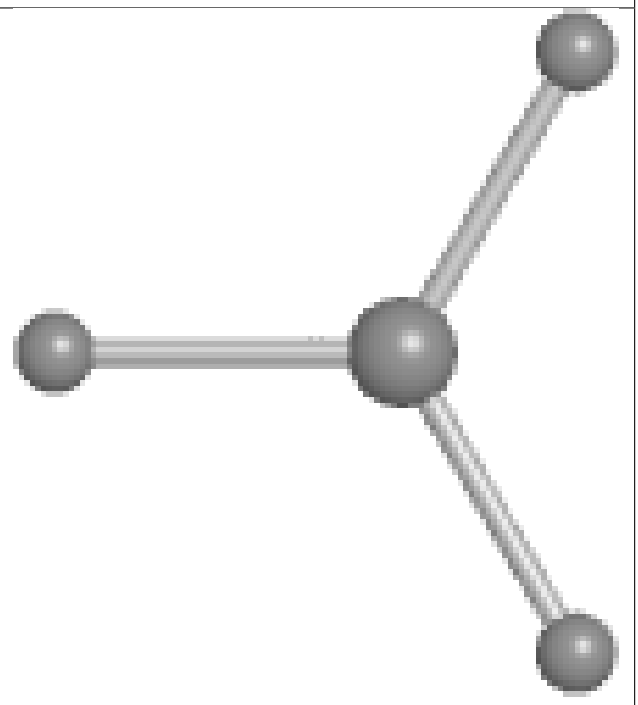
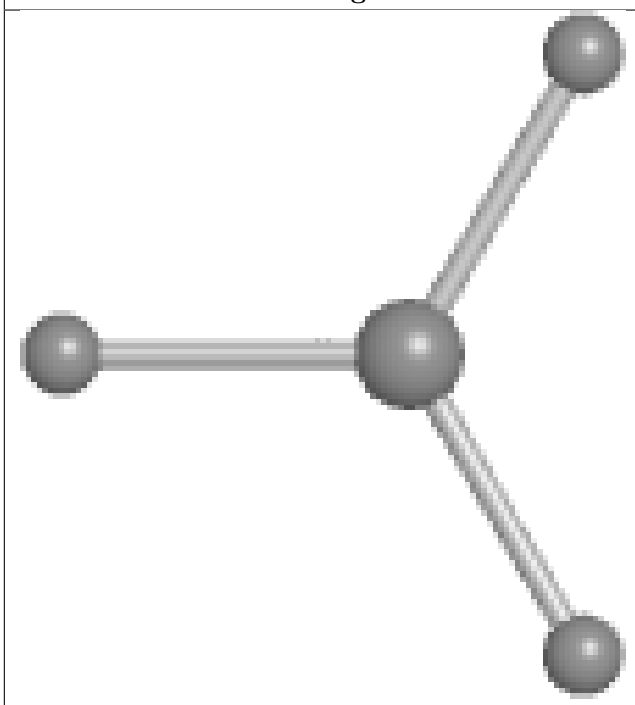


Bond angles



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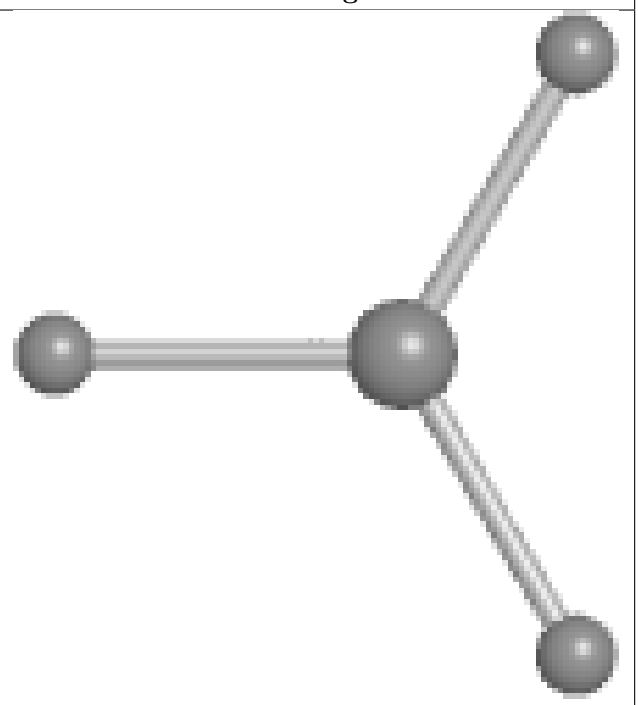
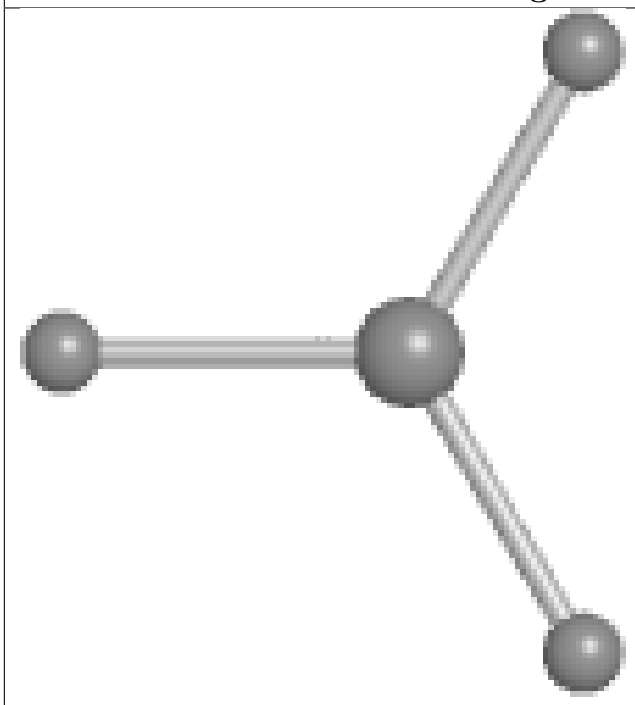


Rings

Ligand AF3 E 603



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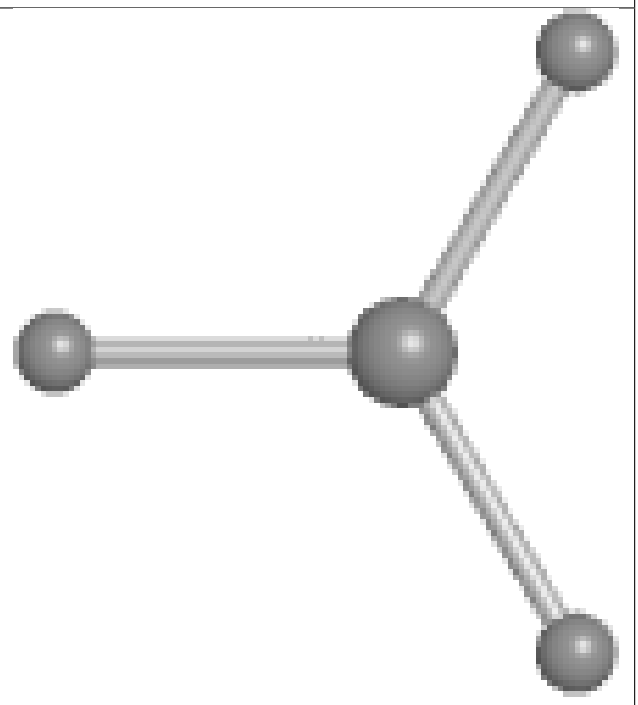

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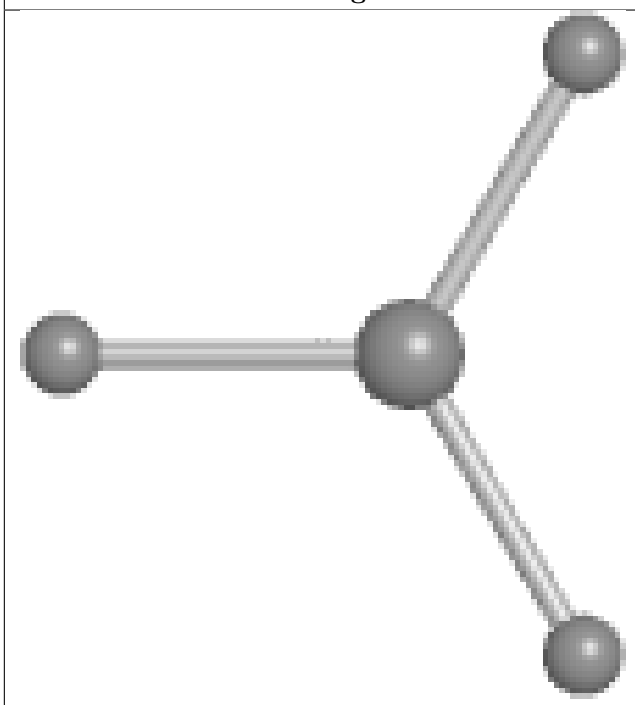

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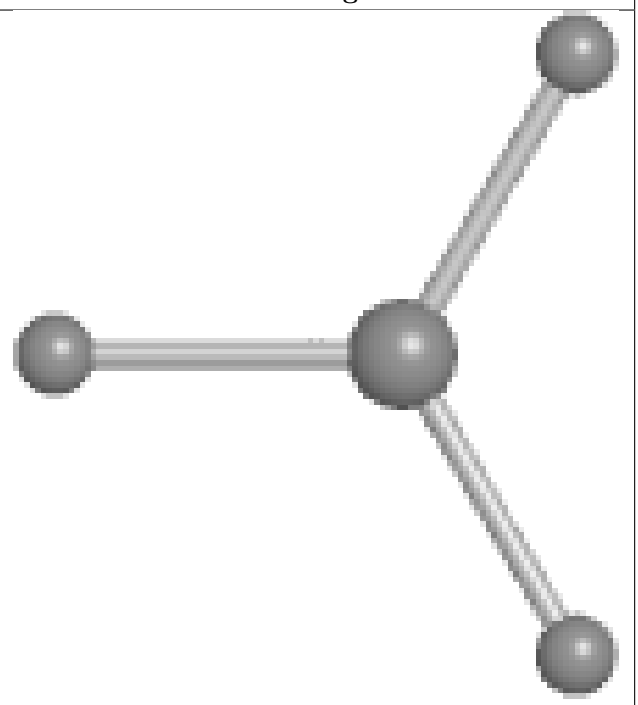
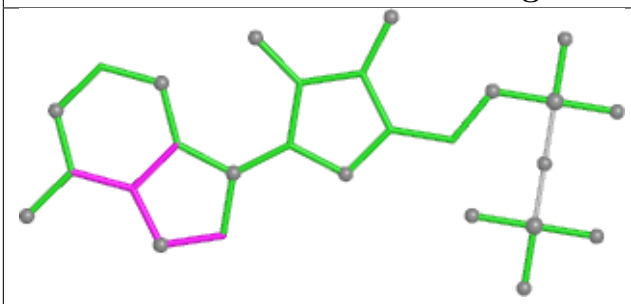


Rings

Ligand ADP C 601



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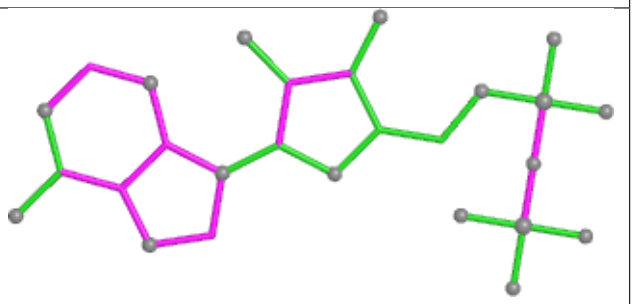

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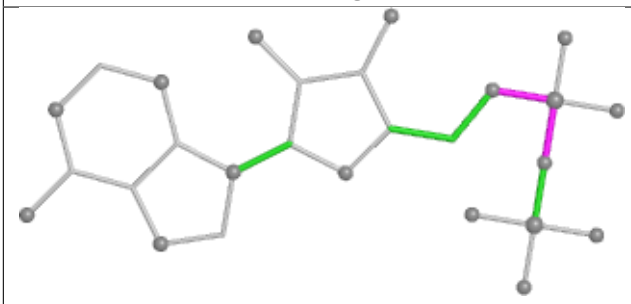

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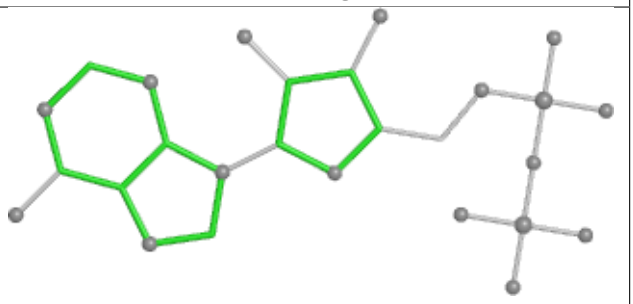
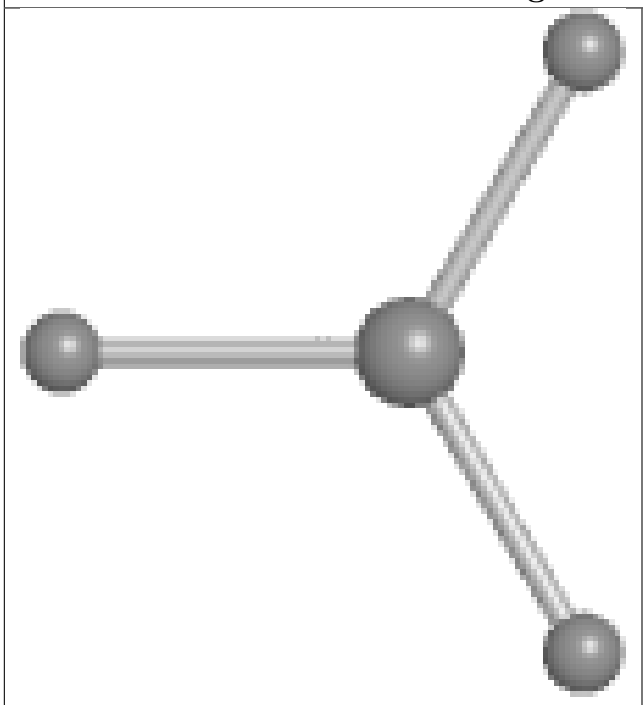


Rings

Ligand AF3 G 603



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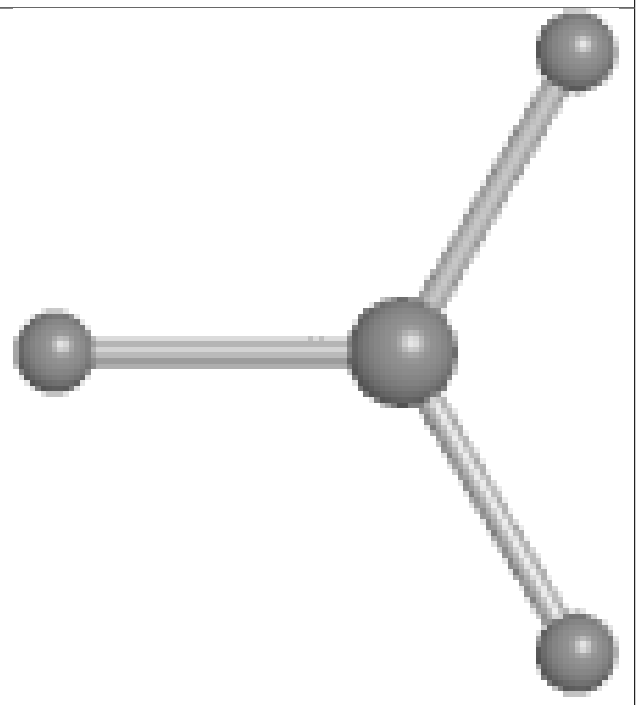

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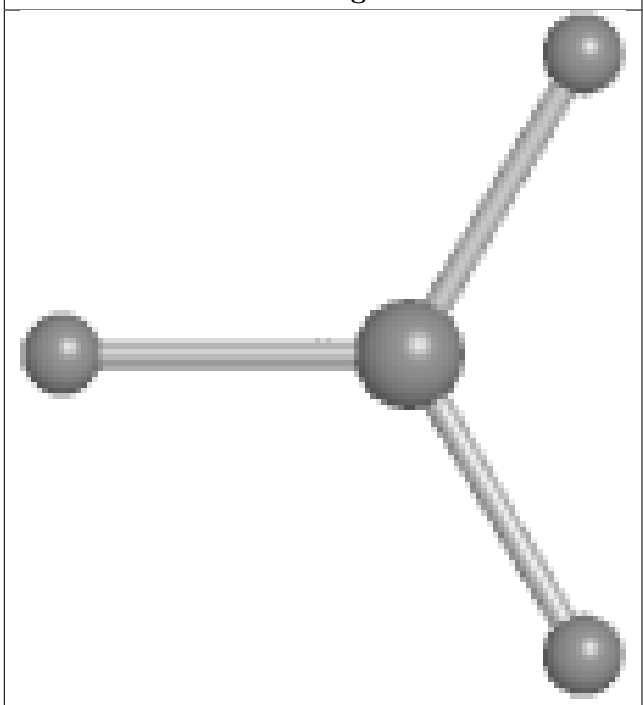

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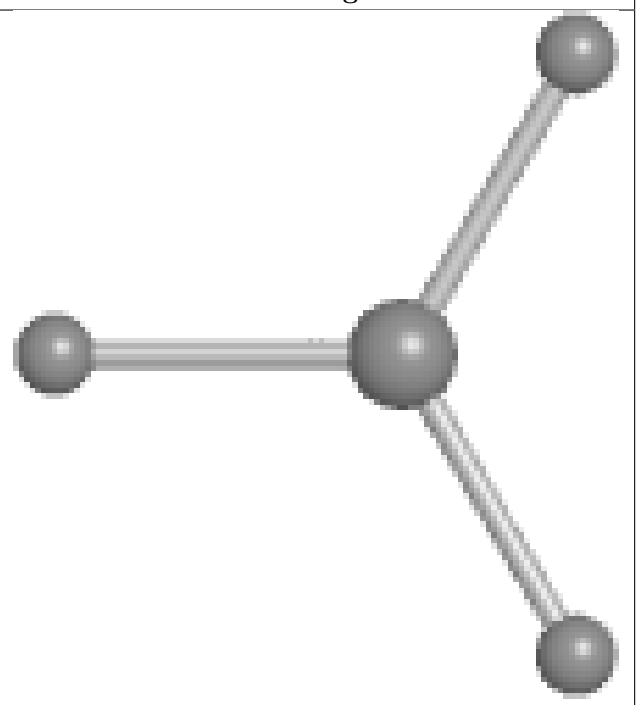
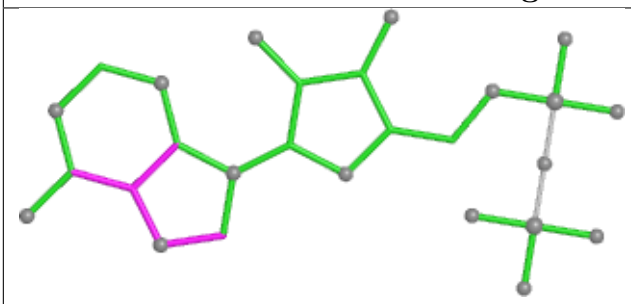


Rings

Ligand ADP A 601



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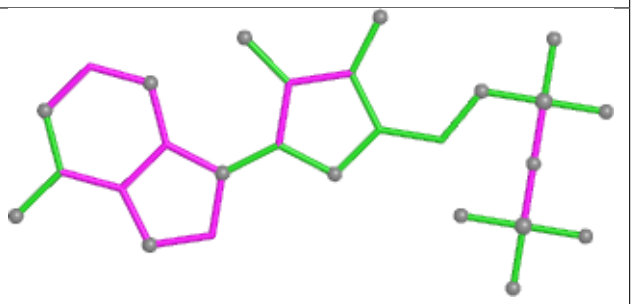

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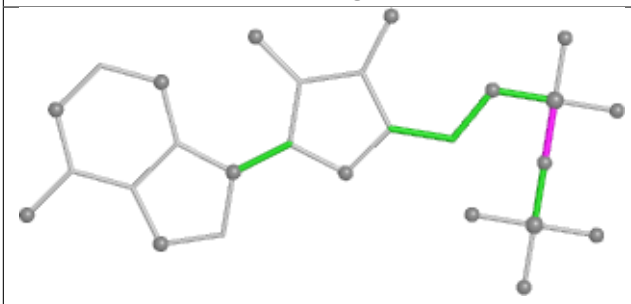

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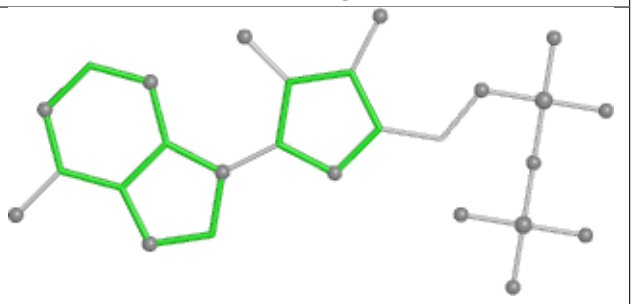
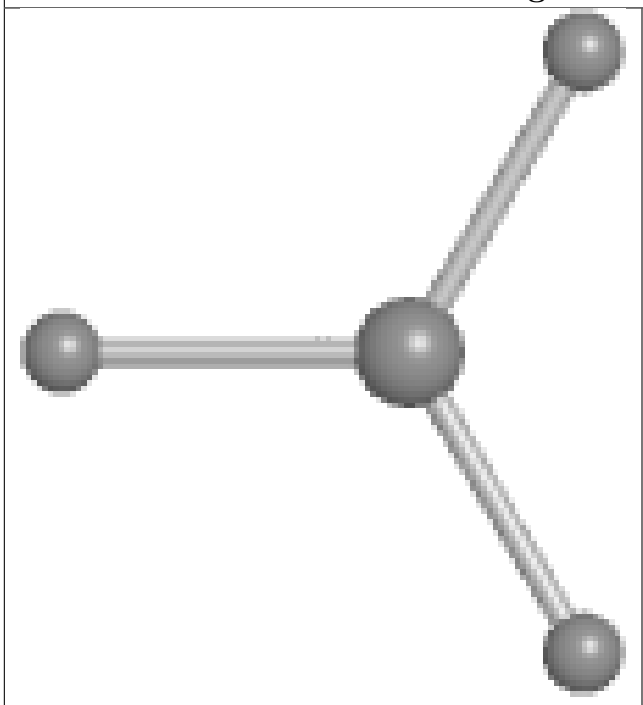


Rings

Ligand AF3 A 603



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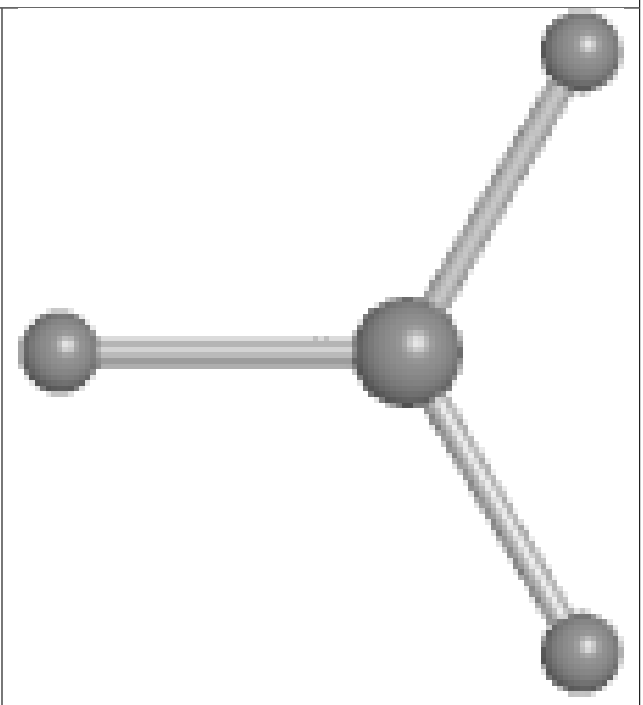
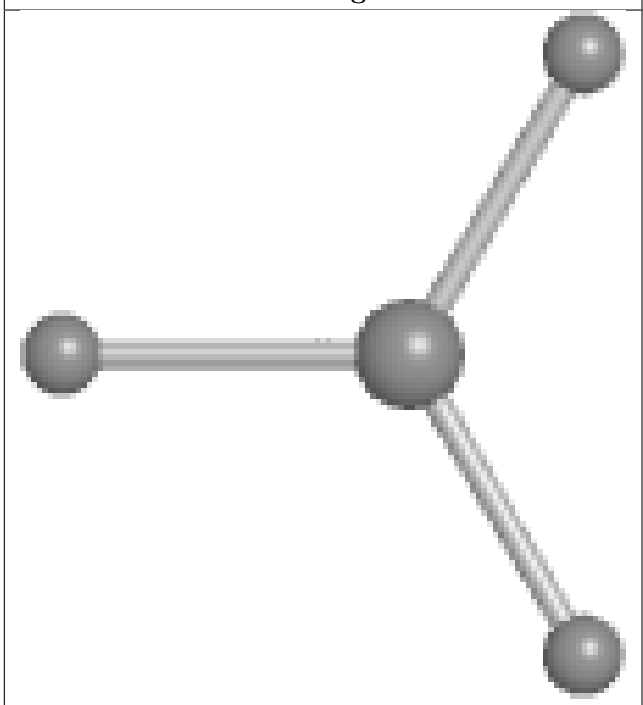


Bond angles



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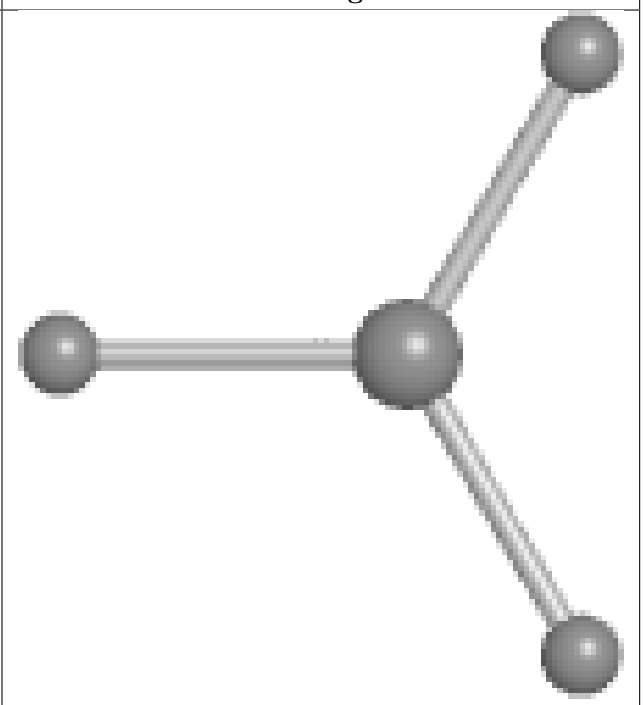
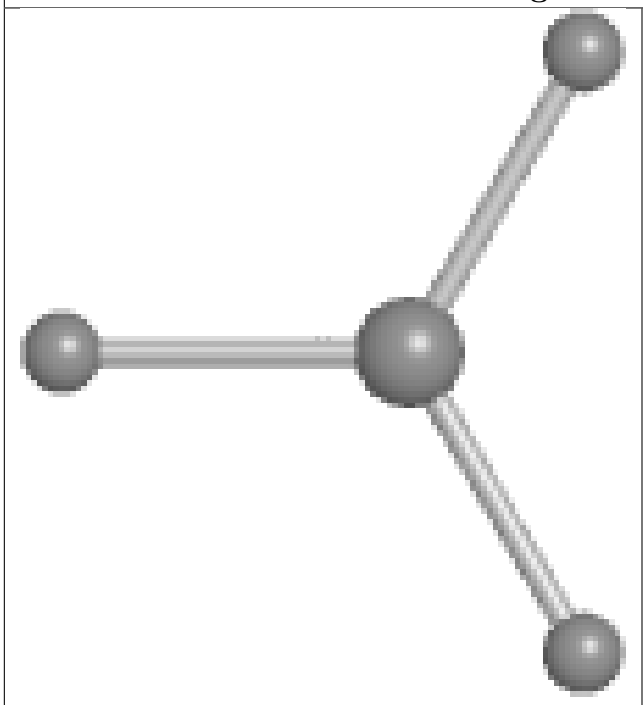


Rings

Ligand AF3 F 603



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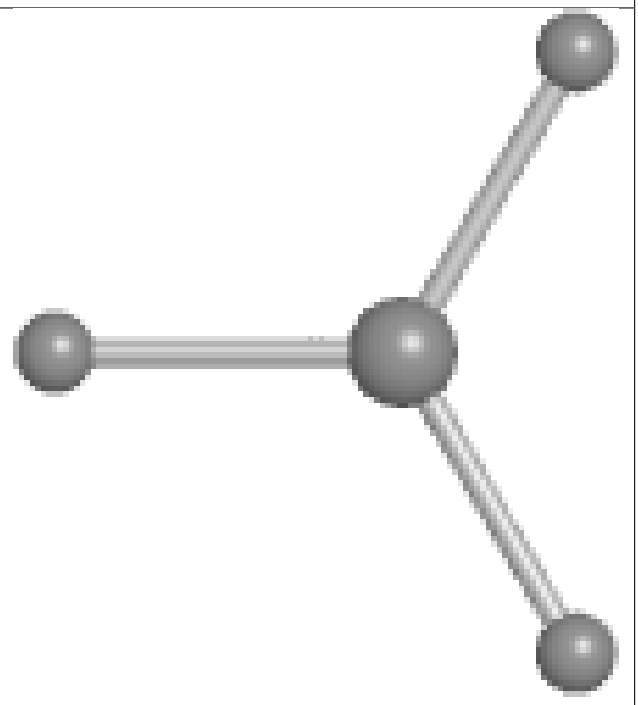

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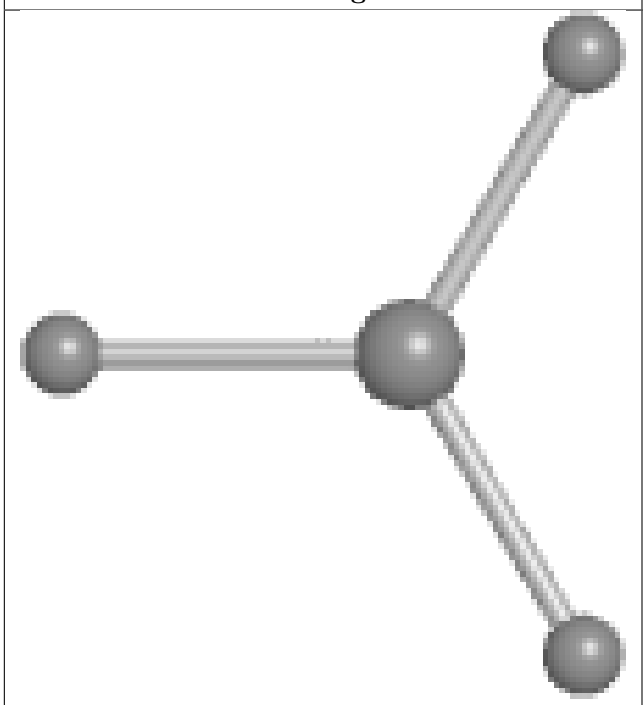

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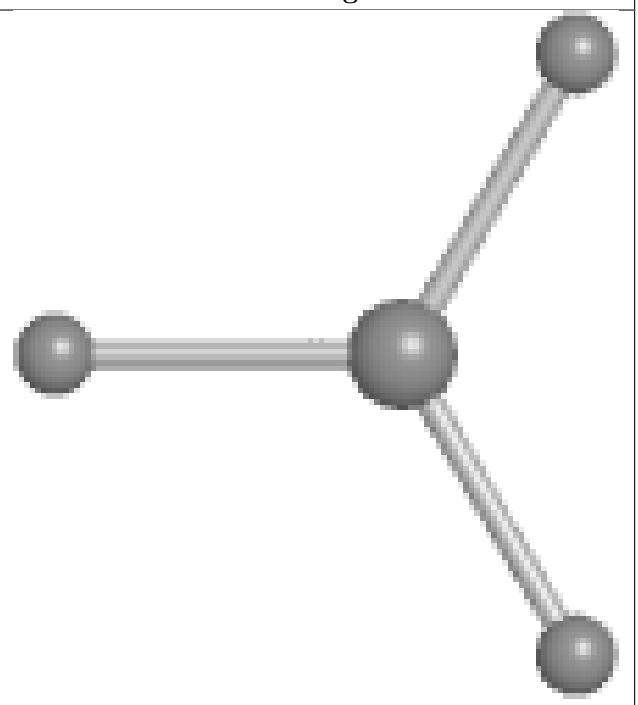
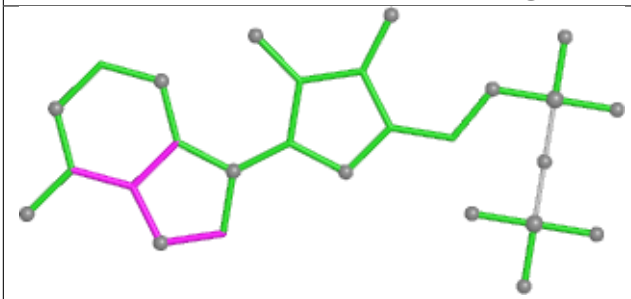
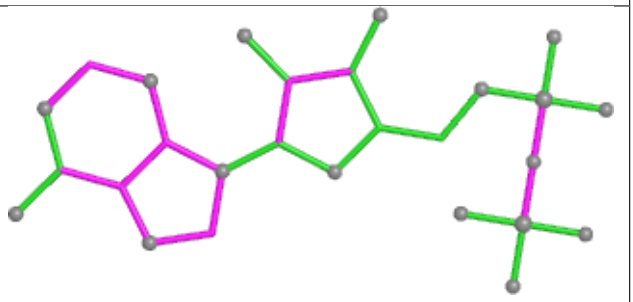


Rings

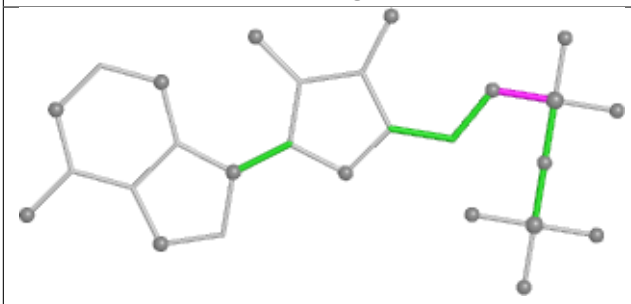
Ligand ADP B 601



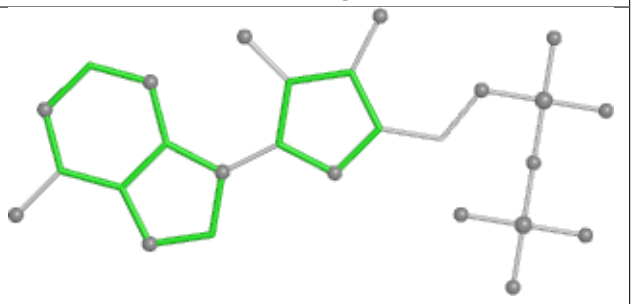
Bond lengths



Bond angles

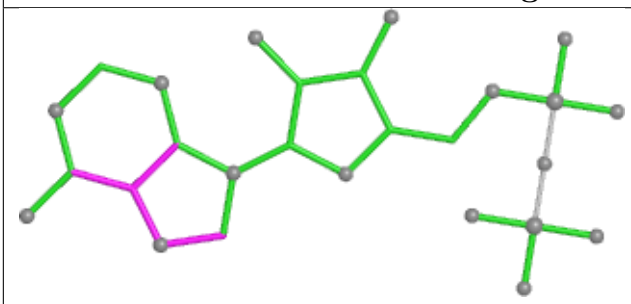


Torsions

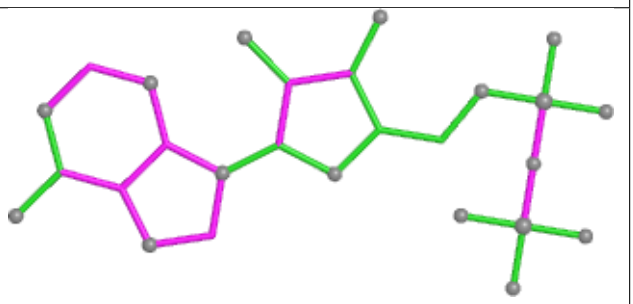


Rings

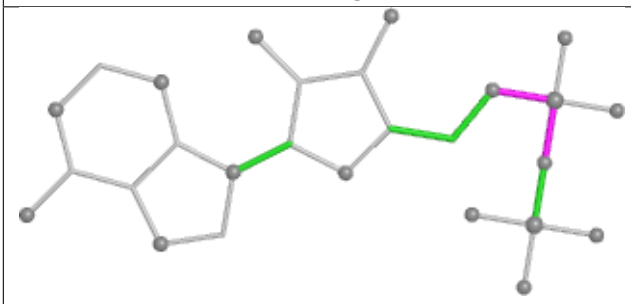
Ligand ADP H 601



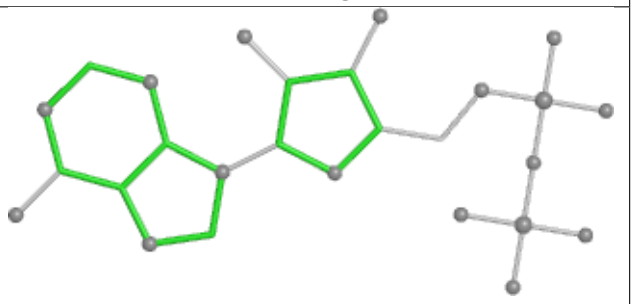
Bond lengths



Bond angles

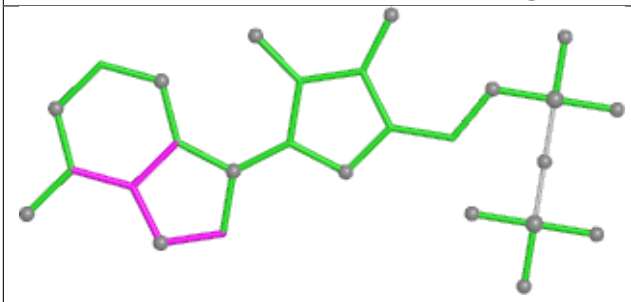


Torsions

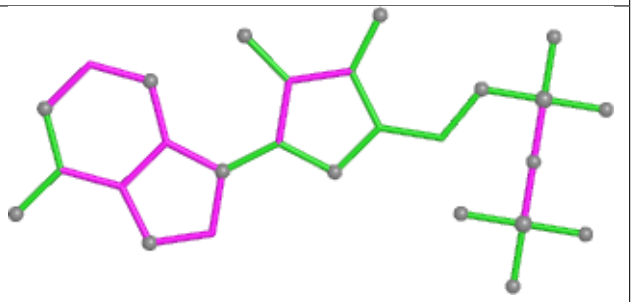


Rings

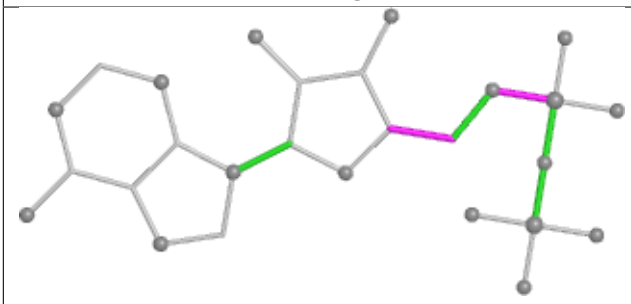
Ligand ADP E 601



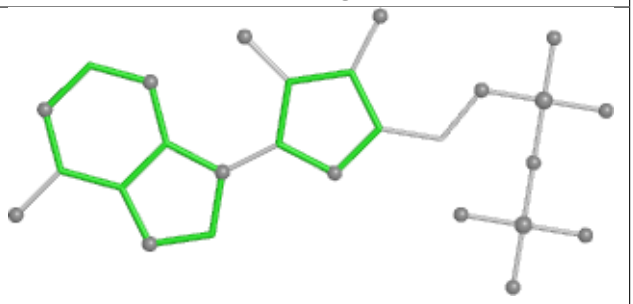
Bond lengths



Bond angles

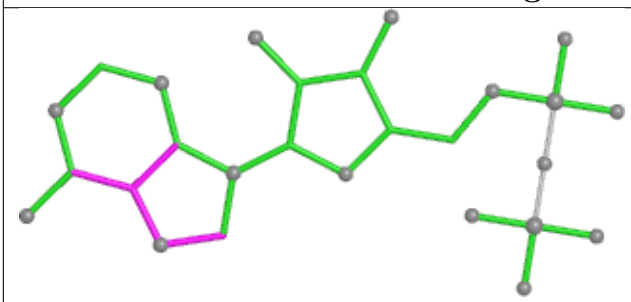


Torsions

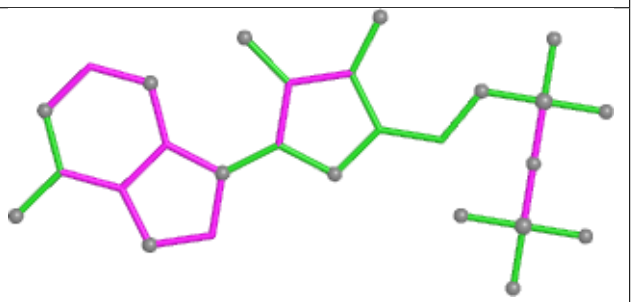


Rings

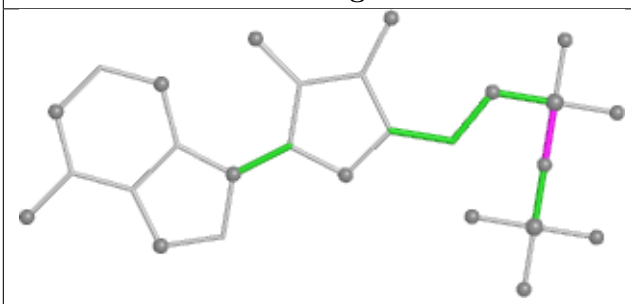
Ligand ADP F 601



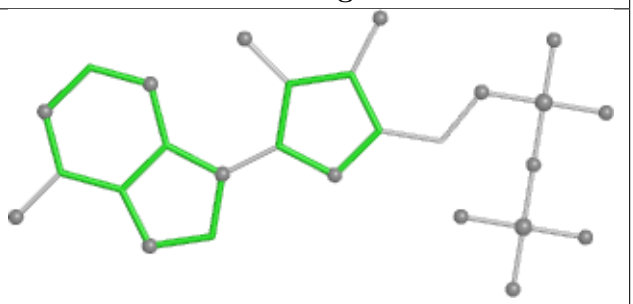
Bond lengths



Bond angles

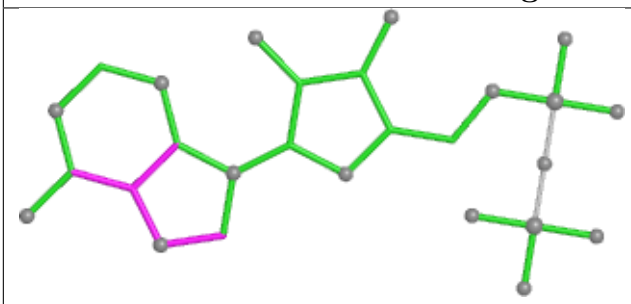


Torsions

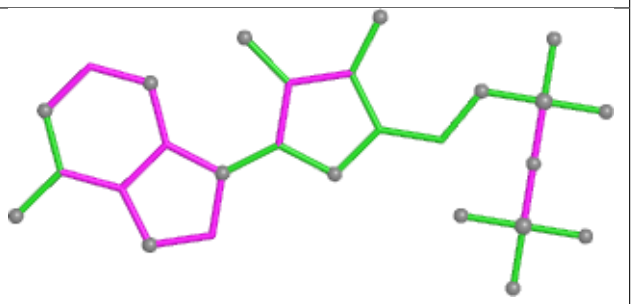


Rings

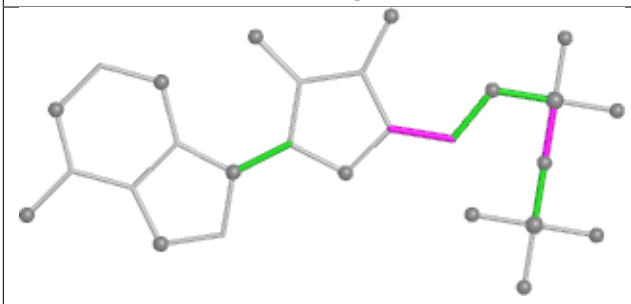
Ligand ADP G 601



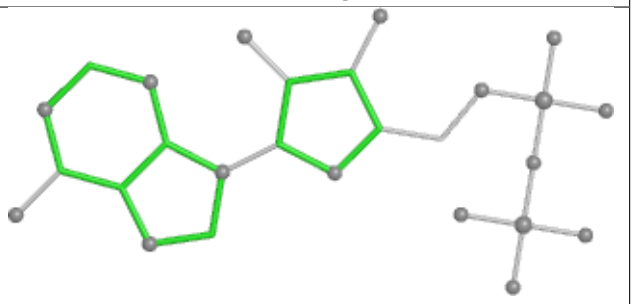
Bond lengths



Bond angles

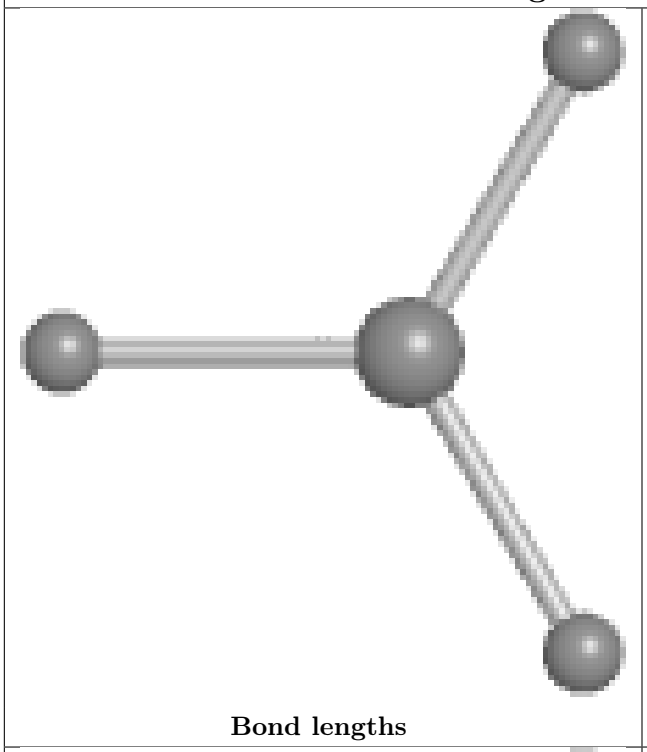


Torsions

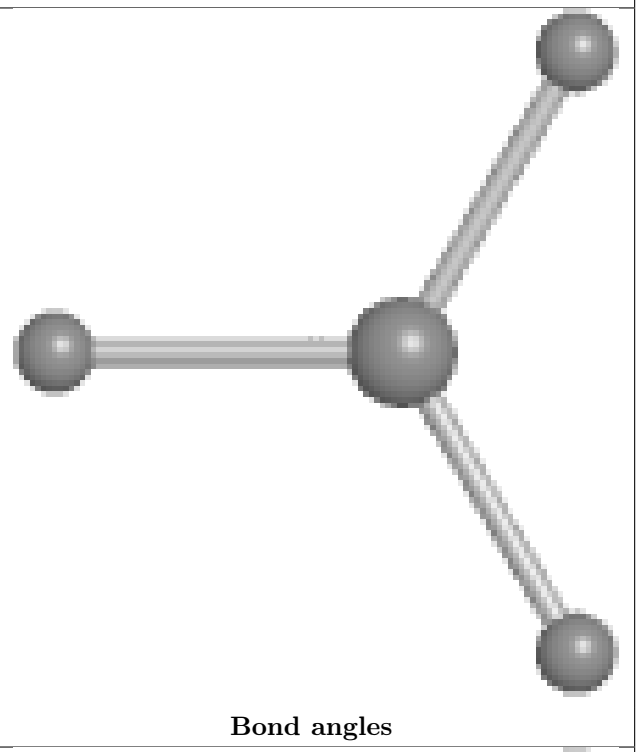


Rings

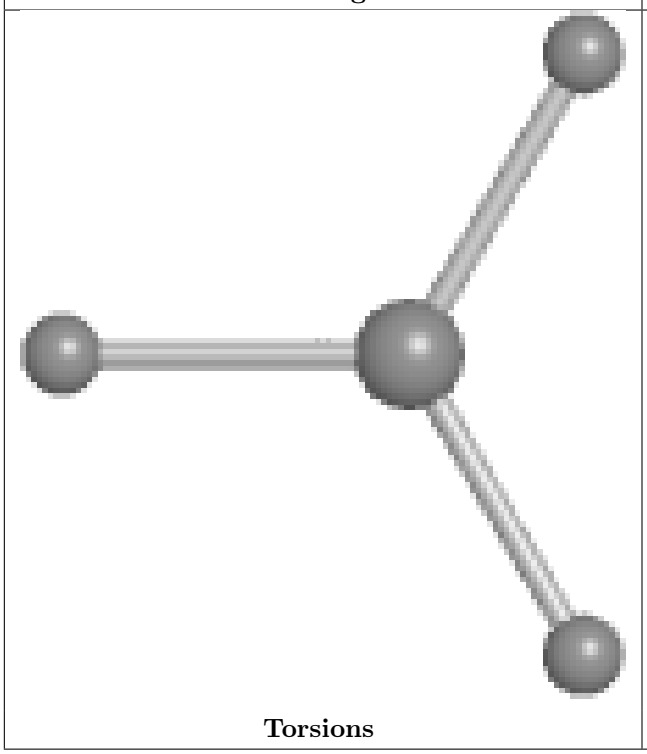
Ligand AF3 C 603



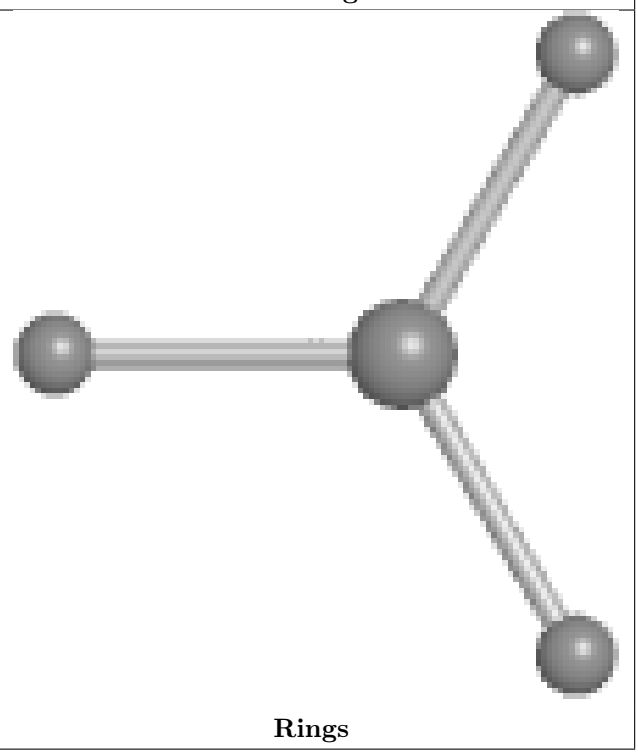
Bond lengths



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.

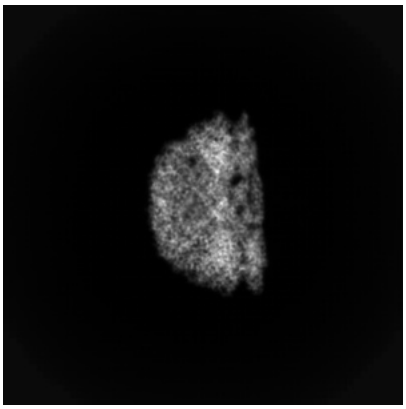
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-64312. These allow visual inspection of the internal detail of the map and identification of artifacts.

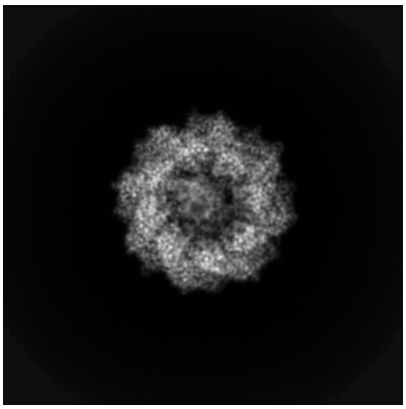
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

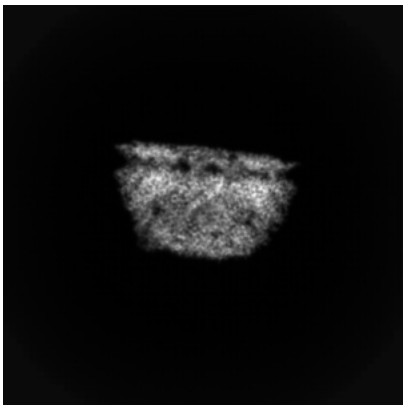
6.1.1 Primary map



X

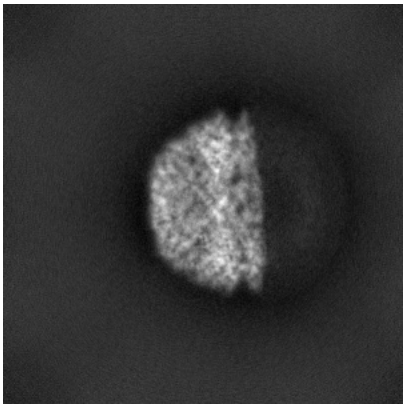


Y

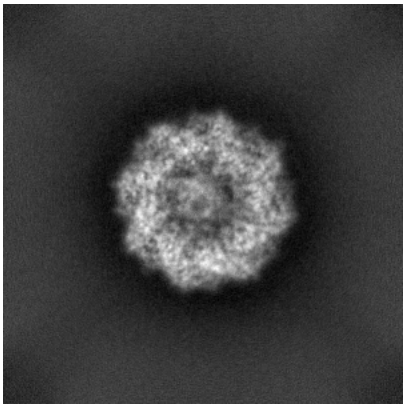


Z

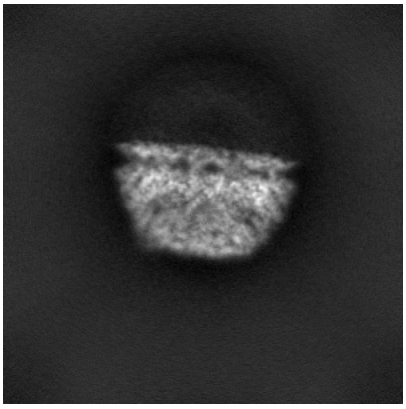
6.1.2 Raw map



X



Y

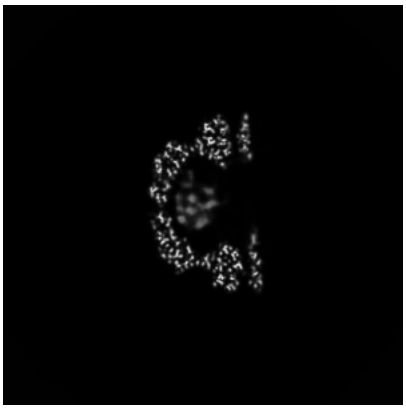


Z

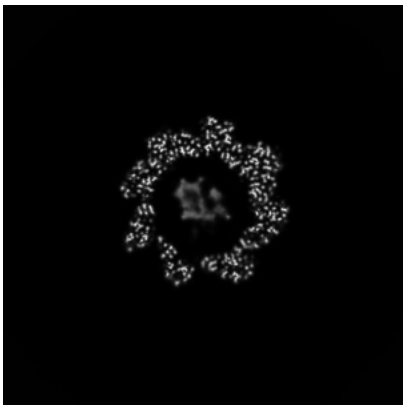
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

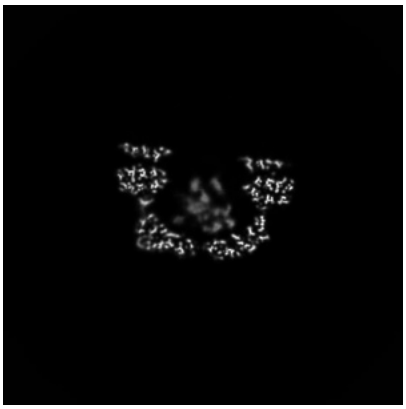
6.2.1 Primary map



X Index: 200

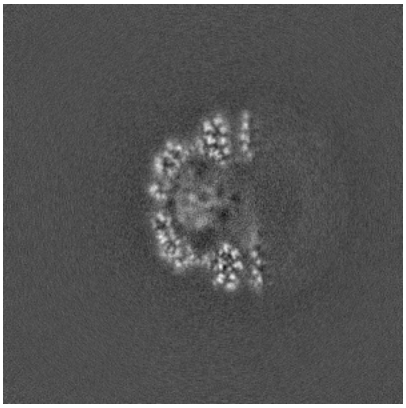


Y Index: 200

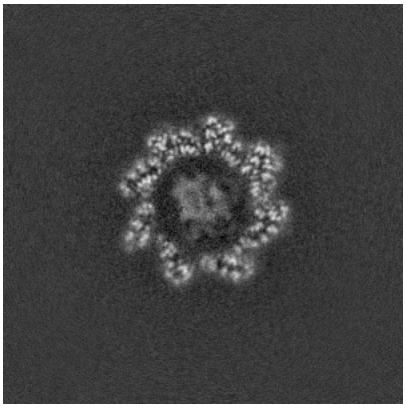


Z Index: 200

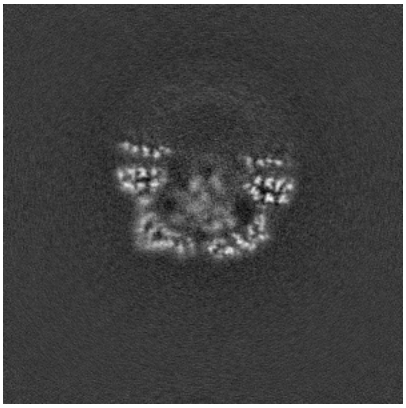
6.2.2 Raw map



X Index: 200



Y Index: 200

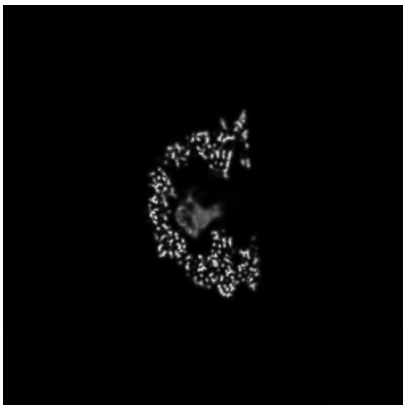


Z Index: 200

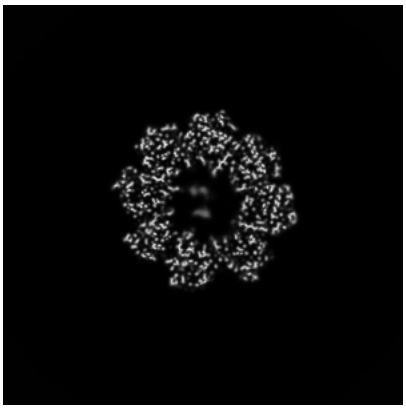
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 219

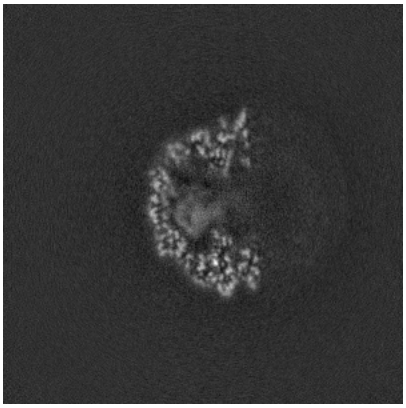


Y Index: 218

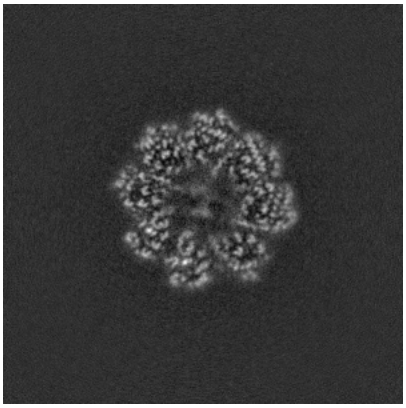


Z Index: 162

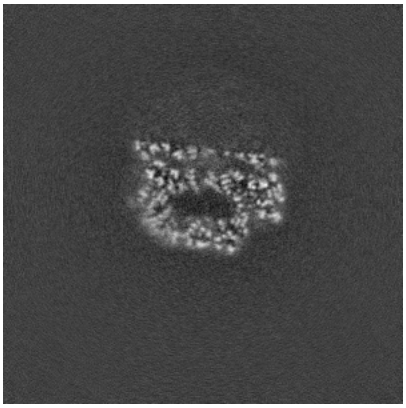
6.3.2 Raw map



X Index: 219



Y Index: 217

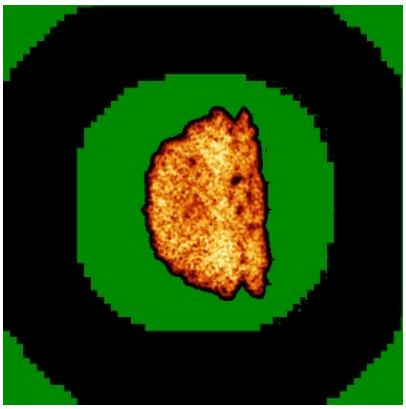


Z Index: 161

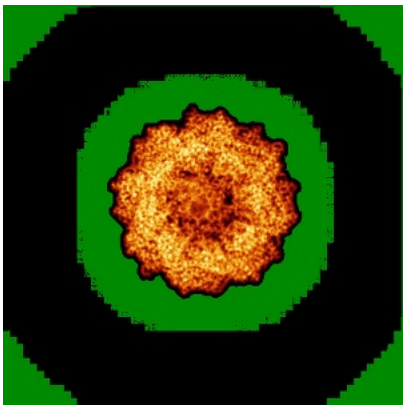
The images above show the largest variance slices of the map in three orthogonal directions.

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

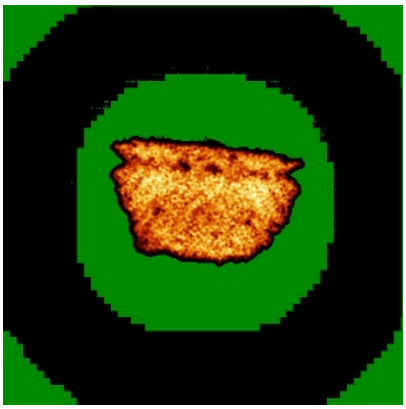
6.4.1 Primary map



X

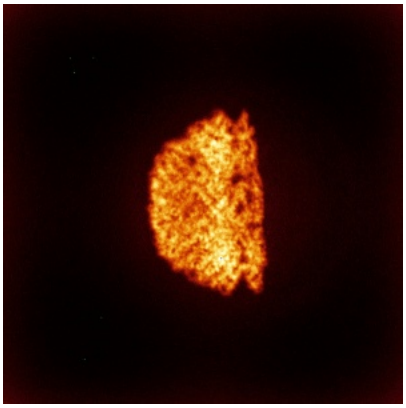


Y

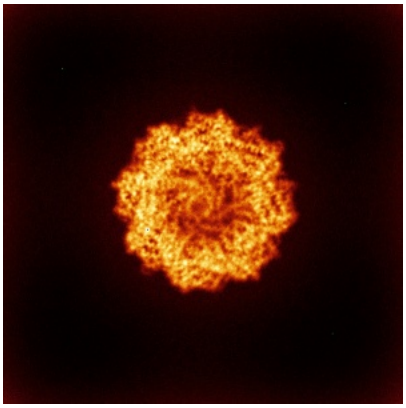


Z

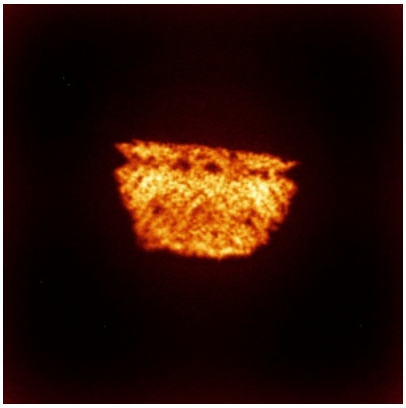
6.4.2 Raw map



X



Y

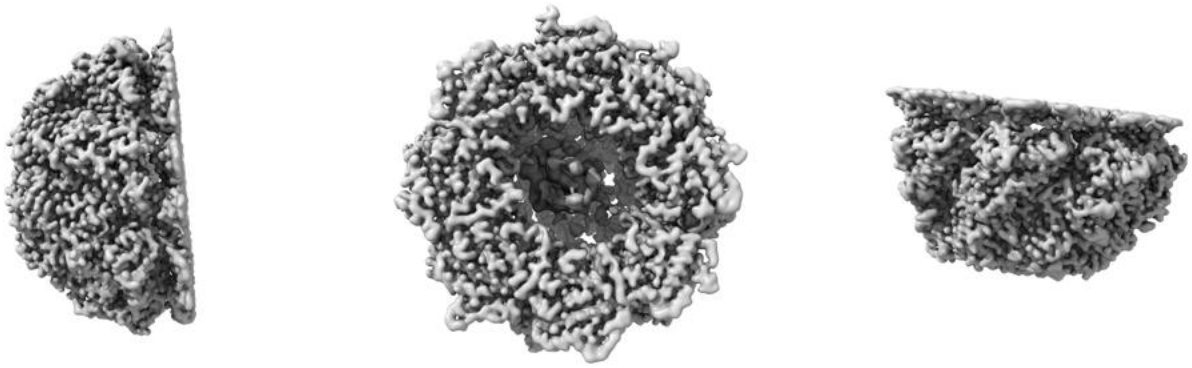


Z

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)

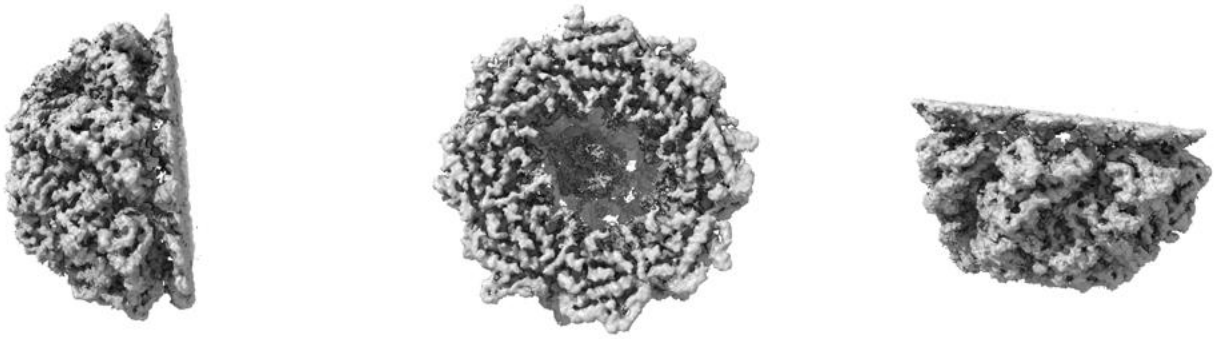
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.5. 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.

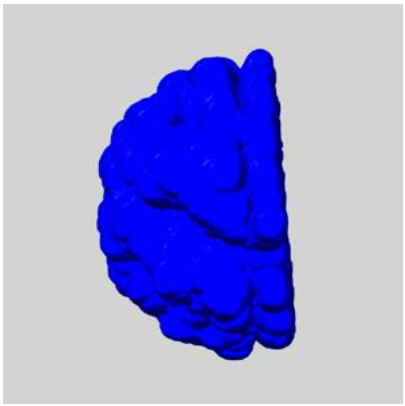
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

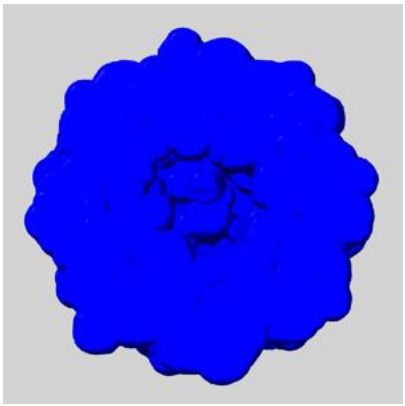
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

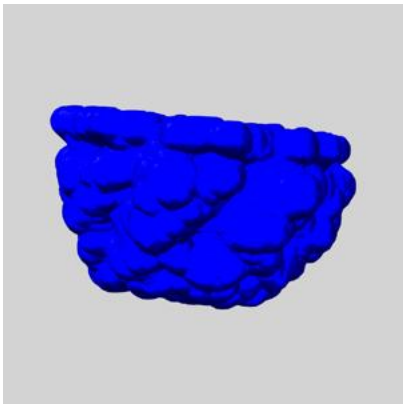
6.6.1 emd_64312_msk_1.map (i)



X



Y

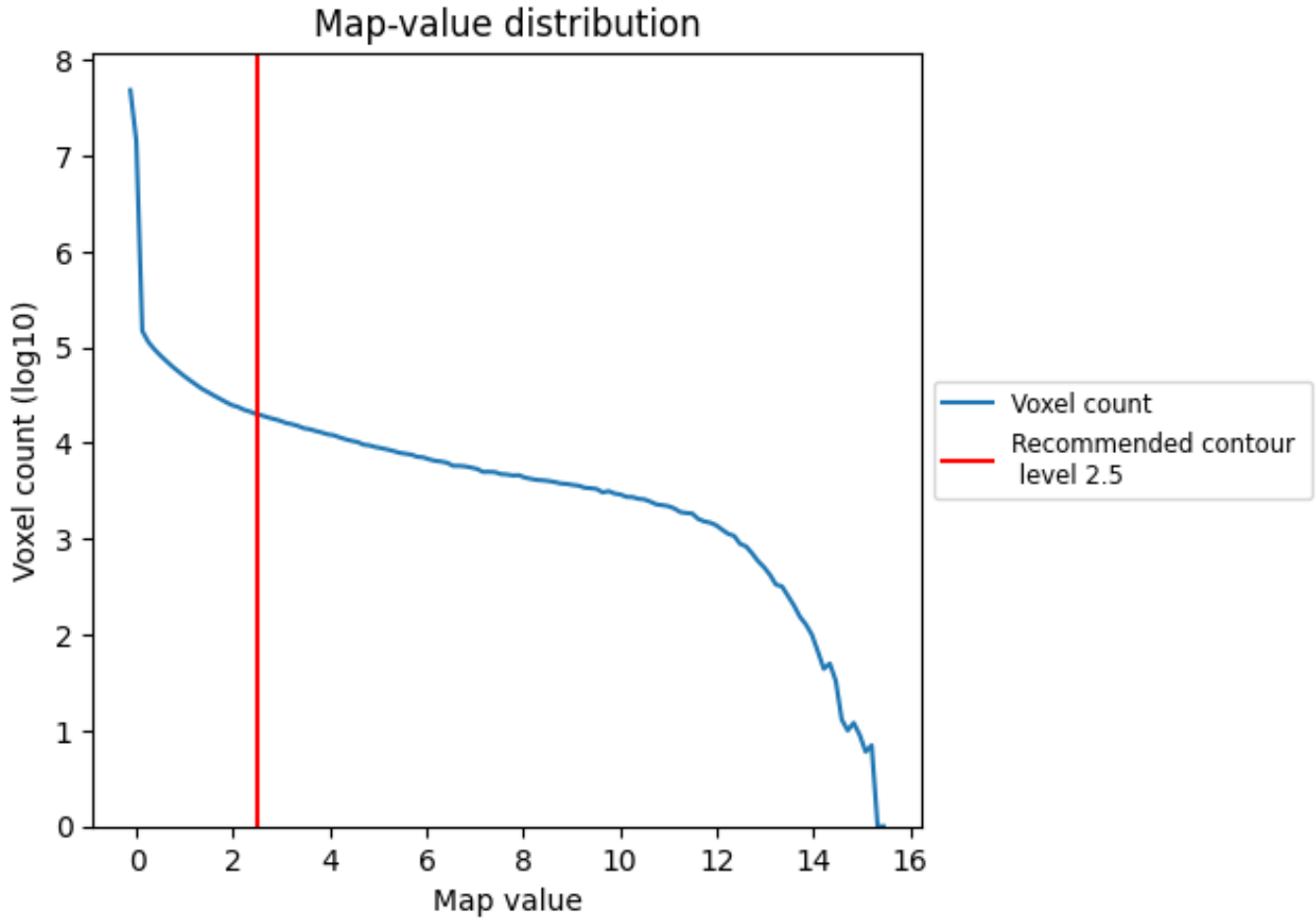


Z

7 Map analysis

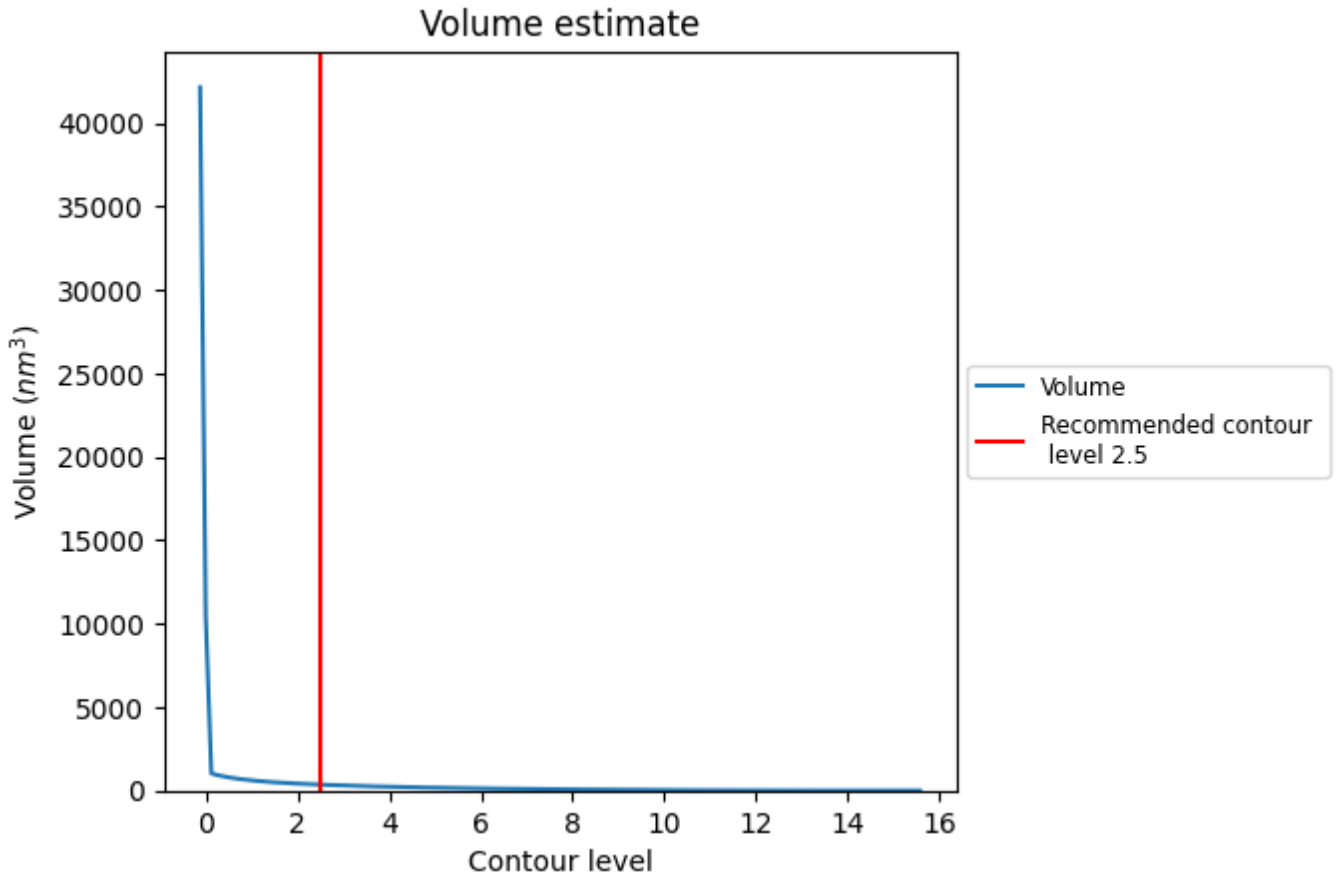
This section contains the results of statistical analysis of the map.

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.

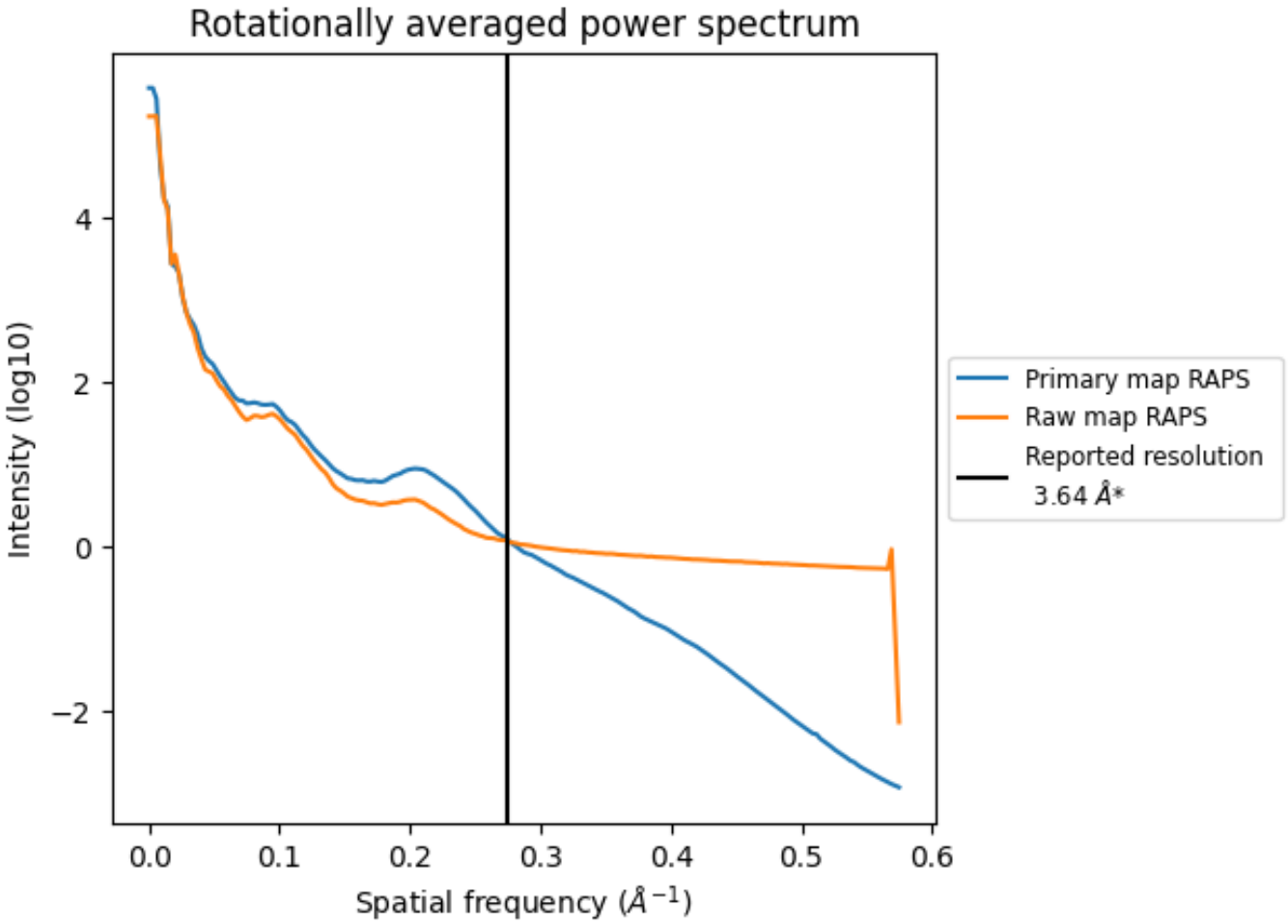
7.2 Volume estimate



The volume at the recommended contour level is 356 nm^3; this corresponds to an approximate mass of 322 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)

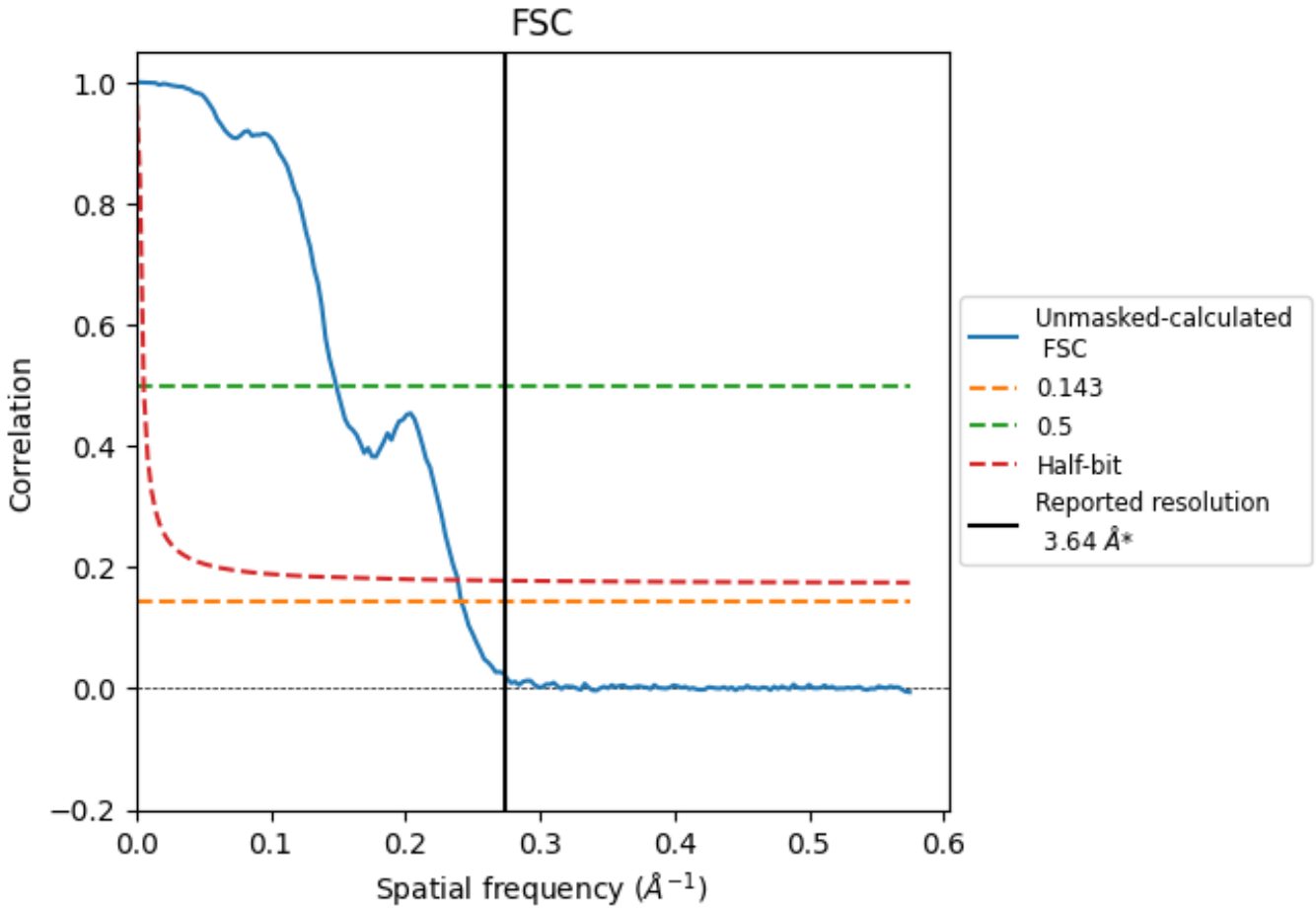


*Reported resolution corresponds to spatial frequency of 0.275 $Å^{-1}$

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 0.275 Å^{-1}

8.2 Resolution estimates (i)

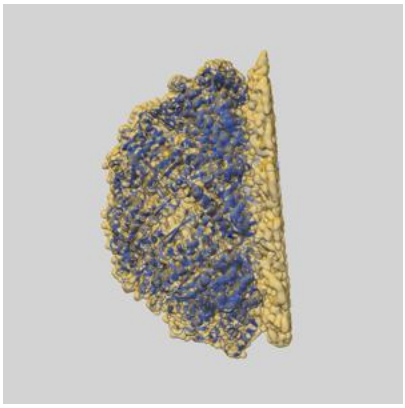
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	6.73	4.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.64 by more than 10 %

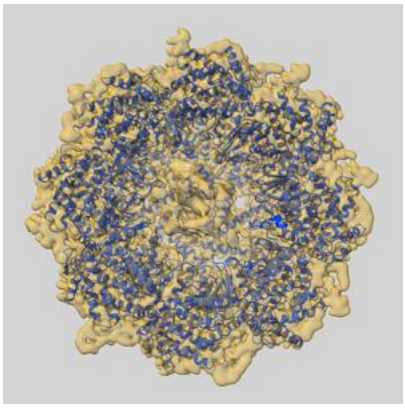
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-64312 and PDB model 9UMT. Per-residue inclusion information can be found in section 3 on page 9.

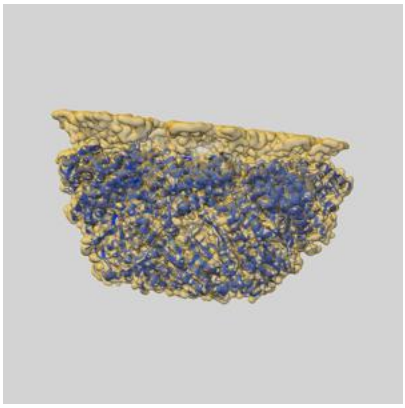
9.1 Map-model overlay



X



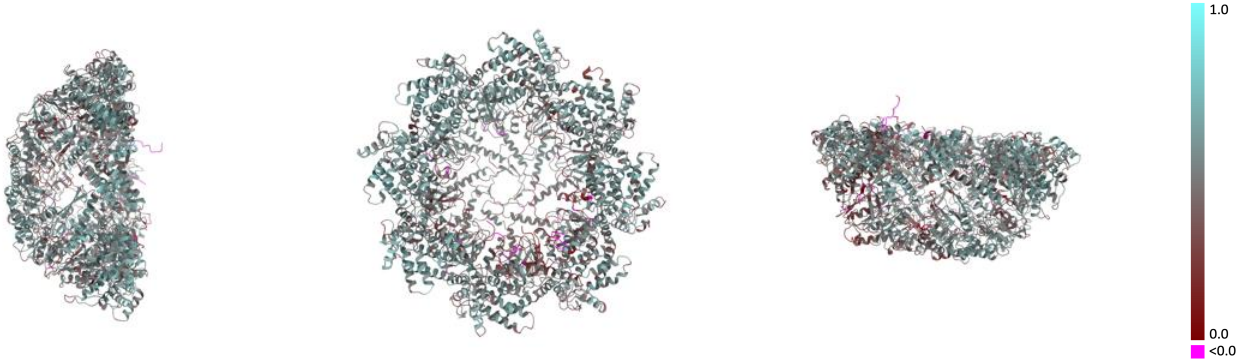
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

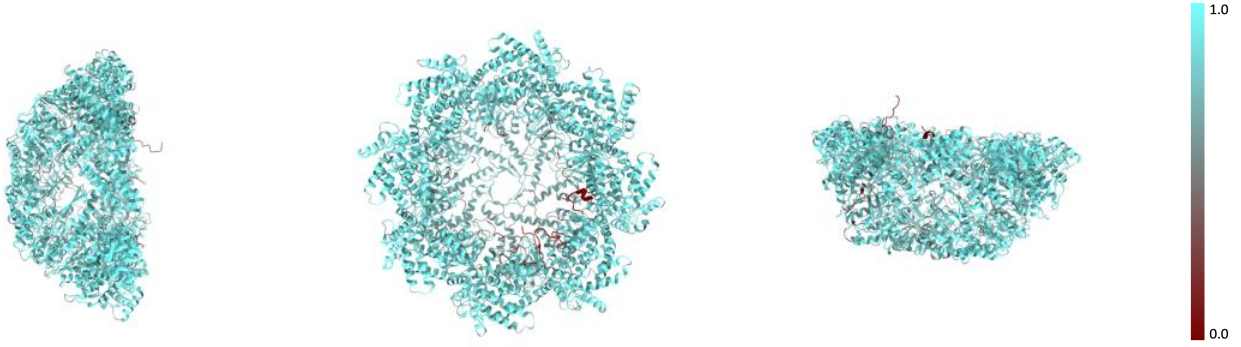
9.2 Q-score mapped to coordinate model



X Y Z

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

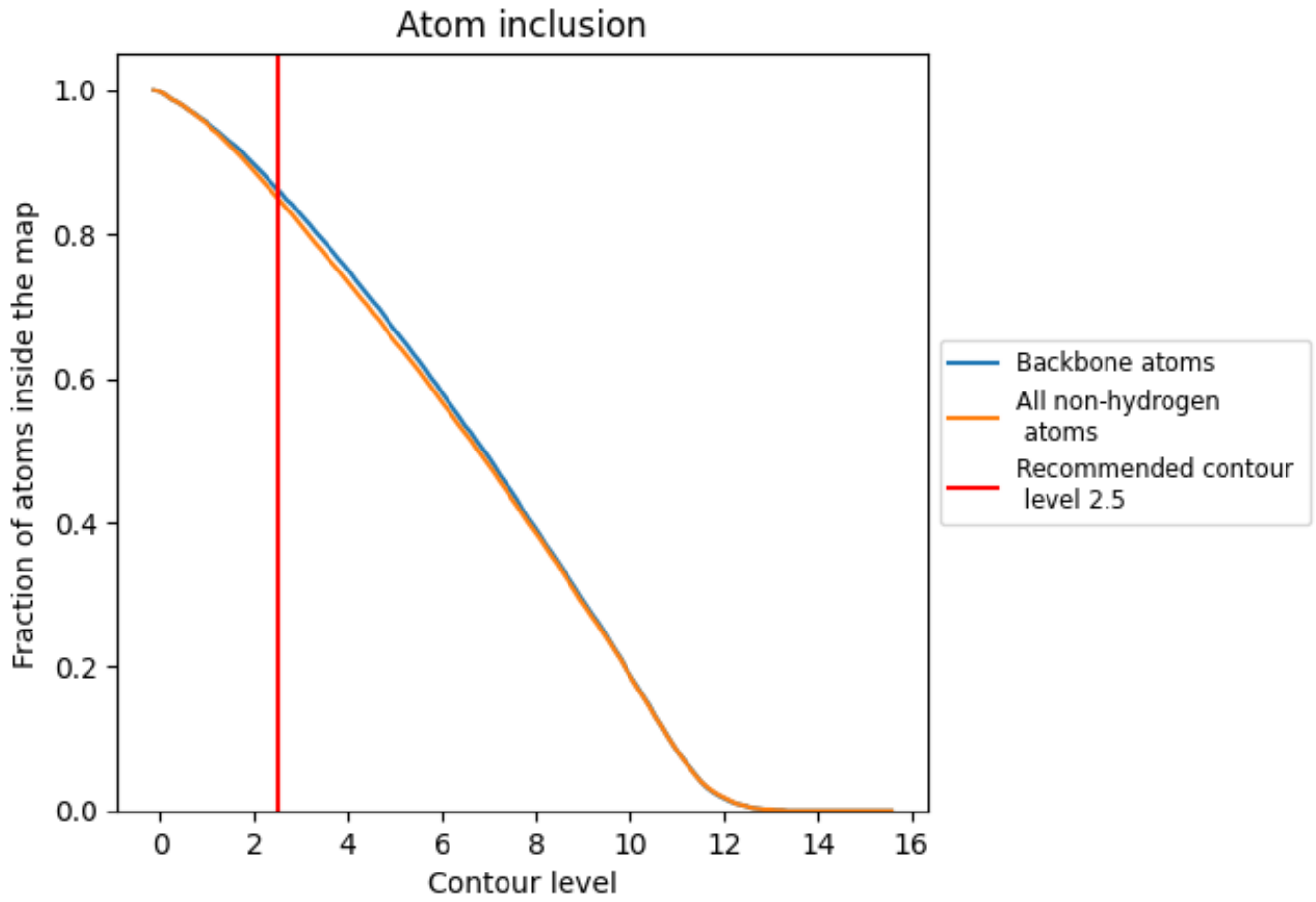
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (2.5).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8500	0.4720
A	0.8900	0.5180
B	0.8860	0.4990
C	0.8510	0.4700
D	0.8670	0.4730
E	0.8180	0.4440
F	0.8630	0.4720
G	0.8880	0.5080
H	0.7900	0.3890

