Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:56 PM EST

PDB ID	:	7R7S
EMDB ID	:	EMD-24302
Title	:	p47-bound p97-R155H mutant with ATPgammaS
Authors	:	Nandi, P.; Li, S.; Coulmbres, R.C.A.; Wang, F.; Williams, D.R.; Malyutin, A.G.; Poh, Y.-P.; Chou, T.-F.; Chiu, P.-L.
Deposited on	:	2021-06-25
Resolution	:	4.23 Å(reported)
Based on initial model	:	5FTN

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:

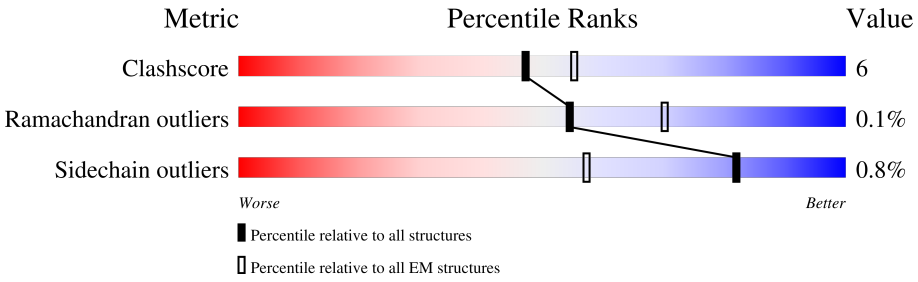
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.23 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	806	72% 17% 10%
1	B	806	58% 11% 32%
1	C	806	57% 11% 32%
1	D	806	10% 74% 15% • 11%
1	E	806	8% 73% 15% • 11%
1	F	806	75% 15% • 9%
2	I	370	21% 26% • 69%
2	J	370	22% 24% • 72%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 33239 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	722	Total	C	N	O	S	0	0
			5680	3577	1012	1061	30		
1	B	551	Total	C	N	O	S	0	0
			4304	2706	766	810	22		
1	C	546	Total	C	N	O	S	0	0
			4272	2689	761	800	22		
1	D	721	Total	C	N	O	S	0	0
			5662	3562	1007	1063	30		
1	E	717	Total	C	N	O	S	0	0
			5632	3543	999	1060	30		
1	F	733	Total	C	N	O	S	0	0
			5757	3624	1024	1079	30		

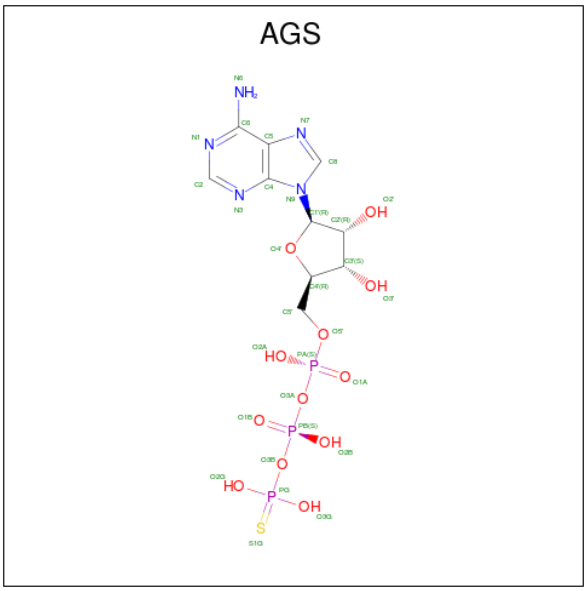
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	HIS	ARG	engineered mutation	UNP P55072
B	155	HIS	ARG	engineered mutation	UNP P55072
C	155	HIS	ARG	engineered mutation	UNP P55072
D	155	HIS	ARG	engineered mutation	UNP P55072
E	155	HIS	ARG	engineered mutation	UNP P55072
F	155	HIS	ARG	engineered mutation	UNP P55072

- Molecule 2 is a protein called NSFL1 cofactor p47.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	113	Total	C	N	O	S	0	0
			802	498	148	154	2		
2	J	104	Total	C	N	O	S	0	0
			758	472	139	145	2		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



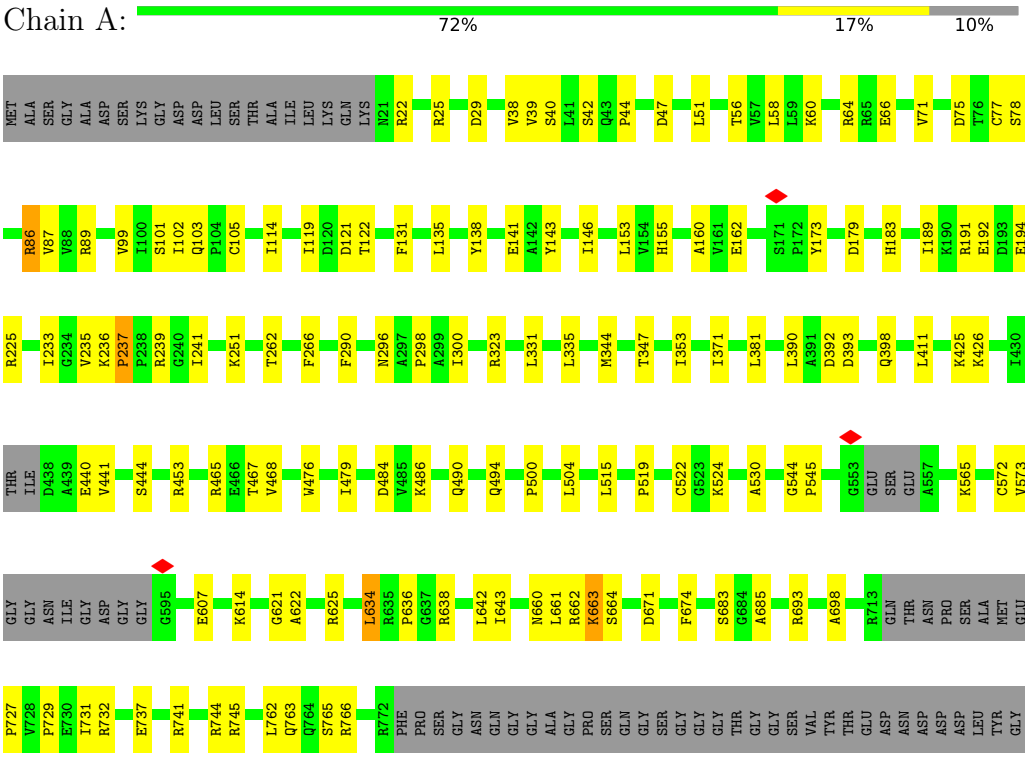
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	B	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	C	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	F	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

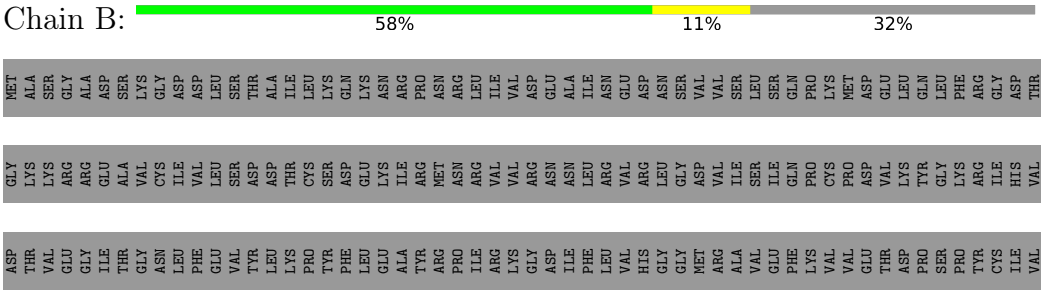
• Molecule 1: Transitional endoplasmic reticulum ATPase

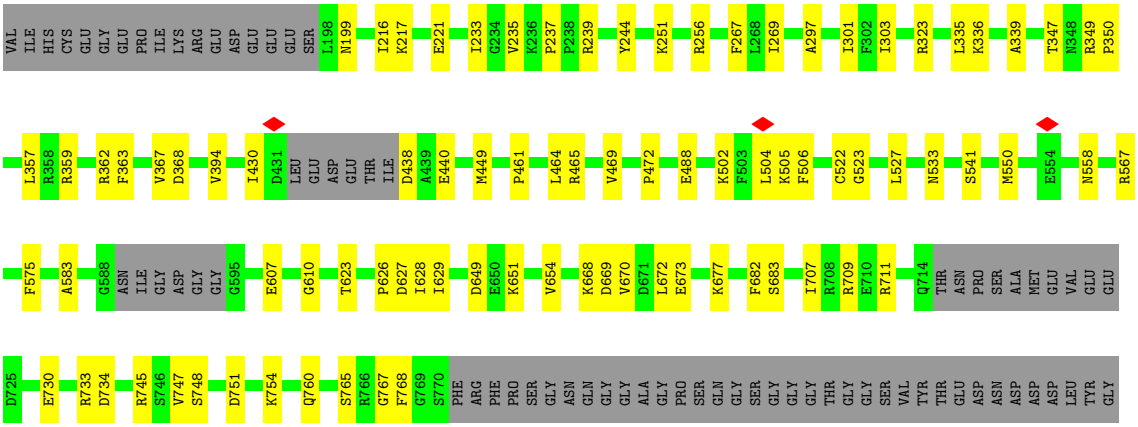
Chain A:



• Molecule 1: Transitional endoplasmic reticulum ATPase

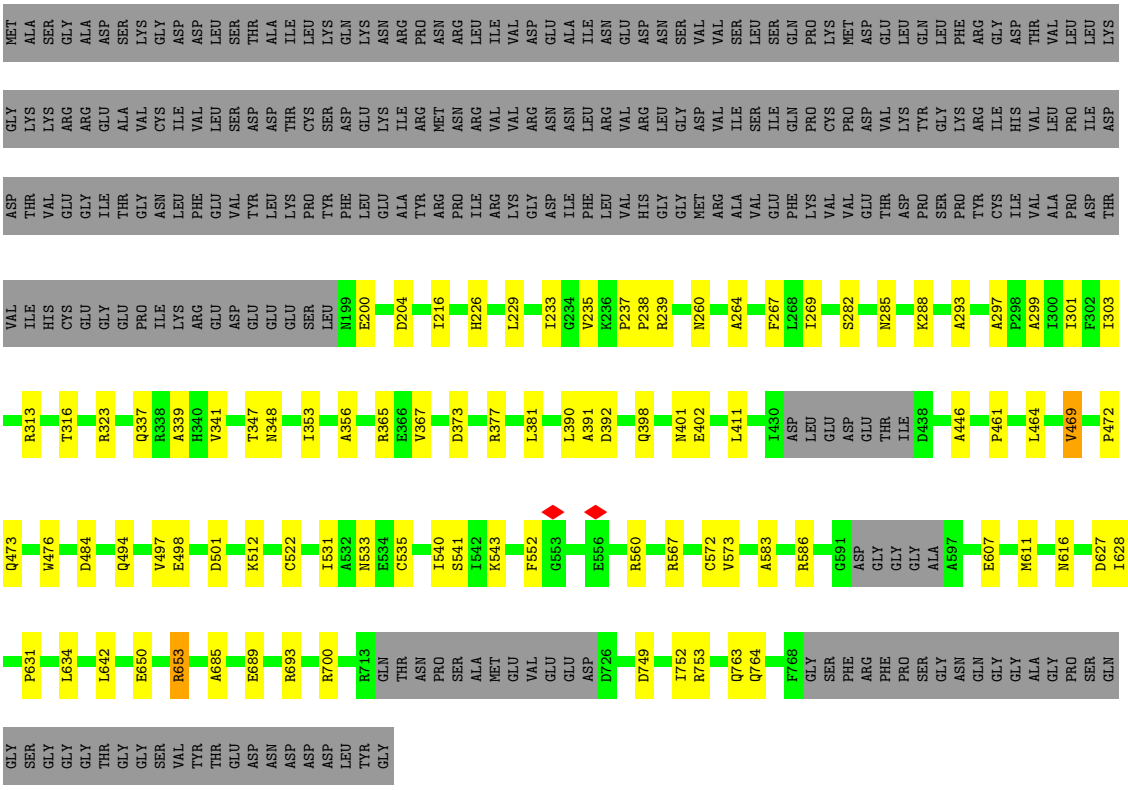
Chain B:





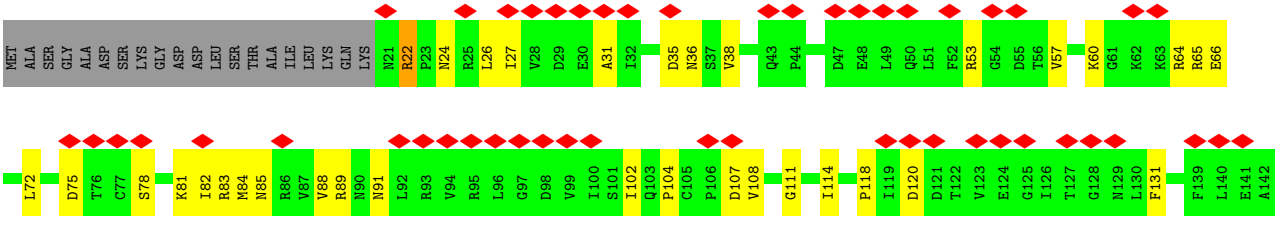
• Molecule 1: Transitional endoplasmic reticulum ATPase

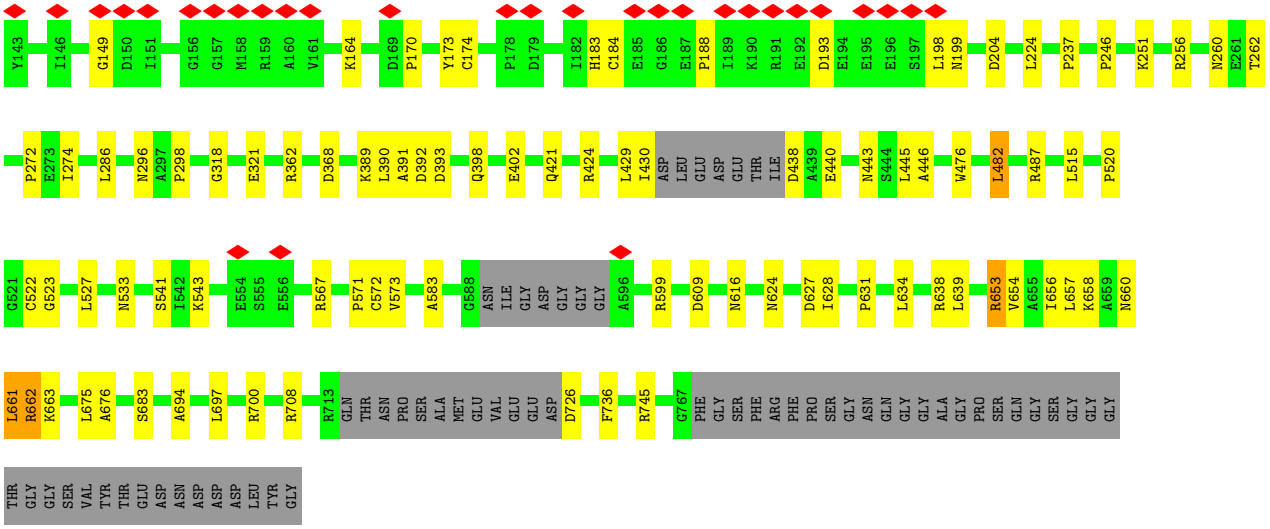
Chain C:



• Molecule 1: Transitional endoplasmic reticulum ATPase

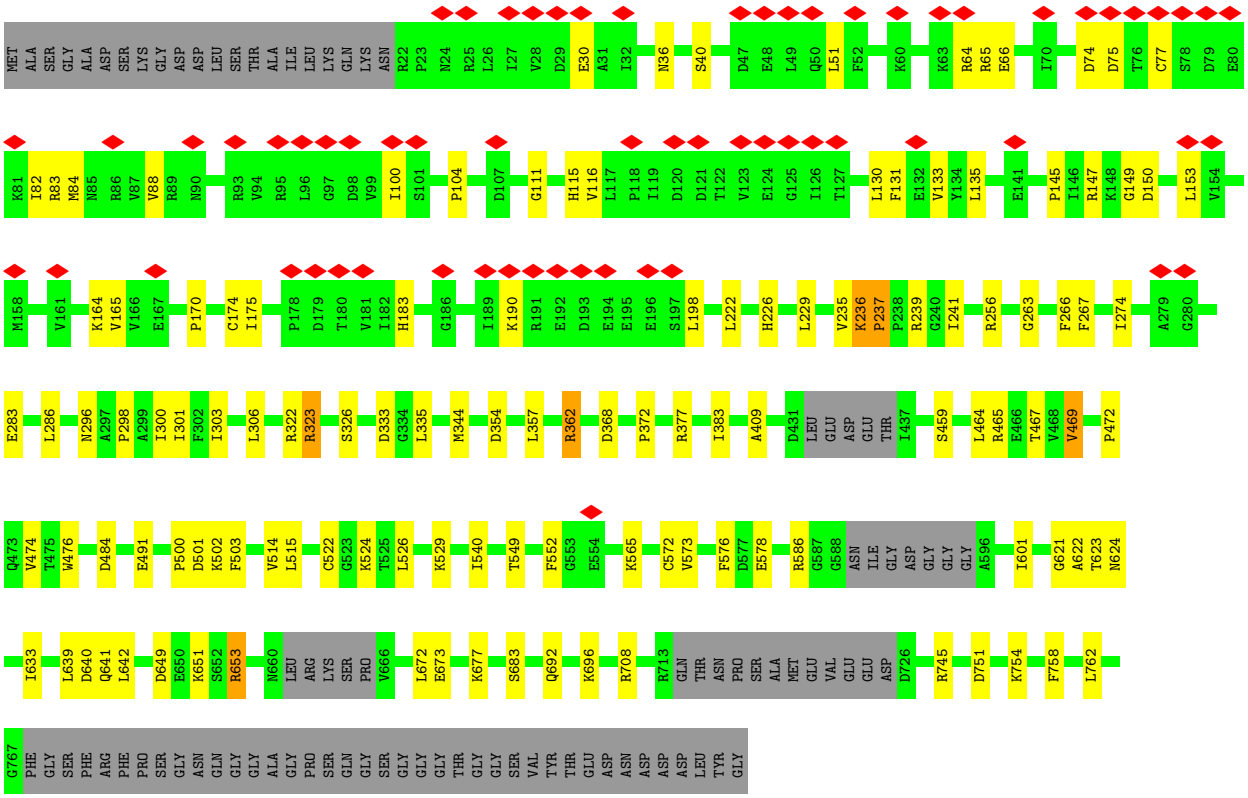
Chain D:





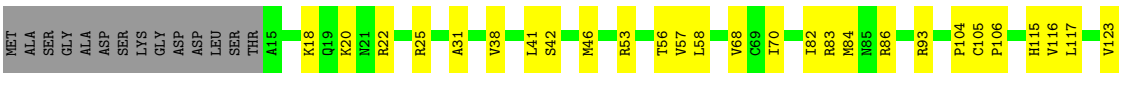
• Molecule 1: Transitional endoplasmic reticulum ATPase

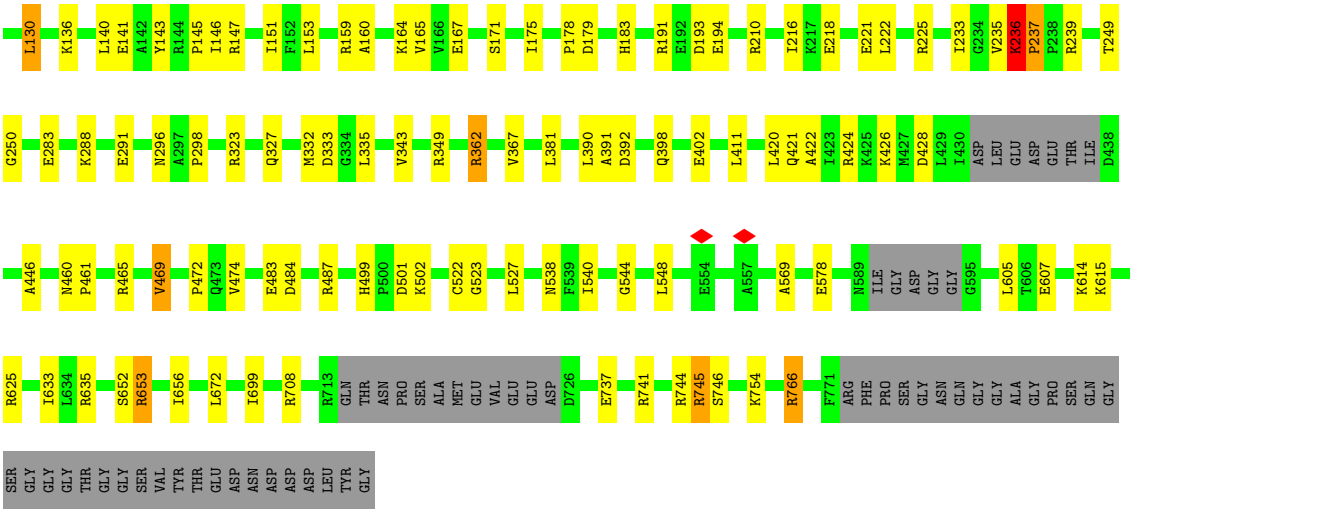
Chain E:



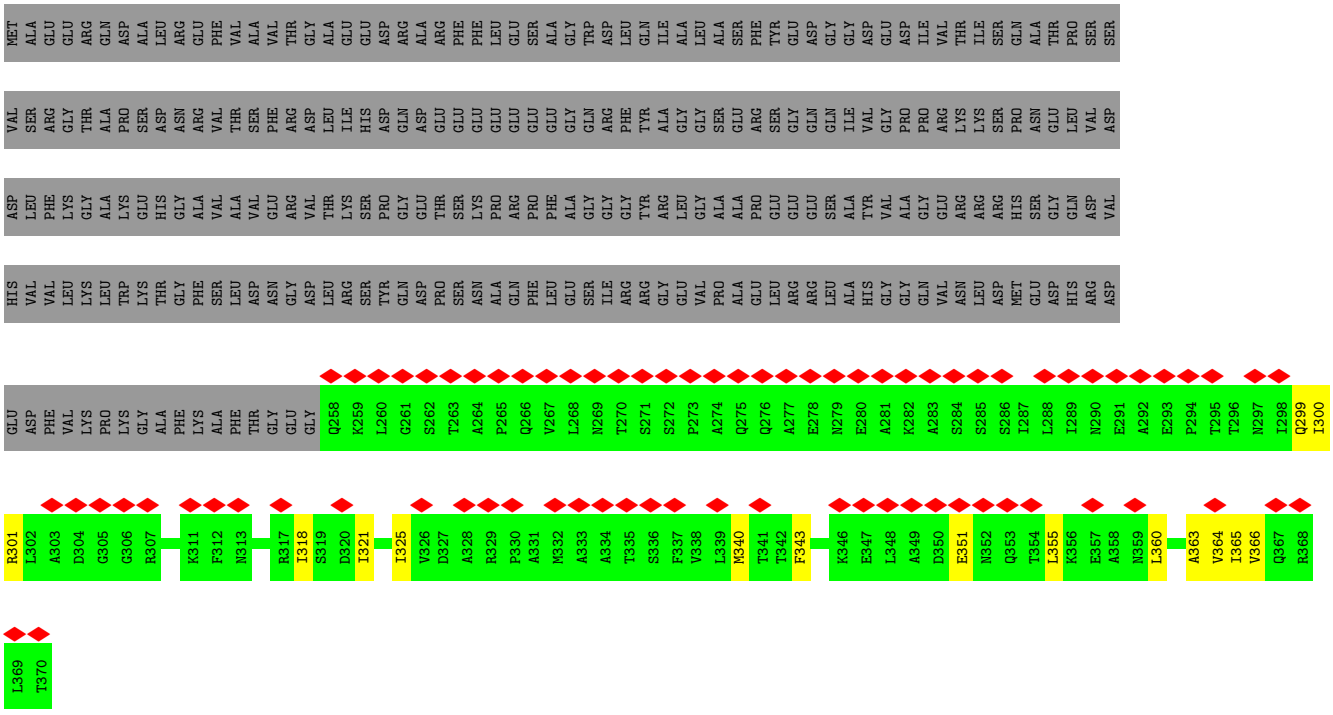
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:

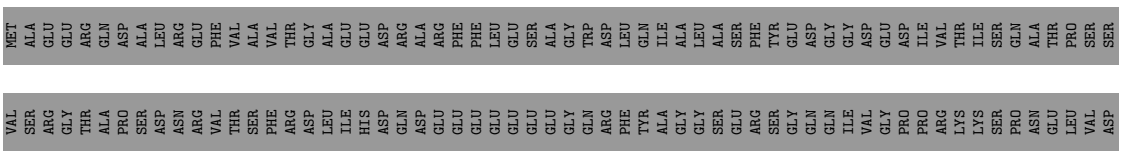


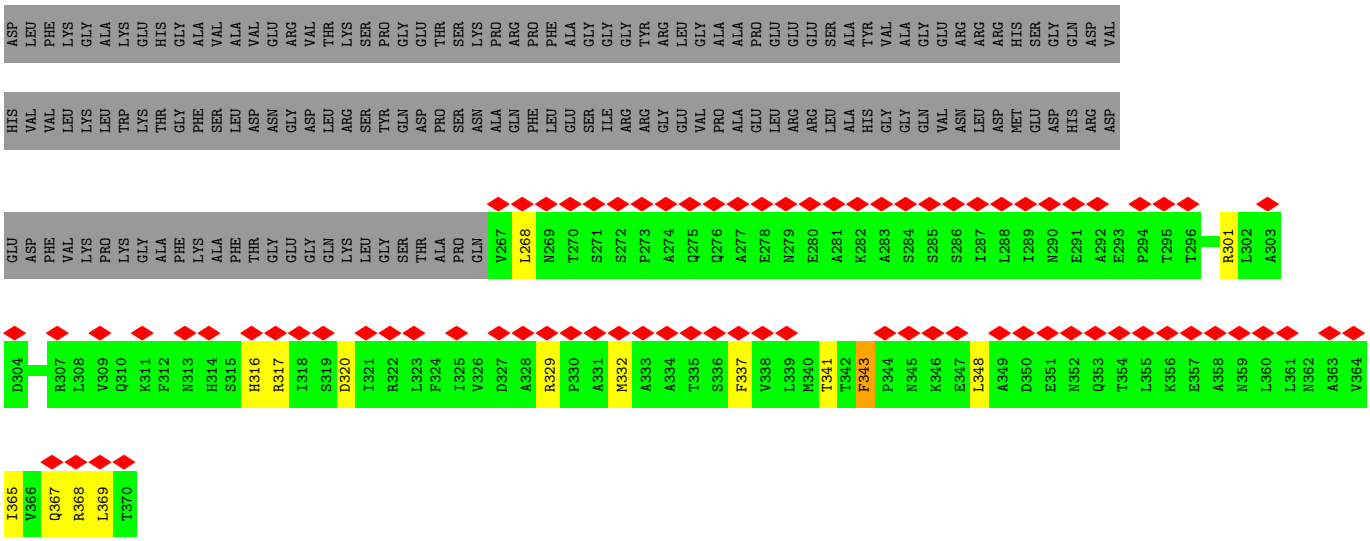


• Molecule 2: NSFL1 cofactor p47



• Molecule 2: NSFL1 cofactor p47




ASP LEU PHE LYS GLY ALA LYS GLU HIS GLY ALA VAL ALA VAL GLU ARG VAL THR LYS SER PRO GLY GLU THR SER LYS PRO ARG PRO PHE ALA GLY GLY GLY TYR ARG LEU GLY ALA ALA PRO GLU GLU GLU SER ALA TYR VAL ALA GLY GLU ARG ARG ARG HIS SER GLY GLN ASP VAL
HIS VAL VAL LEU LYS LEU TRP LYS THR GLY PHE SER LEU ASP ASN GLY ASP LEU ARG SER TYR GLN ASP PRO SER ASN ALA GLN PHE LEU GLU SER ILE ARG ARG GLY GLU VAL PRO ALA GLU LEU ARG ARG LEU ALA HIS GLY GLY GLN VAL ASN LEU ASP MET GLU ASP HIS ARG ASP
GLU ASP PHE VAL LYS PRO LYS GLY ALA PHE LYS ALA PHE THR GLY GLU GLY GLN LYS LEU GLY SER THR ALA PRO GLN V267 L268 N269 T270 S271 S272 P273 A274 Q275 Q276 A277 E278 N279 E280 A281 K282 A283 S284 S285 S286 I287 L288 I289 N290 E291 A292 E293 P294 T295 T296 R301 L302 A303
D304 R307 L308 V309 Q310 K311 F312 N313 H314 S315 H316 R317 I318 S319 D320 I321 R322 L323 F324 I325 V326 D327 A328 R329 P330 A331 M332 A333 A334 T335 S336 F337 V338 L339 M340 T341 T342 F343 P344 N345 K346 E347 L348 A349 D350 E351 N352 Q353 T354 L355 K356 E357 A358 N359 L360 L361 N362 A363 V364
I365 V366 Q367 R368 L369 T370

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44.4	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2500	Depositor
Magnification	48077	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.800	Depositor
Minimum map value	-0.283	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.086	Depositor
Map size (Å)	339.12, 339.12, 339.12	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.413, 1.413, 1.413	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AGS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.29	0/5774	0.59	3/7791 (0.0%)
1	B	0.28	0/4372	0.56	1/5892 (0.0%)
1	C	0.29	0/4342	0.56	1/5855 (0.0%)
1	D	0.27	0/5755	0.56	3/7768 (0.0%)
1	E	0.28	0/5722	0.54	3/7721 (0.0%)
1	F	0.29	0/5852	0.58	4/7896 (0.1%)
2	I	0.26	0/810	0.48	0/1104
2	J	0.25	0/766	0.48	0/1043
All	All	0.28	0/33393	0.56	15/45070 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	3
1	E	0	1
1	F	0	3
2	I	0	1
2	J	0	1
All	All	0	14

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	661	LEU	CA-CB-CG	7.59	132.77	115.30
1	D	482	LEU	CA-CB-CG	7.23	131.92	115.30
1	F	130	LEU	CA-CB-CG	6.86	131.09	115.30
1	C	469	VAL	CG1-CB-CG2	-6.01	101.29	110.90
1	F	469	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	E	235	VAL	CA-CB-CG1	5.64	119.35	110.90
1	F	236	LYS	CA-CB-CG	5.59	125.70	113.40
1	A	634	LEU	CA-CB-CG	5.50	127.95	115.30
1	F	548	LEU	CA-CB-CG	5.45	127.84	115.30
1	E	469	VAL	CG1-CB-CG2	-5.39	102.28	110.90
1	D	22	ARG	CA-CB-CG	5.30	125.05	113.40
1	A	38	VAL	CG1-CB-CG2	-5.29	102.44	110.90
1	E	236	LYS	CA-CB-CG	5.20	124.84	113.40
1	A	661	LEU	CA-CB-CG	5.18	127.21	115.30
1	B	469	VAL	CG1-CB-CG2	-5.07	102.79	110.90

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	LYS	Peptide
1	A	237	PRO	Peptide
1	A	663	LYS	Peptide
1	B	237	PRO	Peptide
1	C	237	PRO	Peptide
1	D	237	PRO	Peptide
1	D	429	LEU	Peptide
1	D	430	ILE	Peptide
1	E	237	PRO	Peptide
1	F	171	SER	Peptide
1	F	236	LYS	Peptide
1	F	237	PRO	Peptide
2	I	343	PHE	Peptide
2	J	343	PHE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5680	0	5762	96	0
1	B	4304	0	4349	58	0
1	C	4272	0	4328	55	0
1	D	5662	0	5740	75	0
1	E	5632	0	5702	77	0
1	F	5757	0	5840	81	0
2	I	802	0	756	9	0
2	J	758	0	735	10	0
3	A	62	0	24	3	0
3	B	62	0	24	3	0
3	C	62	0	24	1	0
3	D	62	0	24	2	0
3	E	62	0	24	2	0
3	F	62	0	24	4	0
All	All	33239	0	33356	426	0

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

All (426) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LYS:H	1:B:505:LYS:H	1.24	0.81
1:A:662:ARG:HB2	1:B:506:PHE:HB2	1.66	0.76
1:B:217:LYS:O	1:B:221:GLU:HB2	1.89	0.71
1:A:29:ASP:HB2	1:A:81:LYS:HB3	1.77	0.66
1:A:663:LYS:HB3	1:B:504:LEU:HB2	1.77	0.66
1:B:349:ARG:HE	1:B:350:PRO:HD2	1.61	0.66
1:A:662:ARG:H	1:B:506:PHE:H	1.44	0.65
1:F:233:ILE:HG13	1:F:235:VAL:H	1.62	0.64
1:A:671:ASP:HB2	1:A:674:PHE:HB2	1.80	0.64
1:F:538:ASN:HD21	1:F:569:ALA:HB1	1.63	0.63
1:D:482:LEU:HD21	1:D:527:LEU:HD21	1.80	0.63
1:D:583:ALA:HB1	1:D:628:ILE:HB	1.82	0.62
1:E:653:ARG:NH2	1:E:672:LEU:O	2.33	0.62
1:B:626:PRO:HA	1:B:629:ILE:HD13	1.82	0.61
1:D:36:ASN:HA	1:D:85:ASN:HD21	1.65	0.61
1:F:333:ASP:HB3	1:F:362:ARG:HD2	1.82	0.61
1:F:222:LEU:HD13	1:F:237:PRO:HD2	1.82	0.61
1:F:141:GLU:H	1:F:178:PRO:HA	1.66	0.61
1:D:571:PRO:HB3	1:D:616:ASN:HB3	1.83	0.60
1:C:634:LEU:HD12	1:C:642:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ILE:HD11	1:F:165:VAL:HG21	1.85	0.59
1:B:267:PHE:HB2	1:B:301:ILE:HG22	1.85	0.58
1:E:409:ALA:HB2	3:E:901:AGS:H5'2	1.85	0.58
1:E:673:GLU:O	1:E:677:LYS:HB2	2.04	0.58
1:A:77:CYS:SG	1:A:78:SER:N	2.76	0.57
1:D:31:ALA:HA	1:D:83:ARG:HB3	1.85	0.57
1:A:25:ARG:HB3	1:A:99:VAL:HB	1.85	0.57
2:I:318:ILE:HB	2:I:351:GLU:HA	1.86	0.57
1:B:550:MET:SD	1:B:558:ASN:ND2	2.76	0.57
1:D:657:LEU:HA	1:D:660:ASN:HB2	1.86	0.57
1:F:390:LEU:HG	1:F:392:ASP:H	1.69	0.57
1:D:522:CYS:SG	1:D:523:GLY:N	2.76	0.57
1:D:675:LEU:HD21	1:D:736:PHE:HB3	1.86	0.57
1:E:469:VAL:HG12	1:E:540:ILE:HG12	1.86	0.57
2:I:299:GLN:HB3	2:I:364:VAL:HG22	1.86	0.57
1:F:56:THR:HB	1:F:70:ILE:HG13	1.87	0.56
1:F:145:PRO:HA	1:F:175:ILE:HA	1.88	0.56
1:B:522:CYS:SG	1:B:523:GLY:N	2.79	0.56
2:J:337:PHE:HB3	2:J:369:LEU:HD23	1.88	0.56
1:A:663:LYS:HA	1:B:505:LYS:HB2	1.88	0.55
1:C:472:PRO:O	1:C:533:ASN:ND2	2.38	0.55
1:C:285:ASN:H	1:C:288:LYS:HE3	1.71	0.55
1:B:465:ARG:NH1	1:C:607:GLU:OE2	2.39	0.55
3:A:901:AGS:S1G	1:B:359:ARG:NH1	2.80	0.55
1:E:601:ILE:HD11	1:E:633:ILE:HD11	1.89	0.55
2:J:332:MET:SD	2:J:367:GLN:NE2	2.79	0.55
1:B:216:ILE:HD11	1:B:367:VAL:HG21	1.88	0.55
1:D:78:SER:HB2	1:D:81:LYS:HB2	1.89	0.55
1:A:347:THR:HG21	1:A:353:ILE:HD11	1.88	0.54
1:A:390:LEU:HG	1:A:392:ASP:H	1.72	0.54
1:B:649:ASP:OD2	1:B:651:LYS:NZ	2.37	0.54
1:D:391:ALA:HB2	1:D:446:ALA:HB1	1.89	0.54
1:A:204:ASP:OD1	1:A:204:ASP:N	2.39	0.54
2:I:301:ARG:HB2	2:I:366:VAL:HA	1.88	0.54
1:A:251:LYS:NZ	3:A:901:AGS:O2B	2.40	0.54
1:D:398:GLN:O	1:D:402:GLU:HB2	2.07	0.54
1:C:239:ARG:HH12	1:C:337:GLN:H	1.55	0.54
1:C:461:PRO:HB2	1:C:464:LEU:HB2	1.88	0.54
1:A:683:SER:HB3	1:A:745:ARG:HD2	1.88	0.54
1:C:572:CYS:SG	1:C:573:VAL:N	2.81	0.54
1:C:689:GLU:OE2	1:C:693:ARG:NH2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:NH2	1:F:428:ASP:OD1	2.40	0.54
1:A:114:ILE:H	1:A:183:HIS:HB3	1.73	0.53
1:C:494:GLN:NE2	1:C:498:GLU:OE1	2.40	0.53
1:C:541:SER:O	1:C:543:LYS:NZ	2.42	0.53
1:A:625:ARG:NH1	1:B:765:SER:O	2.42	0.53
1:D:321:GLU:OE1	1:E:322:ARG:NH1	2.41	0.53
1:D:60:LYS:HG2	1:D:66:GLU:HG2	1.91	0.53
1:F:38:VAL:HG22	1:F:70:ILE:HB	1.91	0.53
1:F:469:VAL:HG12	1:F:540:ILE:HG12	1.91	0.53
1:F:501:ASP:OD1	1:F:501:ASP:N	2.41	0.53
1:A:58:LEU:HB2	1:A:103:GLN:HB3	1.90	0.53
1:A:744:ARG:NH2	1:B:760:GLN:OE1	2.40	0.53
1:C:238:PRO:HD2	1:C:365:ARG:HD2	1.91	0.53
1:A:22:ARG:NH2	1:A:101:SER:OG	2.42	0.53
1:A:296:ASN:ND2	1:A:298:PRO:O	2.42	0.53
1:C:391:ALA:HB2	1:C:446:ALA:HB1	1.90	0.53
1:D:438:ASP:HB3	1:D:440:GLU:H	1.74	0.53
1:E:283:GLU:OE1	1:E:323:ARG:NH2	2.42	0.53
1:F:53:ARG:HB3	2:I:363:ALA:HA	1.91	0.53
1:F:239:ARG:NH1	1:F:335:LEU:O	2.42	0.52
1:C:226:HIS:HB3	1:C:229:LEU:HB2	1.90	0.52
1:E:586:ARG:HH21	1:E:601:ILE:HD13	1.74	0.52
1:D:198:LEU:O	1:D:256:ARG:NH2	2.43	0.52
1:D:296:ASN:ND2	1:D:298:PRO:O	2.43	0.52
1:D:421:GLN:OE1	1:D:424:ARG:NH1	2.43	0.52
1:E:484:ASP:N	1:E:484:ASP:OD1	2.42	0.52
1:E:649:ASP:OD2	1:E:651:LYS:NZ	2.41	0.52
1:B:669:ASP:O	1:B:733:ARG:NH1	2.42	0.52
1:E:467:THR:OG1	1:E:565:LYS:NZ	2.42	0.52
1:F:116:VAL:HG12	1:F:165:VAL:HG22	1.91	0.52
1:D:609:ASP:OD2	1:D:638:ARG:NH1	2.42	0.52
1:E:514:VAL:HG12	1:E:641:GLN:HB2	1.92	0.52
1:A:239:ARG:NH1	1:A:335:LEU:O	2.43	0.52
1:B:233:ILE:HG13	1:B:235:VAL:H	1.73	0.52
1:D:57:VAL:HA	1:D:104:PRO:HA	1.92	0.52
1:D:482:LEU:HD11	1:D:527:LEU:HD11	1.91	0.52
1:B:707:ILE:O	1:B:711:ARG:HB2	2.10	0.51
1:A:577:ASP:HA	1:A:622:ALA:HB3	1.93	0.51
1:D:389:LYS:NZ	1:D:443:ASN:O	2.41	0.51
1:E:572:CYS:SG	1:E:573:VAL:N	2.83	0.51
1:E:36:ASN:ND2	1:E:153:LEU:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:ARG:HH21	1:F:194:GLU:HB3	1.75	0.51
1:A:60:LYS:HD3	1:A:101:SER:HB3	1.93	0.51
1:C:297:ALA:HA	1:C:339:ALA:HB1	1.93	0.51
1:B:654:VAL:HG22	1:B:672:LEU:HD23	1.92	0.51
1:F:68:VAL:HG22	1:F:147:ARG:HD2	1.93	0.51
1:F:522:CYS:SG	1:F:523:GLY:N	2.84	0.51
1:B:567:ARG:NH2	1:B:610:GLY:O	2.44	0.51
1:D:572:CYS:SG	1:D:573:VAL:N	2.83	0.51
1:E:501:ASP:N	1:E:501:ASP:OD1	2.44	0.51
1:D:108:VAL:HA	1:D:173:TYR:HE2	1.76	0.51
1:E:303:ILE:HD12	1:E:306:LEU:HD13	1.93	0.51
1:F:296:ASN:ND2	1:F:298:PRO:O	2.44	0.51
1:A:191:ARG:HB3	1:A:194:GLU:HB3	1.93	0.50
1:F:57:VAL:HG12	1:F:104:PRO:HA	1.93	0.50
1:B:682:PHE:O	1:B:745:ARG:NH2	2.44	0.50
1:C:200:GLU:OE2	1:C:260:ASN:ND2	2.43	0.50
1:F:250:GLY:N	3:F:901:AGS:O2B	2.44	0.50
1:A:698:ALA:HB2	1:A:731:ILE:HD13	1.92	0.50
1:A:763:GLN:NE2	1:F:745:ARG:O	2.44	0.50
1:B:239:ARG:NH1	1:B:335:LEU:O	2.44	0.50
1:D:515:LEU:HG	1:D:639:LEU:HB3	1.93	0.50
1:F:239:ARG:HH12	1:F:335:LEU:HB3	1.77	0.50
1:A:519:PRO:O	1:A:524:LYS:NZ	2.44	0.50
1:D:256:ARG:O	1:D:260:ASN:ND2	2.43	0.50
1:D:654:VAL:O	1:D:658:LYS:N	2.44	0.50
1:E:40:SER:HB3	1:E:74:ASP:HB2	1.92	0.50
1:A:467:THR:O	1:A:565:LYS:NZ	2.43	0.50
1:D:204:ASP:N	1:D:204:ASP:OD1	2.44	0.50
1:E:239:ARG:NH1	1:E:335:LEU:O	2.44	0.50
1:E:333:ASP:HB3	1:E:362:ARG:HD2	1.94	0.50
1:A:233:ILE:HG13	1:A:235:VAL:H	1.76	0.50
1:D:27:ILE:HB	1:D:81:LYS:HG2	1.94	0.50
1:D:541:SER:OG	1:D:543:LYS:NZ	2.41	0.50
1:D:120:ASP:N	1:D:120:ASP:OD1	2.43	0.50
1:A:398:GLN:OE1	1:A:453:ARG:NH2	2.44	0.50
1:D:75:ASP:OD1	1:D:75:ASP:N	2.45	0.50
1:F:151:ILE:HG12	1:F:164:LYS:HG3	1.94	0.50
1:A:25:ARG:HH21	1:A:99:VAL:HG23	1.76	0.49
1:E:66:GLU:HB2	1:E:147:ARG:HE	1.76	0.49
1:F:421:GLN:HA	1:F:424:ARG:HE	1.77	0.49
1:A:576:PHE:HB2	1:A:621:GLY:HA2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ARG:NH1	1:B:488:GLU:OE2	2.45	0.49
1:C:398:GLN:O	1:C:402:GLU:HB2	2.12	0.49
1:A:44:PRO:HA	1:A:47:ASP:HB2	1.94	0.49
1:A:80:GLU:OE2	1:A:81:LYS:NZ	2.45	0.49
1:B:251:LYS:NZ	1:B:347:THR:O	2.45	0.49
1:C:347:THR:OG1	1:C:348:ASN:N	2.45	0.49
1:E:524:LYS:HD3	1:E:622:ALA:HB1	1.94	0.49
1:E:241:ILE:HB	1:E:344:MET:HG2	1.94	0.49
1:E:296:ASN:ND2	1:E:298:PRO:O	2.40	0.49
1:A:60:LYS:HA	1:A:66:GLU:HG2	1.94	0.49
1:B:461:PRO:HB2	1:B:464:LEU:HG	1.93	0.49
1:A:141:GLU:HG2	2:J:368:ARG:HD2	1.95	0.49
1:D:390:LEU:HG	1:D:392:ASP:H	1.77	0.49
1:E:465:ARG:NH1	1:F:607:GLU:OE1	2.45	0.49
1:F:123:VAL:O	1:F:159:ARG:NH1	2.45	0.49
1:E:30:GLU:O	1:E:83:ARG:NH1	2.45	0.49
1:E:515:LEU:HD11	1:E:642:LEU:HD23	1.94	0.49
1:F:499:HIS:HB3	1:F:502:LYS:HD2	1.95	0.49
1:A:179:ASP:OD2	2:J:368:ARG:NH1	2.46	0.49
1:E:74:ASP:HB3	1:E:77:CYS:HB2	1.95	0.49
1:F:41:LEU:HG	1:F:82:ILE:HG12	1.95	0.49
1:A:75:ASP:OD1	1:A:75:ASP:N	2.46	0.49
1:E:372:PRO:O	1:E:377:ARG:NH1	2.46	0.49
1:C:282:SER:OG	1:C:323:ARG:NH1	2.46	0.48
1:E:500:PRO:HA	1:E:503:PHE:HD2	1.77	0.48
1:A:660:ASN:HB3	1:B:505:LYS:HA	1.95	0.48
1:F:544:GLY:H	1:F:578:GLU:HB2	1.78	0.48
1:A:726:ASP:N	1:A:726:ASP:OD1	2.46	0.48
1:C:233:ILE:HG13	1:C:235:VAL:H	1.78	0.48
1:F:283:GLU:HG3	1:F:327:GLN:HG2	1.95	0.48
1:E:65:ARG:NH2	1:E:149:GLY:O	2.46	0.48
1:F:179:ASP:OD1	1:F:179:ASP:N	2.46	0.48
1:F:193:ASP:OD1	1:F:193:ASP:N	2.45	0.48
1:A:155:HIS:HA	1:A:160:ALA:HA	1.95	0.48
1:D:84:MET:O	1:D:89:ARG:NH2	2.47	0.48
1:D:389:LYS:HE2	1:D:445:LEU:HD23	1.95	0.48
1:D:653:ARG:HA	1:D:656:ILE:HG22	1.95	0.48
1:D:683:SER:OG	1:D:745:ARG:NH1	2.46	0.48
1:A:515:LEU:HD11	1:A:642:LEU:HG	1.94	0.48
1:C:285:ASN:HA	1:C:288:LYS:HB2	1.95	0.48
1:C:749:ASP:HA	1:C:752:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:PHE:HD1	1:E:300:ILE:HG23	1.79	0.48
1:D:193:ASP:OD1	1:D:193:ASP:N	2.47	0.48
1:E:459:SER:O	1:F:615:LYS:NZ	2.41	0.48
3:F:902:AGS:O3A	3:F:902:AGS:O2G	2.32	0.48
1:C:631:PRO:HB3	1:C:764:GLN:HB3	1.95	0.47
1:D:224:LEU:HD22	1:D:262:THR:HA	1.96	0.47
1:E:145:PRO:HB3	1:E:175:ILE:HG12	1.96	0.47
1:A:766:ARG:HH21	1:F:754:LYS:HB3	1.79	0.47
1:C:216:ILE:HD11	1:C:367:VAL:HG21	1.96	0.47
1:E:149:GLY:O	1:E:164:LYS:NZ	2.45	0.47
1:A:425:LYS:HG3	1:A:426:LYS:HE3	1.96	0.47
1:D:700:ARG:NE	1:E:491:GLU:OE2	2.43	0.47
1:F:288:LYS:HA	1:F:291:GLU:HB2	1.96	0.47
1:D:368:ASP:OD1	1:D:368:ASP:N	2.47	0.47
1:C:293:ALA:HB1	1:C:341:VAL:HG11	1.96	0.47
1:D:84:MET:HB2	1:D:88:VAL:HB	1.96	0.47
1:E:111:GLY:HA2	1:E:170:PRO:HG2	1.96	0.47
1:D:726:ASP:N	1:D:726:ASP:OD1	2.46	0.47
1:E:198:LEU:O	1:E:256:ARG:NH2	2.48	0.47
1:F:31:ALA:HB2	1:F:83:ARG:HB2	1.97	0.47
1:F:422:ALA:O	1:F:426:LYS:NZ	2.47	0.47
1:A:484:ASP:OD1	1:A:484:ASP:N	2.46	0.47
1:B:522:CYS:O	3:B:902:AGS:O2B	2.32	0.47
1:E:524:LYS:NZ	1:E:623:THR:O	2.48	0.47
1:F:483:GLU:OE1	1:F:487:ARG:NH1	2.47	0.47
1:A:607:GLU:OE2	1:F:465:ARG:NH1	2.48	0.47
1:A:737:GLU:OE2	1:A:741:ARG:NH2	2.48	0.47
1:C:381:LEU:HG	1:C:411:LEU:HD23	1.96	0.47
1:C:497:VAL:HG13	1:C:616:ASN:HD21	1.78	0.47
1:C:650:GLU:O	1:C:653:ARG:NH1	2.45	0.47
1:F:22:ARG:NH1	1:F:25:ARG:O	2.46	0.47
1:B:438:ASP:HB3	1:B:440:GLU:HG2	1.96	0.47
1:B:673:GLU:O	1:B:677:LYS:HB2	2.15	0.47
1:D:64:ARG:HH22	1:D:198:LEU:HD22	1.79	0.47
1:E:642:LEU:HD13	1:E:762:LEU:HB3	1.96	0.47
1:F:605:LEU:HD21	1:F:635:ARG:HH12	1.80	0.47
1:A:39:VAL:HG23	1:A:71:VAL:HG13	1.97	0.46
1:C:347:THR:HG21	1:C:353:ILE:HD11	1.96	0.46
1:C:390:LEU:HG	1:C:392:ASP:H	1.80	0.46
1:A:86:ARG:O	1:A:89:ARG:NH2	2.46	0.46
1:A:143:TYR:O	2:J:301:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LEU:HB3	1:B:363:PHE:HD2	1.79	0.46
3:B:902:AGS:O2B	3:B:902:AGS:O2A	2.32	0.46
1:D:24:ASN:HB2	1:D:102:ILE:H	1.80	0.46
1:F:130:LEU:HD13	1:F:183:HIS:HA	1.97	0.46
1:C:267:PHE:HB2	1:C:301:ILE:HG22	1.98	0.46
1:F:239:ARG:HE	1:F:343:VAL:HG13	1.80	0.46
1:F:522:CYS:O	3:F:902:AGS:O2B	2.32	0.46
1:D:65:ARG:NH1	1:D:91:ASN:O	2.48	0.46
1:F:20:LYS:NZ	1:F:210:ARG:O	2.40	0.46
3:D:901:AGS:O2G	3:D:901:AGS:O1B	2.33	0.46
1:E:274:ILE:HG12	1:E:286:LEU:HG	1.97	0.46
1:F:115:HIS:ND1	1:F:167:GLU:O	2.48	0.46
1:B:670:VAL:HA	1:B:733:ARG:HH11	1.79	0.46
1:A:40:SER:H	1:A:83:ARG:HB2	1.80	0.46
1:A:465:ARG:NH1	1:B:607:GLU:OE2	2.49	0.46
1:D:318:GLY:HA3	1:E:322:ARG:HH12	1.80	0.46
1:A:479:ILE:HD13	1:A:530:ALA:HB2	1.97	0.46
1:B:748:SER:OG	1:C:763:GLN:OE1	2.34	0.46
1:D:111:GLY:HA2	1:D:170:PRO:HG2	1.98	0.46
1:E:170:PRO:HB2	1:E:174:CYS:HB3	1.98	0.46
1:E:751:ASP:HA	1:E:754:LYS:HD2	1.98	0.46
2:I:300:ILE:HG21	2:I:325:ILE:HD11	1.98	0.46
1:A:371:ILE:HD11	1:A:468:VAL:HG12	1.98	0.46
1:B:244:TYR:CZ	1:B:368:ASP:HB3	2.51	0.46
1:B:472:PRO:O	1:B:533:ASN:ND2	2.41	0.45
1:C:469:VAL:HG12	1:C:540:ILE:HG12	1.99	0.45
1:A:80:GLU:HG2	1:A:81:LYS:HG3	1.98	0.45
1:A:479:ILE:O	1:A:486:LYS:NZ	2.41	0.45
1:E:692:GLN:OE1	1:E:696:LYS:NZ	2.44	0.45
1:A:42:SER:HB2	1:A:79:ASP:HA	1.98	0.45
1:A:440:GLU:O	1:A:444:SER:OG	2.34	0.45
1:B:767:GLY:O	1:B:768:PHE:N	2.50	0.45
1:E:75:ASP:OD1	1:E:75:ASP:N	2.49	0.45
2:I:360:LEU:HD13	2:I:365:ILE:HD11	1.97	0.45
1:C:531:ILE:O	1:C:535:CYS:CB	2.65	0.45
1:F:391:ALA:HB2	1:F:446:ALA:HB1	1.99	0.45
2:I:321:ILE:HD11	2:I:355:LEU:HD21	1.97	0.45
1:A:490:GLN:NE2	1:A:494:GLN:OE1	2.44	0.45
1:A:544:GLY:HA3	1:A:545:PRO:HD3	1.81	0.45
1:A:572:CYS:SG	1:A:573:VAL:N	2.89	0.45
1:E:368:ASP:OD1	1:E:368:ASP:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:576:PHE:HB2	1:E:621:GLY:HA2	1.98	0.45
1:E:683:SER:OG	1:E:745:ARG:NH1	2.44	0.45
1:A:237:PRO:HG3	1:F:420:LEU:HD11	1.99	0.45
1:A:727:PRO:HD2	1:A:729:PRO:HG3	1.99	0.45
1:D:609:ASP:N	1:D:609:ASP:OD1	2.49	0.45
1:A:290:PHE:HD2	1:A:331:LEU:HD13	1.82	0.45
1:B:683:SER:HB3	1:B:747:VAL:HG12	1.99	0.45
1:E:226:HIS:HB3	1:E:229:LEU:HB2	1.97	0.45
1:E:267:PHE:HB2	1:E:301:ILE:HG22	1.98	0.45
1:F:218:GLU:HA	1:F:221:GLU:HG3	1.99	0.45
1:A:189:ILE:O	1:A:191:ARG:NH1	2.50	0.45
1:B:523:GLY:O	1:B:527:LEU:N	2.47	0.45
1:C:473:GLN:HA	1:C:533:ASN:HD21	1.81	0.45
1:C:567:ARG:HE	1:C:611:MET:HE1	1.82	0.45
1:F:249:THR:N	3:F:901:AGS:O2B	2.50	0.45
2:J:268:LEU:O	2:J:329:ARG:NH2	2.50	0.45
2:J:301:ARG:N	2:J:365:ILE:O	2.45	0.45
1:B:627:ASP:N	1:B:627:ASP:OD1	2.50	0.44
1:D:661:LEU:HD12	1:D:662:ARG:H	1.82	0.44
1:E:758:PHE:HE2	1:F:766:ARG:HH22	1.65	0.44
1:F:737:GLU:OE2	1:F:741:ARG:NH2	2.50	0.44
1:B:541:SER:HA	1:B:575:PHE:HB3	1.99	0.44
1:D:272:PRO:O	1:E:326:SER:OG	2.34	0.44
2:J:316:HIS:ND1	2:J:320:ASP:OD2	2.48	0.44
1:D:35:ASP:HB3	1:D:38:VAL:HB	1.99	0.44
1:A:51:LEU:HD12	1:A:102:ILE:HD12	1.98	0.44
1:A:634:LEU:HD11	1:A:762:LEU:HA	1.98	0.44
1:B:394:VAL:HG12	1:B:449:MET:HB3	2.00	0.44
1:B:583:ALA:HB1	1:B:628:ILE:HG22	1.99	0.44
2:J:341:THR:HG23	2:J:348:LEU:HD11	1.98	0.44
1:D:393:ASP:OD1	1:D:393:ASP:N	2.50	0.44
1:F:143:TYR:OH	2:I:340:MET:SD	2.72	0.44
1:C:685:ALA:HB1	3:C:902:AGS:H8	1.98	0.44
1:F:472:PRO:HB2	1:F:474:VAL:HG13	2.00	0.44
1:A:56:THR:OG1	1:A:105:CYS:O	2.36	0.44
3:A:901:AGS:O2G	3:A:901:AGS:O1B	2.36	0.44
1:D:520:PRO:HB3	1:D:624:ASN:HB3	2.00	0.44
1:A:241:ILE:HB	1:A:344:MET:HG2	1.98	0.44
1:D:149:GLY:HA2	1:D:164:LYS:HE3	2.00	0.44
1:F:523:GLY:O	1:F:527:LEU:N	2.45	0.44
1:B:199:ASN:O	1:B:256:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:902:AGS:O3A	3:B:902:AGS:O2G	2.36	0.44
1:F:117:LEU:N	1:F:164:LYS:O	2.44	0.44
1:A:500:PRO:O	1:A:504:LEU:N	2.51	0.43
1:D:274:ILE:HG12	1:D:286:LEU:HG	2.00	0.43
1:B:430:ILE:O	1:B:438:ASP:N	2.50	0.43
1:D:26:LEU:HD13	1:D:82:ILE:HB	2.00	0.43
1:D:653:ARG:HH12	1:D:676:ALA:HB2	1.82	0.43
1:E:40:SER:HB2	1:E:83:ARG:HB2	2.00	0.43
1:E:239:ARG:HH12	1:E:335:LEU:HB3	1.83	0.43
1:E:354:ASP:HB3	1:E:357:LEU:HD13	2.00	0.43
1:F:653:ARG:HG2	1:F:672:LEU:HD23	2.00	0.43
1:A:636:PRO:O	1:A:638:ARG:NH1	2.51	0.43
1:A:671:ASP:OD1	1:A:671:ASP:N	2.47	0.43
1:E:522:CYS:HB2	1:E:524:LYS:HE3	2.01	0.43
1:F:283:GLU:OE1	1:F:323:ARG:NH2	2.51	0.43
1:A:122:THR:HG21	1:A:162:GLU:HG3	1.99	0.43
1:A:426:LYS:HG3	1:A:441:VAL:HG21	2.00	0.43
1:D:131:PHE:HB2	1:D:184:CYS:HB3	2.01	0.43
1:A:266:PHE:HD1	1:A:300:ILE:HG23	1.84	0.43
1:B:297:ALA:HA	1:B:339:ALA:HB1	1.99	0.43
1:C:501:ASP:OD1	1:C:501:ASP:N	2.51	0.43
1:E:82:ILE:HG21	1:E:100:ILE:HD11	2.01	0.43
1:E:115:HIS:HA	1:E:183:HIS:HB2	1.99	0.43
1:F:398:GLN:O	1:F:402:GLU:HB2	2.19	0.43
1:F:484:ASP:OD1	1:F:484:ASP:N	2.52	0.43
1:E:64:ARG:HD3	1:E:263:GLY:HA2	2.01	0.43
1:E:131:PHE:HA	1:E:135:LEU:HB2	2.00	0.43
1:A:87:VAL:HG11	1:A:153:LEU:HB3	2.01	0.43
1:A:131:PHE:HA	1:A:135:LEU:HD21	2.01	0.43
1:A:393:ASP:OD1	1:A:393:ASP:N	2.51	0.43
1:D:53:ARG:HH21	1:D:72:LEU:HD22	1.84	0.43
1:D:251:LYS:HB2	1:D:251:LYS:HE2	1.83	0.43
1:D:170:PRO:HB2	1:D:174:CYS:HB3	2.00	0.42
1:D:476:TRP:HE1	1:D:533:ASN:HB3	1.84	0.42
1:D:627:ASP:OD1	1:D:627:ASP:N	2.51	0.42
1:F:381:LEU:HG	1:F:411:LEU:HD21	2.00	0.42
1:A:664:SER:HB2	1:B:506:PHE:CE2	2.54	0.42
1:B:269:ILE:HB	1:B:303:ILE:HG22	2.02	0.42
1:E:65:ARG:HH21	1:E:150:ASP:HA	1.84	0.42
1:F:460:ASN:HA	1:F:461:PRO:HD3	1.84	0.42
1:F:428:ASP:OD2	1:F:428:ASP:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:ASP:OD1	1:C:627:ASP:N	2.43	0.42
1:D:114:ILE:O	1:D:183:HIS:N	2.47	0.42
1:D:694:ALA:HA	1:D:697:LEU:HD12	2.01	0.42
1:E:472:PRO:HB2	1:E:474:VAL:HG13	2.00	0.42
1:F:605:LEU:HD12	1:F:633:ILE:HD13	2.01	0.42
1:D:631:PRO:HA	1:D:634:LEU:HD13	2.01	0.42
1:C:583:ALA:HA	1:C:586:ARG:HG2	2.01	0.42
1:F:42:SER:O	1:F:46:MET:N	2.50	0.42
1:F:699:ILE:HD13	1:F:699:ILE:HA	1.90	0.42
1:A:765:SER:O	1:F:625:ARG:NH1	2.44	0.42
1:B:751:ASP:HA	1:B:754:LYS:HD2	2.01	0.42
1:E:51:LEU:HD11	1:E:104:PRO:HB3	2.02	0.42
1:E:526:LEU:HD23	1:E:529:LYS:HE2	2.02	0.42
1:E:549:THR:HA	1:E:552:PHE:HD2	1.85	0.42
1:E:640:ASP:N	1:E:640:ASP:OD1	2.52	0.42
1:F:18:LYS:HD3	1:F:18:LYS:HA	1.75	0.42
1:C:264:ALA:HB1	1:C:299:ALA:HA	2.00	0.42
1:D:107:ASP:OD1	1:D:107:ASP:N	2.47	0.42
1:E:116:VAL:HG12	1:E:165:VAL:HA	2.01	0.42
1:F:153:LEU:HD11	1:F:160:ALA:HB1	2.02	0.42
1:B:683:SER:OG	1:B:745:ARG:NE	2.53	0.42
1:E:578:GLU:HG2	1:F:635:ARG:HH21	1.85	0.42
1:A:192:GLU:HA	1:A:195:GLU:HB2	2.01	0.41
1:F:349:ARG:HD2	1:F:349:ARG:HA	1.85	0.41
1:A:522:CYS:HA	1:A:685:ALA:HB2	2.02	0.41
1:D:118:PRO:HG2	1:D:188:PRO:HG3	2.02	0.41
1:E:623:THR:OG1	1:E:624:ASN:N	2.53	0.41
1:A:614:LYS:HA	1:A:614:LYS:HD3	1.91	0.41
1:A:762:LEU:O	1:F:746:SER:OG	2.38	0.41
1:C:700:ARG:HH21	1:D:487:ARG:HE	1.67	0.41
1:E:222:LEU:HD21	1:E:237:PRO:HG2	2.02	0.41
1:E:383:ILE:HD11	3:E:901:AGS:H2	2.02	0.41
1:A:138:TYR:HB2	2:J:343:PHE:HE2	1.85	0.41
1:C:313:ARG:O	1:C:316:THR:OG1	2.36	0.41
1:D:520:PRO:O	3:D:902:AGS:O2B	2.37	0.41
1:E:84:MET:HB2	1:E:88:VAL:HB	2.02	0.41
1:A:114:ILE:HD11	1:A:146:ILE:HD11	2.03	0.41
1:B:336:LYS:HA	1:B:336:LYS:HD2	1.92	0.41
1:C:484:ASP:OD1	1:C:484:ASP:N	2.54	0.41
1:D:246:PRO:O	1:D:251:LYS:NZ	2.50	0.41
1:F:58:LEU:HG	1:F:68:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:ILE:HD13	1:A:643:ILE:HA	1.96	0.41
1:C:313:ARG:HH21	1:C:356:ALA:HB2	1.85	0.41
1:C:753:ARG:HA	1:C:753:ARG:HD3	1.89	0.41
1:D:199:ASN:HB3	1:D:256:ARG:HH22	1.86	0.41
1:A:119:ILE:HG22	1:A:121:ASP:H	1.86	0.41
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.91	0.41
1:F:332:MET:HG3	1:F:362:ARG:HG2	2.03	0.41
1:B:465:ARG:HH12	1:C:560:ARG:HG3	1.86	0.41
1:C:204:ASP:OD1	1:C:204:ASP:N	2.45	0.41
1:C:552:PHE:HB2	1:D:599:ARG:HD2	2.02	0.41
1:E:130:LEU:HA	1:E:133:VAL:HB	2.03	0.41
1:E:190:LYS:HA	1:E:190:LYS:HD2	1.87	0.41
1:F:105:CYS:HA	1:F:106:PRO:HD3	1.93	0.41
1:B:527:LEU:HD23	1:B:527:LEU:HA	1.94	0.41
1:C:512:LYS:HB2	1:C:512:LYS:HE3	1.81	0.41
1:C:522:CYS:HA	1:C:685:ALA:HB3	2.03	0.41
1:F:136:LYS:HA	1:F:140:LEU:HD13	2.03	0.41
1:F:216:ILE:HD11	1:F:367:VAL:HG21	2.02	0.41
1:C:583:ALA:HB1	1:C:628:ILE:HG13	2.03	0.41
2:I:301:ARG:HD2	2:I:301:ARG:HA	1.94	0.41
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.96	0.40
1:A:663:LYS:HG2	1:B:502:LYS:HA	2.03	0.40
1:B:734:ASP:N	1:B:734:ASP:OD1	2.54	0.40
1:F:614:LYS:HD3	1:F:614:LYS:HA	1.79	0.40
1:C:464:LEU:HD22	1:D:567:ARG:HH22	1.87	0.40
1:F:652:SER:O	1:F:656:ILE:HB	2.20	0.40
1:A:189:ILE:HG23	1:A:191:ARG:HH11	1.86	0.40
1:B:668:LYS:N	1:B:730:GLU:OE2	2.55	0.40
1:E:515:LEU:HB3	1:E:639:LEU:HD13	2.04	0.40
1:C:269:ILE:HG13	1:C:303:ILE:HG22	2.02	0.40
1:C:373:ASP:O	1:C:377:ARG:N	2.45	0.40
1:A:58:LEU:HD21	1:A:173:TYR:CZ	2.56	0.40
1:A:224:LEU:HD22	1:A:262:THR:HA	2.03	0.40
1:B:623:THR:HG21	1:B:629:ILE:HD11	2.04	0.40
1:C:531:ILE:O	1:C:535:CYS:HB2	2.22	0.40
1:D:663:LYS:NZ	1:E:502:LYS:O	2.47	0.40
1:E:464:LEU:HD23	1:E:464:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	714/806 (89%)	638 (89%)	75 (10%)	1 (0%)	51 85
1	B	541/806 (67%)	483 (89%)	58 (11%)	0	100 100
1	C	540/806 (67%)	486 (90%)	53 (10%)	1 (0%)	47 81
1	D	715/806 (89%)	642 (90%)	72 (10%)	1 (0%)	51 85
1	E	707/806 (88%)	662 (94%)	44 (6%)	1 (0%)	51 85
1	F	727/806 (90%)	658 (90%)	69 (10%)	0	100 100
2	I	111/370 (30%)	105 (95%)	6 (5%)	0	100 100
2	J	102/370 (28%)	94 (92%)	8 (8%)	0	100 100
All	All	4157/5576 (75%)	3768 (91%)	385 (9%)	4 (0%)	54 85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	476	TRP
1	A	476	TRP
1	E	476	TRP
1	D	662	ARG

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	616/678 (91%)	612 (99%)	4 (1%)	86 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	459/678 (68%)	456 (99%)	3 (1%)	84 90
1	C	456/678 (67%)	454 (100%)	2 (0%)	91 94
1	D	614/678 (91%)	610 (99%)	4 (1%)	84 90
1	E	611/678 (90%)	606 (99%)	5 (1%)	81 89
1	F	624/678 (92%)	613 (98%)	11 (2%)	59 77
2	I	75/302 (25%)	75 (100%)	0	100 100
2	J	75/302 (25%)	74 (99%)	1 (1%)	69 82
All	All	3530/4672 (76%)	3500 (99%)	30 (1%)	82 89

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	86	ARG
1	A	323	ARG
1	A	732	ARG
1	B	323	ARG
1	B	362	ARG
1	B	709	ARG
1	C	401	ASN
1	C	653	ARG
1	D	22	ARG
1	D	362	ARG
1	D	653	ARG
1	D	708	ARG
1	E	236	LYS
1	E	323	ARG
1	E	362	ARG
1	E	653	ARG
1	E	708	ARG
1	F	84	MET
1	F	86	ARG
1	F	191	ARG
1	F	225	ARG
1	F	236	LYS
1	F	362	ARG
1	F	653	ARG
1	F	708	ARG
1	F	744	ARG
1	F	745	ARG

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Mol	Chain	Res	Type
1	F	766	ARG
2	J	317	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	764	GLN
1	E	36	ASN
1	F	538	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AGS	F	901	-	26,33,33	0.71	1 (3%)	26,52,52	1.14	2 (7%)
3	AGS	B	901	-	26,33,33	0.71	1 (3%)	26,52,52	1.03	2 (7%)
3	AGS	A	902	-	26,33,33	0.73	1 (3%)	26,52,52	1.09	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	AGS	E	901	-	26,33,33	0.71	1 (3%)	26,52,52	1.13	2 (7%)
3	AGS	C	901	-	26,33,33	0.69	1 (3%)	26,52,52	1.08	2 (7%)
3	AGS	E	902	-	26,33,33	0.72	1 (3%)	26,52,52	1.22	2 (7%)
3	AGS	D	901	-	26,33,33	0.69	0	26,52,52	1.10	2 (7%)
3	AGS	C	902	-	26,33,33	0.70	1 (3%)	26,52,52	1.15	2 (7%)
3	AGS	D	902	-	26,33,33	0.72	1 (3%)	26,52,52	1.16	2 (7%)
3	AGS	A	901	-	26,33,33	0.71	1 (3%)	26,52,52	1.11	2 (7%)
3	AGS	B	902	-	26,33,33	0.71	1 (3%)	26,52,52	1.13	2 (7%)
3	AGS	F	902	-	26,33,33	0.71	1 (3%)	26,52,52	1.12	2 (7%)

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
3	AGS	F	901	-	-	3/17/38/38	0/3/3/3
3	AGS	B	901	-	-	4/17/38/38	0/3/3/3
3	AGS	A	902	-	-	0/17/38/38	0/3/3/3
3	AGS	E	901	-	-	2/17/38/38	0/3/3/3
3	AGS	C	901	-	-	5/17/38/38	0/3/3/3
3	AGS	E	902	-	-	7/17/38/38	0/3/3/3
3	AGS	D	901	-	-	2/17/38/38	0/3/3/3
3	AGS	C	902	-	-	0/17/38/38	0/3/3/3
3	AGS	D	902	-	-	5/17/38/38	0/3/3/3
3	AGS	A	901	-	-	6/17/38/38	0/3/3/3
3	AGS	B	902	-	-	5/17/38/38	0/3/3/3
3	AGS	F	902	-	-	6/17/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	AGS	PG-S1G	2.14	1.95	1.90
3	A	902	AGS	PG-S1G	2.13	1.95	1.90
3	E	902	AGS	PG-S1G	2.13	1.95	1.90
3	B	901	AGS	PG-S1G	2.12	1.95	1.90
3	F	902	AGS	PG-S1G	2.12	1.95	1.90
3	D	902	AGS	PG-S1G	2.12	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	901	AGS	PG-S1G	2.08	1.95	1.90
3	C	902	AGS	PG-S1G	2.08	1.95	1.90
3	C	901	AGS	PG-S1G	2.07	1.95	1.90
3	A	901	AGS	PG-S1G	2.06	1.95	1.90
3	F	901	AGS	PG-S1G	2.03	1.95	1.90

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	902	AGS	PA-O3A-PB	-4.99	115.69	132.83
3	D	902	AGS	PA-O3A-PB	-4.63	116.95	132.83
3	F	901	AGS	PA-O3A-PB	-4.60	117.06	132.83
3	F	902	AGS	PA-O3A-PB	-4.40	117.72	132.83
3	C	902	AGS	PA-O3A-PB	-4.31	118.05	132.83
3	E	901	AGS	PA-O3A-PB	-4.29	118.11	132.83
3	D	901	AGS	PA-O3A-PB	-4.14	118.62	132.83
3	A	901	AGS	PA-O3A-PB	-4.11	118.73	132.83
3	B	902	AGS	PA-O3A-PB	-4.09	118.80	132.83
3	A	902	AGS	PA-O3A-PB	-3.88	119.51	132.83
3	C	901	AGS	PA-O3A-PB	-3.82	119.70	132.83
3	B	901	AGS	PA-O3A-PB	-3.75	119.97	132.83
3	E	901	AGS	C5-C6-N6	2.30	123.85	120.35
3	D	902	AGS	C5-C6-N6	2.30	123.84	120.35
3	C	901	AGS	C5-C6-N6	2.27	123.80	120.35
3	F	902	AGS	C5-C6-N6	2.27	123.80	120.35
3	B	902	AGS	C5-C6-N6	2.27	123.80	120.35
3	A	902	AGS	C5-C6-N6	2.26	123.79	120.35
3	A	901	AGS	C5-C6-N6	2.25	123.77	120.35
3	B	901	AGS	C5-C6-N6	2.24	123.76	120.35
3	E	902	AGS	C5-C6-N6	2.23	123.74	120.35
3	D	901	AGS	C5-C6-N6	2.22	123.73	120.35
3	C	902	AGS	C5-C6-N6	2.19	123.68	120.35
3	F	901	AGS	C5-C6-N6	2.19	123.67	120.35

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	AGS	PB-O3B-PG-O2G
3	A	901	AGS	C5'-O5'-PA-O1A
3	A	901	AGS	C5'-O5'-PA-O2A
3	A	901	AGS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	B	901	AGS	C5'-O5'-PA-O1A
3	B	901	AGS	C5'-O5'-PA-O2A
3	B	901	AGS	C5'-O5'-PA-O3A
3	C	901	AGS	C5'-O5'-PA-O1A
3	C	901	AGS	C5'-O5'-PA-O2A
3	C	901	AGS	C5'-O5'-PA-O3A
3	C	901	AGS	O4'-C4'-C5'-O5'
3	D	901	AGS	C5'-O5'-PA-O3A
3	D	902	AGS	C5'-O5'-PA-O3A
3	E	901	AGS	C5'-O5'-PA-O1A
3	E	902	AGS	C5'-O5'-PA-O1A
3	E	902	AGS	C5'-O5'-PA-O2A
3	F	902	AGS	C5'-O5'-PA-O1A
3	F	902	AGS	C5'-O5'-PA-O3A
3	A	901	AGS	O4'-C4'-C5'-O5'
3	B	901	AGS	O4'-C4'-C5'-O5'
3	E	902	AGS	C3'-C4'-C5'-O5'
3	E	902	AGS	C4'-C5'-O5'-PA
3	D	901	AGS	C5'-O5'-PA-O1A
3	B	902	AGS	PG-O3B-PB-O1B
3	E	902	AGS	O4'-C4'-C5'-O5'
3	B	902	AGS	PB-O3A-PA-O1A
3	B	902	AGS	PB-O3A-PA-O2A
3	D	902	AGS	PA-O3A-PB-O1B
3	F	901	AGS	PA-O3A-PB-O1B
3	E	902	AGS	PG-O3B-PB-O1B
3	F	901	AGS	O4'-C4'-C5'-O5'
3	A	901	AGS	PB-O3B-PG-O3G
3	D	902	AGS	O4'-C4'-C5'-O5'
3	F	902	AGS	PG-O3B-PB-O3A
3	E	901	AGS	O4'-C4'-C5'-O5'
3	B	902	AGS	PG-O3B-PB-O3A
3	F	902	AGS	PG-O3B-PB-O1B
3	F	902	AGS	PG-O3B-PB-O2B
3	E	902	AGS	C5'-O5'-PA-O3A
3	F	901	AGS	C5'-O5'-PA-O3A
3	F	902	AGS	C3'-C4'-C5'-O5'
3	C	901	AGS	PA-O3A-PB-O2B
3	D	902	AGS	C5'-O5'-PA-O1A
3	D	902	AGS	C5'-O5'-PA-O2A
3	B	902	AGS	C4'-C5'-O5'-PA

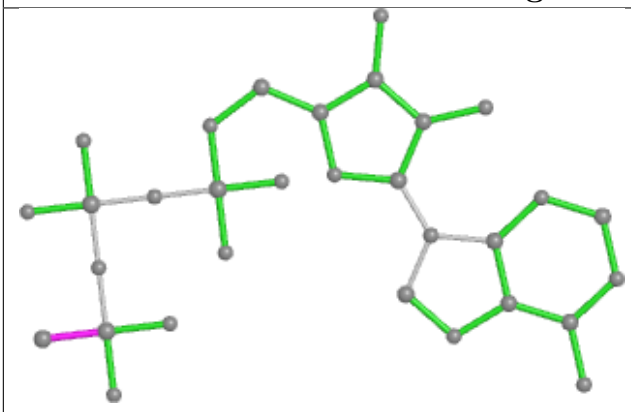
There are no ring outliers.

8 monomers are involved in 15 short contacts:

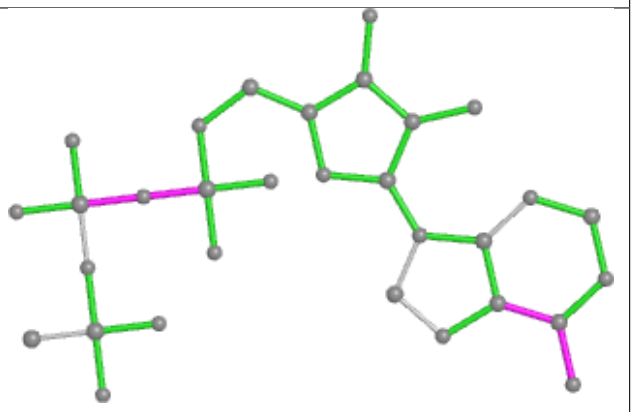
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	901	AGS	2	0
3	E	901	AGS	2	0
3	D	901	AGS	1	0
3	C	902	AGS	1	0
3	D	902	AGS	1	0
3	A	901	AGS	3	0
3	B	902	AGS	3	0
3	F	902	AGS	2	0

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

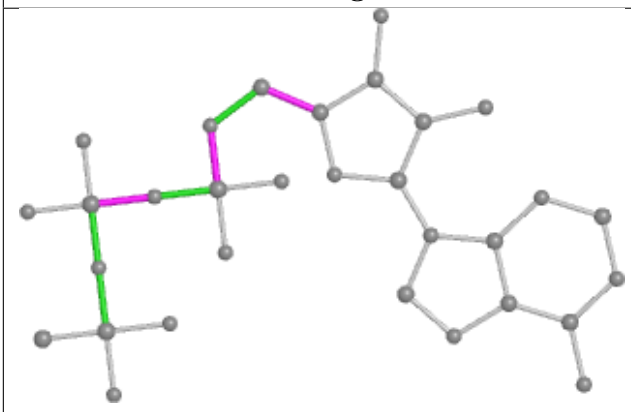
Ligand AGS F 901



Bond lengths



Bond angles



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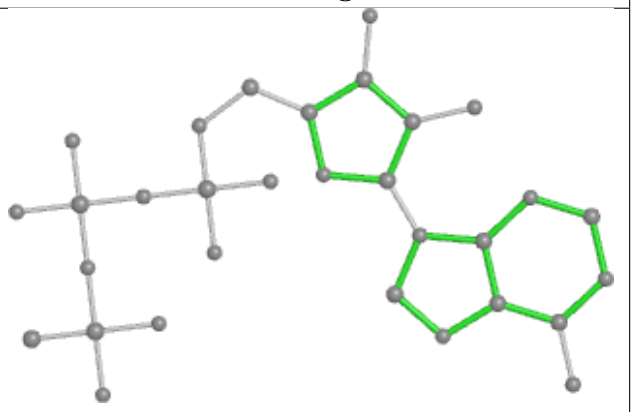
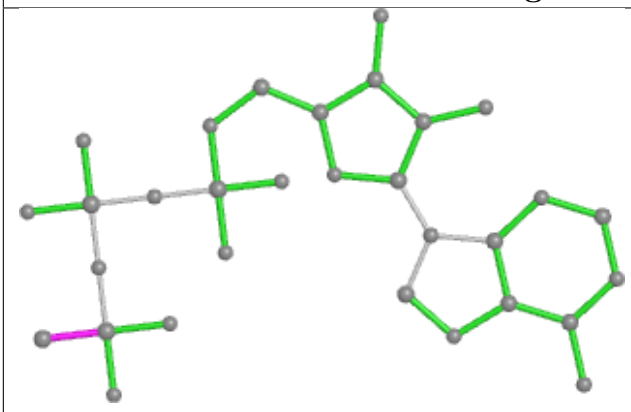
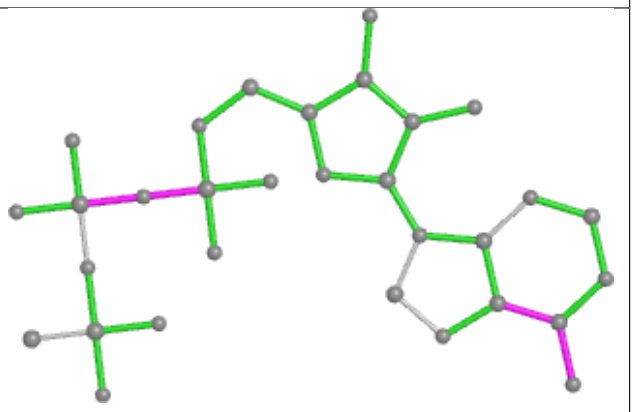


Rings

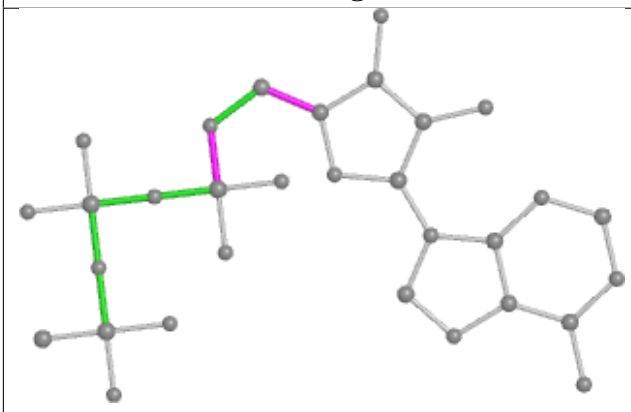
Ligand AGS B 901



Bond lengths



Bond angles



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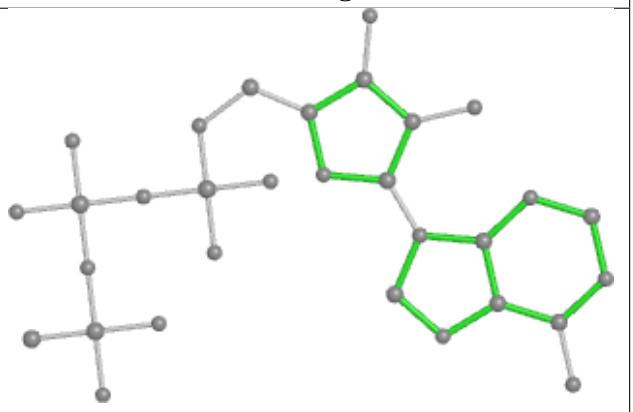
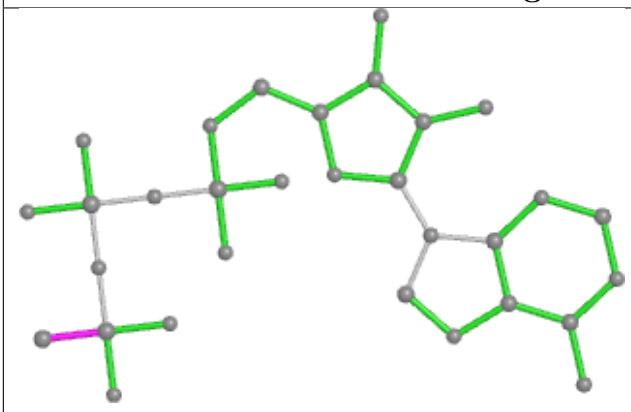


Rings

Ligand AGS A 902



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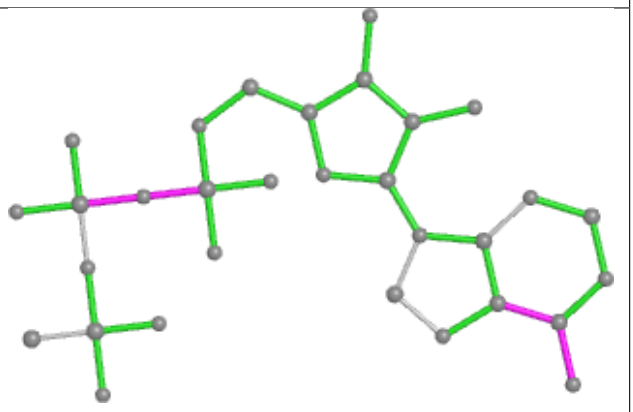

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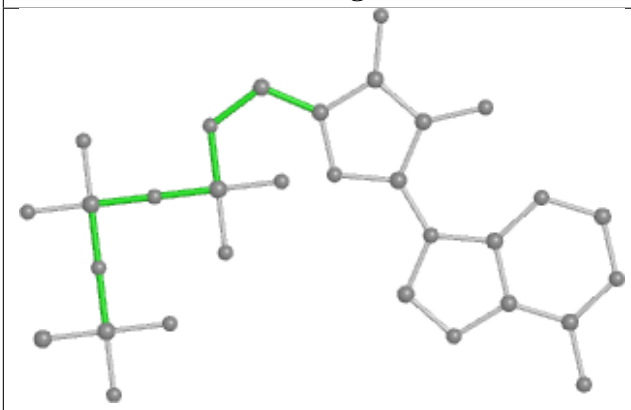

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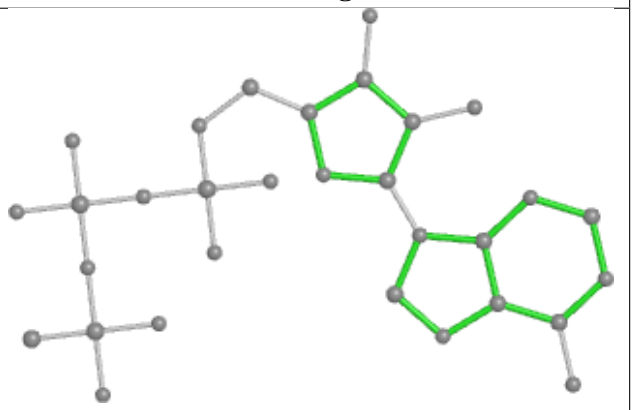
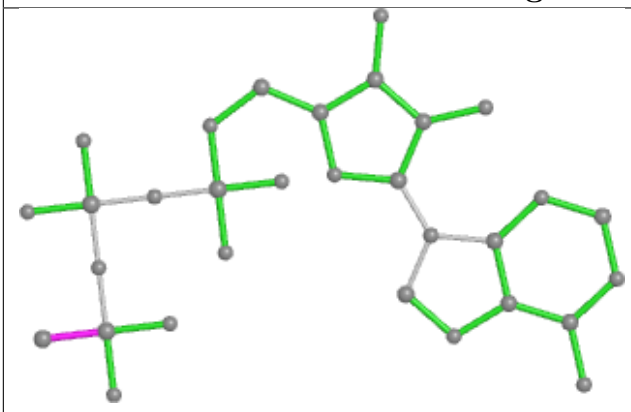


Rings

Ligand AGS E 901



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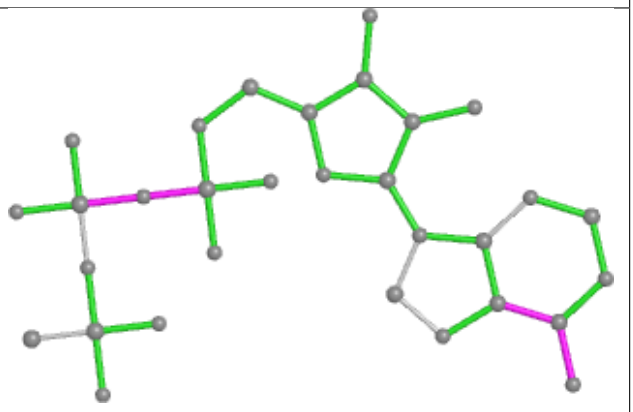
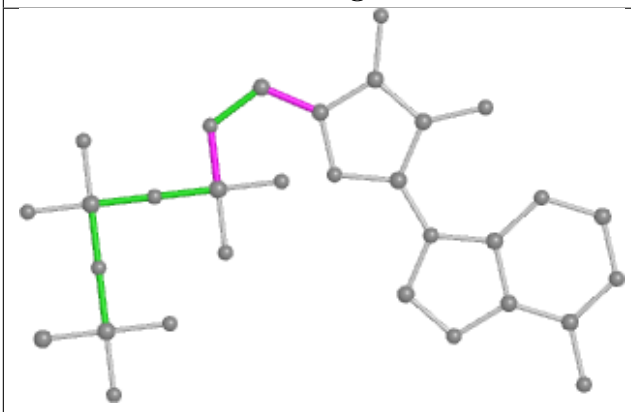


Bond angles



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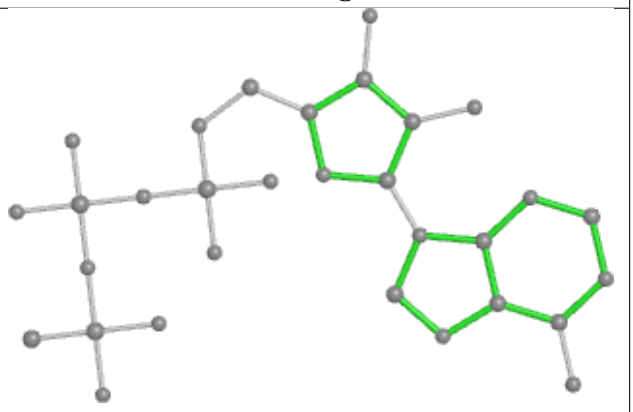
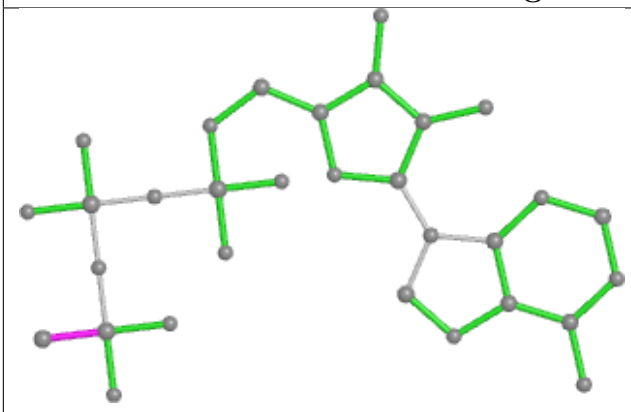


Rings

Ligand AGS C 901



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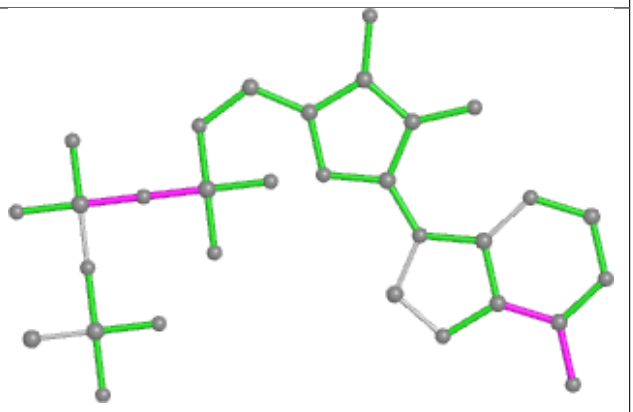

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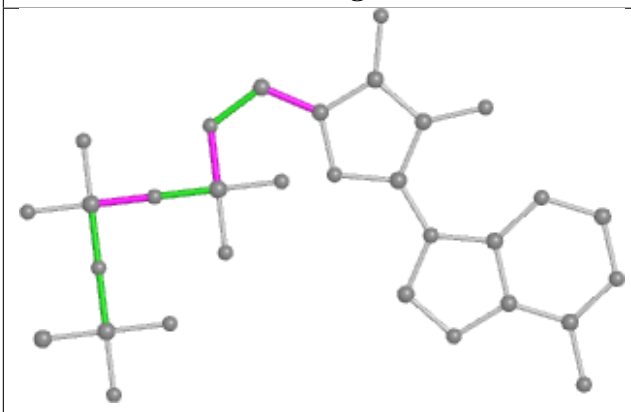

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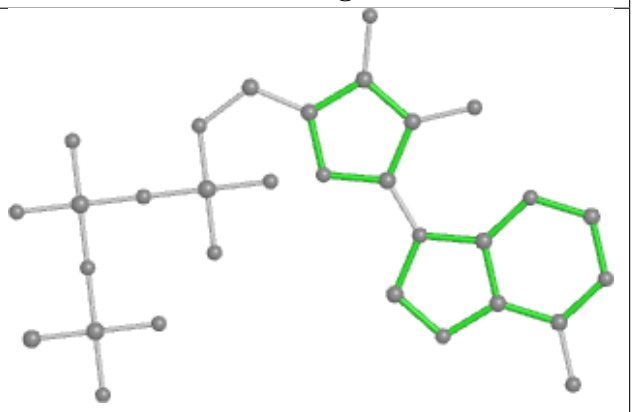
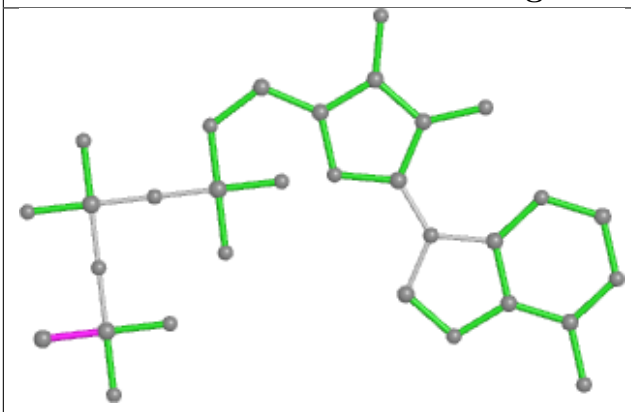


Rings

Ligand AGS E 902



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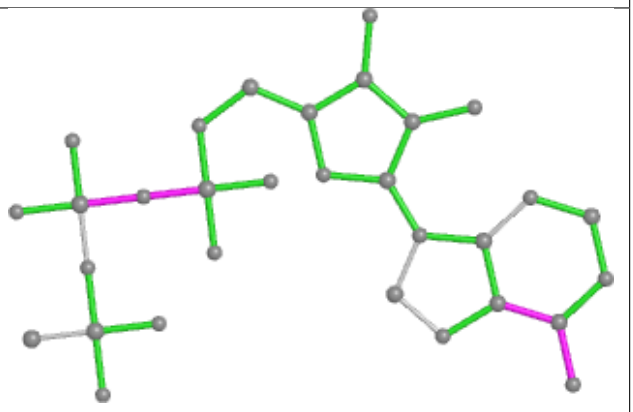
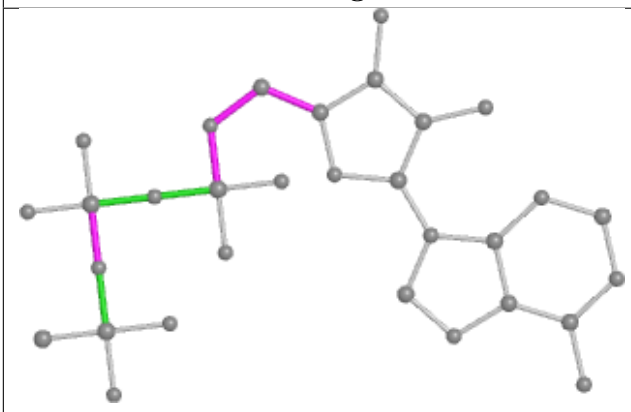


Bond angles



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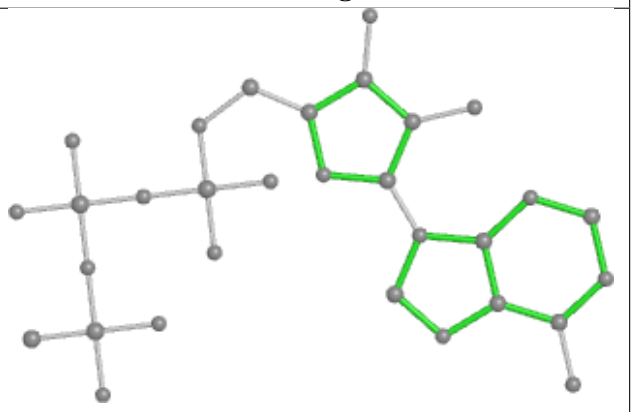
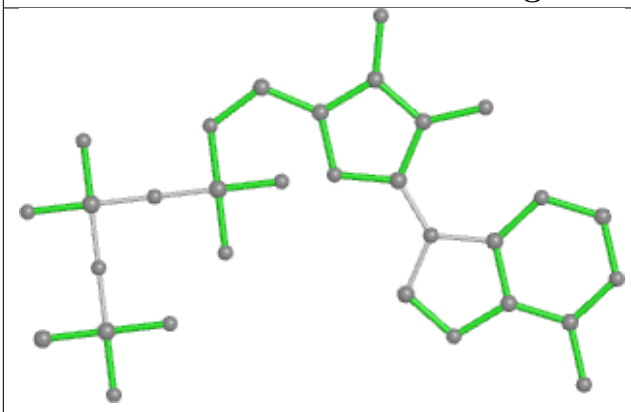


Rings

Ligand AGS D 901



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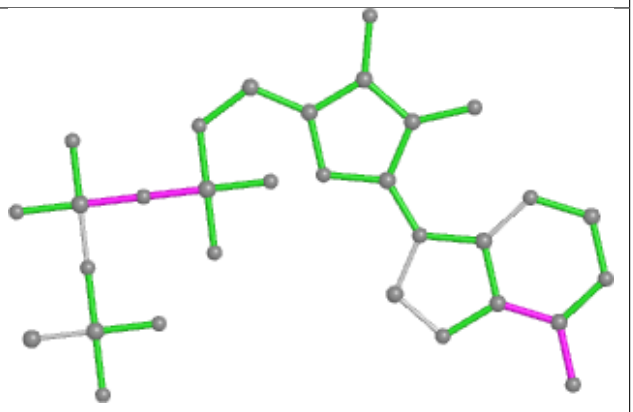

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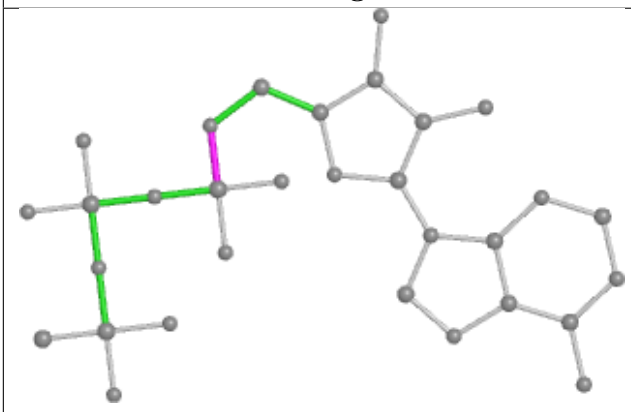

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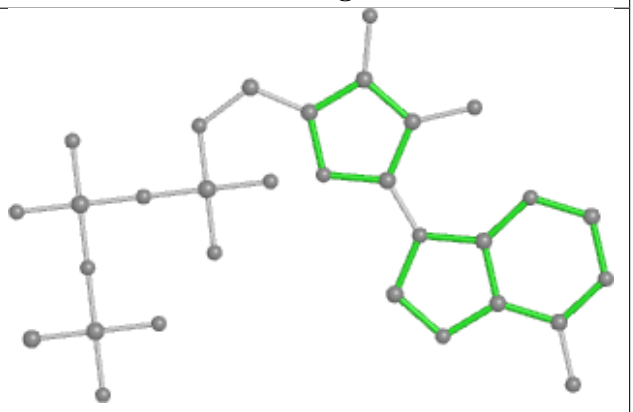
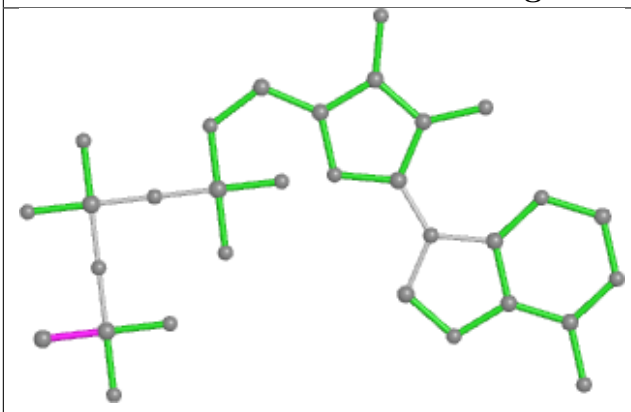


Rings

Ligand AGS C 902



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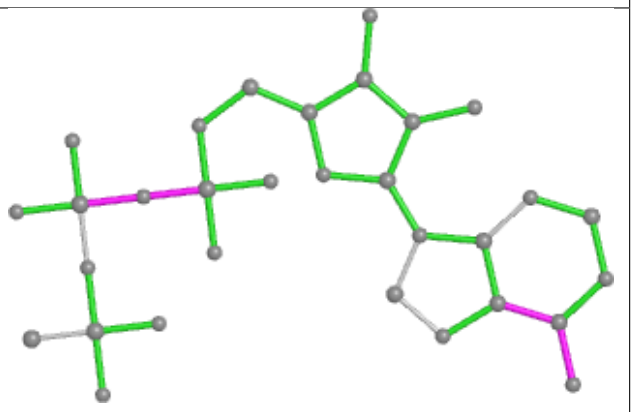
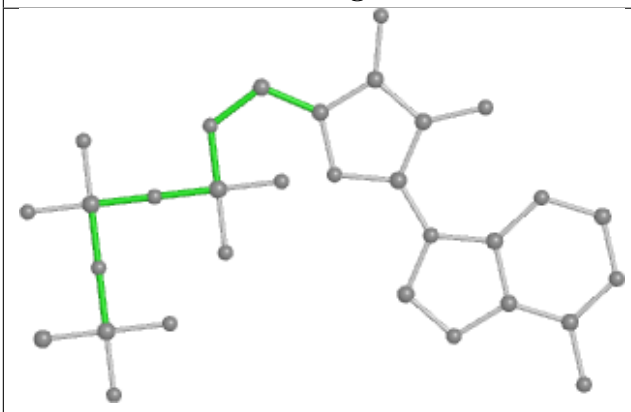


Bond angles



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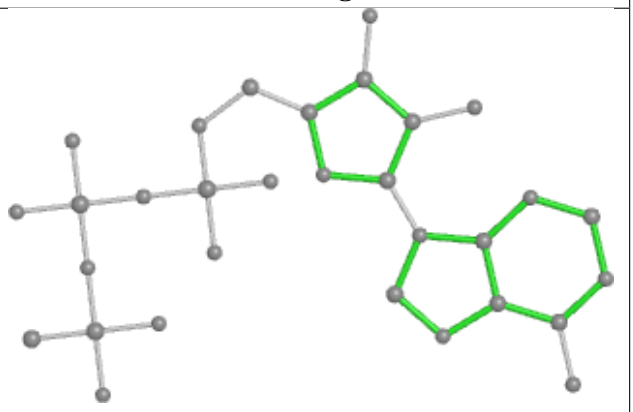
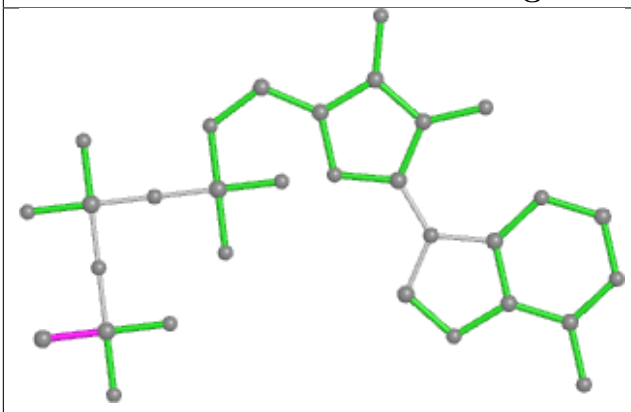
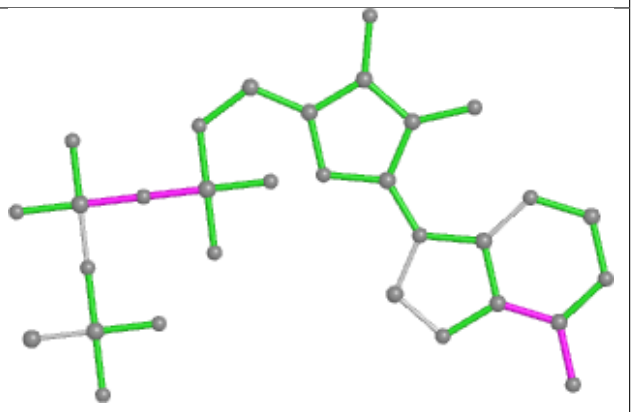


Rings

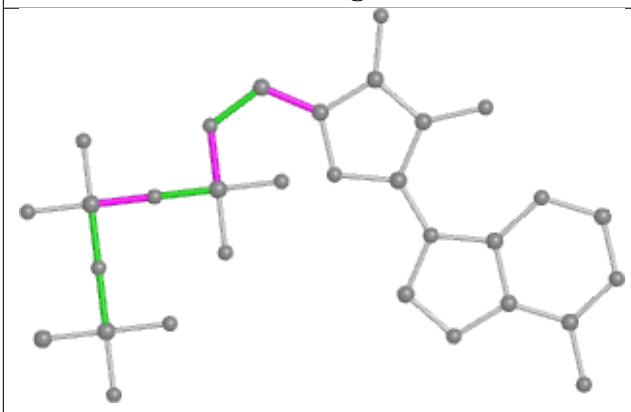
Ligand AGS D 902



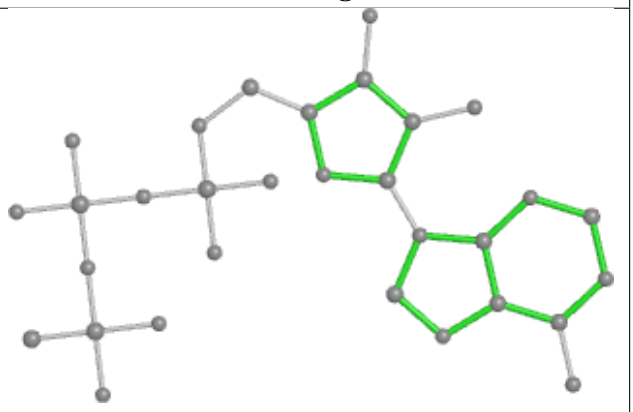
Bond lengths



Bond angles

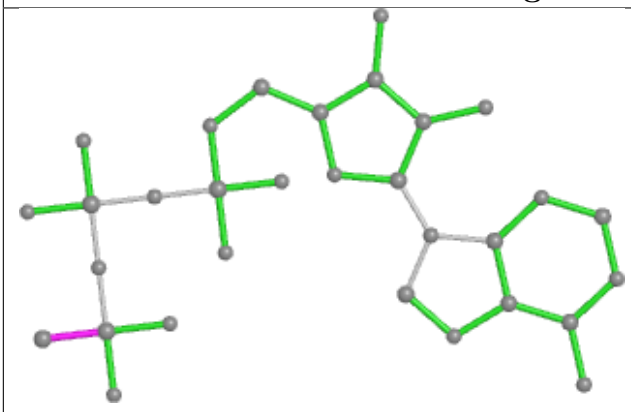


Torsions



Rings

Ligand AGS A 901



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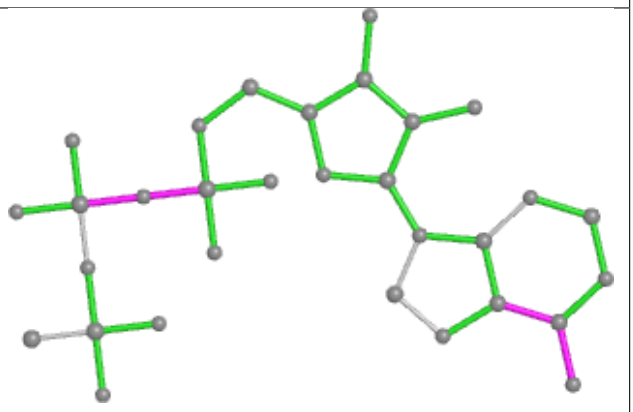

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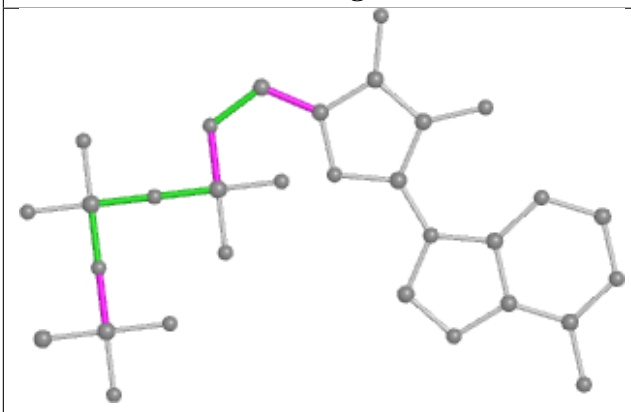

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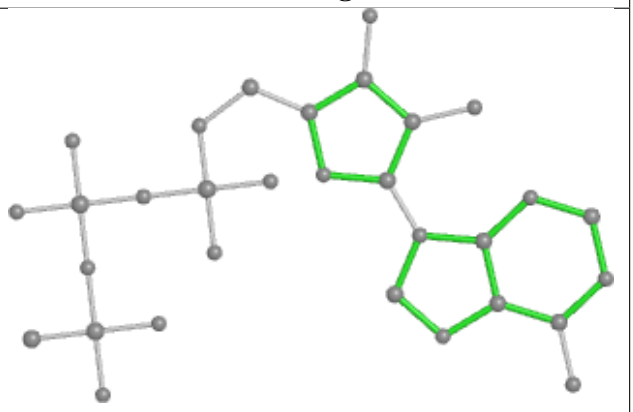
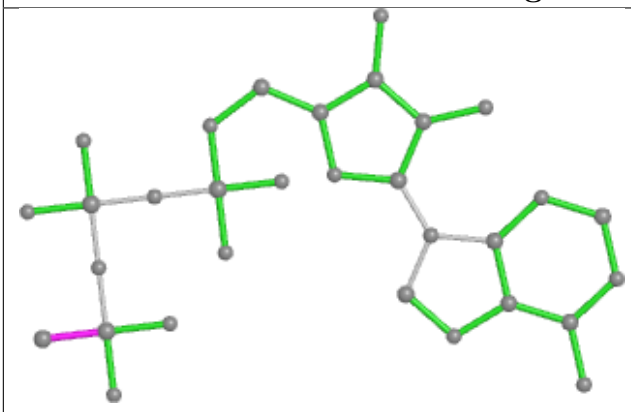
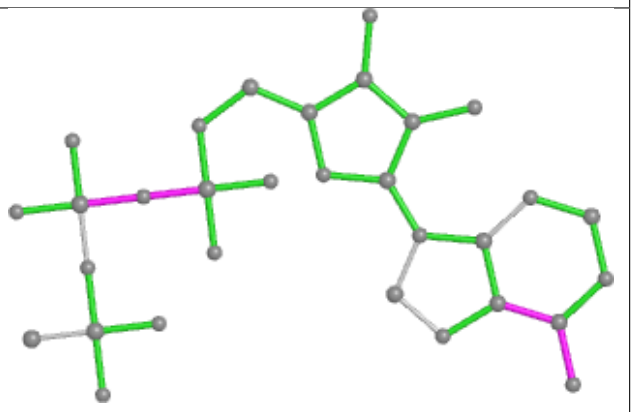


Rings

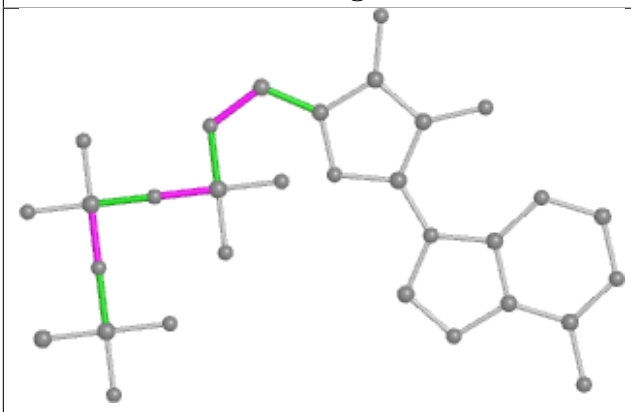
Ligand AGS B 902



Bond lengths



Bond angles



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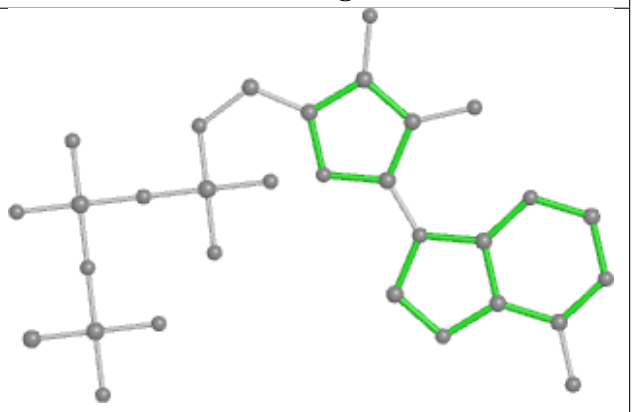
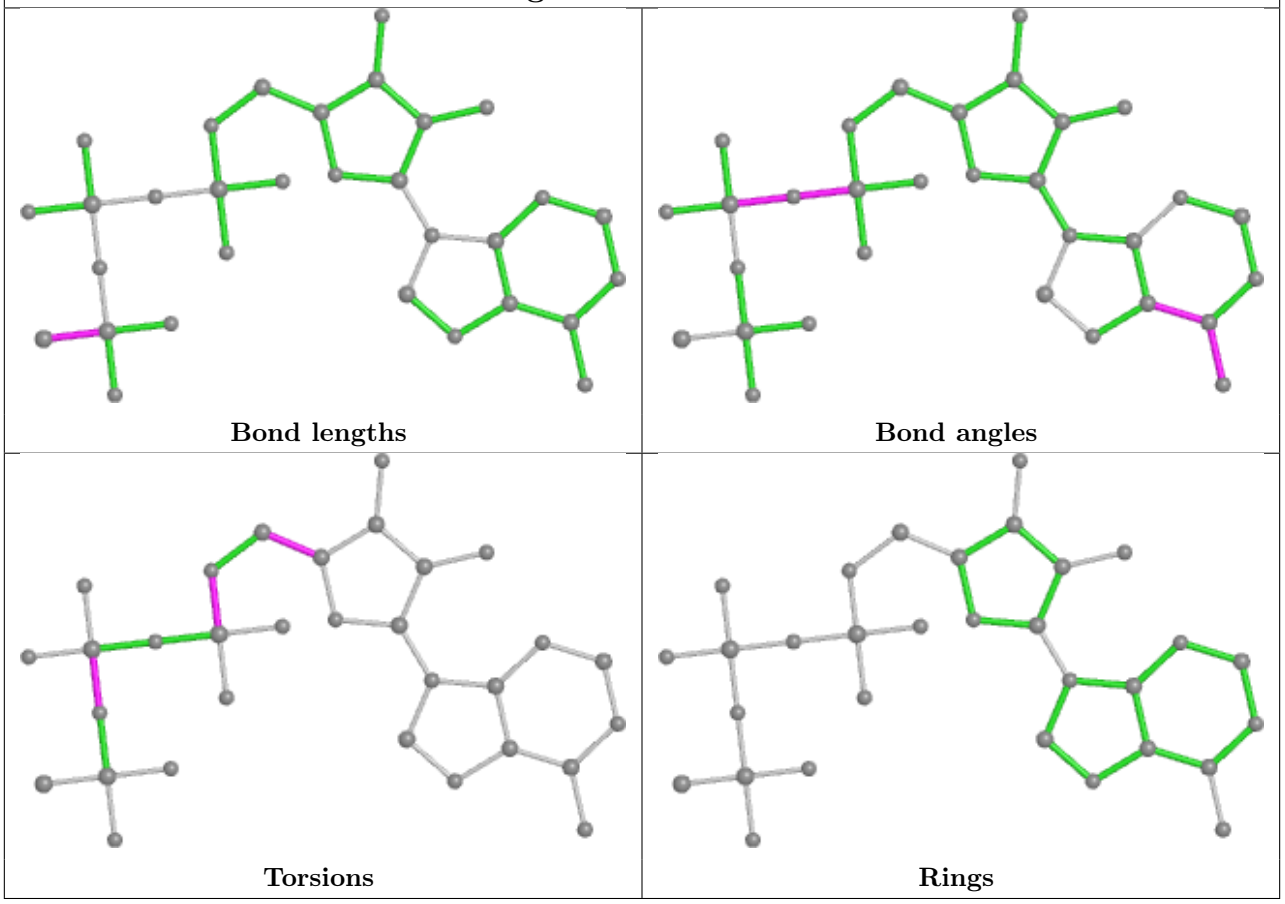


Rings

Ligand AGS F 902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	767:GLY	C	768:PHE	N	3.28

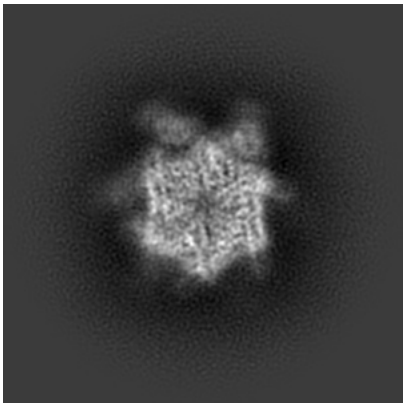
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24302. These allow visual inspection of the internal detail of the map and identification of artifacts.

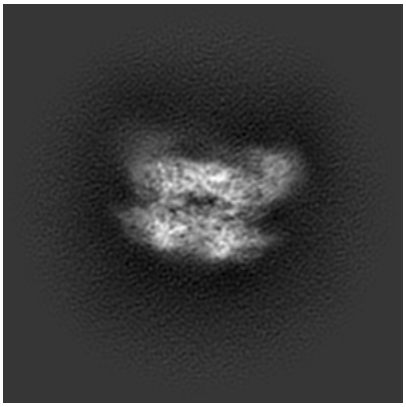
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

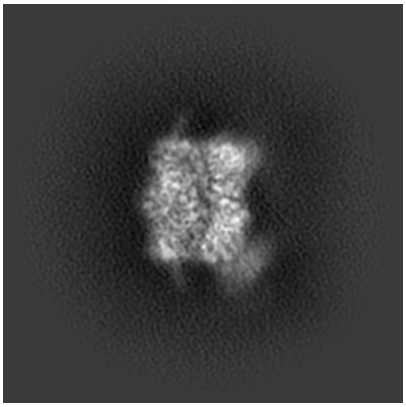
6.1.1 Primary map



X



Y

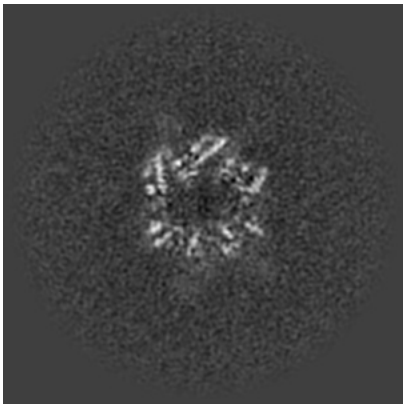


Z

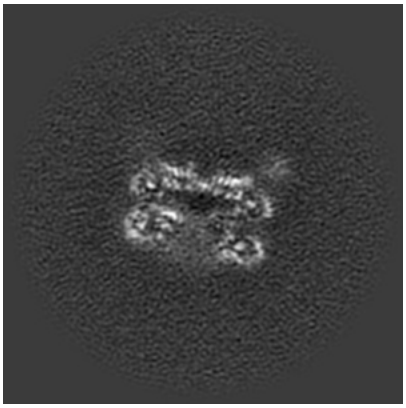
The images above show the map projected in three orthogonal directions.

6.2 Central slices

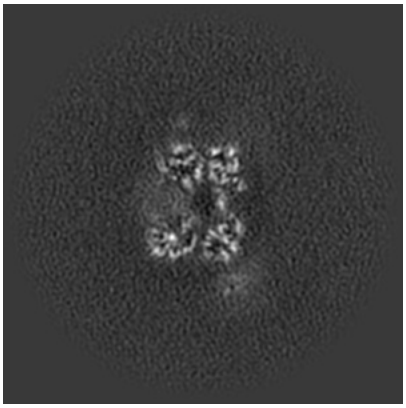
6.2.1 Primary map



X Index: 120



Y Index: 120

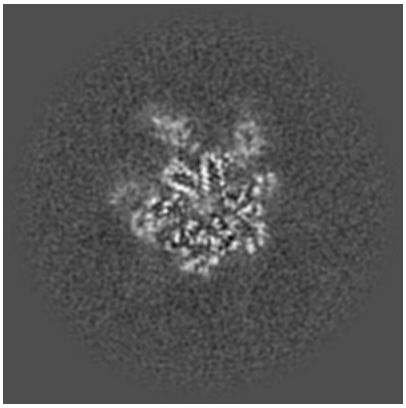


Z Index: 120

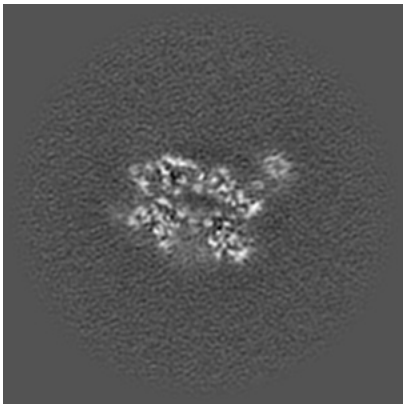
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

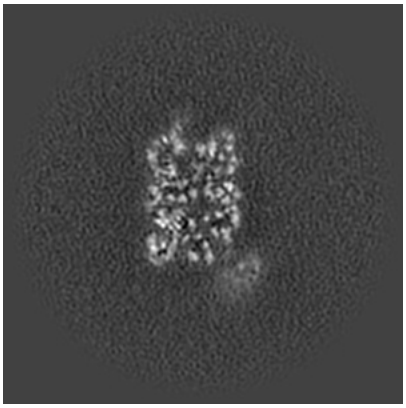
6.3.1 Primary map



X Index: 133



Y Index: 113



Z Index: 132

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.086. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

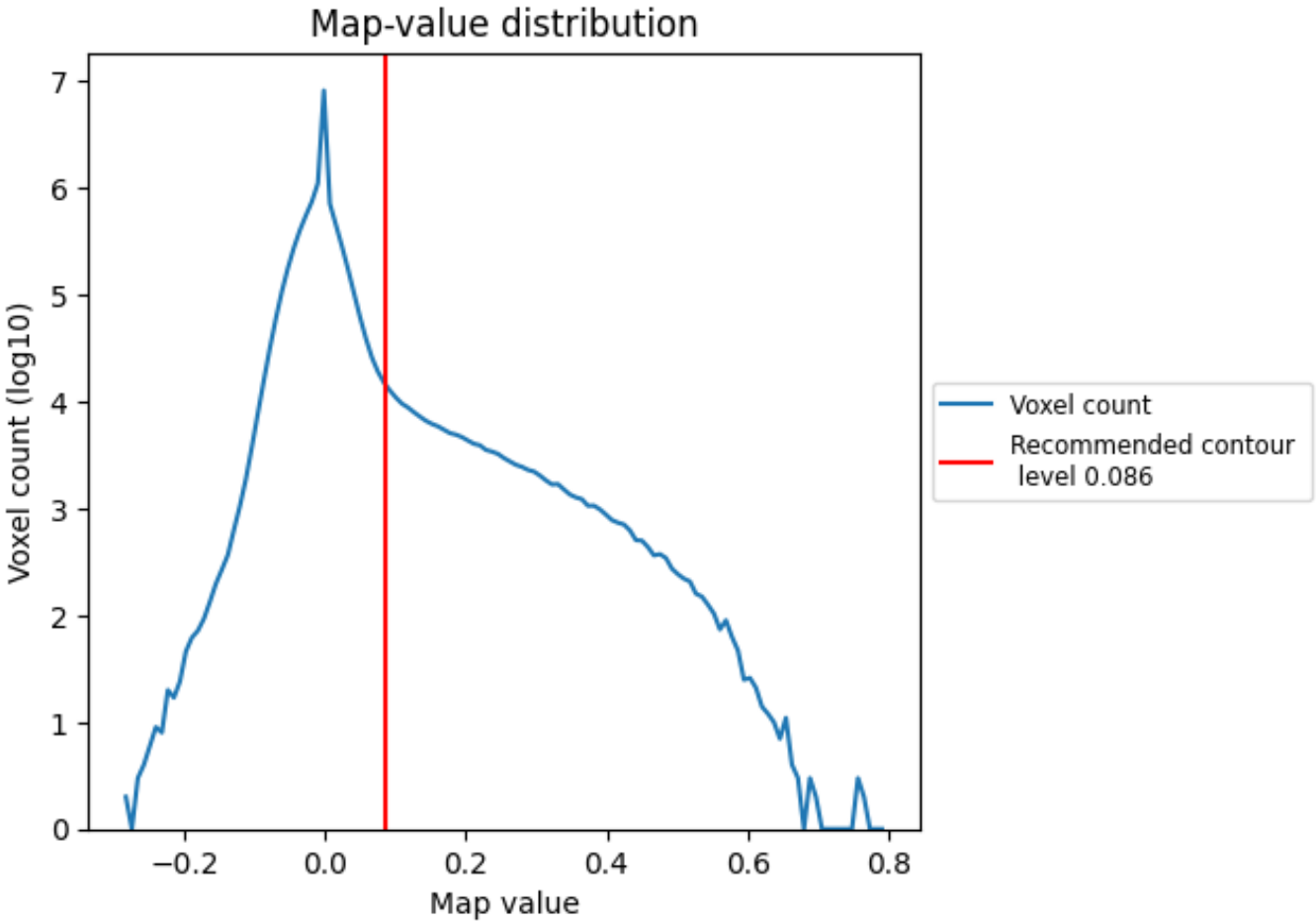
6.5 Mask visualisation (i)

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

7 Map analysis

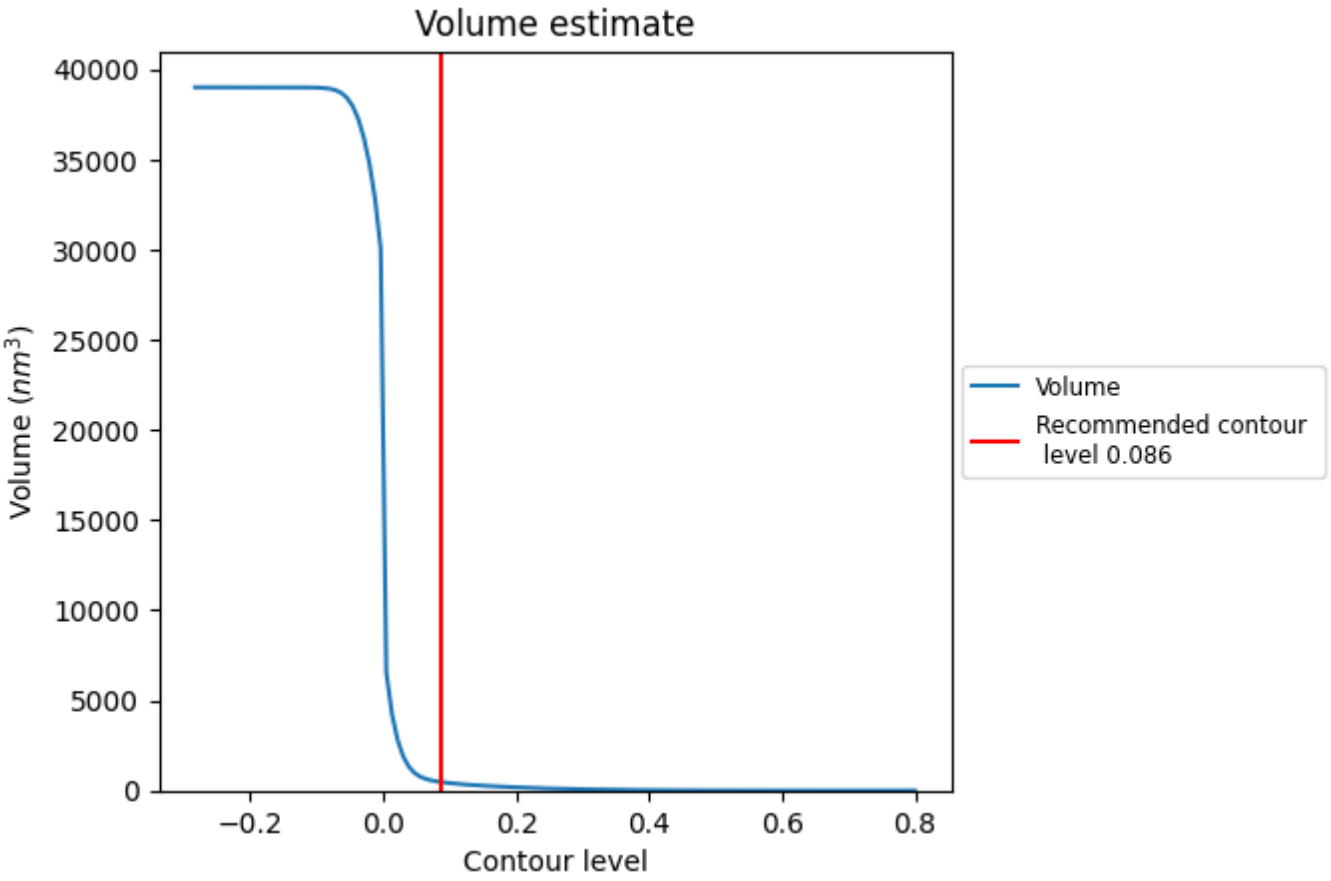
This section contains the results of statistical analysis of the map.

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.

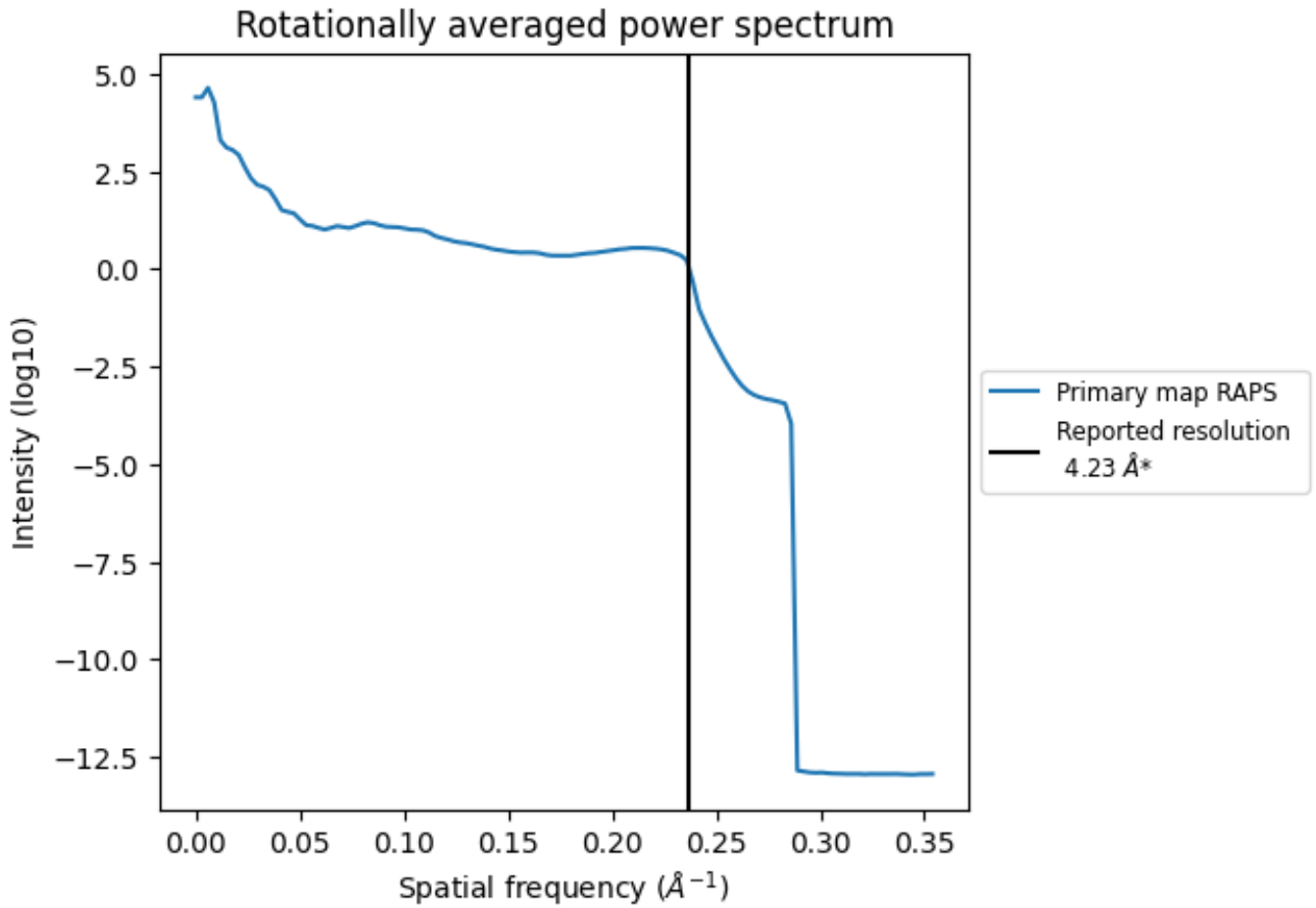
7.2 Volume estimate



The volume at the recommended contour level is 478 nm^3; this corresponds to an approximate mass of 432 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 0.236 $Å^{-1}$

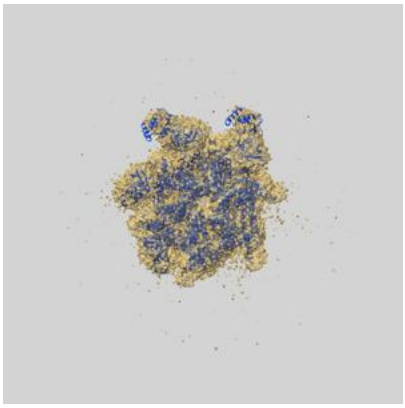
8 Fourier-Shell correlation

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

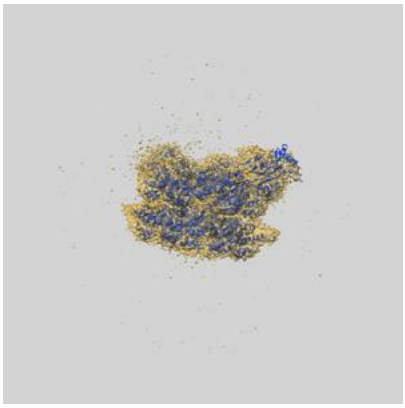
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24302 and PDB model 7R7S. Per-residue inclusion information can be found in section 3 on page 5.

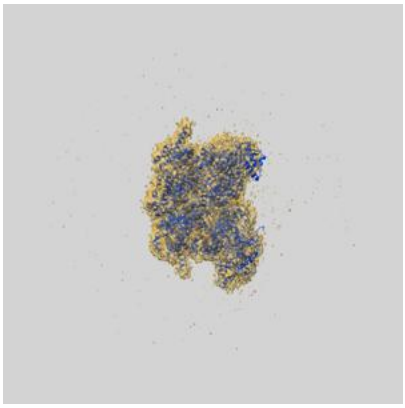
9.1 Map-model overlay



X



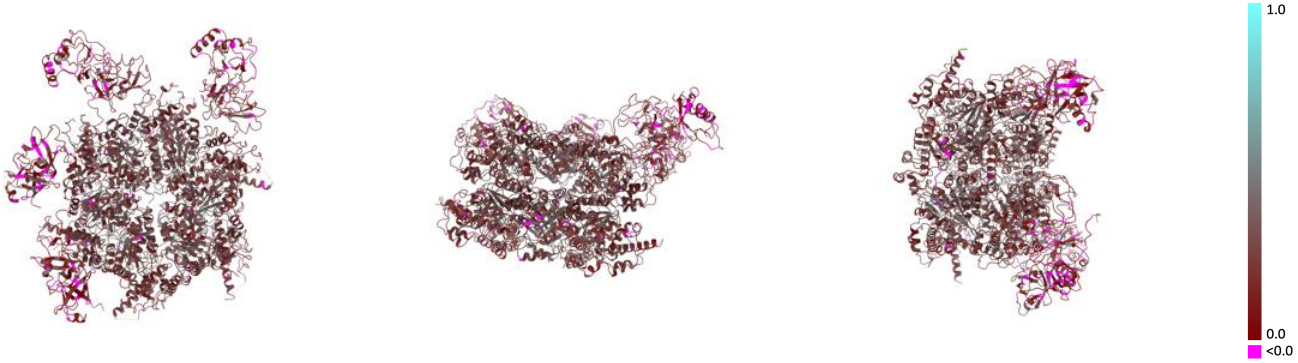
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.086 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.

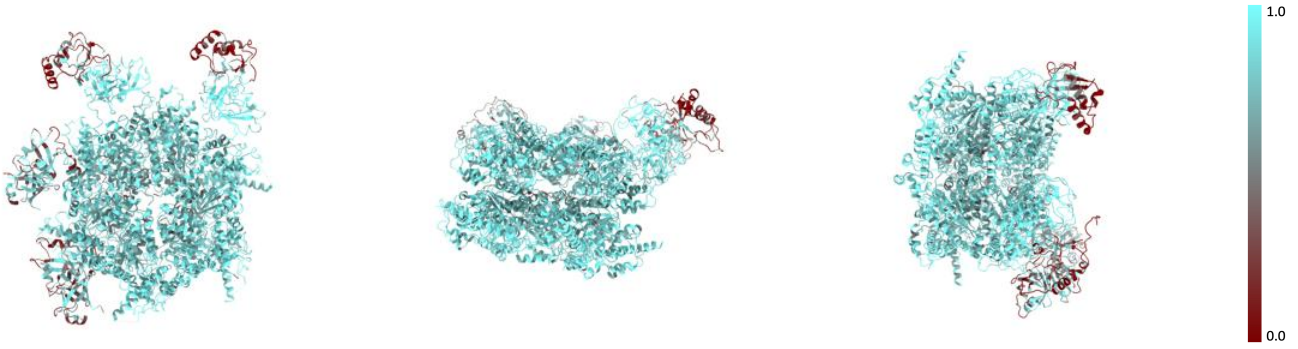
9.2 Q-score mapped to coordinate model (i)



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.

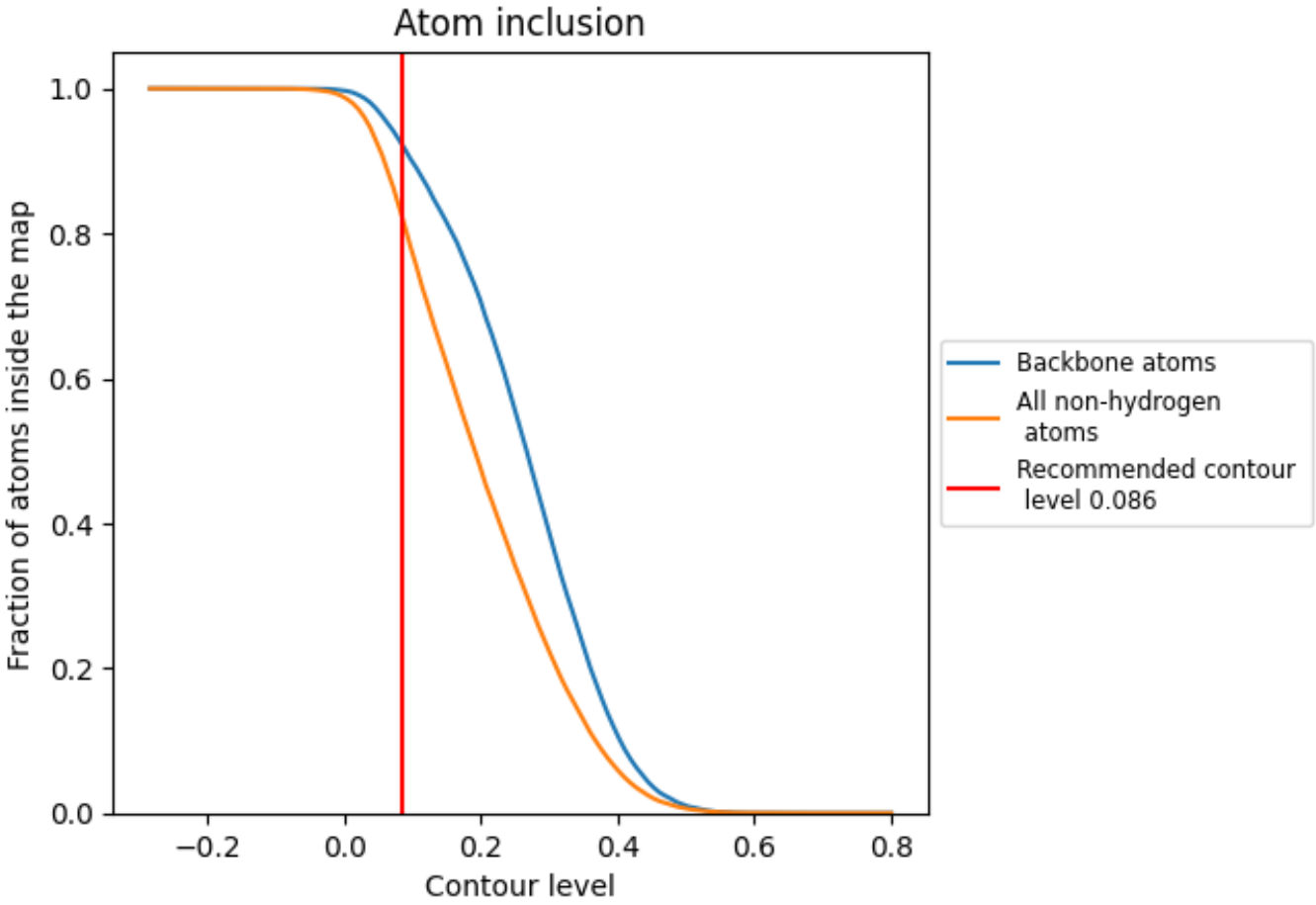
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.086).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.086) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8202	0.2620
A	0.8778	0.2670
B	0.8823	0.2950
C	0.8798	0.2790
D	0.7803	0.2490
E	0.7952	0.2580
F	0.8779	0.2730
I	0.3190	0.1530
J	0.2694	0.1070