Full wwPDB EM Validation Report ⓘ

Aug 12, 2024 – 08:35 AM EDT

PDB ID	:	8UA4
EMDB ID	:	EMD-42050
Title	:	Structure of eastern equine encephalitis virus VLP in complex with VLDLR LA1
Authors	:	Abraham, J.; Yang, P.; Li, W.; Fan, X.; Pan, J.
Deposited on	:	2023-09-20
Resolution	:	3.58 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:

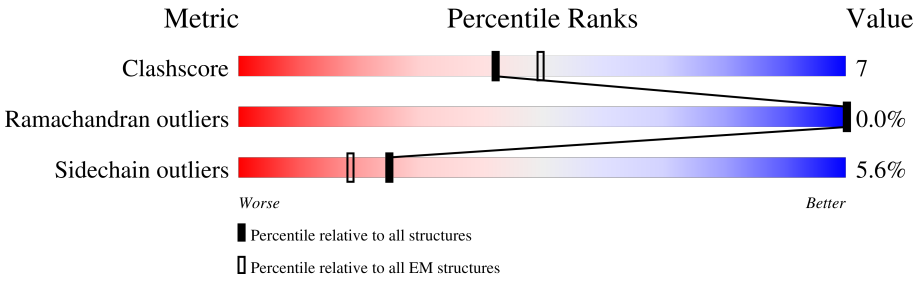
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.58 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	441	77% 22%
1	D	441	81% 18%
1	G	441	84% 15%
1	J	441	78% 22%
2	B	420	68% 25%
2	E	420	78% 19%
2	H	420	82% 14%
2	K	420	76% 21%

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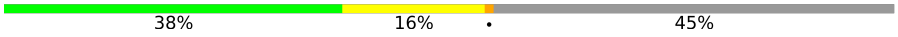
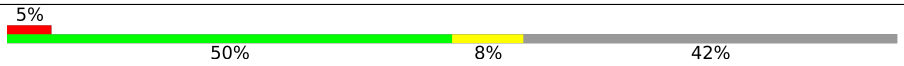
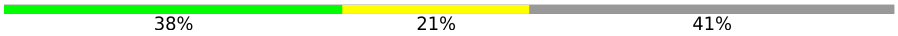
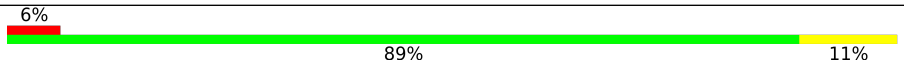
Mol	Chain	Length	Quality of chain
3	C	261	
3	F	261	
3	I	261	
3	L	261	
4	M	63	
4	N	63	
4	O	63	
4	P	63	
5	R	36	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 33292 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 Envelope glycoprotein E1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3371	2152	559	640	20		
1	D	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	G	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		
1	J	441	Total	C	N	O	S	0	0
			3375	2155	560	640	20		

- Molecule 2 is a protein called Envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	402	Total	C	N	O	S	0	0
			3165	2004	576	562	23		
2	E	418	Total	C	N	O	S	0	0
			3287	2081	597	585	24		
2	H	415	Total	C	N	O	S	0	0
			3258	2062	590	583	23		
2	K	419	Total	C	N	O	S	0	0
			3291	2082	597	588	24		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	144	Total	C	N	O	S	0	0
			1110	701	195	210	4		
3	F	155	Total	C	N	O	S	0	0
			1196	754	212	226	4		
3	I	152	Total	C	N	O	S	0	0
			1171	738	207	222	4		
3	L	154	Total	C	N	O	S	0	0
			1187	748	210	225	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	67	ASN	LYS	engineered mutation	UNP Q88678
F	67	ASN	LYS	engineered mutation	UNP Q88678
I	120	ASN	LYS	engineered mutation	UNP Q88678
L	67	ASN	LYS	engineered mutation	UNP Q88678

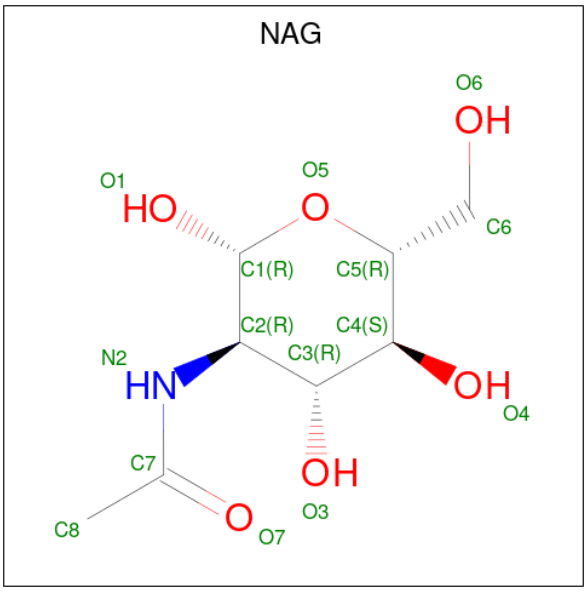
- Molecule 4 is a protein called Envelope glycoprotein E3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	54	Total	C	N	O	S	0	0
			422	262	68	83	9		
4	N	54	Total	C	N	O	S	0	0
			422	262	68	83	9		
4	O	54	Total	C	N	O	S	0	0
			422	262	68	83	9		
4	P	54	Total	C	N	O	S	0	0
			422	262	68	83	9		

- Molecule 5 is a protein called Very low-density lipoprotein receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	36	Total	C	N	O	S	0	0
			274	162	46	60	6		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	
6	E	1	Total	C	N	O	0
			14	8	1	5	
6	G	1	Total	C	N	O	0
			14	8	1	5	
6	H	1	Total	C	N	O	0
			14	8	1	5	
6	J	1	Total	C	N	O	0
			14	8	1	5	
6	K	1	Total	C	N	O	0
			14	8	1	5	
6	M	1	Total	C	N	O	0
			14	8	1	5	
6	N	1	Total	C	N	O	0
			14	8	1	5	
6	O	1	Total	C	N	O	0
			14	8	1	5	
6	P	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

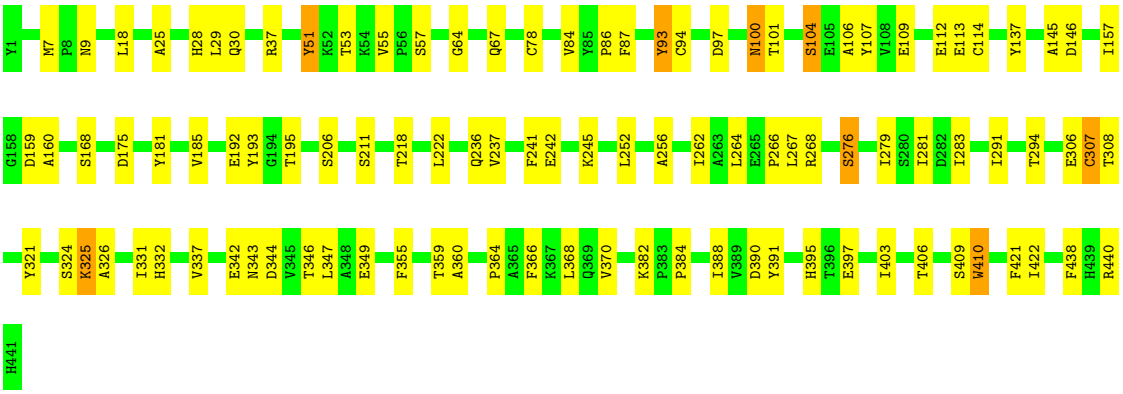
Mol	Chain	Residues	Atoms		AltConf
7	R	1	Total	Ca	0
			1	1	

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.

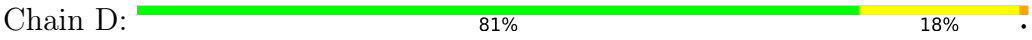
• Molecule 1: Envelope glycoprotein E1

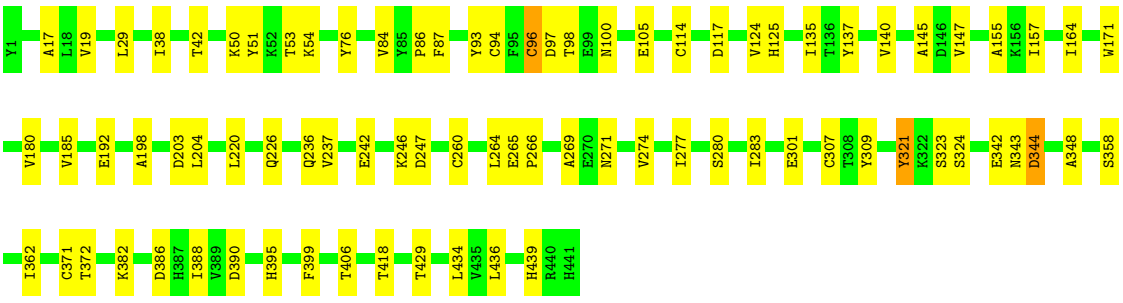
Chain A:



• Molecule 1: Envelope glycoprotein E1

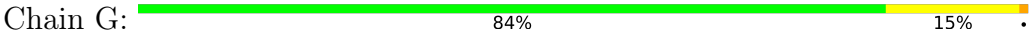
Chain D:

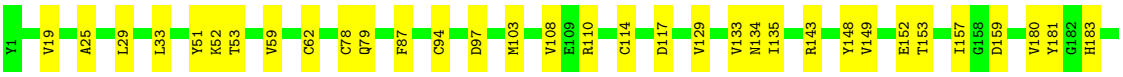


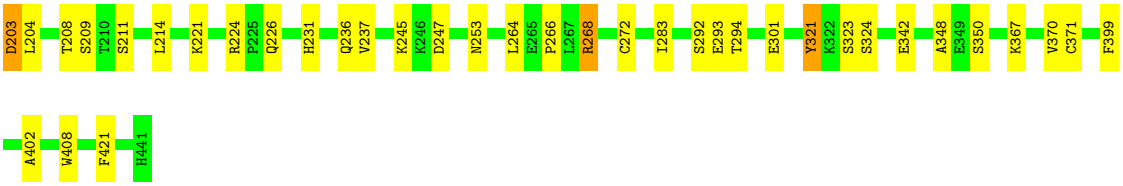


• Molecule 1: Envelope glycoprotein E1

Chain G:

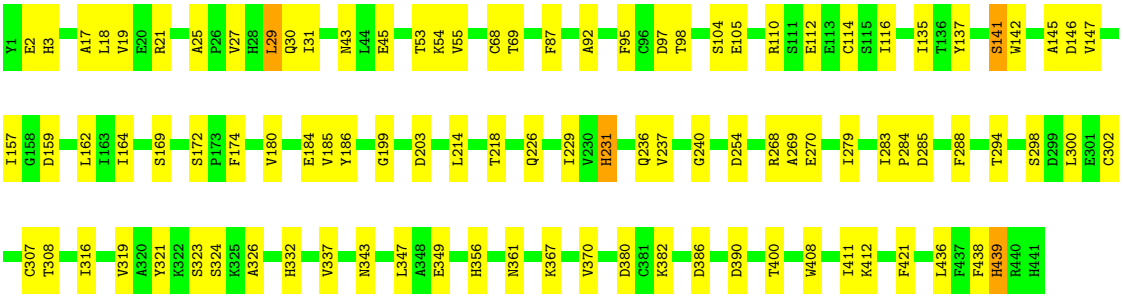






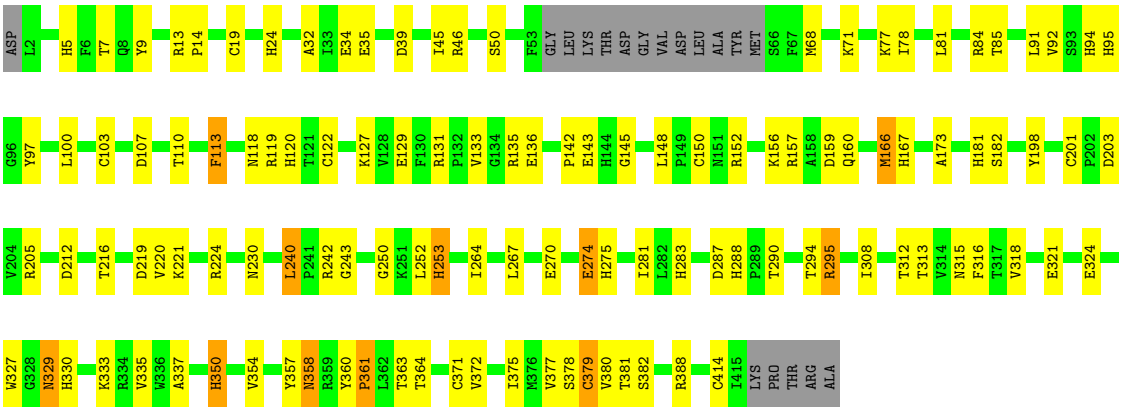
• Molecule 1: Envelope glycoprotein E1

Chain J:



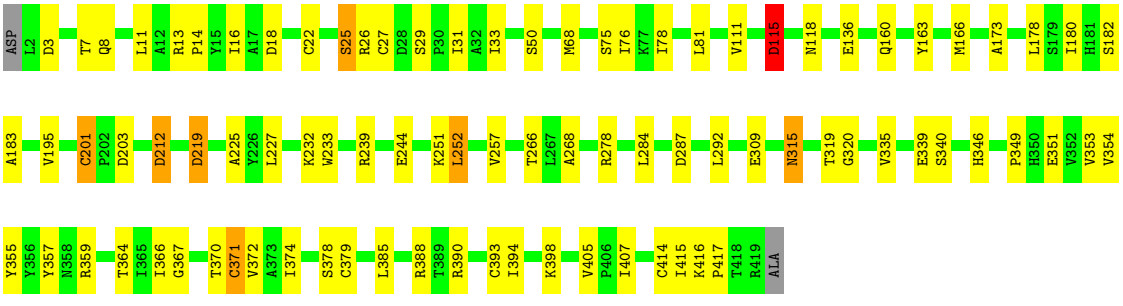
• Molecule 2: Envelope glycoprotein E2

Chain B:



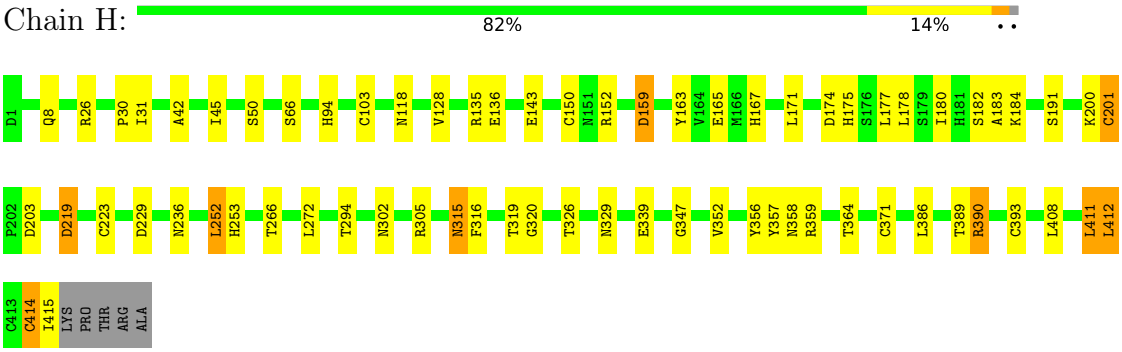
• Molecule 2: Envelope glycoprotein E2

Chain E:



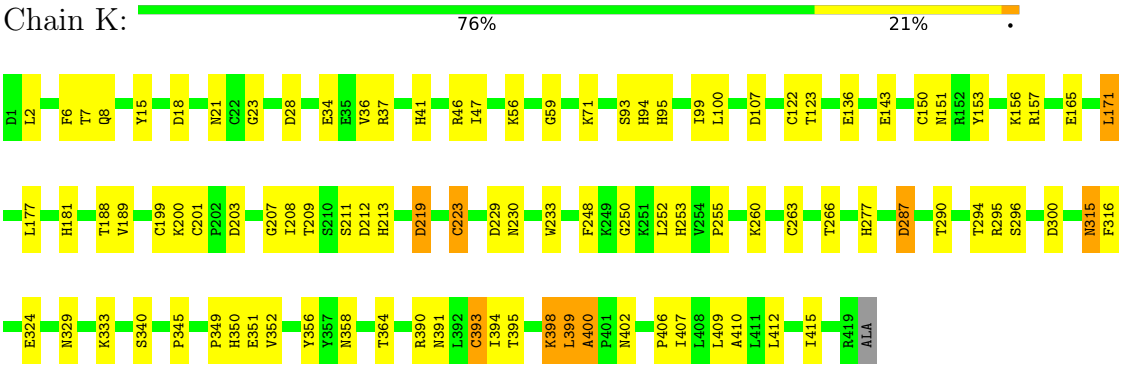
• Molecule 2: Envelope glycoprotein E2

Chain H:



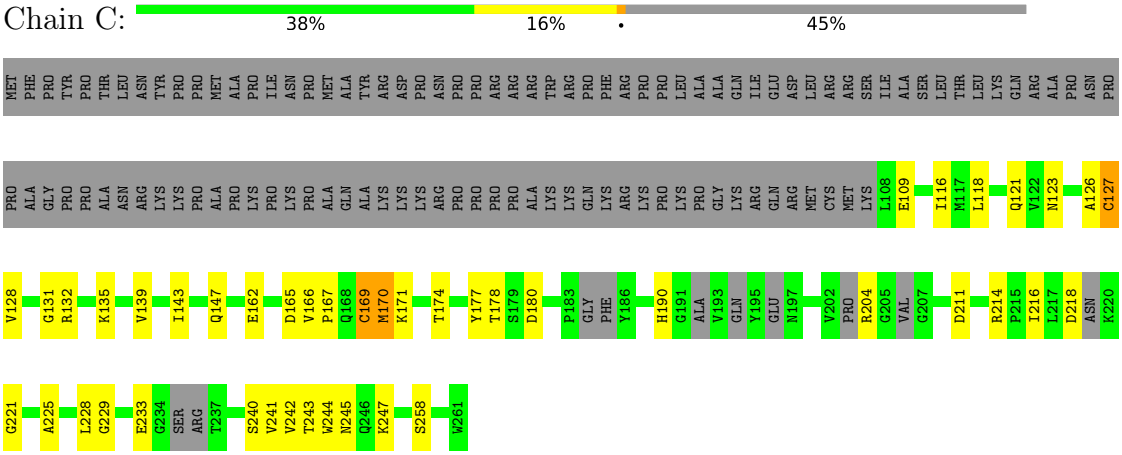
• Molecule 2: Envelope glycoprotein E2

Chain K:



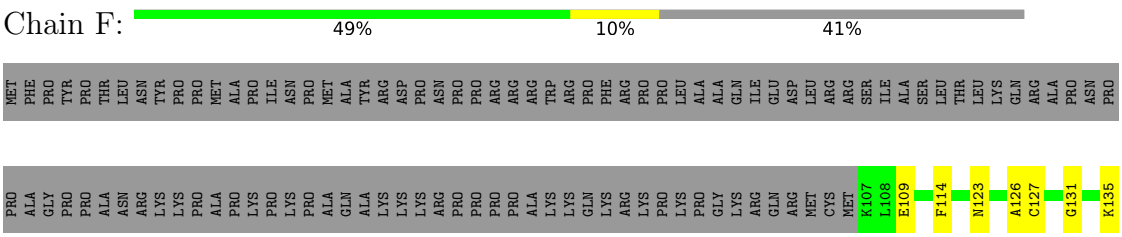
• Molecule 3: Capsid protein

Chain C:

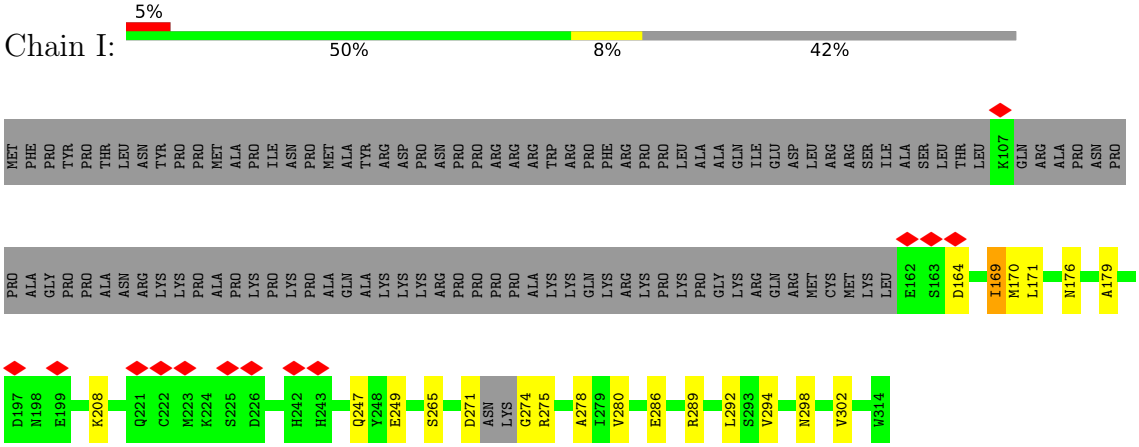


• Molecule 3: Capsid protein

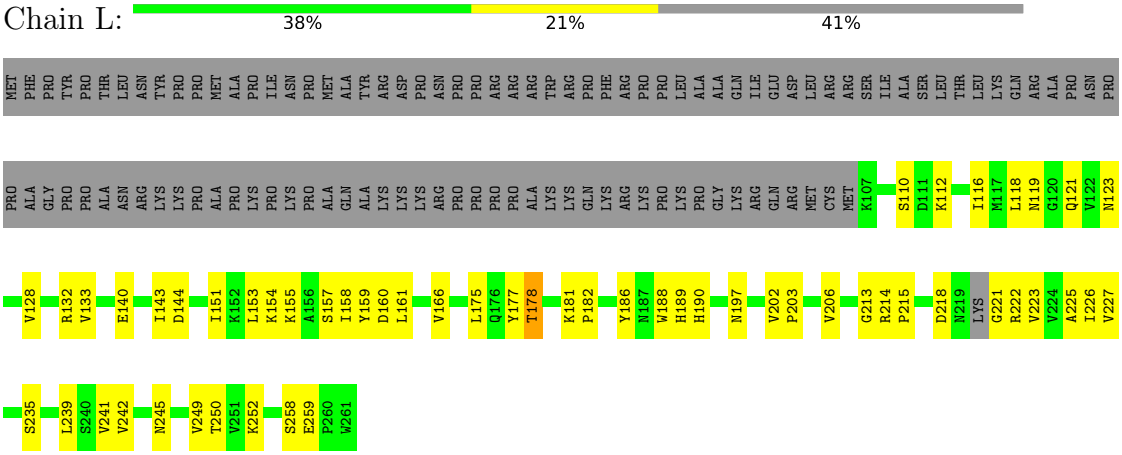
Chain F:



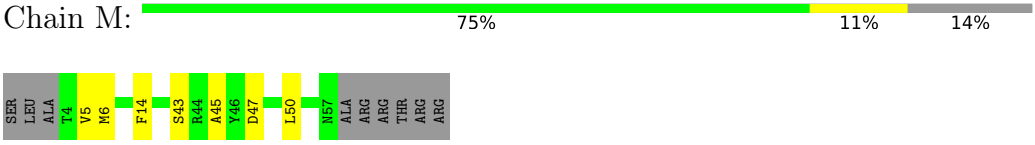
• Molecule 3: Capsid protein



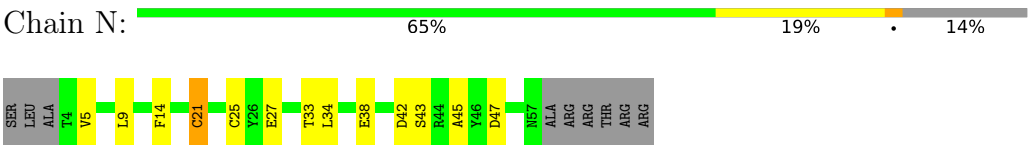
• Molecule 3: Capsid protein



• Molecule 4: Envelope glycoprotein E3

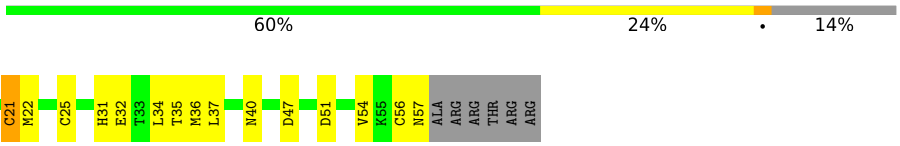


• Molecule 4: Envelope glycoprotein E3



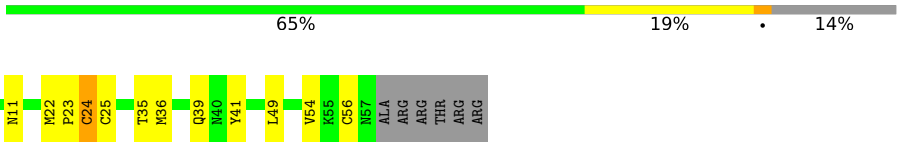
• Molecule 4: Envelope glycoprotein E3

Chain O:



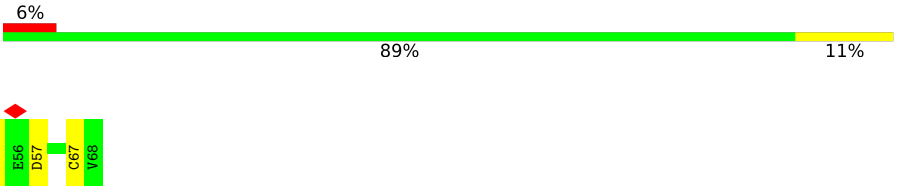
• Molecule 4: Envelope glycoprotein E3

Chain P:



• Molecule 5: Very low-density lipoprotein receptor

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	185420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.075	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.60	0/3465	0.73	1/4730 (0.0%)
1	D	0.73	1/3469 (0.0%)	0.72	4/4734 (0.1%)
1	G	0.74	2/3469 (0.1%)	0.75	4/4734 (0.1%)
1	J	0.69	0/3469	0.71	0/4734
2	B	0.60	0/3257	0.82	3/4442 (0.1%)
2	E	0.67	0/3382	0.76	4/4612 (0.1%)
2	H	0.67	2/3352 (0.1%)	0.78	3/4573 (0.1%)
2	K	0.67	1/3386 (0.0%)	0.80	5/4619 (0.1%)
3	C	0.59	1/1127 (0.1%)	0.82	1/1515 (0.1%)
3	F	0.60	0/1223	0.79	2/1657 (0.1%)
3	I	0.42	0/1196	0.72	0/1618
3	L	0.58	0/1213	0.82	1/1643 (0.1%)
4	M	0.47	0/431	0.66	0/588
4	N	0.50	0/431	0.89	1/588 (0.2%)
4	O	0.68	1/431 (0.2%)	1.02	2/588 (0.3%)
4	P	0.56	1/431 (0.2%)	0.81	1/588 (0.2%)
5	R	0.27	0/277	0.50	0/373
All	All	0.65	9/34009 (0.0%)	0.77	32/46336 (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	A	0	4
2	B	0	4
2	E	0	2
2	H	0	5
2	K	0	4
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1
3	I	0	1
3	L	0	1
4	N	0	1
4	P	0	2
All	All	0	26

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	94	CYS	CB-SG	-9.31	1.66	1.82
4	O	21	CYS	CB-SG	9.19	1.97	1.82
3	C	258	SER	C-N	-5.86	1.20	1.34
1	D	94	CYS	CB-SG	-5.44	1.73	1.81
2	H	393	CYS	CB-SG	5.44	1.91	1.82
4	P	25	CYS	CB-SG	-5.32	1.73	1.81
1	G	152	GLU	CB-CG	5.18	1.61	1.52
2	K	223	CYS	CB-SG	-5.12	1.73	1.81
2	H	150	CYS	CB-SG	-5.08	1.73	1.81

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	21	CYS	CA-CB-SG	13.38	138.09	114.00
4	N	21	CYS	CA-CB-SG	10.69	133.25	114.00
3	L	215	PRO	CA-N-CD	-9.42	98.31	111.50
2	K	107	ASP	CB-CG-OD1	-9.29	109.94	118.30
1	G	117	ASP	CB-CG-OD2	8.89	126.30	118.30
3	F	167	PRO	CA-N-CD	-8.54	99.54	111.50
1	G	62	CYS	CA-CB-SG	-8.49	98.72	114.00
2	H	229	ASP	CB-CG-OD1	8.41	125.87	118.30
2	H	219	ASP	CB-CG-OD1	8.10	125.59	118.30
2	B	361	PRO	CA-N-CD	-7.91	100.42	111.50
2	K	107	ASP	CB-CG-OD2	7.88	125.39	118.30
1	G	159	ASP	CB-CG-OD1	7.87	125.38	118.30
1	G	203	ASP	CB-CG-OD2	7.85	125.37	118.30
2	E	115	ASP	CB-CG-OD1	7.61	125.15	118.30
2	E	417	PRO	CA-N-CD	-7.56	100.92	111.50
1	D	117	ASP	CB-CG-OD1	7.39	124.95	118.30
2	E	219	ASP	CB-CG-OD1	7.29	124.86	118.30
2	B	35	GLU	CA-CB-CG	6.87	128.52	113.40
2	K	219	ASP	CB-CG-OD2	6.63	124.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	255	PRO	CA-N-CD	-6.61	102.24	111.50
4	P	24	CYS	CA-CB-SG	6.09	124.97	114.00
2	B	252	LEU	CA-CB-CG	5.77	128.57	115.30
4	O	22	MET	CA-CB-CG	5.72	123.03	113.30
1	A	18	LEU	CA-CB-CG	5.57	128.11	115.30
3	C	169	CYS	CA-CB-SG	5.50	123.91	114.00
2	K	399	LEU	CA-CB-CG	5.32	127.55	115.30
1	D	260	CYS	CA-CB-SG	5.25	123.45	114.00
1	D	96	CYS	CA-CB-SG	5.21	123.38	114.00
2	K	345	PRO	CA-N-CD	-5.20	104.22	111.50
2	H	412	LEU	CA-CB-CG	5.11	127.05	115.30
1	D	344	ASP	CB-CG-OD1	5.08	122.87	118.30
2	E	393	CYS	CA-CB-SG	5.03	123.05	114.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	THR	Peptide
1	A	349	GLU	Peptide
1	A	384	PRO	Peptide
1	A	93	TYR	Peptide
2	B	181	HIS	Peptide
2	B	182	SER	Peptide
2	B	243	GLY	Peptide
2	B	77	LYS	Peptide
3	C	233	GLU	Peptide
2	E	201	CYS	Peptide
2	E	244	GLU	Peptide
3	F	167	PRO	Peptide
2	H	159	ASP	Peptide
2	H	200	LYS	Peptide
2	H	201	CYS	Peptide
2	H	390	ARG	Sidechain
2	H	411	LEU	Peptide
3	I	169	ILE	Peptide
2	K	181	HIS	Peptide
2	K	200	LYS	Peptide
2	K	250	GLY	Peptide
2	K	400	ALA	Peptide
3	L	235	SER	Peptide
4	N	9	LEU	Peptide

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Mol	Chain	Res	Type	Group
4	P	22	MET	Peptide
4	P	23	PRO	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	3371	0	3269	58	0
1	D	3375	0	3280	45	0
1	G	3375	0	3280	30	0
1	J	3375	0	3280	58	0
2	B	3165	0	3126	64	0
2	E	3287	0	3255	48	0
2	H	3258	0	3215	36	0
2	K	3291	0	3251	57	0
3	C	1110	0	1088	26	0
3	F	1196	0	1181	13	0
3	I	1171	0	1149	13	0
3	L	1187	0	1167	35	0
4	M	422	0	394	5	0
4	N	422	0	396	9	0
4	O	422	0	394	10	0
4	P	422	0	394	5	0
5	R	274	0	238	7	0
6	A	14	0	13	0	0
6	B	14	0	13	2	0
6	D	14	0	13	0	0
6	E	14	0	13	0	0
6	G	14	0	13	2	0
6	H	14	0	13	0	0
6	J	14	0	13	0	0
6	K	14	0	13	1	0
6	M	14	0	13	0	0
6	N	14	0	13	0	0
6	O	14	0	13	0	0
6	P	14	0	13	0	0
7	R	1	0	0	0	0
All	All	33292	0	32513	475	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 7.

All (475) 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)
3:C:228:LEU:HD11	3:C:242:VAL:HG13	1.44	0.99
1:A:218:THR:OG1	1:A:236:GLN:OE1	1.99	0.81
1:D:321:TYR:OH	1:D:348:ALA:O	1.98	0.81
1:D:436:LEU:HD11	3:F:158:ILE:HD12	1.60	0.80
2:K:402:ASN:O	3:L:177:TYR:OH	2.00	0.80
1:G:292:SER:OG	1:G:293:GLU:OE2	2.00	0.80
2:H:414:CYS:SG	2:H:415:ILE:N	2.53	0.79
4:N:25:CYS:SG	4:N:33:THR:OG1	2.41	0.79
1:A:397:GLU:OE2	2:B:360:TYR:OH	2.01	0.79
3:C:118:LEU:O	3:C:121:GLN:NE2	2.17	0.78
3:F:126:ALA:HB3	3:F:143:ILE:HD13	1.65	0.77
1:A:51:TYR:OH	1:A:237:VAL:O	2.01	0.77
1:J:268:ARG:NH1	1:J:270:GLU:OE2	2.19	0.76
2:K:2:LEU:O	2:K:7:THR:OG1	2.04	0.76
3:L:182:PRO:O	3:L:186:TYR:OH	2.03	0.76
1:A:57:SER:OG	2:B:240:LEU:O	2.03	0.75
3:L:123:ASN:ND2	3:L:140:GLU:O	2.19	0.75
1:A:94:CYS:O	2:B:224:ARG:NH1	2.19	0.75
1:A:64:GLY:O	1:A:101:THR:OG1	2.05	0.75
2:H:135:ARG:NH2	2:H:326:THR:OG1	2.19	0.74
3:L:225:ALA:HB1	3:L:241:VAL:HG21	1.68	0.74
4:O:56:CYS:SG	4:O:57:ASN:N	2.60	0.74
2:B:13:ARG:O	2:B:97:TYR:OH	2.06	0.73
4:N:27:GLU:N	4:N:27:GLU:OE1	2.21	0.73
1:D:51:TYR:OH	1:D:237:VAL:O	2.05	0.73
2:H:390:ARG:NH2	2:H:412:LEU:O	2.22	0.72
2:H:26:ARG:NH2	2:K:143:GLU:O	2.22	0.71
1:A:306:GLU:OE1	1:A:307:CYS:N	2.24	0.71
2:E:26:ARG:NH2	2:H:143:GLU:O	2.24	0.71
3:I:280:VAL:HG21	3:I:292:LEU:HD13	1.73	0.71
3:F:142:ARG:NH1	3:F:143:ILE:O	2.24	0.70
2:H:30:PRO:O	2:H:50:SER:OG	2.08	0.70
4:O:36:MET:O	4:O:40:ASN:ND2	2.24	0.70
2:E:390:ARG:NH2	2:E:414:CYS:O	2.23	0.70
1:G:323:SER:OG	1:G:324:SER:N	2.25	0.69
2:B:78:ILE:HG23	2:B:81:LEU:HD13	1.73	0.69
2:E:166:MET:SD	2:E:252:LEU:HD12	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:HIS:O	2:B:354:VAL:HG23	1.92	0.68
1:A:113:GLU:N	1:A:113:GLU:OE1	2.25	0.68
1:G:204:LEU:CD1	1:G:214:LEU:HD13	2.24	0.68
2:B:32:ALA:N	2:B:50:SER:OG	2.27	0.68
2:E:3:ASP:O	2:E:7:THR:OG1	2.11	0.68
3:L:225:ALA:HB1	3:L:241:VAL:CG2	2.24	0.68
2:E:163:TYR:OH	4:O:47:ASP:OD1	2.11	0.67
2:B:274:GLU:OE2	2:B:281:ILE:HD11	1.94	0.67
1:D:323:SER:OG	1:D:324:SER:N	2.25	0.67
3:C:132:ARG:NH1	3:C:165:ASP:OD1	2.28	0.67
2:B:203:ASP:O	2:B:205:ARG:NH1	2.27	0.67
4:N:21:CYS:HB2	4:N:25:CYS:HB2	1.76	0.67
1:G:402:ALA:O	2:H:356:TYR:OH	2.06	0.67
1:A:206:SER:OG	1:A:211:SER:OG	2.13	0.66
3:C:218:ASP:O	3:C:221:GLY:N	2.29	0.66
2:K:15:TYR:OH	2:K:34:GLU:OE2	2.13	0.66
2:B:295:ARG:NH1	2:B:324:GLU:OE2	2.29	0.65
3:I:278:ALA:HB1	3:I:294:VAL:HG21	1.78	0.65
1:D:17:ALA:HB3	1:D:29:LEU:HD21	1.80	0.64
2:B:377:VAL:O	2:B:381:THR:HG23	1.97	0.64
2:K:156:LYS:HZ2	5:R:53:ASP:CG	2.01	0.64
2:B:136:GLU:N	2:B:136:GLU:OE1	2.29	0.64
1:G:53:THR:HG21	1:G:236:GLN:OE1	1.98	0.64
3:L:155:LYS:NZ	3:L:157:SER:OG	2.31	0.64
2:K:156:LYS:HE3	5:R:53:ASP:OD2	1.98	0.64
2:B:118:ASN:OD1	2:B:120:HIS:N	2.31	0.64
2:E:340:SER:O	2:E:340:SER:OG	2.11	0.64
2:E:315:ASN:N	2:E:315:ASN:OD1	2.29	0.64
1:A:25:ALA:HB2	1:A:294:THR:HG21	1.78	0.63
3:C:116:ILE:HD11	3:C:126:ALA:HB2	1.80	0.63
3:C:211:ASP:OD2	3:C:214:ARG:NH1	2.31	0.63
1:J:184:GLU:OE2	1:J:186:TYR:OH	2.15	0.63
2:K:277:HIS:ND1	2:K:340:SER:O	2.31	0.63
1:A:331:ILE:HG23	1:A:368:LEU:HD13	1.80	0.63
2:H:159:ASP:O	2:H:253:HIS:ND1	2.31	0.63
3:I:298:ASN:OD1	3:I:302:VAL:N	2.31	0.63
1:J:411:ILE:HD12	1:J:412:LYS:N	2.14	0.63
3:I:271:ASP:OD1	3:I:274:GLY:N	2.32	0.63
2:E:366:ILE:HD12	2:E:367:GLY:N	2.14	0.62
2:H:136:GLU:OE1	2:H:266:THR:OG1	2.16	0.62
3:C:109:GLU:OE1	3:C:109:GLU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:ARG:NH1	1:J:285:ASP:OD1	2.32	0.62
1:A:192:GLU:O	1:A:195:THR:OG1	2.11	0.62
2:H:315:ASN:OD1	2:H:315:ASN:N	2.32	0.62
2:K:150:CYS:SG	2:K:263:CYS:N	2.72	0.62
1:J:283:ILE:HD12	1:J:284:PRO:HD2	1.82	0.62
2:B:85:THR:OG1	2:B:103:CYS:SG	2.57	0.61
2:B:136:GLU:HG3	2:B:290:THR:HG23	1.81	0.61
1:A:291:ILE:O	1:A:294:THR:OG1	2.13	0.61
3:I:247:GLN:NE2	3:I:249:GLU:OE1	2.33	0.61
2:K:156:LYS:CE	5:R:53:ASP:OD2	2.49	0.61
2:B:143:GLU:OE1	2:B:143:GLU:N	2.32	0.61
1:J:180:VAL:HG22	1:J:185:VAL:HG12	1.83	0.61
1:J:323:SER:OG	1:J:324:SER:N	2.34	0.61
3:L:226:ILE:HG23	3:L:242:VAL:CG1	2.31	0.61
1:A:25:ALA:HB2	1:A:294:THR:CG2	2.30	0.60
1:G:370:VAL:HG22	1:G:371:CYS:SG	2.42	0.60
4:O:34:LEU:O	4:O:37:LEU:N	2.34	0.60
2:K:406:PRO:O	2:K:409:LEU:N	2.34	0.60
3:L:218:ASP:OD1	3:L:221:GLY:N	2.35	0.60
4:O:21:CYS:O	4:O:25:CYS:HB2	2.02	0.60
2:K:296:SER:OG	2:K:300:ASP:O	2.20	0.60
3:C:225:ALA:HB1	3:C:241:VAL:CG2	2.31	0.60
2:B:133:VAL:HG13	2:B:148:LEU:HD11	1.84	0.60
1:A:308:THR:OG1	1:A:382:LYS:O	2.09	0.59
1:G:350:SER:OG	1:G:350:SER:O	2.16	0.59
2:B:13:ARG:NH1	2:B:68:MET:SD	2.74	0.59
3:C:170:MET:SD	3:C:170:MET:N	2.75	0.59
3:F:227:VAL:HA	3:F:241:VAL:HG12	1.84	0.59
2:K:394:ILE:HG22	2:K:415:ILE:HD11	1.85	0.59
2:H:42:ALA:HB3	2:H:152:ARG:HH12	1.68	0.59
1:J:326:ALA:N	1:J:349:GLU:OE2	2.36	0.59
2:K:400:ALA:O	3:L:177:TYR:OH	2.19	0.59
2:E:33:ILE:HD11	2:E:111:VAL:HG23	1.85	0.59
3:L:214:ARG:O	3:L:227:VAL:HG12	2.03	0.58
1:A:325:LYS:NZ	1:A:326:ALA:O	2.31	0.58
1:A:112:GLU:OE2	2:B:46:ARG:NH2	2.35	0.58
2:B:329:ASN:OD1	2:B:329:ASN:N	2.34	0.58
1:G:19:VAL:HG21	1:G:283:ILE:HD11	1.85	0.58
3:C:166:VAL:HG22	3:C:167:PRO:HD2	1.86	0.58
2:K:398:LYS:O	3:L:132:ARG:NH1	2.37	0.58
6:B:501:NAG:O7	6:B:501:NAG:O3	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:399:LEU:HD12	3:L:250:THR:HG21	1.85	0.58
1:J:147:VAL:HG13	1:J:164:ILE:HD11	1.86	0.58
2:K:36:VAL:HG13	2:K:47:ILE:HG22	1.84	0.58
2:E:182:SER:OG	2:E:183:ALA:N	2.38	0.57
1:A:53:THR:OG1	1:A:53:THR:O	2.23	0.57
1:J:18:LEU:HD11	1:J:332:HIS:HB3	1.85	0.57
2:K:409:LEU:HD12	2:K:412:LEU:HD11	1.87	0.57
2:B:107:ASP:OD1	2:B:107:ASP:N	2.38	0.56
1:G:78:CYS:SG	1:G:79:GLN:N	2.78	0.56
1:G:110:ARG:NH2	1:G:211:SER:O	2.38	0.56
1:G:143:ARG:O	1:G:157:ILE:HD11	2.04	0.56
4:O:31:HIS:O	4:O:35:THR:OG1	2.22	0.56
1:J:2:GLU:OE1	1:J:3:HIS:N	2.38	0.56
3:L:202:VAL:HG13	3:L:239:LEU:HD21	1.87	0.56
3:F:202:VAL:HG13	3:F:239:LEU:HD11	1.86	0.56
3:I:170:MET:O	3:I:171:LEU:HD13	2.05	0.56
2:K:295:ARG:NE	2:K:324:GLU:OE1	2.39	0.56
2:H:319:THR:OG1	2:H:320:GLY:N	2.39	0.56
2:H:201:CYS:O	2:H:203:ASP:N	2.39	0.55
3:L:259:GLU:N	3:L:259:GLU:OE1	2.40	0.55
1:A:181:TYR:OH	1:A:245:LYS:NZ	2.34	0.55
1:G:33:LEU:CD2	1:G:133:VAL:HG12	2.36	0.55
1:J:141:SER:OG	1:J:142:TRP:N	2.39	0.55
1:J:229:ILE:HD12	2:K:18:ASP:OD2	2.06	0.55
2:E:349:PRO:O	2:E:353:VAL:HG23	2.06	0.55
3:F:114:PHE:HB2	3:F:143:ILE:HD11	1.88	0.55
1:A:388:ILE:HD11	2:B:275:HIS:CE1	2.42	0.55
1:A:360:ALA:HB2	1:A:395:HIS:NE2	2.22	0.55
2:B:294:THR:HG21	2:B:316:PHE:CE2	2.41	0.55
2:B:205:ARG:NE	2:B:216:THR:OG1	2.40	0.55
1:J:300:LEU:HD21	1:J:370:VAL:CG1	2.37	0.55
1:A:388:ILE:HD13	2:B:335:VAL:CG1	2.37	0.55
6:G:501:NAG:O7	6:G:501:NAG:O3	2.19	0.55
2:K:8:GLN:HG2	2:K:252:LEU:HD22	1.89	0.55
2:K:253:HIS:NE2	4:N:47:ASP:OD1	2.39	0.55
1:A:331:ILE:HG12	1:A:370:VAL:HG22	1.88	0.54
2:E:115:ASP:OD1	2:E:118:ASN:ND2	2.40	0.54
1:A:93:TYR:HD1	2:B:173:ALA:HB2	1.72	0.54
2:B:84:ARG:O	2:B:110:THR:HG22	2.07	0.54
1:D:53:THR:HG21	1:D:220:LEU:HD11	1.88	0.54
2:K:56:LYS:O	2:K:59:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:CD1	1:A:283:ILE:HD11	2.42	0.54
2:E:201:CYS:O	2:E:203:ASP:N	2.40	0.54
2:B:219:ASP:OD1	2:B:220:VAL:N	2.41	0.54
2:K:157:ARG:CZ	5:R:55:ASP:OD1	2.56	0.54
2:K:266:THR:O	2:K:329:ASN:ND2	2.39	0.54
1:J:87:PHE:CE1	1:J:92:ALA:HB2	2.43	0.53
1:D:198:ALA:HB3	2:H:272:LEU:HD11	1.91	0.53
2:E:7:THR:O	4:O:54:VAL:HG11	2.09	0.53
1:G:183:HIS:HA	1:G:264:LEU:HD22	1.89	0.53
1:A:37:ARG:NH2	1:A:146:ASP:OD2	2.41	0.53
2:B:92:VAL:HB	2:B:100:LEU:HD23	1.91	0.53
1:G:143:ARG:C	1:G:157:ILE:HD11	2.28	0.53
2:E:136:GLU:OE1	2:E:266:THR:OG1	2.20	0.53
2:K:233:TRP:CD1	4:N:34:LEU:HD23	2.44	0.53
2:H:408:LEU:HD13	2:H:414:CYS:O	2.09	0.53
3:I:169:ILE:HD11	3:I:179:ALA:HB2	1.91	0.53
1:D:418:THR:HG23	2:E:378:SER:CB	2.38	0.53
3:F:123:ASN:N	3:F:123:ASN:OD1	2.41	0.53
4:P:35:THR:O	4:P:39:GLN:NE2	2.38	0.53
1:A:9:ASN:O	1:A:9:ASN:ND2	2.42	0.52
3:L:133:VAL:HG23	3:L:153:LEU:HD11	1.90	0.52
1:G:59:VAL:HG22	1:G:103:MET:HB2	1.90	0.52
3:C:190:HIS:NE2	3:C:211:ASP:OD2	2.42	0.52
2:H:163:TYR:OH	4:M:47:ASP:OD1	2.23	0.52
2:B:91:LEU:HD23	2:B:92:VAL:N	2.25	0.52
2:B:357:TYR:HA	2:B:364:THR:HG21	1.90	0.52
2:E:160:GLN:HB2	2:E:257:VAL:HG21	1.92	0.52
2:K:136:GLU:HG2	2:K:290:THR:HG23	1.91	0.52
3:L:118:LEU:O	3:L:121:GLN:NE2	2.42	0.52
2:K:100:LEU:HD11	2:K:153:TYR:HB2	1.92	0.52
1:G:51:TYR:OH	1:G:237:VAL:O	2.27	0.52
1:J:400:THR:O	1:J:400:THR:OG1	2.26	0.52
1:A:84:VAL:HG22	1:A:86:PRO:HD3	1.91	0.52
1:A:359:THR:HG21	1:A:364:PRO:HB3	1.92	0.52
1:D:203:ASP:OD1	1:D:203:ASP:N	2.42	0.52
2:B:129:GLU:N	2:B:129:GLU:OE1	2.41	0.51
1:J:199:GLY:N	1:J:203:ASP:OD1	2.42	0.51
3:F:188:TRP:CZ3	3:F:202:VAL:HG11	2.45	0.51
1:A:321:TYR:CE1	1:A:347:LEU:HD11	2.45	0.51
2:H:339:GLU:OE1	2:H:359:ARG:NE	2.44	0.51
3:C:116:ILE:HD11	3:C:126:ALA:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:TYR:OH	1:D:105:GLU:OE1	2.28	0.51
1:A:28:HIS:ND1	1:A:343:ASN:OD1	2.44	0.51
1:A:403:ILE:H	1:A:403:ILE:HD12	1.76	0.51
3:I:247:GLN:OE1	3:I:289:ARG:NH1	2.41	0.51
2:K:391:ASN:O	2:K:395:THR:HG23	2.11	0.51
2:K:315:ASN:OD1	2:K:315:ASN:N	2.41	0.51
3:L:158:ILE:HG23	3:L:159:TYR:CD1	2.45	0.51
1:A:106:ALA:HB2	1:A:222:LEU:HD21	1.92	0.50
2:B:372:VAL:HA	2:B:375:ILE:HG22	1.93	0.50
3:C:123:ASN:ND2	3:C:139:VAL:HG23	2.27	0.50
2:H:174:ASP:OD1	2:H:175:HIS:N	2.44	0.50
3:C:127:CYS:SG	3:C:128:VAL:N	2.84	0.50
3:L:151:ILE:HD12	3:L:151:ILE:H	1.76	0.50
1:D:429:THR:OG1	2:E:385:LEU:HD12	2.12	0.50
1:J:390:ASP:OD1	1:J:390:ASP:N	2.39	0.50
1:A:422:ILE:HD13	2:B:382:SER:HB3	1.94	0.50
1:J:54:LYS:NZ	2:K:165:GLU:OE2	2.35	0.50
1:J:146:ASP:OD1	1:J:147:VAL:N	2.45	0.50
3:L:143:ILE:HD12	3:L:144:ASP:H	1.77	0.50
1:A:109:GLU:N	1:A:109:GLU:OE1	2.44	0.50
2:B:230:ASN:O	2:B:230:ASN:ND2	2.45	0.50
2:H:178:LEU:HD11	2:H:223:CYS:HB3	1.94	0.50
2:B:133:VAL:CG1	2:B:148:LEU:HD11	2.41	0.50
1:D:96:CYS:O	1:D:100:ASN:ND2	2.45	0.50
2:B:287:ASP:OD1	2:B:288:HIS:N	2.45	0.50
2:K:94:HIS:HB3	2:K:99:ILE:HG22	1.93	0.49
3:L:116:ILE:HG22	3:L:143:ILE:HA	1.95	0.49
2:H:386:LEU:O	2:H:389:THR:OG1	2.26	0.49
1:D:180:VAL:HG22	1:D:185:VAL:HG12	1.95	0.49
1:D:436:LEU:HD11	3:F:158:ILE:CD1	2.36	0.49
3:I:280:VAL:CG2	3:I:292:LEU:HD13	2.41	0.49
1:J:174:PHE:CE2	1:J:269:ALA:HB2	2.47	0.49
1:A:137:TYR:OH	1:A:159:ASP:OD1	2.25	0.49
3:F:131:GLY:H	3:F:174:THR:HG21	1.78	0.49
1:A:160:ALA:HB1	1:A:281:ILE:HD11	1.94	0.49
2:E:8:GLN:NE2	2:E:11:LEU:HD12	2.28	0.49
2:E:212:ASP:N	2:E:212:ASP:OD1	2.45	0.49
1:G:19:VAL:HG23	1:G:29:LEU:HD22	1.95	0.49
3:L:226:ILE:HG23	3:L:242:VAL:HG13	1.95	0.49
1:A:337:VAL:O	1:A:359:THR:HG23	2.13	0.49
3:C:216:ILE:HG12	3:C:225:ALA:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:MET:O	2:B:250:GLY:N	2.41	0.49
1:D:42:THR:HG22	1:D:124:VAL:HG12	1.94	0.49
1:J:321:TYR:CE2	1:J:347:LEU:HD22	2.48	0.48
1:A:7:MET:HG2	1:A:279:ILE:HD11	1.95	0.48
1:J:337:VAL:HG23	1:J:361:ASN:OD1	2.13	0.48
1:G:129:VAL:HG13	1:G:149:VAL:HB	1.96	0.48
2:K:188:THR:OG1	2:K:189:VAL:N	2.47	0.48
2:B:13:ARG:NH1	2:B:14:PRO:O	2.47	0.48
3:L:160:ASP:O	3:L:161:LEU:HD23	2.12	0.48
1:D:19:VAL:HG13	1:D:29:LEU:HD22	1.96	0.48
2:E:22:CYS:N	2:E:25:SER:O	2.43	0.48
2:H:180:ILE:HD12	2:H:184:LYS:O	2.14	0.48
1:A:57:SER:O	2:B:242:ARG:NH2	2.47	0.48
2:B:94:HIS:O	2:B:157:ARG:NH1	2.46	0.48
2:H:165:GLU:OE2	2:H:236:ASN:ND2	2.45	0.48
2:K:21:ASN:OD1	2:K:23:GLY:N	2.45	0.48
2:B:159:ASP:OD1	2:B:160:GLN:N	2.46	0.48
1:D:342:GLU:OE1	1:D:342:GLU:N	2.46	0.48
1:J:283:ILE:HD12	1:J:284:PRO:CD	2.43	0.47
2:K:201:CYS:O	2:K:203:ASP:N	2.47	0.47
4:O:31:HIS:O	4:O:31:HIS:ND1	2.43	0.47
2:B:81:LEU:HD12	2:B:113:PHE:HB3	1.95	0.47
1:G:33:LEU:HD23	1:G:133:VAL:HG12	1.96	0.47
2:H:357:TYR:HA	2:H:364:THR:HG21	1.94	0.47
4:N:21:CYS:HB2	4:N:25:CYS:CB	2.43	0.47
2:K:207:GLY:C	2:K:208:ILE:HD12	2.35	0.47
3:C:171:LYS:N	3:I:286:GLU:OE2	2.48	0.47
2:E:13:ARG:NH1	2:E:14:PRO:O	2.47	0.47
1:J:308:THR:OG1	1:J:382:LYS:O	2.17	0.47
1:J:53:THR:HG21	1:J:236:GLN:OE1	2.15	0.47
1:J:53:THR:O	1:J:53:THR:OG1	2.23	0.47
1:J:97:ASP:O	1:J:98:THR:OG1	2.28	0.47
1:J:159:ASP:OD1	1:J:159:ASP:N	2.45	0.47
3:C:229:GLY:N	3:C:240:SER:OG	2.48	0.47
1:J:116:ILE:HD11	2:K:260:LYS:CG	2.45	0.47
2:B:129:GLU:OE2	2:B:131:ARG:NH2	2.48	0.47
2:B:45:ILE:HD11	2:B:103:CYS:SG	2.55	0.47
1:D:220:LEU:HD13	1:D:236:GLN:NE2	2.30	0.47
3:L:213:GLY:HA2	3:L:226:ILE:HD11	1.97	0.46
2:B:34:GLU:OE1	2:B:34:GLU:N	2.48	0.46
1:G:181:TYR:OH	1:G:245:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PRO:HD2	1:A:268:ARG:HE	1.80	0.46
2:E:407:ILE:HD12	2:E:407:ILE:H	1.80	0.46
2:H:45:ILE:HG21	2:H:128:VAL:HG21	1.97	0.46
1:J:19:VAL:HG22	1:J:27:VAL:HG13	1.97	0.46
3:F:216:ILE:HD11	3:F:227:VAL:HG12	1.98	0.46
1:A:324:SER:OG	1:A:325:LYS:N	2.49	0.46
2:E:339:GLU:OE1	2:E:359:ARG:NE	2.41	0.46
2:B:358:ASN:OD1	2:B:358:ASN:N	2.48	0.46
1:A:406:THR:O	1:A:410:TRP:N	2.46	0.46
3:C:228:LEU:HD12	3:C:241:VAL:HA	1.98	0.46
3:I:271:ASP:OD1	3:I:275:ARG:N	2.47	0.46
2:E:284:LEU:HD11	2:E:292:LEU:HD22	1.98	0.46
1:G:19:VAL:HG21	1:G:283:ILE:CD1	2.45	0.46
1:J:203:ASP:OD2	1:J:240:GLY:N	2.45	0.46
3:L:245:ASN:OD1	3:L:249:VAL:N	2.48	0.46
1:A:342:GLU:N	1:A:342:GLU:OE1	2.49	0.46
2:B:7:THR:HG21	4:P:54:VAL:HG11	1.97	0.46
1:A:29:LEU:HD13	1:A:30:GLN:N	2.31	0.45
1:A:264:LEU:O	1:A:267:LEU:N	2.46	0.45
1:G:53:THR:HG22	1:G:108:VAL:HG23	1.98	0.45
2:H:182:SER:OG	2:H:183:ALA:N	2.49	0.45
1:A:307:CYS:SG	1:A:308:THR:N	2.88	0.45
2:B:274:GLU:CD	2:B:281:ILE:HD11	2.37	0.45
2:B:318:VAL:HG13	2:B:337:ALA:HB2	1.99	0.45
1:J:110:ARG:HH11	1:J:214:LEU:HD21	1.81	0.45
1:A:168:SER:HG	1:A:276:SER:H	1.60	0.45
2:B:145:GLY:HA2	2:B:267:LEU:HD23	1.97	0.45
2:H:191:SER:O	2:H:191:SER:OG	2.34	0.45
1:J:31:ILE:HD12	1:J:135:ILE:HD12	1.98	0.45
1:A:185:VAL:HG22	1:A:262:ILE:HD12	1.98	0.45
1:G:53:THR:HG21	1:G:236:GLN:CD	2.37	0.45
2:K:209:THR:OG1	2:K:211:SER:O	2.33	0.45
2:B:9:TYR:OH	2:B:253:HIS:O	2.29	0.45
3:C:245:ASN:OD1	3:C:247:LYS:N	2.49	0.45
1:D:38:ILE:HB	1:D:269:ALA:HB3	1.98	0.45
1:J:25:ALA:CB	1:J:294:THR:HG21	2.46	0.45
4:O:12:ILE:H	4:O:12:ILE:HD12	1.81	0.45
2:E:357:TYR:HA	2:E:364:THR:HG21	1.98	0.45
2:H:178:LEU:HD11	2:H:223:CYS:CB	2.47	0.45
1:J:321:TYR:CZ	1:J:347:LEU:HD22	2.52	0.45
2:K:41:HIS:ND1	2:K:151:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:287:ASP:OD2	2:K:287:ASP:N	2.41	0.45
1:J:68:CYS:SG	1:J:69:THR:N	2.86	0.45
2:K:233:TRP:NE1	4:N:38:GLU:OE2	2.49	0.45
2:H:31:ILE:HG23	2:H:31:ILE:O	2.16	0.45
2:K:94:HIS:CB	2:K:99:ILE:HG22	2.46	0.45
3:L:143:ILE:HD12	3:L:144:ASP:N	2.32	0.45
6:B:501:NAG:HO3	6:B:501:NAG:C7	2.23	0.45
1:G:208:THR:OG1	1:G:209:SER:N	2.49	0.45
2:H:8:GLN:HG3	2:H:252:LEU:HD23	1.99	0.45
2:H:347:GLY:O	2:H:352:VAL:HG23	2.17	0.45
2:K:171:LEU:HD23	2:K:171:LEU:H	1.81	0.45
2:K:349:PRO:HA	2:K:352:VAL:HG12	1.98	0.45
3:C:135:LYS:NZ	3:C:162:GLU:OE1	2.44	0.45
3:C:131:GLY:N	3:C:174:THR:HG21	2.32	0.44
1:G:321:TYR:OH	1:G:348:ALA:O	2.23	0.44
3:L:112:LYS:HE3	3:L:175:LEU:HD13	1.99	0.44
3:L:189:HIS:HB3	3:L:214:ARG:HE	1.82	0.44
2:E:195:VAL:HG22	2:E:227:LEU:HA	1.99	0.44
2:K:8:GLN:CG	2:K:252:LEU:HD22	2.46	0.44
3:L:202:VAL:CG1	3:L:239:LEU:HD21	2.47	0.44
1:A:175:ASP:OD1	1:A:175:ASP:N	2.40	0.44
2:B:379:CYS:SG	2:B:380:VAL:N	2.90	0.44
1:D:242:GLU:N	1:D:242:GLU:OE1	2.50	0.44
1:J:105:GLU:OE1	1:J:105:GLU:N	2.48	0.44
2:K:156:LYS:NZ	5:R:57:ASP:OD2	2.50	0.44
2:E:178:LEU:HD21	2:E:225:ALA:HB2	2.00	0.44
3:L:133:VAL:HG13	3:L:166:VAL:HG12	2.00	0.44
3:C:178:THR:HG22	3:C:180:ASP:H	1.82	0.44
1:D:17:ALA:HB3	1:D:29:LEU:CD2	2.48	0.44
1:D:180:VAL:HG13	1:D:264:LEU:HD11	2.00	0.44
2:K:156:LYS:NZ	5:R:53:ASP:OD2	2.50	0.44
1:D:147:VAL:HG12	1:D:155:ALA:CB	2.48	0.44
1:D:164:ILE:HG22	1:D:277:ILE:HG21	2.00	0.44
2:E:18:ASP:O	2:E:239:ARG:NH1	2.51	0.44
3:L:128:VAL:HG22	3:L:133:VAL:HG12	2.00	0.44
2:B:240:LEU:O	2:B:240:LEU:HD12	2.18	0.44
3:F:186:TYR:O	3:F:193:VAL:HG12	2.18	0.44
1:J:112:GLU:OE2	2:K:46:ARG:NH1	2.47	0.44
2:K:393:CYS:SG	2:K:394:ILE:HG23	2.58	0.44
3:L:178:THR:OG1	3:L:222:ARG:NE	2.51	0.44
2:B:5:HIS:O	2:B:95:HIS:NE2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:O	1:A:256:ALA:N	2.52	0.43
2:B:361:PRO:HD2	2:B:361:PRO:O	2.18	0.43
3:C:131:GLY:H	3:C:174:THR:HG21	1.82	0.43
2:E:7:THR:HG23	4:O:54:VAL:HG12	2.00	0.43
1:G:134:ASN:C	1:G:135:ILE:HD12	2.37	0.43
1:J:226:GLN:OE1	1:J:226:GLN:N	2.47	0.43
1:J:302:CYS:HA	1:J:319:VAL:HG12	1.98	0.43
1:A:440:ARG:CZ	3:I:302:VAL:HG11	2.48	0.43
2:E:319:THR:OG1	2:E:320:GLY:N	2.52	0.43
1:D:137:TYR:CZ	1:D:140:VAL:HG21	2.54	0.43
2:H:94:HIS:O	2:H:94:HIS:ND1	2.51	0.43
1:J:254:ASP:OD1	1:J:254:ASP:N	2.51	0.43
4:M:5:VAL:HG11	4:M:45:ALA:CB	2.49	0.43
2:H:8:GLN:CD	4:M:50:LEU:HD21	2.39	0.43
1:J:218:THR:O	1:J:237:VAL:HG22	2.18	0.43
1:J:283:ILE:CD1	1:J:284:PRO:HD2	2.47	0.43
3:L:203:PRO:O	3:L:206:VAL:HG12	2.19	0.43
4:N:5:VAL:HG23	4:N:5:VAL:O	2.18	0.43
1:A:331:ILE:CG2	1:A:368:LEU:HD13	2.49	0.43
2:E:370:THR:O	2:E:374:ILE:HG23	2.18	0.43
2:H:294:THR:HG21	2:H:316:PHE:CZ	2.54	0.43
1:J:229:ILE:HD11	1:J:231:HIS:CE1	2.54	0.43
1:J:436:LEU:HA	1:J:439:HIS:HB2	2.01	0.43
2:K:93:SER:OG	2:K:94:HIS:N	2.51	0.43
6:K:501:NAG:O7	6:K:501:NAG:O3	2.25	0.43
4:M:47:ASP:OD1	4:M:47:ASP:N	2.51	0.43
1:D:388:ILE:HG23	2:E:335:VAL:HB	2.00	0.42
2:K:356:TYR:O	2:K:364:THR:OG1	2.27	0.42
3:C:243:THR:OG1	3:C:244:TRP:N	2.52	0.42
1:D:147:VAL:HG21	1:D:164:ILE:HD12	2.01	0.42
1:G:148:TYR:HB2	1:G:153:THR:HG21	2.01	0.42
4:P:7:CYS:SG	4:P:49:LEU:HD12	2.58	0.42
2:E:16:ILE:HD11	2:E:68:MET:O	2.19	0.42
1:G:180:VAL:HG13	1:G:264:LEU:HD11	2.00	0.42
1:J:104:SER:O	1:J:104:SER:OG	2.30	0.42
1:D:97:ASP:O	1:D:98:THR:OG1	2.33	0.42
2:K:407:ILE:HD12	2:K:410:ALA:HB3	2.01	0.42
3:C:225:ALA:HB1	3:C:241:VAL:HG23	2.01	0.42
1:D:406:THR:HG21	2:E:346:HIS:HA	2.01	0.42
2:E:78:ILE:HG23	2:E:81:LEU:HB2	2.01	0.42
2:E:180:ILE:O	2:E:180:ILE:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:5:VAL:HG21	4:N:45:ALA:CB	2.49	0.42
2:B:201:CYS:O	2:B:203:ASP:N	2.52	0.42
2:B:308:ILE:HD13	2:B:327:TRP:HZ3	1.83	0.42
1:D:283:ILE:HD12	1:D:283:ILE:N	2.34	0.42
1:J:162:LEU:HD11	1:J:279:ILE:HD11	2.00	0.42
2:B:270:GLU:OE2	2:B:330:HIS:NE2	2.52	0.42
2:B:363:THR:O	2:B:363:THR:HG22	2.19	0.42
1:D:309:TYR:HH	2:E:355:TYR:HH	1.67	0.42
2:E:136:GLU:OE2	2:E:268:ALA:N	2.53	0.42
3:I:164:ASP:N	3:I:164:ASP:OD1	2.52	0.42
2:K:95:HIS:CD2	2:K:255:PRO:HB3	2.55	0.42
1:J:283:ILE:HG23	1:J:288:PHE:HE1	1.84	0.42
1:D:93:TYR:CD2	2:E:173:ALA:HB2	2.55	0.42
1:D:226:GLN:OE1	1:D:226:GLN:N	2.52	0.42
1:D:265:GLU:HB3	1:D:266:PRO:HD3	2.00	0.42
3:L:242:VAL:HG13	3:L:242:VAL:O	2.19	0.42
2:B:267:LEU:HD12	2:B:330:HIS:ND1	2.35	0.42
1:D:271:ASN:OD1	1:D:271:ASN:N	2.53	0.42
2:E:371:CYS:SG	2:E:372:VAL:N	2.93	0.42
2:K:122:CYS:SG	2:K:123:THR:N	2.93	0.42
4:M:5:VAL:HG22	4:M:6:MET:H	1.85	0.42
1:A:104:SER:O	1:A:104:SER:OG	2.32	0.41
1:D:171:TRP:CE3	1:D:274:VAL:HG11	2.55	0.41
1:D:309:TYR:CE1	1:D:362:ILE:HD13	2.55	0.41
1:J:30:GLN:OE1	1:J:343:ASN:ND2	2.51	0.41
3:L:154:LYS:HA	3:L:154:LYS:HE2	2.02	0.41
1:A:344:ASP:OD1	1:A:344:ASP:N	2.53	0.41
1:J:18:LEU:N	1:J:18:LEU:HD12	2.35	0.41
2:B:142:PRO:HD2	2:B:264:ILE:HG23	2.02	0.41
1:D:84:VAL:HG23	1:D:86:PRO:HD3	2.01	0.41
1:D:371:CYS:O	1:D:372:THR:OG1	2.35	0.41
1:D:390:ASP:OD1	1:D:390:ASP:N	2.45	0.41
2:E:394:ILE:HD12	2:E:398:LYS:NZ	2.35	0.41
2:E:405:VAL:HG11	2:E:415:ILE:HG21	2.01	0.41
3:C:116:ILE:HD13	3:C:143:ILE:HD13	2.02	0.41
2:E:351:GLU:HA	2:E:354:VAL:HG12	2.02	0.41
2:H:266:THR:O	2:H:329:ASN:ND2	2.48	0.41
2:K:350:HIS:NE2	2:K:351:GLU:OE1	2.54	0.41
1:G:25:ALA:HB2	1:G:294:THR:HG21	2.03	0.41
6:G:501:NAG:HO3	6:G:501:NAG:C7	2.26	0.41
1:J:17:ALA:HB3	1:J:29:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:ALA:HB3	1:J:157:ILE:HG12	2.01	0.41
2:B:7:THR:CG2	4:P:54:VAL:HG11	2.51	0.41
3:F:109:GLU:OE1	3:F:109:GLU:N	2.47	0.41
1:A:55:VAL:O	1:A:55:VAL:HG23	2.21	0.41
1:D:50:LYS:HG2	1:D:242:GLU:OE1	2.21	0.41
1:D:145:ALA:HB3	1:D:157:ILE:HG12	2.02	0.41
2:H:390:ARG:NE	2:H:411:LEU:O	2.53	0.41
1:J:112:GLU:OE2	2:K:46:ARG:NH2	2.53	0.41
1:A:145:ALA:CB	1:A:157:ILE:HD13	2.51	0.41
1:J:147:VAL:CG1	1:J:164:ILE:HD11	2.51	0.41
2:K:157:ARG:NH1	5:R:55:ASP:OD1	2.54	0.41
1:D:283:ILE:HD12	1:D:283:ILE:H	1.86	0.41
1:J:55:VAL:O	1:J:55:VAL:HG23	2.20	0.41
2:K:294:THR:HG21	2:K:316:PHE:CZ	2.56	0.41
2:E:76:ILE:HD13	2:E:115:ASP:HB2	2.03	0.41
1:J:137:TYR:CD2	1:J:283:ILE:HD11	2.56	0.41
1:A:100:ASN:OD1	1:A:100:ASN:N	2.55	0.40
1:G:266:PRO:CG	1:G:268:ARG:HE	2.34	0.40
2:B:312:THR:OG1	2:B:313:THR:N	2.55	0.40
1:D:135:ILE:HB	1:D:157:ILE:HG21	2.03	0.40
4:P:24:CYS:HB3	4:P:56:CYS:HA	2.03	0.40
1:D:343:ASN:OD1	1:D:343:ASN:N	2.53	0.40
2:E:31:ILE:O	2:E:31:ILE:HG23	2.21	0.40
2:E:339:GLU:OE1	2:E:359:ARG:NH2	2.54	0.40
2:H:45:ILE:HD11	2:H:103:CYS:SG	2.61	0.40
1:J:316:ILE:HD12	1:J:356:HIS:CD2	2.57	0.40
3:L:175:LEU:HG	3:L:223:VAL:HG23	2.03	0.40
2:E:309:GLU:N	2:E:309:GLU:OE1	2.55	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	439/441 (100%)	434 (99%)	5 (1%)	0	100	100
1	D	439/441 (100%)	437 (100%)	2 (0%)	0	100	100
1	G	439/441 (100%)	439 (100%)	0	0	100	100
1	J	439/441 (100%)	437 (100%)	2 (0%)	0	100	100
2	B	398/420 (95%)	397 (100%)	0	1 (0%)	41	74
2	E	416/420 (99%)	415 (100%)	1 (0%)	0	100	100
2	H	413/420 (98%)	408 (99%)	5 (1%)	0	100	100
2	K	417/420 (99%)	413 (99%)	4 (1%)	0	100	100
3	C	128/261 (49%)	128 (100%)	0	0	100	100
3	F	153/261 (59%)	153 (100%)	0	0	100	100
3	I	147/261 (56%)	147 (100%)	0	0	100	100
3	L	150/261 (58%)	150 (100%)	0	0	100	100
4	M	52/63 (82%)	52 (100%)	0	0	100	100
4	N	52/63 (82%)	49 (94%)	3 (6%)	0	100	100
4	O	52/63 (82%)	51 (98%)	1 (2%)	0	100	100
4	P	52/63 (82%)	51 (98%)	1 (2%)	0	100	100
5	R	34/36 (94%)	34 (100%)	0	0	100	100
All	All	4220/4776 (88%)	4195 (99%)	24 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	414	CYS

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	370/371 (100%)	346 (94%)	24 (6%)	17	51
1	D	371/371 (100%)	351 (95%)	20 (5%)	22	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	371/371 (100%)	351 (95%)	20 (5%)	22 57
1	J	371/371 (100%)	353 (95%)	18 (5%)	25 59
2	B	353/367 (96%)	321 (91%)	32 (9%)	9 39
2	E	366/367 (100%)	347 (95%)	19 (5%)	23 58
2	H	362/367 (99%)	349 (96%)	13 (4%)	35 67
2	K	366/367 (100%)	345 (94%)	21 (6%)	20 55
3	C	120/221 (54%)	114 (95%)	6 (5%)	24 59
3	F	129/221 (58%)	120 (93%)	9 (7%)	15 48
3	I	126/221 (57%)	123 (98%)	3 (2%)	49 76
3	L	128/221 (58%)	119 (93%)	9 (7%)	15 48
4	M	50/57 (88%)	48 (96%)	2 (4%)	31 65
4	N	50/57 (88%)	47 (94%)	3 (6%)	19 54
4	O	50/57 (88%)	48 (96%)	2 (4%)	31 65
4	P	50/57 (88%)	47 (94%)	3 (6%)	19 54
5	R	33/33 (100%)	32 (97%)	1 (3%)	41 72
All	All	3666/4097 (90%)	3461 (94%)	205 (6%)	25 56

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	67	GLN
1	A	78	CYS
1	A	87	PHE
1	A	97	ASP
1	A	100	ASN
1	A	104	SER
1	A	107	TYR
1	A	114	CYS
1	A	193	TYR
1	A	241	PHE
1	A	242	GLU
1	A	276	SER
1	A	307	CYS
1	A	325	LYS
1	A	332	HIS
1	A	355	PHE

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Mol	Chain	Res	Type
1	A	366	PHE
1	A	390	ASP
1	A	391	TYR
1	A	409	SER
1	A	410	TRP
1	A	421	PHE
1	A	438	PHE
2	B	19	CYS
2	B	24	HIS
2	B	39	ASP
2	B	71	LYS
2	B	113	PHE
2	B	119	ARG
2	B	122	CYS
2	B	127	LYS
2	B	135	ARG
2	B	150	CYS
2	B	152	ARG
2	B	156	LYS
2	B	166	MET
2	B	167	HIS
2	B	198	TYR
2	B	212	ASP
2	B	221	LYS
2	B	240	LEU
2	B	253	HIS
2	B	274	GLU
2	B	283	HIS
2	B	295	ARG
2	B	315	ASN
2	B	321	GLU
2	B	329	ASN
2	B	333	LYS
2	B	350	HIS
2	B	358	ASN
2	B	371	CYS
2	B	378	SER
2	B	379	CYS
2	B	388	ARG
3	C	127	CYS
3	C	147	GLN
3	C	169	CYS

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Mol	Chain	Res	Type
3	C	170	MET
3	C	177	TYR
3	C	204	ARG
1	D	54	LYS
1	D	87	PHE
1	D	114	CYS
1	D	125	HIS
1	D	192	GLU
1	D	204	LEU
1	D	246	LYS
1	D	247	ASP
1	D	280	SER
1	D	301	GLU
1	D	307	CYS
1	D	321	TYR
1	D	344	ASP
1	D	358	SER
1	D	382	LYS
1	D	386	ASP
1	D	395	HIS
1	D	399	PHE
1	D	434	LEU
1	D	439	HIS
2	E	25	SER
2	E	27	CYS
2	E	29	SER
2	E	50	SER
2	E	75	SER
2	E	115	ASP
2	E	212	ASP
2	E	219	ASP
2	E	232	LYS
2	E	233	TRP
2	E	251	LYS
2	E	252	LEU
2	E	278	ARG
2	E	287	ASP
2	E	315	ASN
2	E	371	CYS
2	E	379	CYS
2	E	388	ARG
2	E	416	LYS

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Mol	Chain	Res	Type
3	F	127	CYS
3	F	135	LYS
3	F	145	ASN
3	F	157	SER
3	F	169	CYS
3	F	170	MET
3	F	209	LYS
3	F	246	GLN
3	F	258	SER
1	G	52	LYS
1	G	87	PHE
1	G	97	ASP
1	G	114	CYS
1	G	203	ASP
1	G	221	LYS
1	G	224	ARG
1	G	226	GLN
1	G	231	HIS
1	G	247	ASP
1	G	253	ASN
1	G	268	ARG
1	G	272	CYS
1	G	301	GLU
1	G	321	TYR
1	G	342	GLU
1	G	367	LYS
1	G	399	PHE
1	G	408	TRP
1	G	421	PHE
2	H	66	SER
2	H	118	ASN
2	H	167	HIS
2	H	171	LEU
2	H	177	LEU
2	H	219	ASP
2	H	252	LEU
2	H	302	ASN
2	H	305	ARG
2	H	315	ASN
2	H	358	ASN
2	H	371	CYS
2	H	414	CYS

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Mol	Chain	Res	Type
3	I	176	ASN
3	I	208	LYS
3	I	265	SER
1	J	29	LEU
1	J	43	ASN
1	J	45	GLU
1	J	95	PHE
1	J	114	CYS
1	J	141	SER
1	J	169	SER
1	J	172	SER
1	J	231	HIS
1	J	298	SER
1	J	307	CYS
1	J	367	LYS
1	J	380	ASP
1	J	386	ASP
1	J	408	TRP
1	J	421	PHE
1	J	438	PHE
1	J	439	HIS
2	K	6	PHE
2	K	28	ASP
2	K	37	ARG
2	K	71	LYS
2	K	171	LEU
2	K	177	LEU
2	K	199	CYS
2	K	212	ASP
2	K	213	HIS
2	K	219	ASP
2	K	223	CYS
2	K	229	ASP
2	K	230	ASN
2	K	248	PHE
2	K	287	ASP
2	K	315	ASN
2	K	333	LYS
2	K	358	ASN
2	K	390	ARG
2	K	393	CYS
2	K	398	LYS

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Mol	Chain	Res	Type
3	L	110	SER
3	L	119	ASN
3	L	178	THR
3	L	181	LYS
3	L	188	TRP
3	L	190	HIS
3	L	197	ASN
3	L	252	LYS
3	L	258	SER
4	M	14	PHE
4	M	43	SER
4	N	14	PHE
4	N	42	ASP
4	N	43	SER
4	O	32	GLU
4	O	51	ASP
4	P	11	ASN
4	P	36	MET
4	P	41	TYR
5	R	67	CYS

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

Mol	Chain	Res	Type
3	F	147	GLN
3	L	123	ASN
4	N	40	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)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	N	101	4	14,14,15	0.24	0	17,19,21	0.52	0
6	NAG	G	501	1	14,14,15	0.75	1 (7%)	17,19,21	0.55	0
6	NAG	K	501	2	14,14,15	0.54	0	17,19,21	0.53	0
6	NAG	B	501	2	14,14,15	0.95	1 (7%)	17,19,21	0.47	0
6	NAG	D	501	1	14,14,15	0.76	1 (7%)	17,19,21	0.53	0
6	NAG	P	101	4	14,14,15	0.25	0	17,19,21	0.37	0
6	NAG	O	101	4	14,14,15	0.22	0	17,19,21	0.43	0
6	NAG	M	101	4	14,14,15	0.20	0	17,19,21	0.74	1 (5%)
6	NAG	A	501	1	14,14,15	0.38	0	17,19,21	0.55	0
6	NAG	J	501	1	14,14,15	0.50	0	17,19,21	0.56	0
6	NAG	E	501	2	14,14,15	0.38	0	17,19,21	0.66	1 (5%)
6	NAG	H	501	2	14,14,15	0.46	0	17,19,21	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	N	101	4	-	2/6/23/26	0/1/1/1
6	NAG	G	501	1	-	2/6/23/26	0/1/1/1
6	NAG	K	501	2	-	2/6/23/26	0/1/1/1
6	NAG	B	501	2	-	2/6/23/26	0/1/1/1
6	NAG	D	501	1	-	2/6/23/26	0/1/1/1
6	NAG	P	101	4	-	2/6/23/26	0/1/1/1
6	NAG	O	101	4	-	0/6/23/26	0/1/1/1
6	NAG	M	101	4	-	0/6/23/26	0/1/1/1
6	NAG	A	501	1	-	1/6/23/26	0/1/1/1
6	NAG	J	501	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	501	2	-	3/6/23/26	0/1/1/1
6	NAG	H	501	2	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	501	NAG	O5-C1	-3.44	1.38	1.43
6	D	501	NAG	O5-C1	-2.61	1.39	1.43
6	G	501	NAG	O5-C1	-2.26	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	101	NAG	C1-O5-C5	2.72	115.88	112.19
6	E	501	NAG	C1-O5-C5	2.29	115.30	112.19

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	501	NAG	O5-C5-C6-O6
6	B	501	NAG	C1-C2-N2-C7
6	K	501	NAG	C1-C2-N2-C7
6	P	101	NAG	C4-C5-C6-O6
6	P	101	NAG	O5-C5-C6-O6
6	G	501	NAG	C1-C2-N2-C7
6	E	501	NAG	C4-C5-C6-O6
6	N	101	NAG	O5-C5-C6-O6
6	N	101	NAG	C4-C5-C6-O6
6	D	501	NAG	O5-C5-C6-O6
6	D	501	NAG	C4-C5-C6-O6
6	A	501	NAG	O5-C5-C6-O6
6	H	501	NAG	C1-C2-N2-C7
6	E	501	NAG	C1-C2-N2-C7
6	B	501	NAG	C3-C2-N2-C7
6	G	501	NAG	C3-C2-N2-C7
6	K	501	NAG	C3-C2-N2-C7

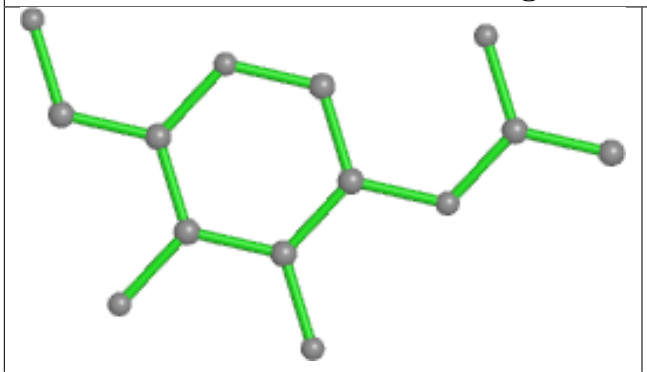
There are no ring outliers.

3 monomers are involved in 5 short contacts:

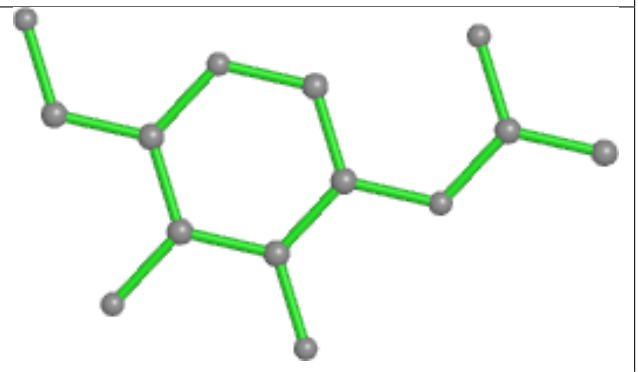
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	501	NAG	2	0
6	K	501	NAG	1	0
6	B	501	NAG	2	0

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.

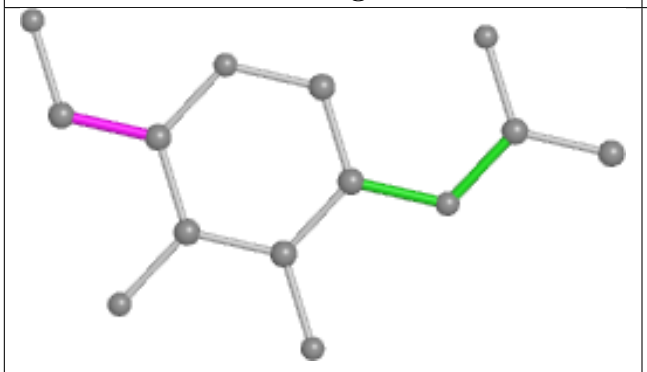
Ligand NAG N 101



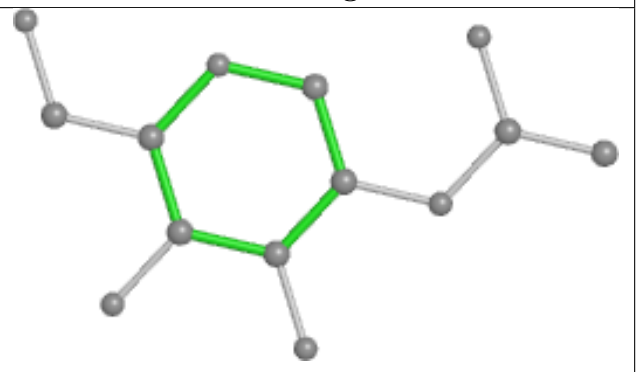
Bond lengths



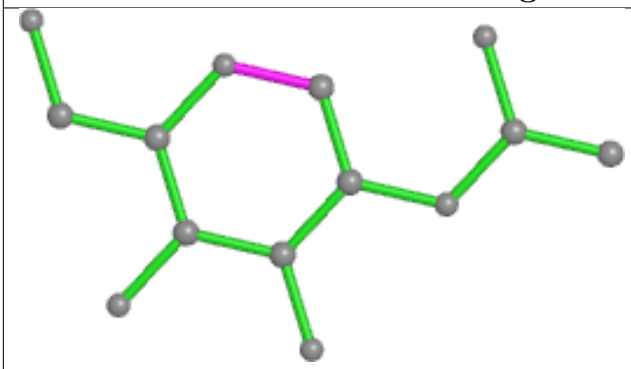
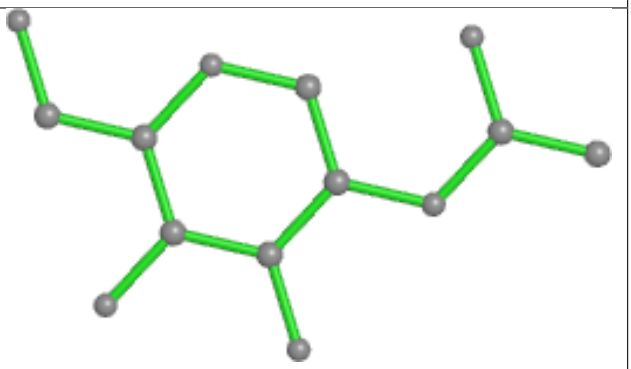
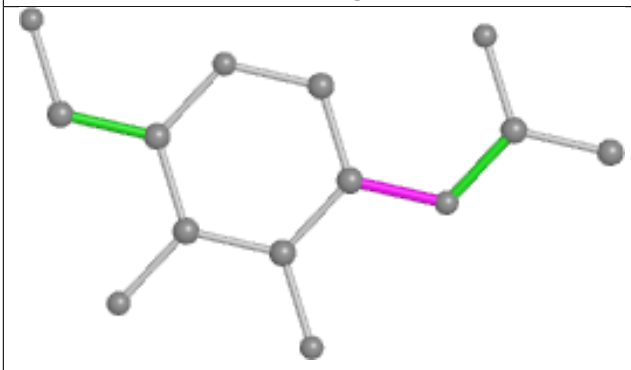
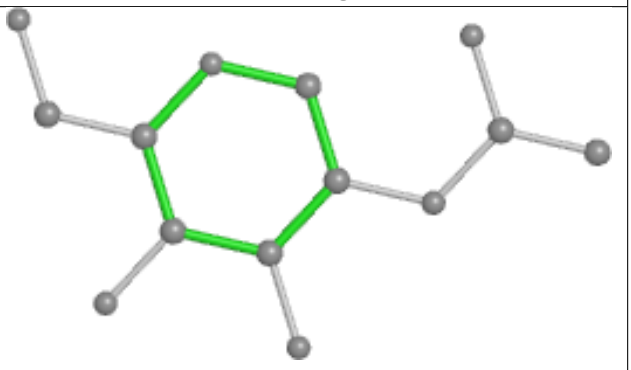
Bond angles

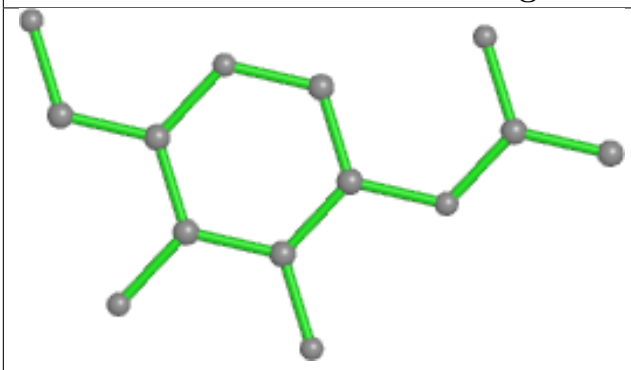
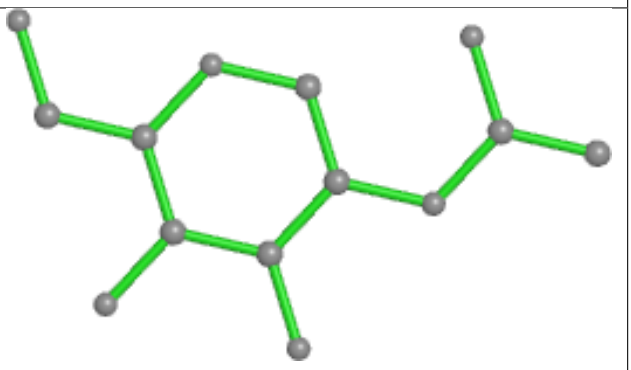
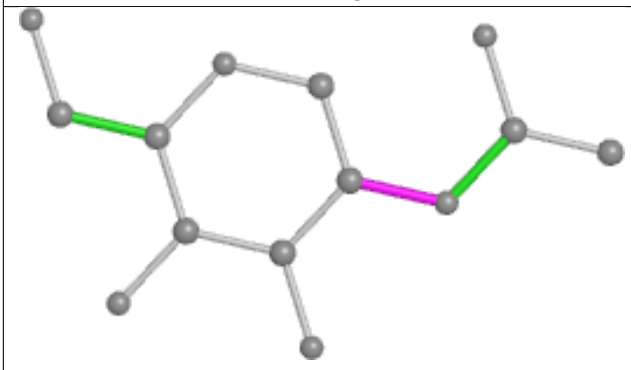
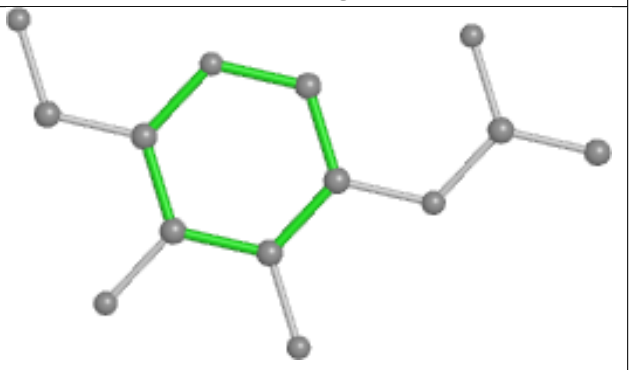


Torsions

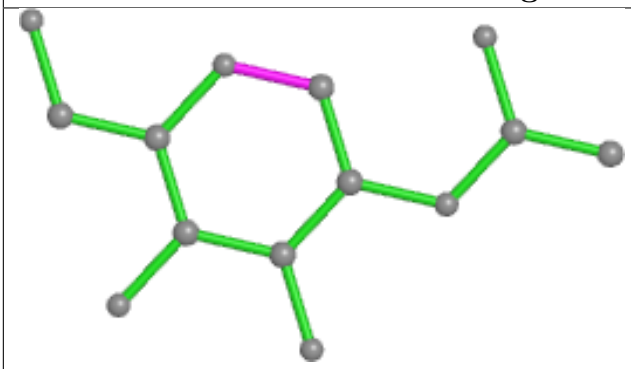


Rings

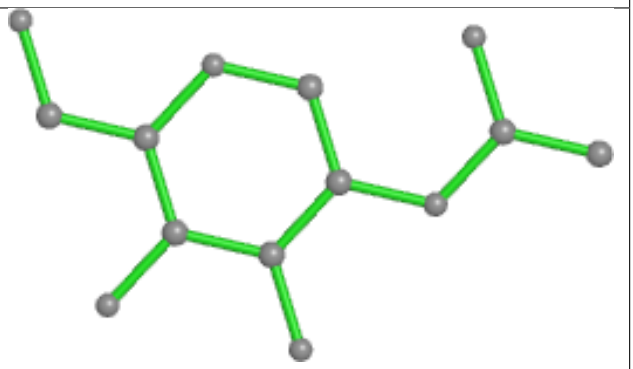
Ligand NAG G 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG K 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

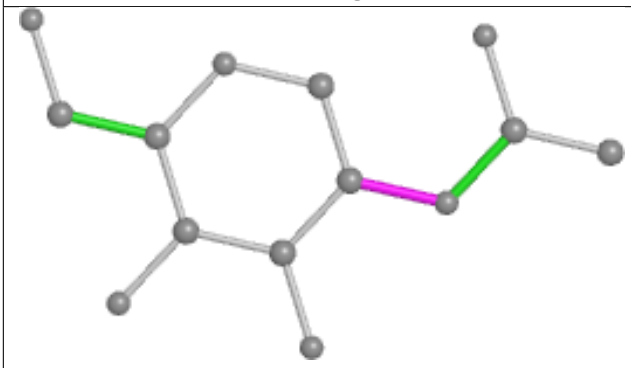
Ligand NAG B 501



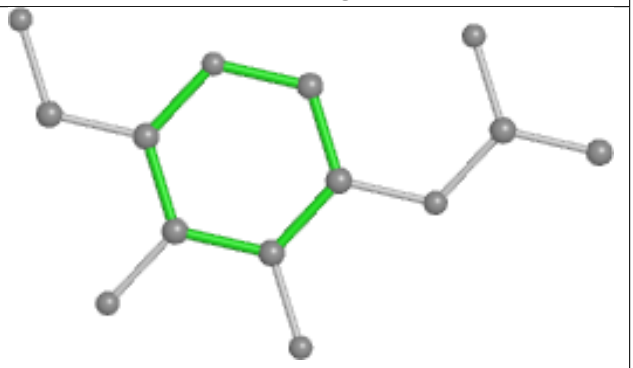
Bond lengths



Bond angles

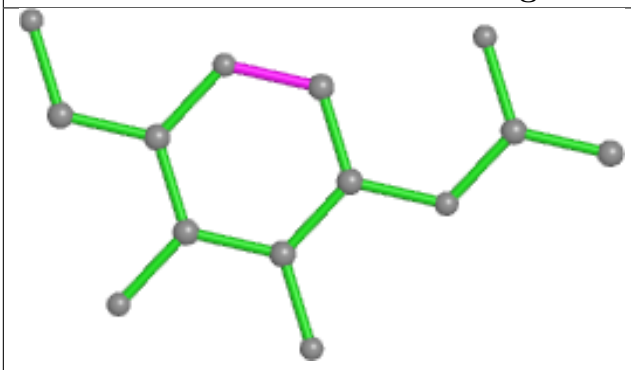


Torsions

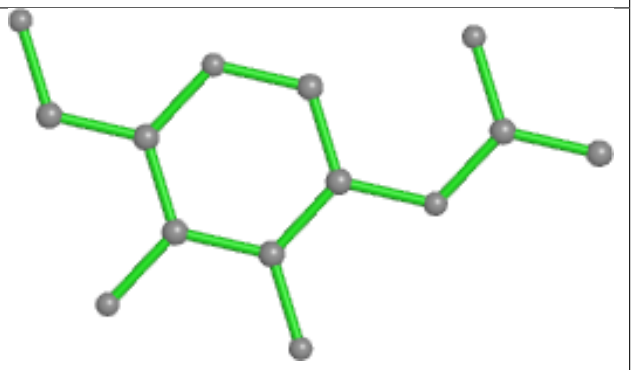


Rings

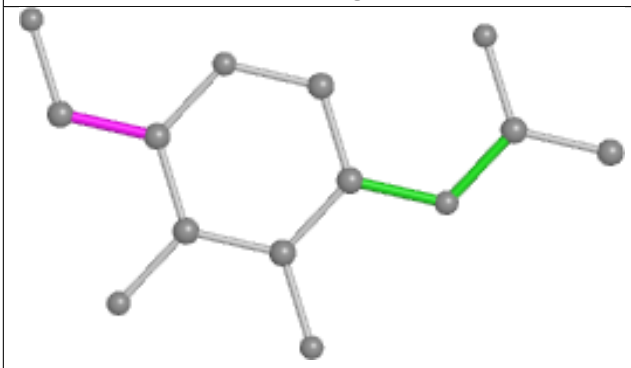
Ligand NAG D 501



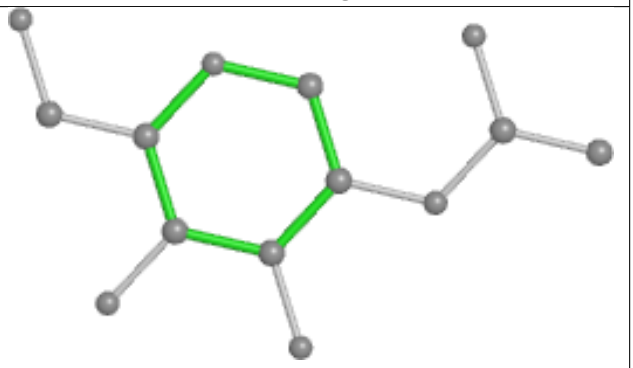
Bond lengths



Bond angles

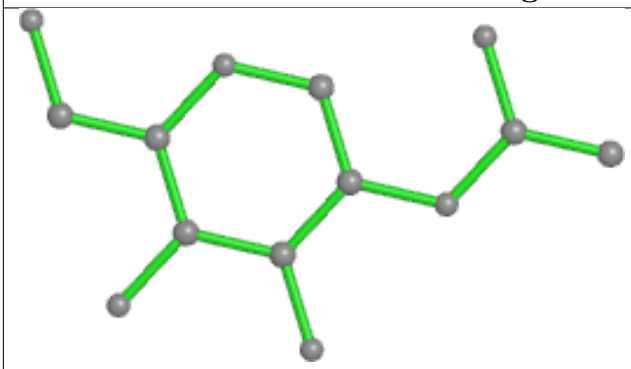


Torsions

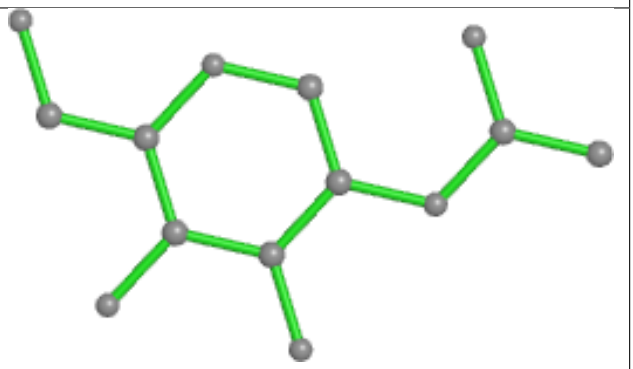


Rings

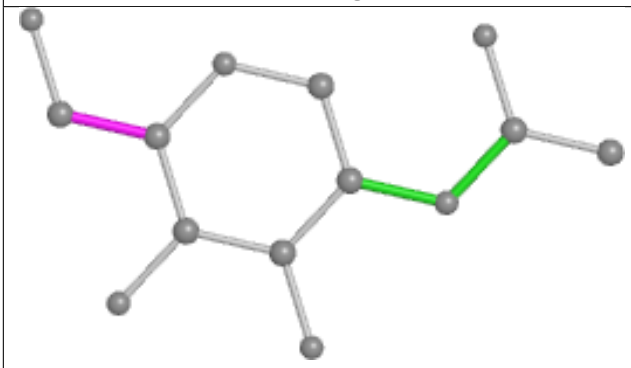
Ligand NAG P 101



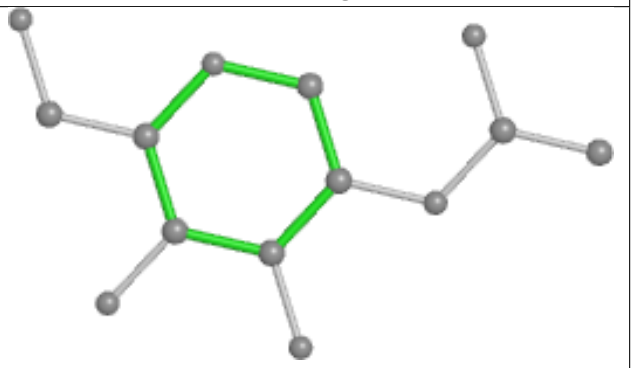
Bond lengths



Bond angles

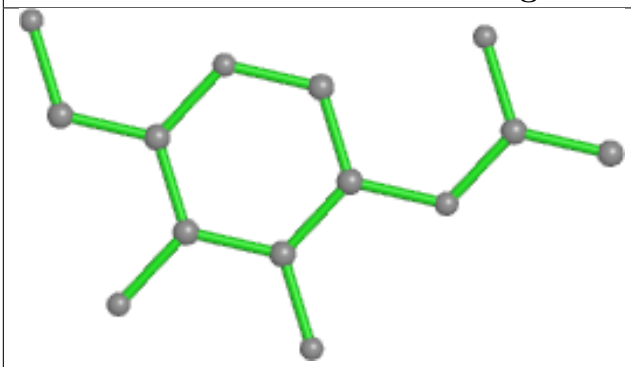


Torsions

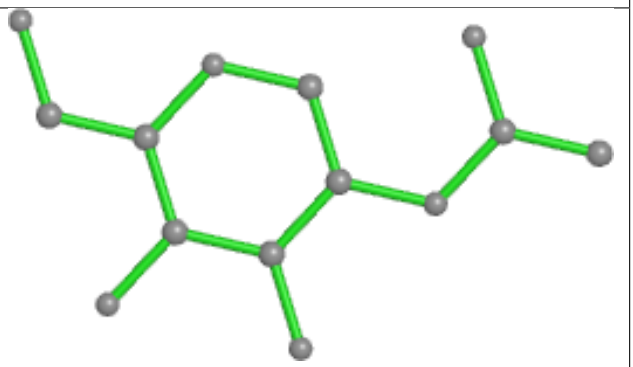


Rings

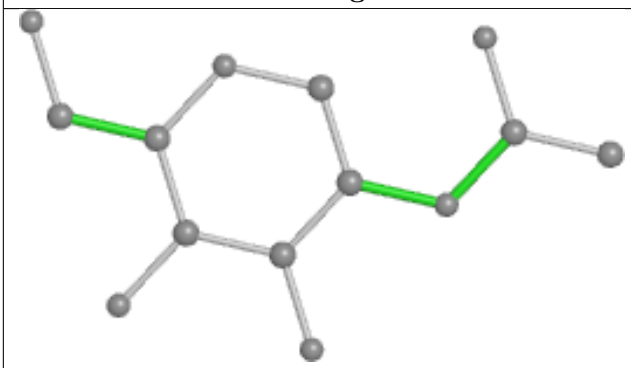
Ligand NAG O 101



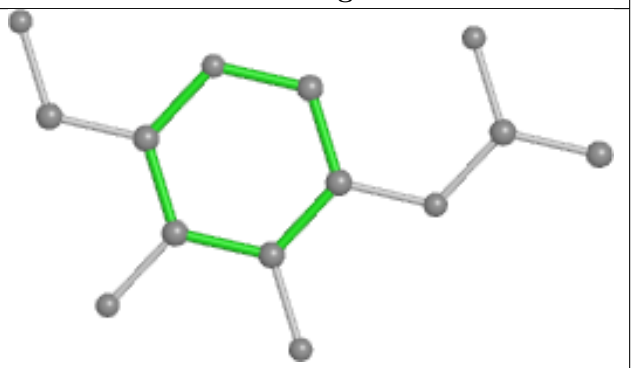
Bond lengths



Bond angles

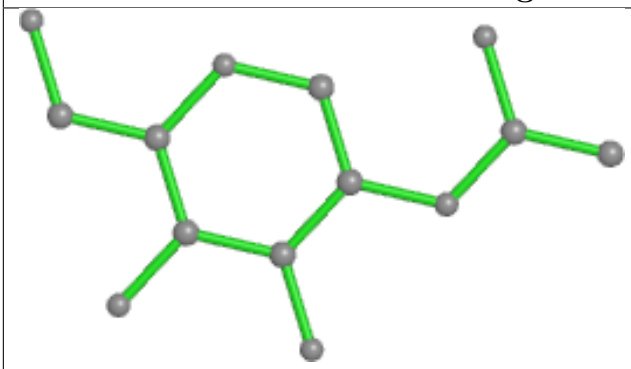


Torsions

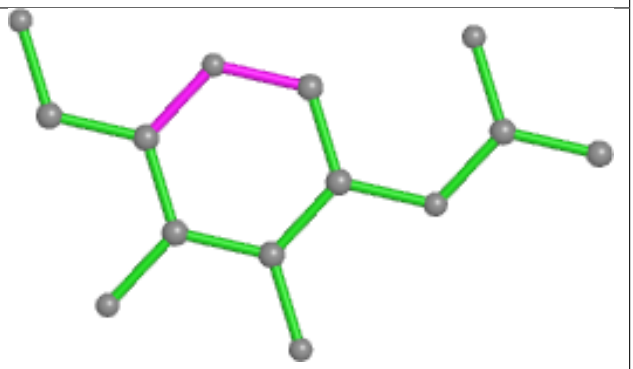


Rings

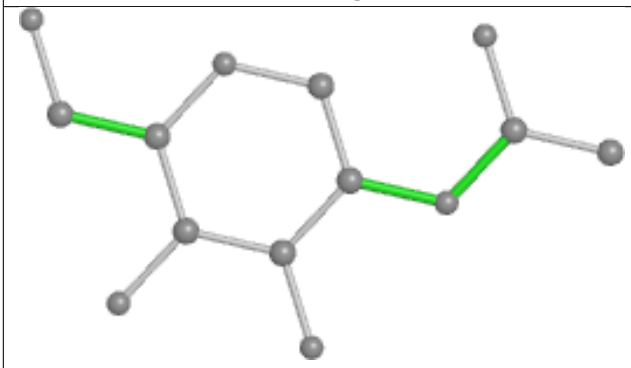
Ligand NAG M 101



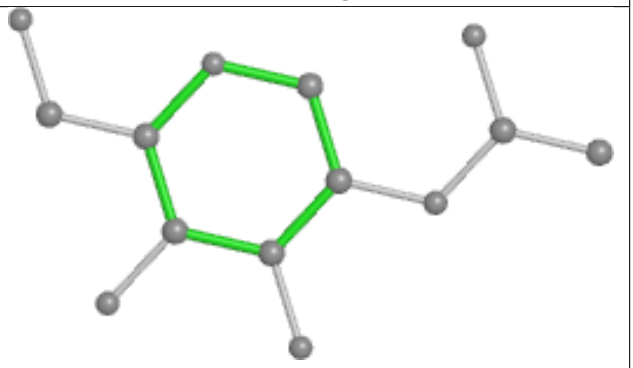
Bond lengths



Bond angles

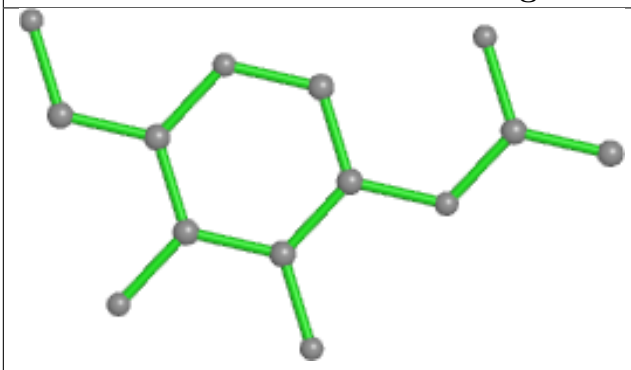


Torsions

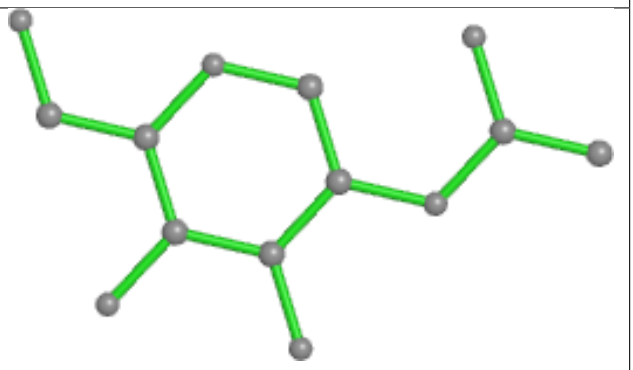


Rings

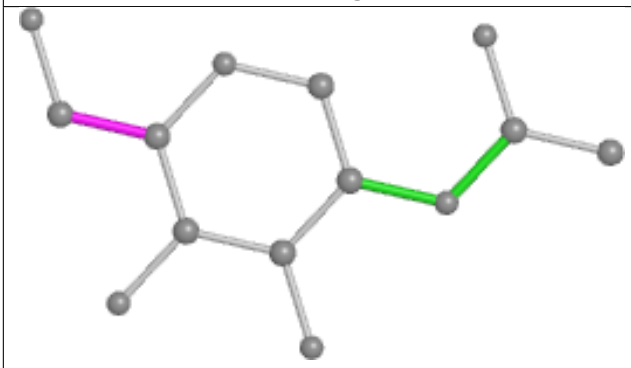
Ligand NAG A 501



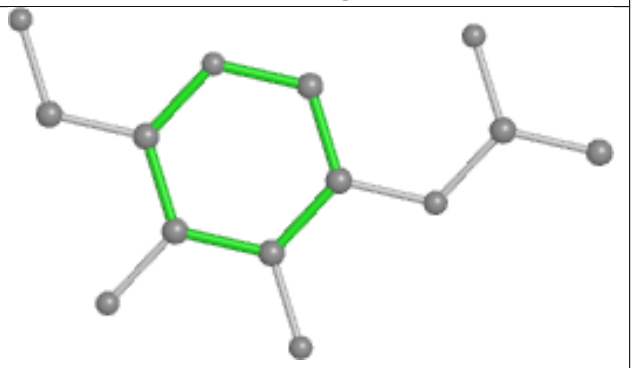
Bond lengths



Bond angles

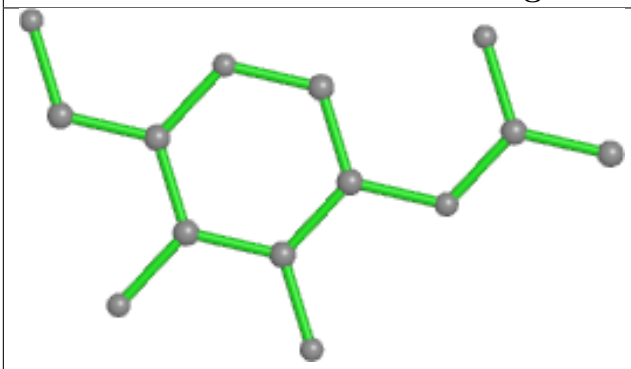


Torsions

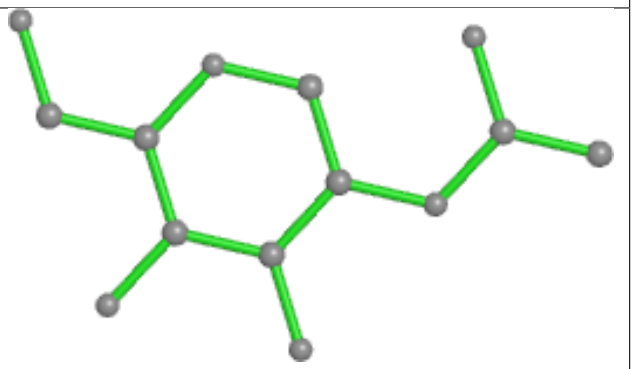


Rings

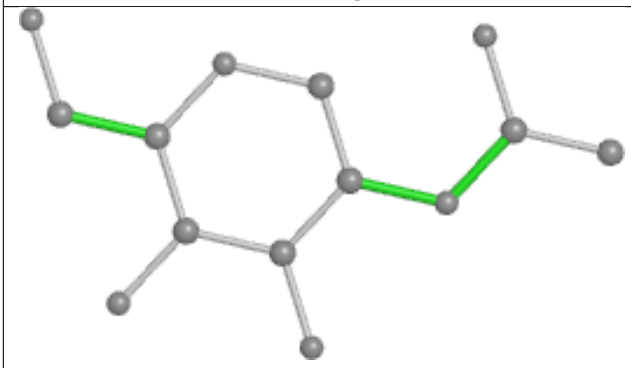
Ligand NAG J 501



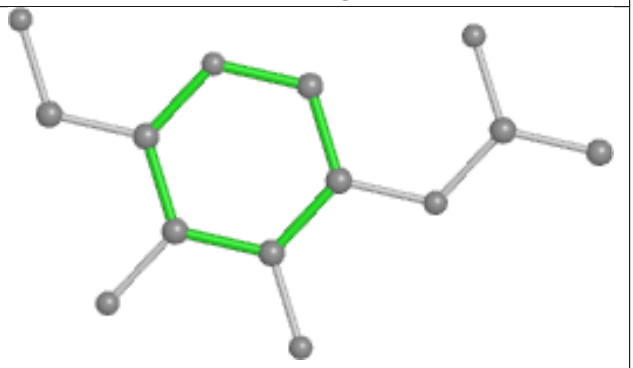
Bond lengths



Bond angles

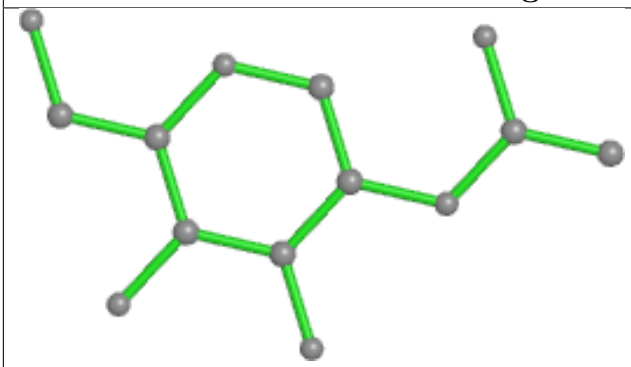


Torsions

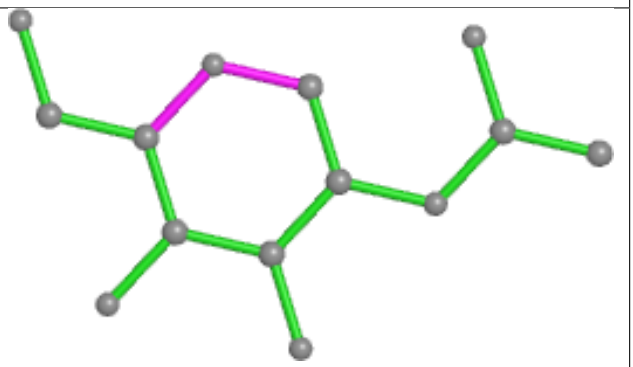


Rings

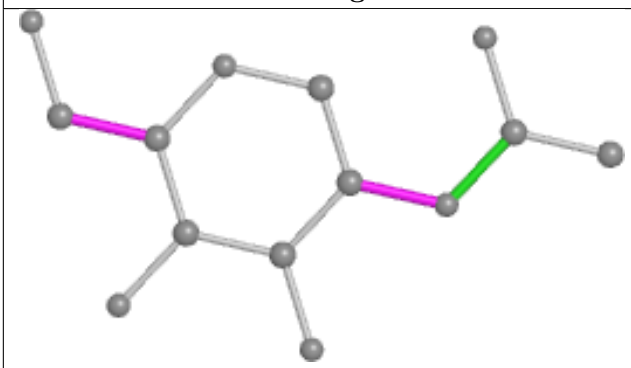
Ligand NAG E 501



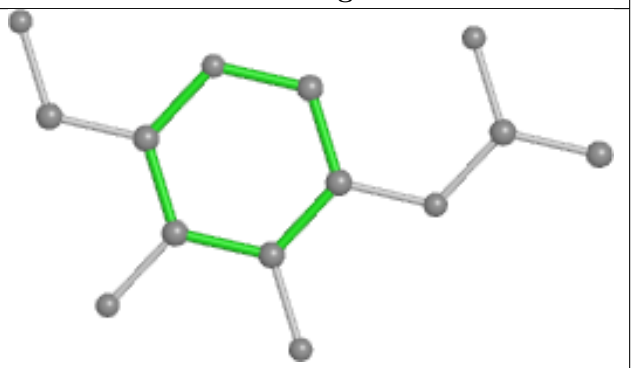
Bond lengths



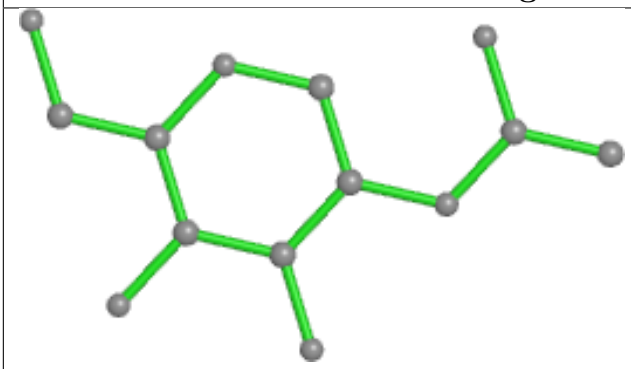
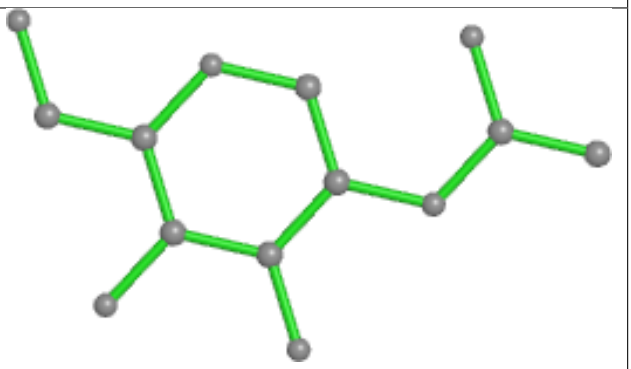
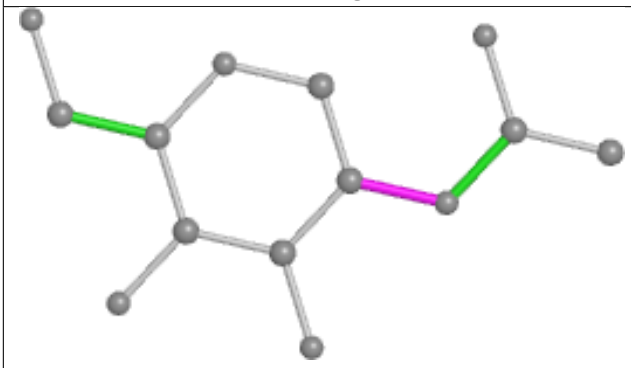
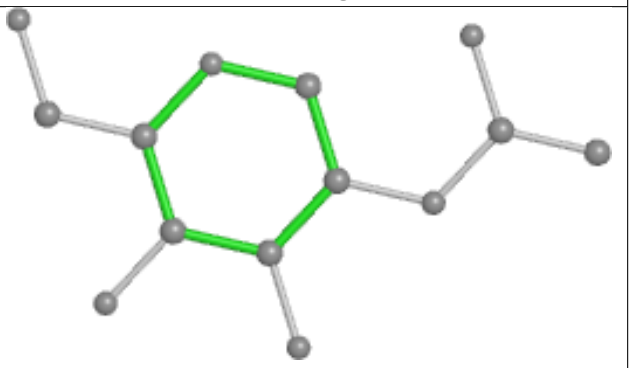
Bond angles



Torsions



Rings

Ligand NAG H 501	
 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.

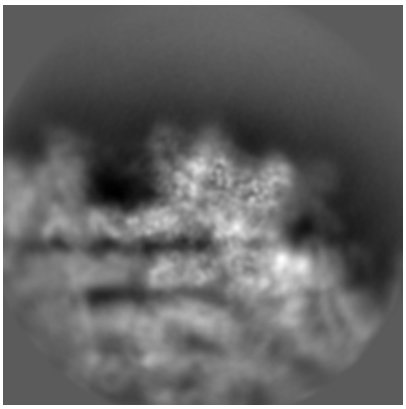
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42050. These allow visual inspection of the internal detail of the map and identification of artifacts.

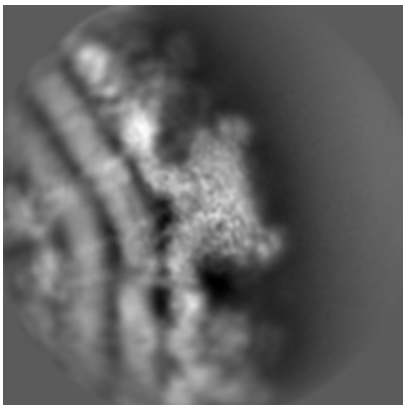
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

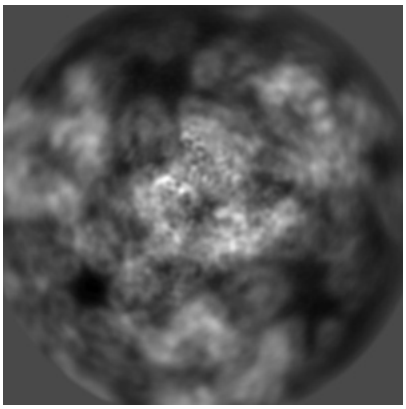
6.1.1 Primary map



X

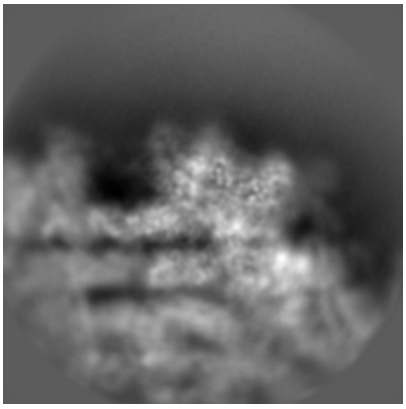


Y

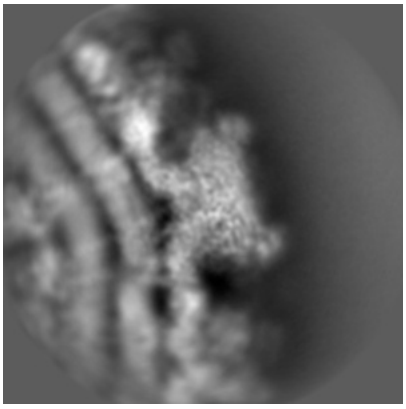


Z

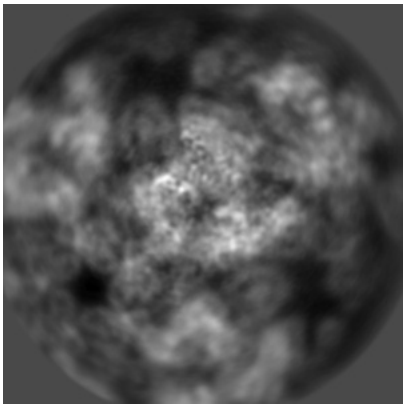
6.1.2 Raw map



X



Y

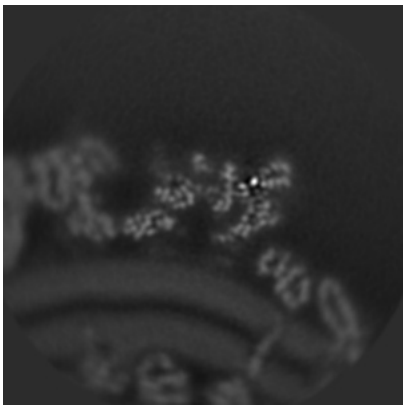


Z

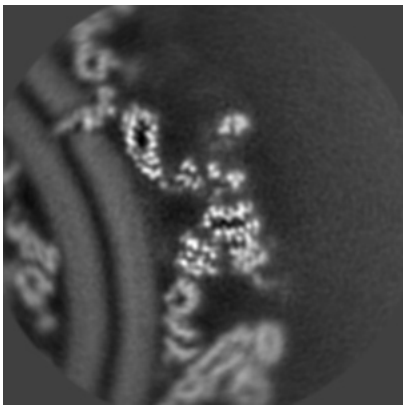
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

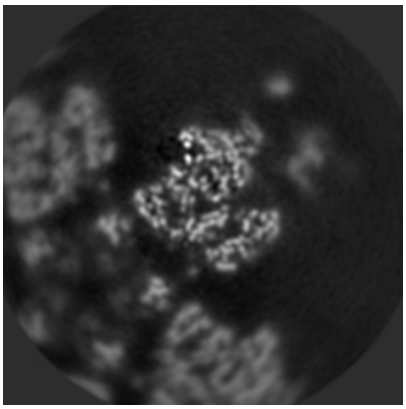
6.2.1 Primary map



X Index: 120

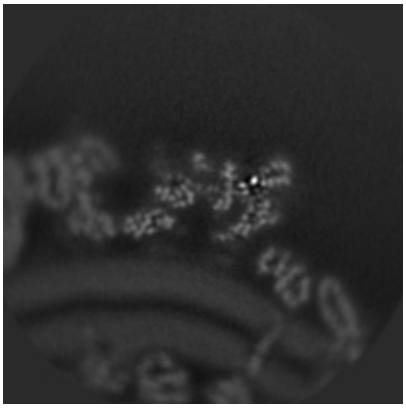


Y Index: 120

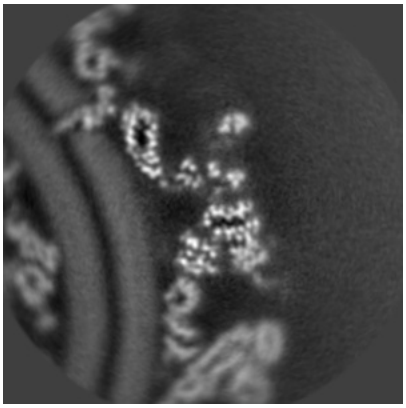


Z Index: 120

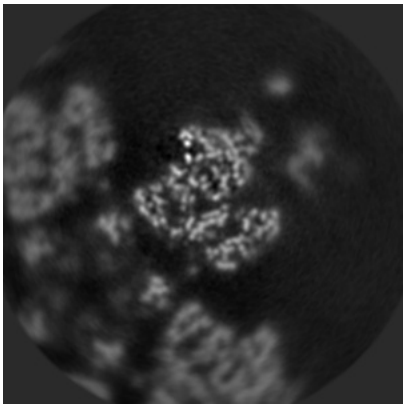
6.2.2 Raw map



X Index: 120



Y Index: 120

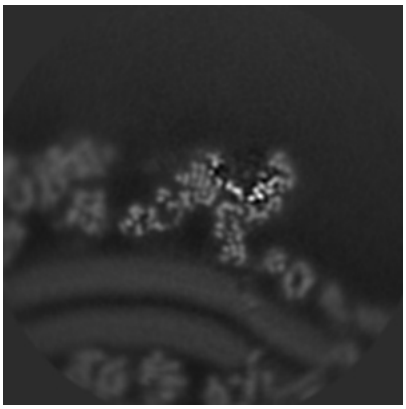


Z Index: 120

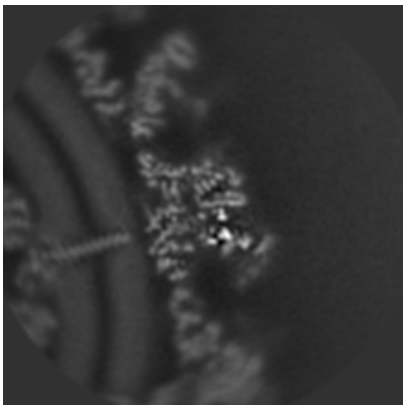
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

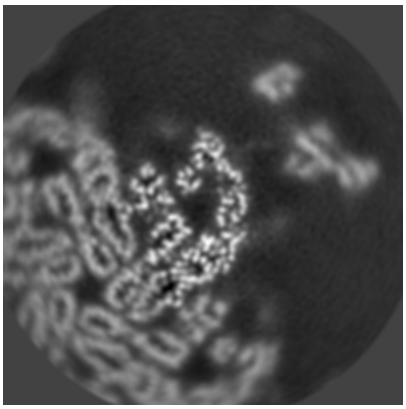
6.3.1 Primary map



X Index: 113

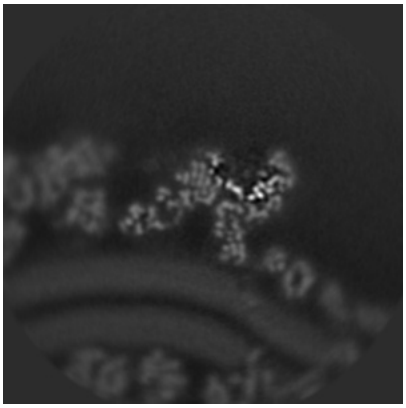


Y Index: 135

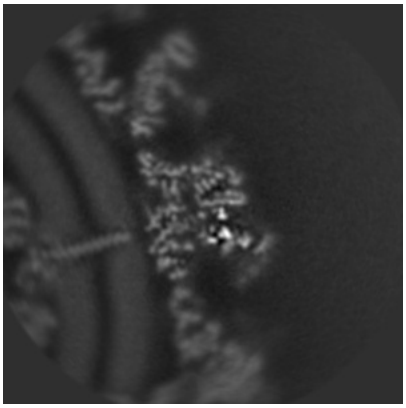


Z Index: 109

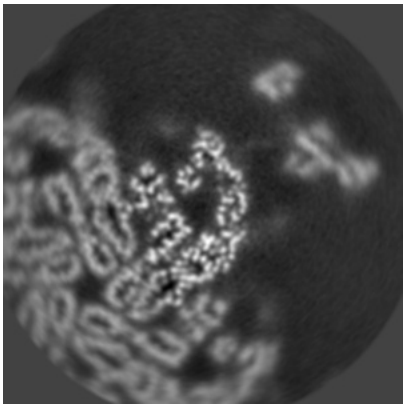
6.3.2 Raw map



X Index: 113



Y Index: 135

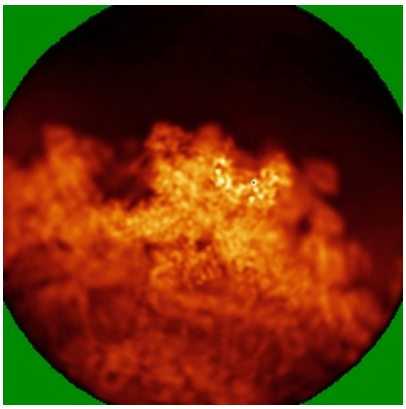


Z Index: 109

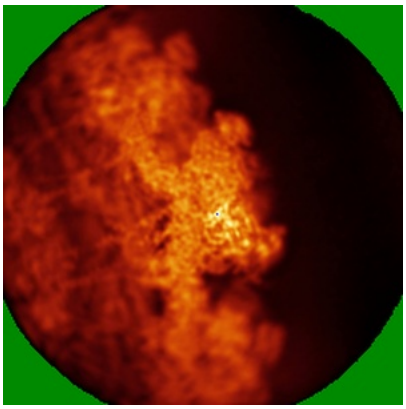
The images above show the largest variance slices of the map in three orthogonal directions.

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

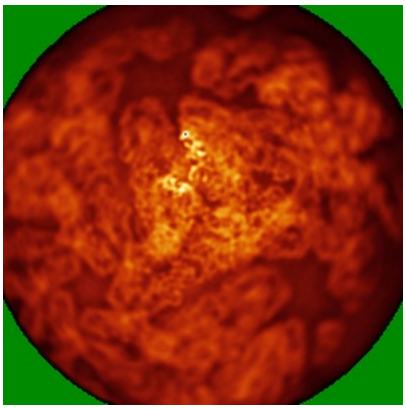
6.4.1 Primary map



X



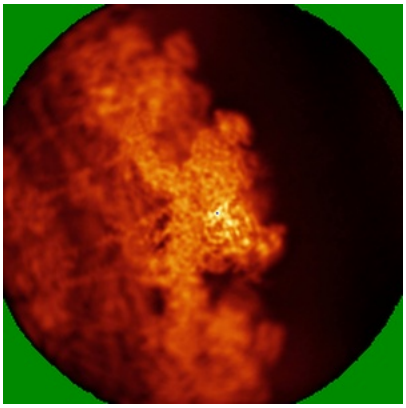
Y



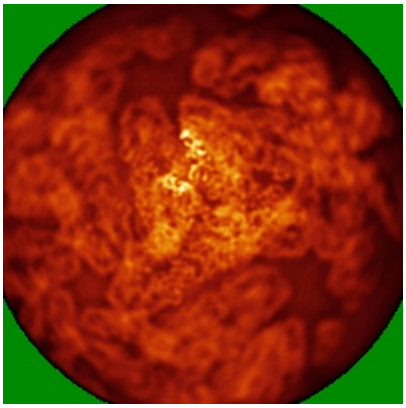
Z

6.4.2 Raw map

X



Y

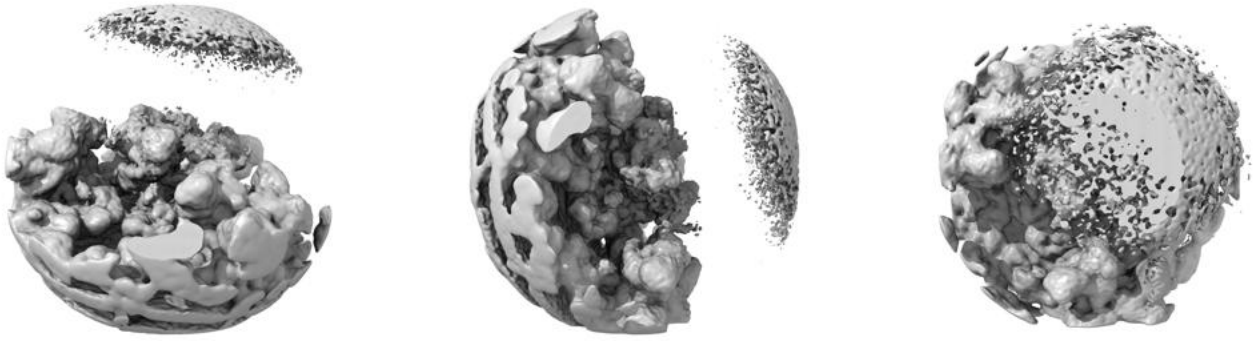


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

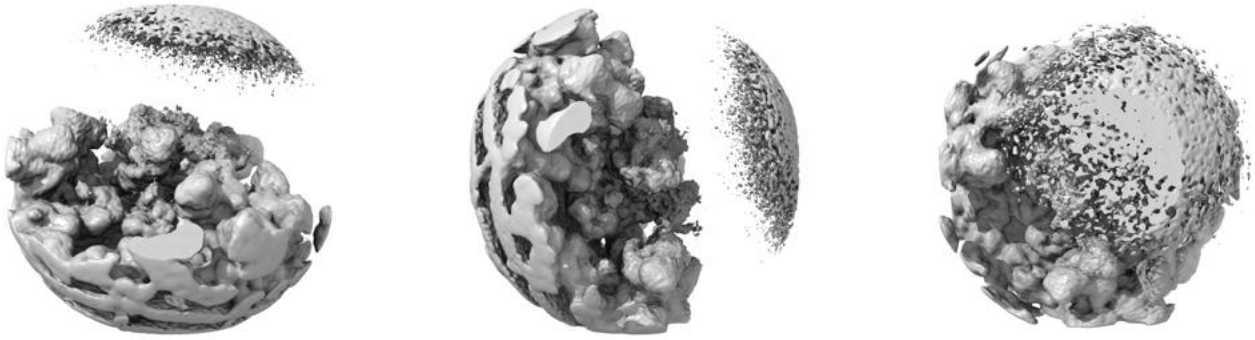
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

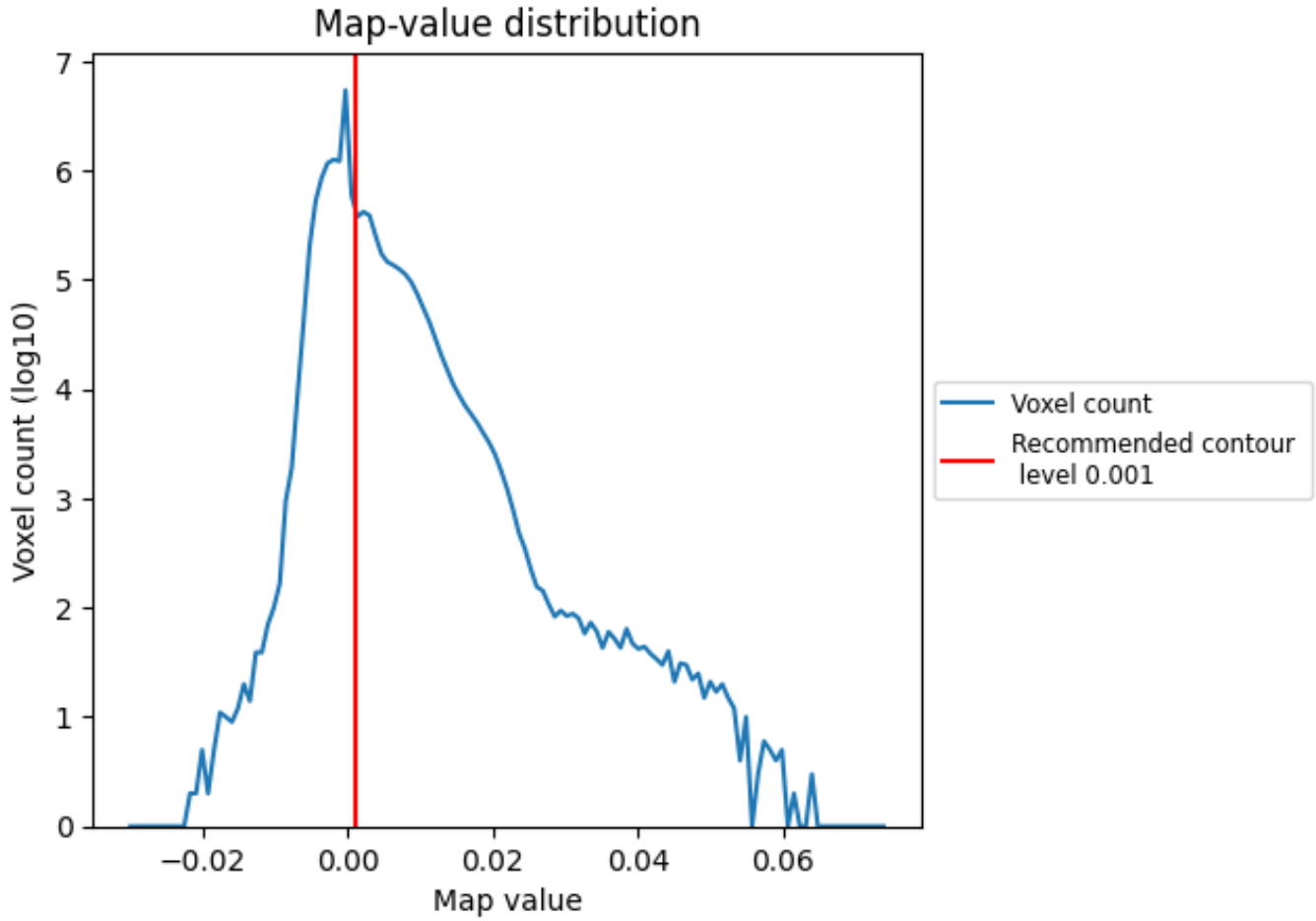
6.6 Mask visualisation (i)

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

7 Map analysis

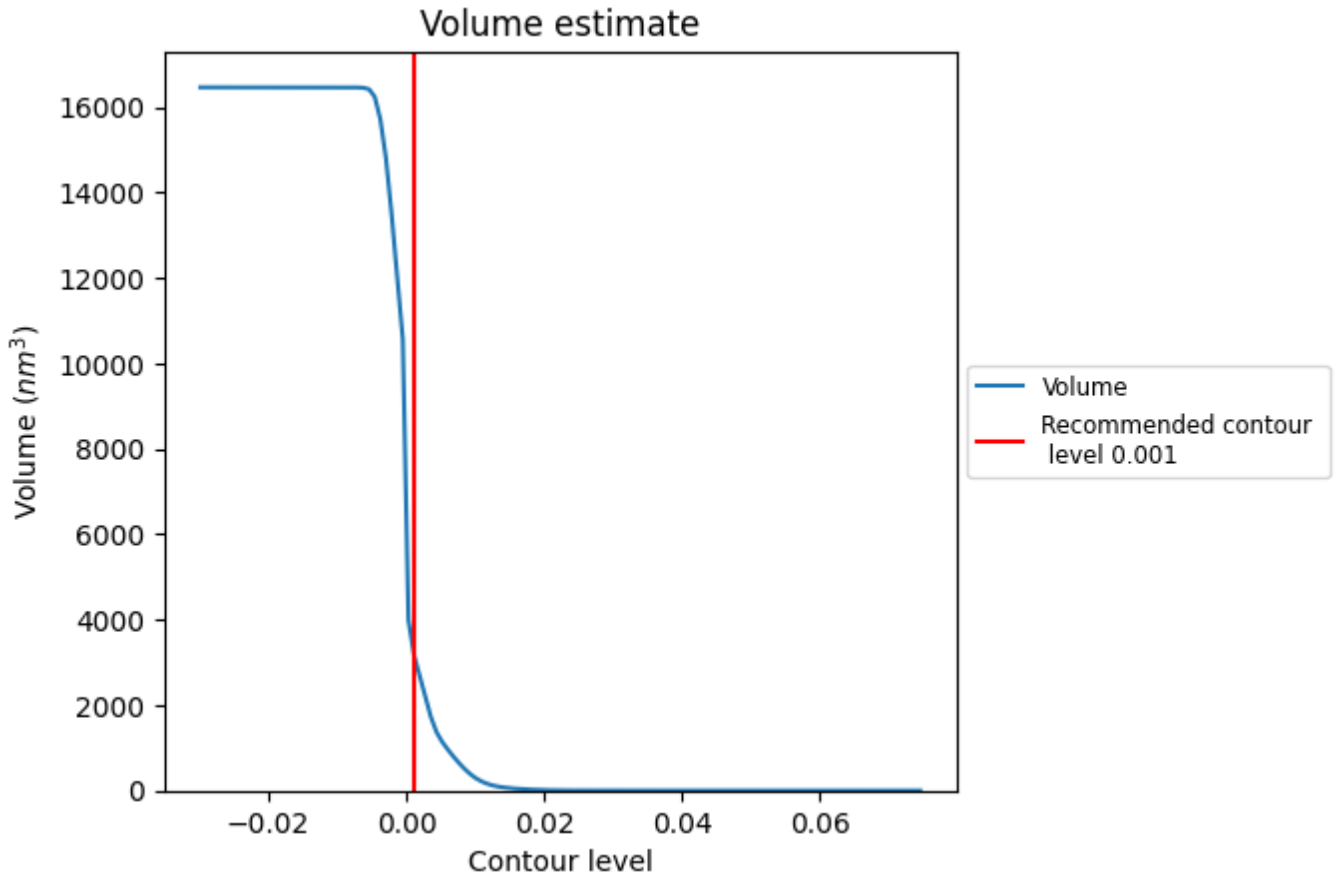
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

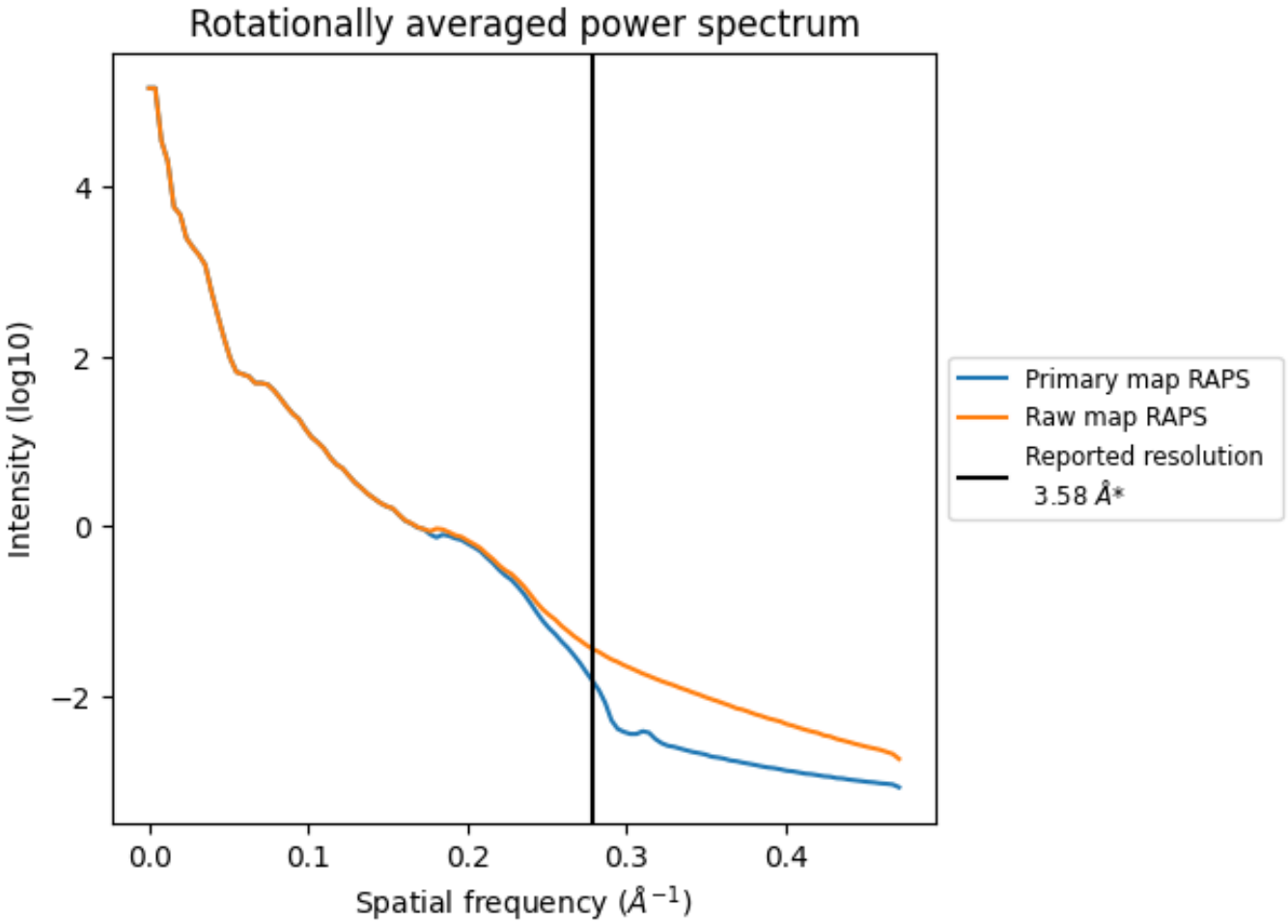
7.2 Volume estimate



The volume at the recommended contour level is 3296 nm^3; this corresponds to an approximate mass of 2978 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)

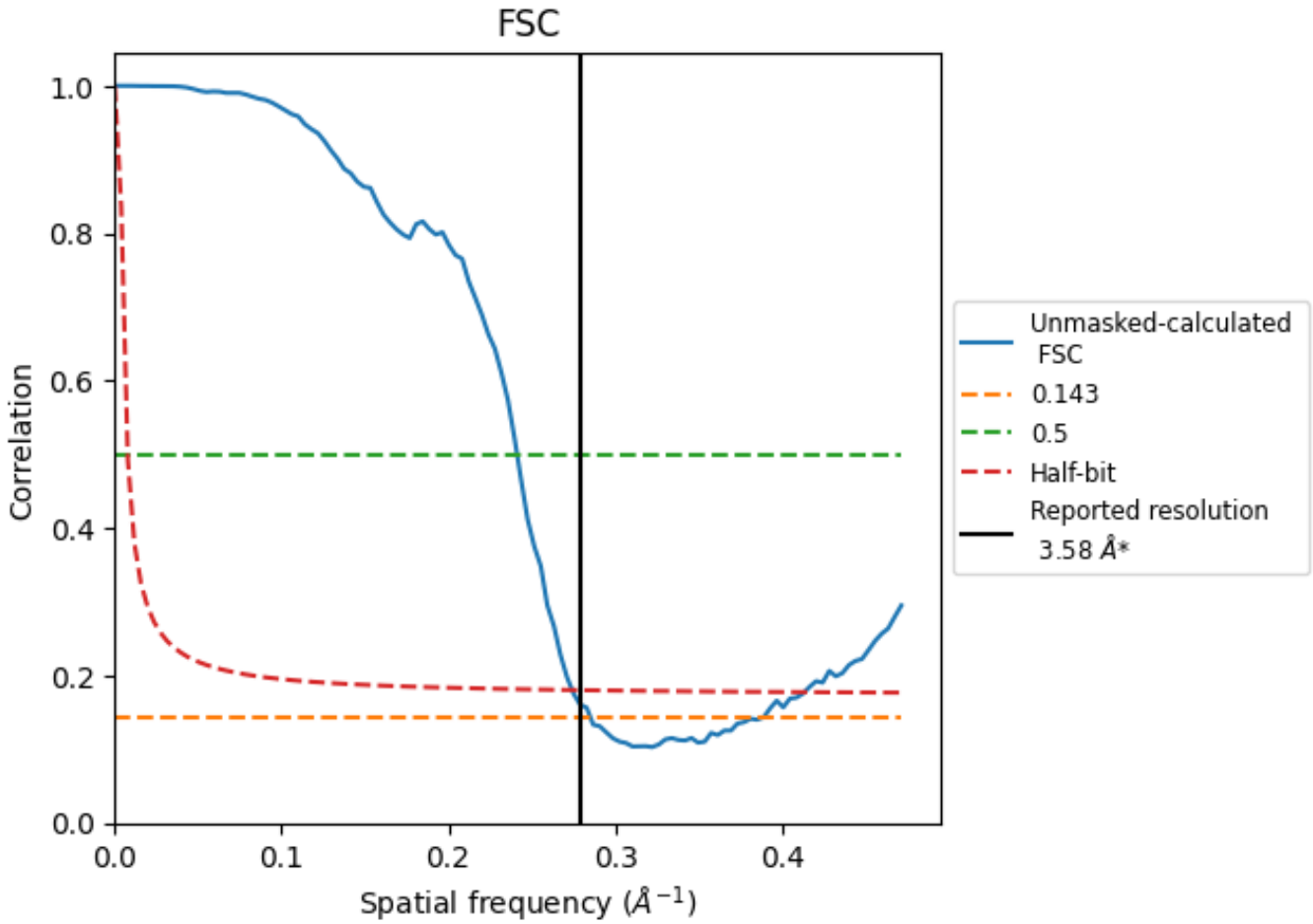


*Reported resolution corresponds to spatial frequency of 0.279 $Å^{-1}$

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 0.279 Å^{-1}

8.2 Resolution estimates (i)

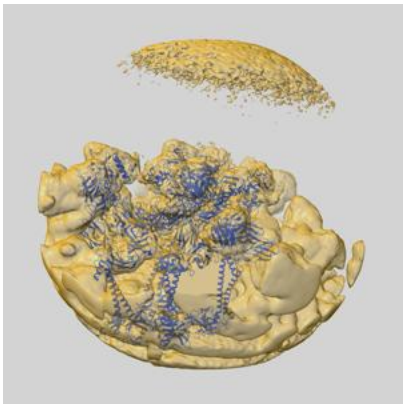
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.14	3.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

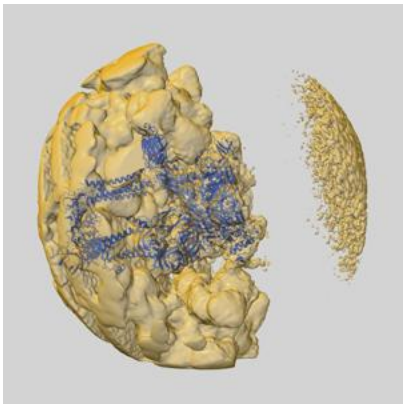
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42050 and PDB model 8UA4. Per-residue inclusion information can be found in section 3 on page 7.

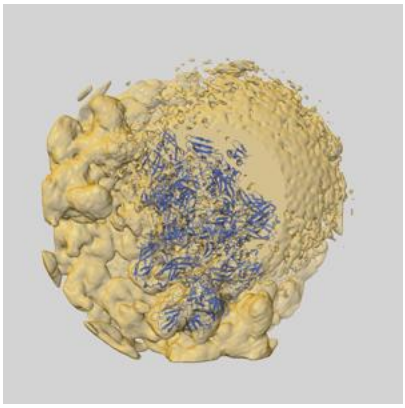
9.1 Map-model overlay



X



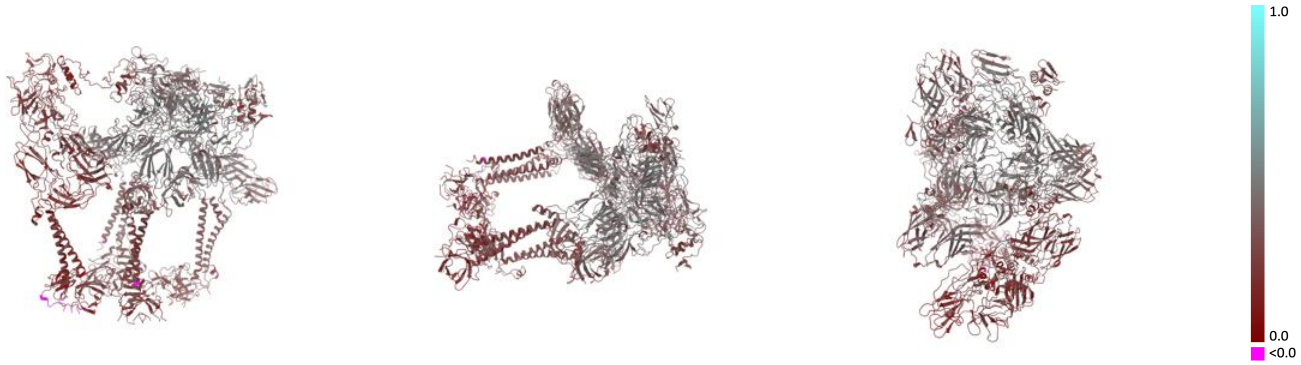
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.001 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.

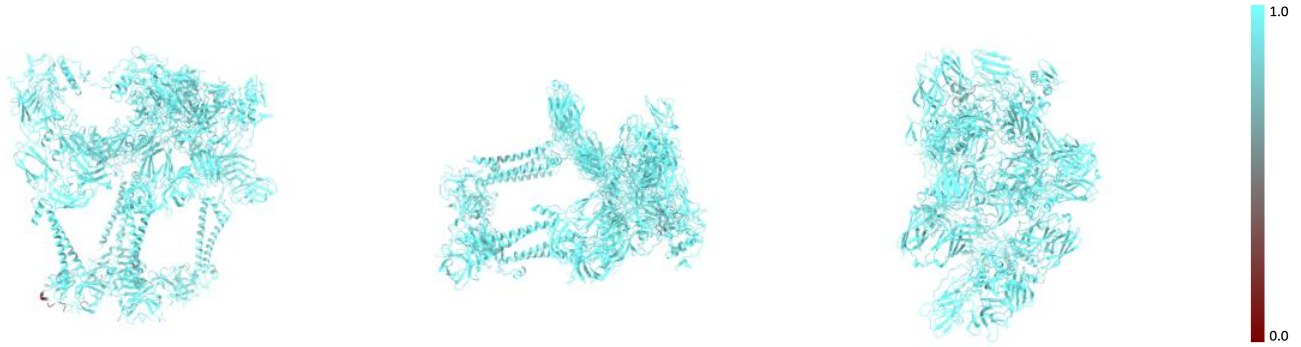
9.2 Q-score mapped to coordinate model (i)



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.

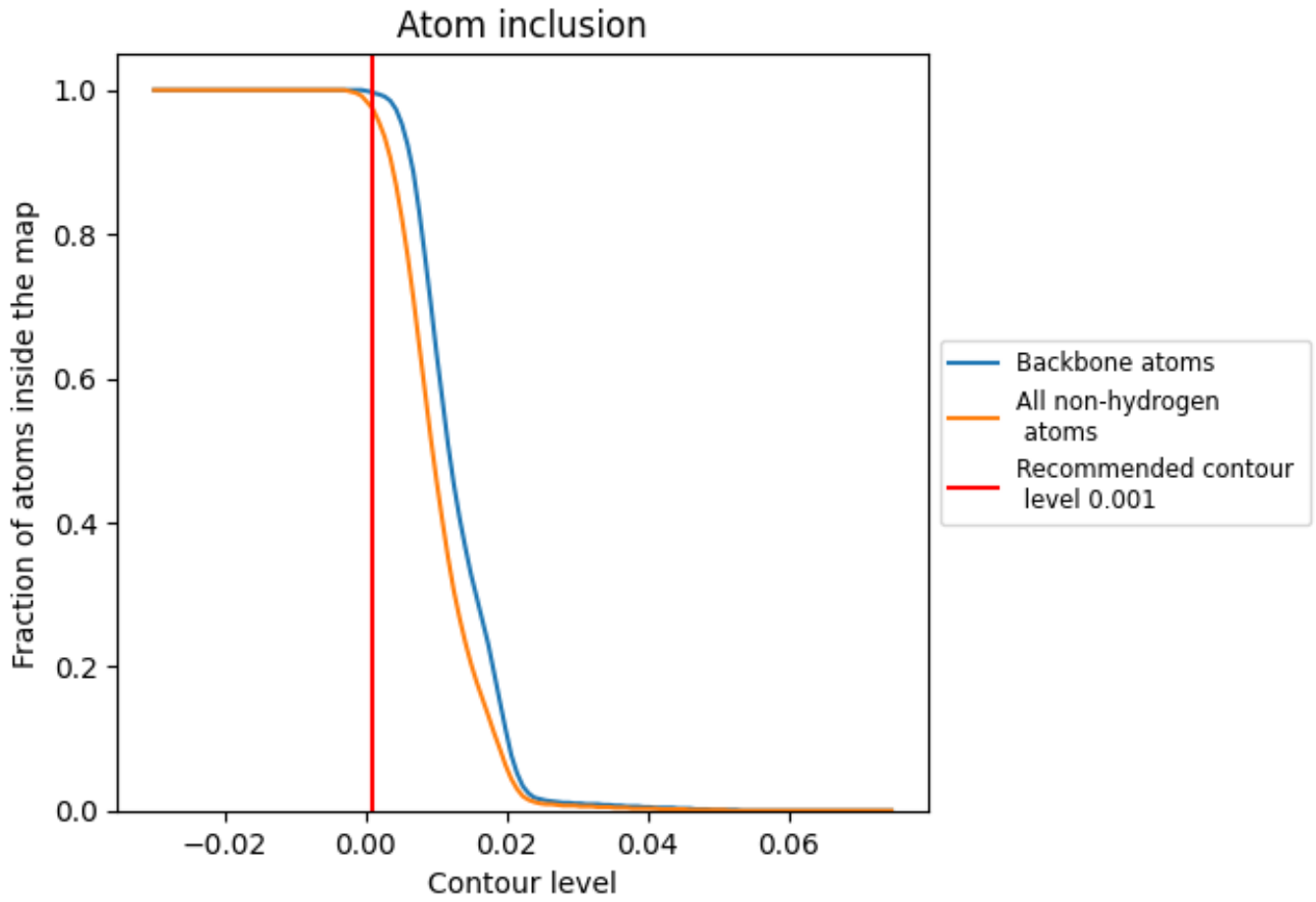
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.001).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9750	0.3300
A	0.9840	0.2500
B	0.9890	0.2160
C	0.9490	0.2380
D	0.9820	0.3810
E	0.9880	0.4000
F	0.9560	0.2440
G	0.9830	0.3980
H	0.9910	0.4070
I	0.8770	0.1510
J	0.9890	0.3780
K	0.9860	0.3950
L	0.9550	0.2280
M	0.9680	0.3130
N	0.9790	0.3150
O	0.9470	0.2810
P	0.9540	0.1910
R	0.6510	0.3140