



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:04 AM UTC

PDB ID : 8UA4 / pdb_00008ua4
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:

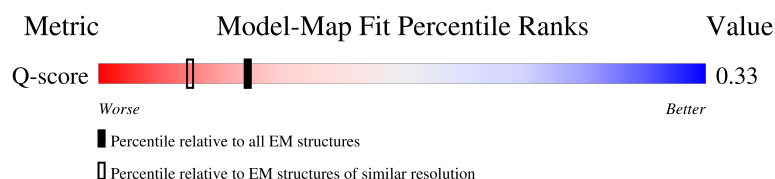
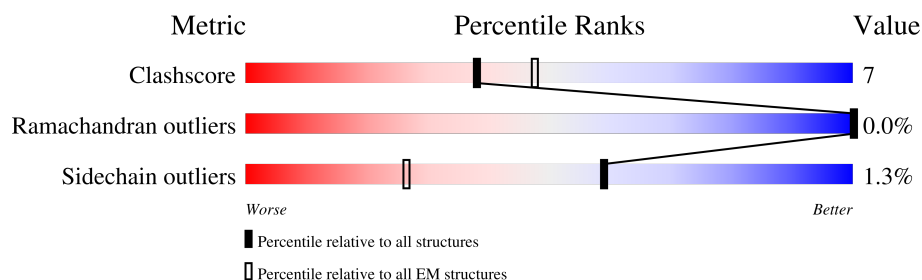
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.58 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.



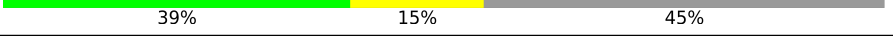
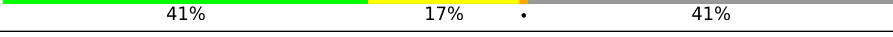
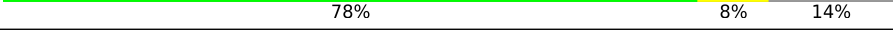
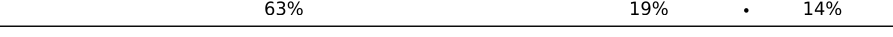
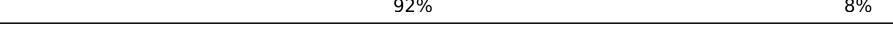
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12629 (3.08 - 4.08)

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 $\leq 5\%$. 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	
1	D	441	
1	G	441	
1	J	441	

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Mol	Chain	Length	Quality of chain
2	B	420	
2	E	420	
2	H	420	
2	K	420	
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

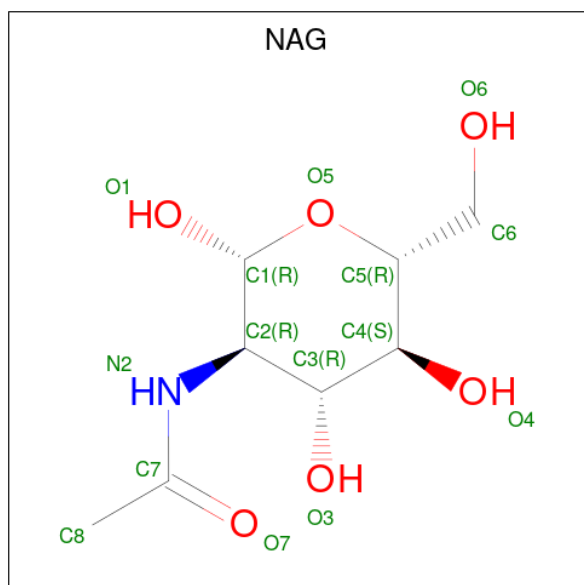
- Molecule 4 is a protein called Envelope glycoprotein E3.

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

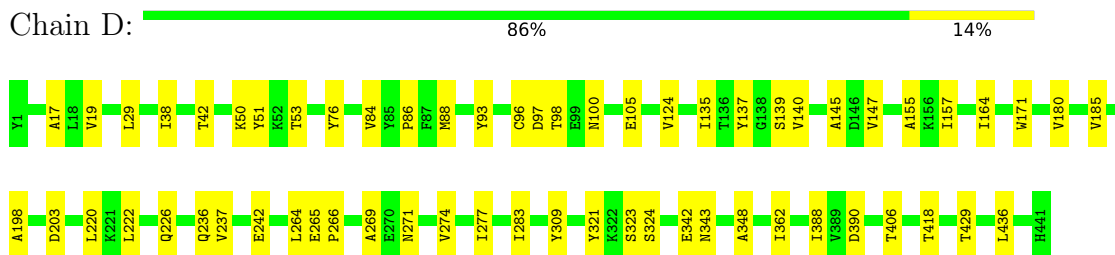
3 Residue-property plots

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.

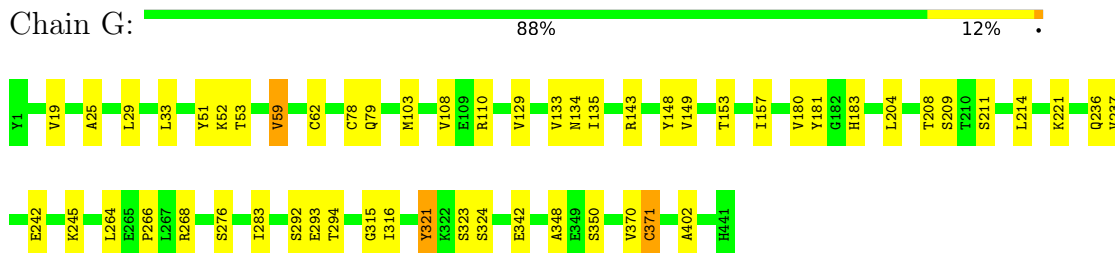
- Molecule 1: Envelope glycoprotein E1



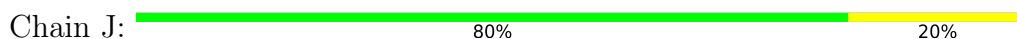
- Molecule 1: Envelope glycoprotein E1

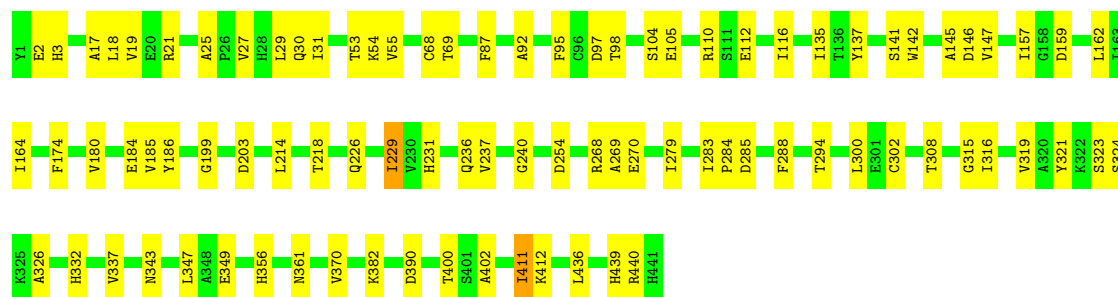


- Molecule 1: Envelope glycoprotein E1



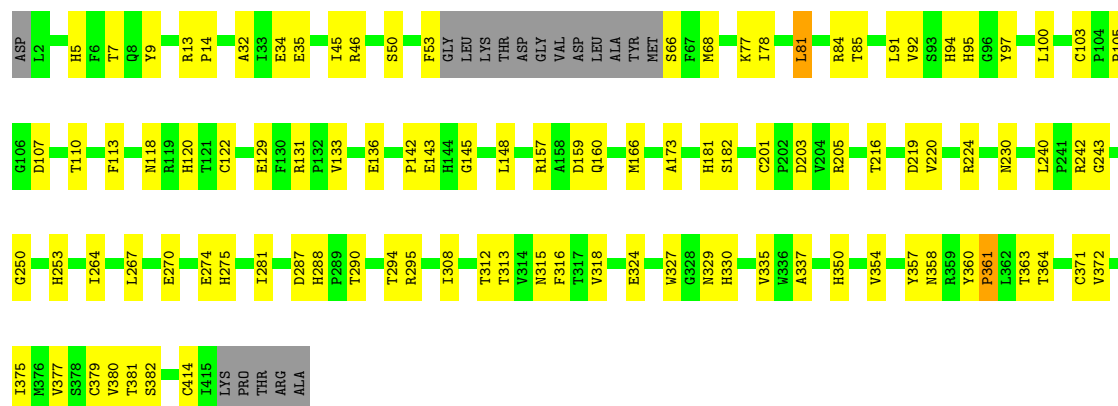
- Molecule 1: Envelope glycoprotein E1





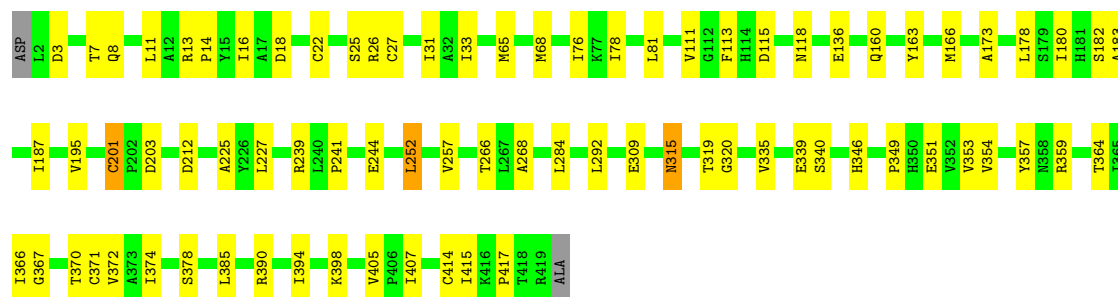
• Molecule 2: Envelope glycoprotein E2

Chain B: 72% 24%



• Molecule 2: Envelope glycoprotein E2

Chain E: 81% 18%



• Molecule 2: Envelope glycoprotein E2

Chain H: 85% 13%



• Molecule 2: Envelope glycoprotein E2

V352	H181	D1
Y356	T188	L2
T364	V189	T7
V372	C199	Q8
N391	K200	Y15
C393	C201	D18
I394	P202	N21
T395	G207	G22
K398	I208	G23
L399	T209	E34
A400	S210	E35
P401	S211	V36
N402	W233	H41
P406	G250	R46
I407	K251	I47
L408	L252	K56
L409	H253	G59
A410	W254	S93
L411	T255	H94
L412	K260	H95
I415	C263	G96
R419	T266	Y97
ALA	H277	Y98
	D287	I99
	T290	L100
	T294	D107
	R295	C122
	S296	T123
	D300	E136
	R305	E143
	N315	C150
	F316	N151
	E324	R152
	N329	Y153
	S340	K156
	P345	R157
	P349	E165
	H350	M166
	F351	H167
		Q168
		L171

Chain C: 39% 15% 45%

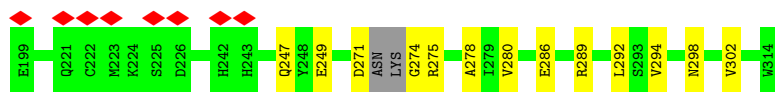
L228	G229	E233	G234	SER	ARG	T237	S240	V241	V242	T243	W244	N245	G246	K247	W251	PRO	ALA	GLY	PRO	PRO	ALA	ASN	ARG	LYS	PRO	ALA	PRO	ALA	PRO	LYS	LYS	PRO	ALA	PRO	ALA	GLN	ALA	ALA	LYS	LYS	ARG	PRO	ASN	PRO	PRO	PRO	ARG	ARG	ARG	TRP	ARG	PRO	PHE	ARG	PRO	ALA	ALA	LEU	LEU	ALA	GLN	ILE	GLU	ASP	LEU	ARG	ARG	ARG	SER	ILE	ALA	SER	LEU	THR	LEU	LYS	GLN	ARG	ALA	PRO	ASN	MET
V128	G131	R132	K135	V139	I143	E162	D165	V166	P167	M170	K171	T174	T178	S179	D180	P183	GLY	PHE	Y186	H190	G191	ALA	V193	Y195	GLU	N197	V202	PRO	R204	G205	VAL	G207	D211	R214	P215	I216	T217	D218	ASN	G220	G221	A225	E109	T116	M117	L118	Q121	V122	N123	A126	G127																															
PRO	ALA	GLY	PRO	PRO	ALA	ASN	ARG	ASN	LYS	LYS	PRO	ALA	PRO	ALA	GLN	ALA	ALA	LYS	LYS	ARG	PRO	PRO	PRO	PRO	LYS	LYS	ARG	GLN	ARG	MET	CYS	MET	LYS	E108	E109	T116	M117	L118	Q121	V122	N123	A126	G127																																							
MET	PHE	PRO	TYR	THR	LEU	ASN	TYR	PRO	PRO	MET	ALA	ILE	ASN	PRO	MET	ALA	TYR	ASP	PRO	ASN	PRO	ARG	ARG	ARG	TRP	ARG	PRO	PHE	PRO	PRO	ALA	ALA	GLN	ILE	GLU	ASP	LEU	ARG	ARG	SER	ILE	ALA	SER	LEU	THR	LEU	LYS	GLN	ARG	ALA	PRO	ASN	PRO																													

Chain F: 51% 8% 41%

R142	R143	I158	V166	P167	M170	T174	P182	Y186	N187	W188	V193	V202	I216	V227	L239	S240	V241	P255	W261																												
PRO	ALA	GLY	PRO	PRO	ALA	ASN	ARG	LYS	LYS	PRO	ALA	GLN	LYS	LYS	ARG	PRO	PRO	ALA	GLY	LYS	ARG	GLN	ARG	MET	K107	L108	E109	F114	M123	A126	G131	K135															
MET	PHE	PRO	TYR	THR	LEU	ASN	TYR	PRO	PRO	MET	ALA	TYR	ASP	ASN	PRO	ARG	ARG	TRP	ARG	PHE	ARG	PRO	PRO	LEU	ALA	ALA	GLN	ILE	GLU	ASP	LEU	ARG	ARG	SER	ILE	ALA	SER	LEU	THR	LEU	LYS	GLN	ARG	ALA	PRO	ASN	PRO

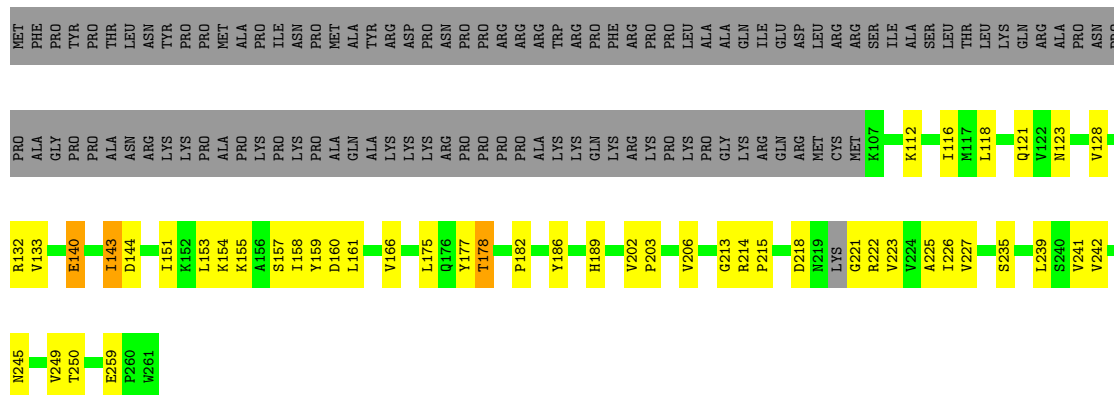
Chain I:

[illegible]



- Molecule 3: Capsid protein

Chain L: 41% 17% 41%



- Molecule 4: Envelope glycoprotein E3

Chain M: 78% 8% 14%



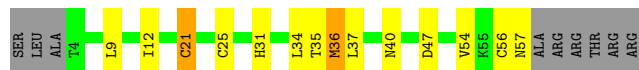
- Molecule 4: Envelope glycoprotein E3

Chain N: 70% 14% 14%



- Molecule 4: Envelope glycoprotein E3

Chain O: 63% 19% 14%

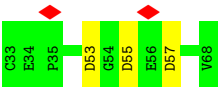
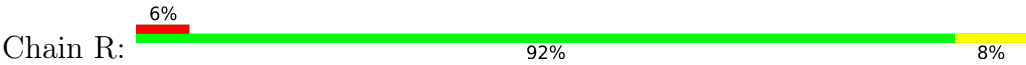


- Molecule 4: Envelope glycoprotein E3

Chain P: 68% 16% 14%



- Molecule 5: Very low-density lipoprotein receptor



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ($\text{\AA}$)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	0.51	0/3465	0.72	2/4730 (0.0%)
1	D	0.63	0/3469	0.69	0/4734
1	G	0.63	0/3469	0.68	1/4734 (0.0%)
1	J	0.59	0/3469	0.70	3/4734 (0.1%)
2	B	0.52	0/3257	0.80	4/4442 (0.1%)
2	E	0.59	0/3382	0.68	1/4612 (0.0%)
2	H	0.59	0/3352	0.71	0/4573
2	K	0.59	0/3386	0.74	3/4619 (0.1%)
3	C	0.47	0/1127	0.78	0/1515
3	F	0.52	0/1223	0.74	2/1657 (0.1%)
3	I	0.37	0/1196	0.68	0/1618
3	L	0.50	0/1213	0.79	2/1643 (0.1%)
4	M	0.37	0/431	0.68	0/588
4	N	0.38	0/431	0.92	1/588 (0.2%)
4	O	0.47	1/431 (0.2%)	0.98	1/588 (0.2%)
4	P	0.37	0/431	0.74	0/588
5	R	0.15	0/277	0.35	0/373
All	All	0.56	1/34009 (0.0%)	0.72	20/46336 (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	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	21	CYS	CB-SG	5.04	1.97	1.81

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	21	CYS	CA-CB-SG	10.30	138.09	114.40
3	L	215	PRO	CA-N-CD	-9.78	98.31	112.00
3	F	167	PRO	CA-N-CD	-8.90	99.54	112.00
2	B	361	PRO	CA-N-CD	-8.27	100.42	112.00
4	N	21	CYS	CA-CB-SG	8.20	133.25	114.40
2	E	417	PRO	CA-N-CD	-7.92	100.92	112.00
2	B	35	GLU	CA-CB-CG	7.21	128.52	114.10
3	F	255	PRO	CA-N-CD	-6.97	102.24	112.00
1	G	62	CYS	CA-CB-SG	-6.82	98.72	114.40
2	B	53	PHE	CA-CB-CG	-6.00	107.80	113.80
1	J	440	ARG	CA-C-N	5.59	131.76	121.70
1	J	440	ARG	C-N-CA	5.59	131.76	121.70
2	K	345	PRO	CA-N-CD	-5.55	104.22	112.00
1	J	411	ILE	CA-CB-CG1	5.51	119.77	110.40
1	A	334	PRO	CA-N-CD	-5.25	104.65	112.00
2	B	105	PRO	CA-N-CD	-5.16	104.78	112.00
2	K	107	ASP	N-CA-CB	-5.08	104.25	111.00
1	A	265	GLU	CA-CB-CG	5.06	124.22	114.10
2	K	251	LYS	CA-CB-CG	5.05	124.19	114.10
3	L	215	PRO	N-CA-C	5.01	119.11	111.34

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	346	THR	Peptide

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Mol	Chain	Res	Type	Group
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
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	59	0
1	D	3375	0	3280	44	0
1	G	3375	0	3280	31	0
1	J	3375	0	3280	60	0
2	B	3165	0	3126	65	0
2	E	3287	0	3255	49	0
2	H	3258	0	3215	35	0
2	K	3291	0	3251	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1110	0	1089	28	0
3	F	1196	0	1181	16	0
3	I	1171	0	1149	13	0
3	L	1187	0	1167	36	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	32514	488	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 (488) 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
4:N:25:CYS:SG	4:N:33:THR:OG1	2.41	0.79
2:H:414:CYS:SG	2:H:415:ILE:N	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:166:MET:HE3	2:K:252:LEU:HD12	1.67	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
2:K:156:LYS:HZ2	5:R:53:ASP:CG	2.00	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
1:A:66:THR:HG23	1:A:103:MET:HE3	1.75	0.69
2:E:166:MET:SD	2:E:252:LEU:HD12	2.32	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:291:ILE:O	1:A:294:THR:OG1	2.13	0.65
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: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
1:J:308:THR:OG1	1:J:382:LYS:O	2.17	0.62
3:C:109:GLU:OE1	3:C:109:GLU:N	2.33	0.62
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
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:A:325:LYS:NZ	1:A:326:ALA:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:TYR:HE2	2:K:166:MET:HE1	1.67	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: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:112:GLU:OE2	2:B:46:ARG:NH2	2.35	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:400:ALA:O	3:L:177:TYR:OH	2.19	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
1:G:143:ARG:C	1:G:157:ILE:HD11	2.28	0.58
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:97:TYR:CE2	2:K:166:MET:HE1	2.39	0.58
2:K:36:VAL:HG13	2:K:47:ILE:HG22	1.84	0.58
1:A:181:TYR:OH	1:A:245:LYS:NZ	2.34	0.57
2:B:329:ASN:OD1	2:B:329:ASN:N	2.34	0.57
2:E:182:SER:OG	2:E:183:ALA:N	2.38	0.57
1:A:53:THR:O	1:A:53:THR:OG1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:117:MET:HE3	3:C:117:MET:HA	1.91	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
2:K:207:GLY:C	2:K:208:ILE:HD12	2.35	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:274:GLU:CD	2:B:281:ILE:HD11	2.37	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
1:G:53:THR:HG21	1:G:236:GLN:CD	2.37	0.50
2:K:315:ASN:OD1	2:K:315:ASN:N	2.41	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
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
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
2:H:386:LEU:O	2:H:389:THR:OG1	2.26	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:134:ASN:C	1:G:135:ILE:HD12	2.37	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:88:MET:HE2	2:E:241:PRO:HD3	1.95	0.48
1:D:342:GLU:OE1	1:D:342:GLU:N	2.46	0.48
2:H:8:GLN:CD	4:M:50:LEU:HD21	2.39	0.47
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
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
3:F:170:MET:HE3	3:F:170:MET:N	2.28	0.47
1:J:53:THR:HG21	1:J:236:GLN:OE1	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:MET:HE1	3:C:122:VAL:HG22	1.98	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: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
2:B:145:GLY:HA2	2:B:267:LEU:HD23	1.97	0.45
3:C:135:LYS:NZ	3:C:162:GLU:OE1	2.44	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
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
1:J:402:ALA:O	2:K:356:TYR:OH	2.29	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
3:F:182:PRO:O	3:F:186:TYR:OH	2.29	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
2:K:287:ASP:OD2	2:K:287:ASP:N	2.41	0.45
1:J:53:THR:O	1:J:53:THR:OG1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:143:ILE:HD12	3:L:144:ASP:N	2.32	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:131:GLY:N	3:C:174:THR:HG21	2.32	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
3:L:213:GLY:C	3:L:226:ILE:HD11	2.42	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:319:THR:OG1	2:E:320:GLY:N	2.52	0.43
1:J:315:GLY:C	1:J:316:ILE:HD13	2.43	0.43
1:A:168:SER:HG	1:A:276:SER:H	1.62	0.43
6:B:501:NAG:HO3	6:B:501:NAG:C7	2.25	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
1:G:321:TYR:OH	1:G:348:ALA:O	2.23	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
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
2:B:148:LEU:C	2:B:148:LEU:HD12	2.43	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
4:M:47:ASP:OD1	4:M:47:ASP:N	2.51	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:GLY:C	1:G:316:ILE:HD13	2.45	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
2:E:65:MET:HE1	2:E:113:PHE:HB2	2.02	0.42
2:E:136:GLU:OE2	2:E:268:ALA:N	2.53	0.42
3:I:164:ASP:OD1	3:I:164:ASP:N	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:131:GLY:C	3:F:166:VAL:HG12	2.46	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
1:J:68:CYS:SG	1:J:69:THR:N	2.86	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%)	36	65
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 ⓘ

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%)	366 (99%)	4 (1%)	65	74
1	D	371/371 (100%)	369 (100%)	2 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	371/371 (100%)	363 (98%)	8 (2%)	45	65
1	J	371/371 (100%)	369 (100%)	2 (0%)	81	80
2	B	353/367 (96%)	348 (99%)	5 (1%)	59	71
2	E	366/367 (100%)	362 (99%)	4 (1%)	65	74
2	H	362/367 (99%)	355 (98%)	7 (2%)	50	67
2	K	366/367 (100%)	361 (99%)	5 (1%)	59	71
3	C	120/221 (54%)	119 (99%)	1 (1%)	73	77
3	F	129/221 (58%)	128 (99%)	1 (1%)	73	77
3	I	126/221 (57%)	126 (100%)	0	100	100
3	L	128/221 (58%)	125 (98%)	3 (2%)	44	64
4	M	50/57 (88%)	50 (100%)	0	100	100
4	N	50/57 (88%)	50 (100%)	0	100	100
4	O	50/57 (88%)	48 (96%)	2 (4%)	28	53
4	P	50/57 (88%)	47 (94%)	3 (6%)	17	44
5	R	33/33 (100%)	33 (100%)	0	100	100
All	All	3666/4097 (90%)	3619 (99%)	47 (1%)	59	72

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	279	ILE
1	A	332	HIS
1	A	367	LYS
1	A	391	TYR
2	B	66	SER
2	B	81	LEU
2	B	122	CYS
2	B	315	ASN
2	B	371	CYS
3	C	162	GLU
1	D	139	SER
1	D	222	LEU
2	E	27	CYS
2	E	187	ILE
2	E	252	LEU
2	E	315	ASN
3	F	135	LYS

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Mol	Chain	Res	Type
1	G	52	LYS
1	G	59	VAL
1	G	221	LYS
1	G	242	GLU
1	G	276	SER
1	G	321	TYR
1	G	342	GLU
1	G	371	CYS
2	H	7	THR
2	H	55	LEU
2	H	99	ILE
2	H	168	GLN
2	H	252	LEU
2	H	315	ASN
2	H	383	VAL
1	J	95	PHE
1	J	229	ILE
2	K	168	GLN
2	K	199	CYS
2	K	305	ARG
2	K	315	ASN
2	K	372	VAL
3	L	140	GLU
3	L	143	ILE
3	L	178	THR
4	O	9	LEU
4	O	36	MET
4	P	11	ASN
4	P	22	MET
4	P	41	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	253	HIS
2	B	346	HIS
3	C	121	GLN
1	D	3	HIS
1	D	43	ASN
2	E	126	HIS
1	G	3	HIS
3	I	198	ASN

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Mol	Chain	Res	Type
3	I	243	HIS
3	I	251	ASN
1	J	3	HIS
1	J	125	HIS
1	J	130	GLN
2	K	24	HIS
2	K	168	GLN
2	K	283	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	P	101	4	14,14,15	0.26	0	17,19,21	0.39	0
6	NAG	G	501	1	14,14,15	0.74	1 (7%)	17,19,21	0.55	0
6	NAG	H	501	2	14,14,15	0.44	0	17,19,21	0.42	0
6	NAG	K	501	2	14,14,15	0.51	0	17,19,21	0.55	0
6	NAG	O	101	4	14,14,15	0.22	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	E	501	2	14,14,15	0.36	0	17,19,21	0.68	1 (5%)
6	NAG	D	501	1	14,14,15	0.73	1 (7%)	17,19,21	0.55	0
6	NAG	B	501	2	14,14,15	0.91	1 (7%)	17,19,21	0.49	0
6	NAG	M	101	4	14,14,15	0.21	0	17,19,21	0.76	1 (5%)
6	NAG	A	501	1	14,14,15	0.37	0	17,19,21	0.57	0
6	NAG	J	501	1	14,14,15	0.49	0	17,19,21	0.58	0
6	NAG	N	101	4	14,14,15	0.25	0	17,19,21	0.54	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	P	101	4	-	2/6/23/26	0/1/1/1
6	NAG	G	501	1	-	1/6/23/26	0/1/1/1
6	NAG	H	501	2	-	0/6/23/26	0/1/1/1
6	NAG	K	501	2	-	2/6/23/26	0/1/1/1
6	NAG	O	101	4	-	0/6/23/26	0/1/1/1
6	NAG	E	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	B	501	2	-	2/6/23/26	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
6	NAG	N	101	4	-	2/6/23/26	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	-3.26	1.38	1.43
6	D	501	NAG	O5-C1	-2.47	1.39	1.43
6	G	501	NAG	O5-C1	-2.14	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	101	NAG	C1-O5-C5	2.76	115.88	112.19
6	E	501	NAG	C1-O5-C5	2.32	115.30	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

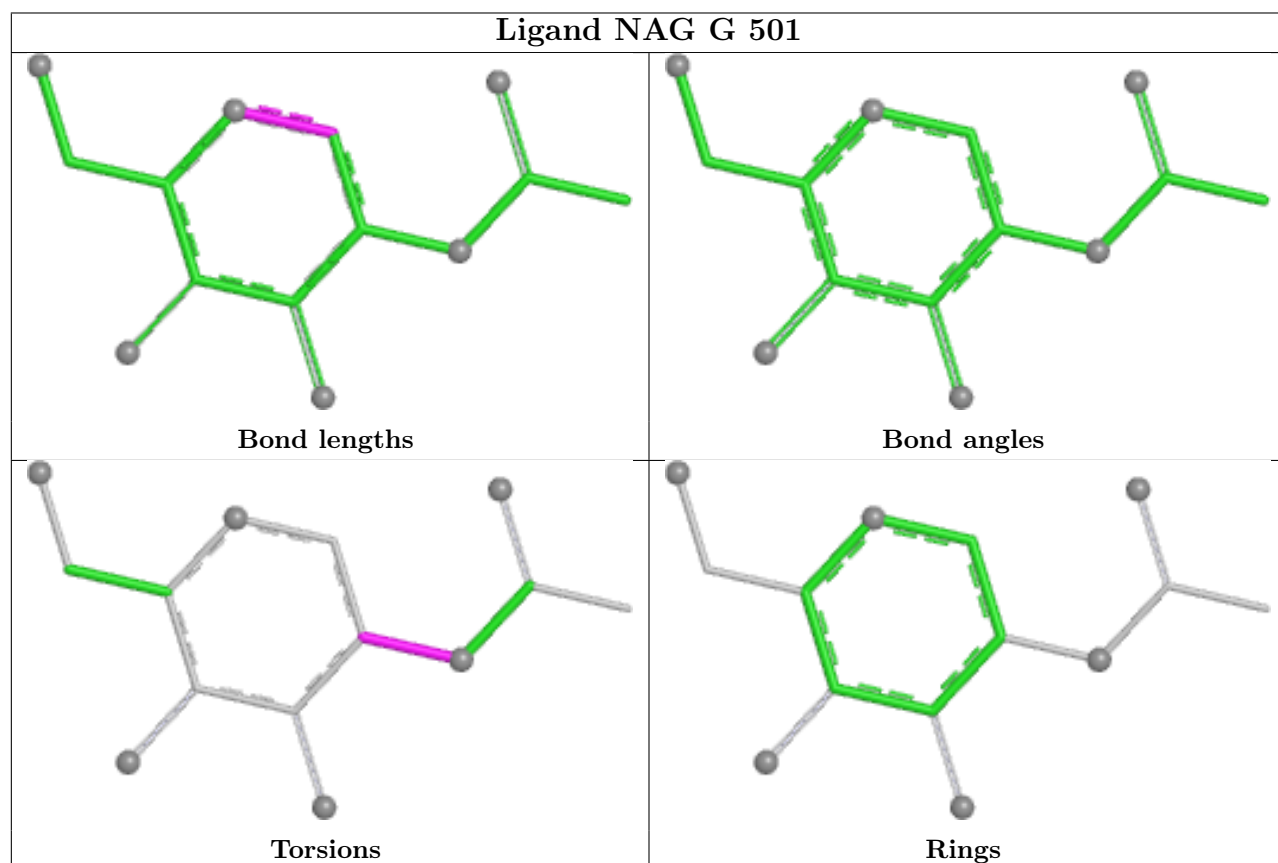
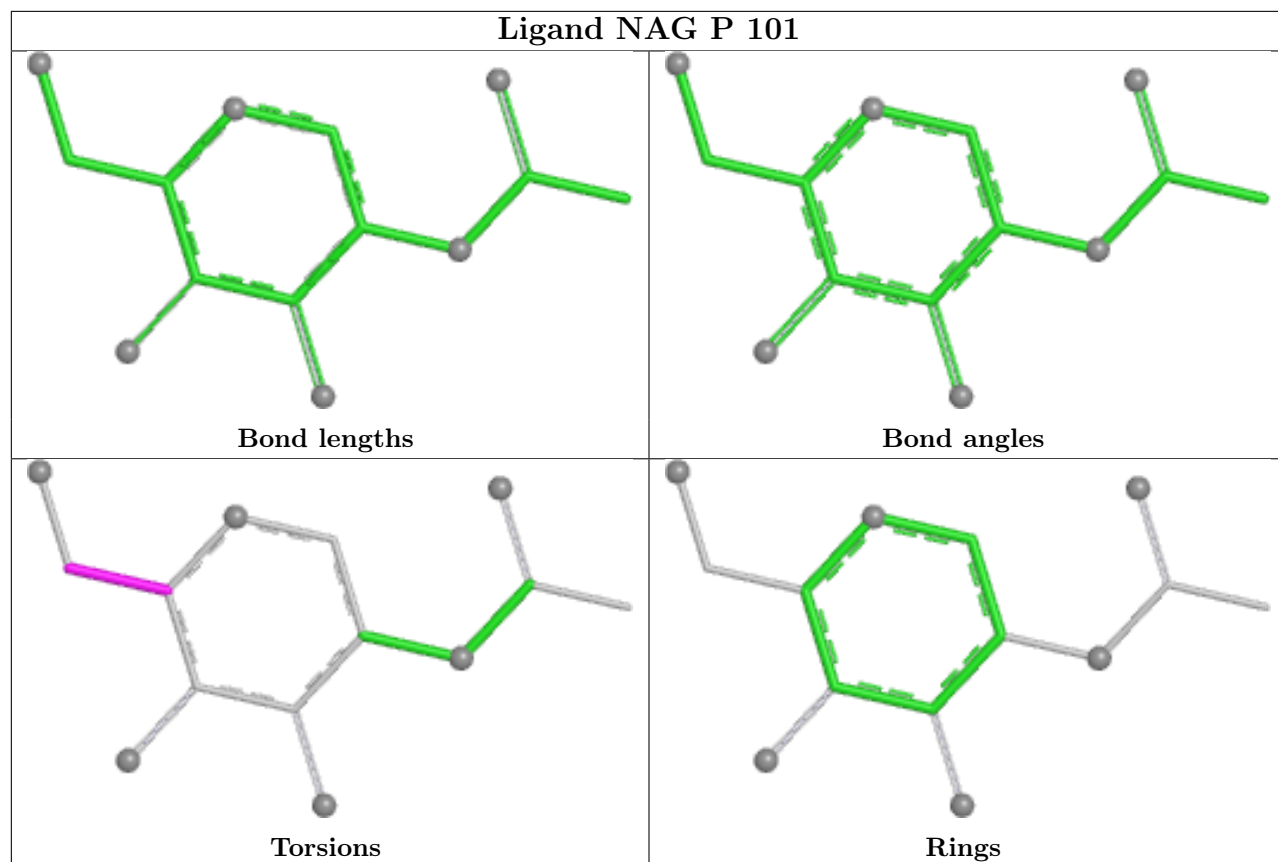
Mol	Chain	Res	Type	Atoms
6	E	501	NAG	O5-C5-C6-O6
6	P	101	NAG	C4-C5-C6-O6
6	P	101	NAG	O5-C5-C6-O6
6	E	501	NAG	C4-C5-C6-O6
6	N	101	NAG	O5-C5-C6-O6
6	N	101	NAG	C4-C5-C6-O6
6	D	501	NAG	O5-C5-C6-O6
6	D	501	NAG	C4-C5-C6-O6
6	A	501	NAG	O5-C5-C6-O6
6	B	501	NAG	C3-C2-N2-C7
6	G	501	NAG	C3-C2-N2-C7
6	K	501	NAG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

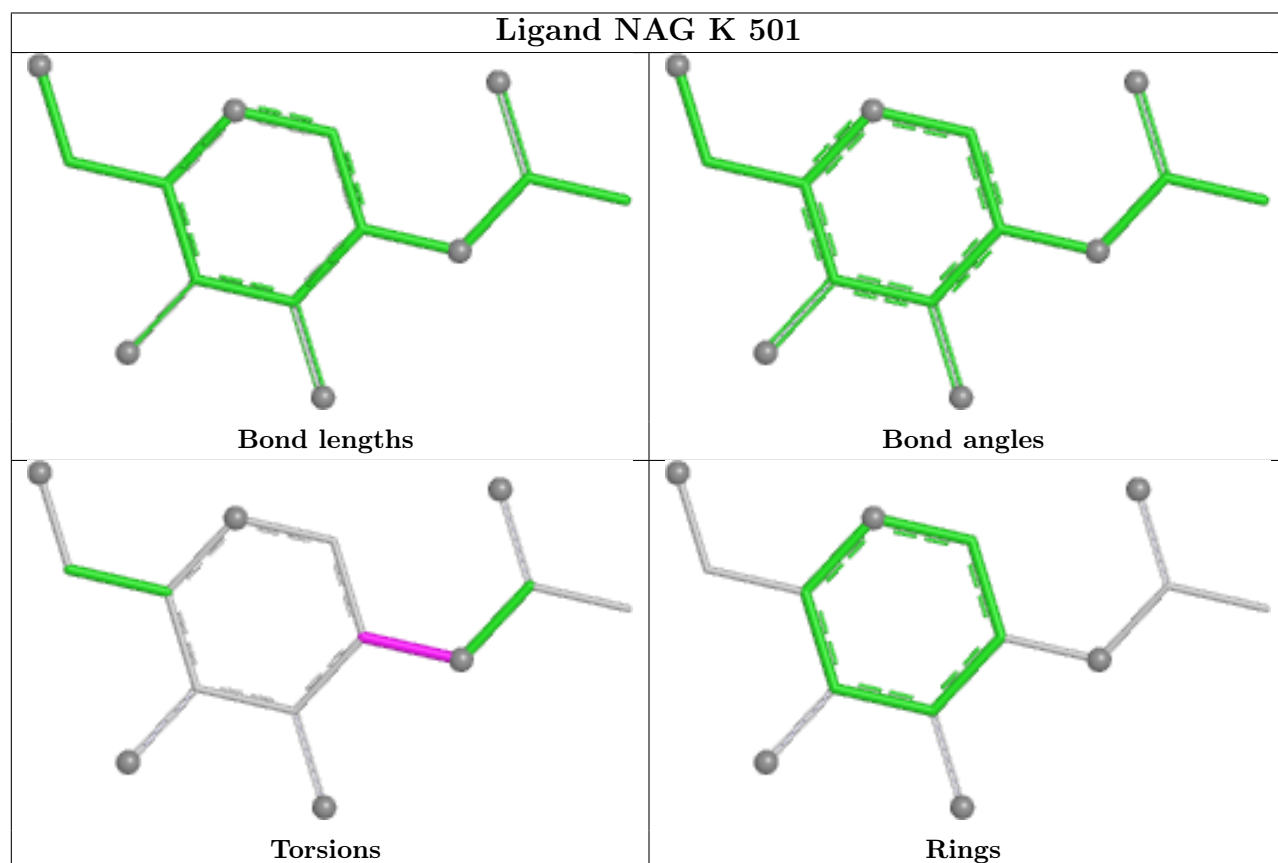
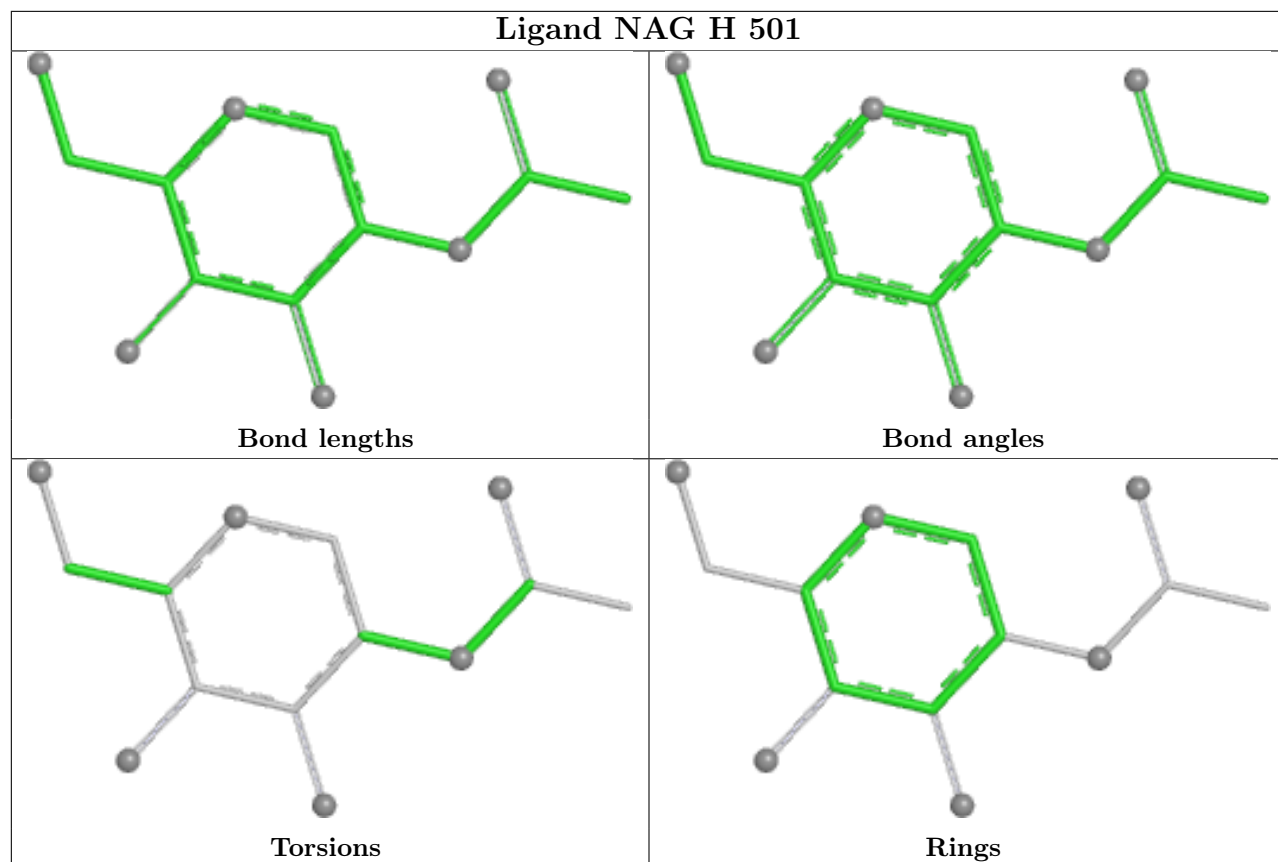
There are no ring outliers.

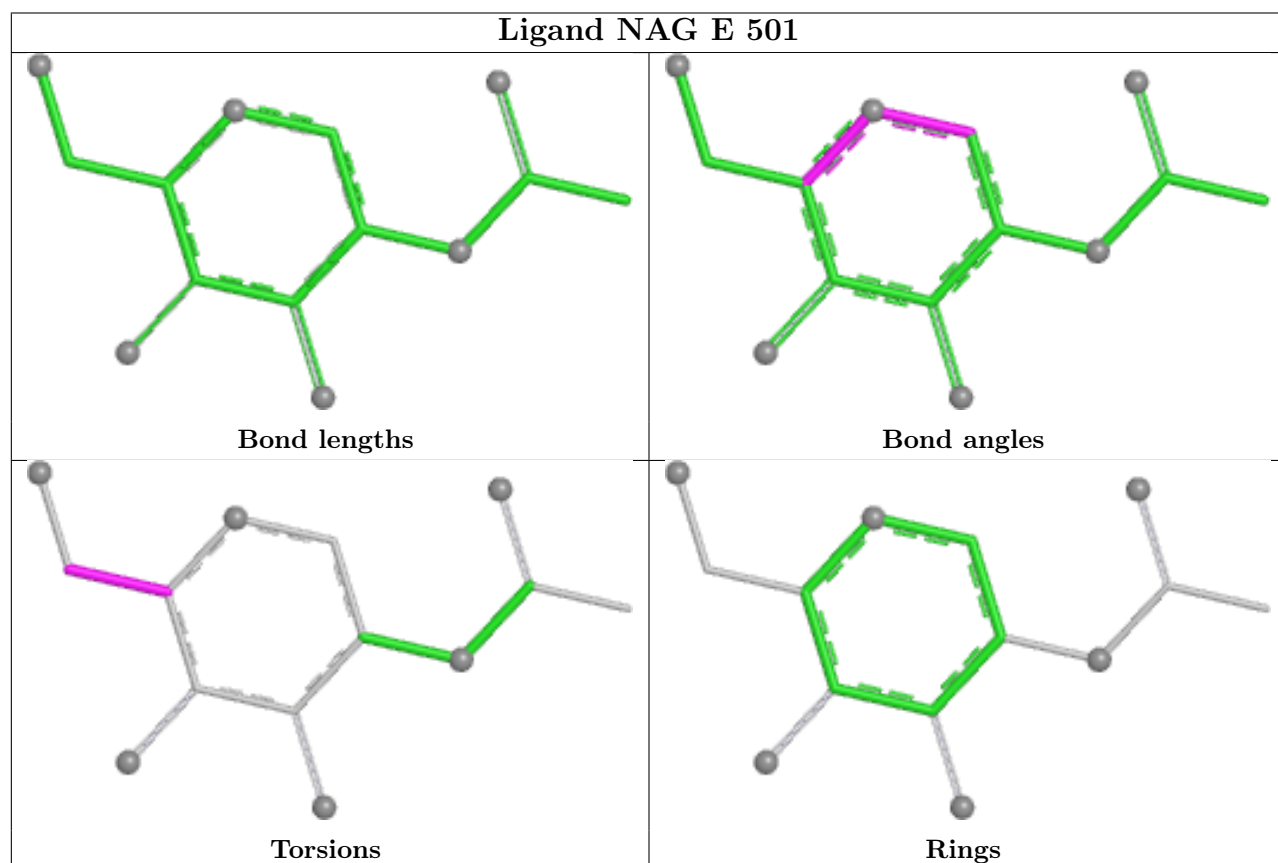
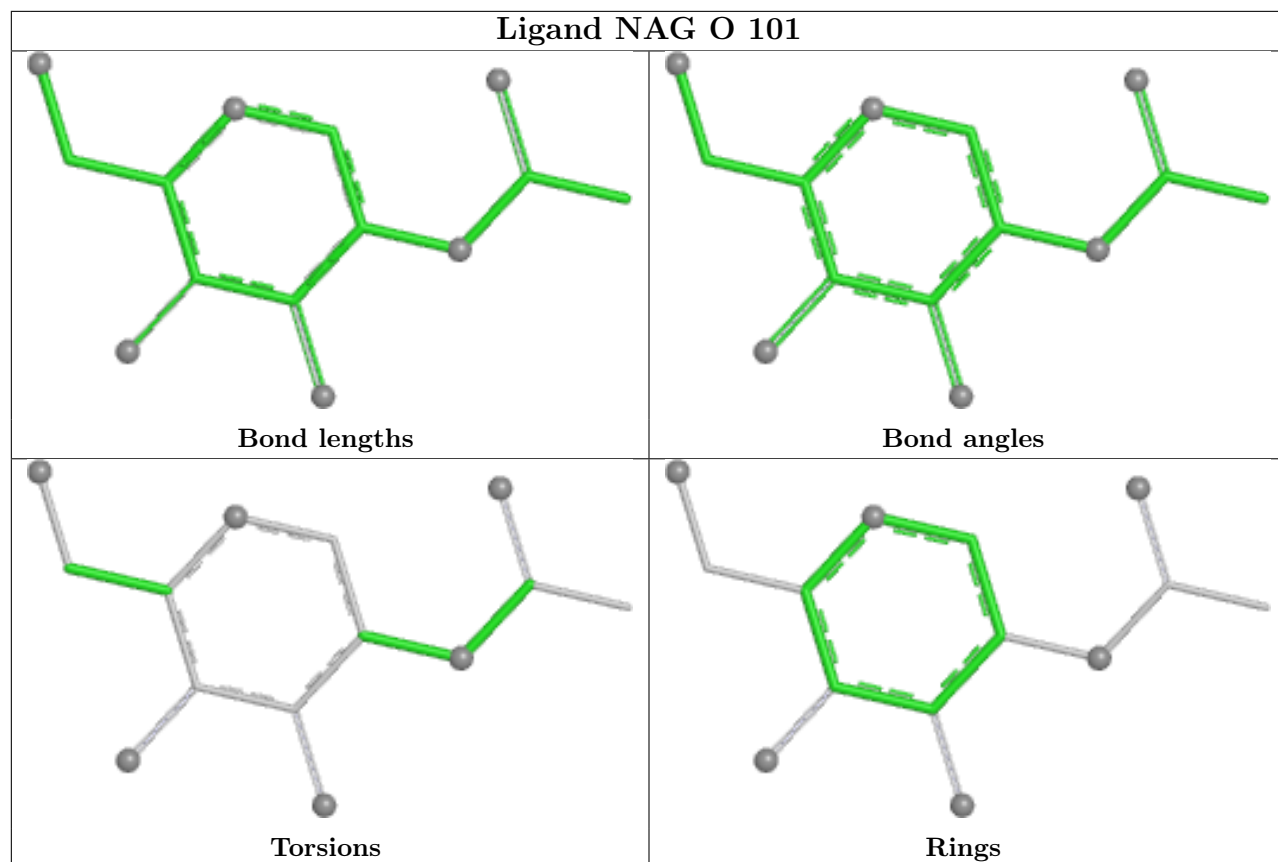
3 monomers are involved in 5 short contacts:

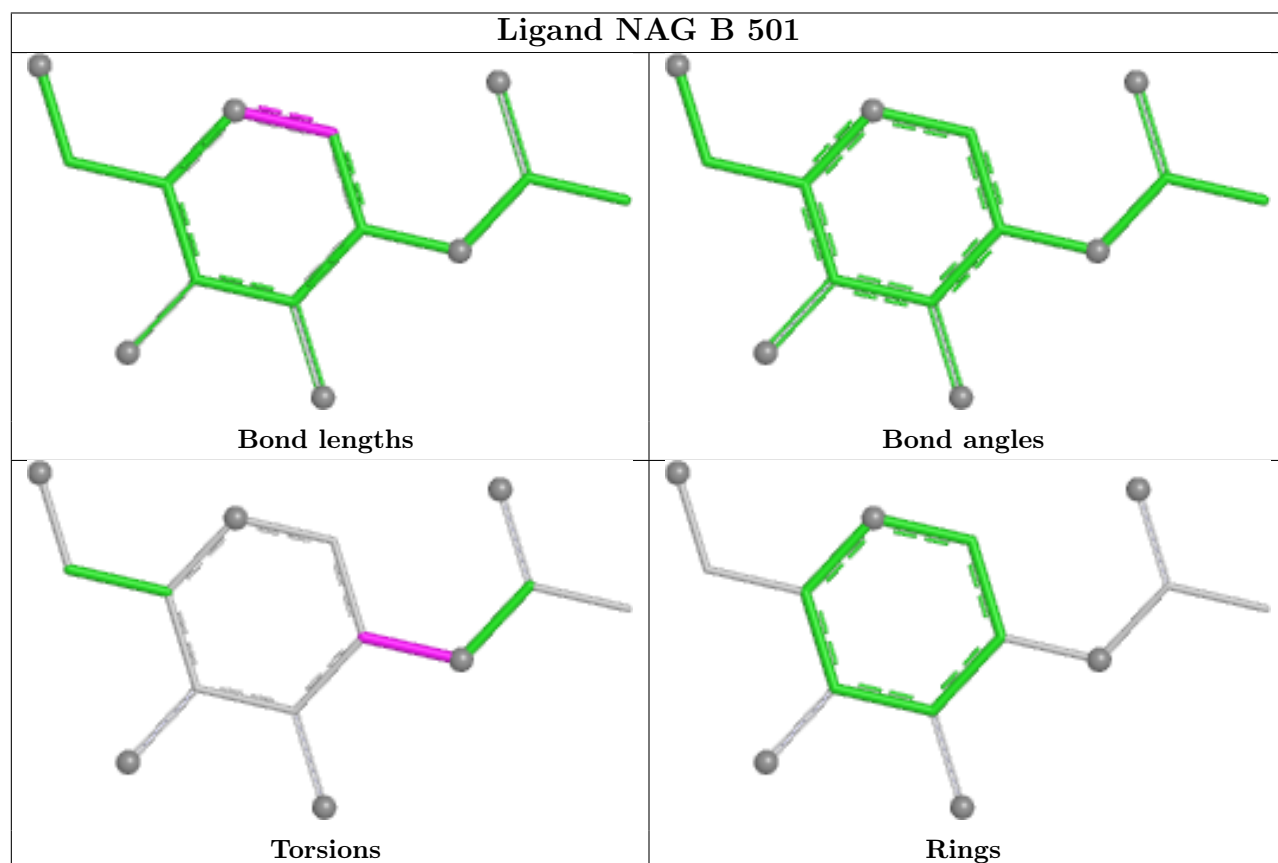
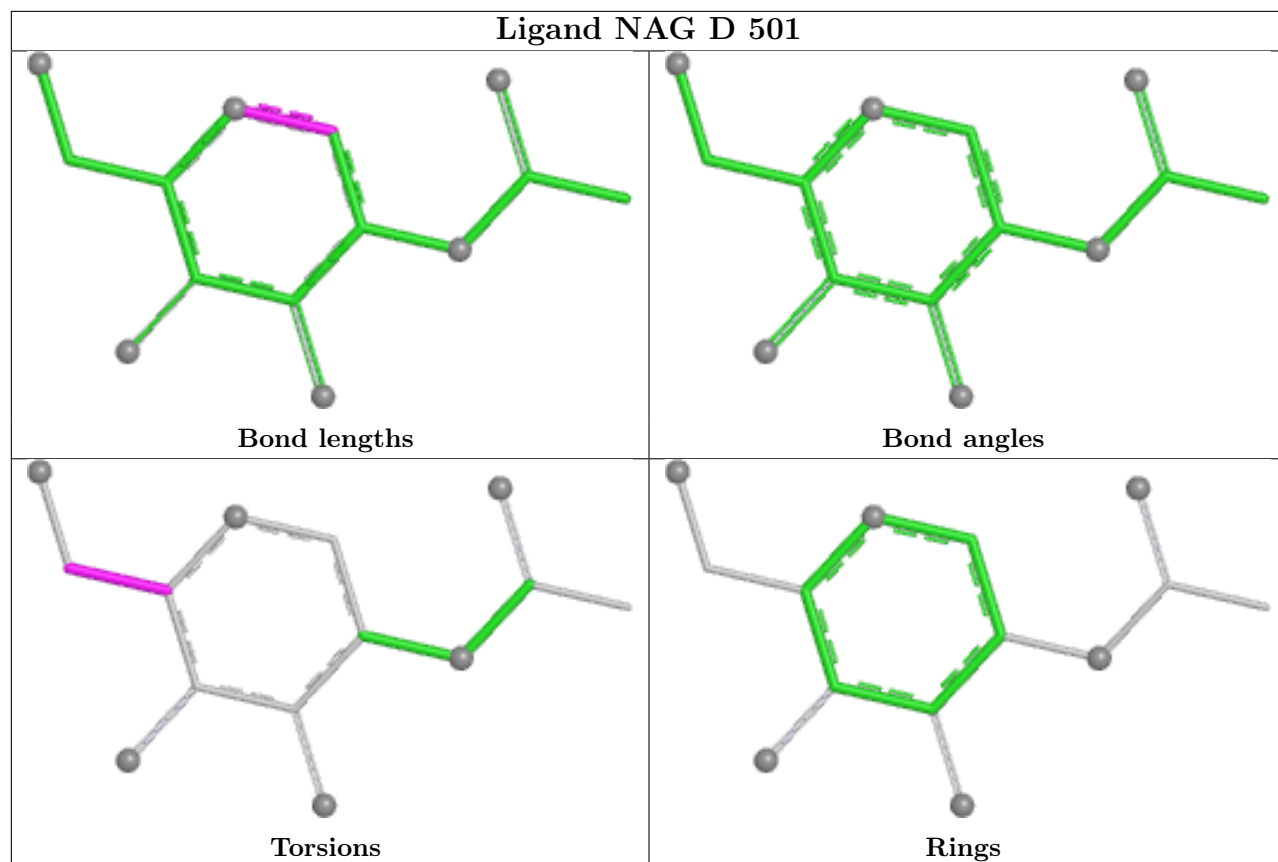
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	501	NAG	2	0
6	K	501	NAG	1	0
6	B	501	NAG	2	0

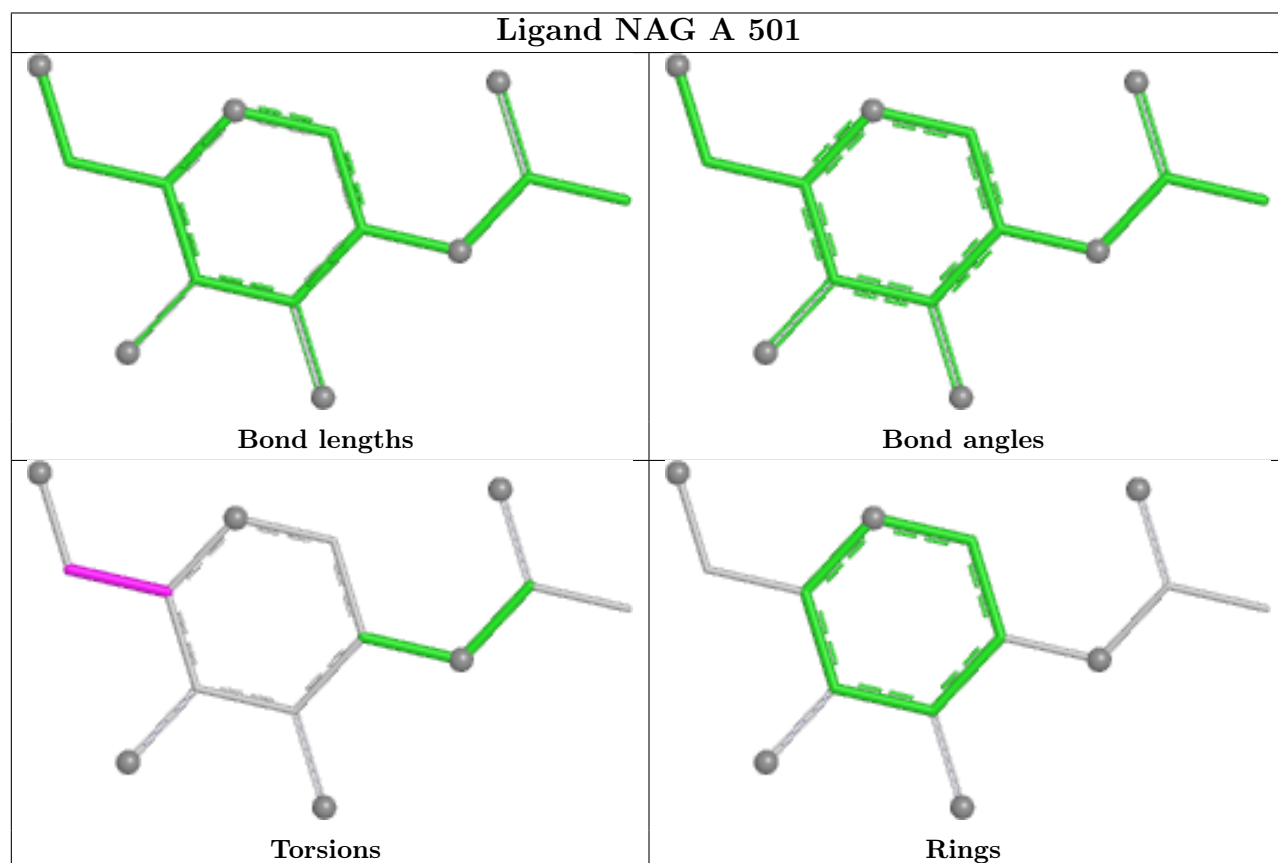
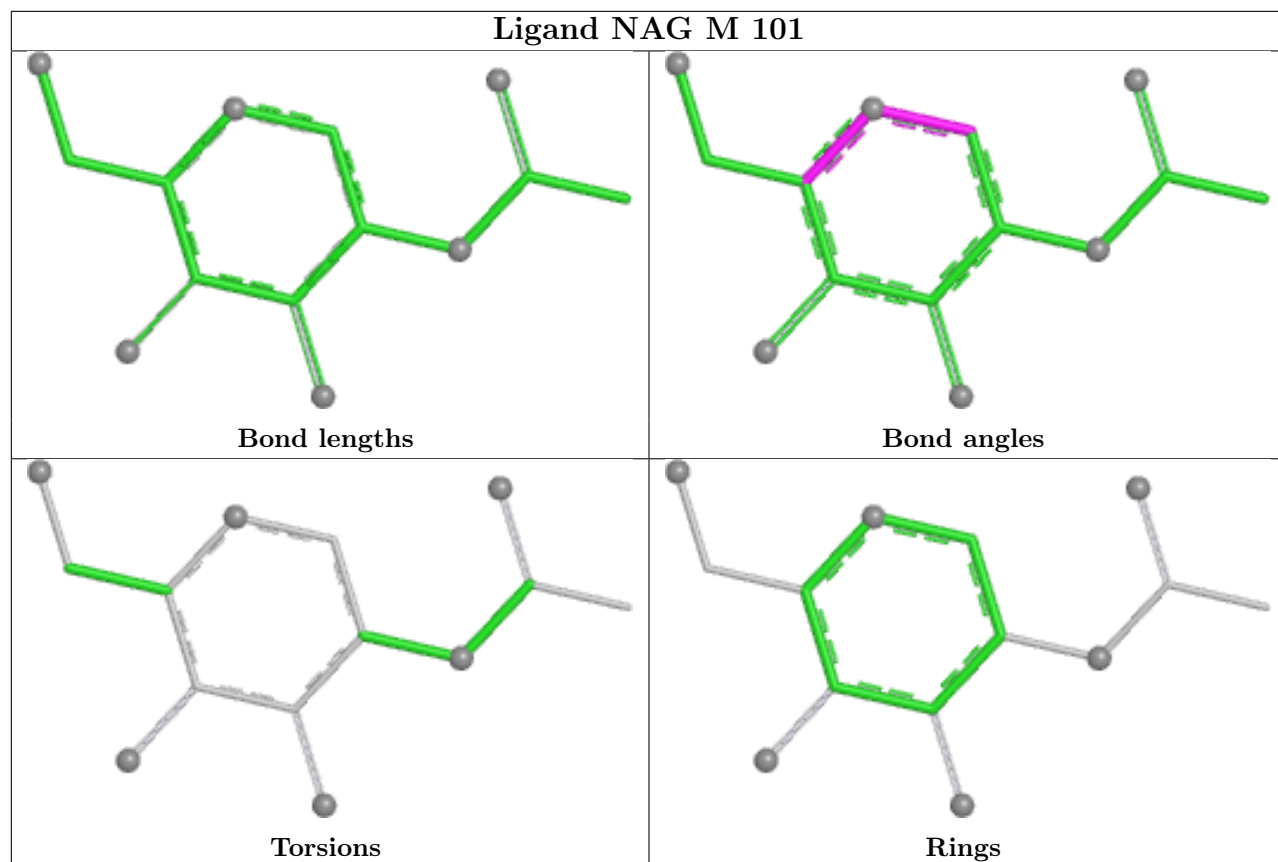
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

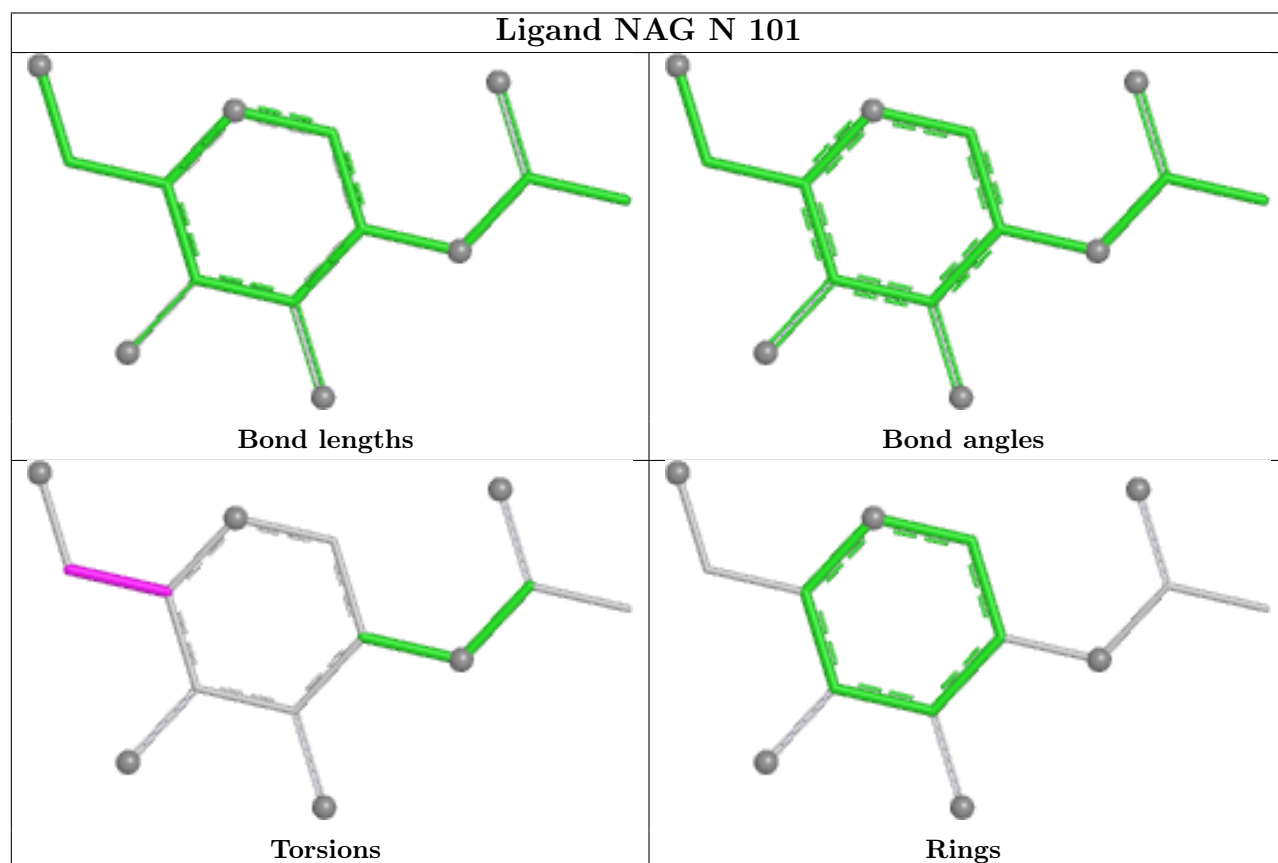
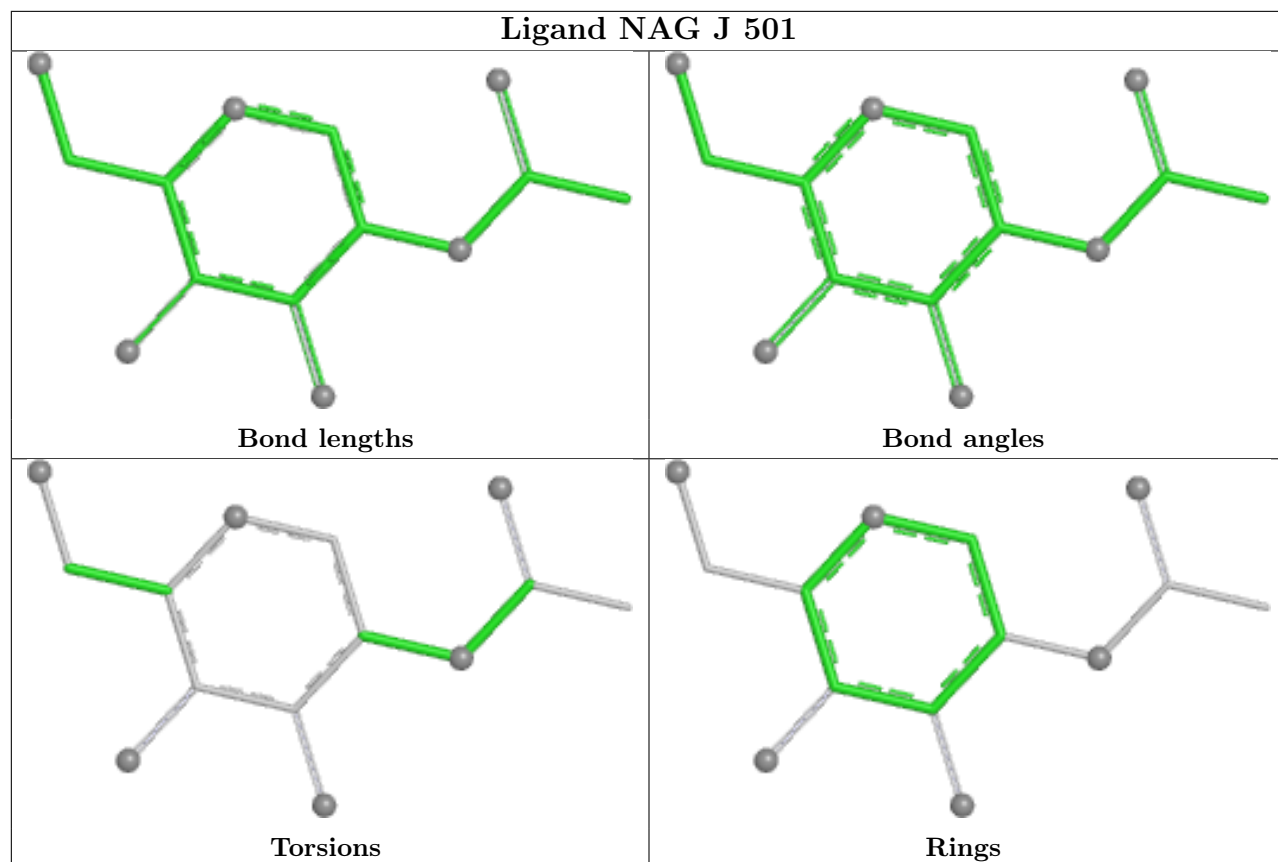












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

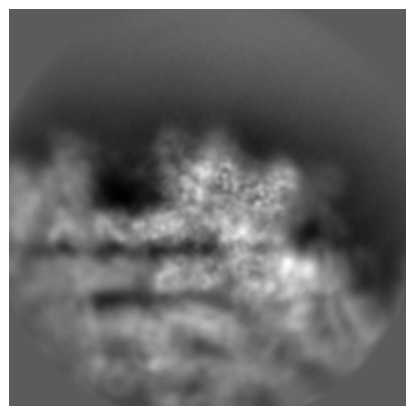
6 Map visualisation [i](#)

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.

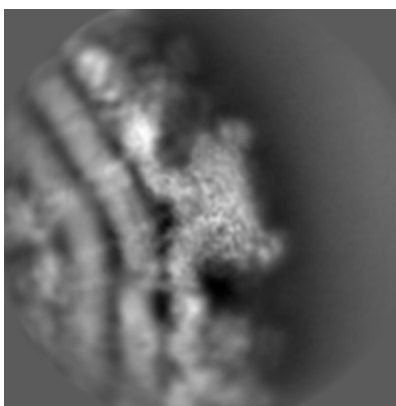
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

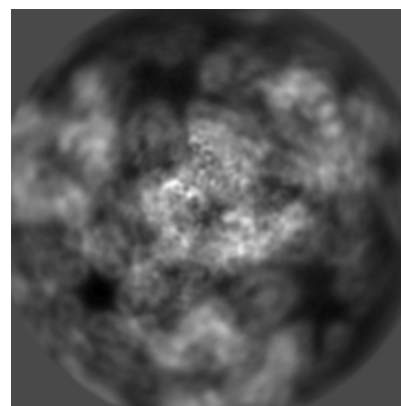
6.1.1 Primary map



X

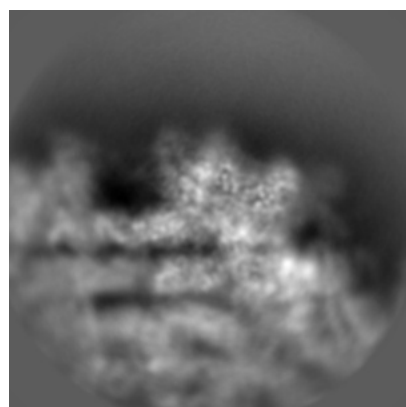


Y

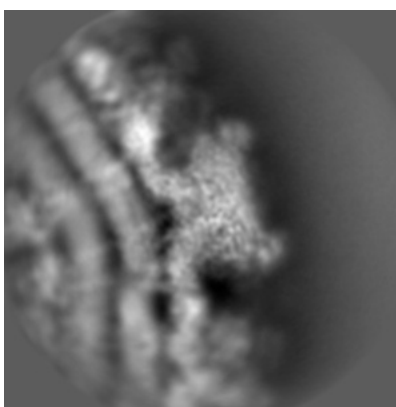


Z

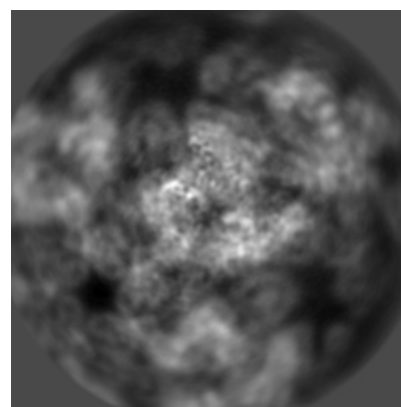
6.1.2 Raw map



X



Y

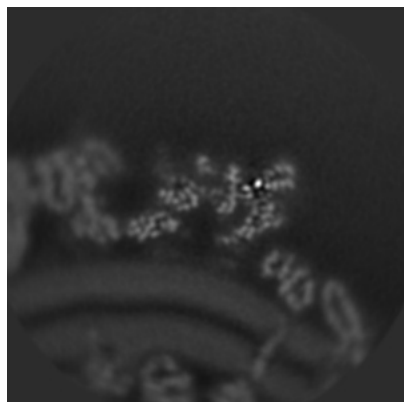


Z

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

6.2 Central slices [i](#)

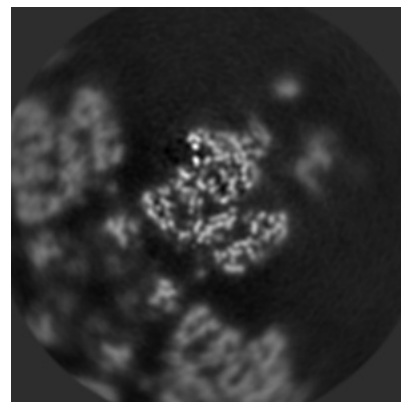
6.2.1 Primary map



X Index: 120

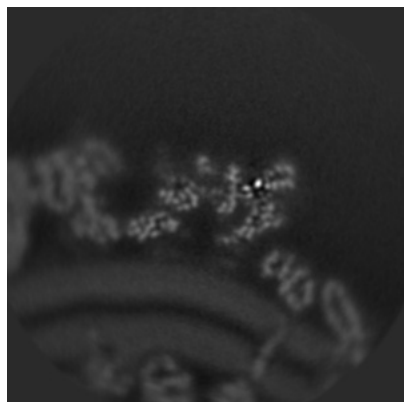


Y Index: 120



Z Index: 120

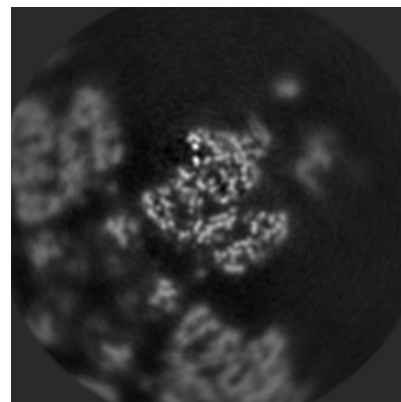
6.2.2 Raw map



X Index: 120



Y Index: 120

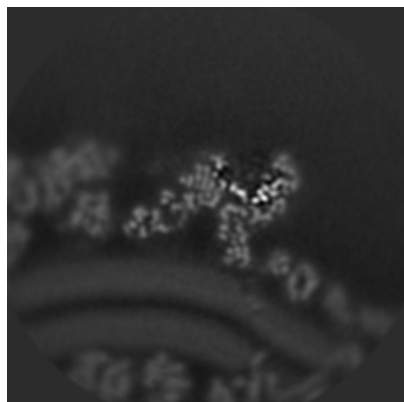


Z Index: 120

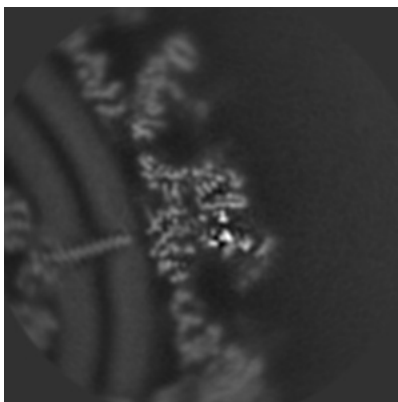
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

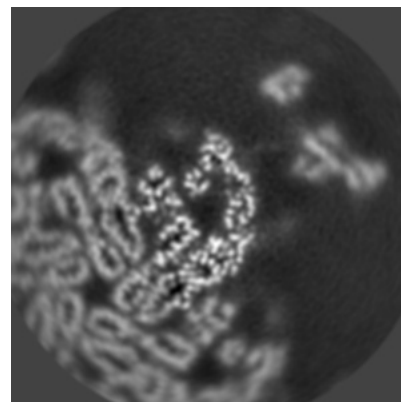
6.3.1 Primary map



X Index: 113

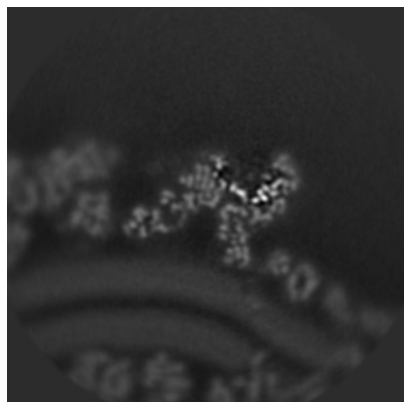


Y Index: 135

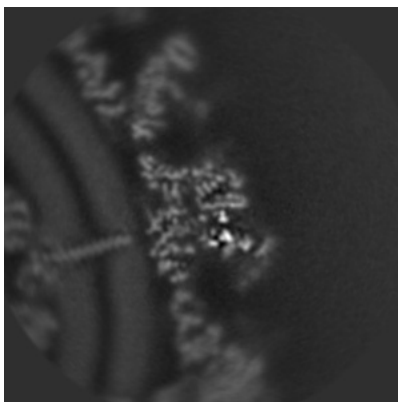


Z Index: 109

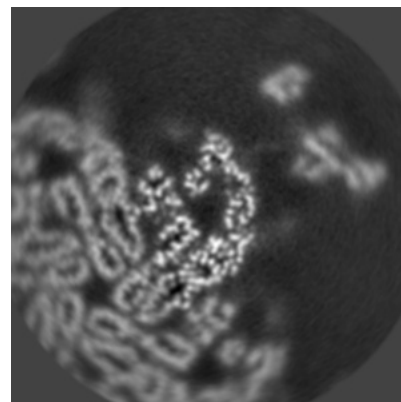
6.3.2 Raw map



X Index: 113



Y Index: 135

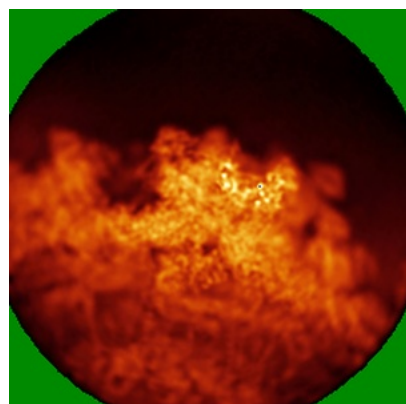


Z Index: 109

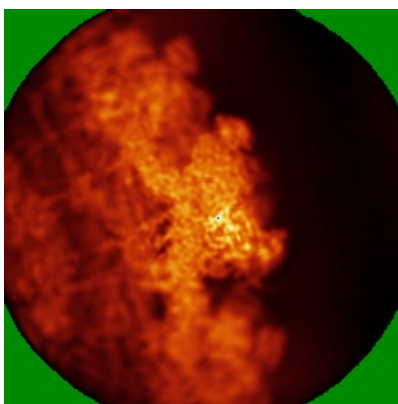
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

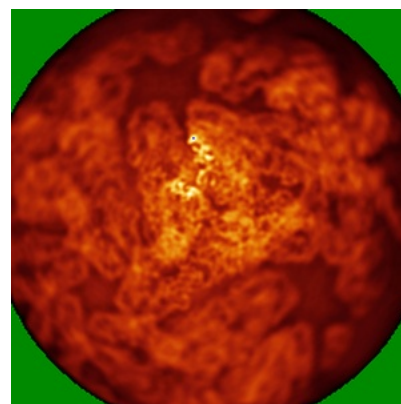
6.4.1 Primary map



X

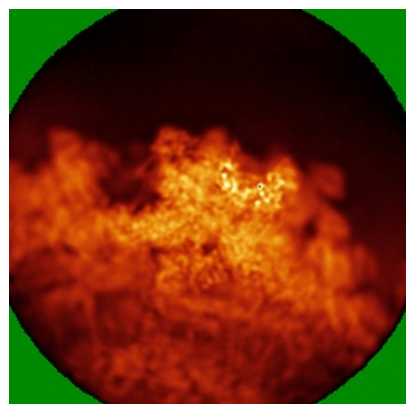


Y

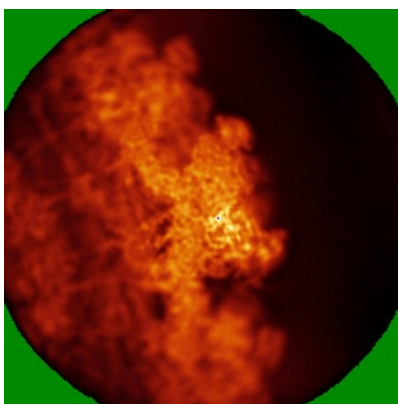


Z

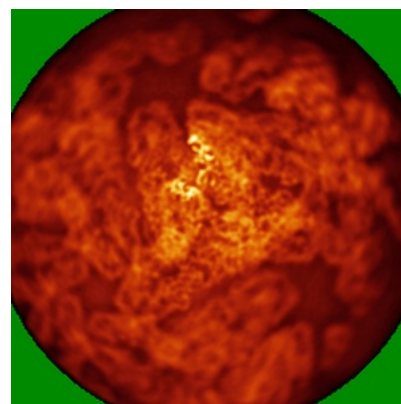
6.4.2 Raw map



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



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.

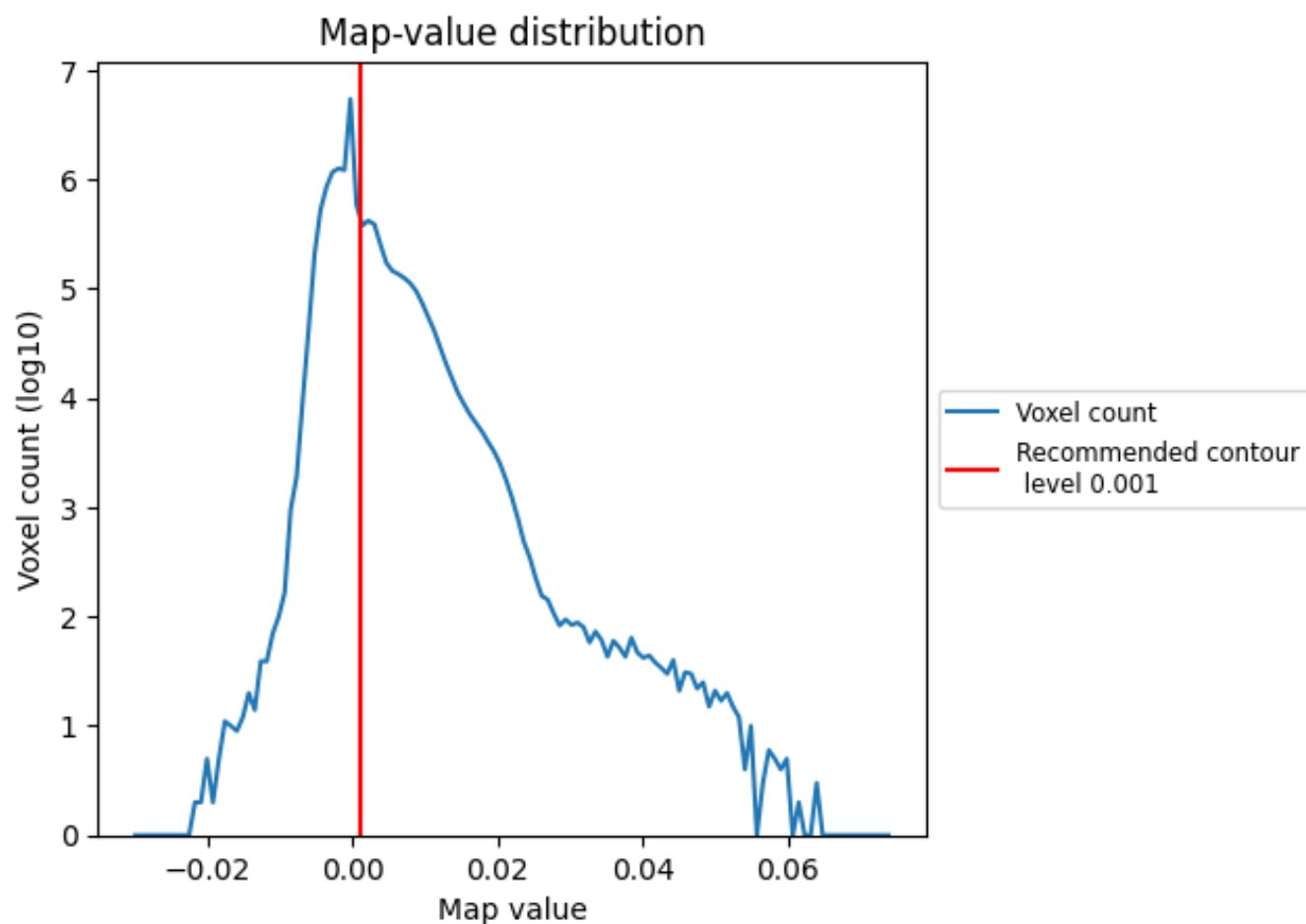
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

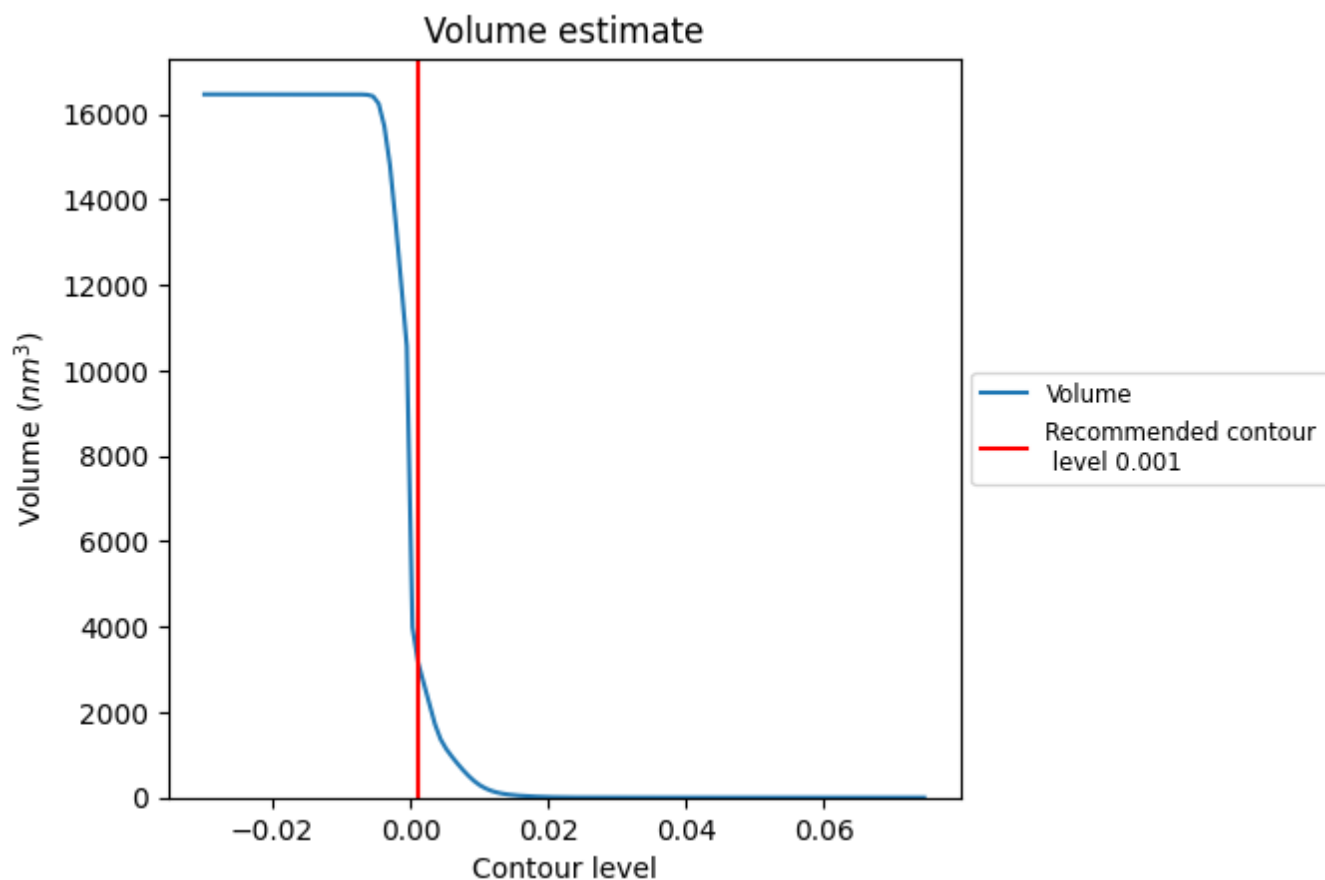
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

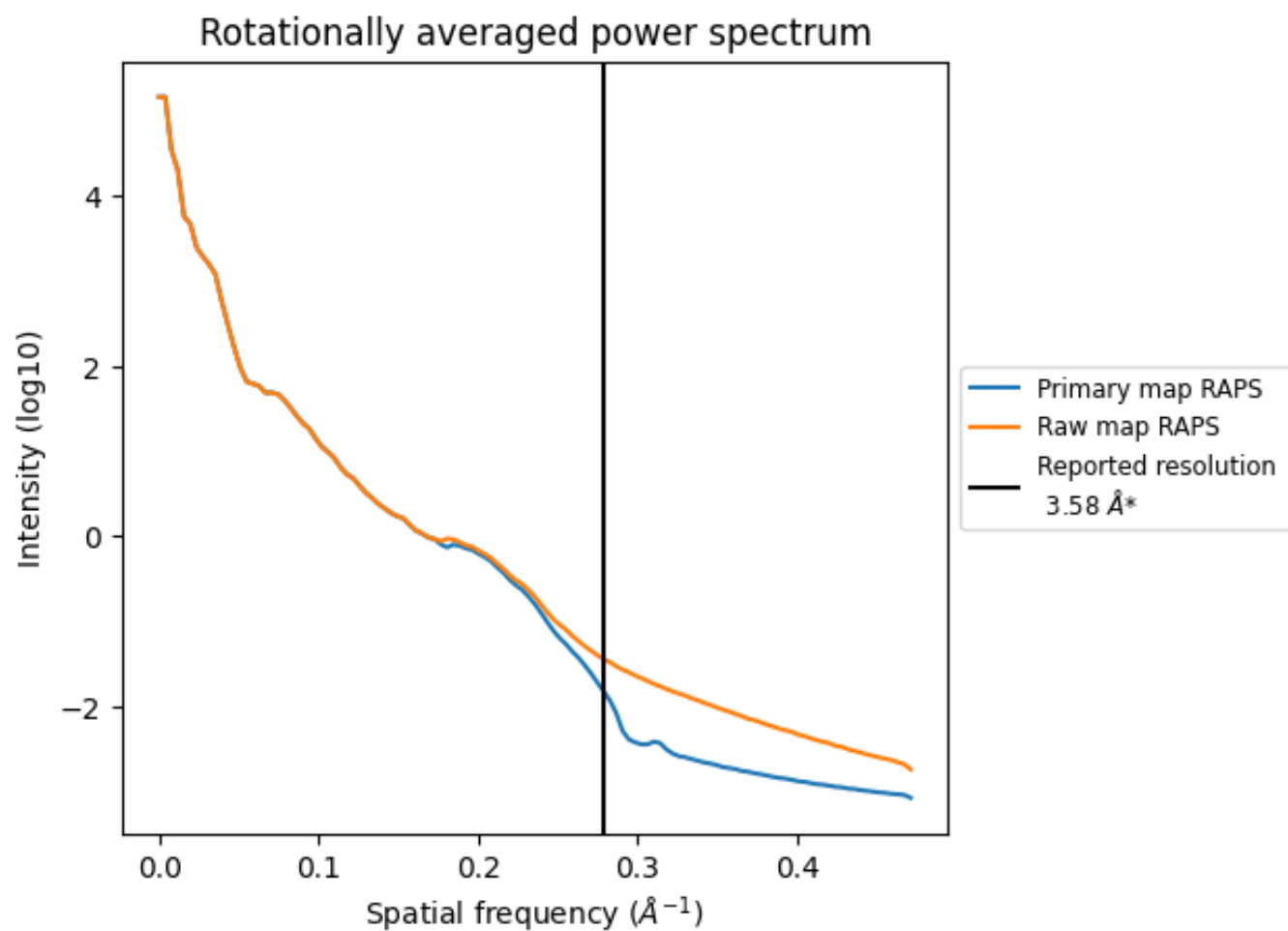
7.2 Volume estimate [i](#)



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 ⓘ

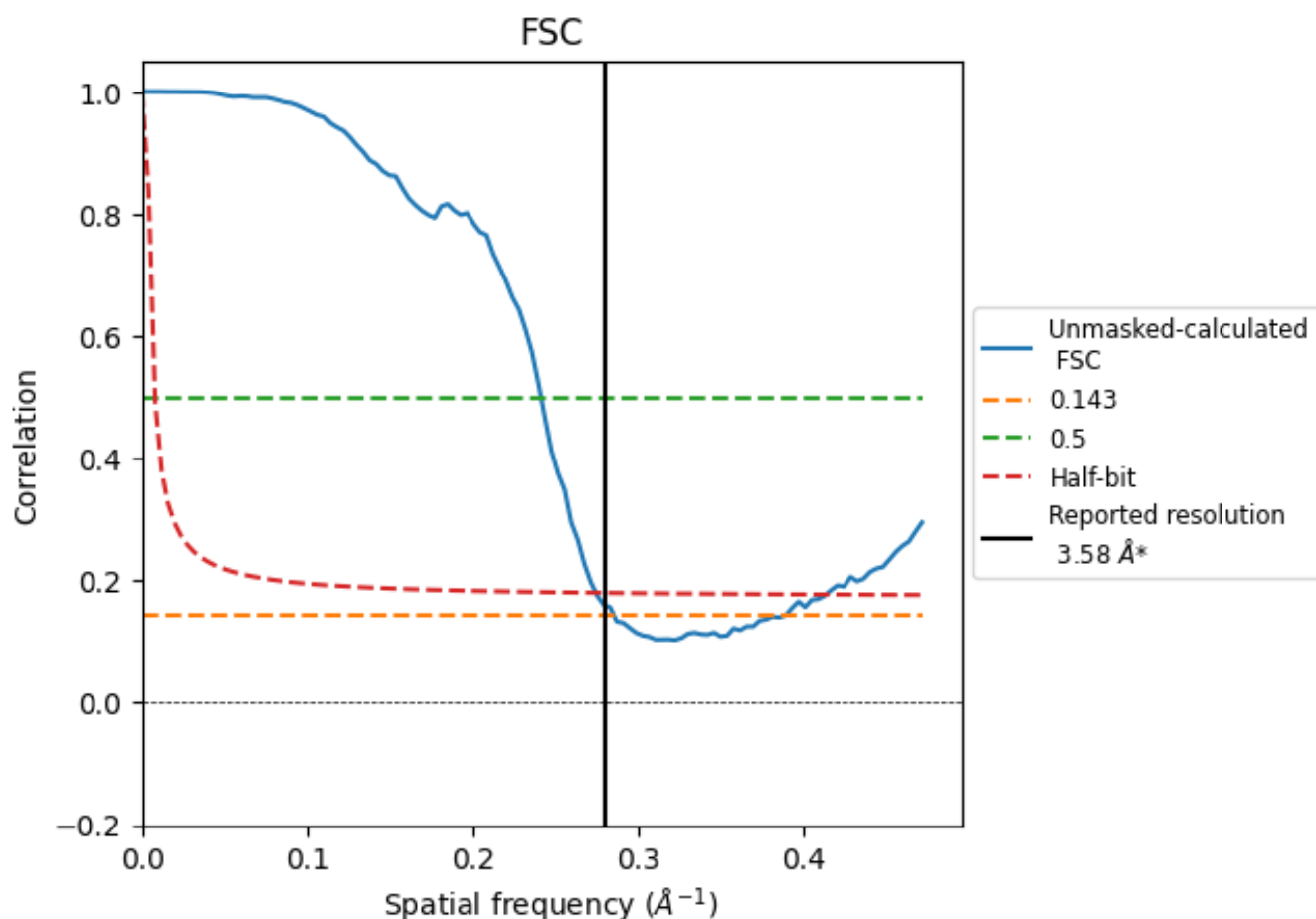


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.279 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

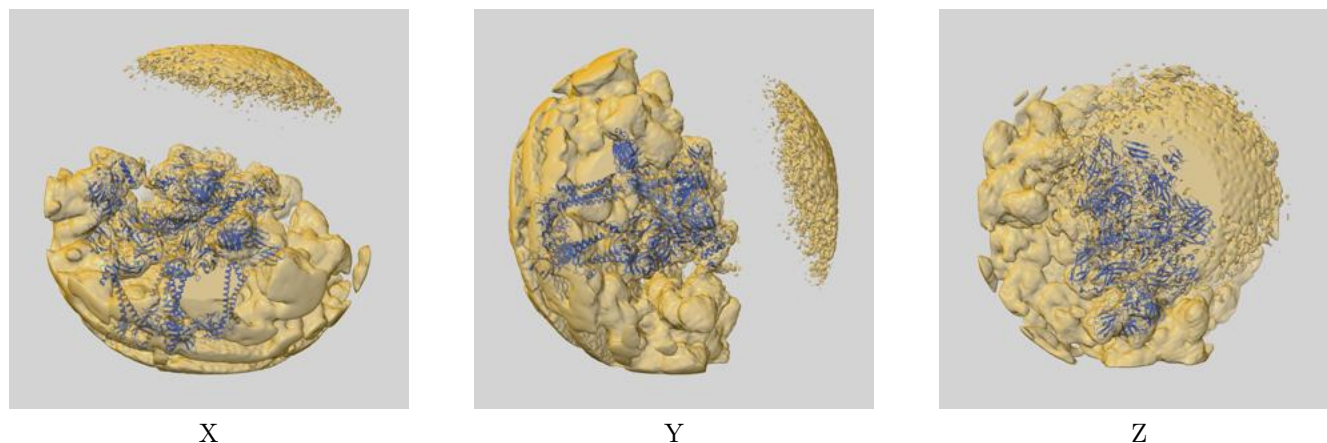
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.14	3.65

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

9 Map-model fit [i](#)

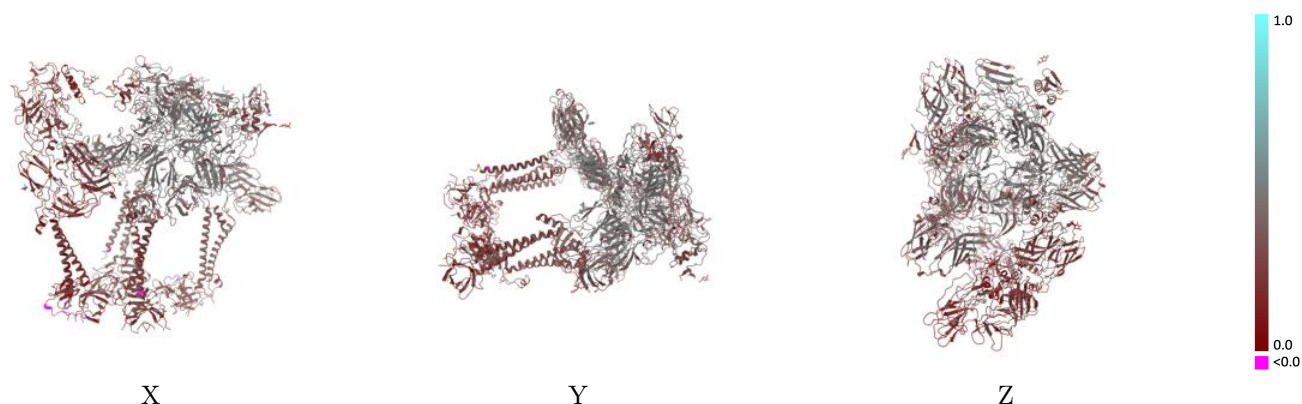
This section contains information regarding the fit between EMDB map EMD-42050 and PDB model 8UA4. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



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](#)

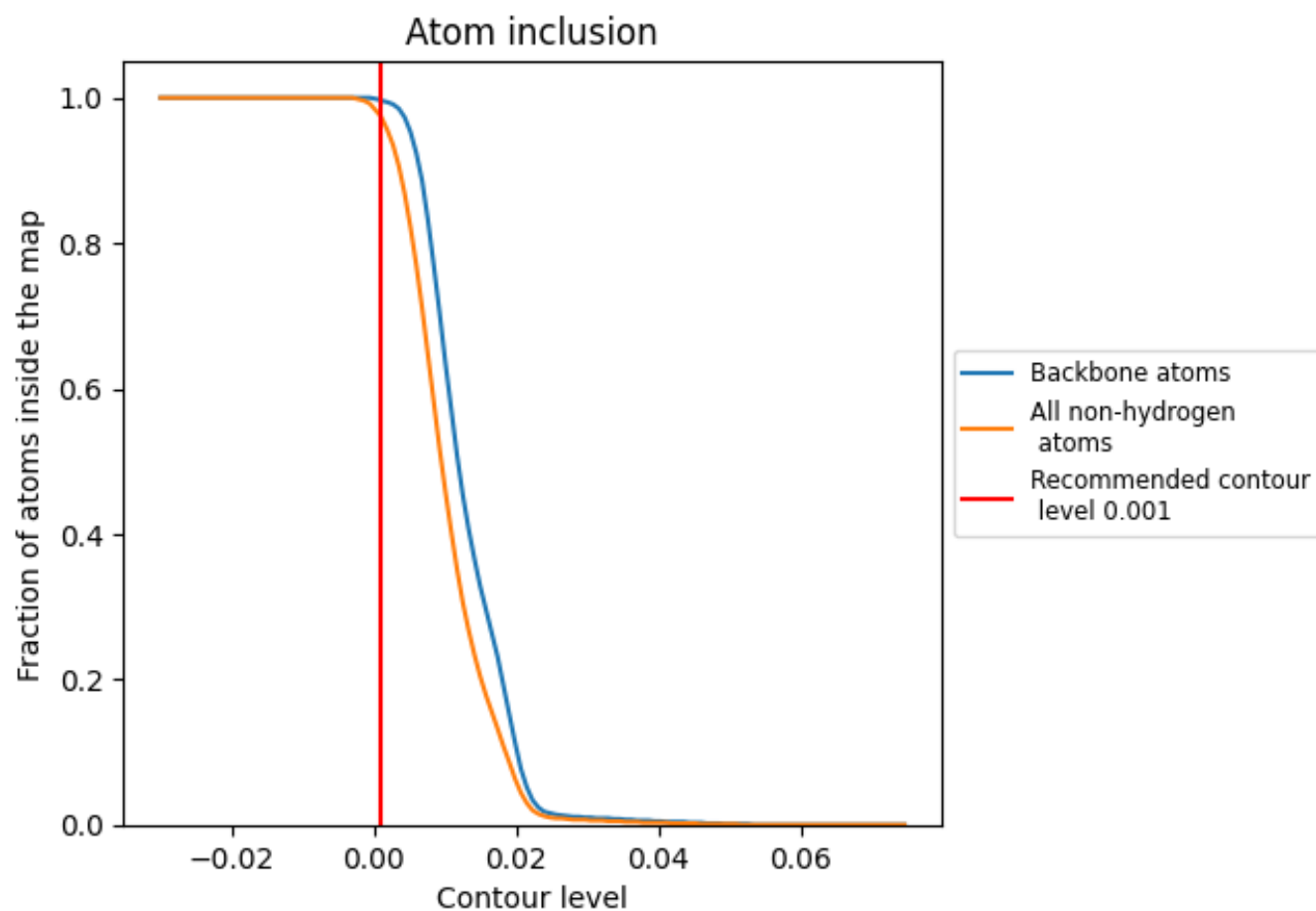


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

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

