Full wwPDB EM Validation Report ⓘ

May 23, 2023 – 08:22 PM JST

PDB ID	:	8H07
EMDB ID	:	EMD-34410
Title	:	SARS-CoV-2 BA.4 variants S ectodomain trimer in complex with neutralizing antibody 10-5B and 6-2C
Authors	:	Wang, X.; Wang, Z.
Deposited on	:	2022-09-28
Resolution	:	2.90 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:

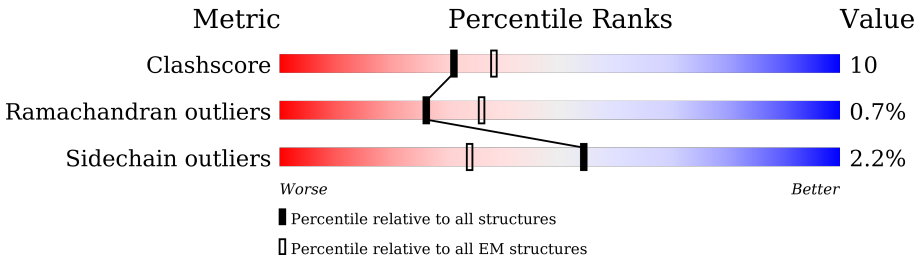
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.90 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	1286	10% 61% 11% 27%
1	B	1286	61% 12% 26%
1	C	1286	11% 62% 11% 26%
2	E	117	99% 72% 27%
2	G	117	87% 68% 31%
2	M	117	99% 73% 26%
3	H	107	85% 64% 36%
3	J	107	100% 71% 29%

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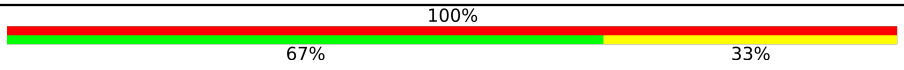
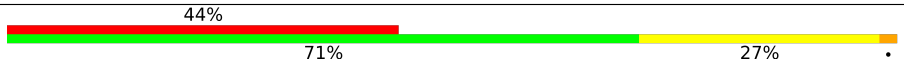
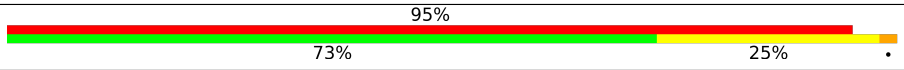
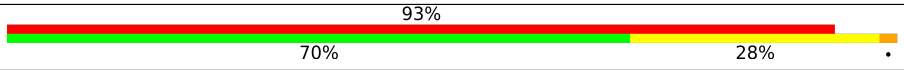
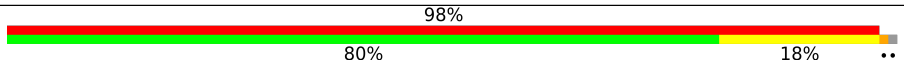
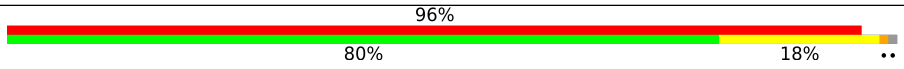
Mol	Chain	Length	Quality of chain
3	P	107	
4	I	122	
4	N	122	
4	Q	122	
5	K	107	
5	O	107	
5	R	107	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 31320 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	939	Total	C	N	O	S	0	0
			7115	4529	1198	1359	29		
1	B	948	Total	C	N	O	S	0	0
			7139	4532	1211	1364	32		
1	C	947	Total	C	N	O	S	0	0
			7188	4574	1208	1375	31		

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	214A	GLU	-	insertion	UNP P0DTC2
A	214B	PRO	-	insertion	UNP P0DTC2
A	214C	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	214A	GLU	-	insertion	UNP P0DTC2
B	214B	PRO	-	insertion	UNP P0DTC2
B	214C	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	214A	GLU	-	insertion	UNP P0DTC2
C	214B	PRO	-	insertion	UNP P0DTC2
C	214C	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called 10-5B H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	116	Total	C	N	O	S	0	0
			837	518	146	168	5		
2	G	116	Total	C	N	O	S	0	0
			847	525	149	168	5		
2	M	116	Total	C	N	O	S	0	0
			838	519	146	168	5		

- Molecule 3 is a protein called 10-5B L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	107	Total	C	N	O	S	0	0
			739	460	129	147	3		
3	H	107	Total	C	N	O	S	0	0
			741	462	129	147	3		
3	P	107	Total	C	N	O	S	0	0
			743	463	129	148	3		

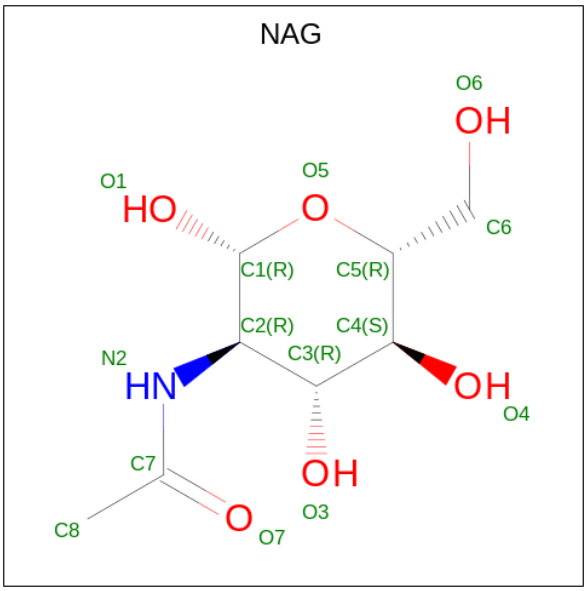
- Molecule 4 is a protein called 6-2C H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	122	Total	C	N	O	S	0	0
			925	579	162	181	3		
4	I	122	Total	C	N	O	S	0	0
			925	579	162	181	3		
4	Q	122	Total	C	N	O	S	0	0
			925	579	162	181	3		

- Molecule 5 is a protein called 6-2C L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	106	Total	C	N	O	S	0	0
			772	488	132	150	2		
5	K	106	Total	C	N	O	S	0	0
			772	488	132	150	2		
5	R	106	Total	C	N	O	S	0	0
			772	488	132	150	2		

- 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).

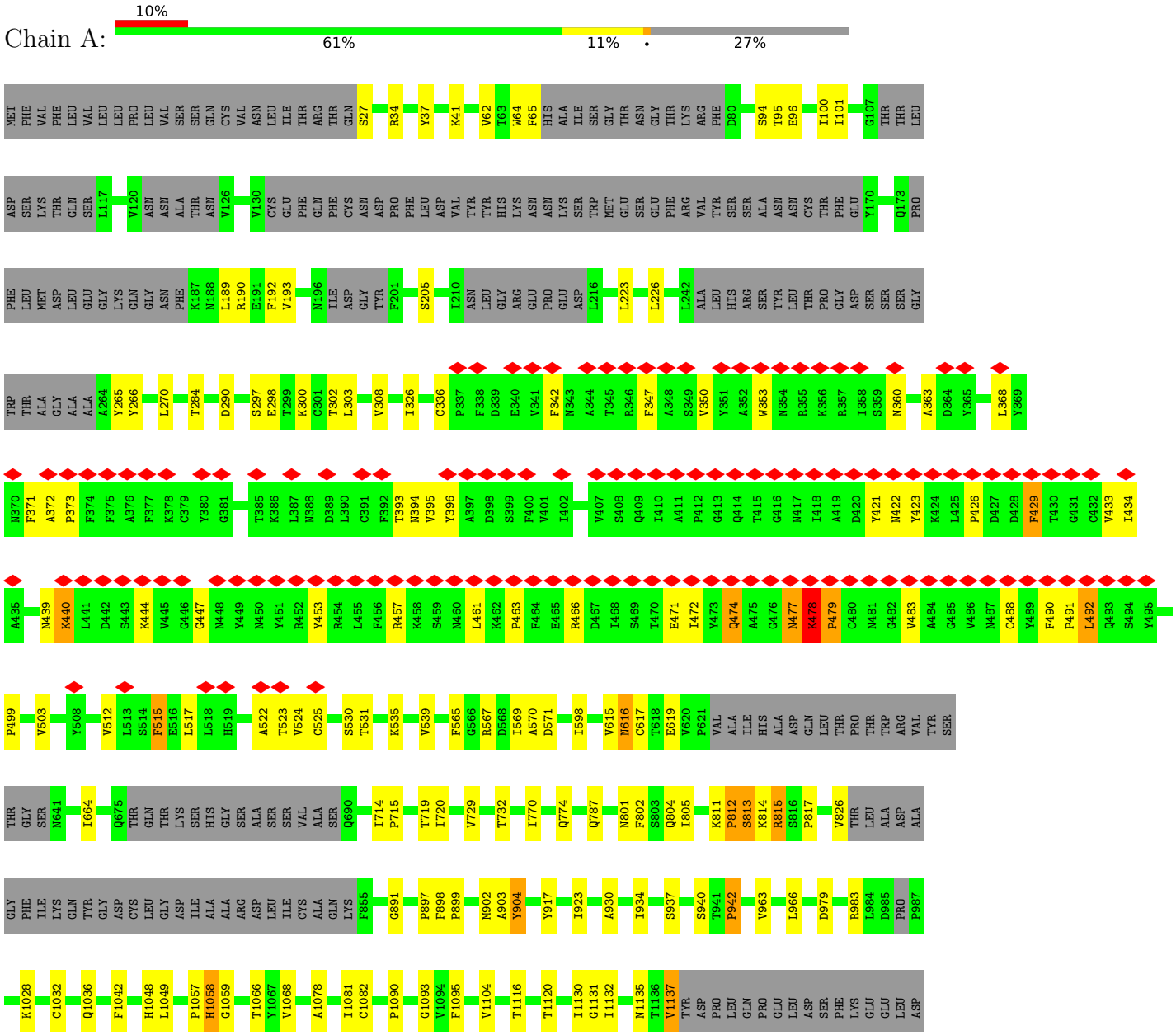


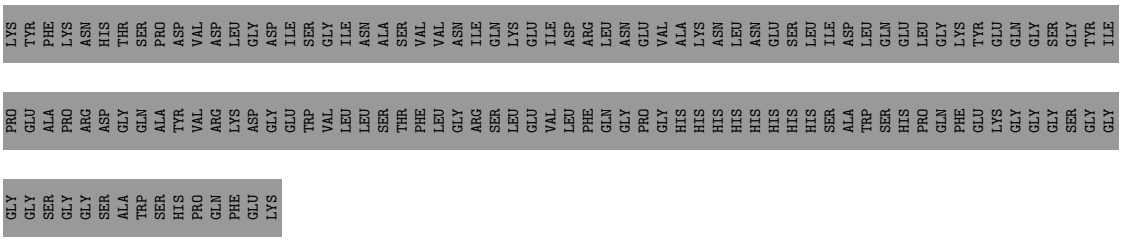
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C N O 14 8 1 5	0
6	B	1	Total C N O 14 8 1 5	0
6	C	1	Total C N O 14 8 1 5	0

3 Residue-property plots (i)

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

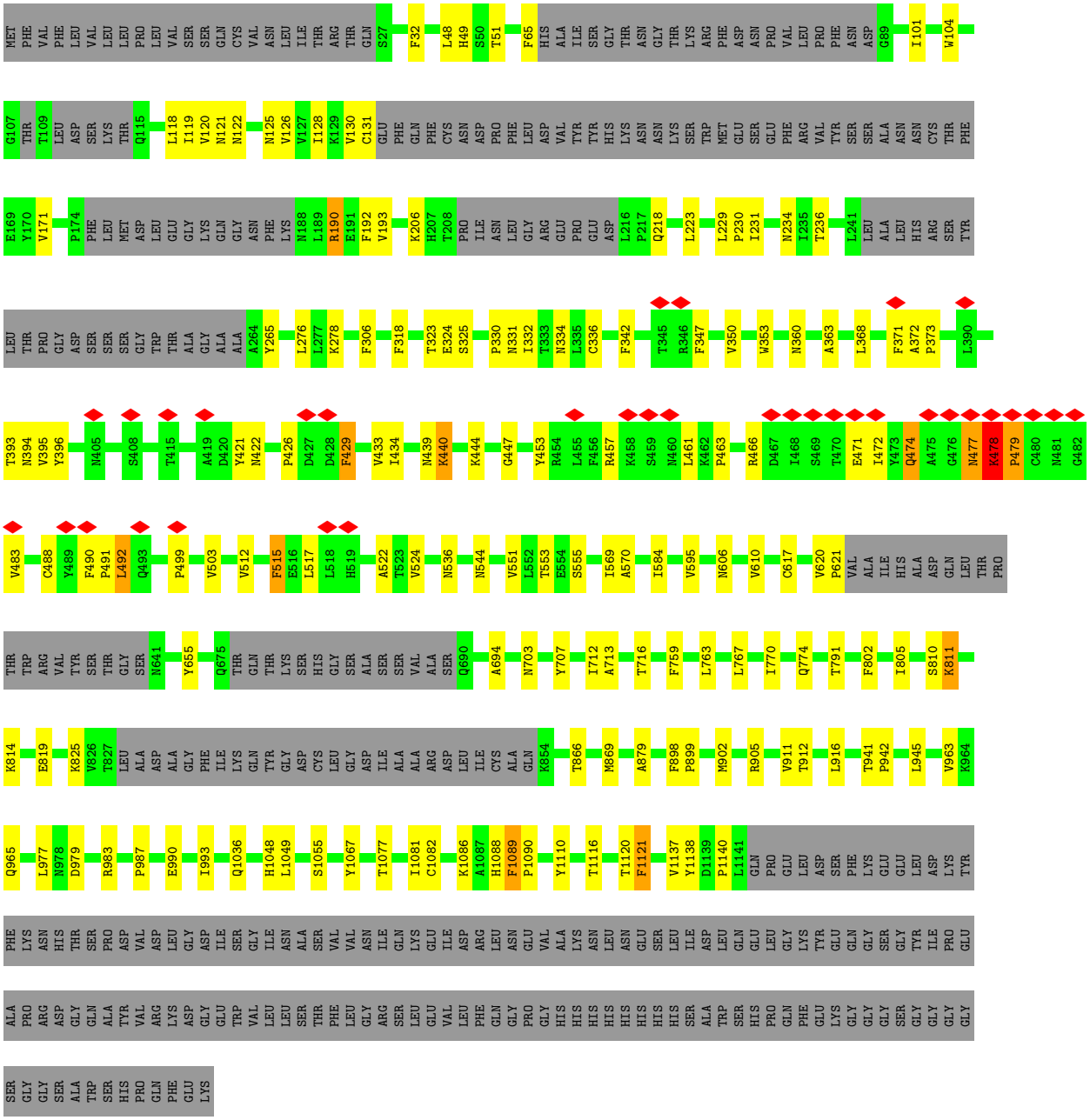
- Molecule 1: Spike glycoprotein





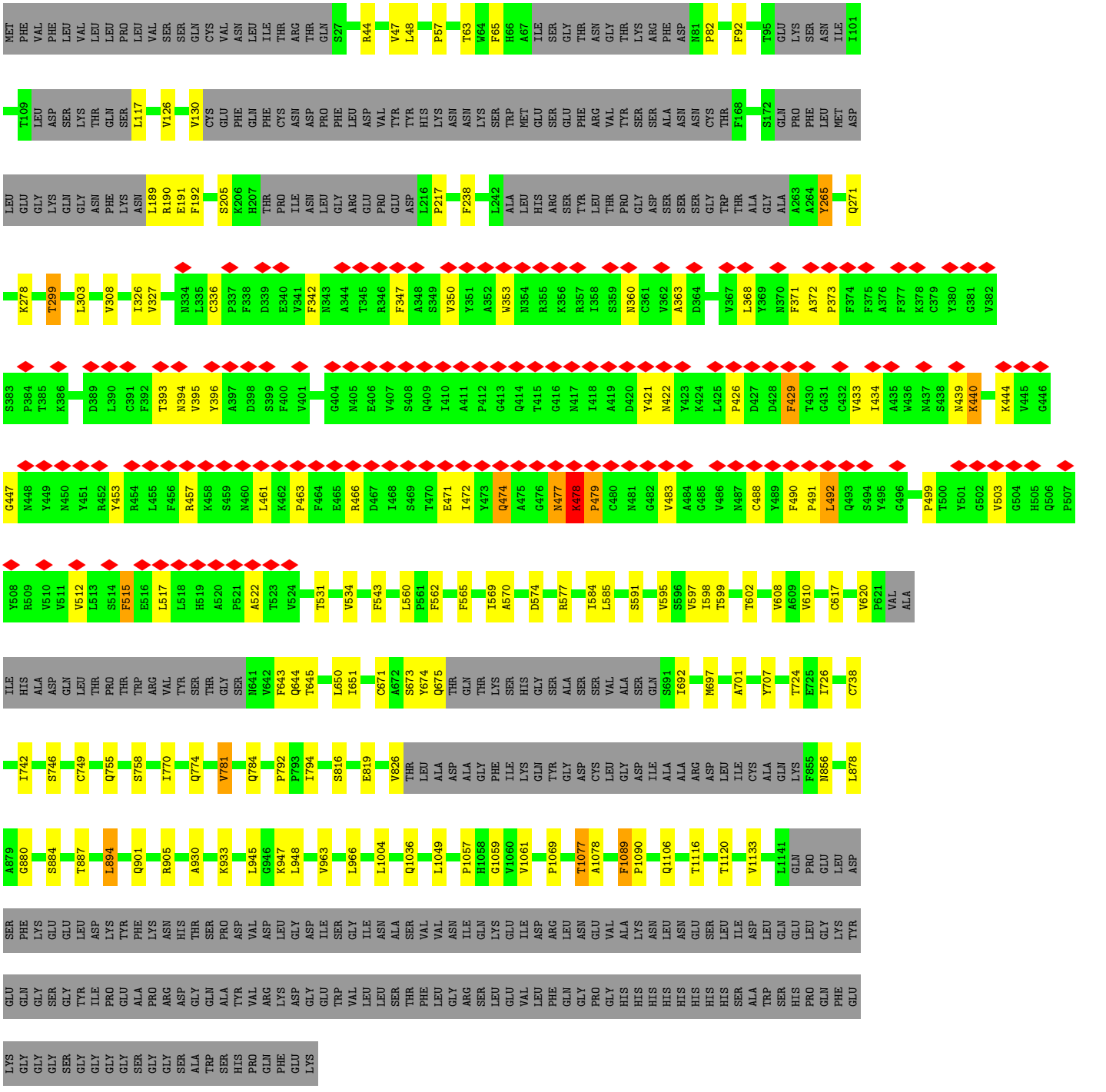
• Molecule 1: Spike glycoprotein

Chain B:



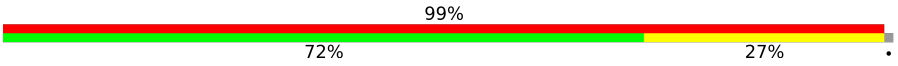
• Molecule 1: Spike glycoprotein

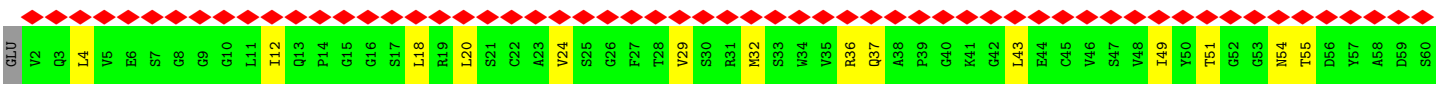
Chain C:

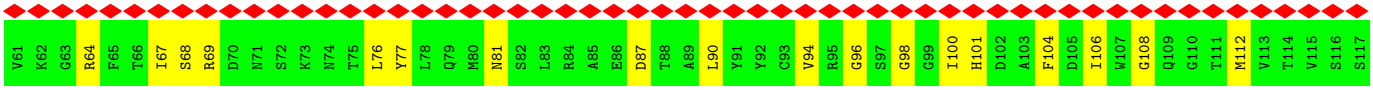


• Molecule 2: 10-5B H chain

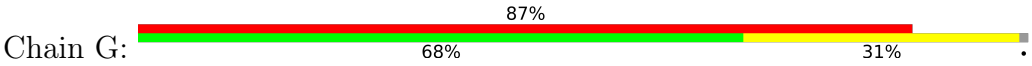
Chain E:

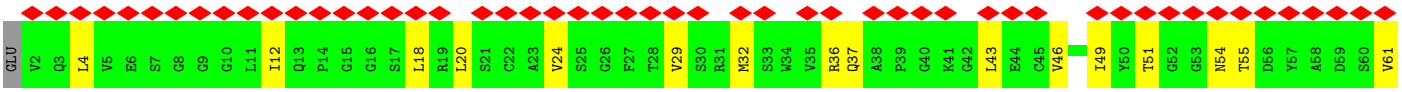


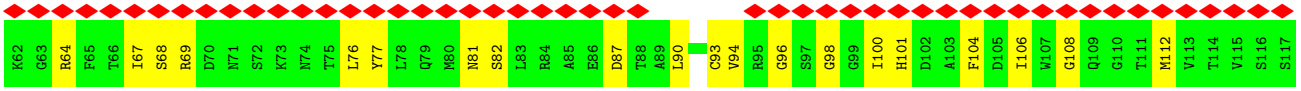




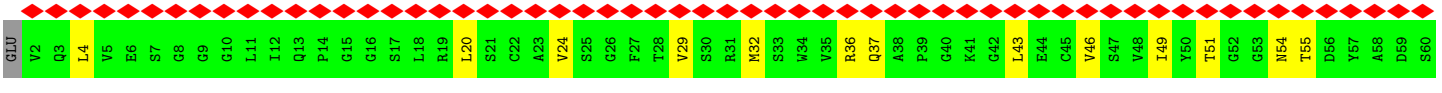
• Molecule 2: 10-5B H chain

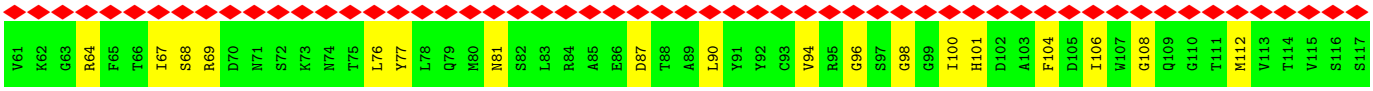




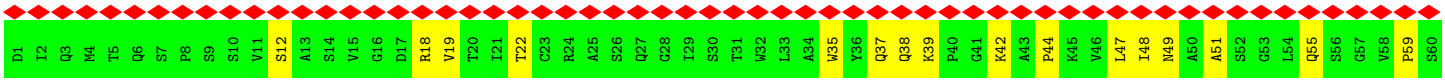


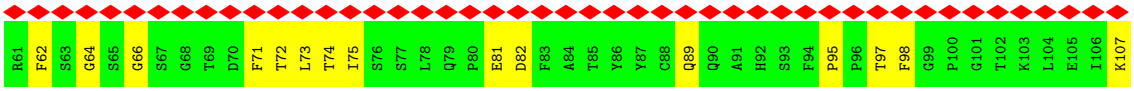
• Molecule 2: 10-5B H chain



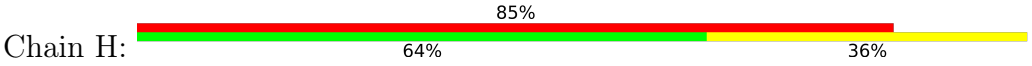


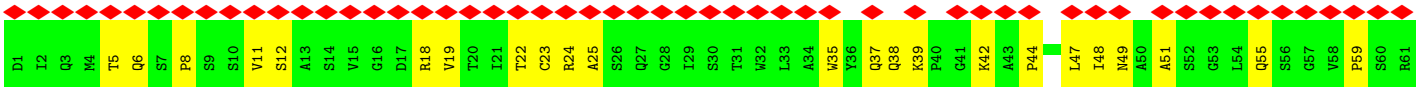
• Molecule 3: 10-5B L chain

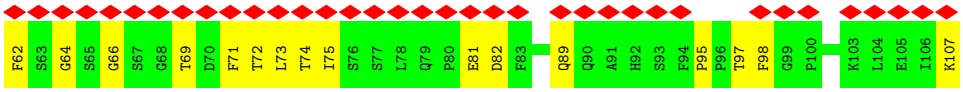




• Molecule 3: 10-5B L chain



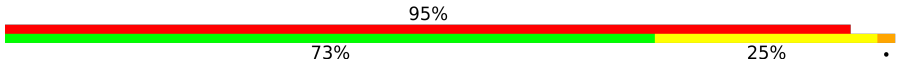




• Molecule 3: 10-5B L chain

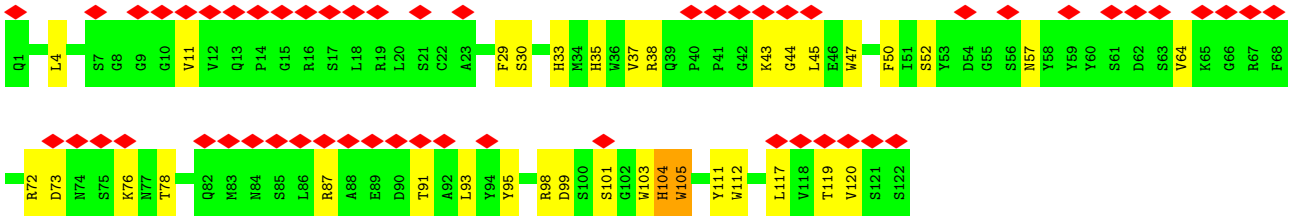
• Molecule 4: 6-2C H chain

Chain N:



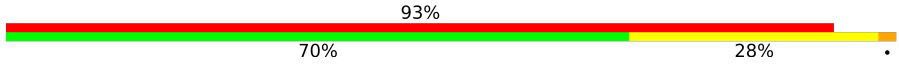
• Molecule 4: 6-2C H chain

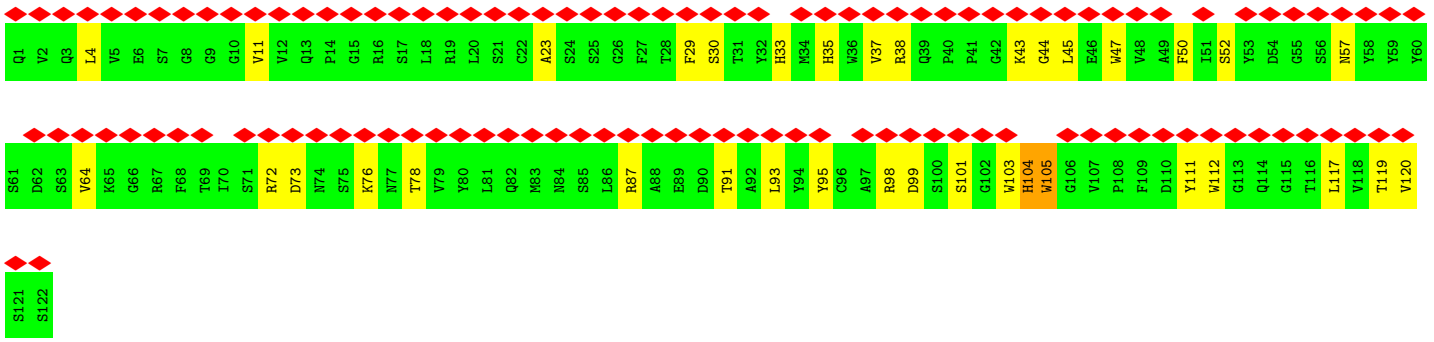
Chain I:



• Molecule 4: 6-2C H chain

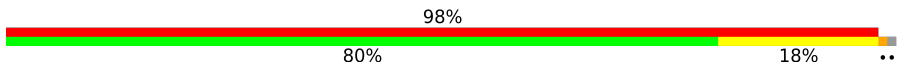
Chain Q:

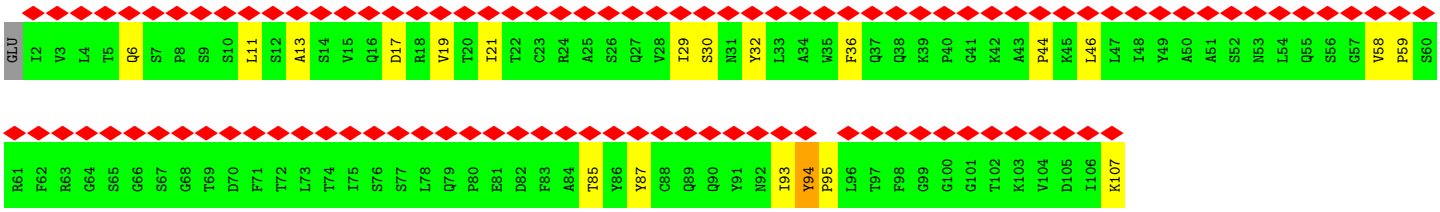




• Molecule 5: 6-2C L chain

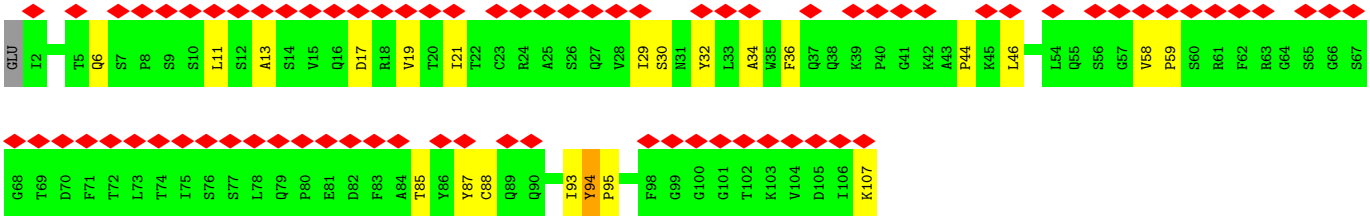
Chain O:





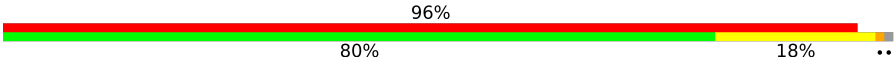
- Molecule 5: 6-2C L chain

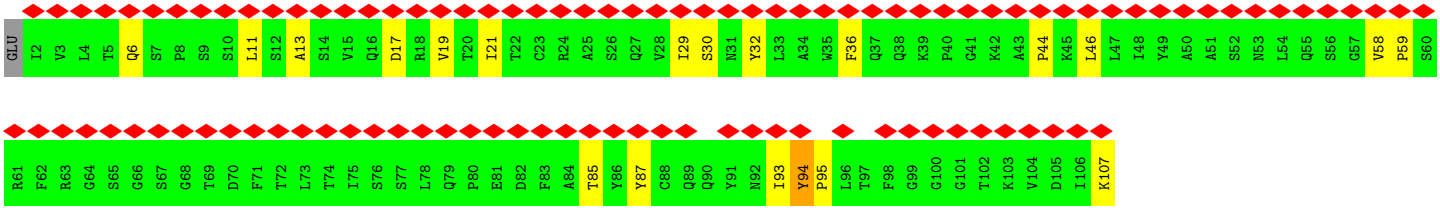
Chain K:



- Molecule 5: 6-2C L chain

Chain R:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	624379	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.466	Depositor
Minimum map value	-2.826	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	329.80002, 329.80002, 329.80002	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.64	1/7274 (0.0%)	0.84	6/9905 (0.1%)
1	B	0.65	1/7293 (0.0%)	0.87	8/9936 (0.1%)
1	C	0.63	1/7356 (0.0%)	0.86	5/10026 (0.0%)
2	E	0.63	0/851	0.73	0/1152
2	G	0.62	0/861	0.73	0/1165
2	M	0.63	0/852	0.73	0/1154
3	H	0.64	0/759	0.75	0/1034
3	J	0.64	0/757	0.75	0/1031
3	P	0.64	0/761	0.74	0/1037
4	I	0.62	0/952	0.82	0/1298
4	N	0.62	0/952	0.82	0/1298
4	Q	0.62	0/952	0.82	0/1298
5	K	0.65	0/789	0.88	1/1074 (0.1%)
5	O	0.65	0/789	0.88	1/1074 (0.1%)
5	R	0.65	0/789	0.88	1/1074 (0.1%)
All	All	0.64	3/31987 (0.0%)	0.84	22/43556 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	PRO	N-CD	-5.46	1.40	1.47
1	B	479	PRO	N-CD	-5.43	1.40	1.47
1	C	479	PRO	N-CD	-5.42	1.40	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1077	THR	CB-CA-C	-11.33	81.00	111.60
1	B	1082	CYS	CB-CA-C	-7.68	95.05	110.40
1	A	440	LYS	CB-CA-C	-6.79	96.81	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	440	LYS	CB-CA-C	-6.78	96.84	110.40
1	C	440	LYS	CB-CA-C	-6.78	96.85	110.40
5	O	94	TYR	CB-CA-C	6.17	122.73	110.40
5	R	94	TYR	CB-CA-C	6.16	122.72	110.40
5	K	94	TYR	CB-CA-C	6.15	122.70	110.40
1	B	1121	PHE	CB-CA-C	6.10	122.60	110.40
1	B	703	ASN	CB-CA-C	6.04	122.47	110.40
1	A	904	TYR	CB-CA-C	5.71	121.82	110.40
1	C	265	TYR	CB-CA-C	5.52	121.45	110.40
1	A	801	ASN	CB-CA-C	5.46	121.32	110.40
1	A	474	GLN	CB-CA-C	-5.29	99.81	110.40
1	C	474	GLN	CB-CA-C	-5.28	99.84	110.40
1	B	474	GLN	CB-CA-C	-5.26	99.88	110.40
1	A	815	ARG	CB-CA-C	5.23	120.86	110.40
1	B	478	LYS	C-N-CD	-5.21	109.14	120.60
1	C	478	LYS	C-N-CD	-5.20	109.17	120.60
1	A	478	LYS	C-N-CD	-5.19	109.18	120.60
1	B	1067	TYR	CB-CA-C	-5.19	100.03	110.40
1	B	1138	TYR	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

There are no planarity outliers.

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	7115	0	6701	105	0
1	B	7139	0	6761	111	0
1	C	7188	0	6752	101	0
2	E	837	0	783	32	0
2	G	847	0	808	40	0
2	M	838	0	788	33	0
3	H	741	0	676	30	0
3	J	739	0	669	22	0
3	P	743	0	681	27	0
4	I	925	0	815	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	925	0	815	31	0
4	Q	925	0	815	33	0
5	K	772	0	726	13	0
5	O	772	0	726	12	0
5	R	772	0	726	12	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
All	All	31320	0	29281	587	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 10.

All (587) 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)
2:E:96:GLY:HA2	2:E:104:PHE:HA	1.45	0.98
2:G:96:GLY:HA2	2:G:104:PHE:HA	1.45	0.95
2:M:96:GLY:HA2	2:M:104:PHE:HA	1.45	0.95
3:P:66:GLY:HA3	3:P:71:PHE:HA	1.62	0.82
4:N:35:HIS:CD2	4:N:47:TRP:HE1	1.99	0.81
4:Q:35:HIS:CD2	4:Q:47:TRP:HE1	1.99	0.80
3:H:66:GLY:HA3	3:H:71:PHE:HA	1.62	0.80
3:J:66:GLY:HA3	3:J:71:PHE:HA	1.62	0.80
4:I:35:HIS:CD2	4:I:47:TRP:HE1	1.99	0.80
2:G:49:ILE:CD1	2:G:55:THR:HG22	2.13	0.79
2:M:49:ILE:CD1	2:M:55:THR:HG22	2.13	0.79
2:E:49:ILE:CD1	2:E:55:THR:HG22	2.13	0.78
1:C:440:LYS:HG3	5:O:94:TYR:CE2	2.19	0.78
1:A:440:LYS:HG3	5:R:94:TYR:CE2	2.19	0.78
1:B:440:LYS:HG3	5:K:94:TYR:CE2	2.19	0.77
3:H:48:ILE:HA	3:H:55:GLN:HB3	1.69	0.74
3:J:48:ILE:HA	3:J:55:GLN:HB3	1.69	0.74
3:H:24:ARG:HA	3:H:69:THR:O	1.88	0.73
2:M:24:VAL:HG21	2:M:29:VAL:HG22	1.70	0.73
3:P:48:ILE:HA	3:P:55:GLN:HB3	1.69	0.73
2:E:24:VAL:HG21	2:E:29:VAL:HG22	1.70	0.72
2:G:24:VAL:HG21	2:G:29:VAL:HG22	1.70	0.72
2:M:36:ARG:HD3	2:M:46:VAL:HG21	1.73	0.70
2:G:36:ARG:HD3	2:G:46:VAL:HG21	1.73	0.70
2:M:29:VAL:HG12	2:M:29:VAL:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:29:VAL:HG12	2:E:29:VAL:O	1.93	0.69
4:Q:30:SER:HA	4:Q:72:ARG:HH22	1.58	0.69
2:G:29:VAL:O	2:G:29:VAL:HG12	1.93	0.68
4:I:30:SER:HA	4:I:72:ARG:HH22	1.58	0.68
5:K:93:ILE:HG22	5:K:95:PRO:HD2	1.75	0.68
5:R:93:ILE:HG22	5:R:95:PRO:HD2	1.75	0.68
1:A:41:LYS:NZ	1:C:562:PHE:HB2	2.09	0.68
4:N:30:SER:HA	4:N:72:ARG:HH22	1.58	0.67
5:O:93:ILE:HG22	5:O:95:PRO:HD2	1.76	0.66
3:P:95:PRO:O	3:P:97:THR:HG23	1.95	0.66
3:J:95:PRO:O	3:J:97:THR:HG23	1.95	0.66
3:H:95:PRO:O	3:H:97:THR:HG23	1.95	0.66
3:P:5:THR:OG1	3:P:24:ARG:HG3	1.96	0.66
3:H:5:THR:OG1	3:H:24:ARG:HG3	1.96	0.65
2:G:61:VAL:HG13	2:G:64:ARG:NE	2.11	0.65
1:C:426:PRO:HD2	1:C:429:PHE:HB2	1.78	0.65
1:A:426:PRO:HD2	1:A:429:PHE:HB2	1.78	0.64
1:B:65:PHE:HB2	1:B:265:TYR:CE1	2.33	0.64
1:C:439:ASN:HD21	1:C:499:PRO:HA	1.63	0.64
1:B:439:ASN:HD21	1:B:499:PRO:HA	1.63	0.63
1:B:426:PRO:HD2	1:B:429:PHE:HB2	1.78	0.63
1:A:439:ASN:HD21	1:A:499:PRO:HA	1.63	0.62
4:Q:4:LEU:HD13	4:Q:98:ARG:HH21	1.64	0.62
1:A:804:GLN:HA	1:A:817:PRO:HG2	1.80	0.62
1:B:866:THR:H	1:B:869:MET:HE3	1.64	0.62
1:B:490:PHE:CD1	2:G:51:THR:CG2	2.83	0.62
1:C:490:PHE:CD1	2:E:51:THR:CG2	2.83	0.62
4:I:4:LEU:HD13	4:I:98:ARG:HH21	1.65	0.62
1:A:393:THR:HA	1:A:522:ALA:HA	1.81	0.62
1:A:490:PHE:CD1	2:M:51:THR:CG2	2.82	0.62
1:A:34:ARG:HH12	1:A:189:LEU:HD21	1.63	0.62
1:B:393:THR:HA	1:B:522:ALA:HA	1.81	0.62
1:A:426:PRO:HD3	1:A:463:PRO:HB3	1.82	0.62
2:M:49:ILE:HD13	2:M:55:THR:HG22	1.82	0.61
3:J:39:LYS:HB2	3:J:42:LYS:HB2	1.83	0.61
1:C:598:ILE:HD12	1:C:650:LEU:HD11	1.81	0.61
2:E:98:GLY:O	2:E:101:HIS:HB2	2.01	0.61
2:E:49:ILE:HD13	2:E:55:THR:HG22	1.82	0.61
2:G:98:GLY:O	2:G:101:HIS:HB2	2.01	0.61
4:I:99:ASP:OD1	4:I:101:SER:HB3	2.00	0.61
4:Q:99:ASP:OD1	4:Q:101:SER:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:61:VAL:HG13	2:G:64:ARG:CZ	2.31	0.61
1:C:393:THR:HA	1:C:522:ALA:HA	1.81	0.60
2:M:98:GLY:O	2:M:101:HIS:HB2	2.01	0.60
3:P:39:LYS:HB2	3:P:42:LYS:HB2	1.83	0.60
1:B:426:PRO:HD3	1:B:463:PRO:HB3	1.81	0.60
4:N:4:LEU:HD13	4:N:98:ARG:HH21	1.64	0.60
1:C:483:VAL:HG13	2:E:54:ASN:HD21	1.66	0.60
4:N:99:ASP:OD1	4:N:101:SER:HB3	2.00	0.60
1:B:483:VAL:HG13	2:G:54:ASN:HD21	1.66	0.60
2:G:49:ILE:HD13	2:G:55:THR:HG22	1.82	0.60
3:H:39:LYS:HB2	3:H:42:LYS:HB2	1.83	0.60
1:B:433:VAL:HG22	1:B:512:VAL:HG13	1.84	0.60
1:C:426:PRO:HD3	1:C:463:PRO:HB3	1.81	0.60
1:A:433:VAL:HG22	1:A:512:VAL:HG13	1.84	0.59
1:A:483:VAL:HG13	2:M:54:ASN:HD21	1.66	0.59
1:C:433:VAL:HG22	1:C:512:VAL:HG13	1.84	0.59
4:N:45:LEU:HD11	5:O:44:PRO:HG2	1.84	0.59
1:A:440:LYS:HG3	5:R:94:TYR:CZ	2.37	0.59
2:E:12:ILE:HG21	2:E:18:LEU:HD11	1.84	0.59
4:N:52:SER:HB2	4:N:57:ASN:HB2	1.84	0.59
4:I:52:SER:HB2	4:I:57:ASN:HB2	1.84	0.59
1:C:342:PHE:HZ	1:C:434:ILE:HD13	1.67	0.59
1:A:205:SER:OG	1:A:226:LEU:HD12	2.03	0.59
1:A:342:PHE:HZ	1:A:434:ILE:HD13	1.67	0.58
1:C:440:LYS:HG3	5:O:94:TYR:CZ	2.38	0.58
1:B:48:LEU:CD2	1:B:278:LYS:HG3	2.32	0.58
2:G:12:ILE:HG21	2:G:18:LEU:HD11	1.84	0.58
1:C:336:CYS:SG	1:C:363:ALA:HB2	2.44	0.58
4:Q:45:LEU:HD11	5:R:44:PRO:HG2	1.84	0.58
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.44	0.58
1:B:353:TRP:CE2	1:B:466:ARG:HB3	2.39	0.58
1:B:440:LYS:HG3	5:K:94:TYR:CZ	2.38	0.58
3:J:22:THR:HG22	3:J:72:THR:HB	1.86	0.58
3:J:59:PRO:HD2	3:J:62:PHE:CD2	2.39	0.58
4:I:45:LEU:HD11	5:K:44:PRO:HG2	1.84	0.58
1:A:353:TRP:CE2	1:A:466:ARG:HB3	2.39	0.58
4:N:35:HIS:HD2	4:N:47:TRP:HE1	1.50	0.58
4:Q:52:SER:HB2	4:Q:57:ASN:HB2	1.84	0.58
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.44	0.58
1:C:82:PRO:HD2	1:C:265:TYR:OH	2.04	0.58
1:B:342:PHE:HZ	1:B:434:ILE:HD13	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20:LEU:O	2:E:77:TYR:HA	2.04	0.57
1:A:284:THR:HG22	1:C:560:LEU:HD11	1.87	0.57
1:A:371:PHE:HB2	1:A:373:PRO:HD3	1.86	0.57
1:A:1082:CYS:HB2	1:A:1132:ILE:HG12	1.87	0.57
4:I:37:VAL:HG21	4:I:112:TRP:CH2	2.39	0.57
3:P:22:THR:HG22	3:P:72:THR:HB	1.86	0.57
4:Q:37:VAL:HG21	4:Q:112:TRP:CH2	2.39	0.57
1:A:1081:ILE:HD11	1:A:1137:VAL:HG23	1.87	0.57
4:N:37:VAL:HG21	4:N:112:TRP:CH2	2.39	0.57
3:H:8:PRO:HG2	3:H:11:VAL:CG2	2.35	0.57
3:H:22:THR:HG22	3:H:72:THR:HB	1.86	0.57
3:P:59:PRO:HD2	3:P:62:PHE:CD2	2.39	0.57
4:Q:35:HIS:HD2	4:Q:47:TRP:HE1	1.50	0.57
2:G:20:LEU:O	2:G:77:TYR:HA	2.04	0.57
1:B:551:VAL:HG12	1:B:553:THR:HG23	1.87	0.57
2:E:29:VAL:HG13	2:E:32:MET:HG3	1.87	0.57
2:M:68:SER:HB2	2:M:77:TYR:HB2	1.86	0.57
3:P:8:PRO:HG2	3:P:11:VAL:CG2	2.35	0.57
1:C:326:ILE:HG21	1:C:534:VAL:HG22	1.86	0.57
1:C:353:TRP:CE2	1:C:466:ARG:HB3	2.39	0.57
3:H:59:PRO:HD2	3:H:62:PHE:CD2	2.39	0.57
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.87	0.56
2:E:68:SER:HB2	2:E:77:TYR:HB2	1.86	0.56
2:G:68:SER:HB2	2:G:77:TYR:HB2	1.86	0.56
2:M:20:LEU:O	2:M:77:TYR:HA	2.04	0.56
4:Q:35:HIS:CD2	4:Q:47:TRP:NE1	2.72	0.56
1:C:48:LEU:HD23	1:C:278:LYS:HA	1.86	0.56
3:J:22:THR:HG22	3:J:72:THR:CB	2.36	0.56
2:M:43:LEU:HB2	3:P:98:PHE:CD2	2.40	0.56
1:B:193:VAL:HG23	1:B:223:LEU:HD12	1.88	0.56
2:G:29:VAL:HG13	2:G:32:MET:HG3	1.87	0.56
2:M:29:VAL:HG13	2:M:32:MET:HG3	1.87	0.56
1:B:371:PHE:HB2	1:B:373:PRO:HD3	1.86	0.56
1:C:371:PHE:HB2	1:C:373:PRO:HD3	1.86	0.56
1:C:595:VAL:HG13	1:C:610:VAL:CG1	2.36	0.56
3:J:37:GLN:HB3	3:J:47:LEU:HD11	1.88	0.56
4:I:35:HIS:CD2	4:I:47:TRP:NE1	2.72	0.56
4:I:35:HIS:HD2	4:I:47:TRP:HE1	1.50	0.56
2:G:43:LEU:HB2	3:H:98:PHE:CD2	2.40	0.56
3:P:22:THR:HG22	3:P:72:THR:CB	2.35	0.56
1:A:37:TYR:HA	1:A:223:LEU:H	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:8:PRO:HG2	3:H:11:VAL:HG22	1.88	0.55
3:H:37:GLN:HB3	3:H:47:LEU:HD11	1.88	0.55
2:E:43:LEU:HB2	3:J:98:PHE:CD2	2.40	0.55
2:E:64:ARG:HA	2:E:81:ASN:HB2	1.88	0.55
1:B:503:VAL:HG11	5:K:30:SER:HB3	1.88	0.55
1:C:880:GLY:O	1:C:884:SER:OG	2.22	0.55
3:P:8:PRO:HG2	3:P:11:VAL:HG22	1.88	0.55
2:G:64:ARG:HA	2:G:81:ASN:HB2	1.88	0.55
1:B:707:TYR:HB3	1:C:792:PRO:HB3	1.87	0.55
4:I:35:HIS:HD2	4:I:47:TRP:NE1	2.05	0.55
4:Q:35:HIS:HD2	4:Q:47:TRP:NE1	2.05	0.55
4:Q:104:HIS:CG	4:Q:104:HIS:O	2.59	0.55
1:A:503:VAL:HG11	5:R:30:SER:HB3	1.88	0.55
3:H:22:THR:HG22	3:H:72:THR:CB	2.35	0.55
2:M:64:ARG:HA	2:M:81:ASN:HB2	1.88	0.55
3:P:37:GLN:HB3	3:P:47:LEU:HD11	1.88	0.55
1:A:720:ILE:HG13	1:A:923:ILE:HG23	1.89	0.54
1:C:673:SER:OG	1:C:674:TYR:N	2.40	0.54
4:N:104:HIS:O	4:N:104:HIS:CG	2.59	0.54
4:N:35:HIS:CD2	4:N:47:TRP:NE1	2.72	0.54
1:C:503:VAL:HG11	5:O:30:SER:HB3	1.89	0.54
4:N:37:VAL:HG21	4:N:112:TRP:CZ3	2.43	0.54
4:I:104:HIS:O	4:I:104:HIS:CG	2.59	0.54
4:N:35:HIS:HD2	4:N:47:TRP:NE1	2.05	0.54
1:B:490:PHE:CD1	2:G:51:THR:HG21	2.43	0.54
1:A:490:PHE:CD1	2:M:51:THR:HG21	2.43	0.54
4:I:37:VAL:HG21	4:I:112:TRP:CZ3	2.43	0.54
4:Q:37:VAL:HG21	4:Q:112:TRP:CZ3	2.43	0.54
1:C:490:PHE:CD1	2:E:51:THR:HG21	2.43	0.53
3:H:25:ALA:H	3:H:69:THR:HA	1.73	0.53
1:A:41:LYS:HZ1	1:C:562:PHE:HB2	1.72	0.53
2:E:29:VAL:CG1	2:E:69:ARG:HG3	2.39	0.53
1:C:395:VAL:HG12	1:C:515:PHE:HA	1.91	0.53
1:C:770:ILE:O	1:C:774:GLN:HG2	2.09	0.53
2:M:29:VAL:CG1	2:M:69:ARG:HG3	2.39	0.53
2:G:96:GLY:HA3	2:G:100:ILE:HD13	1.91	0.52
1:C:65:PHE:CE2	1:C:82:PRO:HG3	2.44	0.52
1:C:595:VAL:HG13	1:C:610:VAL:HG13	1.91	0.52
1:B:655:TYR:HA	1:B:694:ALA:O	2.09	0.52
2:G:29:VAL:CG1	2:G:69:ARG:HG3	2.39	0.52
3:P:5:THR:OG1	3:P:24:ARG:CG	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:VAL:HG12	1:A:515:PHE:HA	1.91	0.52
1:A:598:ILE:HG23	1:A:664:ILE:HD13	1.91	0.52
1:B:395:VAL:HG12	1:B:515:PHE:HA	1.91	0.52
1:A:616:ASN:HD22	1:A:617:CYS:H	1.56	0.52
1:C:620:VAL:HG21	1:C:651:ILE:HD11	1.92	0.52
4:I:33:HIS:HB3	4:I:50:PHE:HE1	1.75	0.52
1:B:32:PHE:CB	1:B:218:GLN:HG3	2.39	0.52
1:C:393:THR:HG23	1:C:517:LEU:HD12	1.92	0.52
1:B:48:LEU:CD2	1:B:278:LYS:CG	2.88	0.52
4:Q:33:HIS:HB3	4:Q:50:PHE:HE1	1.75	0.52
1:C:92:PHE:CE2	1:C:265:TYR:HB2	2.46	0.51
2:M:96:GLY:HA3	2:M:100:ILE:HD13	1.91	0.51
3:P:37:GLN:O	3:P:44:PRO:HA	2.10	0.51
1:B:48:LEU:HD23	1:B:278:LYS:HA	1.91	0.51
3:H:5:THR:OG1	3:H:24:ARG:CG	2.58	0.51
1:B:48:LEU:HD23	1:B:278:LYS:HG3	1.91	0.51
2:E:12:ILE:HG12	2:E:18:LEU:HD11	1.92	0.51
3:H:37:GLN:O	3:H:44:PRO:HA	2.10	0.51
1:A:1081:ILE:HD12	1:A:1135:ASN:HB3	1.91	0.51
1:B:122:ASN:OD1	1:B:125:ASN:O	2.28	0.51
4:N:33:HIS:HB3	4:N:50:PHE:HE1	1.75	0.51
1:A:342:PHE:CZ	1:A:368:LEU:HD13	2.46	0.51
1:B:342:PHE:CZ	1:B:368:LEU:HD13	2.46	0.51
1:C:63:THR:HG1	1:C:65:PHE:HE1	1.58	0.51
1:B:122:ASN:OD1	1:B:125:ASN:N	2.31	0.51
3:J:37:GLN:O	3:J:44:PRO:HA	2.10	0.51
1:C:342:PHE:CZ	1:C:368:LEU:HD13	2.46	0.51
4:I:37:VAL:O	4:I:95:TYR:HB2	2.11	0.51
4:Q:37:VAL:O	4:Q:95:TYR:HB2	2.11	0.51
1:A:393:THR:HG23	1:A:517:LEU:HD12	1.92	0.51
1:A:1090:PRO:HA	1:A:1120:THR:HA	1.92	0.51
1:B:902:MET:HB3	1:B:916:LEU:HD22	1.93	0.51
1:C:92:PHE:CZ	1:C:265:TYR:HB2	2.45	0.51
1:A:41:LYS:HZ3	1:C:562:PHE:HB2	1.75	0.50
1:B:393:THR:HG23	1:B:517:LEU:HD12	1.92	0.50
1:C:190:ARG:HB2	1:C:192:PHE:CZ	2.47	0.50
2:M:49:ILE:HB	2:M:67:ILE:HD13	1.94	0.50
2:E:96:GLY:HA3	2:E:100:ILE:HD13	1.91	0.50
2:G:12:ILE:HG12	2:G:18:LEU:HD11	1.92	0.50
2:G:36:ARG:HA	2:G:90:LEU:O	2.12	0.50
1:A:393:THR:HG22	1:A:522:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:73:ASP:HB3	4:N:76:LYS:HB2	1.94	0.50
2:G:49:ILE:HB	2:G:67:ILE:HD13	1.94	0.50
1:C:724:THR:HG23	1:C:1061:VAL:HG13	1.94	0.50
4:N:37:VAL:O	4:N:95:TYR:HB2	2.11	0.50
2:E:36:ARG:HA	2:E:90:LEU:O	2.12	0.50
2:M:36:ARG:NH2	2:M:87:ASP:HA	2.27	0.50
2:M:36:ARG:HA	2:M:90:LEU:O	2.12	0.49
2:G:36:ARG:NH2	2:G:87:ASP:HA	2.27	0.49
1:B:620:VAL:N	1:B:621:PRO:HD2	2.27	0.49
1:C:884:SER:HB2	1:C:887:THR:OG1	2.11	0.49
1:C:1036:GLN:HE21	1:C:1049:LEU:HA	1.76	0.49
2:E:36:ARG:NH2	2:E:87:ASP:HA	2.27	0.49
1:A:811:LYS:O	1:A:813:SER:N	2.40	0.49
1:B:48:LEU:HD21	1:B:278:LYS:CG	2.42	0.49
5:R:13:ALA:HB1	5:R:17:ASP:HB3	1.94	0.49
1:A:616:ASN:HD22	1:A:617:CYS:N	2.11	0.49
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.93	0.49
1:B:350:VAL:HG12	1:B:422:ASN:ND2	2.28	0.49
4:N:93:LEU:CG	4:N:117:LEU:HD12	2.43	0.49
4:I:73:ASP:HB3	4:I:76:LYS:HB2	1.94	0.49
4:I:93:LEU:CG	4:I:117:LEU:HD12	2.43	0.49
2:E:49:ILE:HB	2:E:67:ILE:HD13	1.94	0.49
1:A:350:VAL:HG12	1:A:422:ASN:ND2	2.28	0.49
1:C:44:ARG:HB3	1:C:47:VAL:HG21	1.95	0.49
1:C:350:VAL:HG12	1:C:422:ASN:ND2	2.28	0.49
1:C:905:ARG:HD3	1:C:1049:LEU:O	2.13	0.49
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.94	0.48
4:N:11:VAL:HG22	4:N:119:THR:HB	1.95	0.48
1:A:979:ASP:O	1:A:983:ARG:HG2	2.13	0.48
1:B:791:THR:HG23	1:B:879:ALA:HB2	1.94	0.48
2:M:94:VAL:HB	2:M:104:PHE:HB3	1.95	0.48
1:B:802:PHE:HB3	1:B:805:ILE:HG12	1.95	0.48
1:B:819:GLU:OE2	1:B:1055:SER:HB3	2.14	0.48
4:Q:11:VAL:HG22	4:Q:119:THR:HB	1.95	0.48
1:C:393:THR:HG22	1:C:522:ALA:HA	1.94	0.48
1:C:617:CYS:N	1:C:644:GLN:OE1	2.46	0.48
4:Q:45:LEU:HD13	4:Q:112:TRP:CH2	2.49	0.48
4:Q:73:ASP:HB3	4:Q:76:LYS:HB2	1.94	0.48
1:C:643:PHE:CE2	1:C:645:THR:HG22	2.49	0.48
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.95	0.48
5:O:13:ALA:HB1	5:O:17:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:94:VAL:HB	2:G:104:PHE:HB3	1.95	0.48
5:K:13:ALA:HB1	5:K:17:ASP:HB3	1.94	0.48
4:Q:93:LEU:CG	4:Q:117:LEU:HD12	2.42	0.48
1:A:444:LYS:HG3	1:A:447:GLY:H	1.79	0.48
1:C:599:THR:HG22	1:C:608:VAL:HG12	1.94	0.48
1:C:816:SER:OG	1:C:819:GLU:HG3	2.14	0.48
1:A:490:PHE:CD1	2:M:51:THR:HG23	2.49	0.48
1:A:902:MET:O	1:A:903:ALA:HB3	2.13	0.48
1:B:393:THR:HG22	1:B:522:ALA:HA	1.94	0.48
4:Q:11:VAL:HA	4:Q:119:THR:HB	1.96	0.48
5:R:58:VAL:HB	5:R:59:PRO:HD3	1.96	0.48
1:B:965:GLN:HE22	1:C:758:SER:H	1.62	0.48
1:C:595:VAL:CG1	1:C:610:VAL:HG13	2.44	0.48
4:I:11:VAL:HA	4:I:119:THR:HB	1.96	0.48
1:B:48:LEU:HD21	1:B:278:LYS:HG3	1.96	0.47
4:N:45:LEU:HD13	4:N:112:TRP:CH2	2.49	0.47
4:I:45:LEU:HD13	4:I:112:TRP:CH2	2.49	0.47
1:B:444:LYS:HG3	1:B:447:GLY:H	1.79	0.47
1:B:490:PHE:CD1	2:G:51:THR:HG23	2.49	0.47
1:B:570:ALA:HB1	1:C:963:VAL:HG11	1.95	0.47
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.95	0.47
4:I:11:VAL:HG22	4:I:119:THR:HB	1.95	0.47
1:A:616:ASN:O	1:A:619:GLU:HG2	2.14	0.47
1:B:372:ALA:N	1:B:373:PRO:HD3	2.30	0.47
1:B:979:ASP:HB2	1:B:983:ARG:HD3	1.97	0.47
2:E:94:VAL:HB	2:E:104:PHE:HB3	1.95	0.47
5:K:58:VAL:HB	5:K:59:PRO:HD3	1.96	0.47
2:M:29:VAL:O	2:M:29:VAL:CG1	2.62	0.47
1:B:595:VAL:HG13	1:B:610:VAL:HG13	1.95	0.47
1:B:1036:GLN:HA	1:B:1048:HIS:CE1	2.49	0.47
1:C:192:PHE:HD1	1:C:205:SER:HB2	1.78	0.47
1:A:27:SER:OG	1:A:64:TRP:HB3	2.14	0.47
1:A:372:ALA:N	1:A:373:PRO:HD3	2.29	0.47
1:A:812:PRO:O	1:A:813:SER:HB2	2.14	0.47
1:B:911:VAL:HG12	1:B:912:THR:N	2.29	0.47
2:E:29:VAL:HG11	2:E:69:ARG:HG3	1.97	0.47
3:J:19:VAL:O	3:J:74:THR:HA	2.15	0.47
2:G:29:VAL:HG11	2:G:69:ARG:HG3	1.97	0.47
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.15	0.47
1:B:1090:PRO:HA	1:B:1120:THR:HA	1.97	0.47
1:C:491:PRO:O	1:C:492:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:87:ARG:HA	4:I:87:ARG:NE	2.30	0.47
2:M:29:VAL:HG11	2:M:69:ARG:HG3	1.97	0.47
4:Q:87:ARG:NE	4:Q:87:ARG:HA	2.30	0.47
1:A:64:TRP:HD1	1:A:65:PHE:H	1.63	0.47
1:A:300:LYS:HG2	1:A:308:VAL:HG23	1.97	0.47
2:G:29:VAL:O	2:G:29:VAL:CG1	2.62	0.47
1:B:48:LEU:CD2	1:B:278:LYS:CB	2.92	0.46
1:B:206:LYS:HB3	1:B:223:LEU:HD22	1.98	0.46
1:B:555:SER:HB3	1:B:584:ILE:HG22	1.97	0.46
1:C:299:THR:OG1	1:C:597:VAL:HG21	2.15	0.46
1:C:490:PHE:CD1	2:E:51:THR:HG23	2.49	0.46
1:B:617:CYS:O	1:B:620:VAL:HG22	2.15	0.46
4:N:11:VAL:HA	4:N:119:THR:HB	1.96	0.46
1:A:326:ILE:HG12	1:A:539:VAL:HG21	1.98	0.46
1:A:491:PRO:O	1:A:492:LEU:HG	2.15	0.46
1:B:1086:LYS:HE3	1:B:1088:HIS:HE1	1.80	0.46
1:C:372:ALA:N	1:C:373:PRO:HD3	2.29	0.46
5:R:85:THR:HG1	5:R:87:TYR:HE2	1.63	0.46
1:A:1078:ALA:HB1	1:A:1131:GLY:O	2.16	0.46
1:B:536:ASN:HA	1:B:551:VAL:HG13	1.97	0.46
3:J:64:GLY:HA3	3:J:73:LEU:HA	1.98	0.46
1:C:48:LEU:HD21	1:C:278:LYS:HD3	1.96	0.46
1:C:746:SER:HB3	1:C:749:CYS:HB3	1.98	0.46
1:C:1004:LEU:HD12	1:C:1004:LEU:HA	1.83	0.46
4:N:87:ARG:HA	4:N:87:ARG:NE	2.30	0.46
1:A:1090:PRO:HG2	1:A:1093:GLY:O	2.16	0.46
1:B:49:HIS:CE1	1:B:51:THR:HG22	2.51	0.46
1:B:977:LEU:HD22	1:B:993:ILE:HD12	1.97	0.46
2:E:29:VAL:O	2:E:29:VAL:CG1	2.62	0.46
1:A:471:GLU:O	1:A:472:ILE:C	2.54	0.46
1:B:1089:PHE:O	1:B:1121:PHE:N	2.46	0.46
3:H:19:VAL:O	3:H:74:THR:HA	2.15	0.46
3:P:19:VAL:O	3:P:74:THR:HA	2.15	0.46
3:P:35:TRP:HD1	3:P:48:ILE:HG13	1.81	0.46
1:C:457:ARG:NH2	1:C:461:LEU:HD13	2.31	0.46
5:O:58:VAL:HB	5:O:59:PRO:HD3	1.96	0.46
1:A:897:PRO:HA	1:C:707:TYR:HE1	1.81	0.46
1:B:48:LEU:CD2	1:B:278:LYS:HB2	2.45	0.46
1:C:444:LYS:HG3	1:C:447:GLY:H	1.79	0.46
1:A:290:ASP:O	1:A:297:SER:HB3	2.15	0.45
1:B:471:GLU:O	1:B:472:ILE:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ILE:O	1:B:774:GLN:HG2	2.15	0.45
2:M:43:LEU:HB2	3:P:98:PHE:CG	2.51	0.45
1:A:615:VAL:HG13	1:A:619:GLU:HG3	1.98	0.45
2:G:43:LEU:HB2	3:H:98:PHE:CG	2.51	0.45
3:H:64:GLY:HA3	3:H:73:LEU:HA	1.98	0.45
1:A:457:ARG:NH2	1:A:461:LEU:HD13	2.31	0.45
1:B:65:PHE:HB2	1:B:265:TYR:CD1	2.51	0.45
1:B:457:ARG:NH2	1:B:461:LEU:HD13	2.31	0.45
1:B:474:GLN:HB2	1:B:488:CYS:SG	2.57	0.45
1:C:491:PRO:C	1:C:492:LEU:HG	2.37	0.45
1:C:474:GLN:HB2	1:C:488:CYS:SG	2.57	0.45
2:E:43:LEU:HB2	3:J:98:PHE:CG	2.51	0.45
3:J:35:TRP:HD1	3:J:48:ILE:HG13	1.81	0.45
3:H:35:TRP:HD1	3:H:48:ILE:HG13	1.81	0.45
4:I:35:HIS:HE1	4:I:99:ASP:HB2	1.82	0.45
1:A:770:ILE:O	1:A:774:GLN:HG2	2.16	0.45
1:B:491:PRO:O	1:B:492:LEU:HG	2.15	0.45
1:C:477:ASN:O	1:C:478:LYS:C	2.55	0.45
4:Q:35:HIS:HE1	4:Q:99:ASP:HB2	1.82	0.45
1:A:298:GLU:O	1:A:302:THR:HG23	2.17	0.45
1:B:371:PHE:C	1:B:373:PRO:HD3	2.38	0.45
1:A:474:GLN:HB2	1:A:488:CYS:SG	2.57	0.45
1:A:897:PRO:HA	1:C:707:TYR:CE1	2.52	0.45
1:A:491:PRO:C	1:A:492:LEU:HG	2.37	0.45
1:B:65:PHE:CB	1:B:265:TYR:CE1	2.99	0.45
1:B:1081:ILE:HD11	1:B:1137:VAL:HG23	1.98	0.45
1:C:189:LEU:CD2	1:C:217:PRO:HG3	2.47	0.45
1:C:471:GLU:O	1:C:472:ILE:C	2.54	0.45
5:O:85:THR:HG1	5:O:87:TYR:HE2	1.64	0.45
2:G:64:ARG:HD3	2:G:82:SER:HB2	1.99	0.45
3:P:64:GLY:HA3	3:P:73:LEU:HA	1.98	0.45
1:A:64:TRP:CD1	1:A:65:PHE:N	2.84	0.44
1:A:95:THR:HG22	1:A:189:LEU:HD13	1.99	0.44
1:A:303:LEU:HD12	1:A:308:VAL:HG22	1.98	0.44
1:A:477:ASN:O	1:A:478:LYS:C	2.55	0.44
1:C:781:VAL:O	1:C:784:GLN:HG3	2.17	0.44
2:E:4:LEU:HB2	2:E:108:GLY:HA2	1.99	0.44
3:J:81:GLU:O	3:J:82:ASP:C	2.56	0.44
1:A:891:GLY:HA3	1:C:1069:PRO:HD2	1.99	0.44
1:B:128:ILE:O	1:B:171:VAL:HA	2.18	0.44
1:C:303:LEU:HD12	1:C:308:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:PHE:C	1:C:373:PRO:HD3	2.38	0.44
4:N:111:TYR:O	4:N:112:TRP:HB2	2.18	0.44
1:B:104:TRP:O	1:B:119:ILE:HG22	2.17	0.44
1:B:477:ASN:O	1:B:478:LYS:C	2.55	0.44
1:B:987:PRO:O	1:B:990:GLU:HG3	2.16	0.44
1:A:1036:GLN:HE21	1:A:1049:LEU:HA	1.82	0.44
4:N:35:HIS:HE1	4:N:99:ASP:HB2	1.82	0.44
1:A:94:SER:HB2	1:A:101:ILE:HD12	1.99	0.44
4:I:111:TYR:O	4:I:112:TRP:HB2	2.17	0.44
3:P:18:ARG:HA	3:P:75:ILE:O	2.18	0.44
1:A:34:ARG:HD3	1:A:34:ARG:HA	1.83	0.44
1:B:811:LYS:HD2	1:B:814:LYS:HG2	1.98	0.44
1:C:963:VAL:O	1:C:966:LEU:HB2	2.18	0.44
2:M:4:LEU:HB2	2:M:108:GLY:HA2	1.99	0.44
1:B:118:LEU:HB3	1:B:120:VAL:HG23	1.99	0.44
1:A:371:PHE:C	1:A:373:PRO:HD3	2.38	0.44
1:A:802:PHE:HB3	1:A:805:ILE:HG12	2.00	0.44
1:A:963:VAL:O	1:A:966:LEU:HB2	2.18	0.44
1:B:905:ARG:HD3	1:B:1049:LEU:O	2.18	0.44
1:C:671:CYS:SG	1:C:697:MET:HB2	2.57	0.44
3:H:81:GLU:O	3:H:82:ASP:C	2.56	0.44
3:P:89:GLN:HA	3:P:97:THR:O	2.18	0.44
1:A:342:PHE:CZ	1:A:368:LEU:CD1	3.01	0.44
1:A:422:ASN:HB3	1:A:423:TYR:H	1.60	0.44
1:B:190:ARG:HB3	1:B:192:PHE:HE1	1.82	0.44
1:B:234:ASN:HD21	1:B:236:THR:HG23	1.82	0.44
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.99	0.44
1:B:101:ILE:HG23	1:B:101:ILE:O	2.17	0.43
1:B:491:PRO:C	1:B:492:LEU:HG	2.37	0.43
3:H:18:ARG:HA	3:H:75:ILE:O	2.18	0.43
3:P:81:GLU:O	3:P:82:ASP:C	2.56	0.43
1:C:327:VAL:H	1:C:531:THR:HG1	1.66	0.43
3:J:89:GLN:HA	3:J:97:THR:O	2.18	0.43
4:N:37:VAL:HG23	4:N:95:TYR:HB2	1.99	0.43
2:G:4:LEU:HB2	2:G:108:GLY:HA2	1.99	0.43
3:H:89:GLN:HA	3:H:97:THR:O	2.18	0.43
4:I:37:VAL:HG23	4:I:95:TYR:HB2	1.99	0.43
5:R:6:GLN:HE21	5:R:21:ILE:CG2	2.31	0.43
2:E:37:GLN:HA	2:E:43:LEU:HA	2.00	0.43
4:N:91:THR:HG22	4:N:120:VAL:H	1.84	0.43
4:Q:37:VAL:HG23	4:Q:95:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:111:TYR:O	4:Q:112:TRP:HB2	2.17	0.43
1:B:759:PHE:O	1:B:763:LEU:HG	2.18	0.43
1:C:945:LEU:O	1:C:947:LYS:N	2.48	0.43
1:C:1078:ALA:HB3	1:C:1133:VAL:HG22	1.99	0.43
3:J:18:ARG:HA	3:J:75:ILE:O	2.18	0.43
4:N:64:VAL:HG23	4:N:64:VAL:O	2.19	0.43
2:G:37:GLN:HA	2:G:43:LEU:HA	2.00	0.43
2:M:37:GLN:HA	2:M:43:LEU:HA	2.00	0.43
4:Q:64:VAL:HG23	4:Q:64:VAL:O	2.19	0.43
4:Q:103:TRP:HB2	4:Q:105:TRP:HE3	1.83	0.43
1:A:567:ARG:HG2	1:A:571:ASP:HA	2.00	0.43
3:P:49:ASN:H	3:P:55:GLN:HB2	1.84	0.43
1:B:483:VAL:HG13	2:G:54:ASN:ND2	2.33	0.43
5:K:6:GLN:HE21	5:K:21:ILE:CG2	2.31	0.43
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.54	0.43
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.54	0.43
1:B:825:LYS:HB3	1:B:945:LEU:HD12	2.01	0.43
1:C:117:LEU:CB	1:C:130:VAL:HA	2.49	0.43
2:G:90:LEU:HG	2:G:112:MET:SD	2.59	0.43
5:K:36:PHE:CD2	5:K:46:LEU:HA	2.54	0.43
5:K:85:THR:HG1	5:K:87:TYR:HE2	1.64	0.43
1:B:342:PHE:CZ	1:B:368:LEU:CD1	3.01	0.43
1:C:421:TYR:CD1	1:C:457:ARG:HB3	2.54	0.43
4:N:76:LYS:HB3	4:N:78:THR:OG1	2.19	0.43
4:N:103:TRP:HB2	4:N:105:TRP:HE3	1.83	0.43
5:O:6:GLN:HE21	5:O:21:ILE:CG2	2.31	0.43
2:M:90:LEU:HG	2:M:112:MET:SD	2.58	0.43
4:Q:33:HIS:HB3	4:Q:50:PHE:CE1	2.54	0.43
1:A:474:GLN:HG3	1:A:488:CYS:SG	2.59	0.43
1:A:729:VAL:HG22	1:A:1059:GLY:HA2	2.00	0.43
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.91	0.43
1:B:1116:THR:HB	1:B:1140:PRO:HD3	2.01	0.43
1:C:342:PHE:CZ	1:C:368:LEU:CD1	3.01	0.43
1:A:96:GLU:CD	1:A:100:ILE:H	2.23	0.42
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.42
1:C:1090:PRO:HA	1:C:1120:THR:HA	2.00	0.42
5:O:36:PHE:CD2	5:O:46:LEU:HA	2.54	0.42
4:I:43:LYS:HB3	4:I:44:GLY:H	1.59	0.42
4:I:64:VAL:HG23	4:I:64:VAL:O	2.19	0.42
4:I:76:LYS:HB3	4:I:78:THR:OG1	2.19	0.42
4:I:91:THR:HG22	4:I:120:VAL:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:91:THR:HG22	4:Q:120:VAL:H	1.84	0.42
1:B:474:GLN:HG3	1:B:488:CYS:SG	2.59	0.42
1:B:898:PHE:N	1:B:899:PRO:HD2	2.34	0.42
2:E:90:LEU:HG	2:E:112:MET:SD	2.58	0.42
2:G:69:ARG:HA	2:G:76:LEU:HD12	2.02	0.42
4:I:103:TRP:HB2	4:I:105:TRP:HE3	1.83	0.42
1:A:394:ASN:OD1	1:A:394:ASN:O	2.38	0.42
3:H:49:ASN:H	3:H:55:GLN:HB2	1.84	0.42
3:H:75:ILE:O	3:H:75:ILE:HG13	2.19	0.42
5:R:36:PHE:CD2	5:R:46:LEU:HA	2.54	0.42
1:A:937:SER:O	1:A:942:PRO:HD3	2.19	0.42
1:B:394:ASN:OD1	1:B:394:ASN:O	2.38	0.42
1:C:474:GLN:HG3	1:C:488:CYS:SG	2.59	0.42
2:G:64:ARG:HG2	2:G:82:SER:HB2	2.00	0.42
4:Q:43:LYS:HB3	4:Q:44:GLY:H	1.59	0.42
1:B:48:LEU:HD23	1:B:278:LYS:CB	2.49	0.42
1:B:342:PHE:CE2	1:B:368:LEU:HD22	2.55	0.42
1:B:814:LYS:HE2	1:B:814:LYS:HB3	1.85	0.42
2:M:69:ARG:HA	2:M:76:LEU:HD12	2.01	0.42
4:Q:76:LYS:HB3	4:Q:78:THR:OG1	2.19	0.42
1:C:569:ILE:O	1:C:570:ALA:HB3	2.20	0.42
3:J:39:LYS:HB2	3:J:42:LYS:CB	2.48	0.42
3:P:12:SER:HB2	3:P:107:LYS:NZ	2.35	0.42
1:B:1081:ILE:HD11	1:B:1137:VAL:CG2	2.50	0.42
1:C:394:ASN:OD1	1:C:394:ASN:O	2.38	0.42
1:C:585:LEU:HD23	1:C:585:LEU:HA	1.87	0.42
1:C:947:LYS:HE2	1:C:947:LYS:HB3	1.84	0.42
4:N:35:HIS:HD2	4:N:47:TRP:CD1	2.37	0.42
1:A:570:ALA:HB1	1:B:963:VAL:HG11	2.02	0.42
3:J:75:ILE:O	3:J:75:ILE:HG13	2.19	0.42
3:P:75:ILE:O	3:P:75:ILE:HG13	2.19	0.42
1:A:719:THR:OG1	1:A:1068:VAL:HB	2.20	0.42
2:E:69:ARG:HA	2:E:76:LEU:HD12	2.02	0.42
4:I:35:HIS:HD2	4:I:47:TRP:CD1	2.37	0.42
1:A:483:VAL:HG13	2:M:54:ASN:ND2	2.33	0.42
1:A:898:PHE:N	1:A:899:PRO:HD2	2.34	0.42
1:A:1093:GLY:HA3	1:A:1104:VAL:HG12	2.02	0.42
5:K:29:ILE:HG22	5:K:32:TYR:HB2	2.02	0.42
2:E:29:VAL:HG12	2:E:69:ARG:HG3	2.02	0.41
3:J:49:ASN:H	3:J:55:GLN:HB2	1.84	0.41
1:A:569:ILE:O	1:A:570:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ALA:O	1:A:934:ILE:HG12	2.19	0.41
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.53	0.41
4:N:103:TRP:CB	4:N:105:TRP:HE3	2.33	0.41
3:H:39:LYS:HB2	3:H:42:LYS:CB	2.48	0.41
3:H:39:LYS:HD2	3:H:42:LYS:HG2	2.03	0.41
1:B:1036:GLN:HE21	1:B:1049:LEU:HA	1.84	0.41
5:O:11:LEU:HD13	5:O:19:VAL:HG13	2.02	0.41
4:I:103:TRP:CB	4:I:105:TRP:HE3	2.33	0.41
1:A:1095:PHE:CE1	1:A:1104:VAL:HG22	2.55	0.41
1:C:342:PHE:CE2	1:C:368:LEU:HD22	2.55	0.41
1:A:62:VAL:HG12	1:A:266:TYR:HB3	2.02	0.41
1:A:472:ILE:H	1:A:472:ILE:HG12	1.60	0.41
1:B:767:LEU:HD23	1:B:770:ILE:HD12	2.01	0.41
2:G:61:VAL:HG13	2:G:64:ARG:CD	2.50	0.41
3:P:39:LYS:HB2	3:P:42:LYS:CB	2.48	0.41
3:P:39:LYS:HD2	3:P:42:LYS:HG2	2.03	0.41
1:A:190:ARG:HB3	1:A:192:PHE:CE2	2.55	0.41
1:B:229:LEU:HA	1:B:230:PRO:HD3	1.87	0.41
3:H:48:ILE:HG22	3:H:51:ALA:H	1.86	0.41
1:B:716:THR:HG22	1:B:1110:TYR:HB3	2.01	0.41
1:B:911:VAL:HG12	1:B:912:THR:H	1.85	0.41
1:B:1077:THR:O	1:B:1077:THR:OG1	2.34	0.41
1:C:598:ILE:CD1	1:C:650:LEU:HD11	2.49	0.41
4:I:33:HIS:HB3	4:I:50:PHE:CE1	2.54	0.41
2:M:49:ILE:HD12	2:M:49:ILE:HA	1.97	0.41
1:A:342:PHE:CE2	1:A:368:LEU:HD22	2.55	0.41
1:A:732:THR:HG22	1:A:1058:HIS:HE1	1.85	0.41
1:B:276:LEU:HD23	1:B:306:PHE:CE1	2.55	0.41
2:M:29:VAL:HG12	2:M:69:ARG:HG3	2.02	0.41
4:Q:35:HIS:HD2	4:Q:47:TRP:CD1	2.37	0.41
1:A:787:GLN:HB3	1:C:701:ALA:O	2.20	0.41
1:B:712:ILE:CB	1:B:1077:THR:CG2	2.99	0.41
1:B:713:ALA:HB3	1:C:894:LEU:HB3	2.02	0.41
1:C:930:ALA:HA	1:C:933:LYS:HE2	2.03	0.41
3:J:12:SER:HB2	3:J:107:LYS:NZ	2.35	0.41
4:N:45:LEU:HD13	4:N:112:TRP:HH2	1.86	0.41
2:G:94:VAL:HA	2:G:106:ILE:O	2.21	0.41
3:H:12:SER:HB2	3:H:107:LYS:NZ	2.35	0.41
3:P:48:ILE:HG22	3:P:51:ALA:H	1.86	0.41
4:Q:103:TRP:CB	4:Q:105:TRP:HE3	2.34	0.41
5:R:11:LEU:HD13	5:R:19:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:TYR:HB2	1:C:1089:PHE:HE2	1.86	0.41
3:J:48:ILE:HG22	3:J:51:ALA:H	1.86	0.41
2:G:61:VAL:CG1	2:G:64:ARG:HB2	2.50	0.41
5:K:11:LEU:HD13	5:K:19:VAL:HG13	2.02	0.41
4:Q:33:HIS:HD2	4:Q:52:SER:HA	1.86	0.41
5:R:29:ILE:HG22	5:R:32:TYR:HB2	2.02	0.41
1:B:331:ASN:O	1:B:332:ILE:HG13	2.20	0.40
4:N:33:HIS:HB3	4:N:50:PHE:CE1	2.54	0.40
5:O:29:ILE:HG22	5:O:32:TYR:HB2	2.02	0.40
1:A:523:THR:O	1:A:525:CYS:N	2.54	0.40
1:A:814:LYS:O	1:A:815:ARG:C	2.60	0.40
1:B:472:ILE:H	1:B:472:ILE:HG12	1.60	0.40
1:C:856:ASN:OD1	1:C:856:ASN:N	2.51	0.40
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.69	0.40
2:E:94:VAL:HA	2:E:106:ILE:O	2.21	0.40
2:G:32:MET:HE1	2:G:93:CYS:HB3	2.02	0.40
4:Q:23:ALA:HA	4:Q:78:THR:HG22	2.04	0.40
1:B:121:ASN:ND2	1:B:126:VAL:HG13	2.36	0.40
1:B:323:THR:OG1	1:B:324:GLU:OE1	2.39	0.40
1:B:866:THR:OG1	1:B:869:MET:HG3	2.21	0.40
3:H:6:GLN:HA	3:H:23:CYS:HA	2.02	0.40
1:A:714:ILE:HA	1:A:715:PRO:HD3	1.95	0.40
5:K:34:ALA:O	5:K:88:CYS:HA	2.21	0.40
2:M:94:VAL:HA	2:M:106:ILE:O	2.21	0.40
1:A:902:MET:O	1:A:903:ALA:CB	2.70	0.40
1:B:130:VAL:HG11	1:B:231:ILE:HG23	2.03	0.40
1:C:57:PRO:HG2	1:C:271:GLN:OE1	2.20	0.40
1:C:577:ARG:HA	1:C:584:ILE:HA	2.02	0.40
1:C:738:CYS:O	1:C:742:ILE:HG12	2.22	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	913/1286 (71%)	859 (94%)	44 (5%)	10 (1%)	14	42
1	B	927/1286 (72%)	866 (93%)	50 (5%)	11 (1%)	13	40
1	C	925/1286 (72%)	870 (94%)	49 (5%)	6 (1%)	25	58
2	E	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
2	G	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
2	M	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
3	H	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	J	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
3	P	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
4	I	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
4	N	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
4	Q	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
5	K	104/107 (97%)	95 (91%)	9 (9%)	0	100	100
5	O	104/107 (97%)	95 (91%)	9 (9%)	0	100	100
5	R	104/107 (97%)	95 (91%)	9 (9%)	0	100	100
All	All	4094/5217 (78%)	3840 (94%)	227 (6%)	27 (1%)	26	54

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	812	PRO
1	A	813	SER
1	B	942	PRO
1	B	810	SER
1	A	477	ASN
1	A	492	LEU
1	A	940	SER
1	A	942	PRO
1	B	330	PRO
1	B	477	ASN
1	B	492	LEU
1	B	941	THR
1	C	477	ASN
1	C	492	LEU
1	C	543	PHE
1	A	479	PRO
1	B	325	SER
1	B	334	ASN

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Mol	Chain	Res	Type
1	B	479	PRO
1	C	479	PRO
1	A	524	VAL
1	A	530	SER
1	B	524	VAL
1	A	478	LYS
1	B	478	LYS
1	C	478	LYS
1	C	126	VAL

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	754/1113 (68%)	738 (98%)	16 (2%)	53 81
1	B	757/1113 (68%)	744 (98%)	13 (2%)	60 86
1	C	762/1113 (68%)	738 (97%)	24 (3%)	40 74
2	E	86/95 (90%)	86 (100%)	0	100 100
2	G	89/95 (94%)	89 (100%)	0	100 100
2	M	87/95 (92%)	87 (100%)	0	100 100
3	H	72/89 (81%)	71 (99%)	1 (1%)	67 89
3	J	71/89 (80%)	70 (99%)	1 (1%)	67 89
3	P	73/89 (82%)	72 (99%)	1 (1%)	67 89
4	I	92/104 (88%)	88 (96%)	4 (4%)	29 62
4	N	92/104 (88%)	88 (96%)	4 (4%)	29 62
4	Q	91/104 (88%)	87 (96%)	4 (4%)	28 61
5	K	79/92 (86%)	78 (99%)	1 (1%)	69 90
5	O	79/92 (86%)	78 (99%)	1 (1%)	69 90
5	R	79/92 (86%)	78 (99%)	1 (1%)	69 90
All	All	3263/4479 (73%)	3192 (98%)	71 (2%)	54 81

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	TYR
1	A	347	PHE
1	A	360	ASN
1	A	396	TYR
1	A	429	PHE
1	A	453	TYR
1	A	515	PHE
1	A	531	THR
1	A	535	LYS
1	A	565	PHE
1	A	616	ASN
1	A	904	TYR
1	A	1058	HIS
1	A	1116	THR
1	A	1130	ILE
1	A	1137	VAL
1	B	131	CYS
1	B	190	ARG
1	B	318	PHE
1	B	347	PHE
1	B	360	ASN
1	B	396	TYR
1	B	429	PHE
1	B	453	TYR
1	B	515	PHE
1	B	544	ASN
1	B	606	ASN
1	B	811	LYS
1	B	1089	PHE
1	C	191	GLU
1	C	238	PHE
1	C	299	THR
1	C	347	PHE
1	C	360	ASN
1	C	396	TYR
1	C	429	PHE
1	C	453	TYR
1	C	515	PHE
1	C	565	PHE
1	C	574	ASP
1	C	591	SER
1	C	602	THR

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Mol	Chain	Res	Type
1	C	675	GLN
1	C	692	ILE
1	C	755	GLN
1	C	781	VAL
1	C	794	ILE
1	C	878	LEU
1	C	894	LEU
1	C	1077	THR
1	C	1089	PHE
1	C	1106	GLN
1	C	1116	THR
3	J	38	GLN
4	N	29	PHE
4	N	38	ARG
4	N	104	HIS
4	N	105	TRP
5	O	107	LYS
3	H	38	GLN
4	I	29	PHE
4	I	38	ARG
4	I	104	HIS
4	I	105	TRP
5	K	107	LYS
3	P	38	GLN
4	Q	29	PHE
4	Q	38	ARG
4	Q	104	HIS
4	Q	105	TRP
5	R	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	ASN
1	A	439	ASN
1	A	505	HIS
1	A	580	GLN
1	A	616	ASN
1	A	709	ASN
1	A	1058	HIS
1	A	1135	ASN
1	B	121	ASN

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	271	GLN
1	B	321	GLN
1	B	360	ASN
1	B	405	ASN
1	B	439	ASN
1	B	505	HIS
1	B	532	ASN
1	B	544	ASN
1	B	606	ASN
1	B	613	GLN
1	B	965	GLN
1	B	1088	HIS
1	B	1113	GLN
1	C	239	GLN
1	C	405	ASN
1	C	439	ASN
1	C	505	HIS
1	C	563	GLN
1	C	895	GLN
1	C	901	GLN
2	E	54	ASN
4	N	35	HIS
5	O	6	GLN
2	G	54	ASN
4	I	35	HIS
5	K	6	GLN
2	M	54	ASN
4	Q	35	HIS
5	R	6	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	C	1301	1	14,14,15	0.42	0	17,19,21	0.77	0
6	NAG	B	1301	1	14,14,15	0.43	0	17,19,21	0.77	0
6	NAG	A	1301	1	14,14,15	0.42	0	17,19,21	0.77	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	C	1301	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

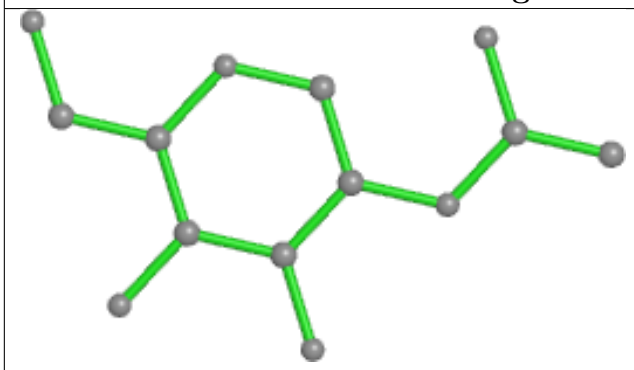
There are no ring outliers.

No monomer is involved in short contacts.

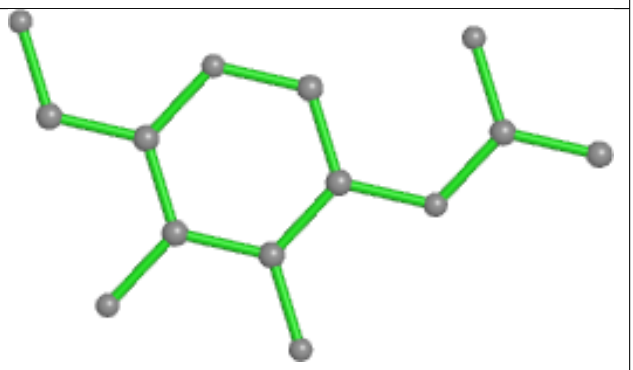
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

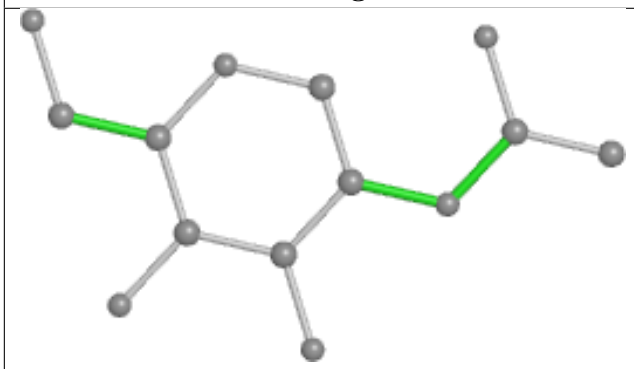
Ligand NAG C 1301



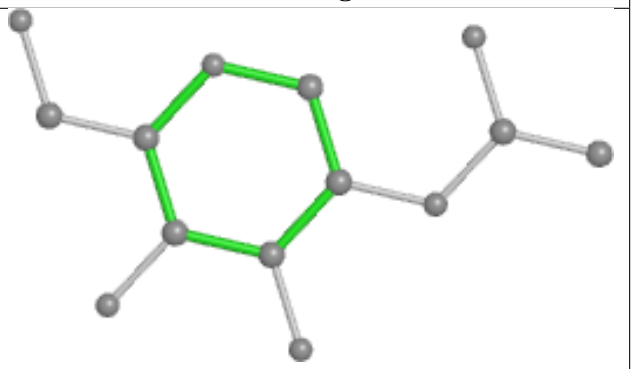
Bond lengths



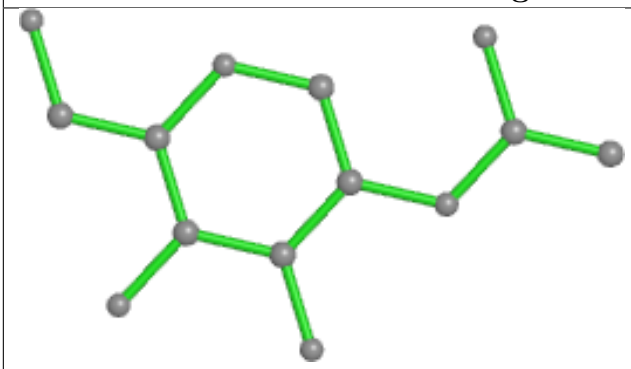
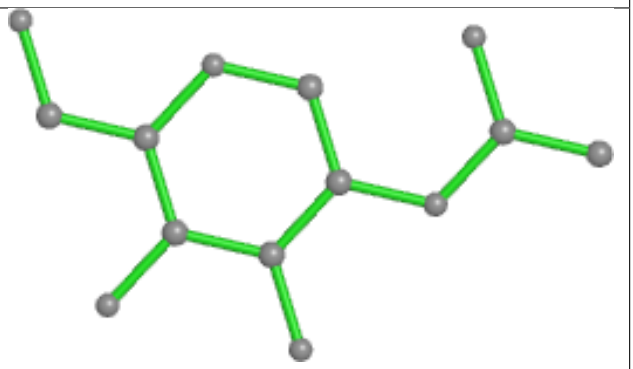
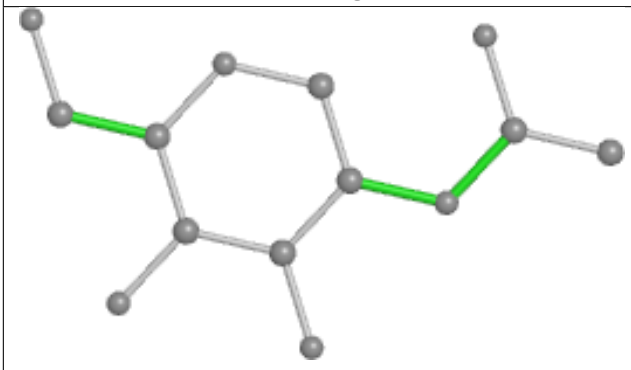
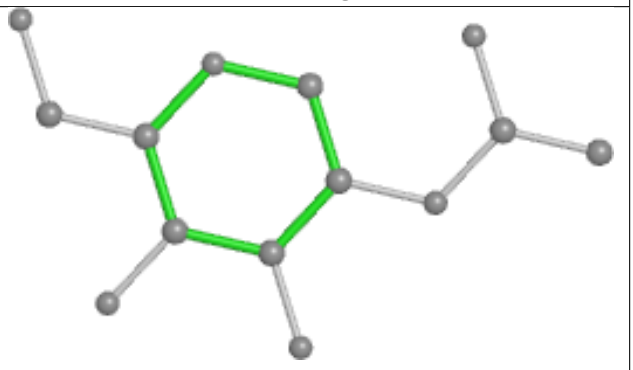
Bond angles

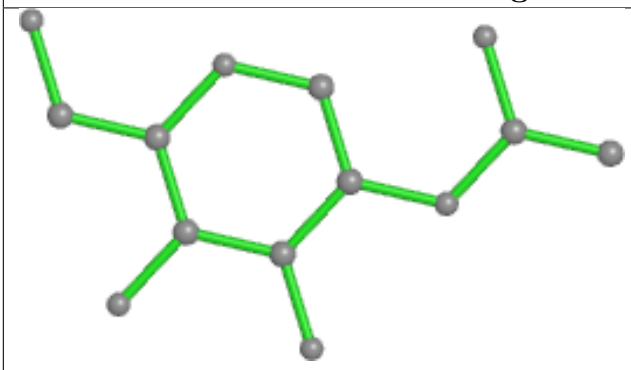
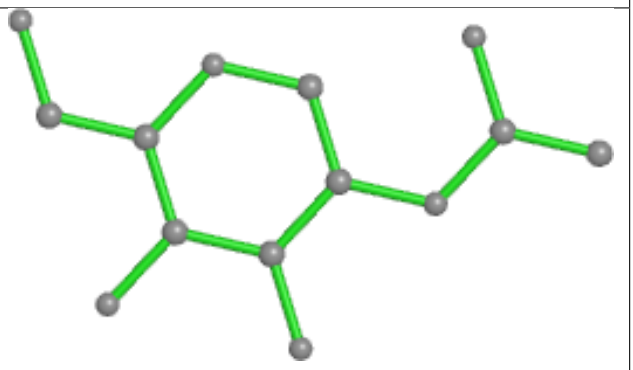
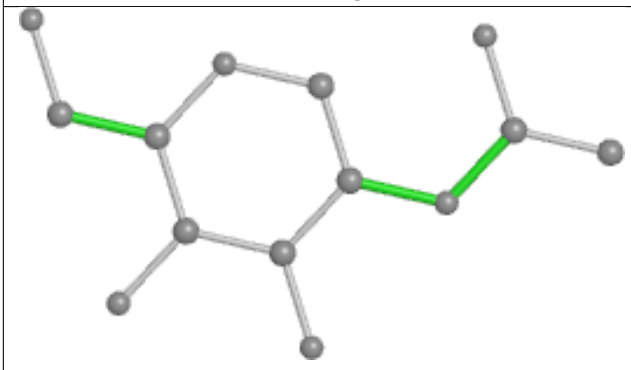
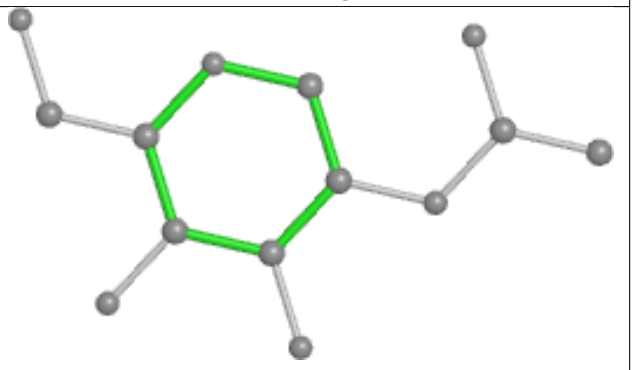


Torsions



Rings

Ligand NAG B 1301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAG A 1301	
 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.

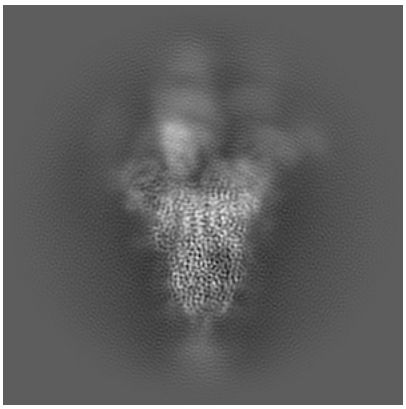
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-34410. These allow visual inspection of the internal detail of the map and identification of artifacts.

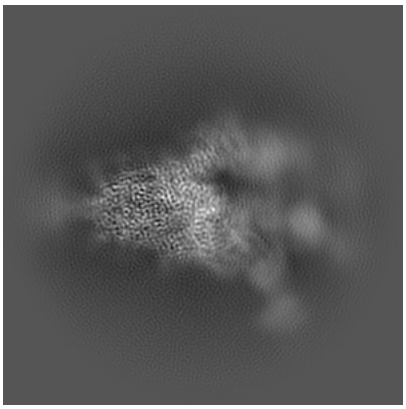
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

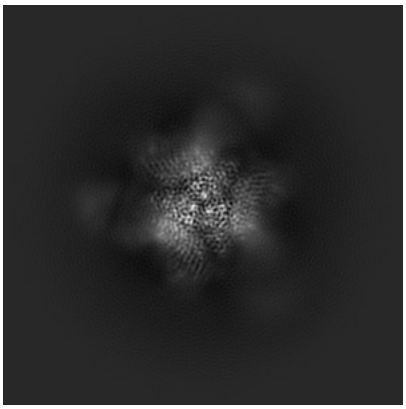
6.1.1 Primary map



X

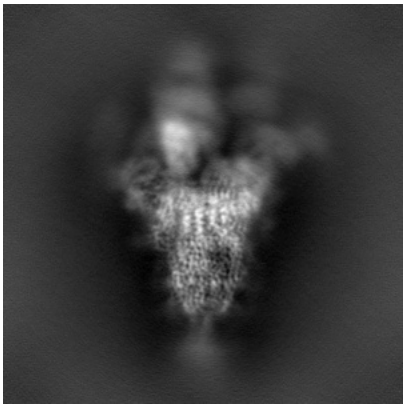


Y

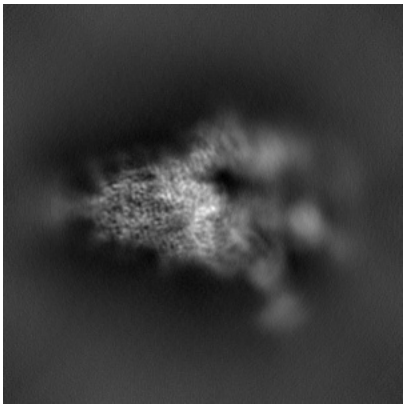


Z

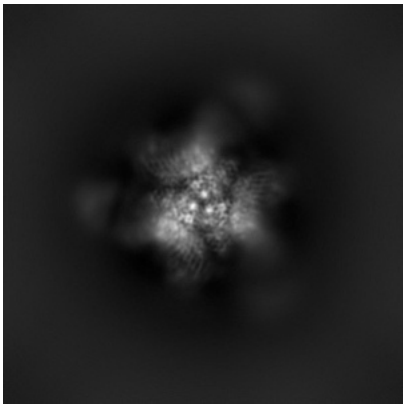
6.1.2 Raw map



X



Y

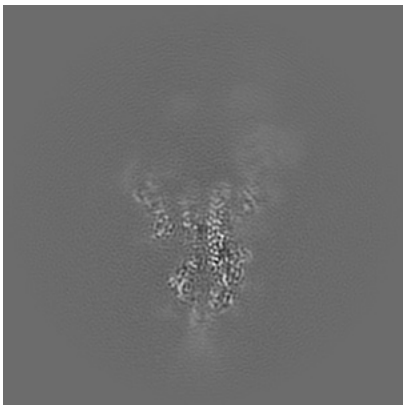


Z

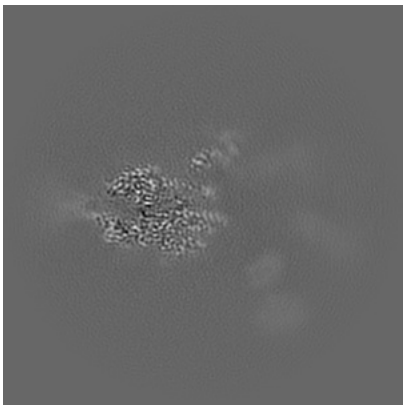
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

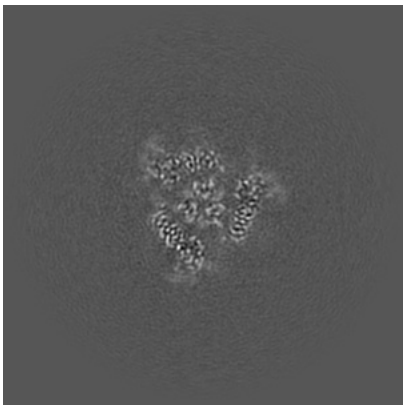
6.2.1 Primary map



X Index: 170

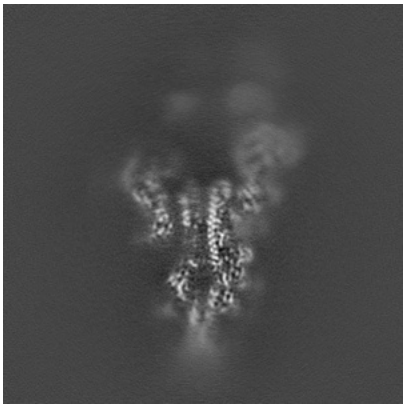


Y Index: 170

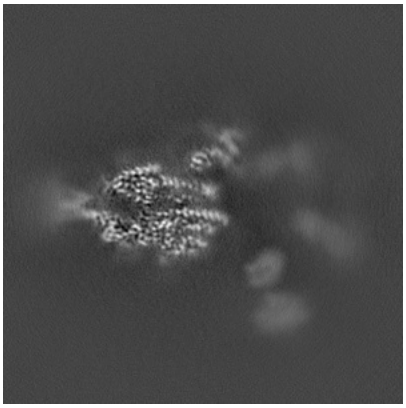


Z Index: 170

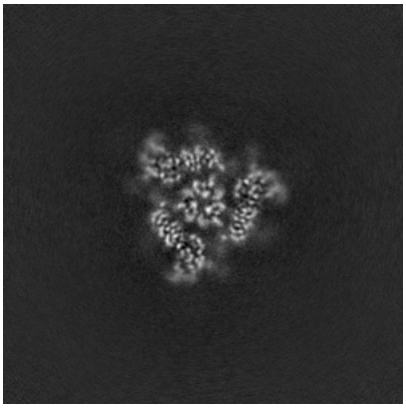
6.2.2 Raw map



X Index: 170



Y Index: 170

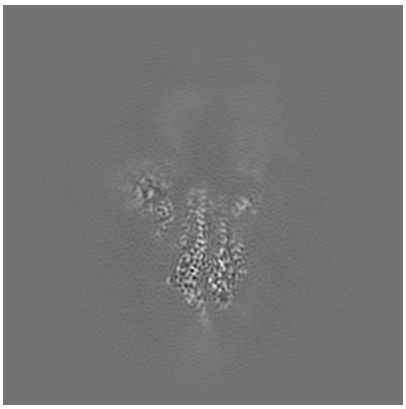


Z Index: 170

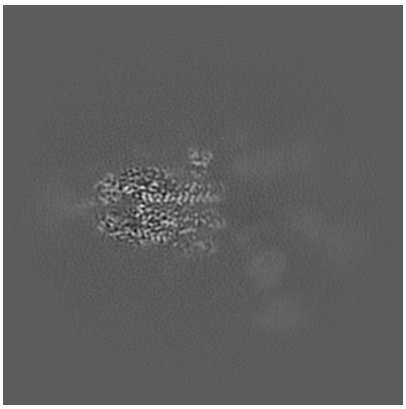
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

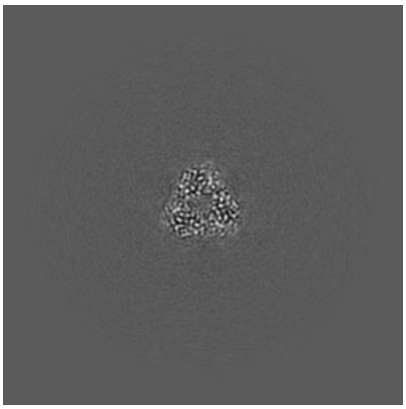
6.3.1 Primary map



X Index: 161

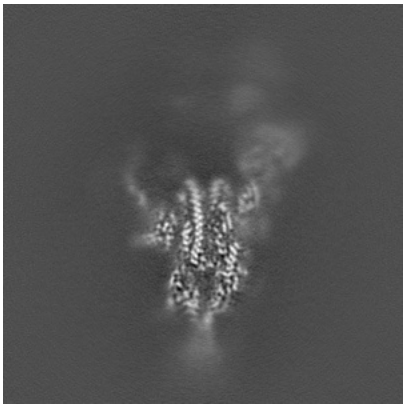


Y Index: 164

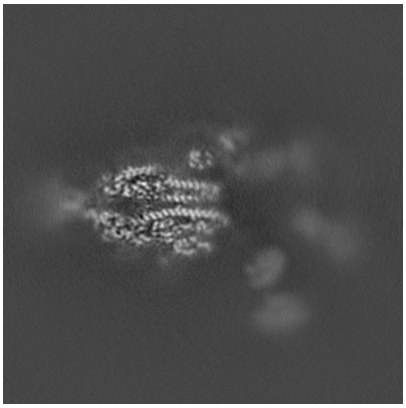


Z Index: 110

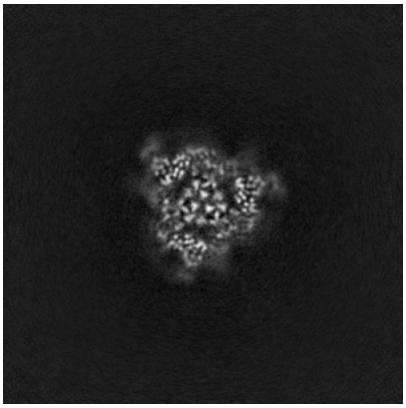
6.3.2 Raw map



X Index: 175



Y Index: 168

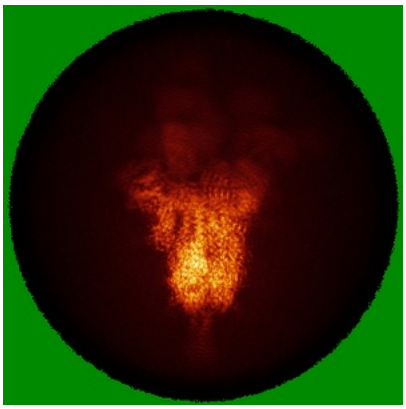


Z Index: 164

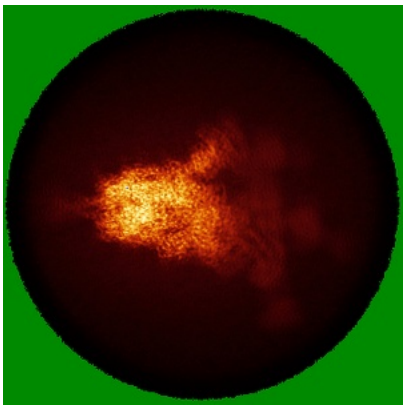
The images above show the largest variance slices of the map in three orthogonal directions.

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

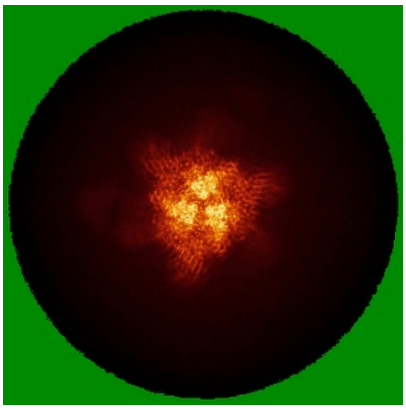
6.4.1 Primary map



X

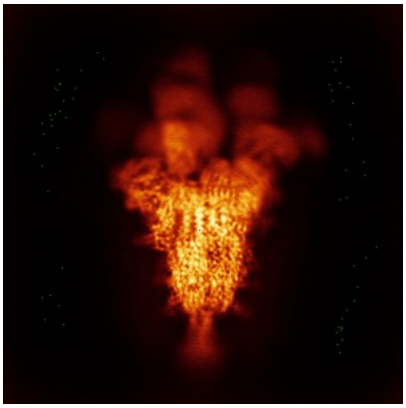


Y

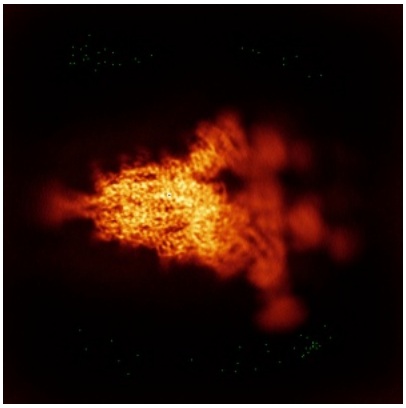


Z

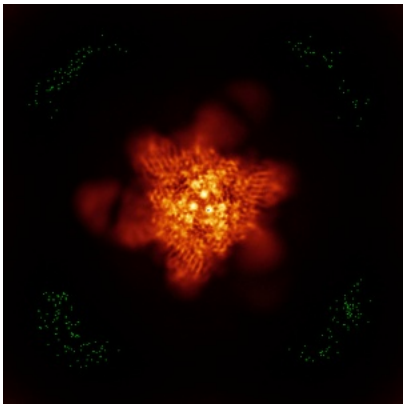
6.4.2 Raw map



X



Y

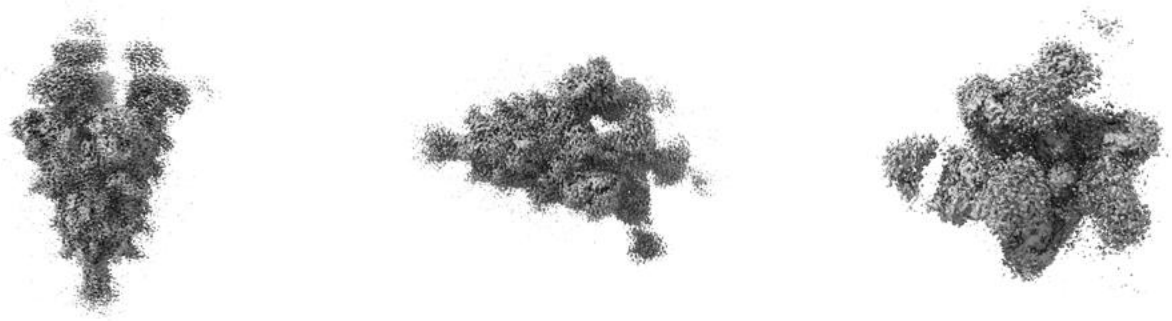


Z

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)

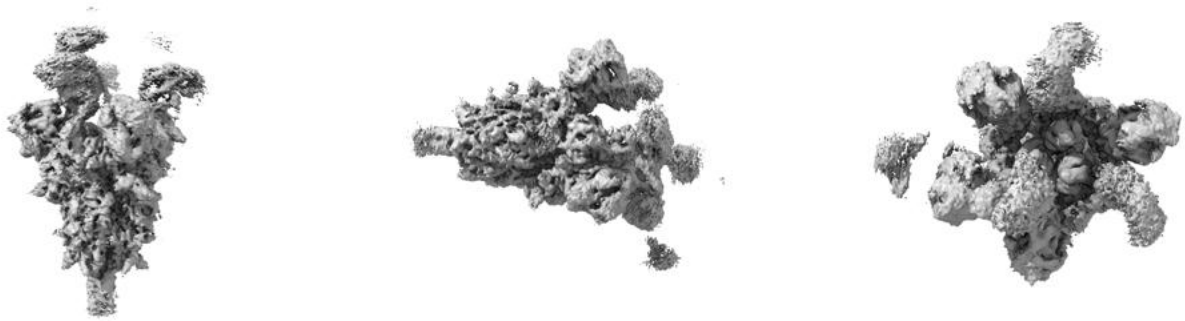
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.17. 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.

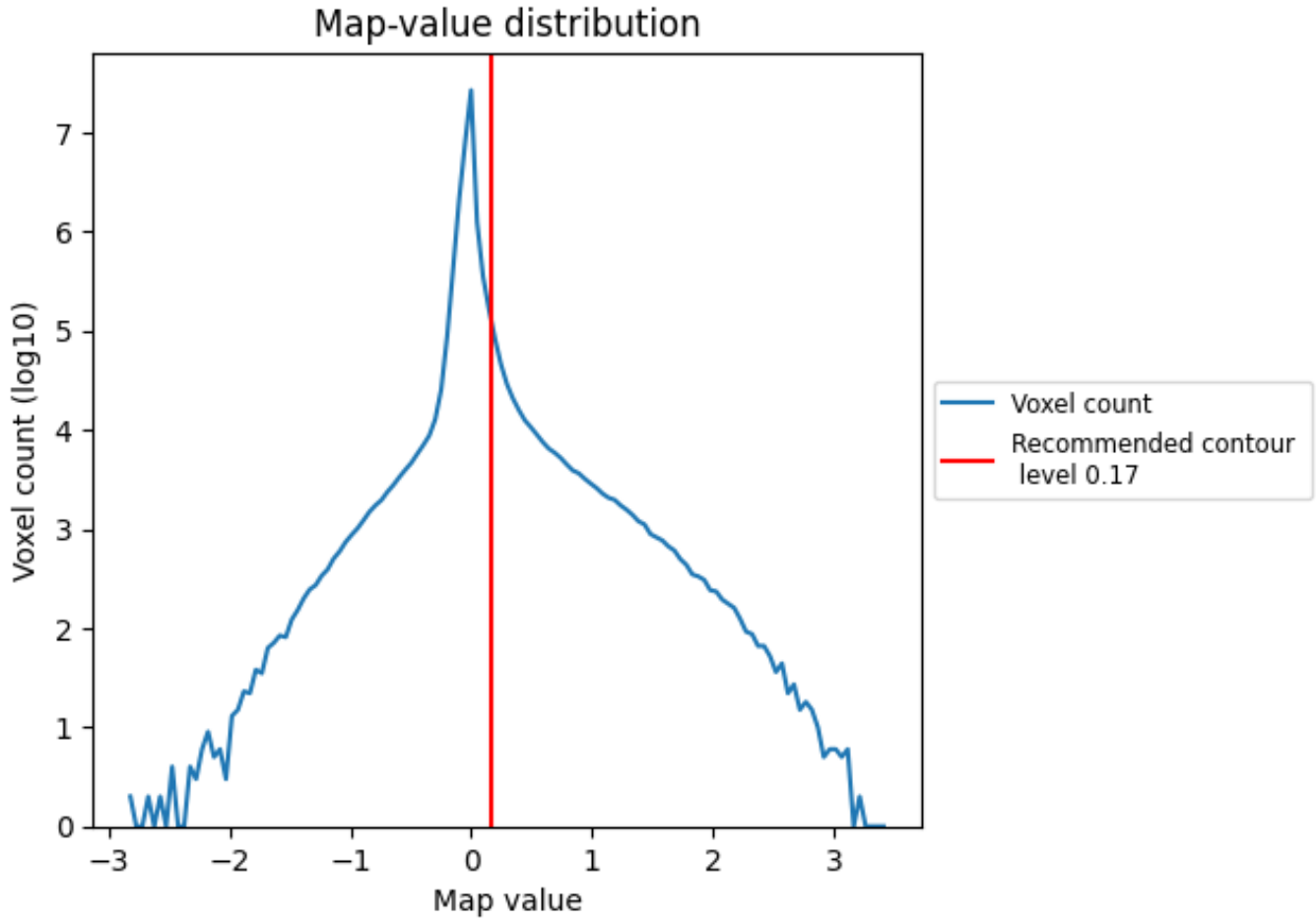
6.6 Mask visualisation (i)

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

7 Map analysis

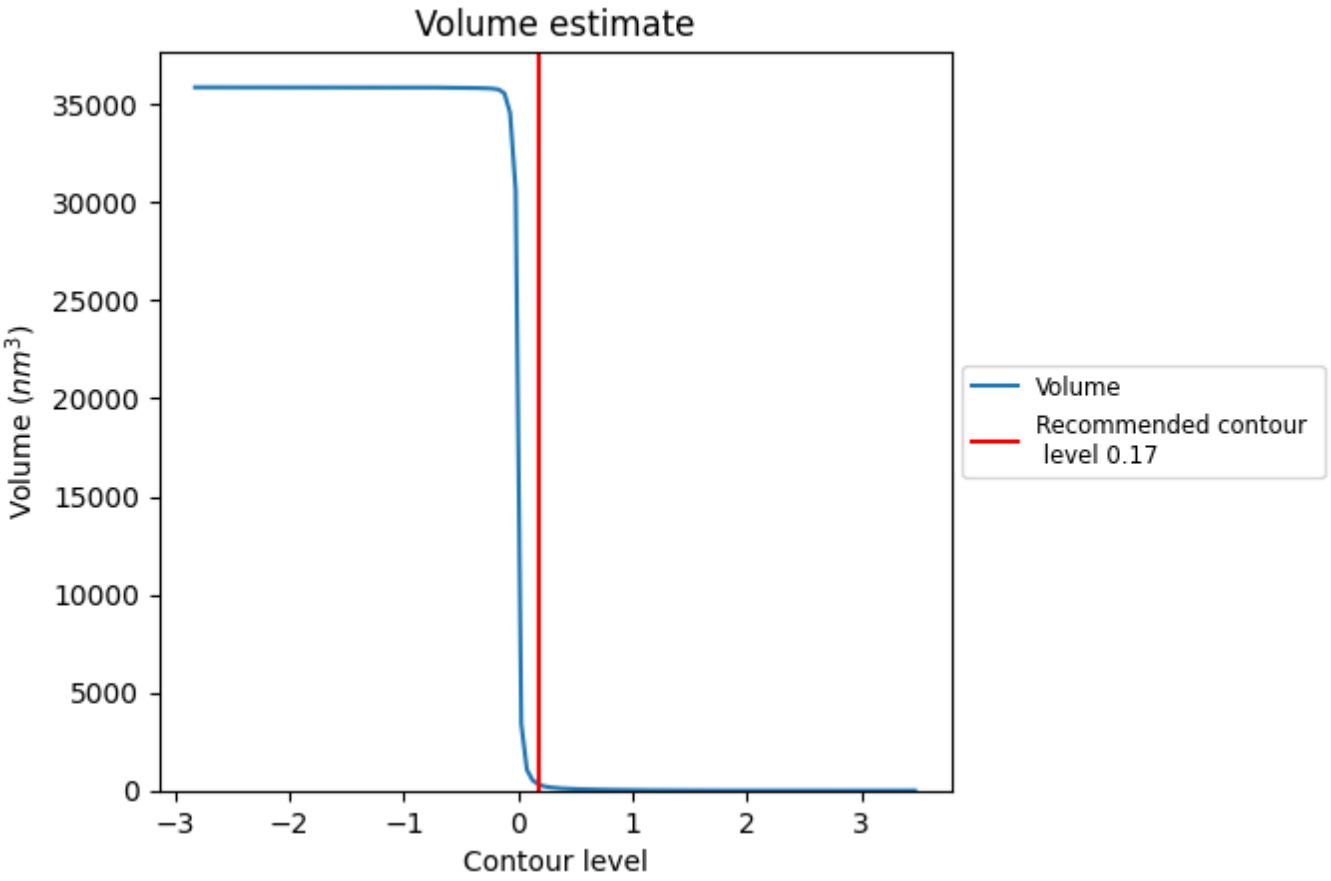
This section contains the results of statistical analysis of the map.

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.

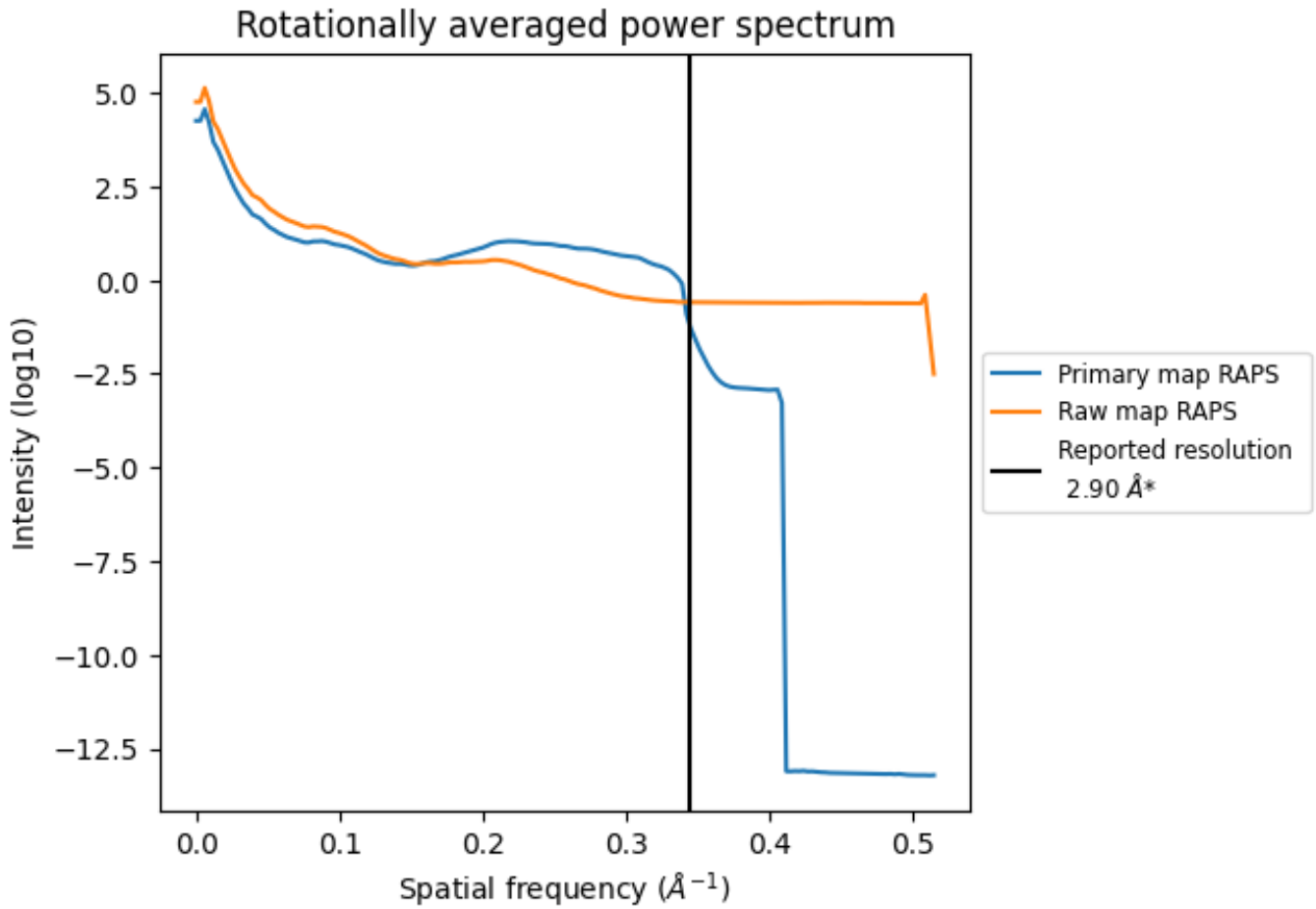
7.2 Volume estimate



The volume at the recommended contour level is 336 nm^3; this corresponds to an approximate mass of 304 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)

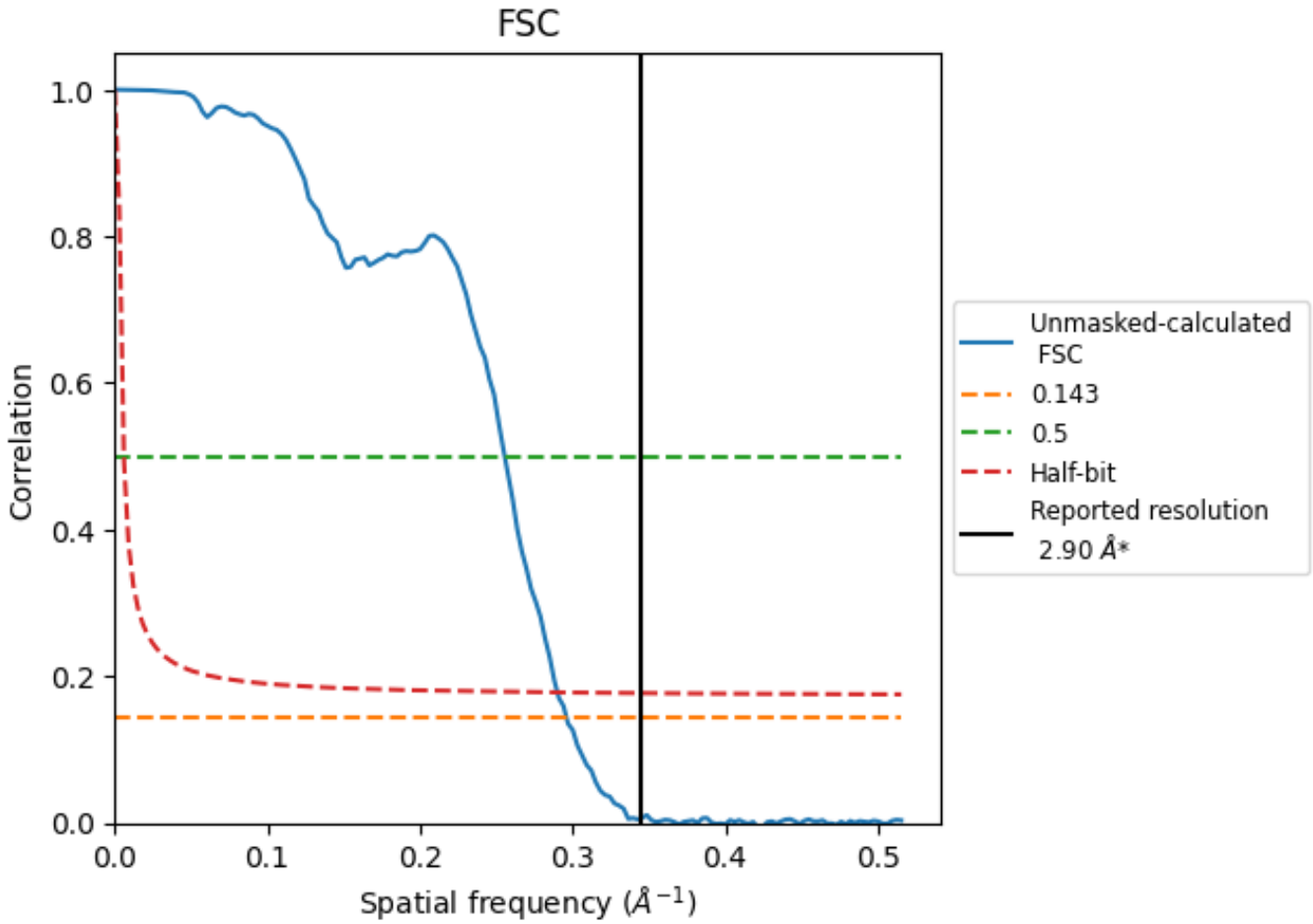


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

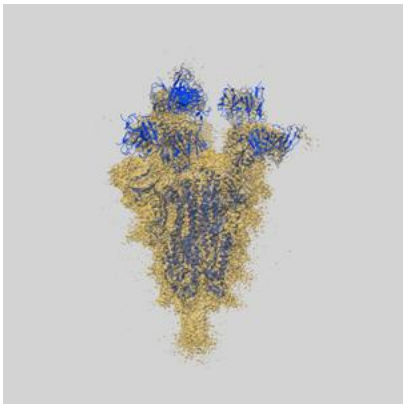
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.91	3.45

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.38 differs from the reported value 2.9 by more than 10 %

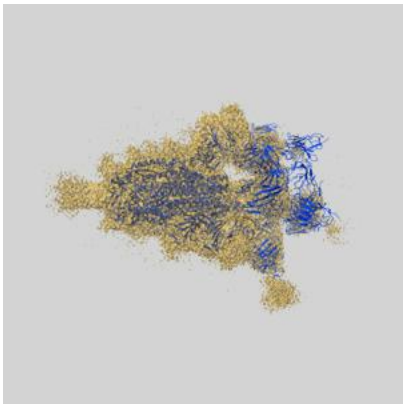
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34410 and PDB model 8H07. Per-residue inclusion information can be found in section 3 on page 10.

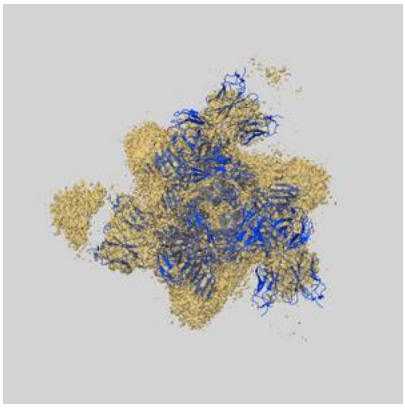
9.1 Map-model overlay



X



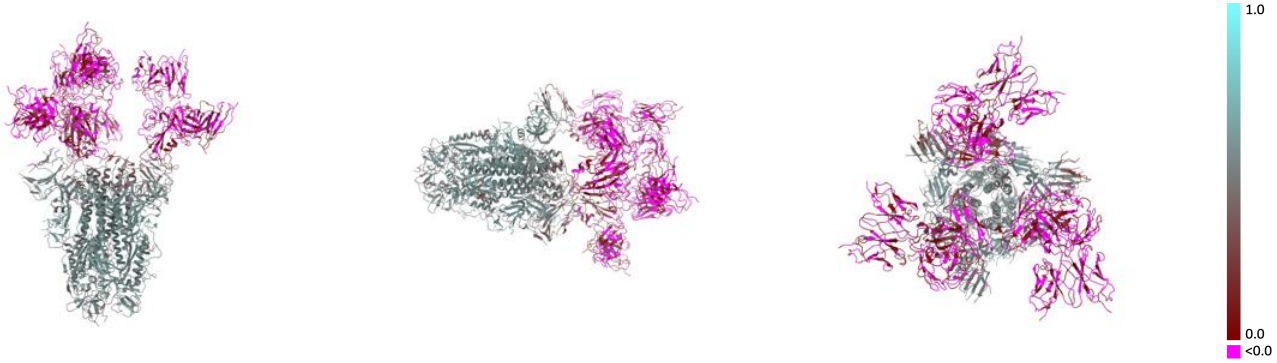
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

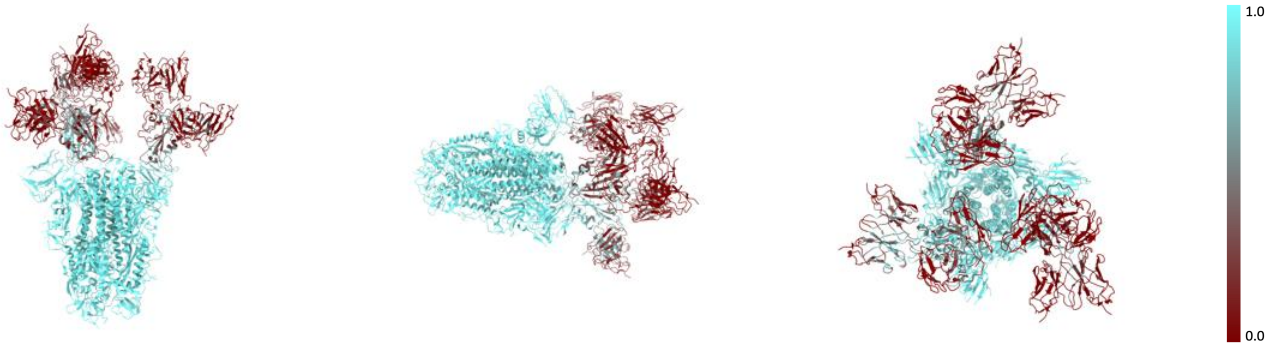
9.2 Q-score mapped to coordinate model



X Y Z

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

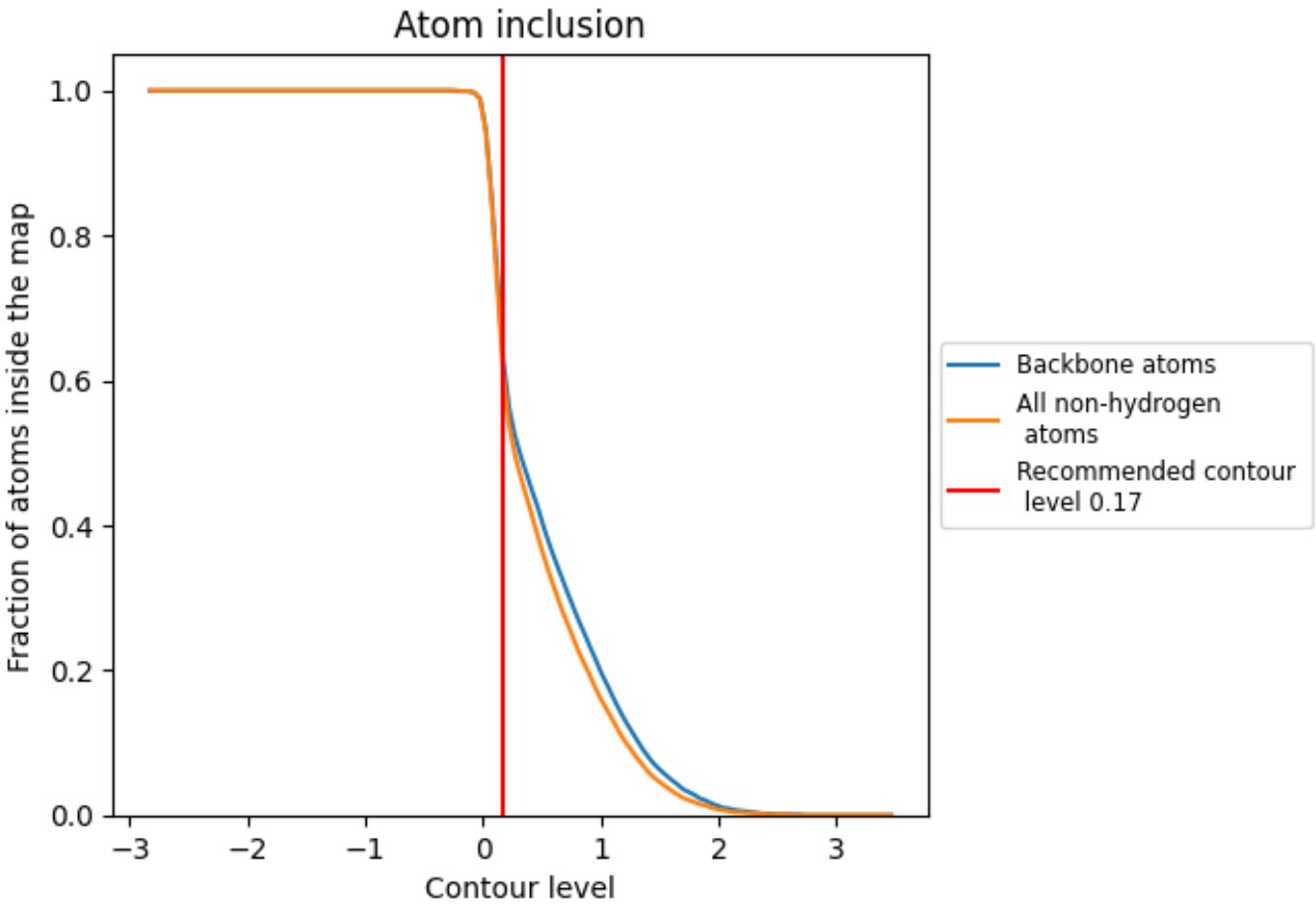
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 61% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6130	0.2980
A	0.8160	0.4240
B	0.8790	0.4360
C	0.8070	0.4260
E	0.0130	0.0120
G	0.1470	0.0060
H	0.1640	0.0170
I	0.4620	0.0860
J	0.0030	0.0070
K	0.2910	0.0420
M	0.0190	-0.0150
N	0.1170	-0.0140
O	0.0300	-0.0220
P	0.0200	0.0030
Q	0.1290	0.0510
R	0.0860	-0.0120