



Full wwPDB EM Validation Report ⓘ

Jun 16, 2026 – 01:40 pm BST

PDB ID : 9RMX / pdb_00009rmx
EMDB ID : EMD-54071
Title : CryoEM reconstruction of integrase filament at the lumen of native HIV-1 cores (box size 34.2 nm)
Authors : Cherepanov, P.; Singer, M.R.; Hope, J.; Zhang, P.
Deposited on : 2025-06-19
Resolution : 4.63 Å (reported)
Based on initial models : 2B4J, 1K6Y, 9C9M, 6SKK, 8A1P

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 : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

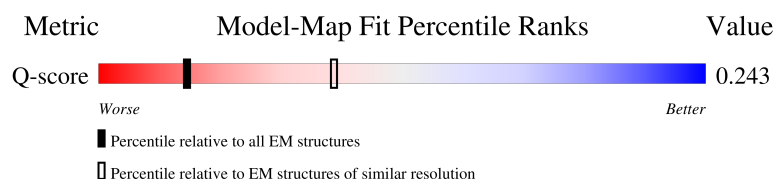
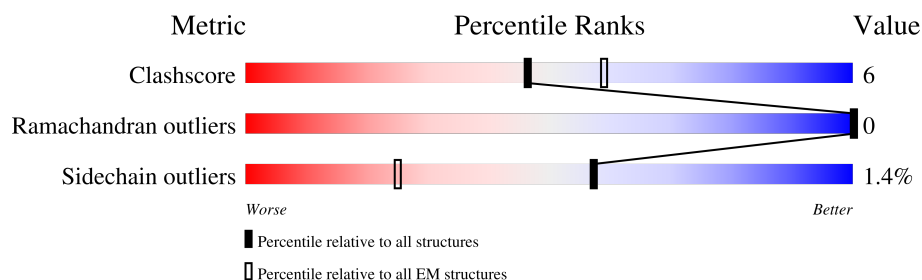
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.63 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	2068 (4.13 - 5.13)

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	288	15% 70% 18% 11%
1	B	288	11% 71% 13% 15%
1	C	288	15% 74% 17% 9%
1	D	288	9% 75% 13% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	288	
1	F	288	
1	G	288	
1	H	288	
1	I	288	
1	J	288	
1	K	288	
1	L	288	
2	U	231	
2	V	231	
2	W	231	
2	X	231	
2	Y	231	
2	Z	231	
2	a	231	
2	b	231	
2	c	231	
2	d	231	
2	e	231	
2	f	231	
2	g	231	
2	h	231	
2	i	231	
2	j	231	
2	k	231	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	l	231	
2	m	231	
2	n	231	
2	o	231	
2	p	231	
2	q	231	
2	r	231	
2	s	231	
2	t	231	
2	u	231	
2	v	231	
2	w	231	
2	x	231	
2	y	231	
2	z	231	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 72751 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 Integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	255	Total	C	N	O	S	0	0
			2006	1277	355	366	8		
1	B	245	Total	C	N	O	S	0	0
			1925	1229	340	348	8		
1	C	263	Total	C	N	O	S	0	0
			2079	1325	367	379	8		
1	D	258	Total	C	N	O	S	0	0
			2036	1299	361	368	8		
1	E	255	Total	C	N	O	S	0	0
			2006	1277	355	366	8		
1	F	245	Total	C	N	O	S	0	0
			1921	1227	339	347	8		
1	G	263	Total	C	N	O	S	0	0
			2075	1323	366	378	8		
1	H	258	Total	C	N	O	S	0	0
			2036	1299	361	368	8		
1	I	43	Total	C	N	O	S	0	0
			342	215	58	66	3		
1	J	44	Total	C	N	O	S	0	0
			351	220	60	68	3		
1	K	44	Total	C	N	O	S	0	0
			351	220	60	68	3		
1	L	44	Total	C	N	O	S	0	0
			347	218	59	67	3		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ASN	ASP	engineered mutation	UNP P12497
A	116	ASN	ASP	engineered mutation	UNP P12497
B	64	ASN	ASP	engineered mutation	UNP P12497
B	116	ASN	ASP	engineered mutation	UNP P12497
C	64	ASN	ASP	engineered mutation	UNP P12497
C	116	ASN	ASP	engineered mutation	UNP P12497

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	64	ASN	ASP	engineered mutation	UNP P12497
D	116	ASN	ASP	engineered mutation	UNP P12497
E	64	ASN	ASP	engineered mutation	UNP P12497
E	116	ASN	ASP	engineered mutation	UNP P12497
F	64	ASN	ASP	engineered mutation	UNP P12497
F	116	ASN	ASP	engineered mutation	UNP P12497
G	64	ASN	ASP	engineered mutation	UNP P12497
G	116	ASN	ASP	engineered mutation	UNP P12497
H	64	ASN	ASP	engineered mutation	UNP P12497
H	116	ASN	ASP	engineered mutation	UNP P12497
I	64	ASN	ASP	engineered mutation	UNP P12497
I	116	ASN	ASP	engineered mutation	UNP P12497
J	64	ASN	ASP	engineered mutation	UNP P12497
J	116	ASN	ASP	engineered mutation	UNP P12497
K	64	ASN	ASP	engineered mutation	UNP P12497
K	116	ASN	ASP	engineered mutation	UNP P12497
L	64	ASN	ASP	engineered mutation	UNP P12497
L	116	ASN	ASP	engineered mutation	UNP P12497

- Molecule 2 is a protein called Gag polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	V	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	W	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	X	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	Y	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	Z	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	a	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	b	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	c	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	d	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	f	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	g	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	h	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	i	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	j	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	k	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	l	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	m	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	n	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	o	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	p	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	q	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	r	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	s	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	t	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	u	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	v	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	w	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	x	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		
2	y	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		

Continued on next page...

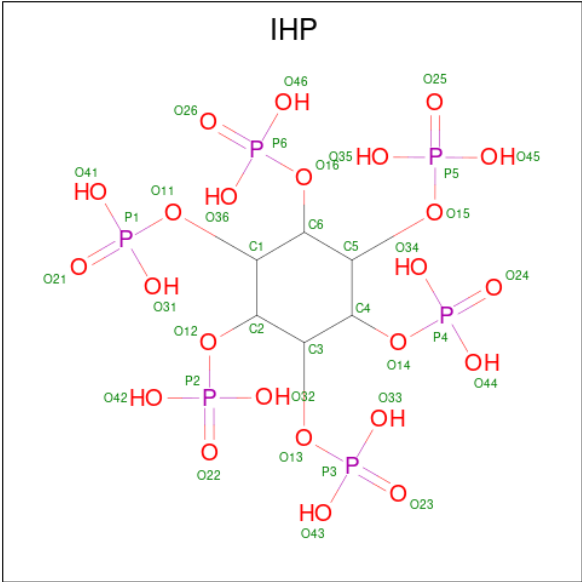
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	z	220	Total	C	N	O	S	0	0
			1718	1083	300	322	13		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	
3	H	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	J	1	Total	Zn	0
			1	1	
3	K	1	Total	Zn	0
			1	1	
3	L	1	Total	Zn	0
			1	1	

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).

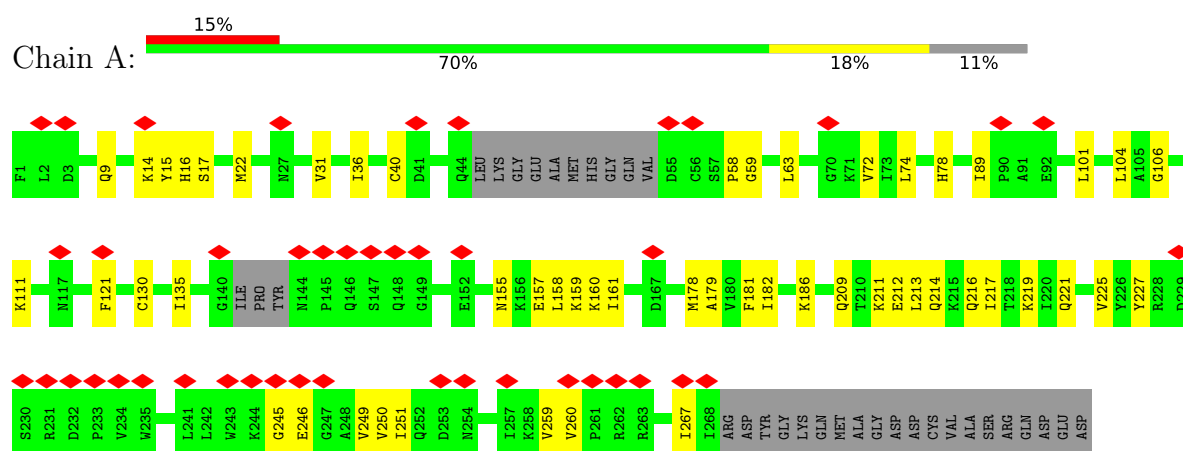


Mol	Chain	Residues	Atoms				AltConf
4	X	1	Total	C	O	P	0
			36	6	24	6	
4	Z	1	Total	C	O	P	0
			36	6	24	6	
4	a	1	Total	C	O	P	0
			36	6	24	6	
4	b	1	Total	C	O	P	0
			36	6	24	6	
4	g	1	Total	C	O	P	0
			36	6	24	6	
4	i	1	Total	C	O	P	0
			36	6	24	6	
4	m	1	Total	C	O	P	0
			36	6	24	6	
4	q	1	Total	C	O	P	0
			36	6	24	6	

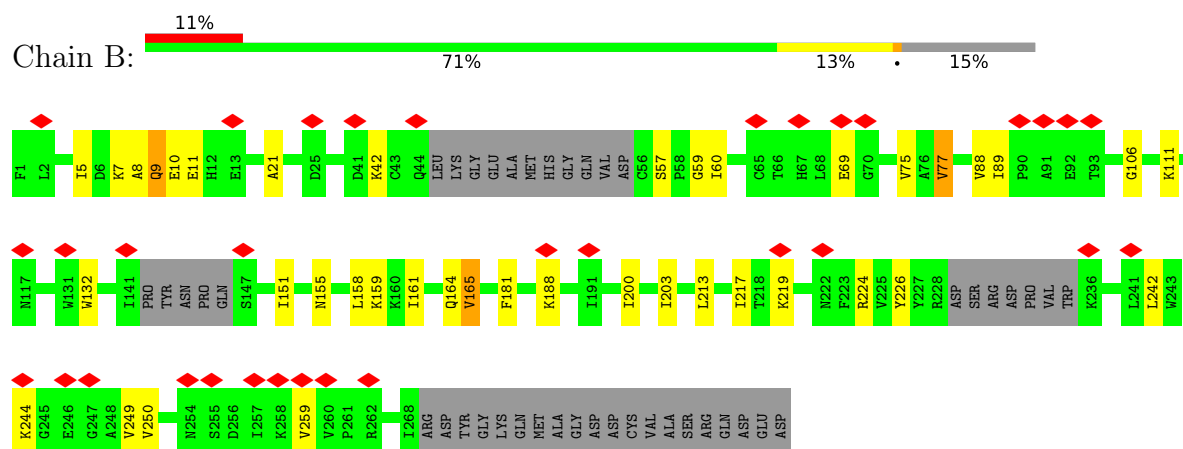
3 Residue-property plots

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.

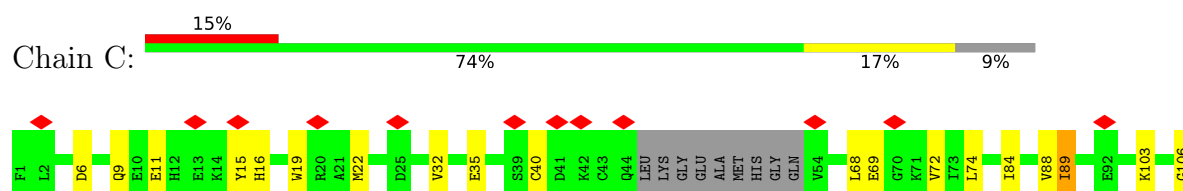
• Molecule 1: Integrase

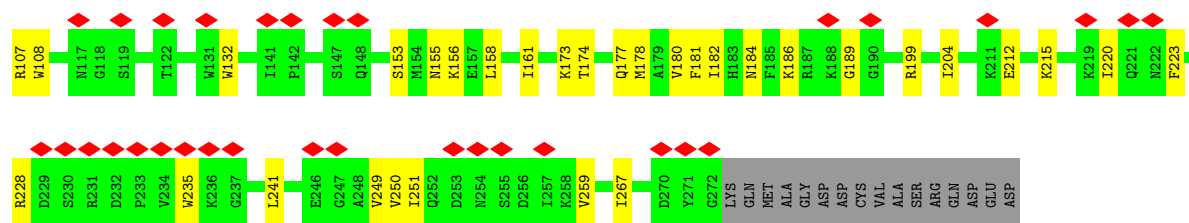


• Molecule 1: Integrase

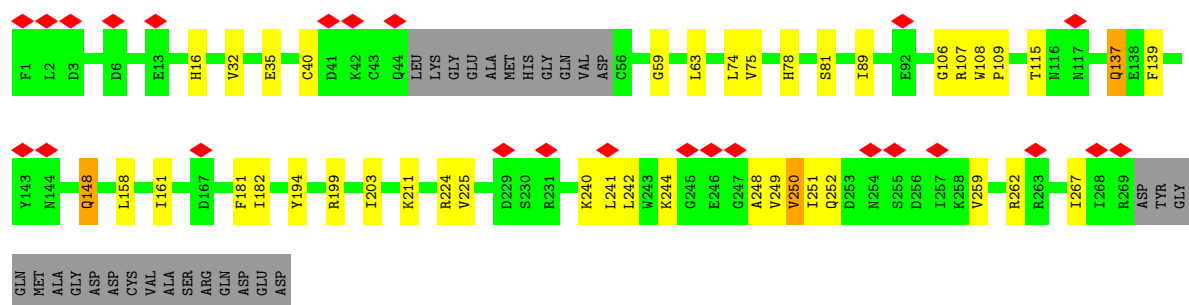
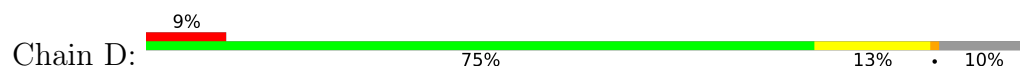


• Molecule 1: Integrase

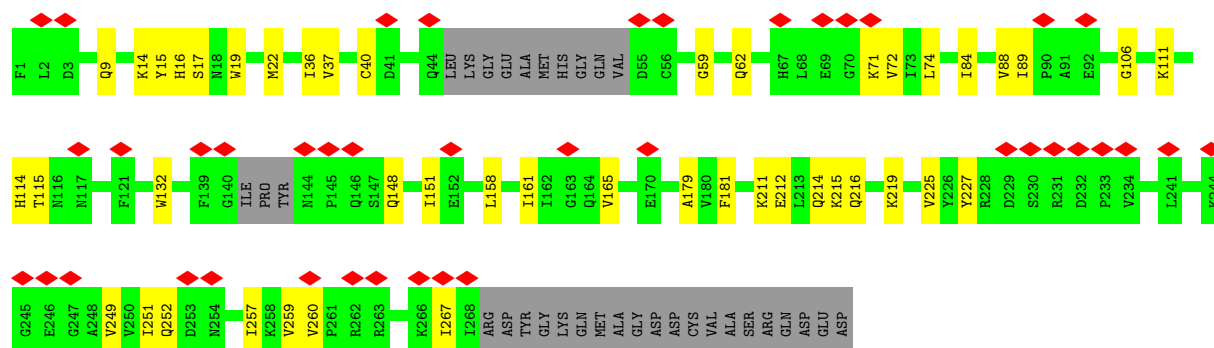
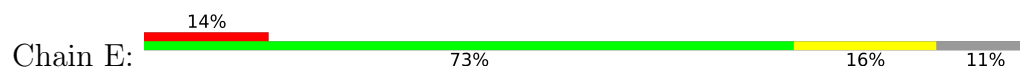




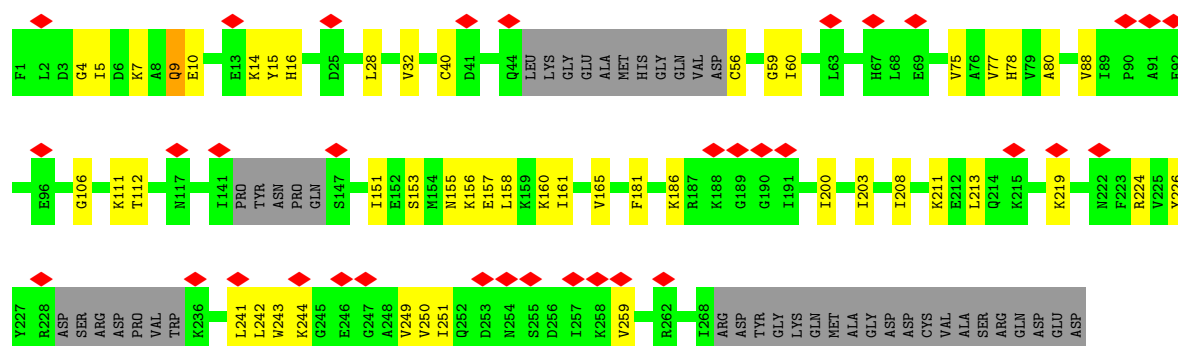
• Molecule 1: Integrase



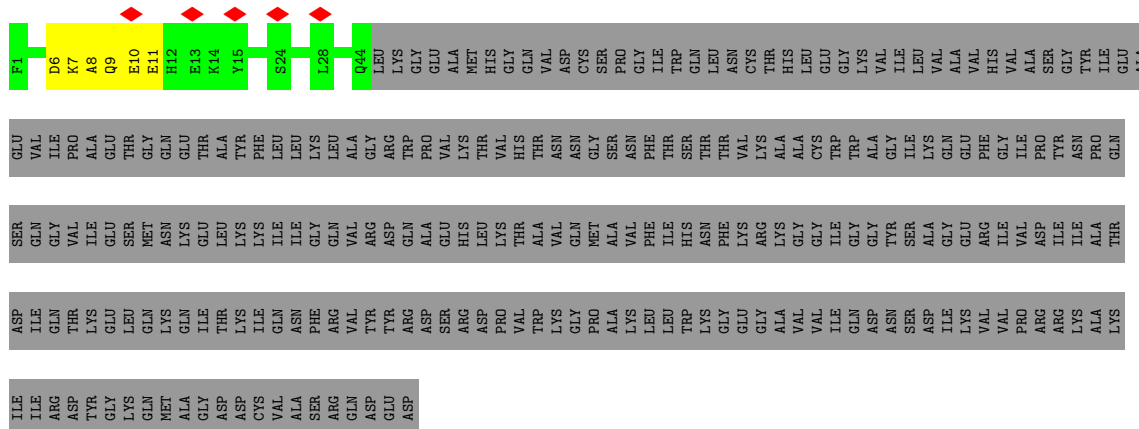
• Molecule 1: Integrase



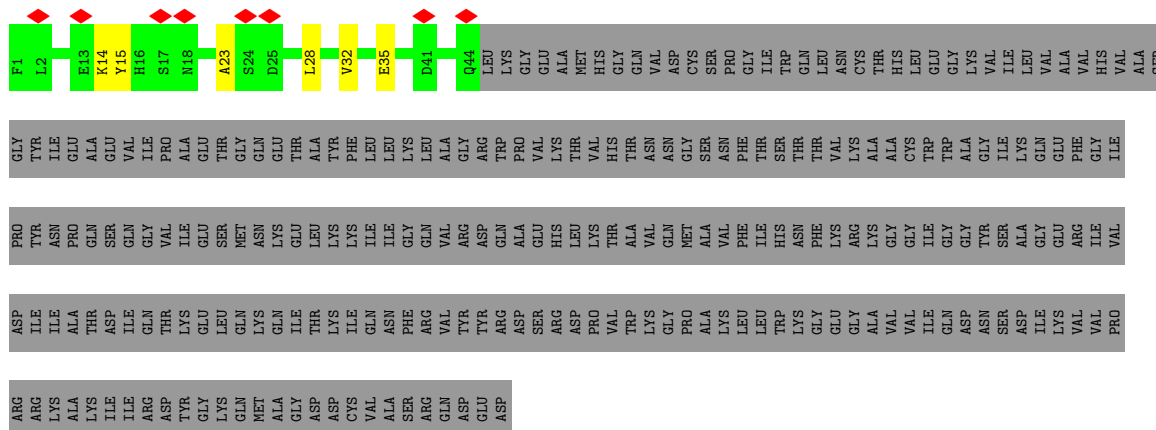
• Molecule 1: Integrase



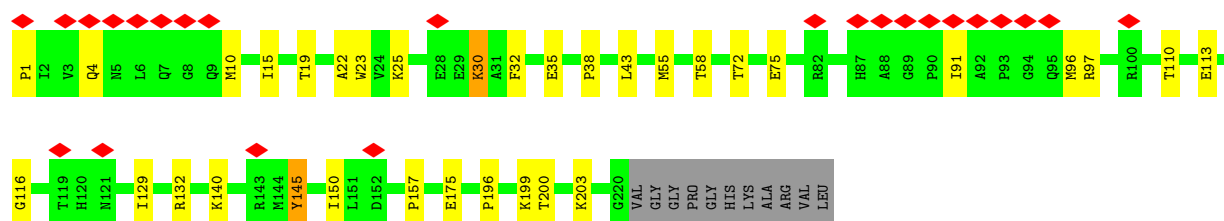
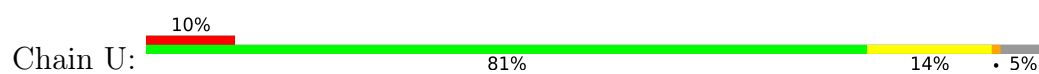
- Molecule 1: Integrase



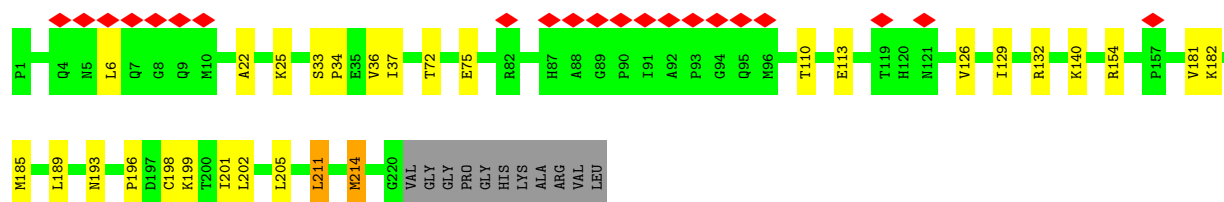
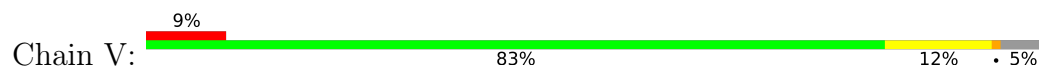
- Molecule 1: Integrase



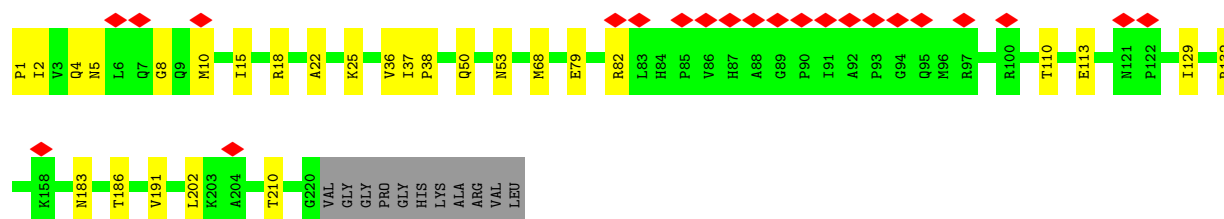
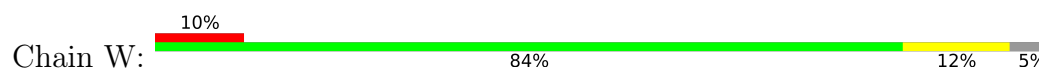
- Molecule 2: Gag polyprotein



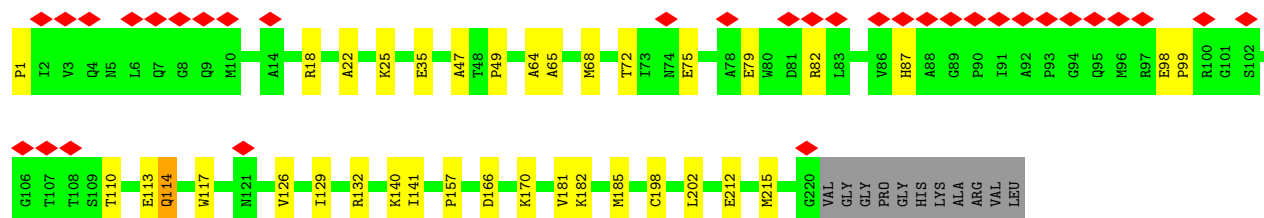
• Molecule 2: Gag polyprotein



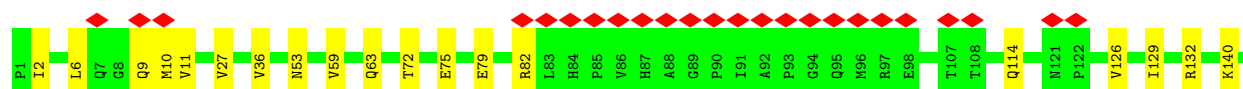
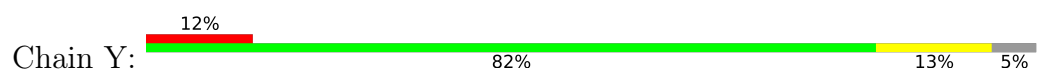
• Molecule 2: Gag polyprotein



• Molecule 2: Gag polyprotein

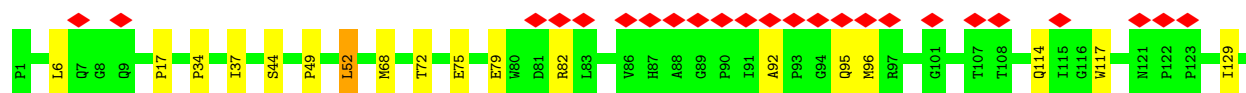
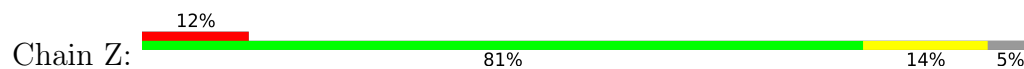


• Molecule 2: Gag polyprotein

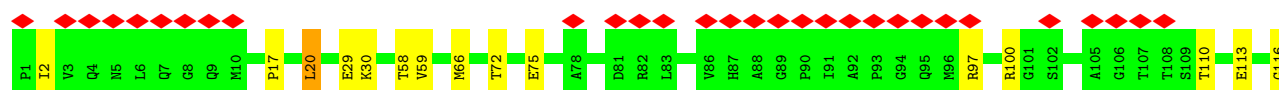
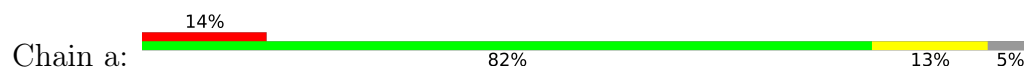




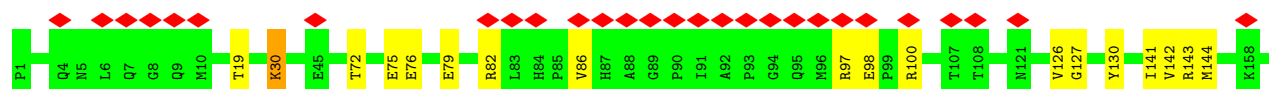
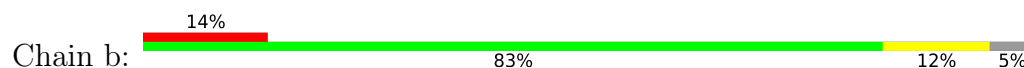
- Molecule 2: Gag polyprotein



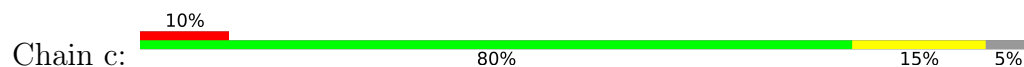
- Molecule 2: Gag polyprotein



- Molecule 2: Gag polyprotein

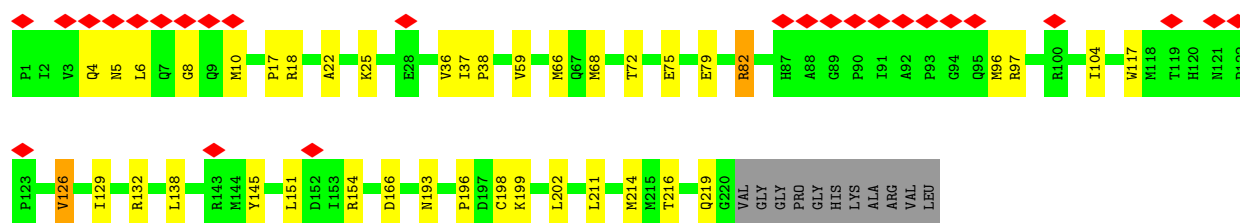


- Molecule 2: Gag polyprotein



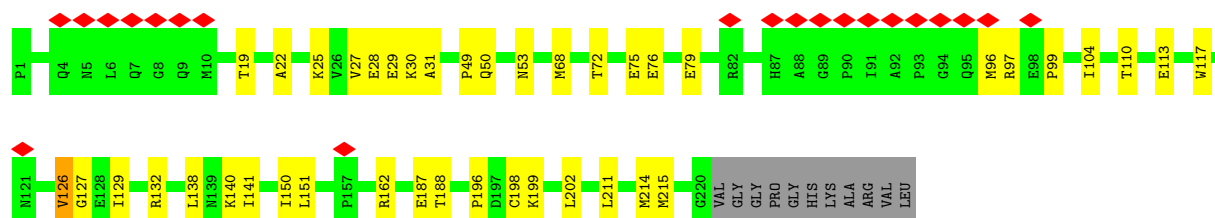
- Molecule 2: Gag polyprotein

Chain d: 



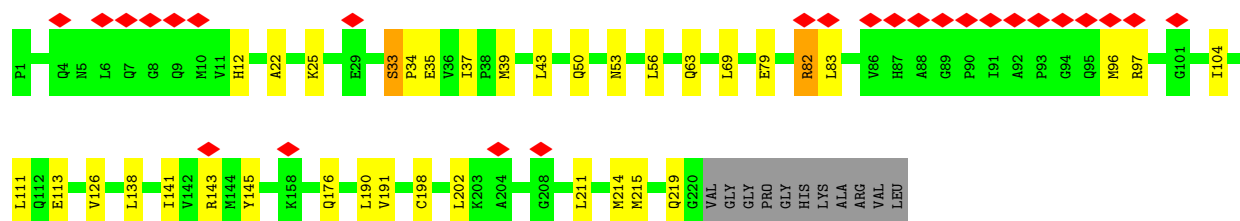
• Molecule 2: Gag polyprotein

Chain e: 



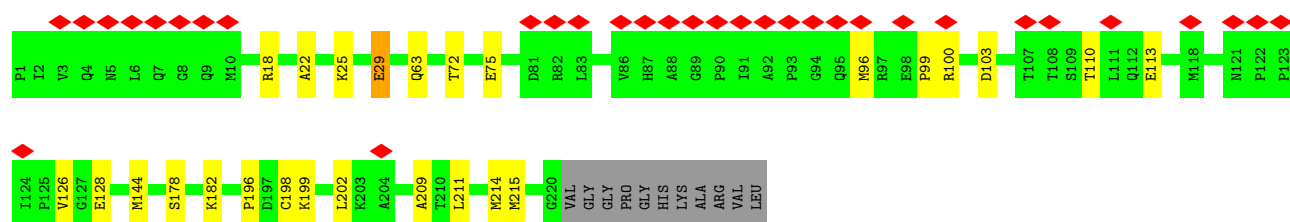
• Molecule 2: Gag polyprotein

Chain f: 



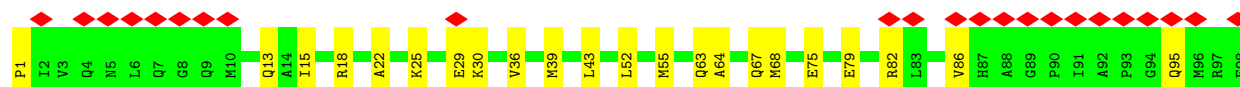
• Molecule 2: Gag polyprotein

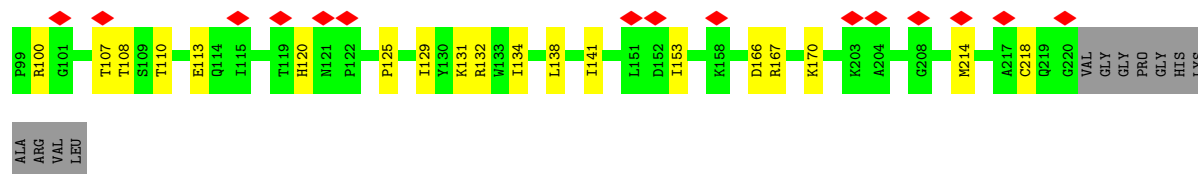
Chain g: 



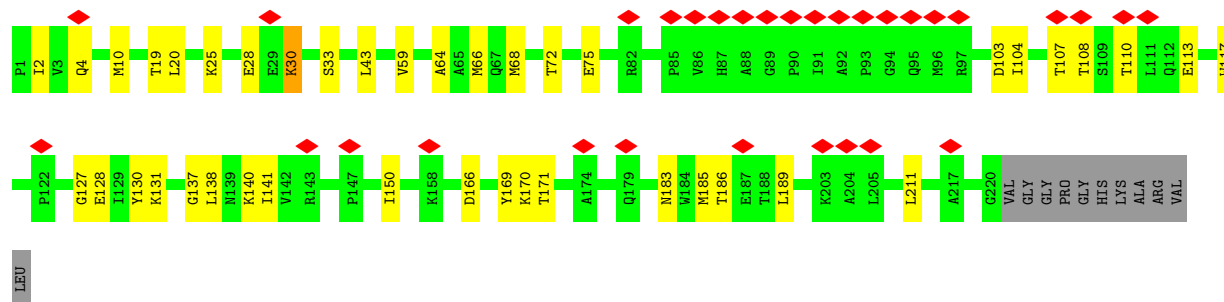
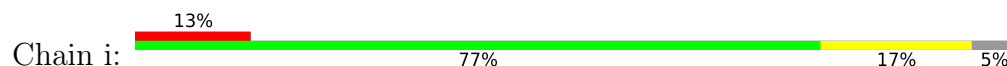
• Molecule 2: Gag polyprotein

Chain h: 

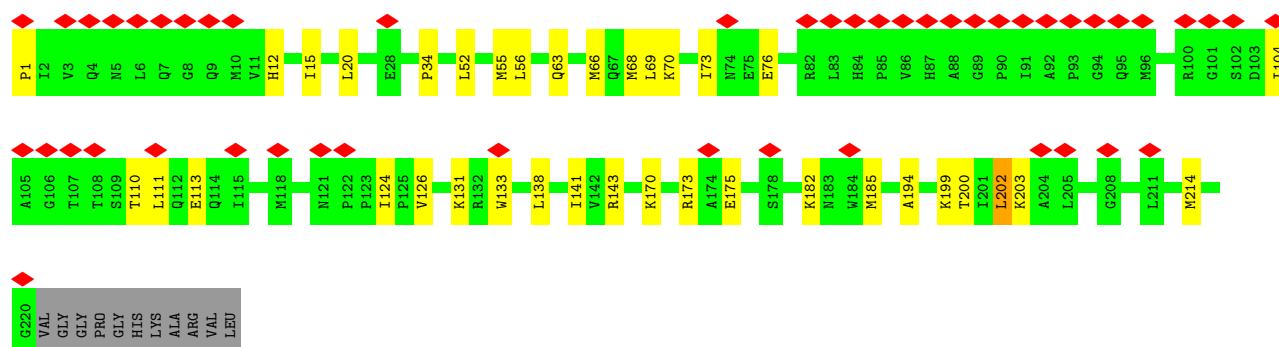
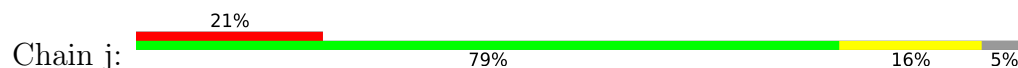




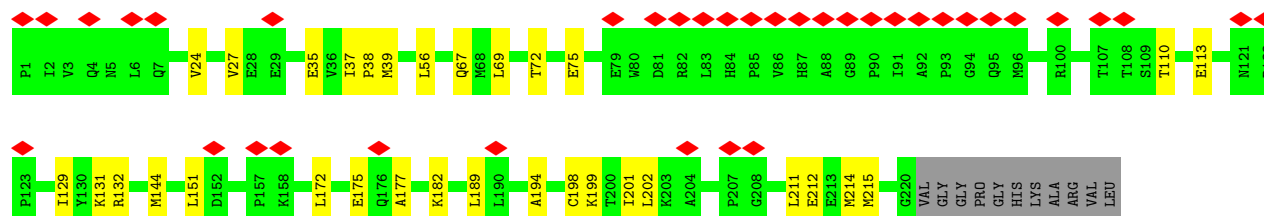
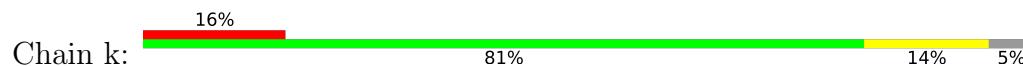
- Molecule 2: Gag polypeptide



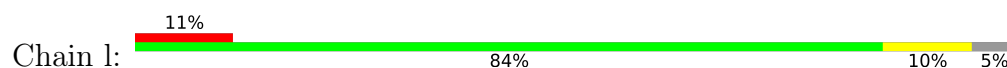
- Molecule 2: Gag polypeptide

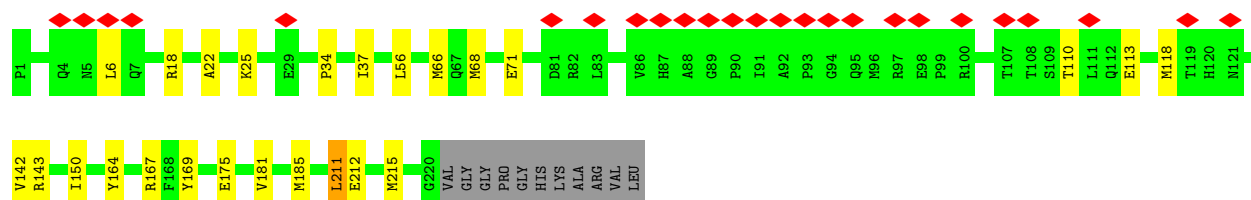


- Molecule 2: Gag polypeptide

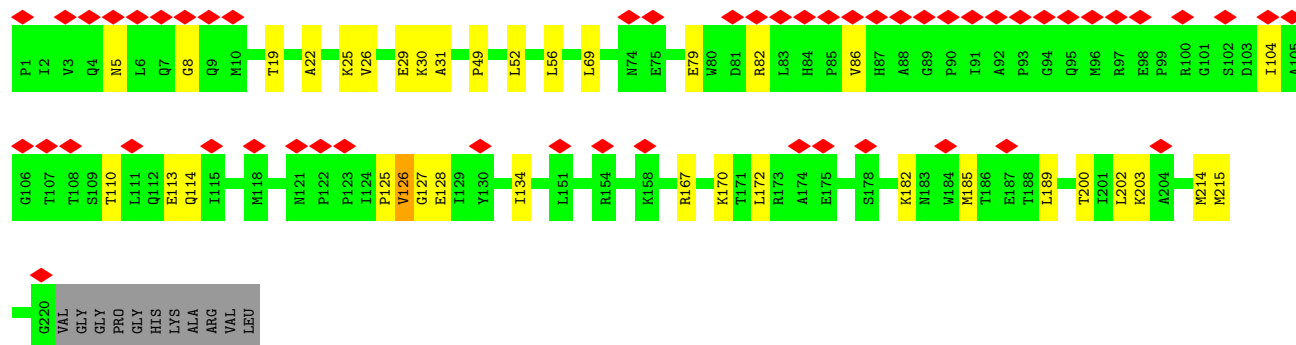
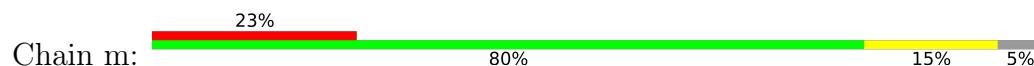


- Molecule 2: Gag polypeptide

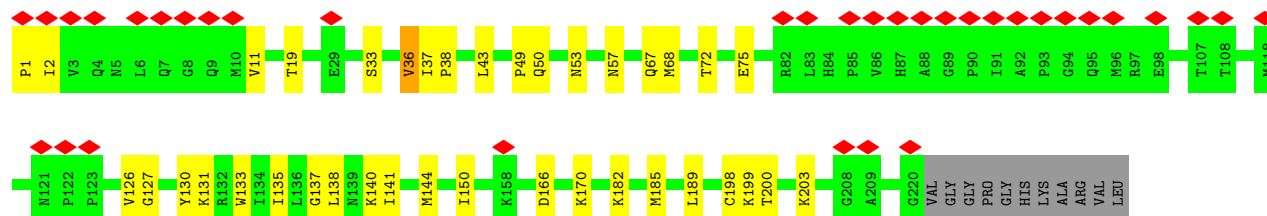




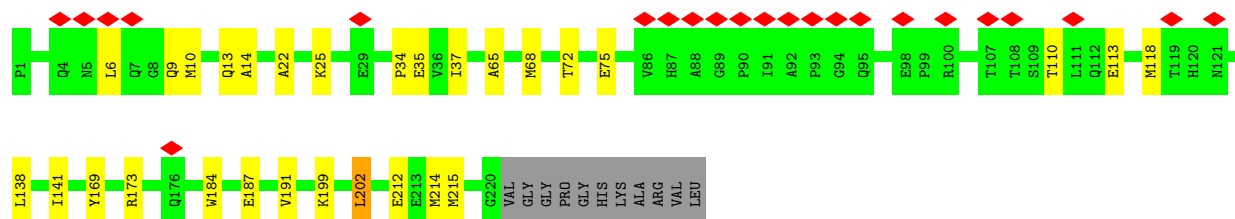
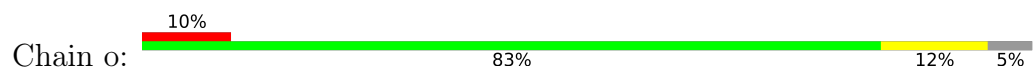
• Molecule 2: Gag polyprotein



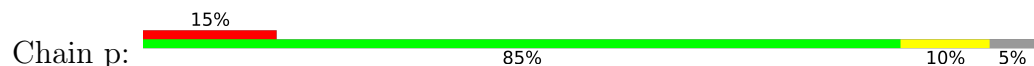
• Molecule 2: Gag polyprotein

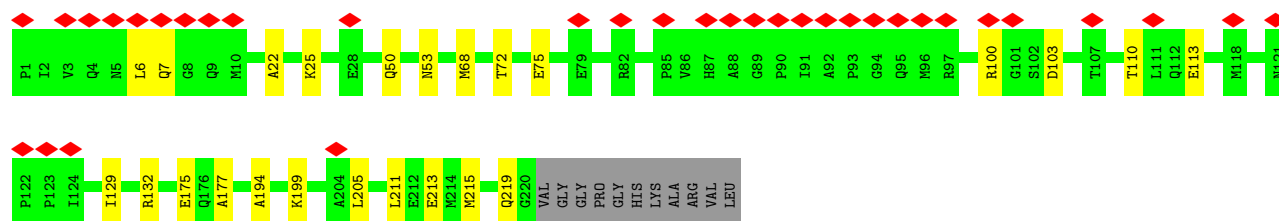


• Molecule 2: Gag polyprotein

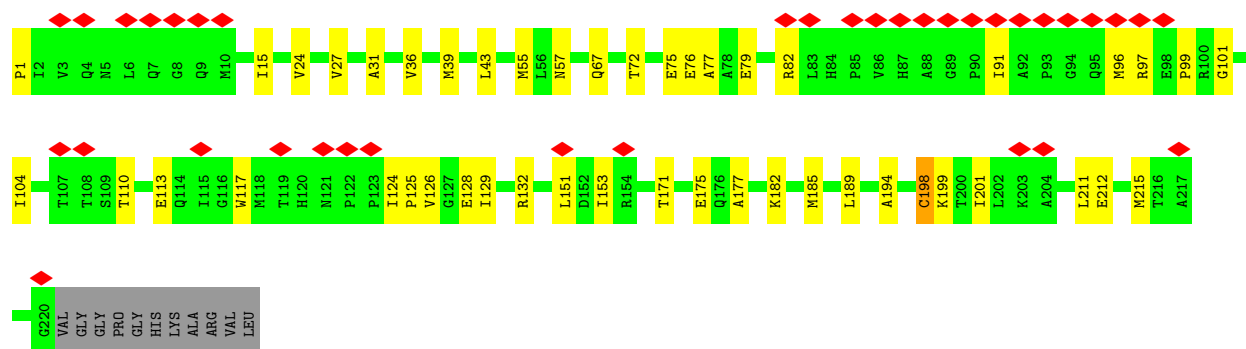
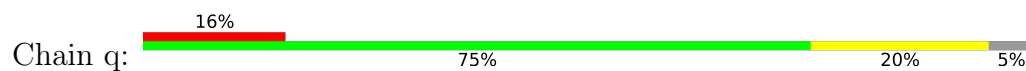


• Molecule 2: Gag polyprotein

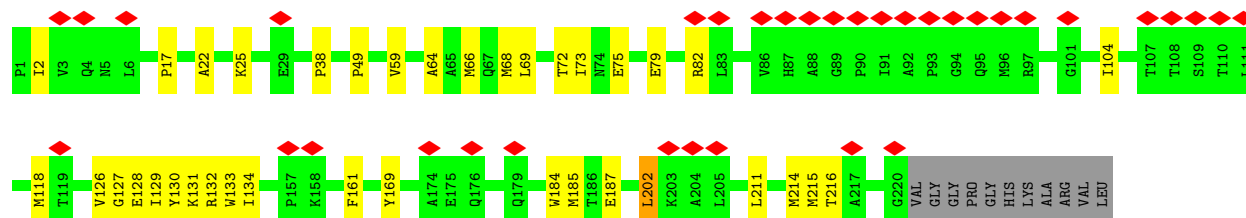
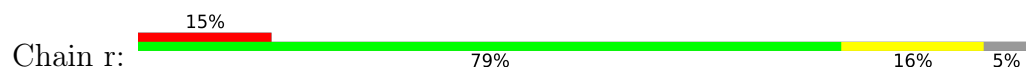




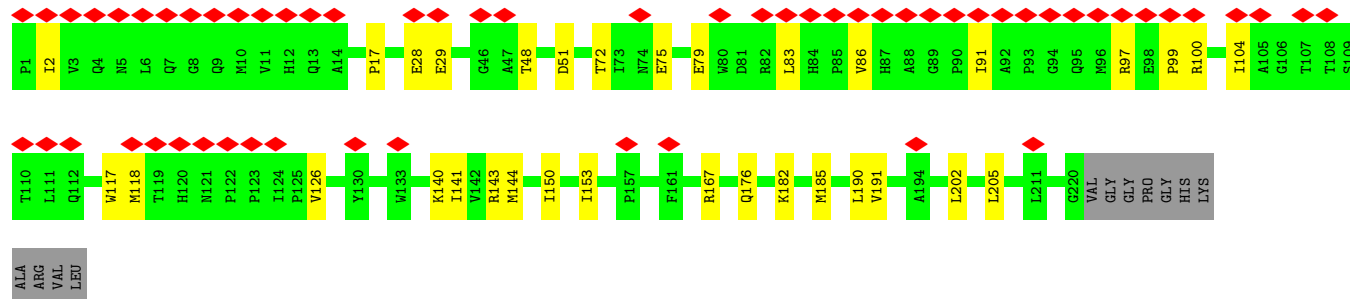
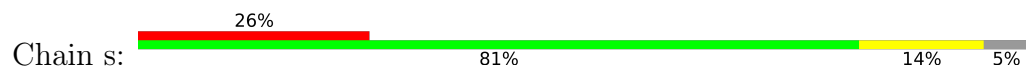
• Molecule 2: Gag polyprotein



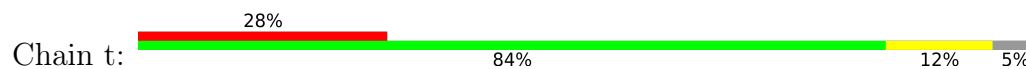
• Molecule 2: Gag polyprotein

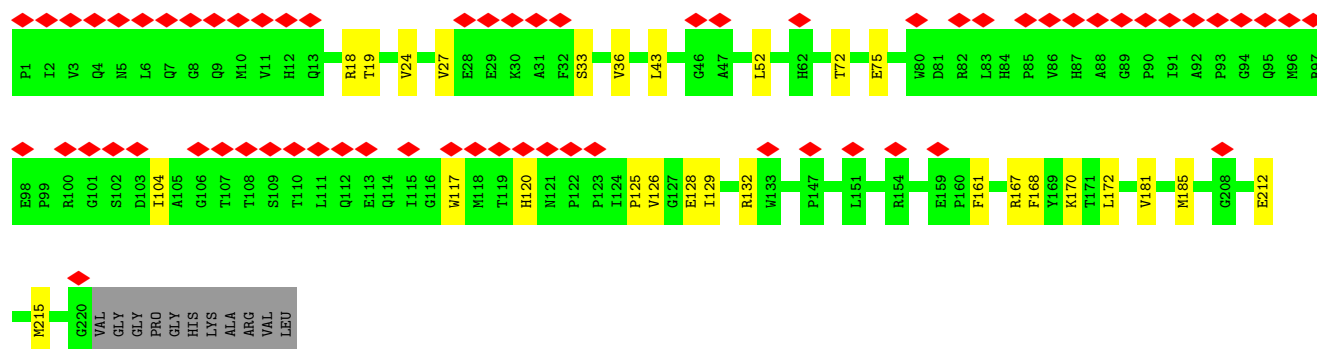


• Molecule 2: Gag polyprotein

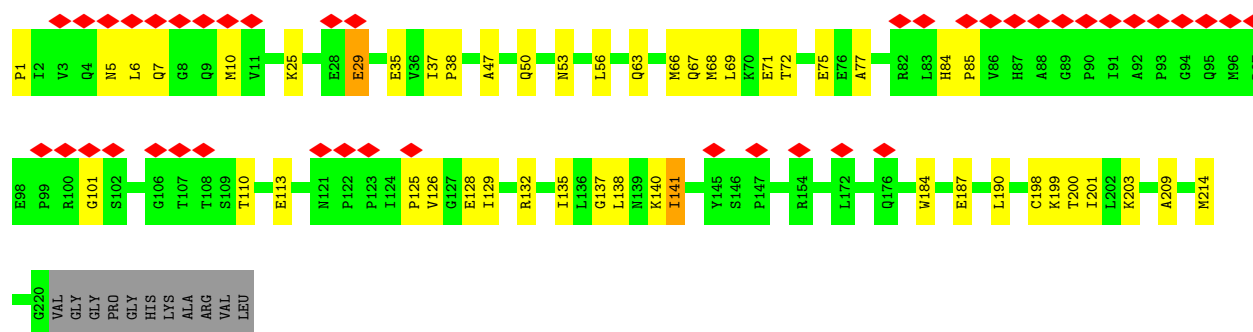
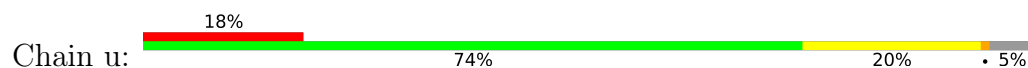


• Molecule 2: Gag polyprotein

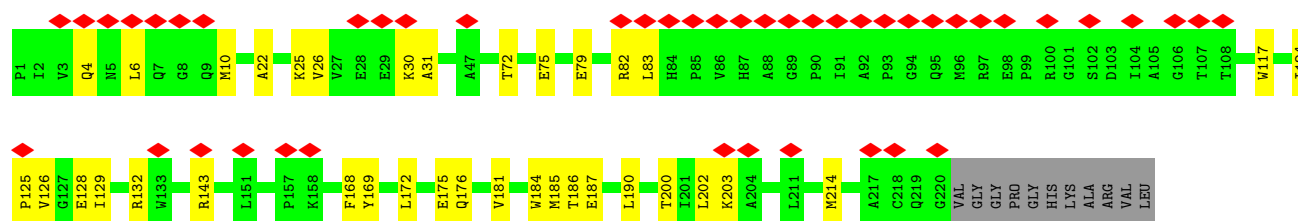
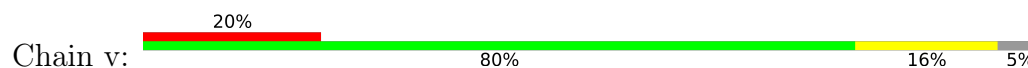




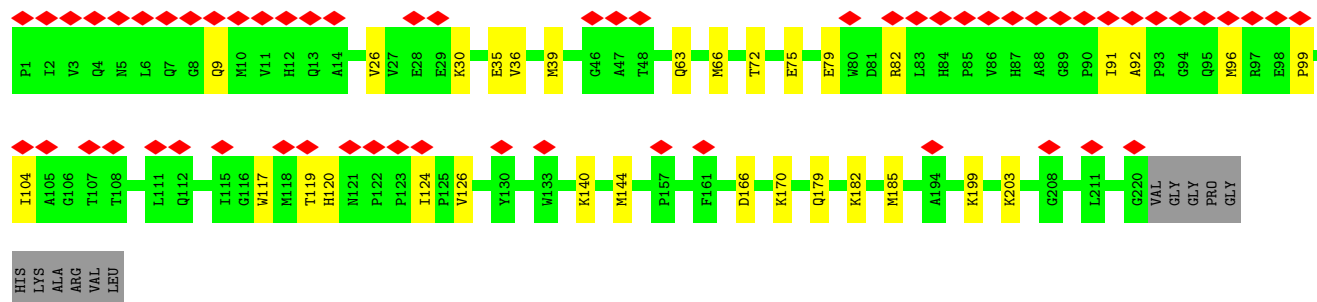
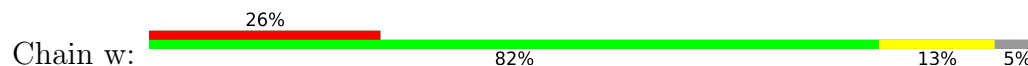
• Molecule 2: Gag polyprotein



• Molecule 2: Gag polyprotein

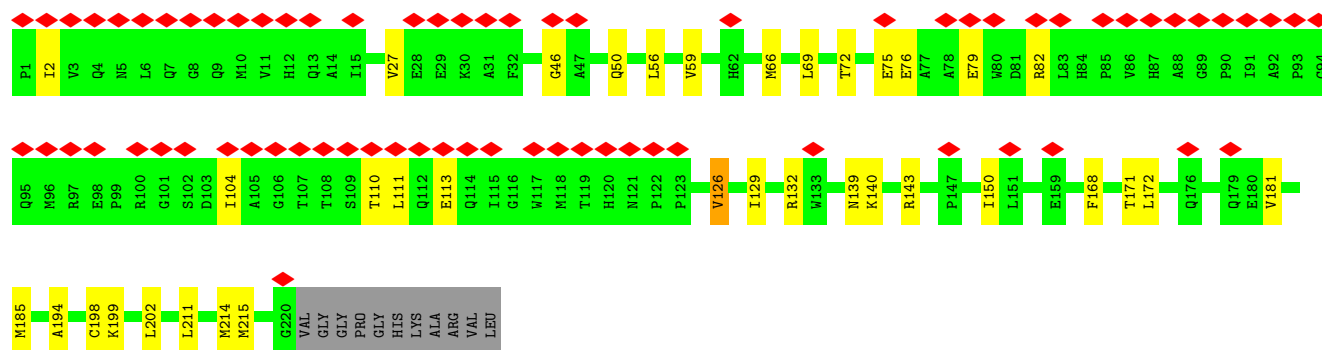


• Molecule 2: Gag polyprotein



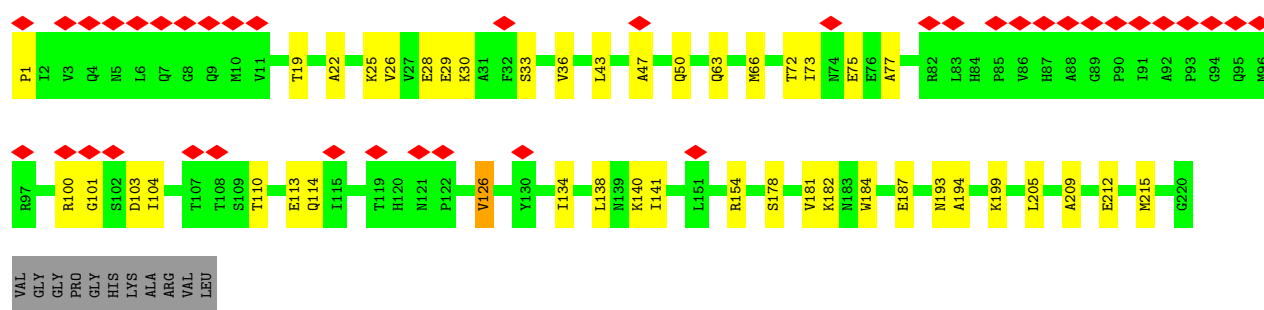
• Molecule 2: Gag polypeptide

Chain x: 



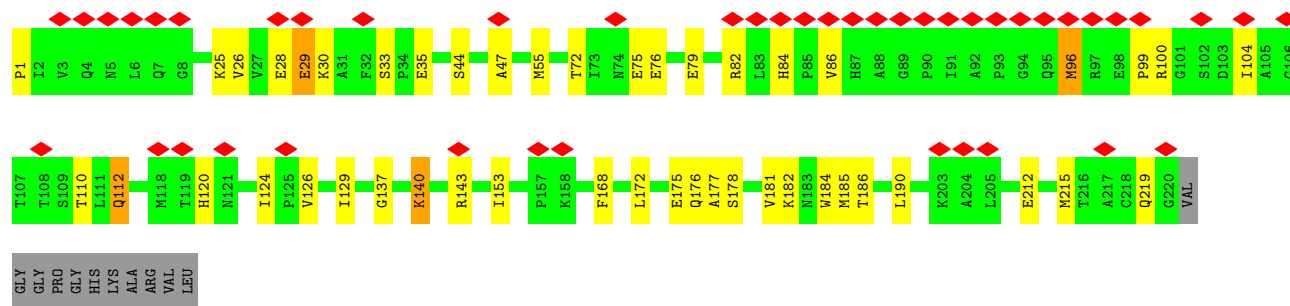
• Molecule 2: Gag polypeptide

Chain y: 



• Molecule 2: Gag polypeptide

Chain z: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	58103	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	11.537	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.201	Depositor
Map value standard deviation	0.905	Depositor
Recommended contour level	3.2	Depositor
Map size ($\text{\AA}$)	342.0, 342.0, 342.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.425, 1.425, 1.425	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.10	0/2047	0.28	0/2765
1	B	0.09	0/1961	0.27	0/2643
1	C	0.09	0/2124	0.25	0/2872
1	D	0.10	0/2080	0.27	0/2812
1	E	0.10	0/2047	0.27	0/2765
1	F	0.10	0/1957	0.26	0/2638
1	G	0.10	0/2120	0.27	0/2867
1	H	0.10	0/2080	0.28	0/2812
1	I	0.09	0/350	0.25	0/472
1	J	0.09	0/359	0.23	0/484
1	K	0.09	0/359	0.21	0/484
1	L	0.10	0/355	0.27	0/479
2	U	0.11	0/1757	0.29	0/2388
2	V	0.11	0/1757	0.30	0/2388
2	W	0.09	0/1757	0.26	0/2388
2	X	0.10	0/1757	0.30	0/2388
2	Y	0.11	0/1757	0.30	0/2388
2	Z	0.11	0/1757	0.28	0/2388
2	a	0.10	0/1757	0.27	0/2388
2	b	0.10	0/1757	0.29	0/2388
2	c	0.10	0/1757	0.30	0/2388
2	d	0.10	0/1757	0.27	0/2388
2	e	0.10	0/1757	0.31	0/2388
2	f	0.10	0/1757	0.30	0/2388
2	g	0.10	0/1757	0.31	0/2388
2	h	0.10	0/1757	0.29	0/2388
2	i	0.11	0/1757	0.30	0/2388
2	j	0.10	0/1757	0.26	0/2388
2	k	0.11	0/1757	0.29	0/2388
2	l	0.10	0/1757	0.29	0/2388
2	m	0.10	0/1757	0.28	0/2388
2	n	0.10	0/1757	0.31	0/2388

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	o	0.11	0/1757	0.31	0/2388
2	p	0.09	0/1757	0.29	0/2388
2	q	0.11	0/1757	0.28	0/2388
2	r	0.10	0/1757	0.26	0/2388
2	s	0.10	0/1757	0.27	0/2388
2	t	0.10	0/1757	0.29	0/2388
2	u	0.11	0/1757	0.29	0/2388
2	v	0.11	0/1757	0.27	0/2388
2	w	0.10	0/1757	0.29	0/2388
2	x	0.10	0/1757	0.27	0/2388
2	y	0.11	0/1757	0.29	0/2388
2	z	0.10	0/1757	0.27	0/2388
All	All	0.10	0/74063	0.28	0/100509

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2006	0	2018	31	0
1	B	1925	0	1957	25	0
1	C	2079	0	2090	34	0
1	D	2036	0	2055	28	0
1	E	2006	0	2018	27	0
1	F	1921	0	1951	32	0
1	G	2075	0	2084	33	0
1	H	2036	0	2055	27	0
1	I	342	0	323	1	0
1	J	351	0	331	2	0
1	K	351	0	331	3	0
1	L	347	0	325	3	0
2	U	1718	0	1716	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	V	1718	0	1716	20	0
2	W	1718	0	1716	15	0
2	X	1718	0	1716	20	0
2	Y	1718	0	1716	18	0
2	Z	1718	0	1716	20	0
2	a	1718	0	1716	19	0
2	b	1718	0	1716	16	0
2	c	1718	0	1716	17	0
2	d	1718	0	1716	24	0
2	e	1718	0	1716	29	0
2	f	1718	0	1716	23	0
2	g	1718	0	1716	16	0
2	h	1718	0	1716	30	0
2	i	1718	0	1716	26	0
2	j	1718	0	1716	25	0
2	k	1718	0	1716	19	0
2	l	1718	0	1716	16	0
2	m	1718	0	1716	20	0
2	n	1718	0	1716	23	0
2	o	1718	0	1716	17	0
2	p	1718	0	1716	15	0
2	q	1718	0	1716	29	0
2	r	1718	0	1716	26	0
2	s	1718	0	1716	23	0
2	t	1718	0	1716	18	0
2	u	1718	0	1716	27	0
2	v	1718	0	1716	22	0
2	w	1718	0	1716	23	0
2	x	1718	0	1716	21	0
2	y	1718	0	1716	26	0
2	z	1718	0	1716	31	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
4	X	36	0	6	0	0
4	Z	36	0	6	0	0
4	a	36	0	6	0	0
4	b	36	0	6	0	0
4	g	36	0	6	1	0
4	i	36	0	6	0	0
4	m	36	0	6	0	0
4	q	36	0	6	0	0
All	All	72751	0	72498	879	0

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

All (879) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:HIS:CE1	1:G:40:CYS:SG	2.73	0.81
1:C:16:HIS:CE1	1:C:40:CYS:SG	2.76	0.78
1:D:16:HIS:CE1	1:D:40:CYS:SG	2.76	0.78
2:x:104:ILE:HG13	2:x:126:VAL:HG23	1.67	0.76
1:F:16:HIS:CE1	1:F:40:CYS:SG	2.79	0.75
1:F:59:GLY:HA3	1:F:111:LYS:HG2	1.69	0.75
1:G:84:ILE:HG13	1:G:180:VAL:HG23	1.69	0.74
2:g:25:LYS:O	2:g:29:GLU:HB2	1.87	0.73
1:E:225:VAL:HG21	1:E:251:ILE:HG21	1.71	0.73
2:s:99:PRO:HG2	2:s:126:VAL:HG11	1.70	0.72
2:v:202:LEU:HD21	2:v:214:MET:HG2	1.73	0.71
1:E:16:HIS:CE1	1:E:40:CYS:SG	2.83	0.70
1:H:16:HIS:CE1	1:H:40:CYS:SG	2.85	0.70
2:a:143:ARG:HH21	2:a:176:GLN:HB2	1.56	0.70
1:A:227:TYR:HB2	1:A:260:VAL:HG11	1.74	0.70
2:s:143:ARG:HH21	2:s:176:GLN:H	1.39	0.70
2:m:19:THR:HG22	2:r:17:PRO:HG3	1.73	0.69
2:j:138:LEU:HD13	2:j:141:ILE:HD11	1.74	0.69
2:k:172:LEU:HD11	2:k:182:LYS:HG3	1.74	0.68
1:G:224:ARG:HG3	1:G:268:ILE:HG13	1.74	0.68
2:b:196:PRO:HA	2:b:199:LYS:HE3	1.75	0.68
2:c:162:ARG:HH22	2:c:215:MET:HB2	1.59	0.67
2:j:194:ALA:H	2:j:199:LYS:HE3	1.61	0.66
1:A:225:VAL:HG21	1:A:251:ILE:HG21	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:i:104:ILE:HG12	2:i:130:TYR:HB2	1.78	0.66
2:k:175:GLU:HG3	2:k:177:ALA:H	1.60	0.65
1:A:158:LEU:HD23	1:A:161:ILE:HD11	1.76	0.65
2:g:63:GLN:HG2	2:h:170:LYS:HZ3	1.61	0.65
2:s:17:PRO:HB2	2:t:18:ARG:HH21	1.62	0.64
1:H:74:LEU:HB2	1:H:89:ILE:HD11	1.80	0.64
2:t:104:ILE:HG13	2:t:126:VAL:HG23	1.79	0.64
2:e:29:GLU:HG3	2:e:30:LYS:HG2	1.79	0.64
2:b:141:ILE:O	2:b:144:MET:HB3	1.98	0.64
2:d:104:ILE:HG13	2:d:126:VAL:HG23	1.79	0.63
1:C:11:GLU:O	1:C:15:TYR:HB2	1.99	0.63
2:o:212:GLU:HA	2:o:215:MET:HE2	1.80	0.63
1:G:17:SER:HA	1:G:187:ARG:HG2	1.79	0.63
1:E:74:LEU:HB2	1:E:89:ILE:HD11	1.80	0.63
2:b:185:MET:HE2	2:b:189:LEU:HD12	1.79	0.63
2:n:37:ILE:HD12	2:n:138:LEU:HD22	1.81	0.63
2:m:202:LEU:HD21	2:m:214:MET:HG2	1.81	0.62
2:y:63:GLN:HA	2:y:66:MET:HE2	1.82	0.62
1:A:250:VAL:HG22	1:A:259:VAL:HG12	1.81	0.62
2:a:17:PRO:HG3	2:b:19:THR:HG22	1.82	0.61
2:V:202:LEU:HD21	2:V:214:MET:HB2	1.82	0.61
2:r:104:ILE:HG12	2:r:130:TYR:HB2	1.81	0.61
2:x:79:GLU:HA	2:x:82:ARG:HG2	1.83	0.61
2:a:2:ILE:HD13	2:a:118:MET:HE3	1.82	0.61
2:Z:49:PRO:HD2	2:Z:114:GLN:HG2	1.83	0.61
2:m:49:PRO:HD2	2:m:114:GLN:HG2	1.83	0.61
1:D:74:LEU:HD23	1:D:89:ILE:HD13	1.82	0.61
2:U:4:GLN:HG3	2:U:10:MET:HG3	1.81	0.61
2:w:104:ILE:HG13	2:w:126:VAL:HB	1.82	0.61
2:f:104:ILE:HG12	2:f:126:VAL:HG23	1.83	0.60
2:l:143:ARG:HE	2:l:175:GLU:HA	1.65	0.60
1:D:241:LEU:HA	1:D:251:ILE:HG22	1.82	0.60
2:u:209:ALA:HB3	2:u:214:MET:HE3	1.82	0.60
1:D:250:VAL:HB	1:D:259:VAL:HG22	1.82	0.60
2:c:202:LEU:HD21	2:c:214:MET:HG2	1.83	0.60
2:f:202:LEU:HD22	2:f:214:MET:HG3	1.84	0.60
2:d:59:VAL:HG21	2:d:66:MET:HE3	1.84	0.60
1:D:108:TRP:HE3	1:D:109:PRO:HD2	1.67	0.60
1:E:225:VAL:HG12	1:E:267:ILE:HG22	1.83	0.59
2:W:1:PRO:HD3	2:W:15:ILE:HD13	1.84	0.59
2:z:104:ILE:HG13	2:z:126:VAL:HB	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:104:ILE:HG13	2:s:126:VAL:HB	1.84	0.59
2:y:36:VAL:HG23	2:y:138:LEU:HD21	1.84	0.59
1:A:63:LEU:HD23	1:A:121:PHE:HE1	1.67	0.59
1:C:15:TYR:HB3	1:C:182:ILE:HD13	1.83	0.59
2:b:212:GLU:HA	2:b:215:MET:HE2	1.83	0.59
2:e:110:THR:HG22	2:e:113:GLU:HG3	1.84	0.59
2:p:175:GLU:HG3	2:p:177:ALA:H	1.67	0.59
1:A:225:VAL:HG12	1:A:267:ILE:HG22	1.85	0.59
2:U:19:THR:HG22	2:Z:17:PRO:HG3	1.85	0.59
2:j:202:LEU:HD11	2:j:214:MET:HA	1.83	0.59
2:y:29:GLU:HG3	2:y:30:LYS:HG2	1.85	0.59
2:X:64:ALA:O	2:X:68:MET:HG2	2.03	0.59
1:B:224:ARG:HH11	1:B:226:TYR:HE2	1.51	0.59
2:a:166:ASP:O	2:a:170:LYS:HG2	2.02	0.58
2:y:77:ALA:HB1	2:y:101:GLY:HA2	1.85	0.58
1:H:182:ILE:HG13	1:H:186:LYS:HB2	1.85	0.58
2:u:1:PRO:HB3	2:u:47:ALA:HA	1.84	0.58
2:w:96:MET:HG2	2:w:120:HIS:HE1	1.69	0.58
1:F:4:GLY:HA2	1:F:7:LYS:HE2	1.86	0.58
2:a:170:LYS:HZ3	2:f:63:GLN:HG2	1.66	0.58
1:F:224:ARG:HH11	1:F:226:TYR:HE2	1.52	0.58
2:i:59:VAL:HG11	2:i:66:MET:HG3	1.86	0.58
2:s:17:PRO:HG3	2:t:19:THR:HG22	1.85	0.58
2:Z:72:THR:HG21	2:Z:140:LYS:HD2	1.86	0.57
2:i:166:ASP:O	2:i:170:LYS:HG2	2.04	0.57
2:x:2:ILE:HB	2:x:46:GLY:HA3	1.86	0.57
2:w:36:VAL:HA	2:w:39:MET:HE2	1.87	0.57
1:H:93:THR:HG22	1:H:95:GLN:H	1.69	0.57
1:E:84:ILE:HD12	1:E:158:LEU:HD12	1.86	0.57
2:X:1:PRO:HB3	2:X:47:ALA:HA	1.87	0.57
1:B:57:SER:HB3	1:B:60:ILE:HG12	1.87	0.56
1:D:224:ARG:HH12	1:D:240:LYS:HA	1.70	0.56
2:V:211:LEU:HD23	2:V:211:LEU:H	1.70	0.56
2:f:39:MET:HE3	2:f:43:LEU:HD11	1.86	0.56
2:v:26:VAL:HG22	2:v:30:LYS:HE3	1.87	0.56
1:G:77:VAL:HG22	1:G:84:ILE:HG22	1.87	0.56
2:a:202:LEU:HD22	2:a:214:MET:HG2	1.86	0.56
2:q:194:ALA:HB3	2:q:199:LYS:HG3	1.88	0.56
2:Y:2:ILE:HG12	2:Y:10:MET:HE3	1.87	0.56
2:u:77:ALA:HB1	2:u:101:GLY:HA2	1.88	0.56
1:A:17:SER:HB2	1:A:22:MET:HE3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:SER:HB3	1:H:203:ILE:HD12	1.87	0.56
2:W:79:GLU:HA	2:W:82:ARG:HD3	1.88	0.55
2:f:79:GLU:HA	2:f:82:ARG:HD3	1.89	0.55
2:p:110:THR:HG23	2:p:113:GLU:H	1.70	0.55
1:D:78:HIS:HD2	1:D:81:SER:H	1.54	0.55
1:E:227:TYR:HB2	1:E:260:VAL:HG11	1.87	0.55
1:A:182:ILE:HD12	1:A:186:LYS:HB2	1.88	0.55
1:C:19:TRP:HA	1:C:22:MET:HE2	1.89	0.55
2:h:166:ASP:O	2:h:170:LYS:HG2	2.07	0.55
1:F:28:LEU:HD12	1:F:32:VAL:HG21	1.88	0.55
1:D:63:LEU:HB3	1:D:115:THR:HG22	1.89	0.55
2:g:99:PRO:HG2	2:g:126:VAL:HG11	1.87	0.55
2:m:104:ILE:HG13	2:m:126:VAL:HG23	1.88	0.55
2:u:63:GLN:HA	2:u:66:MET:HE2	1.89	0.55
2:w:199:LYS:HE2	2:w:203:LYS:HZ2	1.72	0.55
2:b:97:ARG:HG3	2:b:100:ARG:HH21	1.72	0.55
2:y:72:THR:HG21	2:y:140:LYS:HD2	1.88	0.55
2:n:19:THR:HG23	2:n:43:LEU:HD22	1.89	0.55
2:u:110:THR:HG22	2:u:113:GLU:HG3	1.89	0.55
2:y:110:THR:HG23	2:y:113:GLU:H	1.70	0.55
2:q:99:PRO:HG2	2:q:126:VAL:HG11	1.89	0.54
1:F:78:HIS:HE1	1:F:80:ALA:HB3	1.72	0.54
2:m:26:VAL:HA	2:m:29:GLU:HG2	1.89	0.54
1:H:239:ALA:HB1	1:H:251:ILE:HG21	1.88	0.54
2:c:2:ILE:HG22	2:c:10:MET:HG3	1.90	0.54
2:e:150:ILE:HG23	2:e:151:LEU:HD12	1.90	0.54
1:E:132:TRP:CE2	1:F:14:LYS:HE2	2.43	0.54
2:U:32:PHE:HB2	2:U:145:TYR:HD2	1.72	0.54
2:r:202:LEU:HD11	2:r:214:MET:HA	1.90	0.54
2:a:29:GLU:HG3	2:a:30:LYS:HG3	1.90	0.54
2:x:50:GLN:HG3	2:x:111:LEU:HG	1.90	0.54
2:c:72:THR:HG21	2:c:140:LYS:HD2	1.90	0.54
2:p:6:LEU:HD23	2:p:6:LEU:H	1.73	0.54
2:z:30:LYS:HZ3	2:z:35:GLU:HB2	1.72	0.54
2:t:181:VAL:HG12	2:t:185:MET:HE3	1.90	0.53
2:u:56:LEU:HD11	2:u:69:LEU:HD13	1.89	0.53
2:Z:166:ASP:O	2:Z:170:LYS:HG2	2.07	0.53
2:b:86:VAL:HG13	2:b:98:GLU:HB3	1.90	0.53
2:j:20:LEU:HD11	2:j:55:MET:HA	1.89	0.53
2:y:30:LYS:HD2	2:y:33:SER:HB3	1.90	0.53
1:B:59:GLY:HA3	1:B:111:LYS:HG2	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:92:ALA:HB3	2:Z:95:GLN:HB2	1.89	0.53
2:b:86:VAL:HG21	2:b:100:ARG:HD3	1.91	0.53
2:m:185:MET:HB2	2:m:189:LEU:HD23	1.88	0.53
2:z:79:GLU:HA	2:z:82:ARG:HD3	1.89	0.53
1:A:181:PHE:HD1	1:B:106:GLY:HA2	1.74	0.53
2:l:34:PRO:HG3	2:l:142:VAL:HG11	1.91	0.53
2:v:169:TYR:HA	2:v:172:LEU:HD12	1.91	0.53
1:A:16:HIS:CE1	1:A:40:CYS:SG	3.02	0.53
2:g:211:LEU:O	2:g:215:MET:HG2	2.09	0.52
2:w:26:VAL:O	2:w:30:LYS:HB3	2.09	0.52
2:f:97:ARG:HH12	2:f:113:GLU:HB2	1.74	0.52
1:E:181:PHE:HD1	1:F:106:GLY:HA2	1.74	0.52
2:V:34:PRO:HA	2:V:37:ILE:HD13	1.91	0.52
2:j:110:THR:HG22	2:j:113:GLU:HG3	1.91	0.52
2:m:172:LEU:HD11	2:m:182:LYS:HG3	1.91	0.52
2:V:72:THR:HG21	2:V:140:LYS:HD2	1.91	0.52
2:a:138:LEU:HD23	2:a:141:ILE:HD11	1.92	0.52
2:W:50:GLN:HA	2:W:53:ASN:HD21	1.75	0.52
2:m:56:LEU:HD21	2:m:69:LEU:HD11	1.92	0.52
1:H:216:GLN:HA	1:H:219:LYS:HE2	1.91	0.52
2:n:150:ILE:HB	2:n:185:MET:HE1	1.90	0.52
2:r:49:PRO:HG3	2:r:127:GLY:HA3	1.92	0.52
2:V:196:PRO:HA	2:V:199:LYS:HG2	1.92	0.52
2:h:39:MET:HE3	2:h:43:LEU:HD11	1.92	0.52
2:r:69:LEU:HB3	2:r:134:ILE:HD11	1.91	0.52
2:x:72:THR:HG21	2:x:140:LYS:HD3	1.92	0.52
2:i:107:THR:HG23	2:i:108:THR:HG23	1.90	0.51
2:d:22:ALA:HA	2:d:25:LYS:HG2	1.91	0.51
1:H:196:ALA:HA	1:H:199:ARG:HD2	1.93	0.51
2:U:96:MET:HE1	2:U:116:GLY:HA3	1.92	0.51
2:y:72:THR:HA	2:y:75:GLU:HG2	1.93	0.51
2:f:143:ARG:HH21	2:f:176:GLN:HB3	1.74	0.51
2:U:200:THR:HA	2:U:203:LYS:HG2	1.92	0.51
2:V:185:MET:HA	2:V:189:LEU:HD23	1.92	0.51
1:F:157:GLU:O	1:F:160:LYS:HG3	2.10	0.51
2:j:34:PRO:HB2	2:j:173:ARG:HH11	1.75	0.51
2:x:181:VAL:HG12	2:x:185:MET:HE3	1.92	0.51
2:z:44:SER:HB3	2:z:55:MET:HE1	1.91	0.51
1:C:158:LEU:HA	1:C:161:ILE:HG22	1.93	0.51
1:C:181:PHE:HD1	1:D:106:GLY:HA2	1.76	0.51
2:p:50:GLN:HA	2:p:53:ASN:ND2	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:178:SER:HB3	2:Z:181:VAL:HG23	1.92	0.51
2:h:29:GLU:HG3	2:h:30:LYS:HG3	1.93	0.51
2:h:63:GLN:HG2	2:i:170:LYS:HZ3	1.76	0.51
2:j:124:ILE:HG22	2:j:126:VAL:HG13	1.93	0.51
1:C:68:LEU:HG	1:C:69:GLU:HG3	1.91	0.51
1:C:212:GLU:HA	1:C:215:LYS:HG2	1.92	0.51
2:Z:202:LEU:HD21	2:Z:214:MET:HG2	1.93	0.51
2:c:19:THR:HG23	2:c:43:LEU:HD22	1.93	0.51
2:k:56:LEU:HD21	2:k:69:LEU:HD13	1.92	0.51
2:m:52:LEU:HD23	2:m:134:ILE:HD12	1.92	0.51
2:r:2:ILE:HD13	2:r:118:MET:HE2	1.93	0.51
1:E:211:LYS:HG2	1:E:215:LYS:HZ1	1.75	0.51
2:X:72:THR:HA	2:X:75:GLU:HG2	1.93	0.51
2:t:129:ILE:HD13	2:t:132:ARG:HH11	1.75	0.51
2:w:182:LYS:HA	2:w:185:MET:HG2	1.93	0.51
2:y:104:ILE:HG13	2:y:126:VAL:HG23	1.93	0.51
2:k:194:ALA:HB3	2:k:199:LYS:HG3	1.93	0.50
2:v:200:THR:HA	2:v:203:LYS:HG2	1.94	0.50
2:x:139:ASN:O	2:x:143:ARG:HG2	2.11	0.50
2:z:96:MET:HE3	2:z:120:HIS:HB2	1.93	0.50
1:G:73:ILE:HD12	1:G:88:VAL:HG22	1.94	0.50
2:c:72:THR:HA	2:c:75:GLU:HG2	1.94	0.50
2:x:56:LEU:HG	2:x:66:MET:HE1	1.93	0.50
2:v:30:LYS:HG3	2:v:31:ALA:H	1.76	0.50
2:x:110:THR:HG23	2:x:113:GLU:H	1.77	0.50
1:D:81:SER:HB3	1:D:203:ILE:HD12	1.92	0.50
2:i:103:ASP:HB3	2:i:117:TRP:HH2	1.76	0.50
2:j:52:LEU:HD21	2:j:131:LYS:HG2	1.92	0.50
2:o:9:GLN:HG3	2:p:7:GLN:HE21	1.76	0.50
2:s:48:THR:HG23	2:s:51:ASP:H	1.76	0.50
1:E:106:GLY:HA2	1:F:181:PHE:HD1	1.76	0.50
2:k:202:LEU:HD21	2:k:214:MET:HA	1.93	0.50
2:o:65:ALA:HA	2:o:68:MET:HE3	1.94	0.50
2:r:22:ALA:HA	2:r:25:LYS:HG2	1.93	0.50
2:w:179:GLN:HA	2:w:182:LYS:HZ3	1.76	0.50
2:V:110:THR:HG22	2:V:113:GLU:HG3	1.94	0.50
2:p:50:GLN:HA	2:p:53:ASN:HD21	1.76	0.50
2:q:124:ILE:HG22	2:q:126:VAL:HG13	1.92	0.50
2:r:64:ALA:O	2:r:68:MET:HG2	2.12	0.50
2:x:150:ILE:HD13	2:x:171:THR:HB	1.92	0.50
2:y:22:ALA:HA	2:y:25:LYS:HG2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:185:MET:HE2	2:Y:189:LEU:HD21	1.94	0.50
2:g:100:ARG:H	2:g:103:ASP:HB2	1.76	0.50
2:i:138:LEU:O	2:i:141:ILE:HG12	2.12	0.50
2:z:25:LYS:HA	2:z:28:GLU:HG2	1.94	0.50
1:G:74:LEU:HD23	1:G:89:ILE:HD13	1.93	0.49
2:j:104:ILE:HG13	2:j:126:VAL:HB	1.94	0.49
1:G:212:GLU:HA	1:G:215:LYS:HG2	1.92	0.49
2:k:129:ILE:O	2:k:132:ARG:HG2	2.12	0.49
2:l:211:LEU:HD22	2:l:215:MET:HE2	1.93	0.49
1:B:161:ILE:O	1:B:165:VAL:HG23	2.12	0.49
1:F:77:VAL:HG11	1:F:151:ILE:HG13	1.93	0.49
2:m:172:LEU:HG	2:m:182:LYS:HE3	1.93	0.49
2:s:99:PRO:HG3	2:s:117:TRP:CE2	2.47	0.49
1:G:181:PHE:HD1	1:H:106:GLY:HA2	1.77	0.49
1:H:231:ARG:HE	1:H:263:ARG:HH12	1.61	0.49
2:U:129:ILE:O	2:U:132:ARG:HG2	2.13	0.49
2:d:17:PRO:HG2	2:e:19:THR:HG22	1.95	0.49
2:d:196:PRO:HA	2:d:199:LYS:HG2	1.94	0.49
2:g:63:GLN:HG2	2:h:170:LYS:NZ	2.25	0.49
2:h:214:MET:O	2:h:218:CYS:HB2	2.13	0.49
2:o:202:LEU:HD21	2:o:214:MET:HB2	1.93	0.49
1:G:14:LYS:HE3	1:G:15:TYR:CZ	2.47	0.49
2:c:104:ILE:HG12	2:c:126:VAL:HG23	1.95	0.49
2:e:50:GLN:HA	2:e:53:ASN:HD21	1.77	0.49
2:h:1:PRO:H3	2:h:15:ILE:HD13	1.77	0.49
2:r:75:GLU:O	2:r:79:GLU:HG2	2.12	0.49
2:u:200:THR:HA	2:u:203:LYS:HG2	1.95	0.49
1:D:194:TYR:HE1	1:D:199:ARG:HB3	1.76	0.49
1:E:216:GLN:HA	1:E:219:LYS:HG2	1.94	0.49
1:H:63:LEU:HB3	1:H:115:THR:HG22	1.94	0.49
2:U:150:ILE:HD11	2:U:175:GLU:HB2	1.95	0.49
2:j:68:MET:HE3	2:k:211:LEU:HG	1.94	0.49
2:w:30:LYS:HZ1	2:w:35:GLU:HG2	1.77	0.49
2:h:64:ALA:O	2:h:68:MET:HG3	2.13	0.49
2:u:37:ILE:HG23	2:u:135:ILE:HD12	1.95	0.49
1:G:174:THR:O	1:G:178:MET:HG2	2.13	0.49
2:Z:79:GLU:O	2:Z:82:ARG:HG3	2.12	0.49
2:a:129:ILE:O	2:a:132:ARG:HG2	2.12	0.49
2:e:196:PRO:HA	2:e:199:LYS:HE3	1.94	0.49
1:E:72:VAL:HG23	1:E:89:ILE:HB	1.95	0.49
1:G:153:SER:O	1:G:156:LYS:HG3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:129:ILE:O	2:W:132:ARG:HG2	2.12	0.49
2:c:49:PRO:HD2	2:c:114:GLN:HG2	1.94	0.49
2:l:212:GLU:HA	2:l:215:MET:HE3	1.95	0.49
2:n:50:GLN:HA	2:n:53:ASN:HD21	1.77	0.49
2:q:129:ILE:O	2:q:132:ARG:HG2	2.13	0.49
1:H:78:HIS:CE1	1:H:80:ALA:HB3	2.48	0.49
2:X:72:THR:HG21	2:X:140:LYS:HD2	1.95	0.49
2:Y:63:GLN:H	2:Z:170:LYS:HZ3	1.61	0.49
2:i:64:ALA:O	2:i:68:MET:HG2	2.13	0.49
1:C:182:ILE:HD12	1:C:186:LYS:HB2	1.95	0.48
1:D:59:GLY:H	1:D:78:HIS:HE1	1.61	0.48
1:B:158:LEU:HA	1:B:161:ILE:HG12	1.95	0.48
2:V:72:THR:HA	2:V:75:GLU:HG2	1.95	0.48
2:u:50:GLN:HA	2:u:53:ASN:HD21	1.78	0.48
2:w:9:GLN:HE21	2:w:119:THR:HB	1.77	0.48
2:h:63:GLN:H	2:i:170:LYS:HZ3	1.60	0.48
2:w:30:LYS:NZ	2:w:35:GLU:HG2	2.28	0.48
2:z:124:ILE:HG22	2:z:126:VAL:HG13	1.95	0.48
1:D:139:PHE:HZ	2:X:157:PRO:HD2	1.79	0.48
2:m:110:THR:HG22	2:m:113:GLU:HG3	1.95	0.48
2:u:50:GLN:HA	2:u:53:ASN:ND2	2.28	0.48
2:e:72:THR:HA	2:e:75:GLU:HG2	1.95	0.48
1:A:101:LEU:HD23	1:A:104:LEU:HD21	1.95	0.48
2:c:178:SER:HB3	2:c:181:VAL:HG23	1.95	0.48
2:h:67:GLN:HG2	2:i:169:TYR:CZ	2.49	0.48
2:k:211:LEU:HD23	2:k:211:LEU:H	1.78	0.48
2:r:73:ILE:HD11	2:r:134:ILE:HD13	1.95	0.48
2:x:129:ILE:O	2:x:132:ARG:HG2	2.14	0.48
1:C:107:ARG:HD2	1:D:107:ARG:HE	1.79	0.48
1:E:161:ILE:HG13	1:E:179:ALA:HB1	1.95	0.48
1:F:5:ILE:HG22	1:F:9:GLN:HE22	1.78	0.48
2:g:96:MET:HE1	2:g:113:GLU:HA	1.96	0.48
2:n:199:LYS:HG2	2:n:203:LYS:HZ2	1.77	0.48
2:r:59:VAL:HG11	2:r:66:MET:HG3	1.95	0.48
2:v:72:THR:O	2:v:75:GLU:HG3	2.13	0.48
2:x:72:THR:HA	2:x:75:GLU:HG2	1.94	0.48
2:i:2:ILE:HG22	2:i:10:MET:HG3	1.95	0.48
2:q:151:LEU:HA	2:q:189:LEU:HD21	1.96	0.48
2:w:79:GLU:O	2:w:82:ARG:HG3	2.13	0.48
1:A:106:GLY:HA2	1:B:181:PHE:HD1	1.79	0.48
1:G:32:VAL:O	1:G:35:GLU:HG2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:72:THR:HG21	2:a:140:LYS:HD2	1.94	0.48
2:e:138:LEU:HA	2:e:141:ILE:HG22	1.95	0.48
2:i:110:THR:HG22	2:i:113:GLU:HG3	1.95	0.48
2:z:143:ARG:HH21	2:z:176:GLN:H	1.61	0.48
1:A:130:CYS:HB2	1:A:135:ILE:HB	1.96	0.48
1:E:249:VAL:HG22	1:E:251:ILE:HG23	1.95	0.48
2:U:30:LYS:H	2:U:30:LYS:HG3	1.55	0.48
2:X:87:HIS:CE1	2:X:98:GLU:HB2	2.49	0.48
2:d:4:GLN:HA	2:d:10:MET:HA	1.95	0.48
2:u:37:ILE:HB	2:u:38:PRO:HD3	1.96	0.48
2:z:1:PRO:HB3	2:z:47:ALA:HB2	1.96	0.48
2:z:168:PHE:O	2:z:172:LEU:HG	2.14	0.48
1:H:59:GLY:H	1:H:78:HIS:HE2	1.62	0.47
1:H:214:GLN:HA	1:H:217:ILE:HD12	1.96	0.47
2:Y:215:MET:O	2:Y:219:GLN:HG3	2.14	0.47
2:l:56:LEU:HG	2:l:66:MET:HE1	1.96	0.47
2:u:184:TRP:O	2:u:187:GLU:HG3	2.14	0.47
2:v:143:ARG:HH22	2:v:175:GLU:HG2	1.79	0.47
1:H:158:LEU:HA	1:H:161:ILE:HG12	1.96	0.47
2:e:25:LYS:O	2:e:28:GLU:HG3	2.14	0.47
2:i:127:GLY:O	2:i:130:TYR:HB3	2.15	0.47
2:k:24:VAL:HA	2:k:27:VAL:HG22	1.96	0.47
2:l:181:VAL:HG12	2:l:185:MET:HE3	1.97	0.47
2:z:212:GLU:HA	2:z:215:MET:HG2	1.95	0.47
1:C:153:SER:O	1:C:156:LYS:HG3	2.15	0.47
1:F:111:LYS:HG3	1:F:112:THR:HG23	1.96	0.47
2:U:110:THR:HG22	2:U:113:GLU:HG3	1.97	0.47
2:Y:150:ILE:HD12	2:Y:185:MET:HE3	1.94	0.47
2:l:110:THR:HG22	2:l:113:GLU:HG3	1.96	0.47
2:o:191:VAL:HG22	2:o:199:LYS:HD2	1.96	0.47
2:r:130:TYR:O	2:r:133:TRP:HB2	2.14	0.47
2:s:28:GLU:HG3	2:s:29:GLU:HG2	1.96	0.47
2:z:26:VAL:HA	2:z:29:GLU:HG2	1.96	0.47
2:U:91:ILE:HG13	2:U:97:ARG:HB3	1.96	0.47
2:W:50:GLN:HA	2:W:53:ASN:ND2	2.28	0.47
2:m:167:ARG:HA	2:m:170:LYS:HG2	1.95	0.47
2:q:39:MET:HE3	2:q:43:LEU:HD11	1.97	0.47
2:u:6:LEU:O	2:u:7:GLN:HG3	2.15	0.47
2:w:140:LYS:O	2:w:144:MET:HG3	2.13	0.47
2:y:194:ALA:H	2:y:199:LYS:HE2	1.76	0.47
1:B:155:ASN:O	1:B:158:LEU:HG	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:198:CYS:O	2:a:202:LEU:HG	2.14	0.47
2:m:22:ALA:HA	2:m:25:LYS:HG2	1.96	0.47
2:m:30:LYS:HG3	2:m:31:ALA:H	1.79	0.47
2:q:1:PRO:H3	2:q:15:ILE:HD13	1.80	0.47
1:C:6:ASP:O	1:C:9:GLN:HG3	2.14	0.47
2:W:22:ALA:HA	2:W:25:LYS:HG2	1.95	0.47
2:u:72:THR:HA	2:u:75:GLU:HG2	1.96	0.47
1:A:245:GLY:O	1:A:246:GLU:HG3	2.14	0.47
1:C:174:THR:O	1:C:178:MET:HG2	2.14	0.47
1:G:158:LEU:HA	1:G:161:ILE:HG22	1.95	0.47
2:Y:6:LEU:HD23	2:Y:6:LEU:H	1.80	0.47
2:a:97:ARG:HG3	2:a:100:ARG:HH12	1.79	0.47
2:e:72:THR:HG21	2:e:140:LYS:HD2	1.97	0.47
2:f:198:CYS:O	2:f:202:LEU:HG	2.15	0.47
2:z:99:PRO:HG2	2:z:126:VAL:HG11	1.97	0.47
1:A:211:LYS:O	1:A:214:GLN:HG3	2.14	0.47
1:F:244:LYS:HD3	1:F:249:VAL:HG22	1.97	0.47
2:Z:96:MET:HB3	2:Z:117:TRP:HE1	1.78	0.47
2:k:35:GLU:O	2:k:38:PRO:HD2	2.15	0.47
2:q:175:GLU:HG3	2:q:177:ALA:H	1.80	0.47
1:C:106:GLY:HA2	1:D:181:PHE:HD1	1.80	0.47
1:C:189:GLY:HA3	1:C:199:ARG:HH12	1.80	0.47
1:D:32:VAL:O	1:D:35:GLU:HG2	2.14	0.47
2:h:138:LEU:HA	2:h:141:ILE:HG22	1.97	0.47
2:l:164:TYR:O	2:l:167:ARG:HG2	2.15	0.47
2:n:182:LYS:HA	2:n:185:MET:HG2	1.96	0.47
2:s:72:THR:HG21	2:s:140:LYS:HE3	1.97	0.47
1:E:14:LYS:HE3	1:E:15:TYR:CZ	2.50	0.47
1:F:56:CYS:HB3	1:F:60:ILE:HG13	1.97	0.47
2:V:181:VAL:HG12	2:V:185:MET:HE3	1.96	0.47
2:W:68:MET:HE1	2:X:215:MET:HG2	1.96	0.47
2:g:196:PRO:HA	2:g:199:LYS:HE2	1.97	0.47
2:l:22:ALA:HA	2:l:25:LYS:HG2	1.97	0.47
2:m:200:THR:HA	2:m:203:LYS:HZ3	1.80	0.47
2:x:194:ALA:HB3	2:x:199:LYS:HB2	1.97	0.47
1:D:262:ARG:HH22	1:D:267:ILE:HG22	1.80	0.46
2:r:184:TRP:O	2:r:187:GLU:HG3	2.15	0.46
2:w:91:ILE:HG22	2:w:92:ALA:H	1.80	0.46
1:B:77:VAL:HG11	1:B:151:ILE:HD12	1.97	0.46
1:C:241:LEU:HD22	1:C:267:ILE:HD13	1.97	0.46
1:F:155:ASN:O	1:F:158:LEU:HG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:129:ILE:O	2:V:132:ARG:HG2	2.15	0.46
2:b:205:LEU:HD11	2:b:217:ALA:HB2	1.96	0.46
2:e:96:MET:HB3	2:e:117:TRP:HE1	1.81	0.46
2:u:5:ASN:H	2:u:10:MET:HE1	1.80	0.46
1:A:249:VAL:HG22	1:A:251:ILE:HG23	1.97	0.46
2:Z:44:SER:HB2	2:Z:52:LEU:HD11	1.97	0.46
2:m:49:PRO:HG3	2:m:127:GLY:HA2	1.97	0.46
2:n:137:GLY:O	2:n:140:LYS:HG2	2.15	0.46
2:w:124:ILE:HG22	2:w:126:VAL:HG13	1.96	0.46
1:D:242:LEU:HD11	1:D:252:GLN:HB3	1.96	0.46
2:e:50:GLN:HA	2:e:53:ASN:ND2	2.31	0.46
2:e:76:GLU:HA	2:e:79:GLU:HG2	1.98	0.46
2:t:215:MET:HE2	2:t:215:MET:HB2	1.88	0.46
2:u:68:MET:O	2:u:71:GLU:HG3	2.15	0.46
2:v:129:ILE:O	2:v:132:ARG:HG2	2.15	0.46
2:v:181:VAL:HG22	2:v:185:MET:HE3	1.97	0.46
2:h:13:GLN:HG3	2:i:4:GLN:HE22	1.80	0.46
2:w:99:PRO:HG2	2:w:126:VAL:HG11	1.98	0.46
1:E:132:TRP:CD2	1:F:14:LYS:HE2	2.50	0.46
1:F:158:LEU:HA	1:F:161:ILE:HG12	1.96	0.46
2:e:68:MET:HG3	2:f:211:LEU:HD11	1.98	0.46
2:k:110:THR:HG22	2:k:113:GLU:HG3	1.96	0.46
2:q:198:CYS:HA	2:q:201:ILE:HB	1.97	0.46
2:y:154:ARG:HH11	2:y:193:ASN:HA	1.81	0.46
1:C:220:ILE:HA	1:C:223:PHE:HD2	1.80	0.46
2:X:110:THR:HG22	2:X:113:GLU:HG3	1.98	0.46
2:b:30:LYS:H	2:b:30:LYS:HG3	1.62	0.46
2:n:135:ILE:HA	2:n:138:LEU:HG	1.96	0.46
2:t:72:THR:HA	2:t:75:GLU:HG2	1.97	0.46
2:y:30:LYS:HE3	2:y:36:VAL:HG12	1.96	0.46
1:A:157:GLU:HG3	1:A:160:LYS:HZ3	1.81	0.46
2:X:129:ILE:O	2:X:132:ARG:HG2	2.15	0.46
2:a:170:LYS:NZ	2:f:63:GLN:HG2	2.31	0.46
2:h:63:GLN:HG2	2:i:170:LYS:NZ	2.31	0.46
2:r:128:GLU:O	2:r:131:LYS:HB3	2.15	0.46
2:y:73:ILE:HD11	2:y:134:ILE:HG22	1.97	0.46
2:z:178:SER:HB3	2:z:181:VAL:HG23	1.98	0.46
1:G:54:VAL:HG22	1:G:56:CYS:H	1.80	0.46
2:j:200:THR:HA	2:j:203:LYS:HE3	1.98	0.46
2:k:202:LEU:HD11	2:k:214:MET:HG2	1.98	0.46
2:u:198:CYS:HA	2:u:201:ILE:HB	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:r:131:LYS:O	2:r:134:ILE:HG22	2.16	0.46
2:r:161:PHE:HE1	2:r:215:MET:HG3	1.80	0.46
2:s:91:ILE:HG13	2:s:97:ARG:HD2	1.97	0.46
2:u:5:ASN:HB2	2:v:6:LEU:HD23	1.98	0.46
1:B:242:LEU:HB3	1:B:250:VAL:O	2.16	0.45
1:G:6:ASP:O	1:G:9:GLN:HG3	2.16	0.45
2:Y:9:GLN:HE22	2:Y:11:VAL:HB	1.81	0.45
2:Y:129:ILE:O	2:Y:132:ARG:HG2	2.16	0.45
2:a:110:THR:HG22	2:a:113:GLU:HG3	1.98	0.45
2:f:82:ARG:HG2	2:f:83:LEU:N	2.31	0.45
2:k:72:THR:HA	2:k:75:GLU:HG2	1.98	0.45
1:L:32:VAL:O	1:L:35:GLU:HG2	2.16	0.45
2:Z:167:ARG:HA	2:Z:170:LYS:HG2	1.97	0.45
2:u:125:PRO:HB2	2:u:128:GLU:HB2	1.98	0.45
1:A:63:LEU:HD21	1:A:74:LEU:HD21	1.98	0.45
1:C:84:ILE:HG13	1:C:180:VAL:HG23	1.99	0.45
1:E:211:LYS:O	1:E:214:GLN:HG3	2.16	0.45
1:F:241:LEU:HA	1:F:251:ILE:HG22	1.97	0.45
1:H:242:LEU:HD11	1:H:252:GLN:HB3	1.97	0.45
2:V:202:LEU:HD13	2:V:205:LEU:HD12	1.98	0.45
2:c:37:ILE:HB	2:c:38:PRO:HD3	1.99	0.45
2:j:1:PRO:H3	2:j:15:ILE:HD13	1.81	0.45
2:l:34:PRO:HA	2:l:37:ILE:HD13	1.98	0.45
2:r:202:LEU:HD13	2:r:202:LEU:HA	1.80	0.45
1:F:161:ILE:O	1:F:165:VAL:HG23	2.16	0.45
1:G:224:ARG:HD3	1:G:270:ASP:HB2	1.97	0.45
2:c:68:MET:HA	2:c:71:GLU:HG2	1.98	0.45
2:f:138:LEU:HA	2:f:141:ILE:HG22	1.98	0.45
2:n:68:MET:HE1	2:n:144:MET:HE2	1.99	0.45
2:o:72:THR:O	2:o:75:GLU:HG3	2.16	0.45
2:s:150:ILE:HG12	2:s:185:MET:HE2	1.96	0.45
2:v:22:ALA:HA	2:v:25:LYS:HG2	1.99	0.45
1:A:72:VAL:HG23	1:A:89:ILE:HB	1.99	0.45
1:C:72:VAL:HB	1:C:89:ILE:HG23	1.98	0.45
1:F:213:LEU:HD11	1:G:220:ILE:HD13	1.98	0.45
2:X:49:PRO:HD2	2:X:114:GLN:HG2	1.98	0.45
2:Y:212:GLU:HA	2:Y:215:MET:HE2	1.98	0.45
2:n:37:ILE:HB	2:n:38:PRO:HD3	1.98	0.45
2:n:141:ILE:HA	2:n:144:MET:HG2	1.98	0.45
2:q:99:PRO:HB3	2:q:117:TRP:CH2	2.52	0.45
2:v:79:GLU:HA	2:v:82:ARG:HG2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:GLN:HE21	1:D:137:GLN:HB2	1.59	0.45
2:U:72:THR:HA	2:U:75:GLU:HG2	1.99	0.45
2:d:37:ILE:HD12	2:d:138:LEU:HB3	1.98	0.45
2:h:22:ALA:HA	2:h:25:LYS:HG2	1.97	0.45
2:q:125:PRO:HB2	2:q:128:GLU:HG3	1.97	0.45
2:s:2:ILE:HG13	2:s:118:MET:HE3	1.98	0.45
2:Y:144:MET:HE2	2:Y:145:TYR:CE1	2.51	0.45
2:j:202:LEU:HD13	2:j:202:LEU:HA	1.77	0.45
2:z:104:ILE:HD11	2:z:129:ILE:HB	1.97	0.45
1:C:223:PHE:CD1	1:C:267:ILE:HD11	2.52	0.45
1:J:6:ASP:O	1:J:9:GLN:HG3	2.17	0.45
2:z:84:HIS:HB3	2:z:100:ARG:HH22	1.82	0.45
1:B:42:LYS:HB3	1:B:164:GLN:HE22	1.82	0.45
1:F:242:LEU:HB3	1:F:250:VAL:O	2.17	0.45
1:G:177:GLN:HA	1:G:180:VAL:HG12	1.99	0.45
2:X:22:ALA:HA	2:X:25:LYS:HG2	1.99	0.45
2:Y:72:THR:HA	2:Y:75:GLU:HG2	1.99	0.45
2:i:30:LYS:HZ2	2:i:33:SER:HB3	1.82	0.45
2:j:12:HIS:CD2	2:j:111:LEU:HD21	2.51	0.45
2:n:185:MET:HB2	2:n:189:LEU:HD23	1.98	0.45
1:B:5:ILE:HG22	1:B:9:GLN:HE22	1.82	0.45
1:B:21:ALA:HA	1:B:188:LYS:HG2	1.98	0.45
1:B:200:ILE:HA	1:B:203:ILE:HG22	1.97	0.45
1:G:106:GLY:HA2	1:H:181:PHE:HD1	1.82	0.45
1:I:32:VAL:O	1:I:35:GLU:HG3	2.17	0.45
2:g:22:ALA:HA	2:g:25:LYS:HG2	1.99	0.45
2:g:110:THR:HG22	2:g:113:GLU:HG3	1.99	0.45
2:i:25:LYS:HA	2:i:28:GLU:HG2	1.99	0.45
2:o:22:ALA:HA	2:o:25:LYS:HG2	1.99	0.45
2:w:144:MET:HE2	2:x:215:MET:HE2	1.98	0.45
1:E:62:GLN:HE22	1:E:114:HIS:HB2	1.82	0.44
2:V:185:MET:O	2:V:189:LEU:HB2	2.17	0.44
2:a:72:THR:HA	2:a:75:GLU:HG2	1.99	0.44
2:m:79:GLU:HA	2:m:82:ARG:HE	1.82	0.44
2:x:202:LEU:HD22	2:x:214:MET:HB3	2.00	0.44
2:z:72:THR:O	2:z:75:GLU:HG2	2.17	0.44
1:A:157:GLU:HA	1:A:160:LYS:HG2	1.99	0.44
1:C:228:ARG:HG2	1:C:235:TRP:HA	1.99	0.44
1:D:244:LYS:NZ	1:D:262:ARG:HB2	2.31	0.44
1:E:181:PHE:CD1	1:F:106:GLY:HA2	2.52	0.44
2:d:216:THR:HA	2:d:219:GLN:HG3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:p:68:MET:HG2	2:q:211:LEU:HD21	1.98	0.44
2:q:24:VAL:HA	2:q:27:VAL:HG22	1.98	0.44
2:z:76:GLU:O	2:z:79:GLU:HG2	2.17	0.44
1:B:213:LEU:HD11	1:C:220:ILE:HD13	1.97	0.44
1:C:220:ILE:HA	1:C:223:PHE:CD2	2.52	0.44
1:G:147:SER:O	1:G:151:ILE:HG12	2.17	0.44
1:G:198:GLU:HA	1:G:201:VAL:HG12	1.98	0.44
2:W:110:THR:HG22	2:W:113:GLU:HG2	1.99	0.44
2:X:181:VAL:HG12	2:X:185:MET:HE3	1.99	0.44
2:i:185:MET:HG2	2:i:189:LEU:HD13	1.99	0.44
2:n:49:PRO:HG3	2:n:127:GLY:HA2	2.00	0.44
2:v:117:TRP:HB3	2:v:124:ILE:HB	1.99	0.44
2:y:138:LEU:O	2:y:141:ILE:HG22	2.17	0.44
1:G:220:ILE:HA	1:G:223:PHE:HD2	1.83	0.44
1:H:226:TYR:HD2	1:H:266:LYS:HE3	1.82	0.44
2:V:22:ALA:HA	2:V:25:LYS:HE3	2.00	0.44
2:X:198:CYS:O	2:X:202:LEU:HG	2.18	0.44
2:g:18:ARG:HH12	4:g:301:IHP:P2	2.41	0.44
2:g:196:PRO:HA	2:g:199:LYS:HG2	2.00	0.44
2:i:19:THR:HG23	2:i:43:LEU:HD22	1.99	0.44
2:x:211:LEU:HD23	2:x:211:LEU:H	1.82	0.44
2:z:86:VAL:HG13	2:z:100:ARG:HD2	1.99	0.44
1:A:14:LYS:HE3	1:A:15:TYR:CZ	2.52	0.44
1:A:181:PHE:CD1	1:B:106:GLY:HA2	2.53	0.44
1:H:63:LEU:HD11	1:H:74:LEU:HG	2.00	0.44
1:H:103:LYS:O	1:H:107:ARG:HG2	2.17	0.44
2:e:129:ILE:O	2:e:132:ARG:HG2	2.16	0.44
2:f:50:GLN:HA	2:f:53:ASN:HD21	1.83	0.44
2:m:125:PRO:HB2	2:m:128:GLU:HB3	1.99	0.44
2:t:161:PHE:HE2	2:t:215:MET:HE2	1.83	0.44
2:u:129:ILE:HG12	2:u:132:ARG:HH12	1.82	0.44
2:U:72:THR:HG21	2:U:140:LYS:HD2	2.00	0.44
2:V:196:PRO:HA	2:V:199:LYS:HE3	1.99	0.44
2:X:99:PRO:HG3	2:X:117:TRP:CE2	2.53	0.44
2:d:6:LEU:H	2:d:6:LEU:HD12	1.83	0.44
2:n:57:ASN:HB3	2:o:173:ARG:HH22	1.82	0.44
2:s:72:THR:HA	2:s:75:GLU:HG2	2.00	0.44
2:y:205:LEU:HD22	2:y:209:ALA:HB2	2.00	0.44
2:Z:138:LEU:HA	2:Z:141:ILE:HG22	1.99	0.44
2:l:118:MET:HE3	2:l:118:MET:HB3	1.91	0.44
2:r:215:MET:HE3	2:r:216:THR:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:z:182:LYS:HA	2:z:185:MET:HG2	2.00	0.44
2:V:182:LYS:HA	2:V:185:MET:HG2	2.00	0.44
2:f:215:MET:HE2	2:f:215:MET:HB3	1.84	0.44
1:E:19:TRP:HB3	1:E:37:VAL:HG21	2.00	0.44
2:h:167:ARG:HA	2:h:170:LYS:HG2	2.00	0.44
2:p:72:THR:HA	2:p:75:GLU:HG2	1.99	0.44
2:r:72:THR:HA	2:r:75:GLU:HG2	2.00	0.44
2:s:86:VAL:HA	2:s:100:ARG:HH12	1.82	0.44
1:D:211:LYS:HD3	1:D:211:LYS:HA	1.79	0.43
2:d:211:LEU:HD23	2:d:211:LEU:H	1.83	0.43
2:e:49:PRO:HG3	2:e:127:GLY:HA2	2.00	0.43
2:j:56:LEU:HD21	2:j:69:LEU:HD22	1.99	0.43
2:j:63:GLN:HA	2:j:66:MET:HE2	2.00	0.43
2:q:57:ASN:HB3	2:r:38:PRO:HG2	2.00	0.43
2:y:178:SER:HB3	2:y:181:VAL:HG12	1.99	0.43
2:z:153:ILE:HD12	2:z:168:PHE:HD1	1.82	0.43
2:b:79:GLU:O	2:b:82:ARG:HG3	2.18	0.43
2:U:23:TRP:HD1	2:U:43:LEU:HD12	1.83	0.43
2:Z:129:ILE:HG12	2:Z:132:ARG:HH22	1.83	0.43
2:j:68:MET:HA	2:j:68:MET:HE2	2.00	0.43
2:q:77:ALA:HB1	2:q:101:GLY:HA3	2.00	0.43
1:C:103:LYS:HD2	1:C:107:ARG:HH12	1.83	0.43
1:D:78:HIS:CD2	1:D:81:SER:H	2.36	0.43
2:e:104:ILE:HG13	2:e:126:VAL:HG23	2.00	0.43
2:h:75:GLU:O	2:h:79:GLU:HG2	2.19	0.43
2:o:13:GLN:HG2	2:o:14:ALA:H	1.82	0.43
2:w:166:ASP:O	2:w:170:LYS:HG2	2.19	0.43
2:y:194:ALA:HB3	2:y:199:LYS:HG3	2.00	0.43
1:A:9:GLN:HG3	1:A:36:ILE:HD12	2.00	0.43
2:U:1:PRO:HD3	2:U:15:ILE:HD13	2.00	0.43
2:d:5:ASN:HD22	2:d:8:GLY:HA3	1.83	0.43
2:e:187:GLU:HG3	2:e:188:THR:HG23	2.00	0.43
2:g:72:THR:HA	2:g:75:GLU:HG2	2.01	0.43
1:C:132:TRP:HH2	1:D:182:ILE:HD11	1.83	0.43
1:G:78:HIS:CE1	1:G:80:ALA:HB3	2.53	0.43
2:W:2:ILE:HG22	2:W:10:MET:HE3	1.99	0.43
2:Z:34:PRO:HA	2:Z:37:ILE:HD13	2.00	0.43
2:h:95:GLN:HG2	2:h:120:HIS:CE1	2.53	0.43
2:h:153:ILE:HD13	2:h:167:ARG:HG3	2.00	0.43
2:j:143:ARG:HH11	2:j:175:GLU:HA	1.84	0.43
2:q:76:GLU:O	2:q:79:GLU:HG2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:s:17:PRO:HG2	2:t:18:ARG:HE	1.82	0.43
2:x:76:GLU:O	2:x:79:GLU:HG3	2.19	0.43
1:F:78:HIS:CE1	1:F:80:ALA:HB3	2.53	0.43
1:K:6:ASP:O	1:K:9:GLN:HG3	2.19	0.43
2:g:209:ALA:HB3	2:g:214:MET:HE3	1.99	0.43
2:j:68:MET:SD	2:k:212:GLU:HG2	2.58	0.43
2:n:200:THR:HA	2:n:203:LYS:HZ3	1.84	0.43
2:z:137:GLY:O	2:z:140:LYS:HG3	2.18	0.43
1:A:178:MET:HE3	1:B:132:TRP:CH2	2.54	0.43
1:B:155:ASN:O	1:B:159:LYS:HG2	2.19	0.43
1:L:23:ALA:HA	1:L:28:LEU:HB2	2.01	0.43
2:d:37:ILE:HB	2:d:38:PRO:HD3	2.00	0.43
2:e:22:ALA:HA	2:e:25:LYS:HG2	2.01	0.43
2:s:79:GLU:HG3	2:s:83:LEU:HD23	2.00	0.43
2:x:27:VAL:HG11	2:x:59:VAL:HG21	2.01	0.43
2:z:72:THR:HG21	2:z:140:LYS:HE3	2.00	0.43
1:F:200:ILE:HA	1:F:203:ILE:HG22	2.01	0.43
1:H:67:HIS:CE1	1:H:72:VAL:HG22	2.53	0.43
2:a:116:GLY:HA2	2:a:119:THR:HG22	1.99	0.43
2:b:127:GLY:O	2:b:130:TYR:HB3	2.19	0.43
2:c:153:ILE:HG21	2:c:168:PHE:HD1	1.84	0.43
2:m:5:ASN:HD22	2:m:8:GLY:HA3	1.84	0.43
2:p:205:LEU:HD21	2:p:213:GLU:HB3	1.99	0.43
2:q:153:ILE:HD11	2:q:171:THR:HG21	2.01	0.43
2:s:182:LYS:O	2:s:185:MET:HG2	2.19	0.43
2:t:167:ARG:HA	2:t:170:LYS:HG2	2.01	0.43
2:u:25:LYS:O	2:u:29:GLU:HB3	2.18	0.43
2:u:67:GLN:HG2	2:v:169:TYR:CZ	2.54	0.43
2:u:137:GLY:O	2:u:140:LYS:HG2	2.18	0.43
2:v:79:GLU:HG3	2:v:83:LEU:HD23	2.00	0.43
2:v:184:TRP:O	2:v:187:GLU:HG2	2.19	0.43
1:B:250:VAL:HG13	1:B:259:VAL:HG22	2.01	0.43
1:F:7:LYS:HA	1:F:10:GLU:HG2	2.00	0.43
2:U:196:PRO:HA	2:U:199:LYS:HG2	2.00	0.43
2:q:96:MET:HB3	2:q:117:TRP:HE1	1.83	0.43
2:r:129:ILE:O	2:r:132:ARG:HG2	2.19	0.43
2:y:19:THR:HG23	2:y:43:LEU:HD22	2.01	0.43
2:y:184:TRP:O	2:y:187:GLU:HG3	2.18	0.43
2:W:18:ARG:HH22	2:X:18:ARG:CZ	2.32	0.42
2:d:198:CYS:O	2:d:202:LEU:HG	2.19	0.42
2:e:22:ALA:HA	2:e:25:LYS:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:211:LEU:H	2:e:211:LEU:HD23	1.84	0.42
2:n:50:GLN:HA	2:n:53:ASN:ND2	2.34	0.42
2:n:166:ASP:O	2:n:170:LYS:HG2	2.19	0.42
2:s:191:VAL:HG12	2:s:202:LEU:HD13	2.00	0.42
2:v:168:PHE:CE2	2:v:172:LEU:HD11	2.53	0.42
2:x:198:CYS:O	2:x:202:LEU:HG	2.19	0.42
2:z:137:GLY:HA2	2:z:140:LYS:NZ	2.34	0.42
1:F:250:VAL:HG13	1:F:259:VAL:HG22	2.01	0.42
1:G:19:TRP:HA	1:G:22:MET:HE2	2.00	0.42
1:H:77:VAL:HG13	1:H:84:ILE:HG22	2.01	0.42
1:K:7:LYS:HA	1:K:10:GLU:HG2	2.00	0.42
2:d:72:THR:HA	2:d:75:GLU:HG2	2.00	0.42
2:d:154:ARG:HH12	2:d:193:ASN:HB3	1.84	0.42
2:f:12:HIS:NE2	2:f:111:LEU:HD21	2.34	0.42
2:j:138:LEU:HA	2:j:141:ILE:HG12	2.00	0.42
2:p:194:ALA:H	2:p:199:LYS:HD3	1.84	0.42
2:r:185:MET:HE3	2:r:185:MET:HB3	1.85	0.42
1:A:161:ILE:HG13	1:A:179:ALA:HB1	2.01	0.42
2:a:118:MET:HE2	2:a:118:MET:HB2	1.92	0.42
2:h:134:ILE:HD12	2:h:134:ILE:HA	1.93	0.42
2:k:67:GLN:HG3	2:l:169:TYR:CE2	2.53	0.42
2:o:118:MET:HE3	2:o:118:MET:HB3	1.91	0.42
2:z:215:MET:O	2:z:219:GLN:HG3	2.19	0.42
1:A:213:LEU:O	1:A:217:ILE:HG12	2.20	0.42
2:U:22:ALA:HA	2:U:25:LYS:HG2	2.01	0.42
2:b:143:ARG:NH1	2:b:175:GLU:HA	2.34	0.42
2:d:96:MET:HB3	2:d:117:TRP:NE1	2.34	0.42
2:t:168:PHE:O	2:t:172:LEU:HG	2.19	0.42
2:w:72:THR:HA	2:w:75:GLU:HG2	2.01	0.42
1:B:244:LYS:HD3	1:B:249:VAL:HG22	2.00	0.42
2:Y:27:VAL:HG11	2:Y:59:VAL:HG23	2.00	0.42
2:e:196:PRO:HA	2:e:199:LYS:HG2	2.02	0.42
2:k:211:LEU:O	2:k:215:MET:HG2	2.20	0.42
2:v:4:GLN:HA	2:v:10:MET:HG3	2.01	0.42
2:X:166:ASP:O	2:X:170:LYS:HD3	2.19	0.42
2:Y:172:LEU:HD11	2:Y:182:LYS:HG3	2.01	0.42
2:c:22:ALA:HA	2:c:25:LYS:HG2	2.02	0.42
2:c:110:THR:HG22	2:c:113:GLU:HG3	2.02	0.42
2:i:30:LYS:HE2	2:i:30:LYS:O	2.18	0.42
2:q:104:ILE:HG13	2:q:126:VAL:HB	2.02	0.42
2:q:182:LYS:HA	2:q:185:MET:HG2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:117:TRP:HA	2:t:120:HIS:CD2	2.54	0.42
2:z:143:ARG:HH22	2:z:175:GLU:CD	2.27	0.42
1:E:9:GLN:HG3	1:E:36:ILE:HD12	2.02	0.42
1:F:219:LYS:HB3	1:F:219:LYS:HE3	1.83	0.42
2:a:59:VAL:HG21	2:a:66:MET:HE3	2.01	0.42
2:b:72:THR:HA	2:b:75:GLU:HG2	2.00	0.42
2:b:76:GLU:O	2:b:79:GLU:HG2	2.19	0.42
2:i:137:GLY:O	2:i:140:LYS:HG2	2.19	0.42
2:k:37:ILE:HB	2:k:38:PRO:HD3	2.01	0.42
2:k:151:LEU:HA	2:k:189:LEU:HD21	2.02	0.42
2:q:110:THR:HG22	2:q:113:GLU:HG3	2.01	0.42
2:y:212:GLU:HA	2:y:215:MET:HG2	2.02	0.42
1:B:69:GLU:HG2	2:U:157:PRO:HD2	2.01	0.42
1:C:250:VAL:HG22	1:C:259:VAL:HG22	2.02	0.42
1:E:148:GLN:HA	1:E:151:ILE:HG12	2.02	0.42
1:G:228:ARG:HG2	1:G:235:TRP:HA	2.01	0.42
2:Y:72:THR:HG21	2:Y:140:LYS:HD2	2.02	0.42
2:j:170:LYS:HE3	2:j:170:LYS:HB3	1.84	0.42
2:q:96:MET:HB3	2:q:117:TRP:NE1	2.34	0.42
2:u:138:LEU:HA	2:u:141:ILE:HB	2.01	0.42
1:A:59:GLY:HA3	1:A:111:LYS:HE2	2.02	0.42
1:G:114:HIS:HB3	1:G:142:PRO:HG3	2.01	0.42
2:Z:150:ILE:HG13	2:Z:151:LEU:HD22	2.02	0.42
2:f:37:ILE:HD12	2:f:138:LEU:HB3	2.02	0.42
2:i:128:GLU:O	2:i:131:LYS:HB3	2.19	0.42
2:n:130:TYR:O	2:n:133:TRP:HB2	2.20	0.42
2:r:126:VAL:O	2:r:129:ILE:HB	2.20	0.42
2:z:110:THR:HG23	2:z:112:GLN:HG2	2.01	0.42
1:J:8:ALA:O	1:J:11:GLU:HG3	2.20	0.42
2:U:55:MET:O	2:U:58:THR:HG22	2.20	0.42
2:d:211:LEU:HA	2:d:214:MET:HB3	2.01	0.42
2:e:96:MET:HG3	2:e:97:ARG:HD3	2.01	0.42
2:f:22:ALA:HA	2:f:25:LYS:HG2	2.01	0.42
2:h:100:ARG:HD3	2:h:100:ARG:HA	1.79	0.42
2:s:150:ILE:HD12	2:s:153:ILE:HD12	2.02	0.42
2:v:143:ARG:NH2	2:v:176:GLN:H	2.17	0.42
2:w:96:MET:HG3	2:w:117:TRP:NE1	2.34	0.42
2:y:25:LYS:HA	2:y:28:GLU:HG2	2.01	0.42
1:C:88:VAL:HB	1:C:173:LYS:HG3	2.02	0.41
2:X:212:GLU:O	2:X:215:MET:HG3	2.19	0.41
2:Y:129:ILE:HA	2:Y:132:ARG:HE	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:20:LEU:HD12	2:a:58:THR:HG21	2.02	0.41
2:c:166:ASP:O	2:c:170:LYS:HG2	2.20	0.41
2:d:129:ILE:HG12	2:d:132:ARG:NH2	2.35	0.41
2:e:202:LEU:HD21	2:e:214:MET:HA	2.02	0.41
2:h:110:THR:HG22	2:h:113:GLU:HG3	2.02	0.41
2:k:198:CYS:HA	2:k:201:ILE:HB	2.02	0.41
2:q:55:MET:HE3	2:q:55:MET:HB3	1.82	0.41
2:t:125:PRO:HB2	2:t:128:GLU:HG2	2.02	0.41
2:w:75:GLU:O	2:w:79:GLU:HG2	2.20	0.41
2:y:50:GLN:HE22	2:y:114:GLN:HG3	1.85	0.41
2:j:76:GLU:HB3	2:j:133:TRP:CE2	2.55	0.41
2:n:33:SER:O	2:n:36:VAL:HG22	2.20	0.41
2:w:63:GLN:HA	2:w:66:MET:HG2	2.01	0.41
2:w:99:PRO:HG2	2:w:126:VAL:HG21	2.02	0.41
2:y:1:PRO:HB3	2:y:47:ALA:HA	2.03	0.41
1:C:74:LEU:HD23	1:C:89:ILE:HG21	2.02	0.41
2:V:6:LEU:H	2:V:6:LEU:HD23	1.85	0.41
2:W:37:ILE:HB	2:W:38:PRO:HD3	2.02	0.41
2:b:202:LEU:HB2	2:b:214:MET:SD	2.61	0.41
2:e:96:MET:HB3	2:e:117:TRP:NE1	2.35	0.41
2:f:215:MET:O	2:f:219:GLN:HG3	2.21	0.41
2:g:178:SER:O	2:g:182:LYS:HG2	2.20	0.41
2:h:18:ARG:HH12	2:l:18:ARG:HH22	1.68	0.41
2:j:70:LYS:O	2:j:73:ILE:HG22	2.21	0.41
2:l:150:ILE:HG12	2:l:185:MET:SD	2.60	0.41
2:s:202:LEU:HD23	2:s:205:LEU:HD12	2.02	0.41
1:F:15:TYR:CE1	1:F:186:LYS:HE3	2.55	0.41
2:X:79:GLU:O	2:X:82:ARG:HG2	2.20	0.41
2:Z:52:LEU:HD13	2:Z:52:LEU:HA	1.92	0.41
2:g:198:CYS:O	2:g:202:LEU:HG	2.20	0.41
2:i:183:ASN:HA	2:i:186:THR:HG22	2.02	0.41
1:B:8:ALA:O	1:B:11:GLU:HG3	2.20	0.41
1:C:155:ASN:O	1:C:158:LEU:HG	2.20	0.41
1:E:252:GLN:HG3	1:E:257:ILE:HG13	2.01	0.41
2:V:154:ARG:HA	2:V:193:ASN:HB3	2.01	0.41
2:h:107:THR:HG23	2:h:108:THR:HG23	2.01	0.41
2:o:110:THR:HG22	2:o:113:GLU:HG3	2.03	0.41
2:u:84:HIS:HD2	2:u:85:PRO:HD2	1.85	0.41
2:v:125:PRO:HB2	2:v:128:GLU:HB2	2.02	0.41
2:v:186:THR:O	2:v:190:LEU:HD22	2.21	0.41
2:y:26:VAL:HA	2:y:29:GLU:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:GLN:HE21	1:D:148:GLN:HB2	1.68	0.41
2:V:22:ALA:HA	2:V:25:LYS:HG2	2.01	0.41
2:Z:72:THR:O	2:Z:75:GLU:HG2	2.21	0.41
2:Z:151:LEU:HD21	2:z:184:TRP:HH2	1.86	0.41
2:l:68:MET:O	2:l:71:GLU:HG3	2.19	0.41
2:m:215:MET:HE2	2:m:215:MET:HB2	1.94	0.41
2:o:68:MET:HG3	2:p:211:LEU:HD11	2.02	0.41
2:p:100:ARG:H	2:p:103:ASP:HB2	1.84	0.41
2:r:215:MET:HE2	2:r:215:MET:HB3	1.87	0.41
2:z:175:GLU:HG3	2:z:177:ALA:H	1.85	0.41
1:C:108:TRP:HZ3	1:C:204:ILE:HG13	1.86	0.41
1:D:81:SER:HB2	1:D:199:ARG:HG3	2.02	0.41
1:E:212:GLU:HA	1:E:215:LYS:HG2	2.02	0.41
1:G:155:ASN:O	1:G:158:LEU:HG	2.21	0.41
1:G:161:ILE:HD12	1:G:161:ILE:HA	1.96	0.41
1:H:240:LYS:HB3	1:H:252:GLN:HE21	1.85	0.41
2:Y:144:MET:HE3	2:Z:162:ARG:NH1	2.35	0.41
2:d:75:GLU:O	2:d:79:GLU:HG2	2.20	0.41
2:d:96:MET:HG3	2:d:97:ARG:HD3	2.02	0.41
2:h:86:VAL:HA	2:h:100:ARG:HH22	1.85	0.41
2:i:72:THR:HA	2:i:75:GLU:HG2	2.03	0.41
2:n:72:THR:O	2:n:75:GLU:HG2	2.21	0.41
2:p:129:ILE:HG12	2:p:132:ARG:NH2	2.36	0.41
1:C:32:VAL:HA	1:C:35:GLU:HG2	2.03	0.41
1:E:17:SER:HB2	1:E:22:MET:HE3	2.02	0.41
1:F:153:SER:O	1:F:156:LYS:HG2	2.20	0.41
2:h:131:LYS:HE3	2:h:131:LYS:HB3	1.83	0.41
2:j:185:MET:HE2	2:j:185:MET:HB2	1.81	0.41
2:n:199:LYS:HG2	2:n:203:LYS:NZ	2.35	0.41
2:p:22:ALA:HA	2:p:25:LYS:HG2	2.02	0.41
2:r:211:LEU:H	2:r:211:LEU:HD23	1.85	0.41
2:s:141:ILE:HA	2:s:144:MET:HG2	2.02	0.41
2:t:33:SER:O	2:t:36:VAL:HG22	2.19	0.41
2:u:35:GLU:C	2:u:38:PRO:HD2	2.46	0.41
1:A:209:GLN:O	1:A:212:GLU:HG3	2.21	0.41
1:C:180:VAL:HG22	1:C:184:ASN:ND2	2.36	0.41
1:D:158:LEU:HA	1:D:161:ILE:HG12	2.02	0.41
1:E:59:GLY:HA3	1:E:111:LYS:HE2	2.03	0.41
1:E:71:LYS:HE2	1:E:71:LYS:HB3	1.91	0.41
1:G:10:GLU:O	1:G:13:GLU:HG3	2.21	0.41
1:H:240:LYS:HB3	1:H:252:GLN:NE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:14:LYS:HE3	1:L:15:TYR:CZ	2.56	0.41
2:U:35:GLU:O	2:U:38:PRO:HD2	2.21	0.41
2:V:129:ILE:HA	2:V:132:ARG:HE	1.86	0.41
2:W:4:GLN:HB3	2:W:10:MET:SD	2.61	0.41
2:W:5:ASN:HB3	2:W:8:GLY:HA3	2.02	0.41
2:X:65:ALA:HB1	2:X:141:ILE:HD13	2.03	0.41
2:c:18:ARG:HH21	2:d:18:ARG:NH1	2.19	0.41
2:d:145:TYR:HE1	2:e:162:ARG:HH22	1.68	0.41
2:e:99:PRO:HG3	2:e:117:TRP:CD2	2.56	0.41
2:f:56:LEU:HD21	2:f:69:LEU:HD13	2.02	0.41
2:f:141:ILE:HD12	2:f:141:ILE:HA	1.93	0.41
2:f:190:LEU:HD12	2:f:191:VAL:N	2.35	0.41
2:h:52:LEU:O	2:h:55:MET:HG3	2.20	0.41
2:h:125:PRO:O	2:h:129:ILE:HG12	2.21	0.41
2:l:22:ALA:HA	2:l:25:LYS:HE2	2.02	0.41
2:o:34:PRO:HA	2:o:37:ILE:HD13	2.02	0.41
2:o:138:LEU:HA	2:o:141:ILE:HG22	2.03	0.41
2:o:184:TRP:O	2:o:187:GLU:HG2	2.21	0.41
2:p:215:MET:O	2:p:219:GLN:HG3	2.21	0.41
2:q:72:THR:HA	2:q:75:GLU:HG2	2.03	0.41
2:q:79:GLU:O	2:q:82:ARG:HG3	2.20	0.41
2:t:19:THR:HB	2:t:43:LEU:HD11	2.03	0.41
2:t:24:VAL:HA	2:t:27:VAL:HG22	2.03	0.41
2:u:125:PRO:O	2:u:128:GLU:HB2	2.21	0.41
2:v:124:ILE:HG22	2:v:126:VAL:HG13	2.03	0.41
2:w:96:MET:HG2	2:w:120:HIS:CE1	2.52	0.41
2:x:168:PHE:O	2:x:172:LEU:HG	2.20	0.41
2:y:100:ARG:H	2:y:103:ASP:HB2	1.85	0.41
1:A:155:ASN:O	1:A:159:LYS:HG2	2.20	0.41
1:C:249:VAL:HG22	1:C:251:ILE:HG23	2.02	0.41
1:G:223:PHE:HA	1:G:269:ARG:HD2	2.03	0.41
2:d:68:MET:HE1	2:e:215:MET:SD	2.61	0.41
2:h:129:ILE:O	2:h:132:ARG:HG2	2.20	0.41
2:q:27:VAL:O	2:q:31:ALA:HB2	2.21	0.41
2:q:67:GLN:HG2	2:r:169:TYR:OH	2.21	0.41
1:A:216:GLN:O	1:A:219:LYS:HG3	2.20	0.40
1:B:7:LYS:HA	1:B:10:GLU:HG2	2.03	0.40
1:F:208:ILE:HA	1:F:211:LYS:HZ2	1.86	0.40
1:F:243:TRP:CD2	1:G:242:LEU:HD13	2.56	0.40
1:K:8:ALA:O	1:K:11:GLU:HG3	2.21	0.40
2:d:79:GLU:HA	2:d:82:ARG:HD3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:68:MET:HE3	2:i:211:LEU:HG	2.02	0.40
2:n:1:PRO:HB2	2:n:2:ILE:H	1.73	0.40
2:o:10:MET:HE3	2:o:10:MET:HB3	1.93	0.40
2:q:212:GLU:O	2:q:215:MET:HG2	2.21	0.40
2:s:153:ILE:HG23	2:s:167:ARG:NH1	2.36	0.40
2:x:66:MET:O	2:x:69:LEU:HG	2.21	0.40
1:B:219:LYS:HE3	1:B:219:LYS:HB3	1.88	0.40
1:D:244:LYS:HD2	1:D:248:ALA:O	2.21	0.40
1:G:42:LYS:HD3	1:G:164:GLN:HB3	2.02	0.40
1:H:63:LEU:HD21	1:H:74:LEU:HD21	2.03	0.40
2:W:183:ASN:HA	2:W:186:THR:HG22	2.03	0.40
2:W:191:VAL:HG23	2:W:202:LEU:HD12	2.03	0.40
2:Y:191:VAL:O	2:Y:199:LYS:HG2	2.21	0.40
2:c:35:GLU:O	2:c:38:PRO:HD2	2.22	0.40
2:f:211:LEU:HA	2:f:214:MET:HE2	2.02	0.40
2:t:212:GLU:O	2:t:215:MET:HG3	2.21	0.40
1:H:146:GLN:HG3	1:H:147:SER:H	1.86	0.40
2:q:91:ILE:HD12	2:q:97:ARG:HB3	2.03	0.40
2:s:190:LEU:HD23	2:s:191:VAL:H	1.86	0.40
2:z:30:LYS:NZ	2:z:33:SER:HB3	2.36	0.40
1:B:217:ILE:C	1:B:219:LYS:H	2.30	0.40
1:C:177:GLN:O	1:C:180:VAL:HG12	2.22	0.40
1:D:225:VAL:HG22	1:D:267:ILE:HA	2.04	0.40
1:H:153:SER:HA	1:H:156:LYS:HG2	2.04	0.40
2:V:198:CYS:HA	2:V:201:ILE:HB	2.03	0.40
2:X:182:LYS:HA	2:X:185:MET:HG2	2.03	0.40
2:Y:79:GLU:HA	2:Y:82:ARG:HG2	2.02	0.40
2:e:27:VAL:O	2:e:31:ALA:HA	2.21	0.40
2:f:33:SER:OG	2:f:34:PRO:HD2	2.22	0.40
2:n:67:GLN:HG2	2:o:169:TYR:CZ	2.57	0.40
2:t:167:ARG:O	2:t:170:LYS:HG2	2.21	0.40
1:A:58:PRO:HA	1:A:78:HIS:NE2	2.37	0.40
2:i:150:ILE:HD13	2:i:171:THR:HB	2.02	0.40
2:j:182:LYS:O	2:j:185:MET:HG3	2.21	0.40
2:z:186:THR:O	2:z:190:LEU:HD22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	249/288 (86%)	243 (98%)	6 (2%)	0	100	100
1	B	237/288 (82%)	230 (97%)	7 (3%)	0	100	100
1	C	259/288 (90%)	254 (98%)	5 (2%)	0	100	100
1	D	254/288 (88%)	250 (98%)	4 (2%)	0	100	100
1	E	249/288 (86%)	242 (97%)	7 (3%)	0	100	100
1	F	237/288 (82%)	229 (97%)	8 (3%)	0	100	100
1	G	259/288 (90%)	254 (98%)	5 (2%)	0	100	100
1	H	254/288 (88%)	248 (98%)	6 (2%)	0	100	100
1	I	41/288 (14%)	41 (100%)	0	0	100	100
1	J	42/288 (15%)	41 (98%)	1 (2%)	0	100	100
1	K	42/288 (15%)	41 (98%)	1 (2%)	0	100	100
1	L	42/288 (15%)	40 (95%)	2 (5%)	0	100	100
2	U	218/231 (94%)	216 (99%)	2 (1%)	0	100	100
2	V	218/231 (94%)	215 (99%)	3 (1%)	0	100	100
2	W	218/231 (94%)	217 (100%)	1 (0%)	0	100	100
2	X	218/231 (94%)	209 (96%)	9 (4%)	0	100	100
2	Y	218/231 (94%)	211 (97%)	7 (3%)	0	100	100
2	Z	218/231 (94%)	214 (98%)	4 (2%)	0	100	100
2	a	218/231 (94%)	216 (99%)	2 (1%)	0	100	100
2	b	218/231 (94%)	211 (97%)	7 (3%)	0	100	100
2	c	218/231 (94%)	214 (98%)	4 (2%)	0	100	100
2	d	218/231 (94%)	218 (100%)	0	0	100	100
2	e	218/231 (94%)	214 (98%)	4 (2%)	0	100	100
2	f	218/231 (94%)	213 (98%)	5 (2%)	0	100	100
2	g	218/231 (94%)	211 (97%)	7 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h	218/231 (94%)	215 (99%)	3 (1%)	0	100	100
2	i	218/231 (94%)	209 (96%)	9 (4%)	0	100	100
2	j	218/231 (94%)	215 (99%)	3 (1%)	0	100	100
2	k	218/231 (94%)	208 (95%)	10 (5%)	0	100	100
2	l	218/231 (94%)	214 (98%)	4 (2%)	0	100	100
2	m	218/231 (94%)	214 (98%)	4 (2%)	0	100	100
2	n	218/231 (94%)	210 (96%)	8 (4%)	0	100	100
2	o	218/231 (94%)	212 (97%)	6 (3%)	0	100	100
2	p	218/231 (94%)	215 (99%)	3 (1%)	0	100	100
2	q	218/231 (94%)	213 (98%)	5 (2%)	0	100	100
2	r	218/231 (94%)	215 (99%)	3 (1%)	0	100	100
2	s	218/231 (94%)	211 (97%)	7 (3%)	0	100	100
2	t	218/231 (94%)	215 (99%)	3 (1%)	0	100	100
2	u	218/231 (94%)	212 (97%)	6 (3%)	0	100	100
2	v	218/231 (94%)	209 (96%)	9 (4%)	0	100	100
2	w	218/231 (94%)	209 (96%)	9 (4%)	0	100	100
2	x	218/231 (94%)	212 (97%)	6 (3%)	0	100	100
2	y	218/231 (94%)	213 (98%)	5 (2%)	0	100	100
2	z	218/231 (94%)	213 (98%)	5 (2%)	0	100	100
All	All	9141/10848 (84%)	8926 (98%)	215 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	213/240 (89%)	211 (99%)	2 (1%)	70	76
1	B	204/240 (85%)	198 (97%)	6 (3%)	37	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	221/240 (92%)	220 (100%)	1 (0%)	81	81
1	D	216/240 (90%)	211 (98%)	5 (2%)	44	63
1	E	213/240 (89%)	209 (98%)	4 (2%)	50	66
1	F	203/240 (85%)	200 (98%)	3 (2%)	57	70
1	G	220/240 (92%)	220 (100%)	0	100	100
1	H	216/240 (90%)	213 (99%)	3 (1%)	59	71
1	I	37/240 (15%)	37 (100%)	0	100	100
1	J	38/240 (16%)	37 (97%)	1 (3%)	40	60
1	K	38/240 (16%)	38 (100%)	0	100	100
1	L	37/240 (15%)	37 (100%)	0	100	100
2	U	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	V	187/194 (96%)	182 (97%)	5 (3%)	39	59
2	W	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	X	187/194 (96%)	184 (98%)	3 (2%)	55	69
2	Y	187/194 (96%)	183 (98%)	4 (2%)	47	65
2	Z	187/194 (96%)	183 (98%)	4 (2%)	47	65
2	a	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	b	187/194 (96%)	184 (98%)	3 (2%)	55	69
2	c	187/194 (96%)	183 (98%)	4 (2%)	47	65
2	d	187/194 (96%)	182 (97%)	5 (3%)	39	59
2	e	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	f	187/194 (96%)	182 (97%)	5 (3%)	39	59
2	g	187/194 (96%)	184 (98%)	3 (2%)	55	69
2	h	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	i	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	j	187/194 (96%)	186 (100%)	1 (0%)	81	81
2	k	187/194 (96%)	184 (98%)	3 (2%)	55	69
2	l	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	m	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	n	187/194 (96%)	182 (97%)	5 (3%)	39	59
2	o	187/194 (96%)	184 (98%)	3 (2%)	55	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	p	187/194 (96%)	187 (100%)	0	100	100
2	q	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	r	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	s	187/194 (96%)	187 (100%)	0	100	100
2	t	187/194 (96%)	186 (100%)	1 (0%)	81	81
2	u	187/194 (96%)	182 (97%)	5 (3%)	39	59
2	v	187/194 (96%)	187 (100%)	0	100	100
2	w	187/194 (96%)	187 (100%)	0	100	100
2	x	187/194 (96%)	186 (100%)	1 (0%)	81	81
2	y	187/194 (96%)	185 (99%)	2 (1%)	65	74
2	z	187/194 (96%)	183 (98%)	4 (2%)	47	65
All	All	7840/9088 (86%)	7734 (99%)	106 (1%)	57	71

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	221	GLN
1	B	9	GLN
1	B	75	VAL
1	B	77	VAL
1	B	88	VAL
1	B	89	ILE
1	B	165	VAL
1	C	89	ILE
1	D	75	VAL
1	D	137	GLN
1	D	148	GLN
1	D	249	VAL
1	D	250	VAL
1	E	88	VAL
1	E	115	THR
1	E	165	VAL
1	E	259	VAL
1	F	9	GLN
1	F	75	VAL
1	F	88	VAL
1	H	5	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	152	GLU
1	H	250	VAL
1	J	35	GLU
2	U	30	LYS
2	U	145	TYR
2	V	33	SER
2	V	36	VAL
2	V	126	VAL
2	V	211	LEU
2	V	214	MET
2	W	36	VAL
2	W	210	THR
2	X	35	GLU
2	X	114	GLN
2	X	126	VAL
2	Y	36	VAL
2	Y	53	ASN
2	Y	114	GLN
2	Y	126	VAL
2	Z	6	LEU
2	Z	52	LEU
2	Z	68	MET
2	Z	185	MET
2	a	20	LEU
2	a	193	ASN
2	b	30	LYS
2	b	126	VAL
2	b	142	VAL
2	c	6	LEU
2	c	82	ARG
2	c	185	MET
2	c	211	LEU
2	d	36	VAL
2	d	82	ARG
2	d	126	VAL
2	d	151	LEU
2	d	166	ASP
2	e	126	VAL
2	e	198	CYS
2	f	33	SER
2	f	35	GLU
2	f	82	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	f	96	MET
2	f	145	TYR
2	g	29	GLU
2	g	128	GLU
2	g	144	MET
2	h	36	VAL
2	h	82	ARG
2	i	20	LEU
2	i	30	LYS
2	j	202	LEU
2	k	39	MET
2	k	131	LYS
2	k	144	MET
2	l	6	LEU
2	l	211	LEU
2	m	86	VAL
2	m	126	VAL
2	n	11	VAL
2	n	36	VAL
2	n	126	VAL
2	n	131	LYS
2	n	198	CYS
2	o	6	LEU
2	o	35	GLU
2	o	202	LEU
2	q	36	VAL
2	q	198	CYS
2	r	82	ARG
2	r	202	LEU
2	t	52	LEU
2	u	29	GLU
2	u	126	VAL
2	u	141	ILE
2	u	190	LEU
2	u	199	LYS
2	x	126	VAL
2	y	126	VAL
2	y	182	LYS
2	z	29	GLU
2	z	96	MET
2	z	112	GLN
2	z	140	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	GLN
1	B	148	GLN
1	B	164	GLN
1	C	27	ASN
1	C	78	HIS
1	C	137	GLN
1	C	144	ASN
1	C	146	GLN
1	C	148	GLN
1	C	177	GLN
1	C	184	ASN
1	C	222	ASN
1	C	252	GLN
1	D	78	HIS
1	E	137	GLN
1	E	155	ASN
1	F	9	GLN
1	F	171	HIS
1	F	221	GLN
1	G	177	GLN
1	G	216	GLN
2	U	53	ASN
2	U	139	ASN
2	U	179	GLN
2	U	192	GLN
2	V	84	HIS
2	V	120	HIS
2	V	139	ASN
2	W	7	GLN
2	W	74	ASN
2	W	84	HIS
2	X	12	HIS
2	X	21	ASN
2	X	112	GLN
2	X	183	ASN
2	Y	9	GLN
2	Y	155	GLN
2	Y	179	GLN
2	Z	12	HIS
2	Z	53	ASN
2	Z	74	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Z	139	ASN
2	Z	155	GLN
2	Z	179	GLN
2	Z	183	ASN
2	a	53	ASN
2	a	74	ASN
2	a	139	ASN
2	b	63	GLN
2	c	74	ASN
2	c	139	ASN
2	c	183	ASN
2	d	21	ASN
2	d	74	ASN
2	d	139	ASN
2	d	176	GLN
2	d	183	ASN
2	d	192	GLN
2	e	12	HIS
2	e	74	ASN
2	e	139	ASN
2	f	7	GLN
2	f	53	ASN
2	f	74	ASN
2	f	139	ASN
2	f	183	ASN
2	f	193	ASN
2	f	195	ASN
2	g	63	GLN
2	g	139	ASN
2	h	5	ASN
2	h	12	HIS
2	h	62	HIS
2	h	120	HIS
2	h	139	ASN
2	i	13	GLN
2	i	57	ASN
2	i	63	GLN
2	j	63	GLN
2	k	67	GLN
2	k	74	ASN
2	k	176	GLN
2	k	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	l	67	GLN
2	l	74	ASN
2	l	84	HIS
2	l	87	HIS
2	n	74	ASN
2	n	155	GLN
2	n	195	ASN
2	o	74	ASN
2	p	155	GLN
2	p	193	ASN
2	q	62	HIS
2	q	74	ASN
2	q	95	GLN
2	q	139	ASN
2	q	176	GLN
2	q	183	ASN
2	r	5	ASN
2	r	67	GLN
2	r	74	ASN
2	r	120	HIS
2	s	50	GLN
2	s	57	ASN
2	s	183	ASN
2	t	120	HIS
2	t	179	GLN
2	u	21	ASN
2	u	53	ASN
2	u	74	ASN
2	u	84	HIS
2	u	120	HIS
2	v	7	GLN
2	v	12	HIS
2	v	74	ASN
2	v	139	ASN
2	w	9	GLN
2	w	139	ASN
2	x	7	GLN
2	x	179	GLN
2	y	4	GLN
2	y	74	ASN
2	y	139	ASN
2	y	195	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	z	57	ASN
2	z	63	GLN
2	z	87	HIS
2	z	183	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	$\# Z > 2$
4	IHP	X	301	-	36,36,36	1.94	6 (16%)	54,60,60	0.85	0
4	IHP	g	301	-	36,36,36	1.94	6 (16%)	54,60,60	0.90	0
4	IHP	b	301	-	36,36,36	1.94	6 (16%)	54,60,60	0.93	0
4	IHP	Z	301	-	36,36,36	1.94	6 (16%)	54,60,60	0.88	0
4	IHP	m	301	-	36,36,36	1.94	6 (16%)	54,60,60	0.87	0
4	IHP	a	301	-	36,36,36	1.94	6 (16%)	54,60,60	0.91	0
4	IHP	q	301	-	36,36,36	1.93	6 (16%)	54,60,60	0.88	0
4	IHP	i	301	-	36,36,36	1.94	6 (16%)	54,60,60	0.94	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
4	IHP	X	301	-	-	1/30/54/54	0/1/1/1
4	IHP	g	301	-	-	2/30/54/54	0/1/1/1
4	IHP	b	301	-	-	1/30/54/54	0/1/1/1
4	IHP	Z	301	-	-	1/30/54/54	0/1/1/1
4	IHP	m	301	-	-	0/30/54/54	0/1/1/1
4	IHP	a	301	-	-	2/30/54/54	0/1/1/1
4	IHP	q	301	-	-	0/30/54/54	0/1/1/1
4	IHP	i	301	-	-	2/30/54/54	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Z	301	IHP	P5-O15	4.61	1.68	1.59
4	b	301	IHP	P2-O12	4.60	1.68	1.59
4	m	301	IHP	P5-O15	4.59	1.68	1.59
4	a	301	IHP	P5-O15	4.59	1.68	1.59
4	Z	301	IHP	P2-O12	4.59	1.68	1.59
4	i	301	IHP	P2-O12	4.59	1.68	1.59
4	m	301	IHP	P2-O12	4.58	1.68	1.59
4	i	301	IHP	P5-O15	4.58	1.68	1.59
4	X	301	IHP	P2-O12	4.58	1.68	1.59
4	b	301	IHP	P5-O15	4.58	1.68	1.59
4	X	301	IHP	P5-O15	4.56	1.67	1.59
4	q	301	IHP	P5-O15	4.55	1.67	1.59
4	g	301	IHP	P5-O15	4.55	1.67	1.59
4	g	301	IHP	P2-O12	4.52	1.67	1.59
4	q	301	IHP	P2-O12	4.50	1.67	1.59
4	a	301	IHP	P2-O12	4.46	1.67	1.59
4	a	301	IHP	P6-O16	4.43	1.67	1.59
4	g	301	IHP	P6-O16	4.43	1.67	1.59
4	i	301	IHP	P6-O16	4.42	1.67	1.59
4	q	301	IHP	P6-O16	4.42	1.67	1.59
4	Z	301	IHP	P6-O16	4.40	1.67	1.59
4	i	301	IHP	P4-O14	4.40	1.67	1.59
4	X	301	IHP	P6-O16	4.39	1.67	1.59
4	m	301	IHP	P6-O16	4.39	1.67	1.59
4	a	301	IHP	P4-O14	4.38	1.67	1.59
4	Z	301	IHP	P4-O14	4.37	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	301	IHP	P6-O16	4.37	1.67	1.59
4	g	301	IHP	P4-O14	4.36	1.67	1.59
4	q	301	IHP	P4-O14	4.35	1.67	1.59
4	b	301	IHP	P4-O14	4.35	1.67	1.59
4	b	301	IHP	P3-O13	4.33	1.67	1.59
4	X	301	IHP	P4-O14	4.32	1.67	1.59
4	g	301	IHP	P3-O13	4.32	1.67	1.59
4	m	301	IHP	P4-O14	4.30	1.67	1.59
4	m	301	IHP	P3-O13	4.29	1.67	1.59
4	Z	301	IHP	P3-O13	4.29	1.67	1.59
4	q	301	IHP	P3-O13	4.28	1.67	1.59
4	a	301	IHP	P3-O13	4.28	1.67	1.59
4	i	301	IHP	P3-O13	4.27	1.67	1.59
4	X	301	IHP	P3-O13	4.25	1.67	1.59
4	a	301	IHP	P1-O11	4.14	1.67	1.59
4	X	301	IHP	P1-O11	4.12	1.67	1.59
4	m	301	IHP	P1-O11	4.11	1.67	1.59
4	b	301	IHP	P1-O11	4.10	1.67	1.59
4	Z	301	IHP	P1-O11	4.09	1.67	1.59
4	q	301	IHP	P1-O11	4.09	1.67	1.59
4	g	301	IHP	P1-O11	4.09	1.67	1.59
4	i	301	IHP	P1-O11	4.06	1.67	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	g	301	IHP	C2-O12-P2-O32
4	b	301	IHP	C3-O13-P3-O23
4	X	301	IHP	C2-O12-P2-O32
4	a	301	IHP	C6-O16-P6-O36
4	g	301	IHP	C6-O16-P6-O36
4	Z	301	IHP	C4-O14-P4-O44
4	a	301	IHP	C4-O14-P4-O44
4	i	301	IHP	C2-O12-P2-O42
4	i	301	IHP	C4-O14-P4-O44

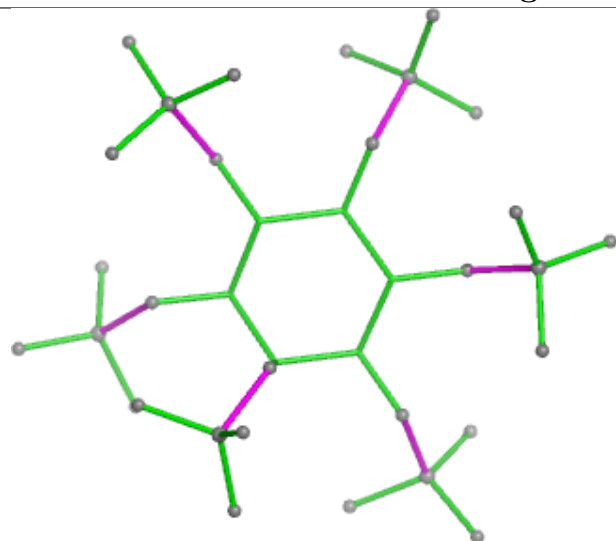
There are no ring outliers.

1 monomer is involved in 1 short contact:

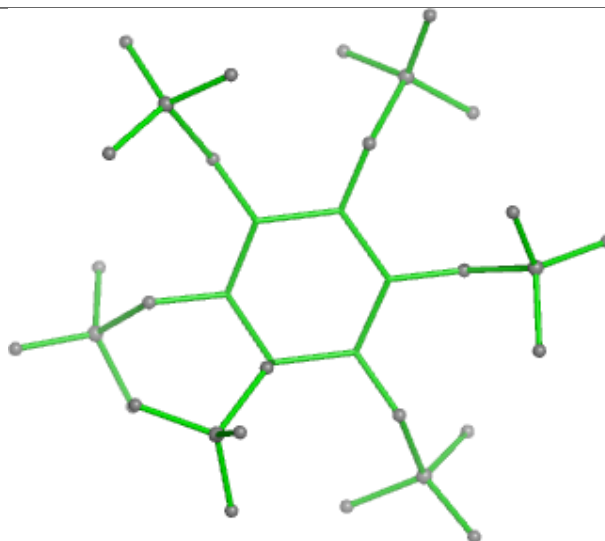
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	g	301	IHP	1	0

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

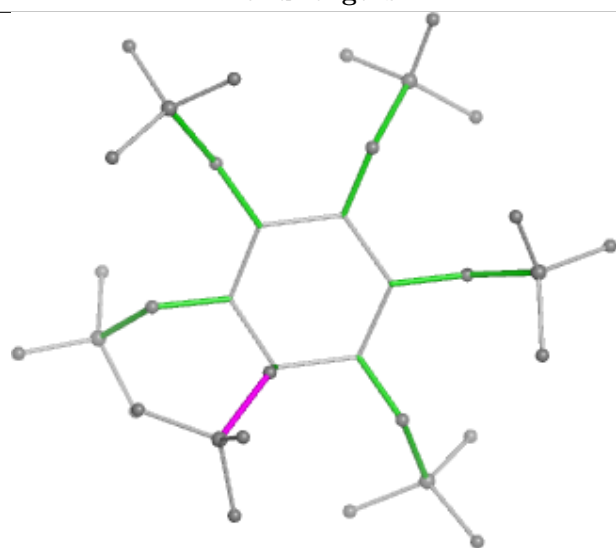
Ligand IHP X 301



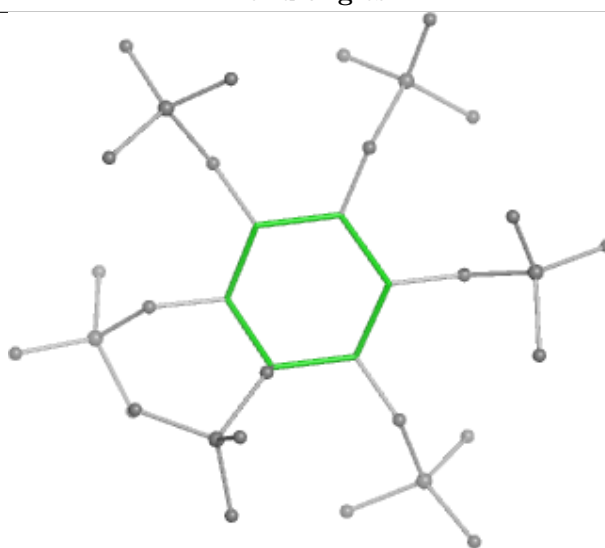
Bond lengths



Bond angles

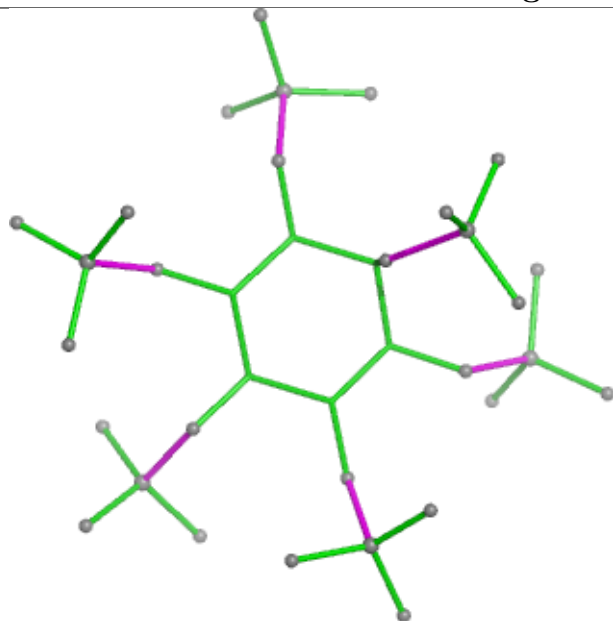


Torsions

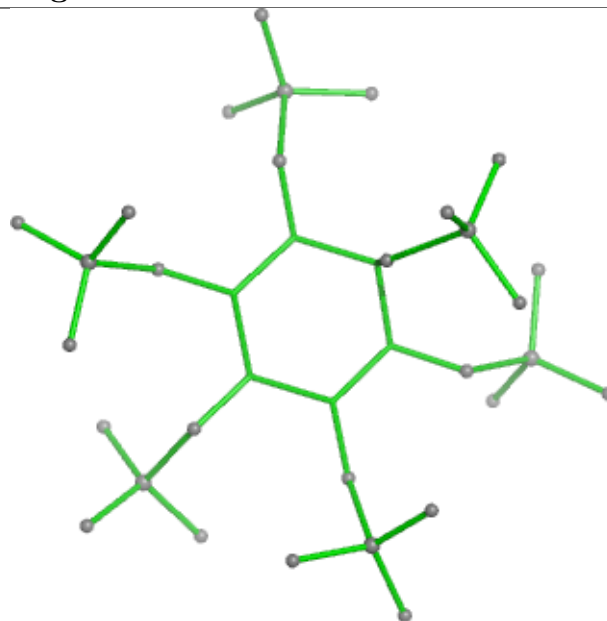


Rings

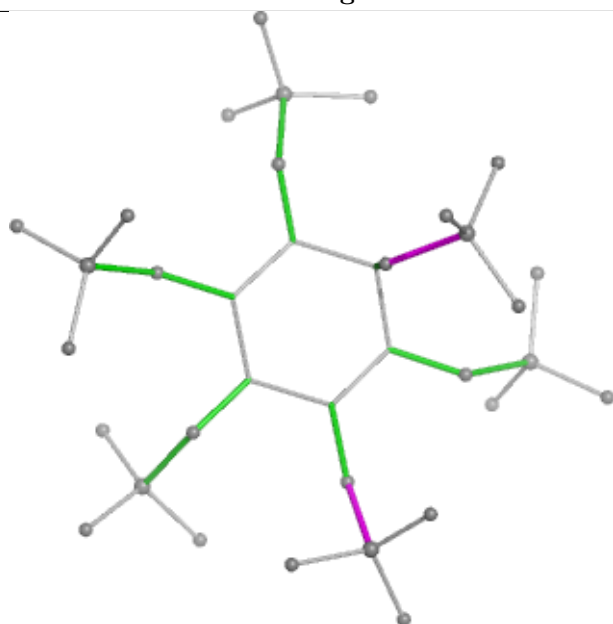
Ligand IHP g 301



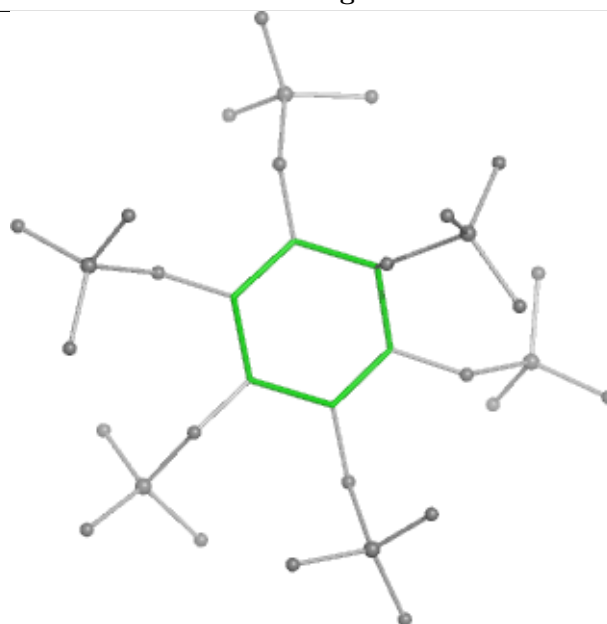
Bond lengths



Bond angles

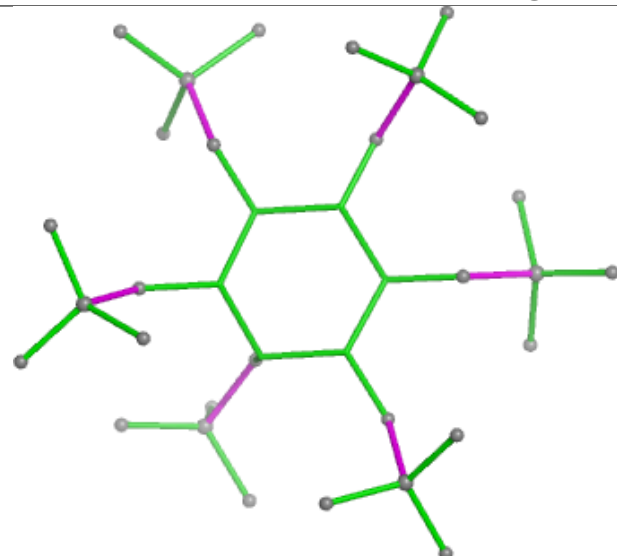


Torsions

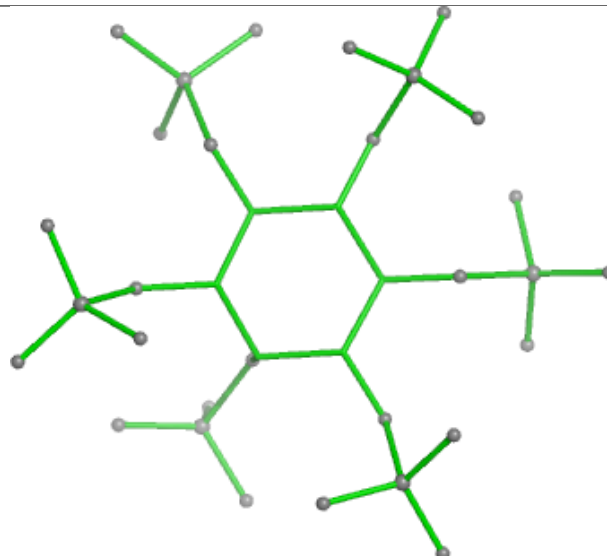


Rings

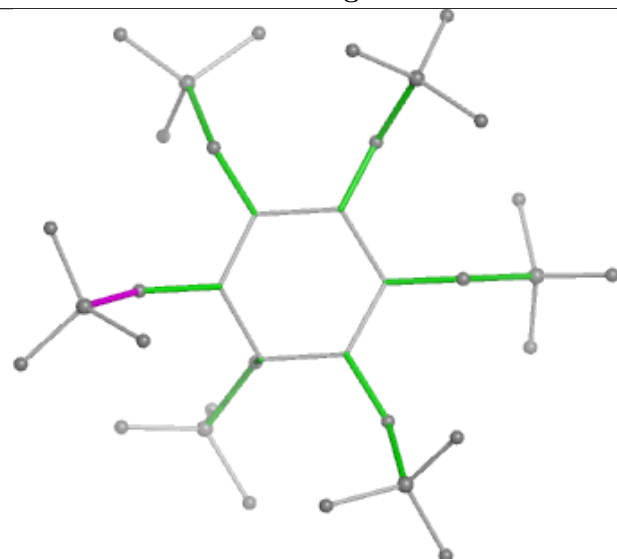
Ligand IHP b 301



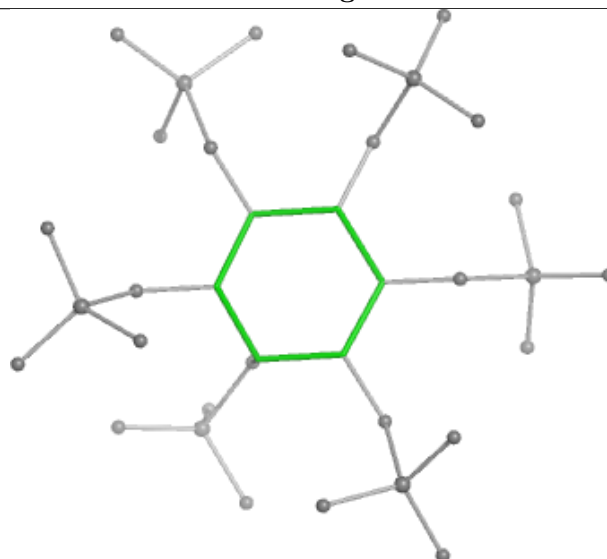
Bond lengths



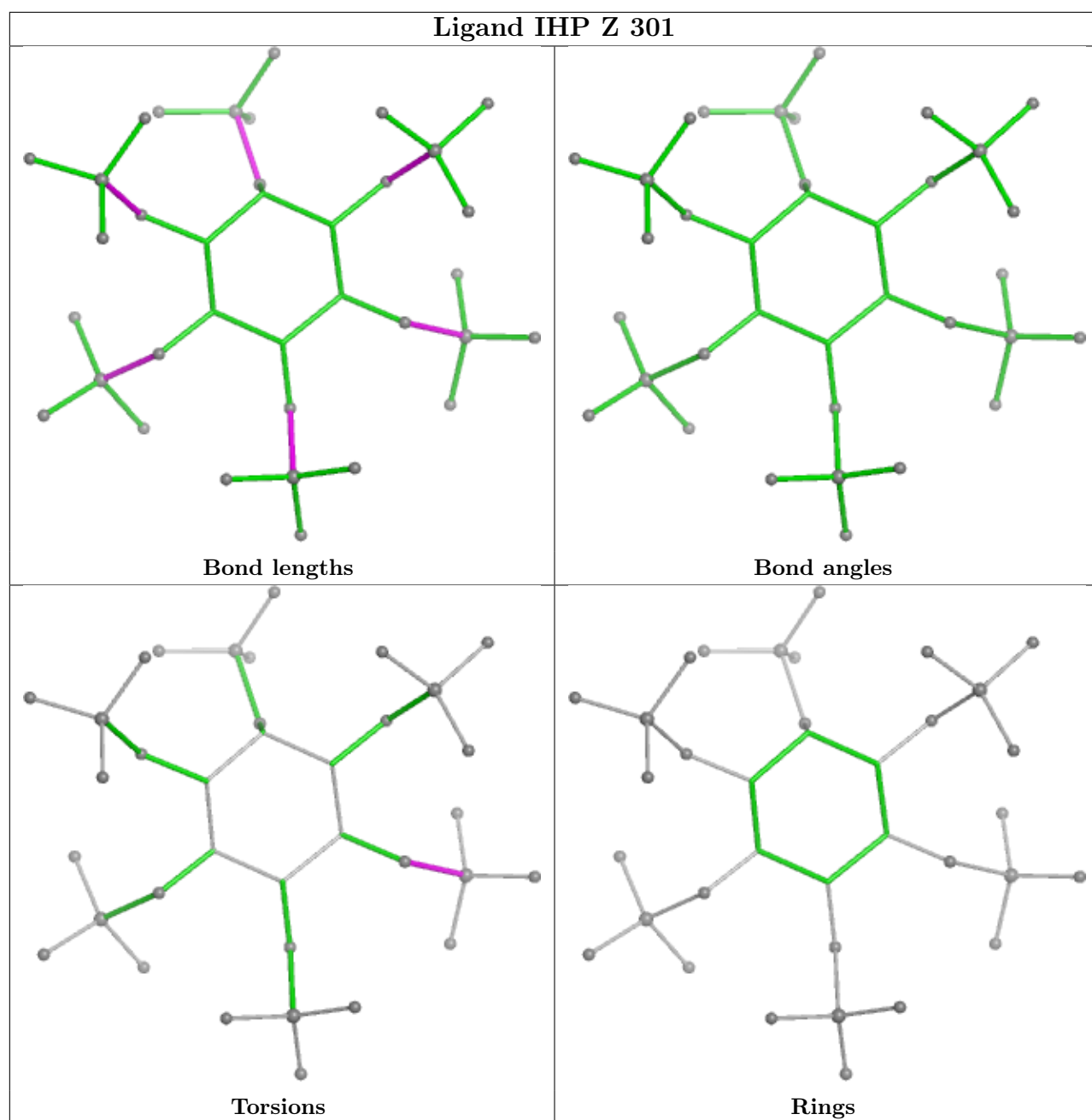
Bond angles



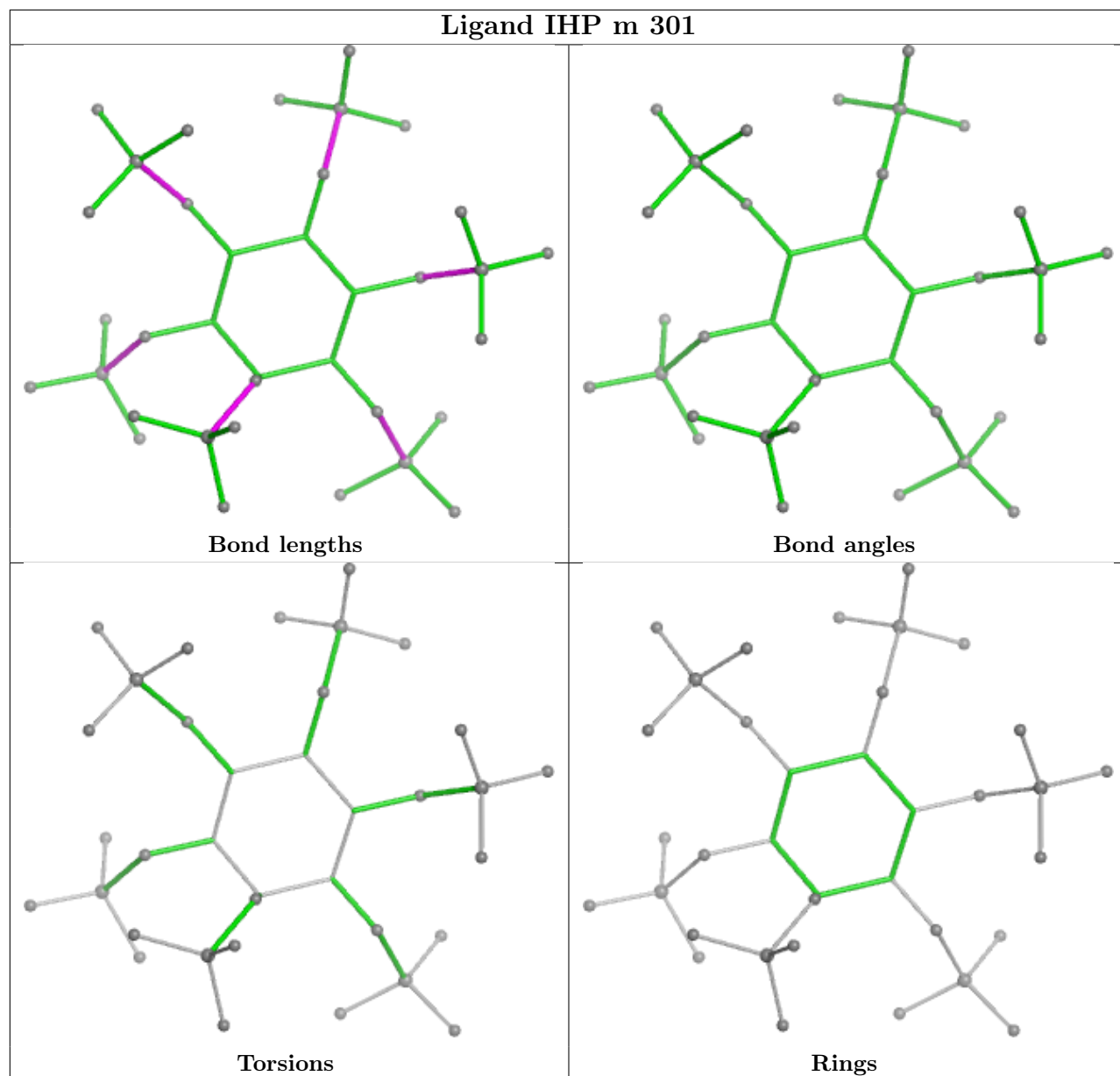
Torsions



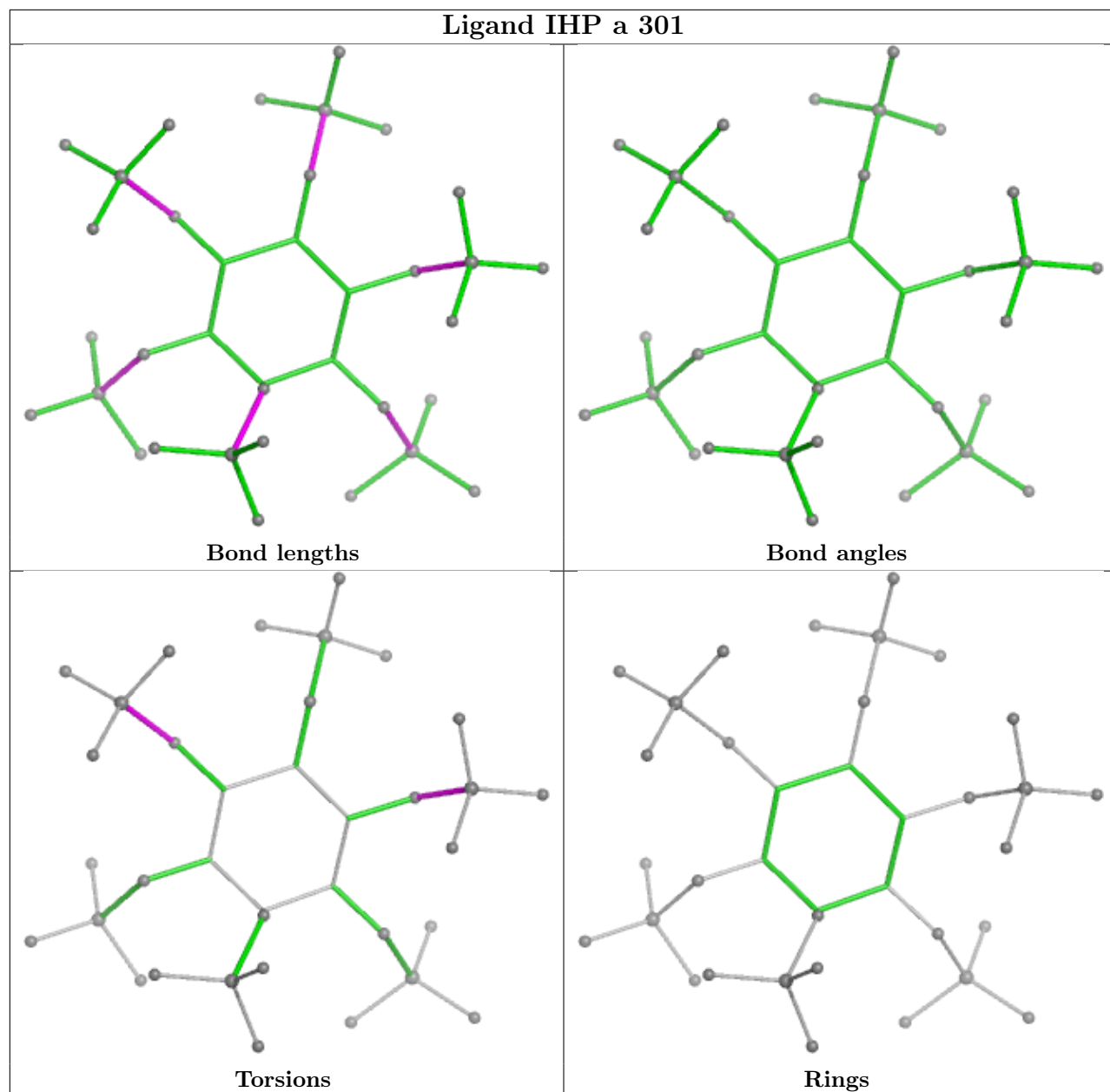
Rings

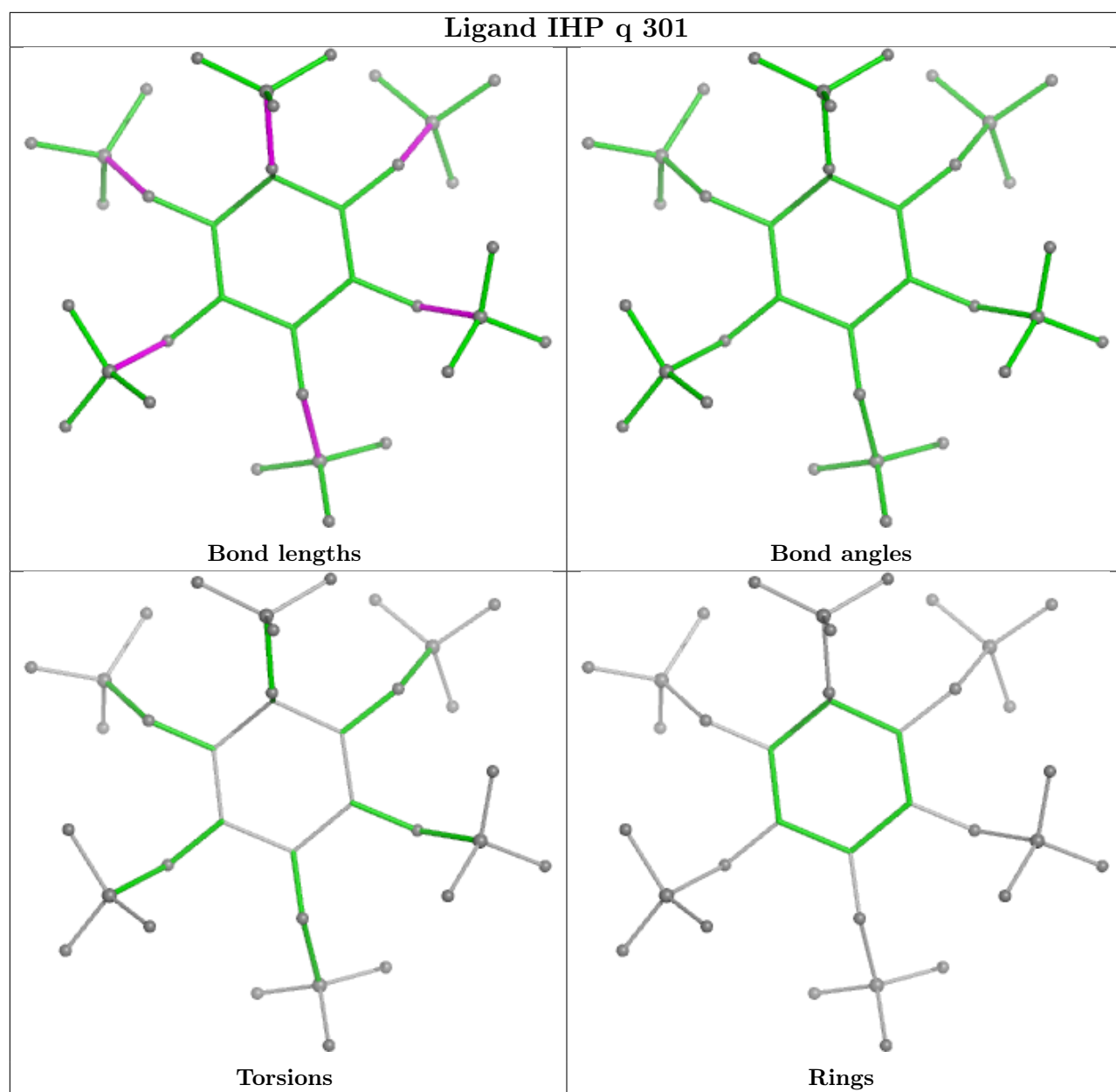


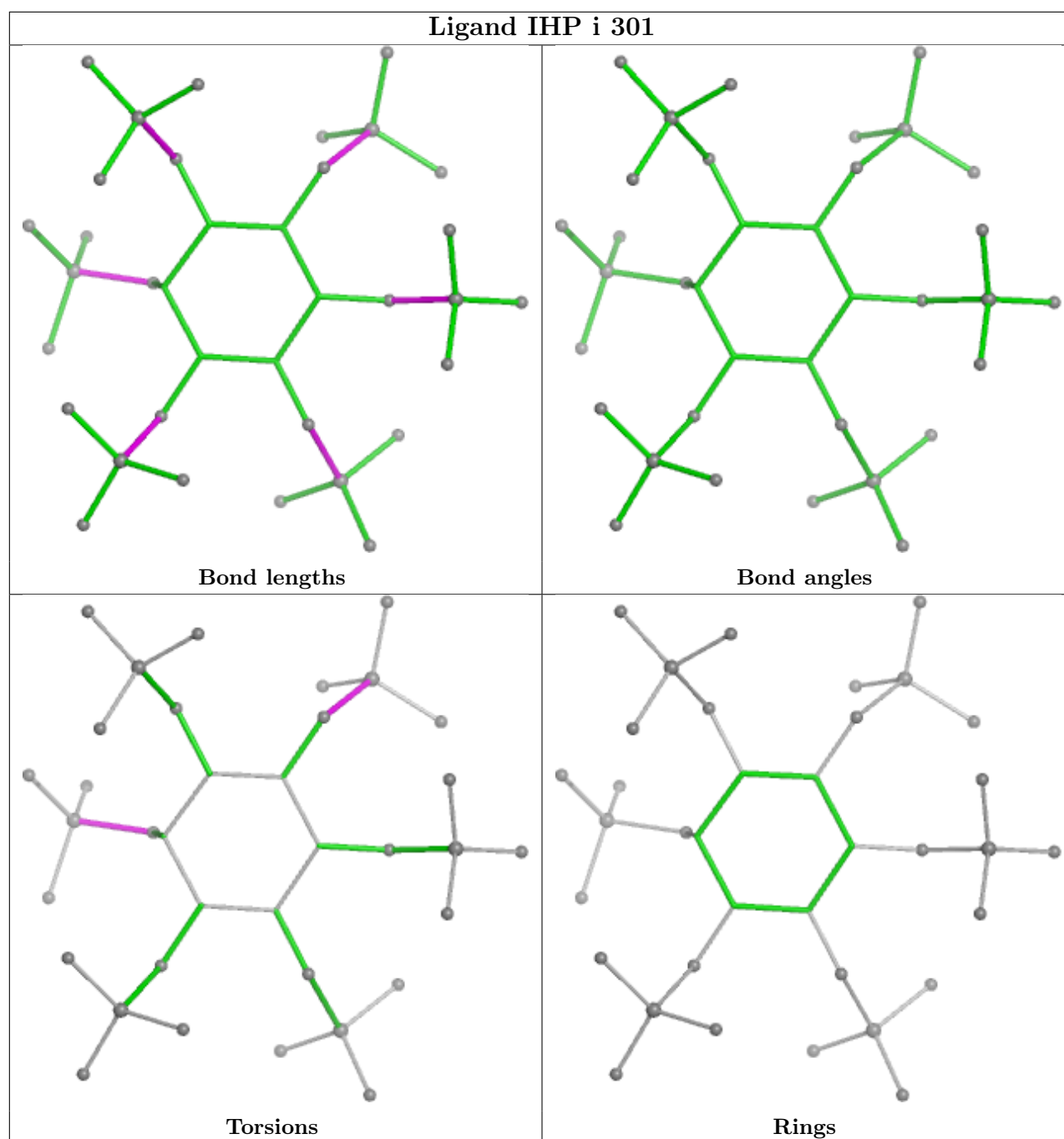
Ligand IHP m 301



Ligand IHP a 301







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.

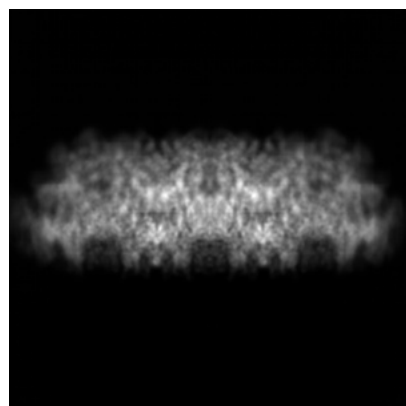
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54071. These allow visual inspection of the internal detail of the map and identification of artifacts.

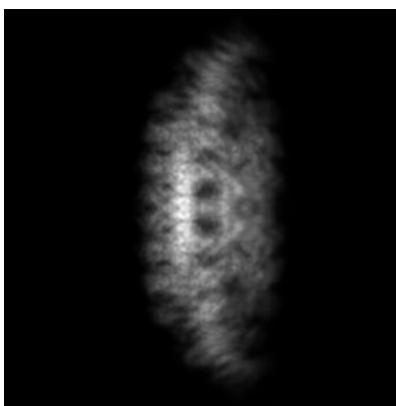
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

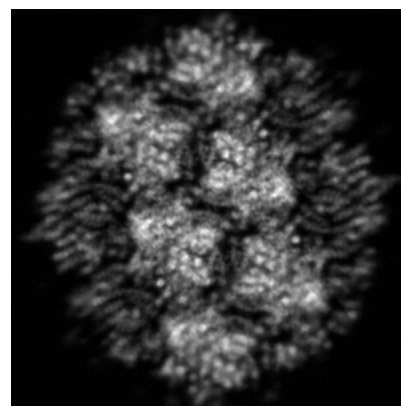
6.1.1 Primary map



X

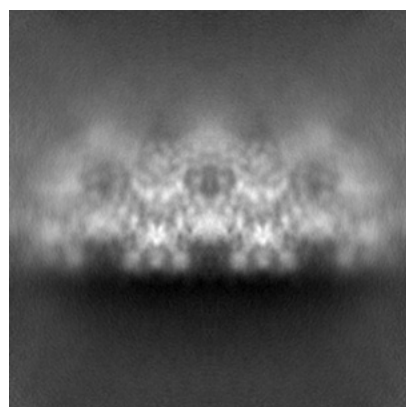


Y

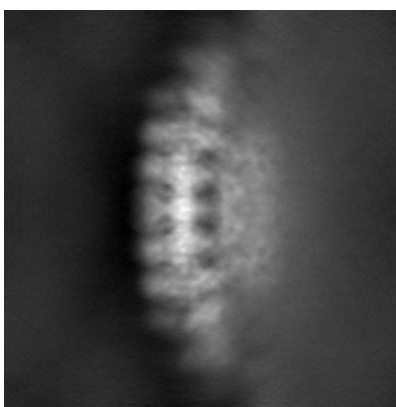


Z

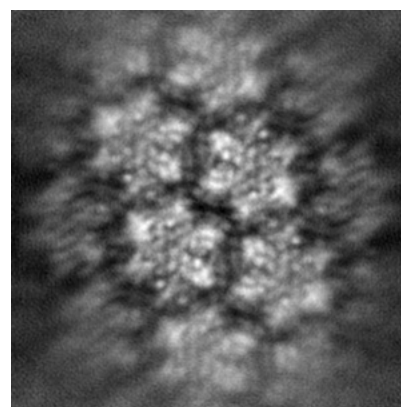
6.1.2 Raw map



X



Y

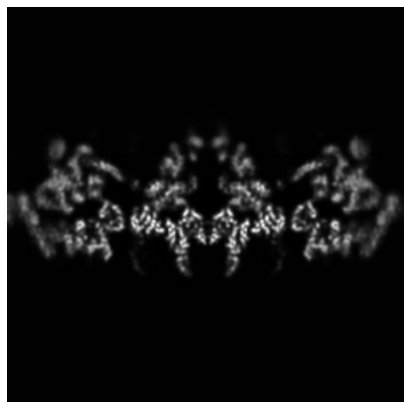


Z

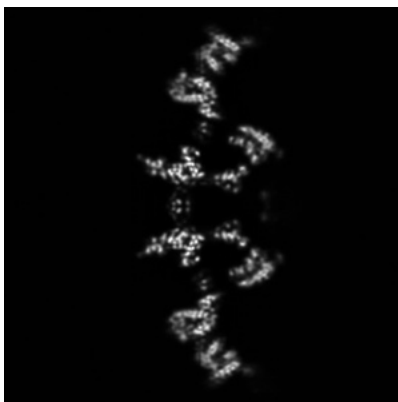
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

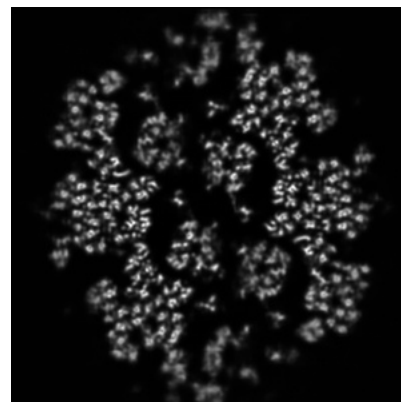
6.2.1 Primary map



X Index: 120

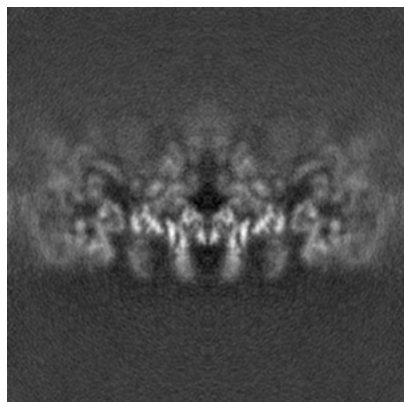


Y Index: 120

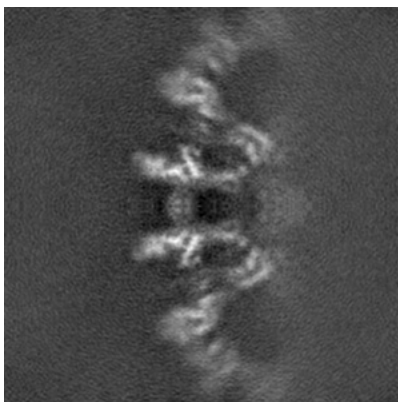


Z Index: 120

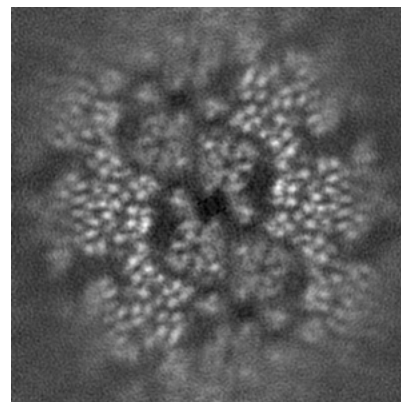
6.2.2 Raw map



X Index: 120



Y Index: 120

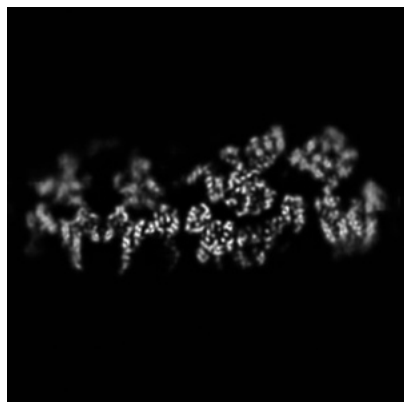


Z Index: 120

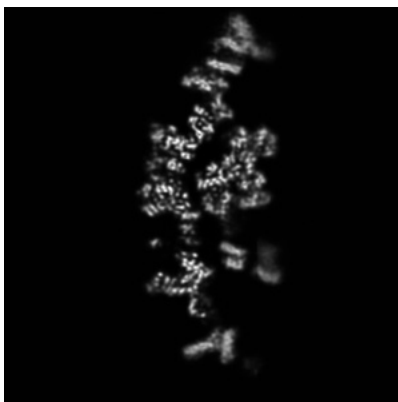
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

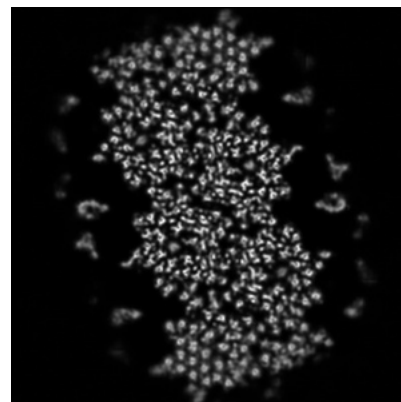
6.3.1 Primary map



X Index: 139

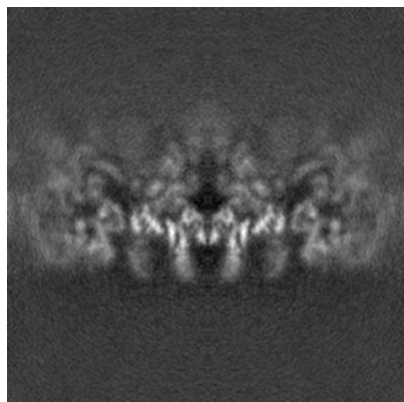


Y Index: 137

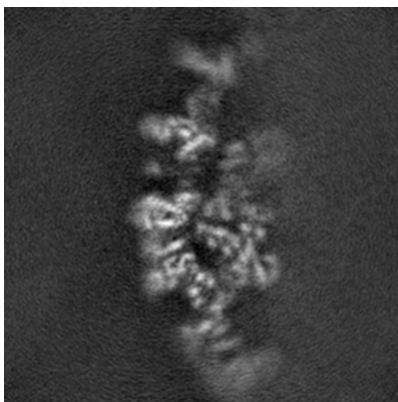


Z Index: 107

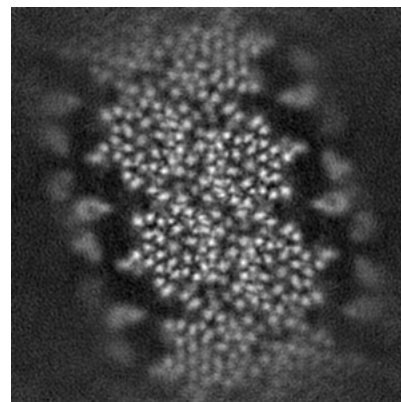
6.3.2 Raw map



X Index: 120



Y Index: 104

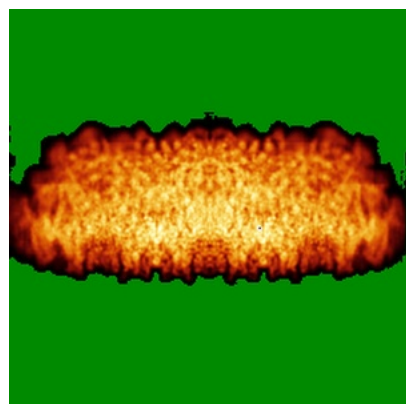


Z Index: 106

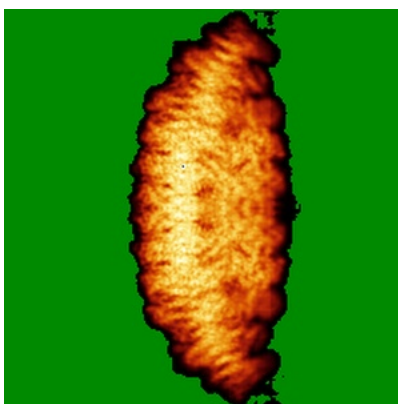
The images above show the largest variance slices of the map in three orthogonal directions.

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

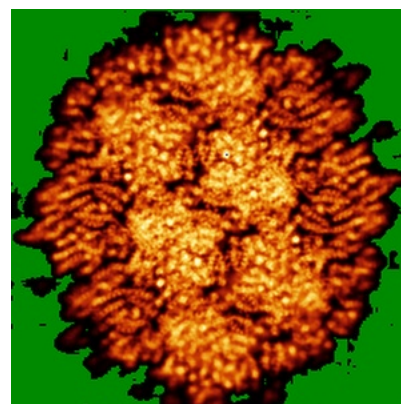
6.4.1 Primary map



X

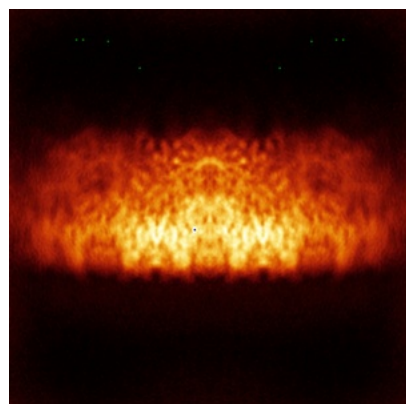


Y

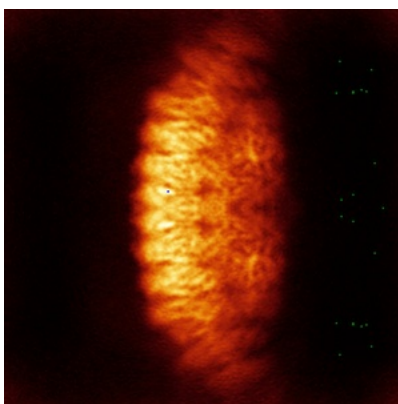


Z

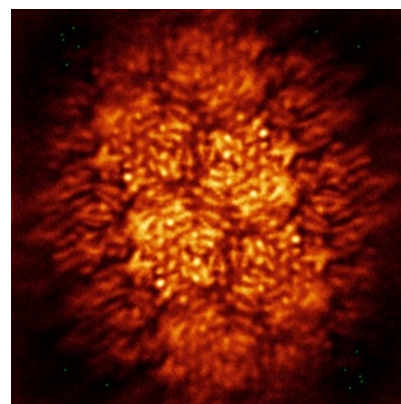
6.4.2 Raw map



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 3.2. 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



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

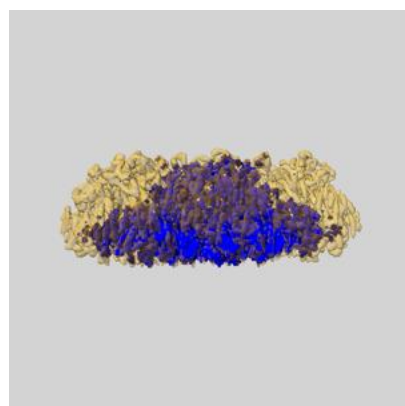
6.6 Mask visualisation [i](#)

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

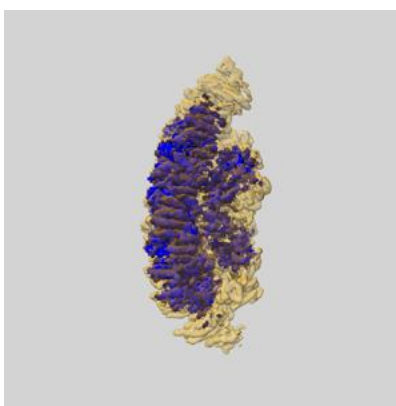
A mask typically either:

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

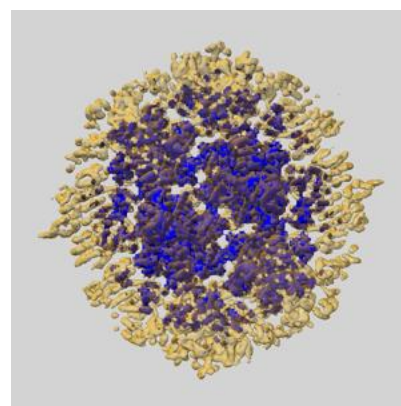
6.6.1 emd_54071_msk_1.map [i](#)



X



Y

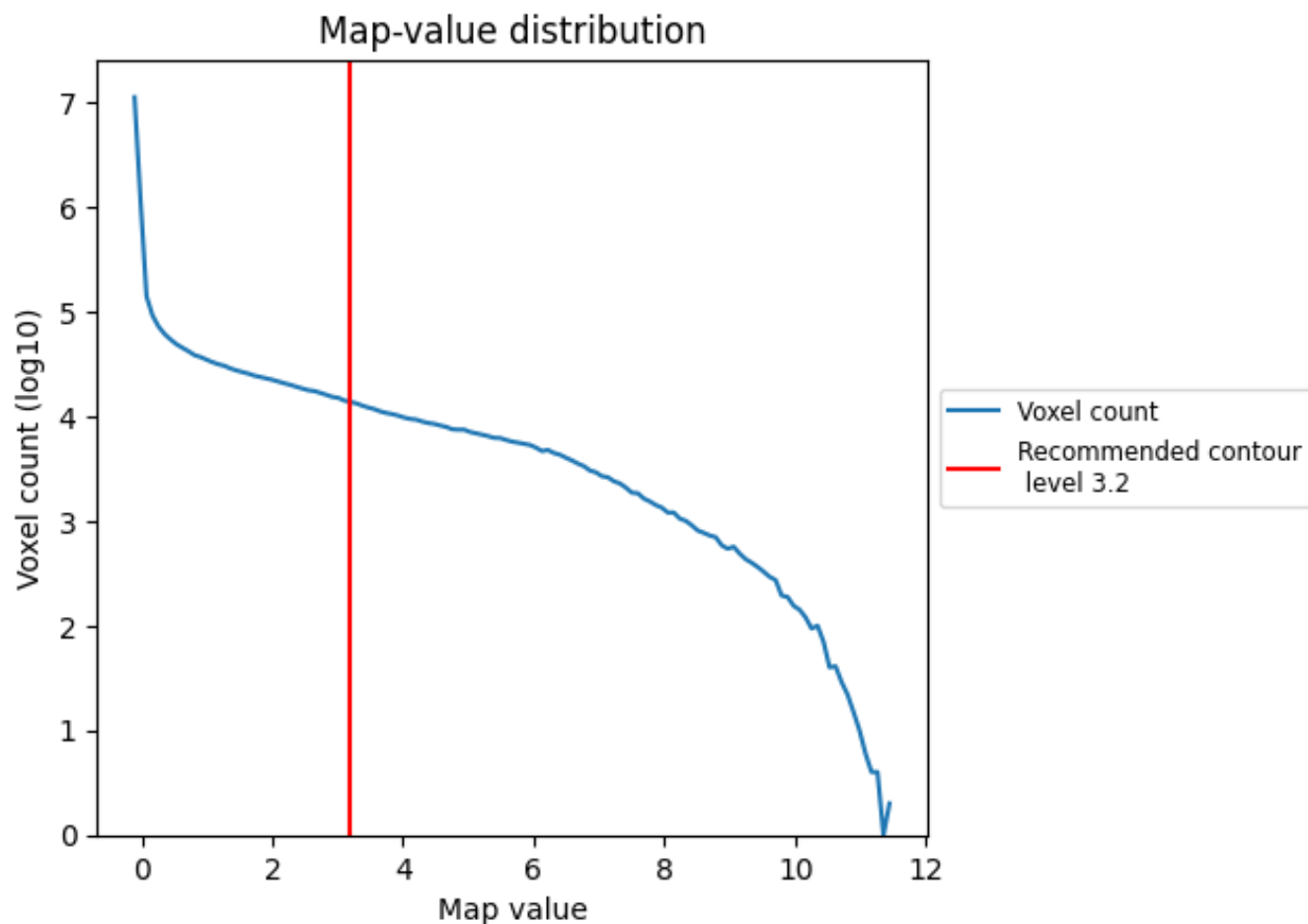


Z

7 Map analysis [i](#)

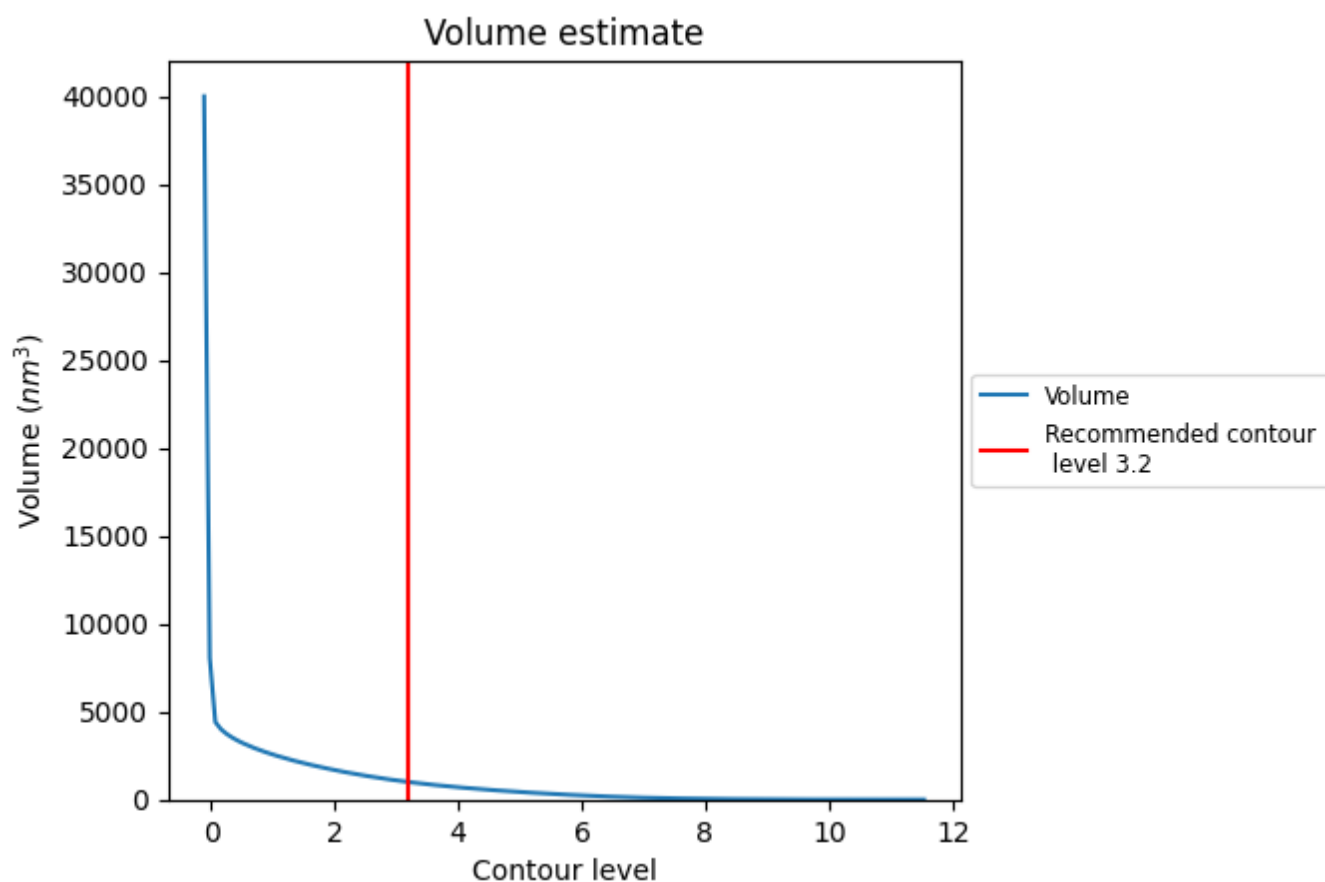
This section contains the results of statistical analysis of the map.

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.

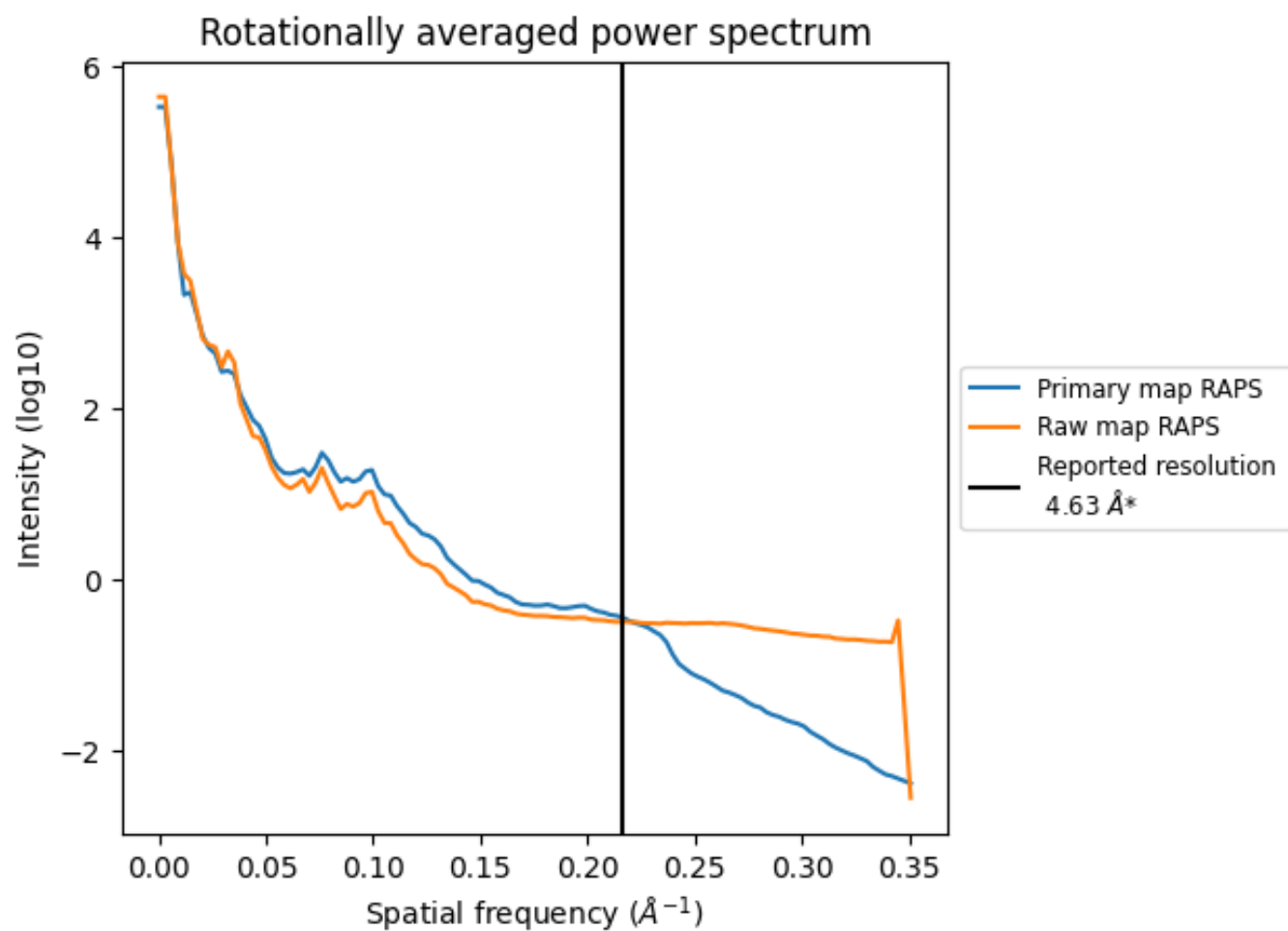
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 999 nm^3 ; this corresponds to an approximate mass of 903 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 ⓘ

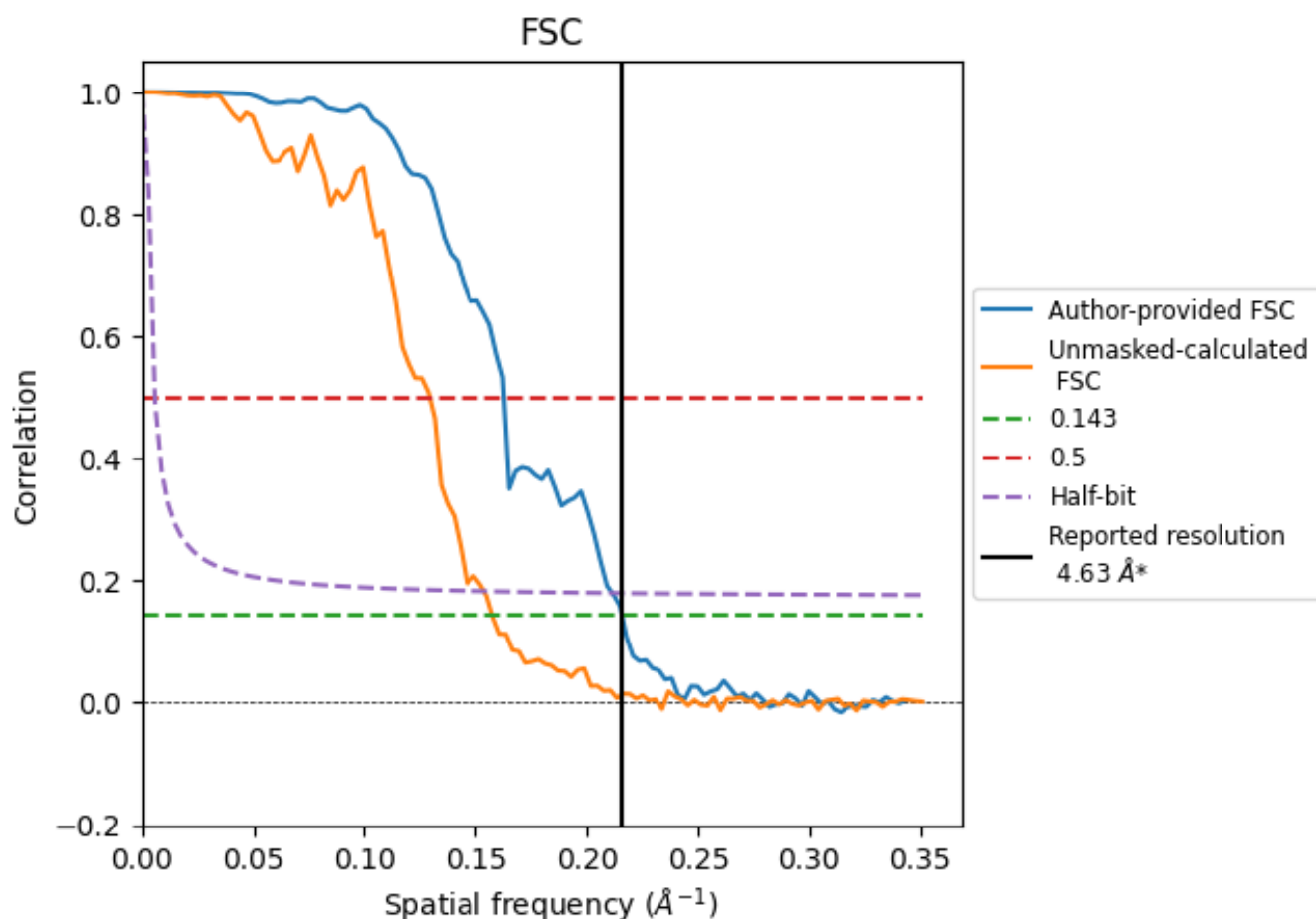


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

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 $0.216 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

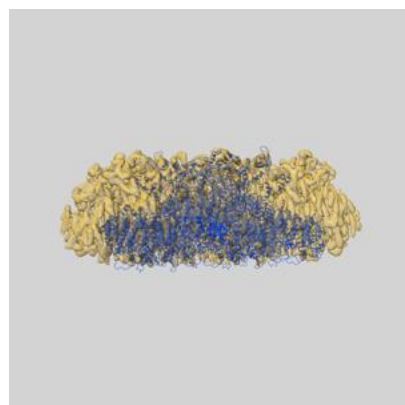
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	6.14	4.73
Unmasked-calculated*	6.35	7.74	6.50

*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 6.35 differs from the reported value 4.63 by more than 10 %

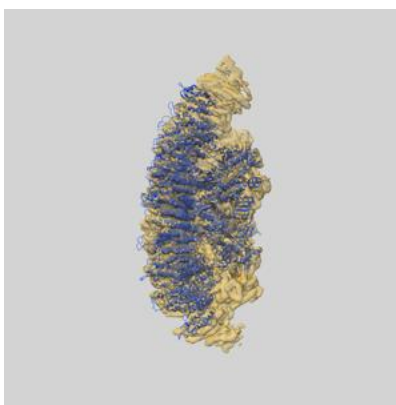
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54071 and PDB model 9RMX. Per-residue inclusion information can be found in section [3](#) on page [10](#).

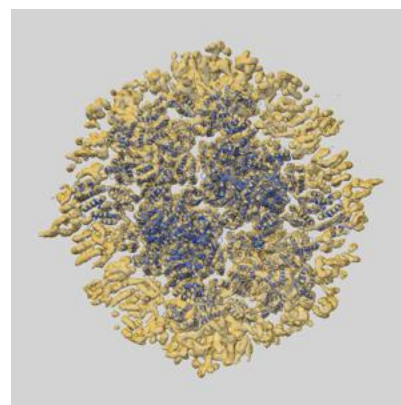
9.1 Map-model overlay [i](#)



X



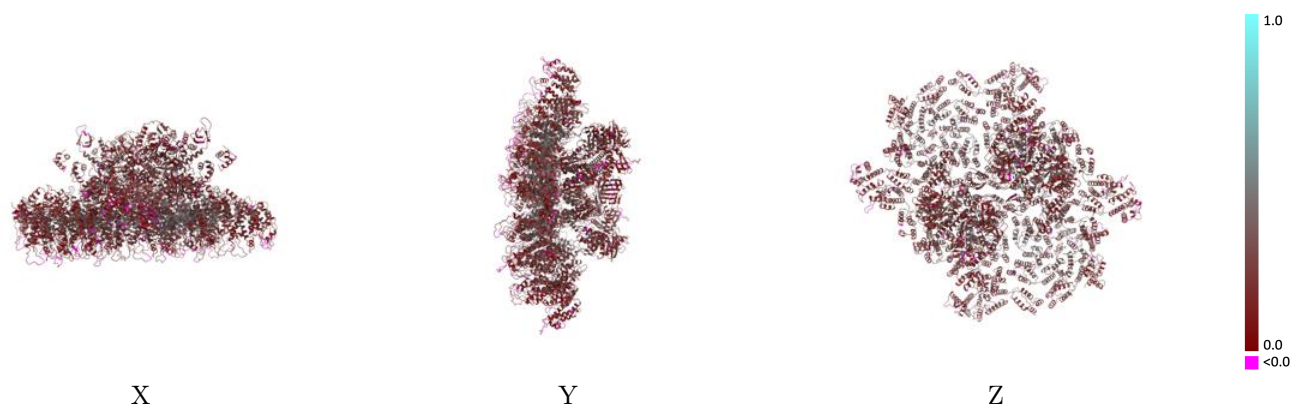
Y



Z

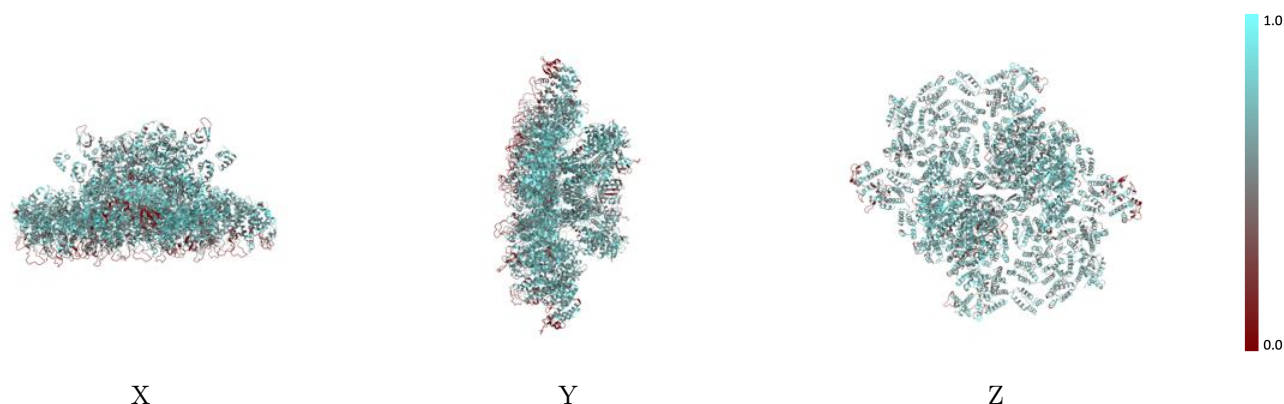
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



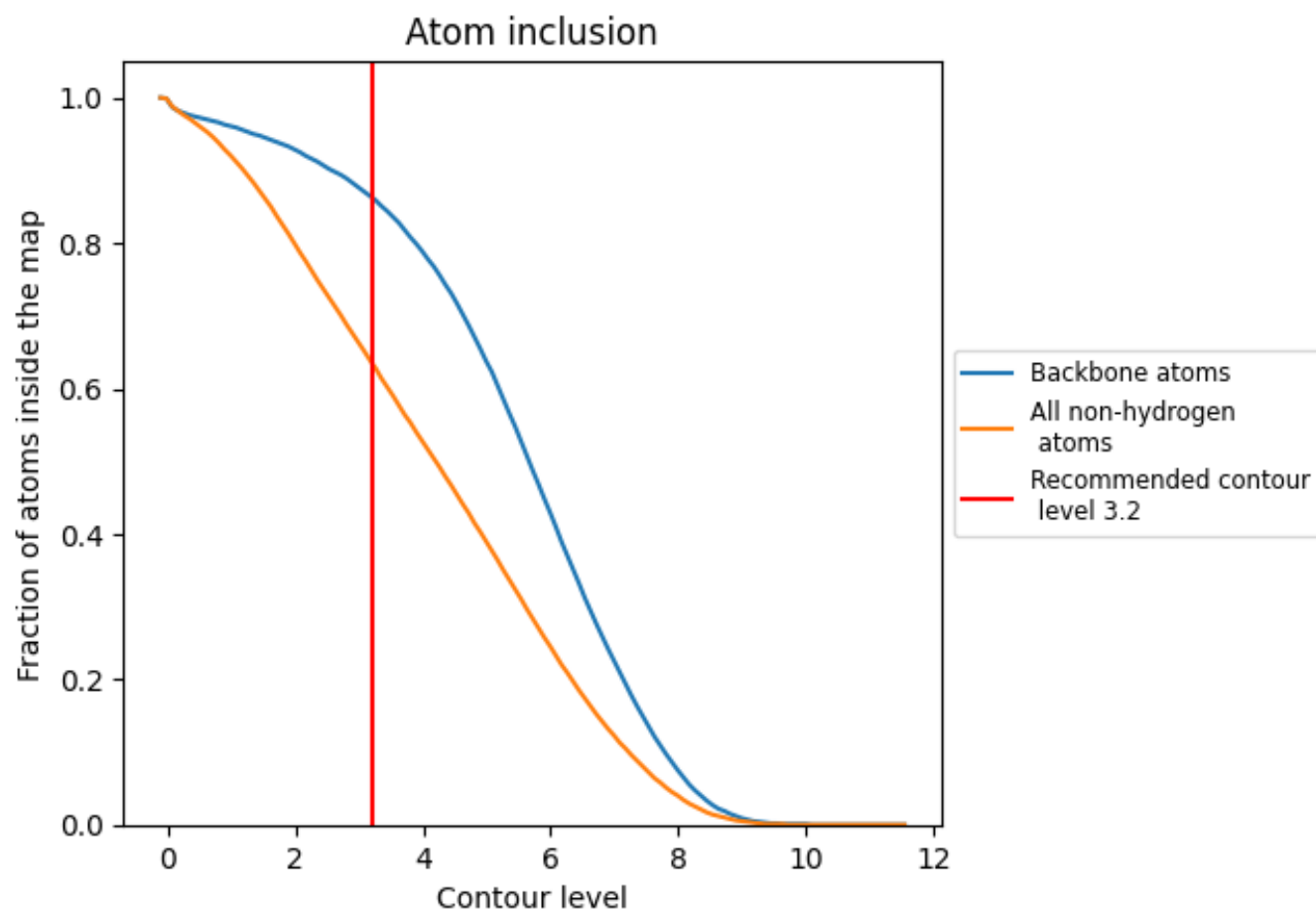
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (3.2).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 64% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6350	 0.2430
A	 0.6360	 0.2400
B	 0.6310	 0.2220
C	 0.6030	 0.2000
D	 0.6640	 0.2400
E	 0.6210	 0.2390
F	 0.6310	 0.2220
G	 0.6110	 0.2010
H	 0.6720	 0.2410
I	 0.6490	 0.1780
J	 0.6870	 0.1920
K	 0.6750	 0.1870
L	 0.6160	 0.1730
U	 0.7290	 0.3060
V	 0.7390	 0.3130
W	 0.7280	 0.3210
X	 0.6790	 0.2830
Y	 0.6640	 0.2710
Z	 0.6930	 0.2970
a	 0.6820	 0.2920
b	 0.6560	 0.2700
c	 0.7140	 0.3050
d	 0.7140	 0.3070
e	 0.7380	 0.3160
f	 0.7150	 0.3160
g	 0.6640	 0.2710
h	 0.6020	 0.2280
i	 0.6140	 0.2270
j	 0.5730	 0.1860
k	 0.6180	 0.2340
l	 0.7090	 0.3030
m	 0.5610	 0.1790
n	 0.6180	 0.2380
o	 0.6990	 0.3000
p	 0.6460	 0.2740



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
q	 0.6120	 0.2330
r	 0.6100	 0.2320
s	 0.5220	 0.1890
t	 0.5050	 0.1690
u	 0.5740	 0.1930
v	 0.5780	 0.1940
w	 0.5190	 0.1920
x	 0.4990	 0.1690
y	 0.5800	 0.1960
z	 0.5790	 0.1950