



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 11:22 AM UTC

PDB ID : 6NK6 / pdb_00006nk6
EMDB ID : EMD-9394
Title : Electron Cryo-Microscopy Of Chikungunya VLP in complex with mouse Mxra8 receptor
Authors : Basore, K.; Kim, A.S.; Nelson, C.A.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-01-04
Resolution : 4.06 Å (reported)
Based on initial models : 3N42, 3J0C, 6NK3, 5H23

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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

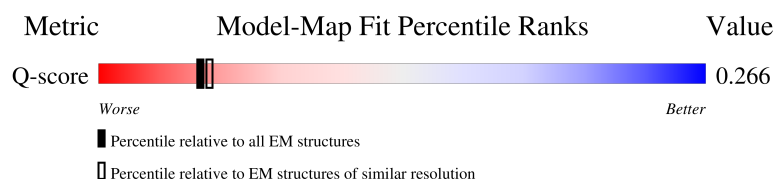
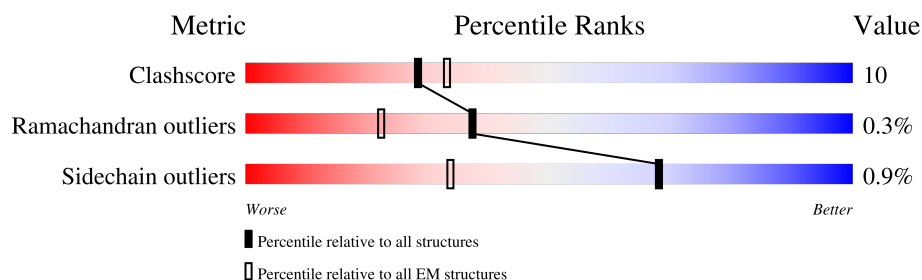
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.06 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.



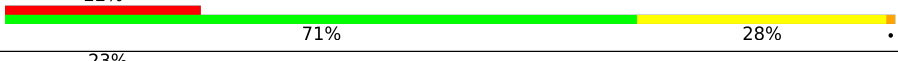
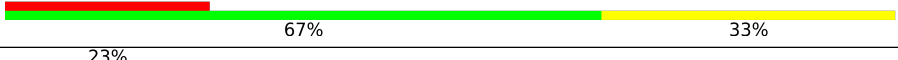
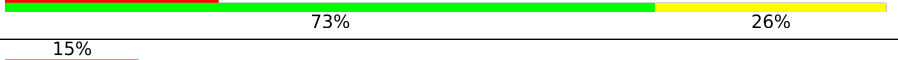
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6515 (3.56 - 4.56)

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	M	269	
1	N	269	
1	O	269	
1	P	269	

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Mol	Chain	Length	Quality of chain
2	A	439	
2	B	439	
2	C	439	
2	D	439	
3	E	419	
3	F	419	
3	G	419	
3	H	419	
4	I	151	
4	J	151	
4	K	151	
4	L	151	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 39805 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 Matrix remodeling-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	269	Total	C	N	O	S	0	0
			2169	1344	416	400	9		
1	N	261	Total	C	N	O	S	0	0
			2111	1306	408	388	9		
1	O	269	Total	C	N	O	S	0	0
			2168	1344	416	399	9		
1	P	269	Total	C	N	O	S	0	0
			2169	1344	416	400	9		

- Molecule 2 is a protein called E1 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		
2	B	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		
2	C	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		
2	D	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		

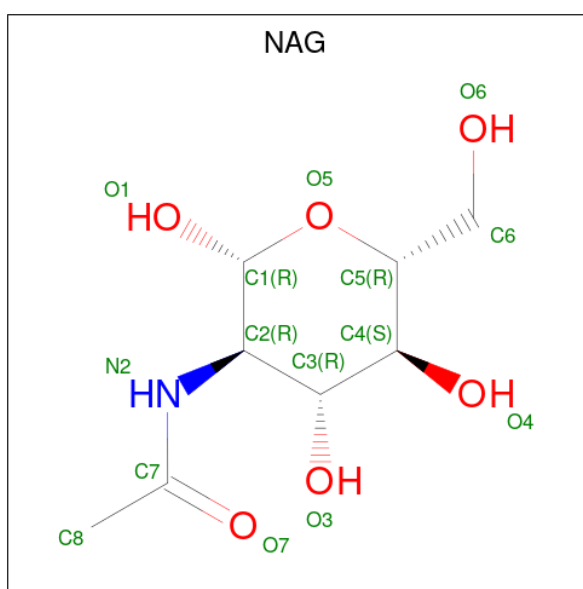
- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		
3	F	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		
3	G	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		
3	H	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		

- Molecule 4 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		
4	J	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		
4	K	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		
4	L	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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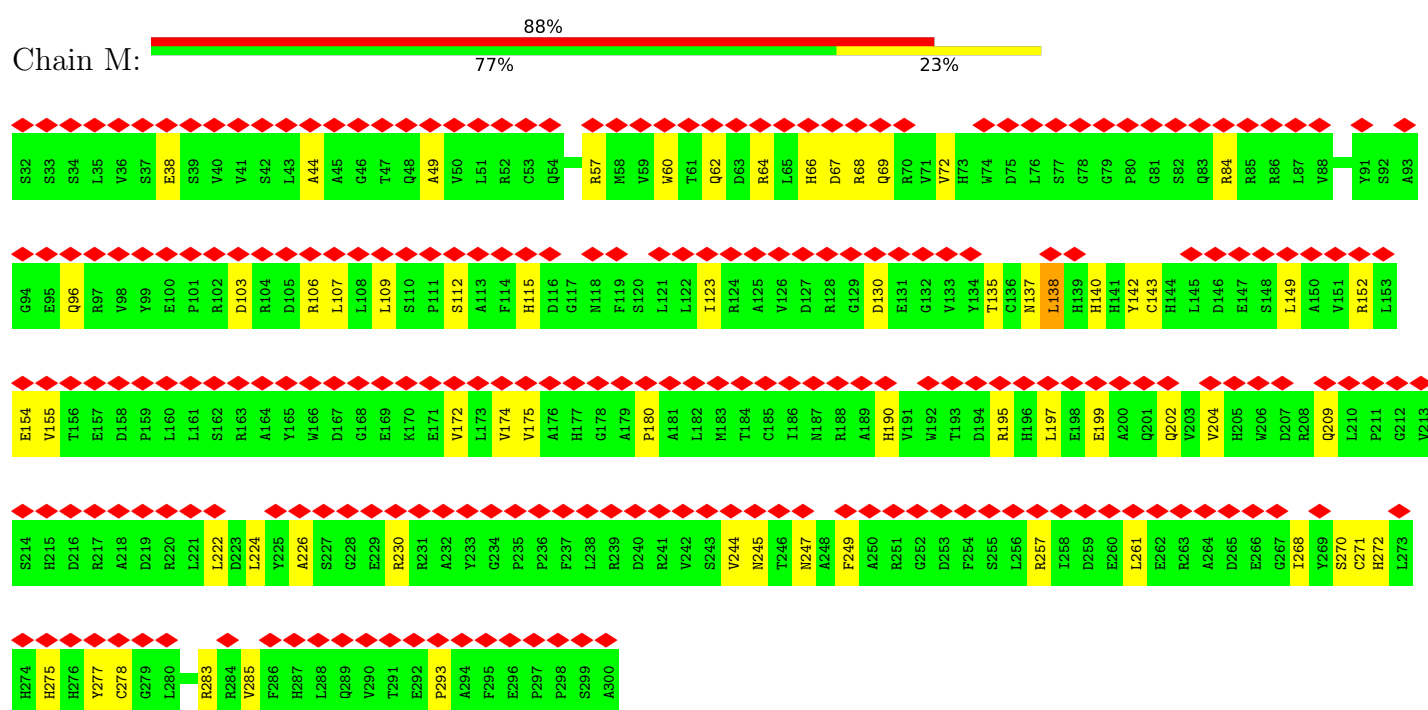
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Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

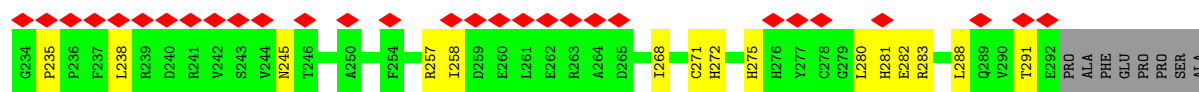
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Matrix remodeling-associated protein 8



• Molecule 1: Matrix remodeling-associated protein 8

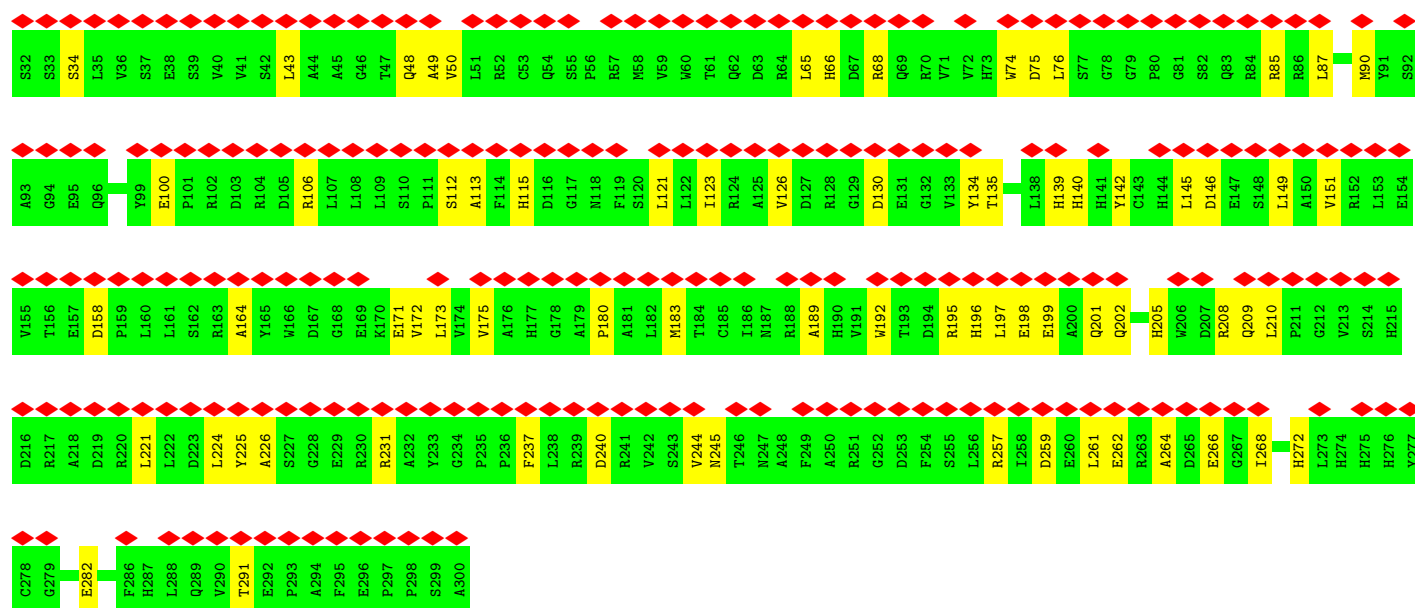
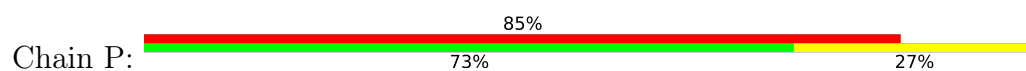




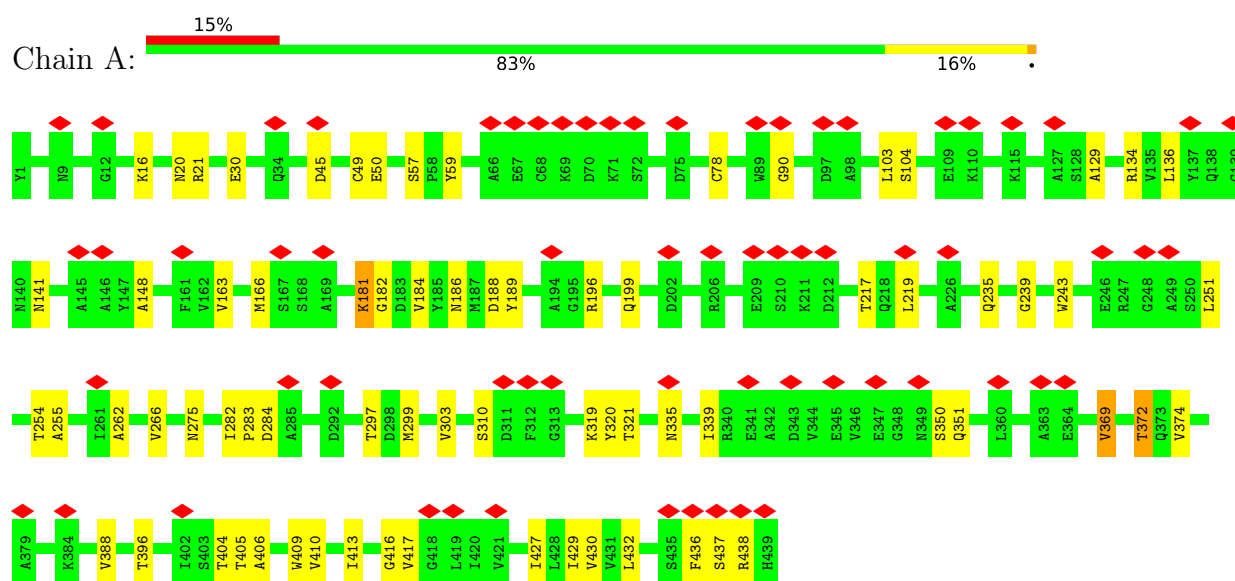
• Molecule 1: Matrix remodeling-associated protein 8



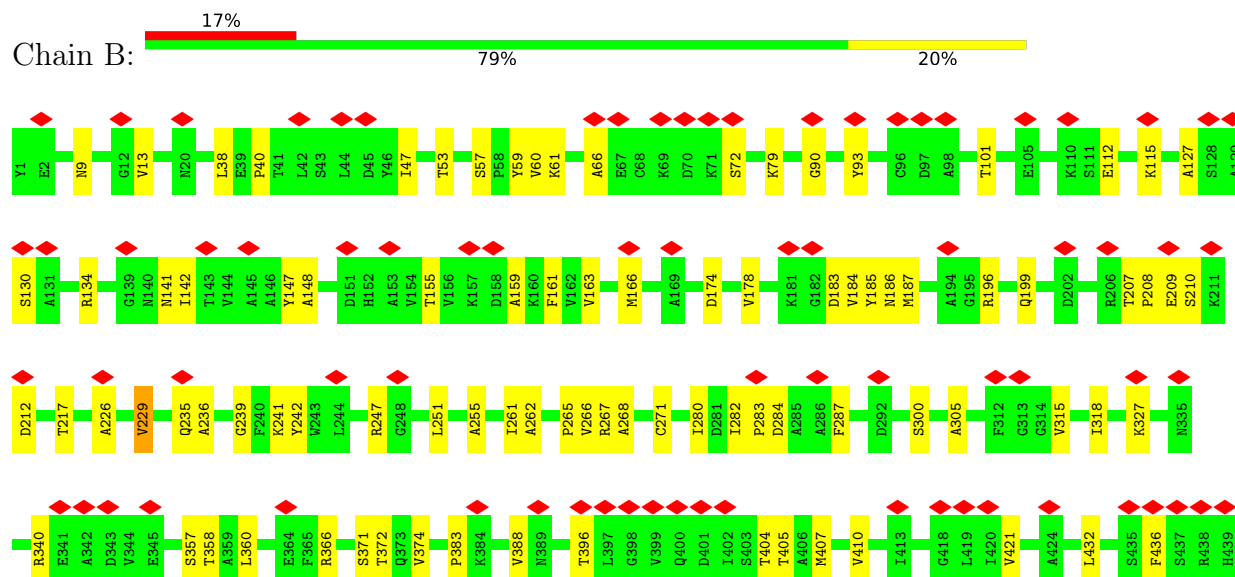
• Molecule 1: Matrix remodeling-associated protein 8



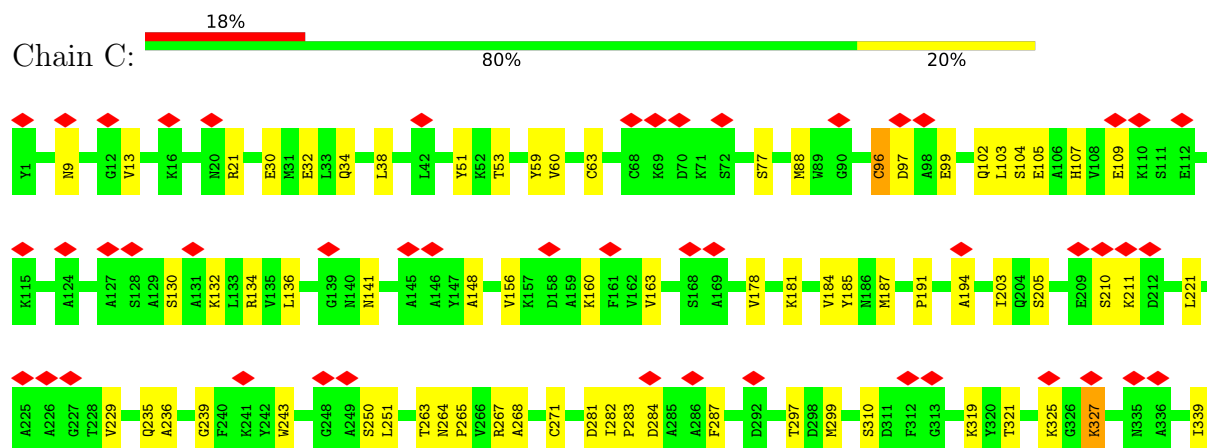
• Molecule 2: E1 glycoprotein

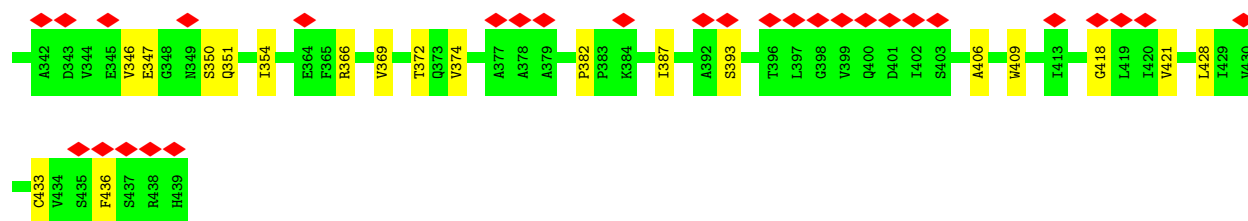


• Molecule 2: E1 glycoprotein

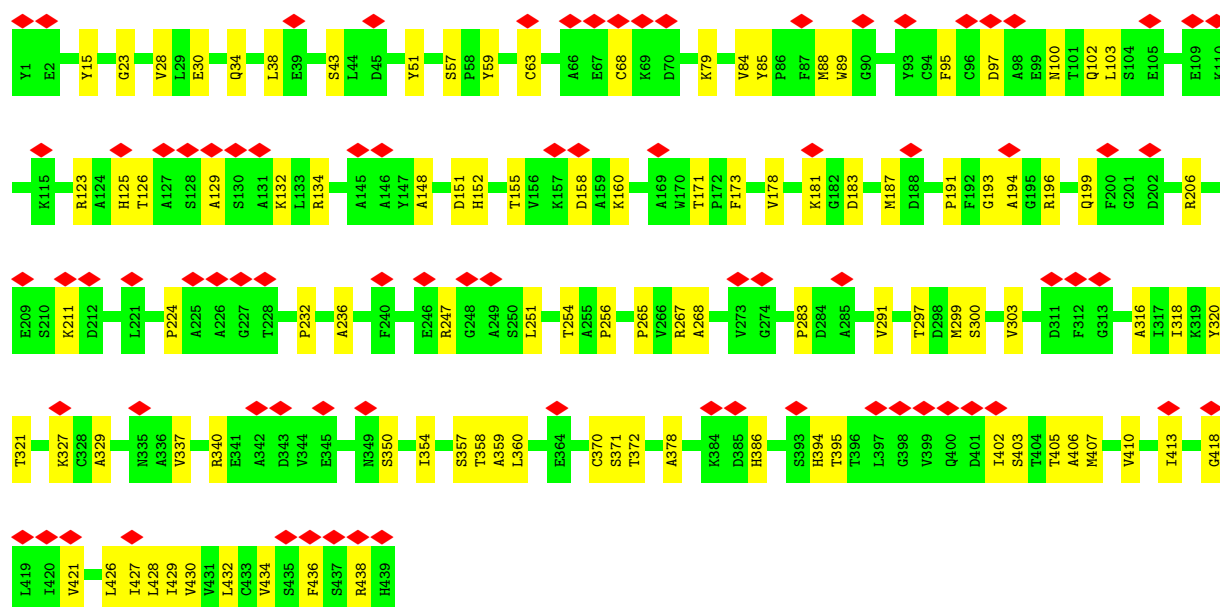
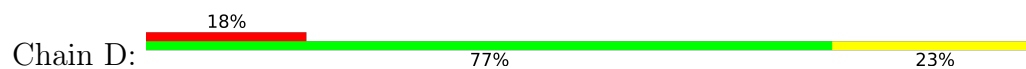


• Molecule 2: E1 glycoprotein

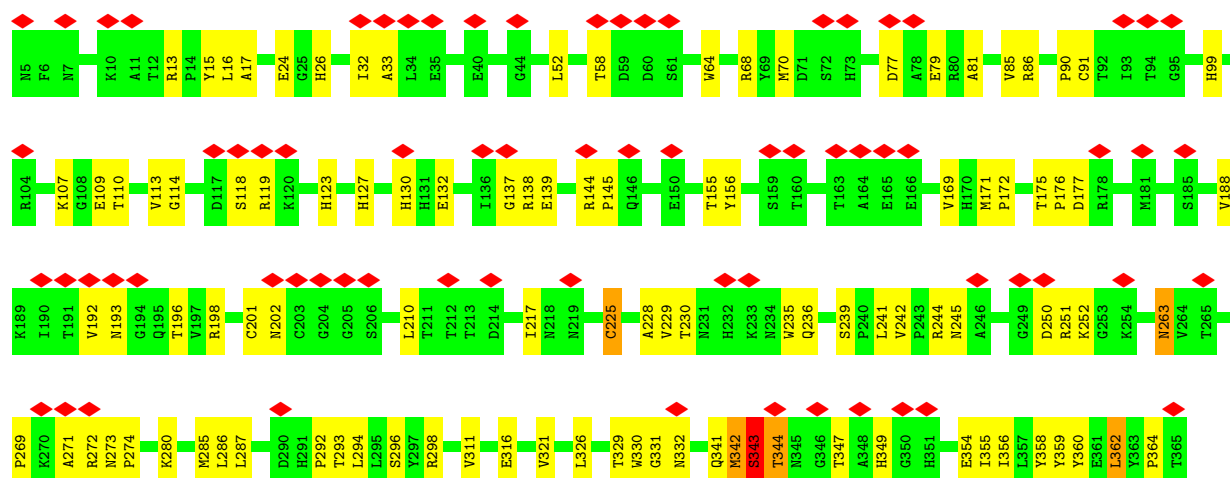


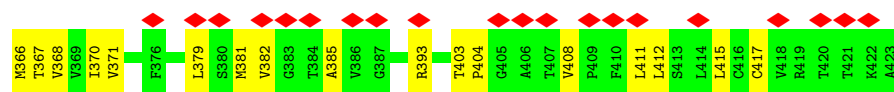


• Molecule 2: E1 glycoprotein



• Molecule 3: E2 glycoprotein

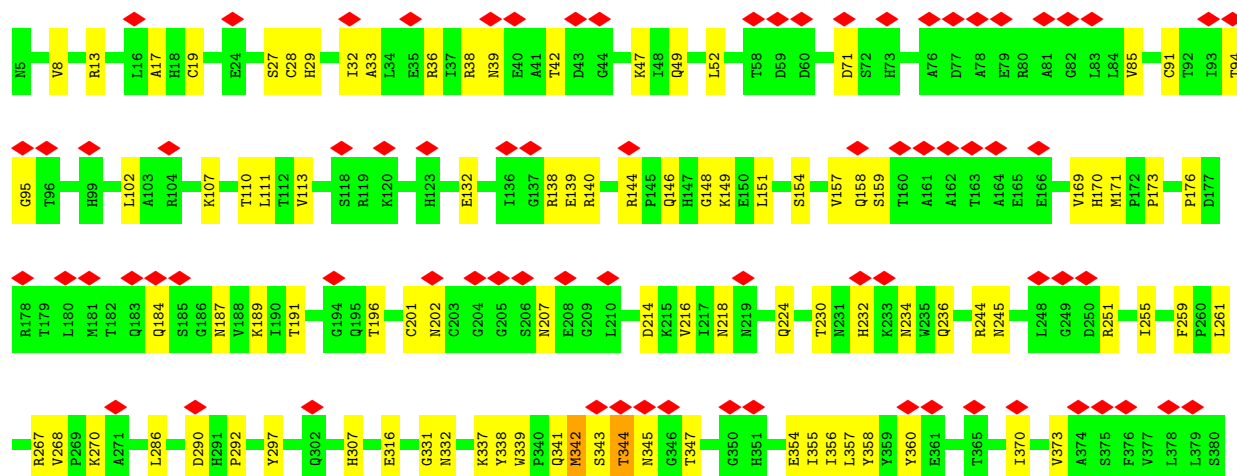
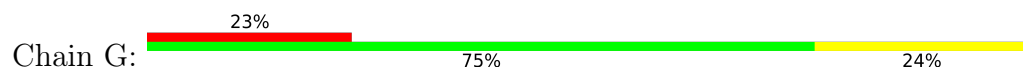


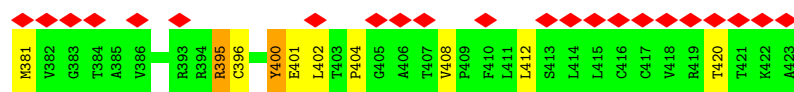


• Molecule 3: E2 glycoprotein

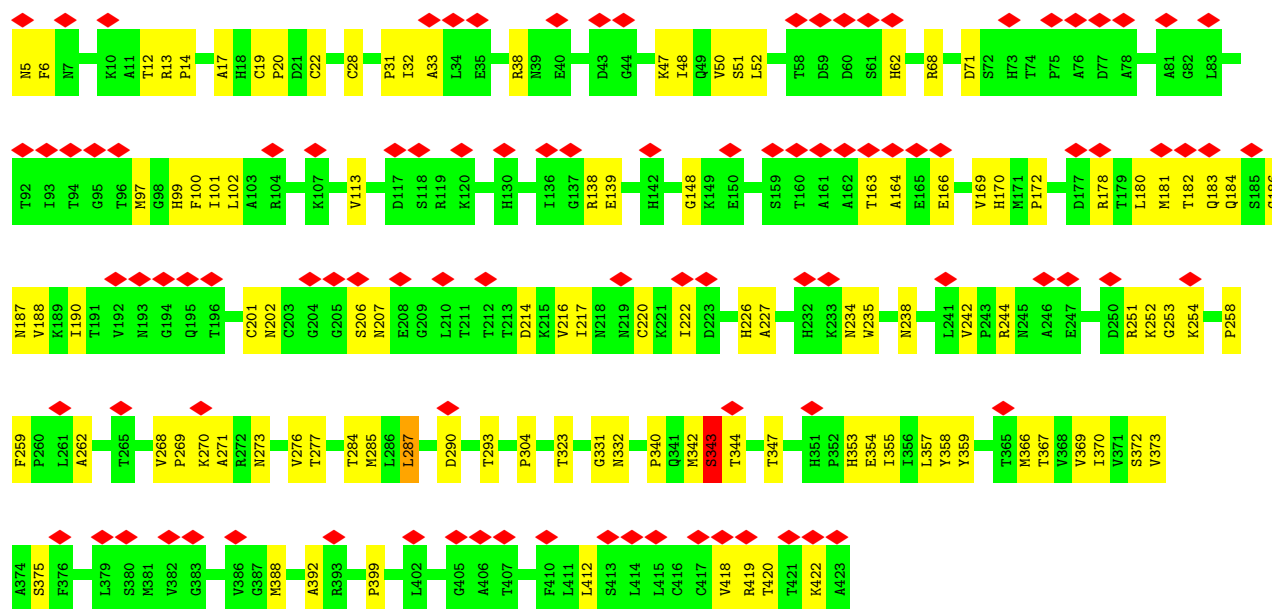
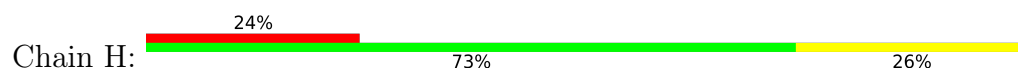


• Molecule 3: E2 glycoprotein

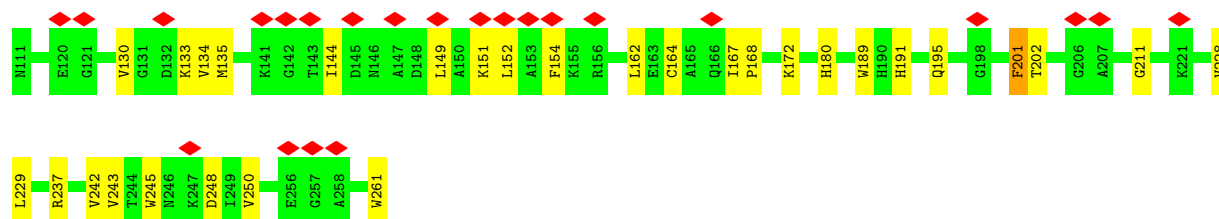




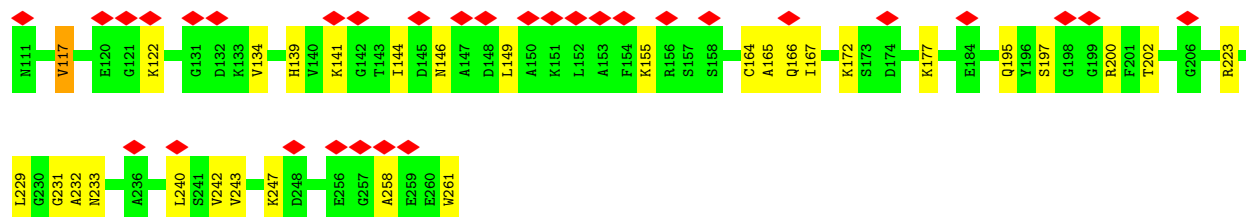
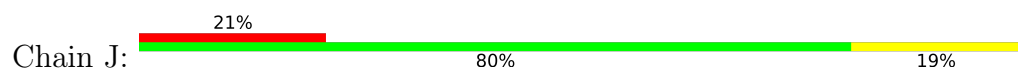
• Molecule 3: E2 glycoprotein



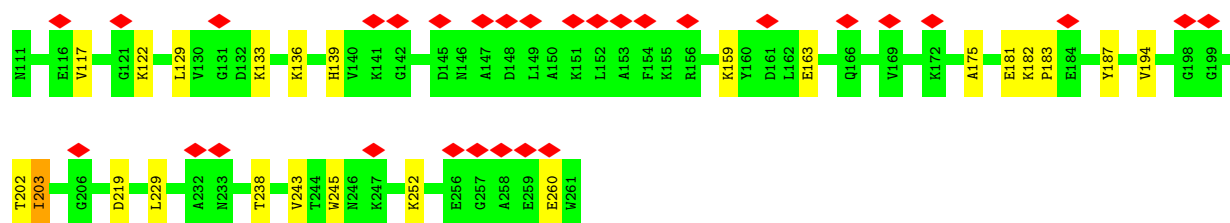
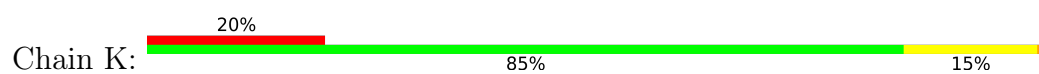
• Molecule 4: Capsid protein



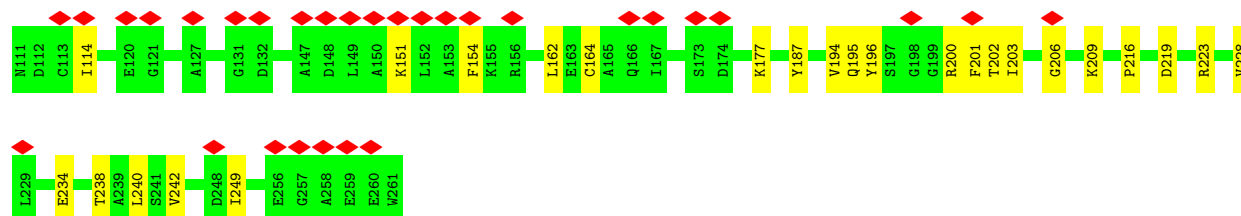
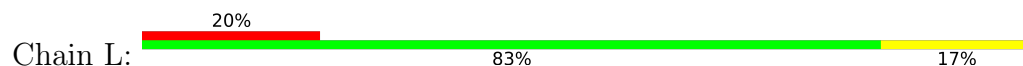
• Molecule 4: Capsid protein



• Molecule 4: Capsid protein



• Molecule 4: Capsid protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	22486	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	6.303	Depositor
Minimum map value	-3.983	Depositor
Average map value	0.055	Depositor
Map value standard deviation	0.636	Depositor
Recommended contour level	2	Depositor
Map size (Å)	841.8, 841.8, 841.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.403, 1.403, 1.403	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	M	0.29	0/2224	0.77	0/3020
1	N	0.28	0/2162	0.76	2/2932 (0.1%)
1	O	0.30	0/2223	0.80	2/3018 (0.1%)
1	P	0.30	0/2224	0.79	0/3020
2	A	0.30	0/3400	0.70	0/4643
2	B	0.29	0/3400	0.72	0/4643
2	C	0.30	0/3400	0.75	2/4643 (0.0%)
2	D	0.30	0/3400	0.75	2/4643 (0.0%)
3	E	0.31	0/3367	0.74	5/4592 (0.1%)
3	F	0.28	0/3367	0.71	2/4592 (0.0%)
3	G	0.30	0/3367	0.70	4/4592 (0.1%)
3	H	0.29	0/3367	0.71	5/4592 (0.1%)
4	I	0.30	0/1185	0.78	0/1599
4	J	0.29	0/1185	0.82	0/1599
4	K	0.36	0/1185	0.87	0/1599
4	L	0.28	0/1185	0.77	0/1599
All	All	0.30	0/40641	0.75	24/55326 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	GLU	CA-C-N	6.53	134.01	121.54
3	F	401	GLU	C-N-CA	6.53	134.01	121.54
3	H	343	SER	N-CA-C	6.50	124.64	110.80
2	D	370	CYS	CA-CB-SG	-6.19	100.17	114.40
3	E	342	MET	CA-C-N	5.96	132.93	121.54
3	E	342	MET	C-N-CA	5.96	132.93	121.54
1	O	215	HIS	CA-C-N	5.94	132.89	121.54
1	O	215	HIS	C-N-CA	5.94	132.89	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	96	CYS	CA-CB-SG	5.89	127.95	114.40
3	H	366	MET	CA-C-N	5.81	132.63	121.54
3	H	366	MET	C-N-CA	5.81	132.63	121.54
3	H	342	MET	CA-C-N	5.75	132.51	121.54
3	H	342	MET	C-N-CA	5.75	132.51	121.54
1	N	215	HIS	CA-C-N	5.48	132.01	121.54
1	N	215	HIS	C-N-CA	5.48	132.01	121.54
3	G	400	TYR	CA-C-N	5.48	132.00	121.54
3	G	400	TYR	C-N-CA	5.48	132.00	121.54
3	E	225	CYS	CA-CB-SG	5.37	126.76	114.40
3	E	344	THR	N-CA-C	5.24	121.95	110.80
2	D	63	CYS	CA-CB-SG	5.22	126.41	114.40
2	C	97	ASP	N-CA-C	5.19	117.73	111.40
3	G	343	SER	CA-C-N	5.09	131.26	121.54
3	G	343	SER	C-N-CA	5.09	131.26	121.54
3	E	362	LEU	CA-CB-CG	5.05	133.96	116.30

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	M	2169	0	2062	41	0
1	N	2111	0	2011	46	0
1	O	2168	0	2062	53	0
1	P	2169	0	2062	46	0
2	A	3318	0	3246	52	0
2	B	3318	0	3246	57	0
2	C	3318	0	3246	55	0
2	D	3318	0	3246	68	0
3	E	3280	0	3210	85	0
3	F	3280	0	3210	92	0
3	G	3280	0	3210	68	0
3	H	3280	0	3210	77	0
4	I	1157	0	1137	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	1157	0	1137	20	0
4	K	1157	0	1137	14	0
4	L	1157	0	1137	18	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
5	G	14	0	13	0	0
5	H	14	0	13	1	0
5	M	14	0	13	0	0
5	N	14	0	13	0	0
5	O	14	0	13	0	0
5	P	14	0	13	0	0
All	All	39805	0	38725	746	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (746) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:169:VAL:O	3:F:253:GLY:HA3	1.59	1.02
3:E:355:ILE:O	3:E:358:TYR:HB2	1.72	0.90
3:F:356:ILE:O	3:F:359:TYR:HB3	1.72	0.90
3:H:148:GLY:HA3	3:H:268:VAL:O	1.74	0.87
2:C:299:MET:HA	2:C:319:LYS:O	1.79	0.83
3:H:187:ASN:HA	3:H:217:ILE:O	1.81	0.80
4:I:154:PHE:HA	4:I:164:CYS:O	1.82	0.80
1:N:44:ALA:HA	1:N:291:THR:O	1.82	0.79
2:A:432:LEU:O	2:A:436:PHE:HB2	1.86	0.76
3:F:169:VAL:O	3:F:253:GLY:CA	2.35	0.75
3:H:14:PRO:HD3	3:H:68:ARG:HH21	1.54	0.72
1:O:204:VAL:HA	1:O:272:HIS:O	1.89	0.72
2:A:49:CYS:SG	2:A:50:GLU:N	2.63	0.72
1:N:64:ARG:HH12	1:N:200:ALA:HB2	1.55	0.71
3:F:83:LEU:HA	3:F:114:GLY:O	1.90	0.71
2:D:360:LEU:HD11	2:D:402:ILE:H	1.55	0.70
1:M:64:ARG:HE	3:F:26:HIS:HB3	1.57	0.68
2:D:428:LEU:HD11	3:H:392:ALA:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:30:GLU:HB3	2:A:136:LEU:HB3	1.76	0.68
2:B:262:ALA:O	2:B:266:VAL:HA	1.95	0.67
4:K:229:LEU:HD11	4:K:243:VAL:HG23	1.77	0.67
2:A:196:ARG:HH12	2:A:199:GLN:HE21	1.43	0.66
1:N:143:CYS:SG	1:N:275:HIS:NE2	2.68	0.66
1:O:84:ARG:HH22	3:E:193:ASN:H	1.43	0.66
2:B:340:ARG:HH12	2:B:357:SER:HB2	1.61	0.66
3:H:183:GLN:HE21	3:H:222:ILE:H	1.42	0.66
1:P:196:HIS:NE2	1:P:198:GLU:O	2.29	0.65
3:E:272:ARG:NH1	3:E:273:ASN:OD1	2.29	0.65
1:O:151:VAL:HA	1:O:171:GLU:O	1.96	0.65
1:M:123:ILE:O	1:M:180:PRO:HA	1.96	0.65
2:B:183:ASP:OD2	2:B:247:ARG:NH2	2.29	0.65
4:I:133:LYS:NZ	4:I:134:VAL:O	2.29	0.64
1:N:96:GLN:HG2	1:N:109:LEU:HB3	1.78	0.64
1:P:151:VAL:HG11	1:P:183:MET:HG2	1.80	0.64
2:B:90:GLY:HA3	3:F:177:ASP:HA	1.79	0.64
2:B:196:ARG:HH21	2:B:199:GLN:HE21	1.46	0.64
1:P:123:ILE:O	1:P:180:PRO:HA	1.97	0.63
4:I:228:VAL:HA	4:I:242:VAL:HG22	1.80	0.63
1:O:223:ASP:O	1:O:230:ARG:HA	1.99	0.63
1:N:202:GLN:HB2	1:N:226:ALA:HB2	1.80	0.63
3:F:421:THR:HB	2:D:438:ARG:HB3	1.81	0.63
1:P:106:ARG:NH2	1:P:130:ASP:OD2	2.32	0.63
2:D:178:VAL:HG11	2:D:187:MET:HE2	1.79	0.63
3:H:138:ARG:NH1	3:H:331:GLY:O	2.32	0.63
3:H:271:ALA:HB2	3:H:331:GLY:HA3	1.80	0.62
3:H:269:PRO:O	3:H:332:ASN:ND2	2.33	0.62
1:M:230:ARG:HH12	1:M:244:VAL:H	1.46	0.62
1:O:151:VAL:HG22	1:O:171:GLU:HB2	1.81	0.62
3:E:144:ARG:NH1	3:F:25:GLY:O	2.33	0.62
2:C:160:LYS:HB2	2:C:281:ASP:HB3	1.82	0.62
2:A:59:TYR:HB3	2:A:103:LEU:HB3	1.82	0.61
2:A:416:GLY:HA2	3:E:381:MET:HE1	1.81	0.61
2:C:30:GLU:HB3	2:C:136:LEU:HB2	1.81	0.61
2:D:299:MET:HE1	2:D:372:THR:HB	1.82	0.61
2:D:340:ARG:NH2	2:D:357:SER:OG	2.33	0.61
2:C:428:LEU:HD22	3:G:395:ARG:HG2	1.83	0.61
3:G:337:LYS:HZ3	3:G:339:TRP:HB2	1.65	0.61
1:M:209:GLN:HB2	1:M:268:ILE:HB	1.82	0.60
3:H:184:GLN:HB2	3:H:187:ASN:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:181:GLU:HG3	4:K:183:PRO:HD3	1.83	0.60
2:D:403:SER:HG	2:D:406:ALA:H	1.49	0.60
3:H:190:ILE:O	3:H:214:ASP:HA	2.02	0.60
3:H:370:ILE:HA	3:H:373:VAL:HG12	1.82	0.60
2:A:57:SER:HB3	3:E:244:ARG:HG3	1.84	0.60
1:O:51:LEU:O	1:O:255:SER:HA	2.01	0.60
2:B:229:VAL:HG21	3:F:243:PRO:HD3	1.83	0.60
1:M:112:SER:O	1:M:115:HIS:ND1	2.30	0.60
1:O:209:GLN:HB2	1:O:268:ILE:HB	1.83	0.60
1:P:262:GLU:HG3	1:P:264:ALA:H	1.66	0.60
2:A:90:GLY:HA3	3:E:177:ASP:HA	1.83	0.60
4:I:135:MET:HE2	4:I:162:LEU:HD22	1.84	0.60
3:H:14:PRO:HG3	3:H:68:ARG:HB3	1.82	0.60
1:P:50:VAL:HG22	1:P:257:ARG:HG2	1.85	0.59
2:C:130:SER:HA	2:C:148:ALA:H	1.67	0.59
3:G:401:GLU:HG2	3:G:402:LEU:H	1.67	0.59
1:N:245:ASN:HB3	1:N:257:ARG:HH22	1.68	0.59
3:F:274:PRO:HB3	3:F:287:LEU:HD12	1.84	0.59
2:D:97:ASP:O	2:D:100:ASN:ND2	2.35	0.59
3:F:248:LEU:HD11	3:F:251:ARG:HH11	1.68	0.59
1:P:225:TYR:HE1	1:P:231:ARG:HH12	1.50	0.59
4:J:195:GLN:NE2	4:J:197:SER:OG	2.36	0.59
1:N:34:SER:HB2	1:N:281:HIS:O	2.02	0.58
2:A:297:THR:O	2:A:321:THR:OG1	2.22	0.58
4:K:159:LYS:O	4:K:252:LYS:NZ	2.35	0.58
1:M:64:ARG:NH2	3:F:24:GLU:O	2.37	0.58
4:J:166:GLN:NE2	4:J:167:ILE:O	2.36	0.58
2:C:13:VAL:HG11	2:C:393:SER:HB3	1.84	0.58
2:A:404:THR:OG1	2:A:405:THR:N	2.37	0.58
3:F:322:PRO:HG2	3:F:325:GLY:H	1.68	0.58
3:G:173:PRO:HB3	3:G:245:ASN:HA	1.84	0.58
3:G:214:ASP:OD1	3:G:214:ASP:N	2.36	0.58
3:E:201:CYS:HB3	3:E:225:CYS:HA	1.84	0.58
1:M:67:ASP:HB3	1:M:199:GLU:HG2	1.86	0.58
3:F:280:LYS:HZ3	3:F:281:ASN:HB2	1.69	0.58
3:G:412:LEU:HD22	3:G:420:THR:HG22	1.86	0.58
3:H:48:ILE:HB	3:H:101:ILE:HB	1.86	0.58
1:P:266:GLU:O	2:C:211:LYS:NZ	2.37	0.58
3:E:296:SER:HG	3:E:329:THR:HG1	1.50	0.58
1:N:75:ASP:OD2	1:N:84:ARG:NH1	2.37	0.58
3:F:167:ILE:HG13	3:F:255:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:13:ARG:HH22	3:E:172:PRO:HG3	1.70	0.57
2:A:134:ARG:NH1	2:A:141:ASN:OD1	2.35	0.57
2:C:339:ILE:HD11	2:C:354:ILE:HB	1.86	0.57
3:H:355:ILE:O	3:H:359:TYR:N	2.38	0.57
1:P:151:VAL:HA	1:P:171:GLU:O	2.04	0.57
3:F:178:ARG:NH1	3:F:225:CYS:O	2.38	0.57
1:M:96:GLN:NE2	1:M:109:LEU:O	2.38	0.57
1:O:208:ARG:NH1	1:O:264:ALA:O	2.38	0.57
3:F:272:ARG:HG2	3:F:288:TYR:HB2	1.85	0.57
1:M:106:ARG:NH2	1:M:130:ASP:OD2	2.38	0.57
1:P:199:GLU:HG2	1:P:201:GLN:HG3	1.87	0.57
3:H:412:LEU:HD22	3:H:420:THR:HG22	1.87	0.57
2:A:57:SER:OG	3:E:242:VAL:O	2.22	0.57
3:E:176:PRO:HA	3:E:228:ALA:HA	1.87	0.56
1:N:64:ARG:HG2	1:N:67:ASP:HB2	1.88	0.56
1:N:271:CYS:O	1:N:283:ARG:HA	2.05	0.56
3:E:272:ARG:HD3	2:B:235:GLN:HE21	1.71	0.56
3:E:349:HIS:ND1	3:E:358:TYR:OH	2.31	0.56
3:E:355:ILE:HG23	3:E:356:ILE:HD12	1.87	0.56
2:B:207:THR:HG22	2:B:210:SER:HB3	1.88	0.56
3:G:138:ARG:NH1	3:G:331:GLY:O	2.38	0.56
4:L:114:ILE:HG22	4:L:216:PRO:HD2	1.88	0.56
1:M:222:LEU:HD11	1:M:230:ARG:HB3	1.87	0.56
1:O:116:ASP:O	1:O:188:ARG:NH1	2.39	0.56
2:B:134:ARG:NH1	2:B:141:ASN:OD1	2.38	0.56
2:B:148:ALA:HA	2:B:163:VAL:HG23	1.87	0.56
2:D:59:TYR:HB3	2:D:103:LEU:HB3	1.86	0.56
4:L:203:ILE:HG23	4:L:240:LEU:HD11	1.86	0.56
1:N:60:TRP:NE1	1:N:67:ASP:OD2	2.38	0.56
1:N:34:SER:O	1:N:282:GLU:HA	2.04	0.56
3:E:272:ARG:NH1	3:E:273:ASN:O	2.39	0.56
3:F:69:TYR:OH	3:F:119:ARG:NH2	2.32	0.56
3:G:171:MET:HE3	3:G:232:HIS:HB3	1.86	0.56
3:G:171:MET:SD	3:G:245:ASN:ND2	2.79	0.56
1:P:112:SER:O	1:P:115:HIS:ND1	2.36	0.56
3:E:86:ARG:HG2	3:E:90:PRO:HA	1.88	0.56
1:N:66:HIS:HB3	1:N:69:GLN:HB2	1.88	0.56
3:F:201:CYS:HA	3:F:225:CYS:HA	1.88	0.56
2:C:387:ILE:HD11	3:G:338:TYR:HB3	1.87	0.56
3:E:139:GLU:OE1	3:E:332:ASN:ND2	2.39	0.56
2:A:299:MET:HA	2:A:319:LYS:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:GLY:O	2:C:243:TRP:HB2	2.07	0.55
3:H:169:VAL:O	3:H:253:GLY:HA3	2.05	0.55
2:B:166:MET:SD	2:B:166:MET:N	2.77	0.55
3:G:148:GLY:HA2	3:G:270:LYS:HG2	1.87	0.55
1:O:86:ARG:NH1	1:O:89:ASP:OD2	2.39	0.55
1:O:112:SER:O	1:O:115:HIS:ND1	2.34	0.55
3:E:367:THR:HG23	3:E:370:ILE:HD12	1.87	0.55
4:I:144:ILE:HG12	4:I:149:LEU:HD12	1.89	0.55
3:F:296:SER:HB2	3:F:308:GLU:HG3	1.88	0.55
4:J:139:HIS:NE2	4:J:261:TRP:OXT	2.40	0.55
2:B:174:ASP:HB2	2:B:186:ASN:HD21	1.70	0.55
2:C:9:ASN:ND2	2:C:271:CYS:O	2.40	0.55
2:A:350:SER:OG	2:A:351:GLN:N	2.38	0.55
3:E:198:ARG:HB2	3:E:210:LEU:HD12	1.87	0.55
3:F:46:LEU:HB3	3:F:48:ILE:HD11	1.89	0.55
1:N:204:VAL:HG13	1:N:224:LEU:HB3	1.88	0.55
1:O:76:LEU:HD23	1:O:87:LEU:HD22	1.89	0.55
2:D:410:VAL:HA	2:D:413:ILE:HG22	1.87	0.55
1:N:223:ASP:HB2	1:N:231:ARG:HB2	1.88	0.55
2:B:155:THR:HA	2:B:159:ALA:O	2.07	0.55
3:F:66:LYS:NZ	3:F:79:GLU:OE1	2.37	0.55
2:D:57:SER:HB3	3:H:244:ARG:HG3	1.89	0.55
3:E:85:VAL:HG23	3:E:91:CYS:HB2	1.89	0.55
2:D:183:ASP:OD2	2:D:247:ARG:NH1	2.40	0.55
1:O:264:ALA:HA	2:D:211:LYS:HD3	1.89	0.54
3:E:274:PRO:HG3	3:E:285:MET:HE3	1.88	0.54
4:I:133:LYS:HZ3	4:I:164:CYS:HA	1.73	0.54
1:O:139:HIS:ND1	1:O:145:LEU:O	2.40	0.54
3:G:404:PRO:HD3	4:K:133:LYS:HE3	1.89	0.54
2:A:427:ILE:HA	2:A:430:VAL:HG22	1.90	0.54
2:B:112:GLU:OE1	2:B:115:LYS:NZ	2.41	0.54
3:G:202:ASN:O	3:G:224:GLN:NE2	2.40	0.54
1:N:77:SER:HB3	1:N:84:ARG:HB3	1.90	0.54
1:O:70:ARG:NH2	1:O:194:ASP:OD1	2.39	0.54
3:G:144:ARG:HH21	3:G:267:ARG:HE	1.54	0.54
4:K:182:LYS:NZ	4:K:245:TRP:O	2.39	0.54
3:H:182:THR:OG1	3:H:184:GLN:NE2	2.38	0.54
2:B:183:ASP:N	2:B:183:ASP:OD1	2.35	0.54
2:B:130:SER:HA	2:B:147:TYR:HA	1.89	0.54
3:G:157:VAL:HG13	3:G:159:SER:H	1.73	0.54
4:I:195:GLN:O	4:I:201:PHE:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:285:MET:HE1	3:H:287:LEU:HD23	1.90	0.54
1:N:32:SER:OG	1:N:33:SER:N	2.40	0.53
1:O:206:TRP:HB2	1:O:222:LEU:HB3	1.90	0.53
2:C:105:GLU:OE1	3:G:244:ARG:NH1	2.42	0.53
4:I:152:LEU:HD11	4:I:168:PRO:HG3	1.89	0.53
3:H:13:ARG:HH11	3:H:234:ASN:HB3	1.73	0.53
3:H:178:ARG:HH12	3:H:226:HIS:HA	1.74	0.53
3:F:153:CYS:O	3:F:263:ASN:HA	2.08	0.53
2:C:51:TYR:HB3	2:C:203:ILE:HD13	1.90	0.53
1:O:42:SER:HG	1:O:291:THR:HG1	1.56	0.53
1:O:115:HIS:HA	1:O:194:ASP:HB2	1.89	0.53
3:E:412:LEU:HA	3:E:415:LEU:HB2	1.89	0.53
2:C:263:THR:O	2:C:267:ARG:NH2	2.41	0.53
3:G:95:GLY:H	3:G:102:LEU:HB2	1.74	0.53
2:D:88:MET:HE3	2:D:89:TRP:HD1	1.73	0.53
3:H:188:VAL:O	3:H:216:VAL:HA	2.08	0.53
1:M:66:HIS:HB3	1:M:69:GLN:HB2	1.89	0.53
2:B:40:PRO:HA	2:B:127:ALA:HA	1.90	0.53
2:B:178:VAL:HG11	2:B:187:MET:HE2	1.91	0.53
3:F:183:GLN:HE21	3:F:222:ILE:HG12	1.74	0.53
3:H:170:HIS:HB2	3:H:251:ARG:HB3	1.90	0.53
1:N:72:VAL:HG12	1:N:138:LEU:HD23	1.91	0.53
3:E:169:VAL:O	3:E:252:LYS:O	2.26	0.53
3:F:183:GLN:HE22	3:F:221:LYS:HB3	1.73	0.53
3:E:17:ALA:HB3	3:E:33:ALA:HB3	1.90	0.53
1:O:142:TYR:OH	1:O:202:GLN:NE2	2.41	0.53
1:M:62:GLN:HG2	1:M:249:PHE:HZ	1.74	0.52
1:P:209:GLN:HB2	1:P:268:ILE:HB	1.91	0.52
3:F:118:SER:OG	3:F:119:ARG:NH1	2.42	0.52
3:F:43:ASP:OD1	3:F:43:ASP:N	2.41	0.52
2:D:407:MET:SD	2:D:407:MET:N	2.80	0.52
1:M:72:VAL:HA	1:M:137:ASN:O	2.09	0.52
3:E:354:GLU:O	3:E:358:TYR:N	2.42	0.52
2:B:66:ALA:H	2:B:101:THR:HG21	1.73	0.52
3:F:201:CYS:O	3:F:207:ASN:ND2	2.42	0.52
3:G:32:ILE:HD12	3:G:113:VAL:HG23	1.91	0.52
2:C:239:GLY:O	2:C:243:TRP:CB	2.58	0.52
3:G:184:GLN:O	3:G:187:ASN:ND2	2.42	0.52
3:G:27:SER:OG	3:G:28:CYS:N	2.43	0.52
2:D:95:PHE:HZ	3:H:202:ASN:HB2	1.74	0.52
1:N:163:ARG:H	1:N:174:VAL:HB	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:13:ARG:HH22	3:H:172:PRO:HG3	1.74	0.52
1:N:72:VAL:HA	1:N:137:ASN:O	2.10	0.52
3:E:24:GLU:OE2	3:E:26:HIS:NE2	2.42	0.52
3:F:412:LEU:HA	3:F:415:LEU:HG	1.91	0.52
3:H:180:LEU:HD12	3:H:227:ALA:HB1	1.92	0.52
2:A:282:ILE:HD12	2:A:283:PRO:HD2	1.92	0.52
3:F:163:THR:OG1	3:F:164:ALA:N	2.43	0.52
4:J:172:LYS:HB2	4:L:234:GLU:HB2	1.92	0.52
2:D:129:ALA:O	2:D:148:ALA:N	2.43	0.52
3:H:262:ALA:HA	5:H:501:NAG:H82	1.91	0.52
2:A:310:SER:H	3:E:341:GLN:HE21	1.58	0.52
4:J:134:VAL:O	4:J:164:CYS:HA	2.10	0.52
4:L:219:ASP:OD1	4:L:223:ARG:N	2.43	0.52
3:G:146:GLN:O	3:G:267:ARG:NH1	2.43	0.51
2:D:265:PRO:O	2:D:267:ARG:NH1	2.41	0.51
4:L:194:VAL:HG12	4:L:203:ILE:HG22	1.92	0.51
1:N:136:CYS:O	1:N:148:SER:HA	2.10	0.51
2:C:191:PRO:HG2	2:C:194:ALA:HB3	1.93	0.51
2:C:433:CYS:HA	2:C:436:PHE:HB3	1.93	0.51
3:G:148:GLY:HA3	3:G:268:VAL:O	2.10	0.51
1:O:247:ASN:HB2	1:O:251:ARG:HH11	1.75	0.51
4:J:200:ARG:NH2	4:J:240:LEU:O	2.44	0.51
2:D:51:TYR:OH	2:D:236:ALA:O	2.29	0.51
1:P:85:ARG:HH22	1:P:100:GLU:HB2	1.75	0.51
1:P:202:GLN:HB3	1:P:226:ALA:HB2	1.93	0.51
2:C:34:GLN:HB2	2:C:132:LYS:HB3	1.91	0.51
2:C:107:HIS:NE2	2:C:109:GLU:OE2	2.43	0.51
3:G:347:THR:OG1	3:G:354:GLU:O	2.28	0.51
2:D:316:ALA:HB3	2:D:354:ILE:HG22	1.91	0.51
2:B:265:PRO:O	2:B:267:ARG:NH1	2.43	0.51
3:F:169:VAL:HA	3:F:237:TYR:HA	1.92	0.51
3:G:17:ALA:HB3	3:G:33:ALA:HB3	1.93	0.51
1:O:207:ASP:O	1:O:269:TYR:HA	2.11	0.51
1:P:245:ASN:HB3	1:P:257:ARG:HH11	1.76	0.51
2:C:418:GLY:HA2	2:C:421:VAL:HG12	1.93	0.51
3:H:186:GLY:O	3:H:220:CYS:N	2.40	0.51
1:N:49:ALA:HB3	1:N:258:ILE:HB	1.93	0.51
1:O:163:ARG:H	1:O:174:VAL:HB	1.76	0.51
4:K:139:HIS:NE2	4:K:260:GLU:OE2	2.44	0.51
2:D:337:VAL:HG23	2:D:358:THR:HB	1.92	0.51
2:D:394:HIS:HD2	2:D:395:THR:HG23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:68:ARG:HE	1:N:197:LEU:HG	1.76	0.51
3:F:102:LEU:HD21	3:F:156:TYR:HB2	1.93	0.51
3:F:171:MET:HE1	3:F:245:ASN:HD22	1.76	0.51
1:N:84:ARG:NH2	3:G:191:THR:OG1	2.45	0.50
2:A:410:VAL:HA	2:A:413:ILE:HG12	1.93	0.50
2:A:432:LEU:O	2:A:436:PHE:CB	2.57	0.50
3:E:359:TYR:HA	3:E:362:LEU:HG	1.93	0.50
3:F:16:LEU:HD21	3:F:71:ASP:HA	1.92	0.50
2:C:77:SER:O	2:C:105:GLU:HA	2.10	0.50
3:G:400:TYR:HE1	3:G:408:VAL:HG22	1.76	0.50
3:E:360:TYR:HA	3:E:364:PRO:HB3	1.92	0.50
3:G:355:ILE:O	3:G:358:TYR:HB2	2.10	0.50
4:K:136:LYS:O	4:K:163:GLU:HB2	2.11	0.50
3:H:188:VAL:HG22	3:H:217:ILE:HB	1.93	0.50
2:B:388:VAL:HG21	3:F:341:GLN:HE21	1.77	0.50
3:G:154:SER:HB2	3:G:261:LEU:HD21	1.93	0.50
3:E:271:ALA:HB2	3:E:331:GLY:HA3	1.94	0.50
2:B:184:VAL:HG12	2:B:251:LEU:HD12	1.93	0.50
3:F:201:CYS:HB2	3:F:207:ASN:HB2	1.92	0.50
2:C:191:PRO:HB3	2:D:151:ASP:HB2	1.94	0.50
3:F:193:ASN:O	3:F:195:GLN:NE2	2.45	0.50
2:C:88:MET:HG2	3:G:176:PRO:HD2	1.93	0.50
3:H:139:GLU:HG3	3:H:293:THR:HG23	1.93	0.50
4:J:195:GLN:OE1	4:J:202:THR:OG1	2.23	0.49
2:D:155:THR:HB	2:D:160:LYS:HG2	1.94	0.49
3:H:412:LEU:HD13	3:H:420:THR:HA	1.94	0.49
1:P:199:GLU:OE2	1:P:201:GLN:NE2	2.42	0.49
3:F:139:GLU:HG3	3:F:293:THR:HG23	1.95	0.49
2:C:160:LYS:NZ	2:D:193:GLY:O	2.40	0.49
3:G:356:ILE:O	3:G:360:TYR:N	2.41	0.49
3:G:370:ILE:HA	3:G:373:VAL:HG12	1.94	0.49
1:O:190:HIS:HB3	1:O:195:ARG:HH21	1.77	0.49
2:B:284:ASP:HA	2:B:287:PHE:HD2	1.77	0.49
4:J:177:LYS:HB2	4:J:223:ARG:HG2	1.94	0.49
2:C:325:LYS:HA	2:C:346:VAL:O	2.12	0.49
1:O:215:HIS:CD2	1:O:216:ASP:H	2.30	0.49
2:C:347:GLU:OE2	2:C:350:SER:OG	2.29	0.49
1:O:275:HIS:HB3	1:O:280:LEU:HB2	1.93	0.49
2:C:102:GLN:HE22	2:C:104:SER:HB3	1.77	0.49
3:H:12:THR:O	3:H:68:ARG:NH2	2.45	0.49
1:O:49:ALA:HB2	1:O:261:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:167:ILE:O	4:I:172:LYS:NZ	2.38	0.49
4:I:180:HIS:CE1	4:I:248:ASP:H	2.29	0.49
2:B:282:ILE:HD12	2:B:283:PRO:HD2	1.95	0.49
3:G:13:ARG:HH21	3:G:234:ASN:HB2	1.77	0.49
2:D:171:THR:HG22	2:D:173:PHE:H	1.76	0.49
1:N:199:GLU:HG2	1:N:201:GLN:HB2	1.94	0.49
3:F:39:ASN:OD1	3:F:39:ASN:N	2.44	0.49
2:A:184:VAL:HG23	2:A:251:LEU:HD12	1.93	0.49
1:M:60:TRP:NE1	1:M:67:ASP:OD2	2.45	0.49
2:B:38:LEU:HB2	2:B:268:ALA:HB3	1.93	0.49
1:O:112:SER:HG	1:O:115:HIS:HD1	1.61	0.49
3:E:198:ARG:HA	3:E:210:LEU:HA	1.95	0.49
2:B:358:THR:HG22	2:B:360:LEU:H	1.78	0.49
2:C:134:ARG:NH1	2:C:141:ASN:OD1	2.38	0.49
2:A:410:VAL:HG23	2:A:413:ILE:HD11	1.95	0.48
2:D:158:ASP:HB3	2:D:283:PRO:HG3	1.94	0.48
2:D:418:GLY:HA2	2:D:421:VAL:HG22	1.95	0.48
1:O:50:VAL:HG12	1:O:257:ARG:HG2	1.94	0.48
2:C:406:ALA:HA	2:C:409:TRP:HB2	1.95	0.48
3:G:110:THR:OG1	3:G:111:LEU:N	2.45	0.48
2:A:217:THR:O	2:A:235:GLN:NE2	2.46	0.48
3:F:42:THR:HG1	3:F:154:SER:H	1.55	0.48
4:J:134:VAL:HB	4:J:165:ALA:HB3	1.95	0.48
3:G:47:LYS:NZ	3:G:259:PHE:O	2.42	0.48
2:D:256:PRO:HG3	3:H:304:PRO:HD3	1.96	0.48
1:M:60:TRP:HD1	1:M:142:TYR:HE1	1.60	0.48
1:O:195:ARG:H	1:O:197:LEU:HD13	1.78	0.48
2:A:78:CYS:HA	2:A:104:SER:O	2.12	0.48
1:N:156:THR:OG1	1:N:158:ASP:OD1	2.29	0.48
1:O:120:SER:HB2	1:O:184:THR:HA	1.94	0.48
2:A:16:LYS:HE3	2:A:339:ILE:O	2.13	0.48
3:E:77:ASP:O	3:E:118:SER:OG	2.30	0.48
2:D:432:LEU:O	2:D:436:PHE:HB2	2.14	0.48
3:H:22:CYS:SG	3:H:28:CYS:N	2.86	0.48
3:H:181:MET:HE3	3:H:222:ILE:HG23	1.95	0.48
3:H:277:THR:HG1	3:H:284:THR:HG1	1.53	0.48
4:J:233:ASN:OD1	4:J:233:ASN:N	2.47	0.48
2:D:57:SER:OG	3:H:242:VAL:O	2.28	0.48
1:P:205:HIS:HB2	1:P:272:HIS:HB2	1.96	0.48
3:E:107:LYS:HE2	3:E:132:GLU:HG3	1.94	0.48
3:F:148:GLY:HA2	3:F:270:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:355:ILE:HA	3:F:358:TYR:HB2	1.96	0.48
3:G:19:CYS:O	3:G:27:SER:OG	2.28	0.48
1:M:195:ARG:HE	3:E:64:TRP:HZ2	1.60	0.48
1:O:136:CYS:O	1:O:148:SER:HA	2.13	0.48
1:O:236:PRO:HA	1:O:239:ARG:HG2	1.96	0.48
3:E:347:THR:HG21	3:E:358:TYR:HA	1.95	0.48
2:C:59:TYR:HB3	2:C:103:LEU:HB3	1.94	0.48
2:D:43:SER:HB2	2:D:123:ARG:HB2	1.95	0.48
2:A:21:ARG:NH2	2:A:284:ASP:OD1	2.46	0.48
3:F:14:PRO:O	3:F:236:GLN:NE2	2.47	0.48
3:F:154:SER:HA	3:F:262:ALA:O	2.14	0.48
2:A:186:ASN:HB2	2:A:251:LEU:HD21	1.96	0.47
2:B:57:SER:N	3:F:238:ASN:OD1	2.46	0.47
2:B:178:VAL:HG13	2:B:185:TYR:HB2	1.97	0.47
2:B:407:MET:HA	2:B:410:VAL:HG22	1.95	0.47
3:F:364:PRO:C	3:F:366:MET:H	2.22	0.47
3:F:412:LEU:HD23	3:F:415:LEU:HD11	1.95	0.47
3:H:19:CYS:HA	3:H:20:PRO:HD3	1.76	0.47
3:E:32:ILE:HD12	3:E:113:VAL:HG13	1.95	0.47
4:J:117:VAL:HG23	4:J:144:ILE:HA	1.96	0.47
2:C:21:ARG:NH1	2:C:284:ASP:OD1	2.48	0.47
1:M:135:THR:HA	1:M:149:LEU:O	2.15	0.47
1:P:224:LEU:HD21	1:P:244:VAL:HG11	1.97	0.47
2:C:53:THR:HG21	2:C:235:GLN:HE22	1.79	0.47
2:D:426:LEU:HA	2:D:429:ILE:HG22	1.96	0.47
2:A:369:VAL:O	2:A:372:THR:HB	2.15	0.47
3:E:145:PRO:HG3	3:E:269:PRO:HB3	1.96	0.47
4:J:122:LYS:HB3	4:J:122:LYS:HE3	1.73	0.47
2:D:125:HIS:ND1	2:D:126:THR:OG1	2.43	0.47
4:L:196:TYR:HA	4:L:200:ARG:O	2.14	0.47
1:N:131:GLU:HG2	1:N:154:GLU:HA	1.95	0.47
2:A:262:ALA:O	2:A:266:VAL:HA	2.15	0.47
1:M:68:ARG:HE	1:M:197:LEU:HB2	1.78	0.47
3:F:12:THR:HB	3:F:53:GLN:HE22	1.78	0.47
3:F:114:GLY:HA2	3:F:123:HIS:O	2.15	0.47
3:G:347:THR:HB	3:G:357:LEU:HB2	1.96	0.47
2:D:38:LEU:HB2	2:D:268:ALA:HB3	1.96	0.47
2:D:79:LYS:HA	2:D:79:LYS:HD3	1.69	0.47
3:H:201:CYS:HB2	3:H:207:ASN:HA	1.97	0.47
1:O:205:HIS:HB3	1:O:220:ARG:NH2	2.30	0.47
3:E:155:THR:OG1	3:E:156:TYR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:17:ALA:O	3:G:29:HIS:HA	2.15	0.47
3:G:169:VAL:HA	3:G:236:GLN:O	2.15	0.47
2:A:239:GLY:O	2:A:243:TRP:HB2	2.15	0.47
3:E:109:GLU:OE2	3:E:130:HIS:ND1	2.40	0.47
2:B:161:PHE:HB3	2:B:280:ILE:HG23	1.97	0.47
3:G:85:VAL:HG23	3:G:91:CYS:HB2	1.97	0.47
3:H:273:ASN:OD1	3:H:273:ASN:N	2.48	0.47
3:F:36:ARG:HH12	3:F:38:ARG:HB3	1.80	0.47
3:F:202:ASN:HB3	3:F:224:GLN:HG2	1.97	0.47
3:F:290:ASP:OD2	3:F:291:HIS:ND1	2.47	0.47
3:H:206:SER:O	3:H:206:SER:OG	2.31	0.47
3:E:408:VAL:HG12	3:E:411:LEU:HB3	1.97	0.46
2:D:191:PRO:HG2	2:D:194:ALA:HB3	1.97	0.46
4:L:195:GLN:O	4:L:201:PHE:HA	2.14	0.46
1:N:204:VAL:HA	1:N:272:HIS:O	2.15	0.46
1:P:210:LEU:HD23	2:C:211:LYS:HD2	1.97	0.46
1:O:158:ASP:OD1	1:O:158:ASP:N	2.40	0.46
3:E:403:THR:HG22	4:I:250:VAL:HG13	1.98	0.46
2:C:310:SER:HB2	3:G:341:GLN:HE22	1.80	0.46
2:C:369:VAL:O	2:C:372:THR:OG1	2.24	0.46
3:H:13:ARG:HB2	3:H:234:ASN:HD22	1.80	0.46
3:H:97:MET:O	3:H:100:PHE:HB2	2.15	0.46
1:N:275:HIS:HB3	1:N:280:LEU:HB2	1.96	0.46
2:A:188:ASP:OD1	2:A:188:ASP:N	2.42	0.46
3:E:273:ASN:OD1	3:E:273:ASN:N	2.41	0.46
4:J:229:LEU:HD22	4:J:243:VAL:HG13	1.98	0.46
2:C:282:ILE:HD12	2:C:283:PRO:HD2	1.96	0.46
2:C:366:ARG:HA	2:C:374:VAL:O	2.16	0.46
3:H:290:ASP:OD1	3:H:290:ASP:N	2.46	0.46
3:H:355:ILE:O	3:H:358:TYR:HB3	2.15	0.46
1:O:63:ASP:HB3	1:O:65:LEU:HD22	1.96	0.46
3:E:287:LEU:HD11	3:E:330:TRP:CE2	2.51	0.46
2:B:207:THR:HG23	2:B:209:GLU:H	1.79	0.46
2:C:382:PRO:O	3:G:345:ASN:ND2	2.47	0.46
1:O:96:GLN:HE22	1:O:109:LEU:H	1.62	0.46
2:C:178:VAL:HG23	2:C:185:TYR:HB2	1.97	0.46
3:G:189:LYS:HG3	3:G:216:VAL:HG22	1.98	0.46
3:G:344:THR:OG1	3:G:345:ASN:N	2.49	0.46
2:D:303:VAL:HG11	2:D:378:ALA:HA	1.97	0.46
1:M:140:HIS:CE1	1:M:142:TYR:HB3	2.49	0.46
2:D:28:VAL:HG22	2:D:329:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:74:TRP:HA	1:N:135:THR:O	2.15	0.46
1:P:237:PHE:HE2	2:D:152:HIS:HE1	1.64	0.46
2:C:327:LYS:HD3	2:C:327:LYS:HA	1.65	0.46
3:H:97:MET:HE2	3:H:258:PRO:HG2	1.96	0.46
3:E:280:LYS:HZ3	3:E:343:SER:HG	1.59	0.46
3:G:144:ARG:HH21	3:G:267:ARG:NE	2.14	0.46
3:H:71:ASP:N	3:H:71:ASP:OD1	2.48	0.46
1:M:247:ASN:HD22	2:B:226:ALA:HB1	1.80	0.46
1:P:34:SER:H	1:P:282:GLU:HA	1.81	0.46
1:P:139:HIS:ND1	1:P:146:ASP:OD1	2.49	0.46
3:E:196:THR:OG1	3:E:230:THR:O	2.32	0.46
3:F:15:TYR:HB2	3:F:51:SER:HB2	1.97	0.46
3:G:139:GLU:OE2	3:G:332:ASN:N	2.46	0.46
3:G:187:ASN:HA	3:G:218:ASN:HA	1.98	0.46
3:H:238:ASN:OD1	3:H:238:ASN:N	2.48	0.46
1:M:84:ARG:HH12	3:F:193:ASN:ND2	2.14	0.45
3:E:292:PRO:HA	3:E:311:VAL:O	2.15	0.45
3:G:107:LYS:HE3	3:G:132:GLU:HG3	1.98	0.45
2:D:125:HIS:HD1	2:D:126:THR:HG1	1.64	0.45
4:L:154:PHE:HA	4:L:164:CYS:O	2.16	0.45
4:L:228:VAL:HA	4:L:242:VAL:HG22	1.97	0.45
1:M:190:HIS:O	1:M:277:TYR:OH	2.34	0.45
1:P:76:LEU:HB2	1:P:87:LEU:HD21	1.98	0.45
1:P:208:ARG:HD3	1:P:221:LEU:HD11	1.98	0.45
3:E:251:ARG:HD2	3:E:252:LYS:H	1.81	0.45
3:G:38:ARG:HB2	3:G:47:LYS:HB3	1.98	0.45
3:H:148:GLY:HA2	3:H:270:LYS:HG2	1.98	0.45
2:B:212:ASP:OD1	2:B:212:ASP:N	2.46	0.45
2:B:327:LYS:HD2	2:B:327:LYS:HA	1.79	0.45
3:G:42:THR:OG1	3:G:154:SER:N	2.50	0.45
3:G:140:ARG:HB2	3:G:292:PRO:HB2	1.98	0.45
1:M:57:ARG:NH2	1:M:143:CYS:SG	2.83	0.45
3:E:114:GLY:HA2	3:E:123:HIS:O	2.15	0.45
3:F:166:GLU:OE2	3:F:255:ILE:N	2.49	0.45
3:F:196:THR:HB	3:F:210:LEU:HD11	1.97	0.45
3:E:263:ASN:OD1	3:E:263:ASN:N	2.49	0.45
4:K:117:VAL:HG11	4:K:136:LYS:HE2	1.97	0.45
1:M:64:ARG:HB2	3:F:26:HIS:CG	2.52	0.45
2:B:59:TYR:HE1	2:B:61:LYS:HE3	1.81	0.45
3:H:17:ALA:HB3	3:H:33:ALA:HB3	1.98	0.45
3:E:321:VAL:HG12	3:E:326:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:LEU:HB2	2:C:268:ALA:HB3	1.98	0.45
2:C:51:TYR:OH	2:C:236:ALA:O	2.35	0.45
2:D:371:SER:O	2:D:371:SER:OG	2.29	0.45
1:P:135:THR:HA	1:P:149:LEU:O	2.16	0.45
2:B:142:ILE:HD12	2:B:142:ILE:HA	1.87	0.45
2:C:184:VAL:HG23	2:C:251:LEU:HD12	1.99	0.45
2:D:84:VAL:HG11	2:D:102:GLN:HB2	1.98	0.45
3:H:50:VAL:O	3:H:99:HIS:ND1	2.44	0.45
2:A:335:ASN:N	2:A:335:ASN:OD1	2.48	0.45
3:F:370:ILE:HA	3:F:373:VAL:HG12	1.99	0.45
3:H:38:ARG:HB2	3:H:47:LYS:HB3	1.99	0.45
3:H:418:VAL:HG22	3:H:419:ARG:HG3	1.98	0.45
2:B:305:ALA:HB1	2:D:23:GLY:HA2	1.99	0.45
3:F:13:ARG:HH11	3:F:70:MET:HE3	1.82	0.45
3:G:32:ILE:HG22	3:G:52:LEU:HD22	1.99	0.45
3:G:196:THR:O	3:G:230:THR:N	2.48	0.45
2:D:68:CYS:HB3	2:D:103:LEU:HD11	1.99	0.45
4:L:206:GLY:O	4:L:209:LYS:NZ	2.41	0.45
1:M:154:GLU:O	1:M:174:VAL:HA	2.16	0.44
1:P:68:ARG:NH1	1:P:196:HIS:O	2.50	0.44
3:F:71:ASP:OD1	3:F:74:THR:OG1	2.36	0.44
2:C:319:LYS:HD2	2:C:351:GLN:HB3	1.98	0.44
1:P:240:ASP:OD2	2:D:132:LYS:NZ	2.43	0.44
2:A:45:ASP:OD2	2:A:189:TYR:OH	2.28	0.44
3:G:36:ARG:HB3	3:G:49:GLN:HG2	2.00	0.44
2:D:407:MET:HE3	2:D:407:MET:HB3	1.83	0.44
1:N:205:HIS:ND1	1:N:223:ASP:OD1	2.48	0.44
3:E:272:ARG:NH2	2:B:235:GLN:O	2.51	0.44
4:I:229:LEU:HD23	4:I:243:VAL:HG13	2.00	0.44
2:B:371:SER:O	2:B:371:SER:OG	2.33	0.44
2:C:265:PRO:O	2:C:267:ARG:NE	2.46	0.44
2:A:299:MET:HB2	2:A:374:VAL:HG11	2.00	0.44
2:A:396:THR:O	2:A:396:THR:OG1	2.33	0.44
2:A:429:ILE:HD12	2:A:432:LEU:HB2	1.99	0.44
3:E:17:ALA:HB1	3:E:241:LEU:HD22	1.99	0.44
3:E:144:ARG:NH1	3:F:21:ASP:OD1	2.51	0.44
2:B:241:LYS:NZ	3:F:39:ASN:O	2.45	0.44
2:B:383:PRO:HD2	3:F:342:MET:HB2	2.00	0.44
2:C:284:ASP:HA	2:C:287:PHE:HD2	1.83	0.44
3:G:94:THR:C	3:G:158:GLN:HE22	2.26	0.44
3:H:399:PRO:HB2	4:L:249:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:204:VAL:HG13	1:M:224:LEU:HB3	2.00	0.44
1:O:112:SER:OG	1:O:115:HIS:ND1	2.50	0.44
1:P:65:LEU:O	1:P:66:HIS:ND1	2.51	0.44
2:A:166:MET:HE2	2:A:166:MET:HB2	1.83	0.44
3:E:175:THR:HB	3:E:229:VAL:HB	2.00	0.44
2:B:255:ALA:O	3:F:298:ARG:NH1	2.51	0.44
4:K:122:LYS:HB2	4:K:122:LYS:HE3	1.80	0.44
1:M:195:ARG:HA	1:M:195:ARG:HD3	1.83	0.44
1:N:76:LEU:HB2	1:N:87:LEU:HD11	1.99	0.44
1:P:85:ARG:NH2	1:P:100:GLU:HB2	2.33	0.44
3:E:296:SER:OG	3:E:329:THR:OG1	2.25	0.44
2:B:184:VAL:HB	2:B:261:ILE:HD12	2.00	0.44
2:C:63:CYS:HA	2:C:99:GLU:HB3	1.99	0.44
3:H:169:VAL:HG22	3:H:235:TRP:HB3	2.00	0.44
3:F:269:PRO:O	3:F:332:ASN:ND2	2.49	0.44
3:F:272:ARG:O	3:F:330:TRP:NE1	2.48	0.44
1:N:152:ARG:HB3	1:N:172:VAL:HG22	1.99	0.44
2:A:166:MET:SD	2:A:166:MET:N	2.88	0.44
4:I:151:LYS:HB3	4:I:151:LYS:HE3	1.80	0.44
3:F:63:ASP:OD2	3:F:66:LYS:N	2.48	0.44
2:C:205:SER:OG	2:C:210:SER:OG	2.35	0.44
3:G:71:ASP:OD1	3:G:71:ASP:N	2.50	0.44
2:D:85:TYR:HE1	2:D:97:ASP:HB2	1.83	0.44
4:K:129:LEU:HD12	4:K:175:ALA:HA	2.00	0.43
2:D:251:LEU:HA	2:D:254:THR:HG22	1.98	0.43
2:D:421:VAL:HG23	3:H:388:MET:HE3	2.00	0.43
2:D:427:ILE:HA	2:D:430:VAL:HG22	1.99	0.43
1:M:275:HIS:ND1	1:M:278:CYS:SG	2.92	0.43
2:A:148:ALA:HA	2:A:163:VAL:HG23	2.00	0.43
2:A:239:GLY:O	2:A:243:TRP:CB	2.67	0.43
3:F:314:LYS:HE2	3:F:314:LYS:HB3	1.72	0.43
1:N:65:LEU:HG	3:G:28:CYS:HA	2.00	0.43
1:O:234:GLY:O	1:O:239:ARG:NH2	2.37	0.43
1:P:49:ALA:HB2	1:P:261:LEU:HD11	2.00	0.43
3:E:58:THR:HA	3:E:68:ARG:HH11	1.83	0.43
3:F:40:GLU:OE1	3:F:156:TYR:OH	2.36	0.43
3:H:148:GLY:CA	3:H:268:VAL:O	2.57	0.43
1:N:75:ASP:O	1:N:134:TYR:HA	2.18	0.43
1:P:195:ARG:HH22	3:H:6:PHE:HB2	1.84	0.43
2:A:251:LEU:HA	2:A:254:THR:HG22	2.00	0.43
3:F:223:ASP:OD1	3:F:223:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:247:LYS:HD2	4:J:247:LYS:HA	1.70	0.43
1:O:106:ARG:NH2	1:O:130:ASP:OD2	2.51	0.43
1:P:164:ALA:HA	1:P:172:VAL:O	2.18	0.43
3:E:343:SER:HB3	3:E:344:THR:H	1.64	0.43
3:F:252:LYS:HA	3:F:252:LYS:HD3	1.80	0.43
2:C:263:THR:OG1	2:C:264:ASN:N	2.52	0.43
3:H:372:SER:O	3:H:375:SER:OG	2.32	0.43
1:P:189:ALA:HB3	1:P:192:TRP:HD1	1.84	0.43
2:A:129:ALA:O	2:A:148:ALA:N	2.50	0.43
3:F:11:ALA:O	3:F:235:TRP:N	2.48	0.43
2:D:386:HIS:CE1	3:H:344:THR:H	2.37	0.43
1:M:49:ALA:HB2	1:M:261:LEU:HD11	2.00	0.43
1:M:202:GLN:HG2	1:M:226:ALA:HB2	2.00	0.43
3:H:5:ASN:O	3:H:62:HIS:NE2	2.52	0.43
3:H:102:LEU:HD11	3:H:259:PHE:CG	2.53	0.43
1:M:152:ARG:HB3	1:M:172:VAL:HG22	1.99	0.43
1:O:231:ARG:HD2	1:O:231:ARG:HA	1.77	0.43
2:A:275:ASN:OD1	2:A:275:ASN:N	2.52	0.43
3:E:355:ILE:HA	3:E:358:TYR:CD2	2.54	0.43
2:B:432:LEU:O	2:B:436:PHE:HB2	2.19	0.43
3:G:39:ASN:OD1	3:G:39:ASN:N	2.49	0.43
3:G:297:TYR:CZ	3:G:307:HIS:HB2	2.53	0.43
3:H:323:THR:HA	3:H:340:PRO:HG3	2.00	0.43
1:M:103:ASP:OD1	1:M:106:ARG:NH1	2.51	0.43
3:E:139:GLU:HG3	3:E:293:THR:HG23	2.00	0.43
3:E:366:MET:SD	3:E:366:MET:N	2.91	0.43
2:D:15:TYR:O	2:D:30:GLU:HA	2.19	0.43
3:H:163:THR:HG22	3:H:164:ALA:H	1.82	0.43
3:H:422:LYS:HD2	3:H:422:LYS:HA	1.79	0.43
1:P:126:VAL:HG11	1:P:175:VAL:HG13	2.00	0.43
1:N:51:LEU:HD21	1:N:288:LEU:HD21	2.00	0.42
1:N:116:ASP:HB2	1:N:188:ARG:HH12	1.84	0.42
3:E:250:ASP:OD1	3:E:250:ASP:N	2.52	0.42
2:D:196:ARG:HH12	2:D:199:GLN:HG3	1.83	0.42
3:H:183:GLN:HG3	3:H:222:ILE:HG13	2.00	0.42
2:A:219:LEU:HD12	2:A:235:GLN:HE22	1.84	0.42
3:E:286:LEU:HD13	3:E:316:GLU:HB3	2.00	0.42
3:F:152:PRO:HA	3:F:265:THR:HA	2.01	0.42
4:J:146:ASN:HD22	4:J:149:LEU:H	1.65	0.42
3:G:286:LEU:HD13	3:G:316:GLU:HB3	1.99	0.42
2:D:394:HIS:CD2	2:D:395:THR:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:177:LYS:HG3	4:L:223:ARG:HG2	2.00	0.42
1:M:72:VAL:HG12	1:M:138:LEU:HD13	2.00	0.42
1:P:74:TRP:CE2	1:P:121:LEU:HB2	2.54	0.42
3:E:52:LEU:O	3:E:99:HIS:ND1	2.53	0.42
3:E:130:HIS:CD2	3:G:290:ASP:HB2	2.55	0.42
3:E:201:CYS:HB2	3:E:202:ASN:H	1.74	0.42
2:B:9:ASN:ND2	2:B:271:CYS:O	2.52	0.42
1:O:32:SER:O	1:O:32:SER:OG	2.34	0.42
4:I:130:VAL:O	4:I:133:LYS:HB3	2.19	0.42
4:I:189:TRP:CE2	4:I:191:HIS:HB2	2.54	0.42
3:G:149:LYS:HE2	3:G:270:LYS:HE3	2.00	0.42
1:O:63:ASP:OD1	1:O:64:ARG:N	2.52	0.42
1:O:273:LEU:HG	1:O:282:GLU:HB2	2.01	0.42
1:P:76:LEU:HG	1:P:87:LEU:HD11	2.00	0.42
3:E:393:ARG:HE	3:E:417:CYS:HB3	1.85	0.42
2:B:239:GLY:HA2	2:B:242:TYR:CE1	2.54	0.42
3:F:10:LYS:HA	3:F:10:LYS:HD3	1.86	0.42
3:F:112:THR:HB	3:F:126:THR:HG22	2.00	0.42
3:F:287:LEU:HD23	3:F:311:VAL:HG21	2.01	0.42
2:C:136:LEU:HD23	2:C:136:LEU:HA	1.89	0.42
1:M:38:GLU:HG3	1:M:285:VAL:HB	2.01	0.42
1:P:291:THR:O	1:P:291:THR:OG1	2.32	0.42
2:A:20:ASN:OD1	2:A:20:ASN:N	2.52	0.42
3:E:379:LEU:HA	3:E:382:VAL:HG22	2.01	0.42
2:B:315:VAL:HG11	2:D:291:VAL:HG11	2.01	0.42
3:F:17:ALA:HB3	3:F:33:ALA:HB3	2.01	0.42
3:F:203:CYS:O	3:F:207:ASN:ND2	2.52	0.42
3:F:315:LYS:HZ3	3:F:315:LYS:HG2	1.61	0.42
2:C:32:GLU:HB3	2:C:134:ARG:HB3	2.01	0.42
3:G:170:HIS:HB2	3:G:251:ARG:HD3	2.01	0.42
1:P:259:ASP:OD1	1:P:259:ASP:N	2.47	0.42
3:H:32:ILE:HD12	3:H:113:VAL:HG13	2.02	0.42
3:F:409:PRO:O	3:F:413:SER:OG	2.28	0.42
4:J:240:LEU:HD12	4:J:242:VAL:HB	2.02	0.42
3:G:151:LEU:HD23	3:G:268:VAL:HG11	2.02	0.42
3:H:50:VAL:HG13	3:H:52:LEU:H	1.85	0.42
1:O:97:ARG:HB2	3:E:119:ARG:HE	1.83	0.42
3:E:171:MET:HB2	3:E:245:ASN:HD21	1.85	0.42
4:I:211:GLY:N	4:I:261:TRP:O	2.46	0.42
2:C:250:SER:OG	2:C:251:LEU:N	2.53	0.42
1:M:44:ALA:HB2	1:M:293:PRO:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:89:ASP:OD1	1:O:90:MET:N	2.53	0.42
1:P:140:HIS:CE1	1:P:142:TYR:HB3	2.55	0.42
2:A:255:ALA:O	3:E:298:ARG:NH1	2.53	0.42
2:A:417:VAL:HG21	3:E:385:ALA:HB2	2.02	0.42
3:F:175:THR:HB	3:F:229:VAL:HG12	2.00	0.42
2:D:224:PRO:HA	2:D:232:PRO:HG3	2.02	0.42
3:H:367:THR:H	3:H:369:VAL:HG22	1.85	0.42
1:M:204:VAL:HA	1:M:272:HIS:O	2.20	0.41
1:O:241:ARG:NE	1:O:265:ASP:OD1	2.52	0.41
1:P:48:GLN:HE21	1:P:259:ASP:HB3	1.85	0.41
3:G:201:CYS:HB2	3:G:207:ASN:HA	2.01	0.41
4:K:194:VAL:HG22	4:K:203:ILE:HD11	2.02	0.41
2:D:30:GLU:OE2	2:D:134:ARG:NH1	2.53	0.41
1:M:103:ASP:HB3	1:M:107:LEU:HG	2.01	0.41
1:O:173:LEU:HG	1:O:175:VAL:HG13	2.02	0.41
2:A:299:MET:HE3	2:A:320:TYR:HB3	2.02	0.41
2:A:406:ALA:HA	2:A:409:TRP:HB2	2.02	0.41
3:E:138:ARG:HG2	3:E:294:LEU:HD21	2.02	0.41
3:E:239:SER:HB3	3:E:242:VAL:HB	2.01	0.41
4:J:232:ALA:HB2	4:J:258:ALA:HA	2.02	0.41
3:G:8:VAL:HG12	3:G:255:ILE:HG22	2.01	0.41
1:N:106:ARG:HA	1:N:124:ARG:HG2	2.01	0.41
1:N:173:LEU:HG	1:N:175:VAL:HG13	2.02	0.41
3:E:79:GLU:HG3	3:E:81:ALA:H	1.85	0.41
3:E:169:VAL:HG22	3:E:235:TRP:HE3	1.85	0.41
3:H:276:VAL:HG12	3:H:285:MET:HG2	2.02	0.41
3:E:16:LEU:HD21	3:E:70:MET:HB3	2.02	0.41
3:E:188:VAL:HB	3:E:217:ILE:HB	2.02	0.41
4:L:202:THR:HA	4:L:238:THR:O	2.20	0.41
1:P:142:TYR:OH	1:P:202:GLN:OE1	2.38	0.41
3:G:381:MET:HE2	3:G:381:MET:HB3	1.86	0.41
2:D:206:ARG:HD2	2:D:206:ARG:HA	1.86	0.41
1:N:33:SER:HB2	1:N:283:ARG:HB3	2.01	0.41
1:O:96:GLN:NE2	1:O:109:LEU:H	2.18	0.41
3:F:22:CYS:HB3	3:F:28:CYS:HB2	1.85	0.41
3:F:363:TYR:HB3	3:F:366:MET:HB2	2.01	0.41
2:C:148:ALA:HA	2:C:163:VAL:HG23	2.01	0.41
1:P:90:MET:HE1	1:P:113:ALA:HB3	2.03	0.41
2:A:181:LYS:HB3	2:A:182:GLY:H	1.77	0.41
3:E:15:TYR:CZ	3:E:236:GLN:HA	2.54	0.41
4:J:141:LYS:HB2	4:J:141:LYS:HE2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:155:LYS:HB3	4:J:164:CYS:SG	2.61	0.41
4:L:162:LEU:HA	4:L:162:LEU:HD12	1.85	0.41
1:P:158:ASP:OD1	1:P:158:ASP:N	2.48	0.41
2:B:57:SER:OG	3:F:239:SER:O	2.33	0.41
2:B:79:LYS:HD2	2:B:79:LYS:HA	1.67	0.41
3:F:147:HIS:HA	3:F:267:ARG:HH21	1.85	0.41
3:F:170:HIS:HB2	3:F:251:ARG:HG2	2.03	0.41
2:C:297:THR:HG23	2:C:321:THR:HB	2.03	0.41
2:D:403:SER:OG	2:D:405:THR:N	2.49	0.41
1:M:155:VAL:HA	1:M:175:VAL:O	2.21	0.41
1:N:195:ARG:HA	1:N:195:ARG:HD3	1.36	0.41
1:O:162:SER:OG	1:O:174:VAL:O	2.34	0.41
3:E:393:ARG:NE	3:E:417:CYS:HB3	2.36	0.41
3:E:404:PRO:HG2	4:I:245:TRP:CE2	2.55	0.41
2:D:95:PHE:HB2	3:H:226:HIS:HB2	2.02	0.41
3:H:31:PRO:O	3:H:51:SER:OG	2.36	0.41
3:H:254:LYS:HE3	3:H:254:LYS:HB2	1.87	0.41
4:L:209:LYS:HE2	4:L:209:LYS:HB2	1.84	0.41
4:L:249:ILE:HD12	4:L:249:ILE:HA	1.86	0.41
1:P:173:LEU:HD11	1:P:183:MET:HB2	2.03	0.41
3:F:13:ARG:HD3	3:F:234:ASN:HB2	2.02	0.41
3:F:95:GLY:O	3:F:101:ILE:HA	2.21	0.41
3:F:192:VAL:HG13	3:F:194:GLY:H	1.86	0.41
4:J:231:GLY:HA2	4:J:240:LEU:HA	2.02	0.41
2:D:320:TYR:HH	2:D:350:SER:HG	1.68	0.41
2:D:359:ALA:HB2	2:D:395:THR:HB	2.03	0.41
3:H:347:THR:HG23	3:H:357:LEU:HD23	2.03	0.41
1:M:271:CYS:O	1:M:283:ARG:HA	2.21	0.40
1:N:88:VAL:HG22	1:N:98:VAL:HA	2.03	0.40
1:N:235:PRO:HD2	1:N:238:LEU:HD12	2.02	0.40
1:O:84:ARG:NH2	3:E:192:VAL:H	2.19	0.40
1:P:75:ASP:O	1:P:134:TYR:HA	2.21	0.40
2:A:299:MET:HG2	2:A:320:TYR:HA	2.02	0.40
3:E:137:GLY:HA3	3:E:332:ASN:HD21	1.85	0.40
3:E:368:VAL:HA	3:E:371:VAL:HG22	2.02	0.40
4:I:202:THR:HG23	4:I:237:ARG:HH21	1.86	0.40
2:B:300:SER:O	2:B:318:ILE:HA	2.20	0.40
3:F:213:THR:OG1	3:F:214:ASP:N	2.54	0.40
1:N:58:MET:HE1	1:N:275:HIS:HB2	2.03	0.40
1:N:206:TRP:CH2	1:N:271:CYS:HB2	2.56	0.40
1:N:209:GLN:HB3	1:N:268:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:88:VAL:HG12	1:O:98:VAL:HA	2.03	0.40
1:P:189:ALA:HB3	1:P:192:TRP:CD1	2.56	0.40
2:A:299:MET:HE1	2:A:369:VAL:HG11	2.03	0.40
2:B:366:ARG:HA	2:B:374:VAL:O	2.21	0.40
2:D:300:SER:O	2:D:318:ILE:HA	2.21	0.40
1:M:245:ASN:HB3	1:M:257:ARG:HH22	1.87	0.40
1:M:270:SER:HG	1:M:272:HIS:CE1	2.39	0.40
1:O:212:GLY:HA2	3:H:166:GLU:HG3	2.04	0.40
4:K:129:LEU:HA	4:K:133:LYS:O	2.22	0.40
4:K:187:TYR:HD1	4:K:219:ASP:HA	1.86	0.40
4:L:151:LYS:HE3	4:L:151:LYS:HB3	1.76	0.40
4:L:187:TYR:HB2	4:L:194:VAL:HG23	2.03	0.40
3:E:110:THR:OG1	3:E:127:HIS:O	2.33	0.40
2:B:47:ILE:HD12	2:B:208:PRO:HG3	2.04	0.40
2:B:72:SER:O	2:B:72:SER:OG	2.32	0.40
2:B:421:VAL:HA	3:F:388:MET:HG3	2.03	0.40
2:C:185:TYR:HB3	2:C:187:MET:HE3	2.04	0.40
3:G:408:VAL:HG12	3:G:412:LEU:H	1.86	0.40
4:K:202:THR:HA	4:K:238:THR:O	2.21	0.40
2:D:34:GLN:HB2	2:D:132:LYS:HB3	2.03	0.40
2:D:97:ASP:OD1	2:D:97:ASP:N	2.53	0.40
1:O:222:LEU:HD11	1:O:230:ARG:HB2	2.04	0.40
2:A:437:SER:OG	2:A:438:ARG:NH1	2.55	0.40
2:B:93:TYR:HD1	3:F:176:PRO:HG3	1.87	0.40
2:B:217:THR:HB	2:B:236:ALA:HB1	2.02	0.40
2:B:251:LEU:HB2	2:B:261:ILE:HD13	2.02	0.40
3:G:85:VAL:HG12	3:G:113:VAL:HG12	2.04	0.40
2:D:297:THR:O	2:D:321:THR:OG1	2.39	0.40
2:D:327:LYS:HD3	2:D:327:LYS:HA	1.92	0.40
3:H:252:LYS:HD3	3:H:252:LYS:HA	1.88	0.40
3:H:353:HIS:CG	3:H:354:GLU:H	2.39	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	M	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	N	259/269 (96%)	242 (93%)	15 (6%)	2 (1%)	16	52
1	O	267/269 (99%)	250 (94%)	17 (6%)	0	100	100
1	P	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	30	65
2	A	437/439 (100%)	413 (94%)	23 (5%)	1 (0%)	43	75
2	B	437/439 (100%)	413 (94%)	23 (5%)	1 (0%)	43	75
2	C	437/439 (100%)	410 (94%)	26 (6%)	1 (0%)	43	75
2	D	437/439 (100%)	417 (95%)	19 (4%)	1 (0%)	43	75
3	E	417/419 (100%)	360 (86%)	56 (13%)	1 (0%)	43	75
3	F	417/419 (100%)	363 (87%)	51 (12%)	3 (1%)	18	55
3	G	417/419 (100%)	361 (87%)	54 (13%)	2 (0%)	24	61
3	H	417/419 (100%)	361 (87%)	55 (13%)	1 (0%)	43	75
4	I	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
4	J	149/151 (99%)	146 (98%)	3 (2%)	0	100	100
4	K	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
4	L	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
All	All	5072/5112 (99%)	4674 (92%)	384 (8%)	14 (0%)	37	70

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	181	LYS
3	F	402	LEU
2	C	181	LYS
3	G	342	MET
3	G	344	THR
2	D	181	LYS
3	H	343	SER
1	N	195	ARG
1	P	197	LEU
2	B	405	THR
3	E	343	SER
3	F	367	THR
1	N	197	LEU
3	F	173	PRO

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	M	232/232 (100%)	231 (100%)	1 (0%)	84	83
1	N	226/232 (97%)	223 (99%)	3 (1%)	61	72
1	O	232/232 (100%)	232 (100%)	0	100	100
1	P	232/232 (100%)	230 (99%)	2 (1%)	70	77
2	A	366/366 (100%)	362 (99%)	4 (1%)	65	74
2	B	366/366 (100%)	359 (98%)	7 (2%)	50	67
2	C	366/366 (100%)	360 (98%)	6 (2%)	55	70
2	D	366/366 (100%)	365 (100%)	1 (0%)	86	85
3	E	369/369 (100%)	366 (99%)	3 (1%)	73	78
3	F	369/369 (100%)	367 (100%)	2 (0%)	81	82
3	G	369/369 (100%)	366 (99%)	3 (1%)	73	78
3	H	369/369 (100%)	367 (100%)	2 (0%)	81	82
4	I	120/120 (100%)	119 (99%)	1 (1%)	73	78
4	J	120/120 (100%)	119 (99%)	1 (1%)	73	78
4	K	120/120 (100%)	119 (99%)	1 (1%)	73	78
4	L	120/120 (100%)	120 (100%)	0	100	100
All	All	4342/4348 (100%)	4305 (99%)	37 (1%)	68	77

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	138	LEU
1	N	37	SER
1	N	50	VAL
1	N	195	ARG
1	P	43	LEU
1	P	145	LEU
2	A	303	VAL
2	A	369	VAL

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Mol	Chain	Res	Type
2	A	372	THR
2	A	388	VAL
3	E	263	ASN
3	E	342	MET
3	E	343	SER
4	I	201	PHE
2	B	13	VAL
2	B	53	THR
2	B	60	VAL
2	B	229	VAL
2	B	372	THR
2	B	396	THR
2	B	404	THR
3	F	113	VAL
3	F	404	PRO
4	J	117	VAL
2	C	60	VAL
2	C	96	CYS
2	C	156	VAL
2	C	221	LEU
2	C	229	VAL
2	C	327	LYS
3	G	342	MET
3	G	395	ARG
3	G	396	CYS
4	K	203	ILE
2	D	434	VAL
3	H	287	LEU
3	H	343	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	48	GLN
1	M	144	HIS
1	M	190	HIS
1	M	245	ASN
1	M	281	HIS
1	N	209	GLN
1	N	245	ASN
1	N	247	ASN
1	O	48	GLN

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Mol	Chain	Res	Type
1	O	83	GLN
1	O	144	HIS
1	O	202	GLN
1	O	215	HIS
1	O	245	ASN
1	O	281	HIS
1	P	48	GLN
1	P	187	ASN
1	P	281	HIS
2	A	152	HIS
2	A	199	GLN
2	A	260	GLN
2	A	373	GLN
2	A	439	HIS
3	E	73	HIS
3	E	147	HIS
3	E	183	GLN
3	E	195	GLN
3	E	238	ASN
3	E	281	ASN
3	E	332	ASN
3	E	341	GLN
2	B	20	ASN
2	B	102	GLN
2	B	199	GLN
2	B	216	ASN
2	B	235	GLN
2	B	260	GLN
2	B	308	HIS
2	B	375	HIS
2	B	381	HIS
3	F	29	HIS
3	F	147	HIS
3	F	219	ASN
3	F	234	ASN
3	F	245	ASN
3	F	341	GLN
4	J	111	ASN
4	J	146	ASN
4	J	180	HIS
2	C	20	ASN
2	C	34	GLN

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Mol	Chain	Res	Type
2	C	138	GLN
2	C	140	ASN
2	C	152	HIS
2	C	230	HIS
2	C	373	GLN
3	G	7	ASN
3	G	53	GLN
3	G	142	HIS
3	G	158	GLN
3	G	184	GLN
3	G	187	ASN
3	G	202	ASN
4	K	188	ASN
2	D	34	GLN
2	D	100	ASN
2	D	102	GLN
2	D	199	GLN
2	D	230	HIS
2	D	260	GLN
2	D	270	ASN
2	D	275	ASN
2	D	368	GLN
2	D	411	GLN
2	D	439	HIS
3	H	127	HIS
3	H	183	GLN
3	H	184	GLN
3	H	226	HIS
3	H	232	HIS
3	H	234	ASN
3	H	245	ASN
3	H	302	GLN
3	H	313	HIS
4	L	195	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	D	501	2	14,14,15	0.26	0	17,19,21	0.60	0
5	NAG	B	501	2	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
5	NAG	N	401	1	14,14,15	0.36	0	17,19,21	0.68	1 (5%)
5	NAG	C	501	2	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
5	NAG	O	501	1	14,14,15	0.34	0	17,19,21	0.61	1 (5%)
5	NAG	M	501	1	14,14,15	0.51	0	17,19,21	0.51	0
5	NAG	F	501	3	14,14,15	0.56	0	17,19,21	0.62	0
5	NAG	H	501	3	14,14,15	0.23	0	17,19,21	0.68	1 (5%)
5	NAG	E	501	3	14,14,15	0.39	0	17,19,21	0.57	0
5	NAG	A	501	2	14,14,15	0.29	0	17,19,21	0.72	1 (5%)
5	NAG	G	501	3	14,14,15	0.48	0	17,19,21	0.68	1 (5%)
5	NAG	P	501	1	14,14,15	0.47	0	17,19,21	0.73	1 (5%)

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
5	NAG	D	501	2	-	2/6/23/26	0/1/1/1
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1
5	NAG	N	401	1	-	1/6/23/26	0/1/1/1
5	NAG	C	501	2	-	1/6/23/26	0/1/1/1
5	NAG	O	501	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	M	501	1	-	3/6/23/26	0/1/1/1
5	NAG	F	501	3	-	2/6/23/26	0/1/1/1
5	NAG	H	501	3	-	2/6/23/26	0/1/1/1
5	NAG	E	501	3	-	0/6/23/26	0/1/1/1
5	NAG	A	501	2	-	0/6/23/26	0/1/1/1
5	NAG	G	501	3	-	2/6/23/26	0/1/1/1
5	NAG	P	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	NAG	C1-O5-C5	2.68	115.78	112.19
5	P	501	NAG	C1-O5-C5	2.56	115.61	112.19
5	B	501	NAG	C1-O5-C5	2.46	115.49	112.19
5	N	401	NAG	C1-O5-C5	2.35	115.33	112.19
5	C	501	NAG	C1-O5-C5	2.28	115.24	112.19
5	G	501	NAG	C1-O5-C5	2.23	115.18	112.19
5	H	501	NAG	C1-O5-C5	2.18	115.10	112.19
5	O	501	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	501	NAG	C4-C5-C6-O6
5	M	501	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	M	501	NAG	O5-C5-C6-O6
5	F	501	NAG	O5-C5-C6-O6
5	H	501	NAG	O5-C5-C6-O6
5	G	501	NAG	O5-C5-C6-O6
5	F	501	NAG	C4-C5-C6-O6
5	G	501	NAG	C4-C5-C6-O6
5	D	501	NAG	C4-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
5	N	401	NAG	O5-C5-C6-O6
5	M	501	NAG	C1-C2-N2-C7
5	C	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	501	NAG	1	0

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.

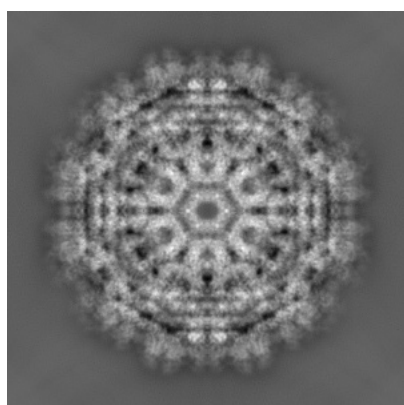
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9394. These allow visual inspection of the internal detail of the map and identification of artifacts.

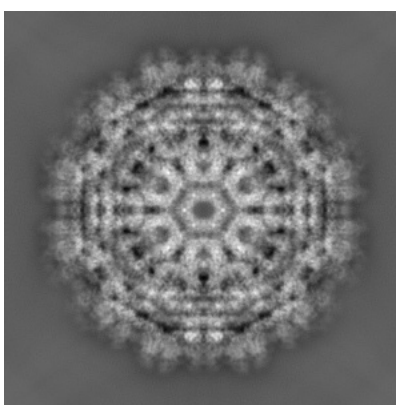
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

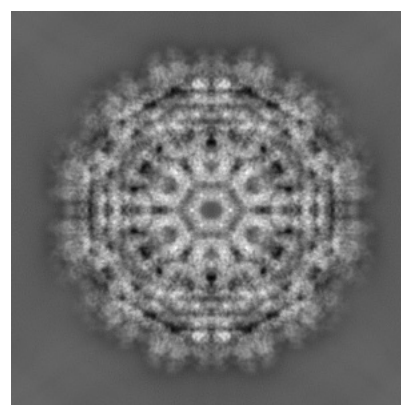
6.1.1 Primary map



X



Y

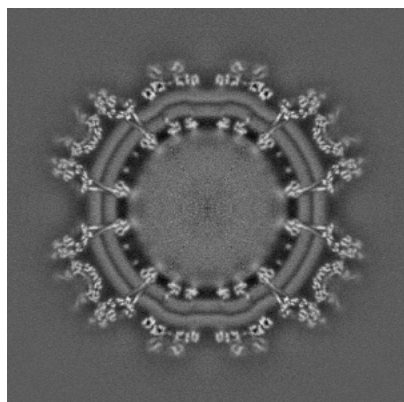


Z

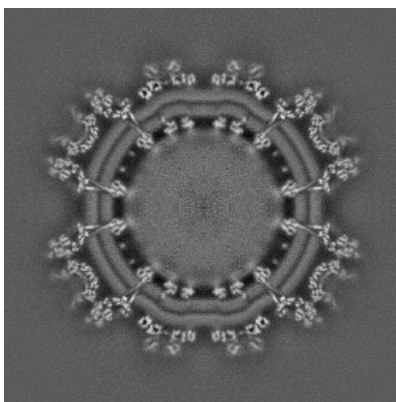
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

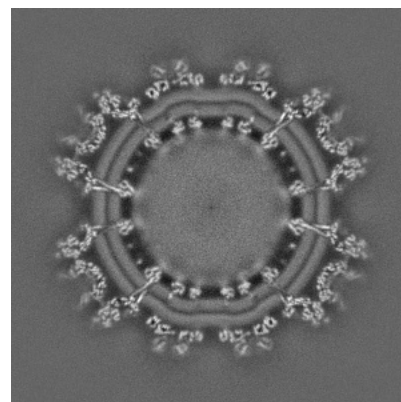
6.2.1 Primary map



X Index: 300



Y Index: 300

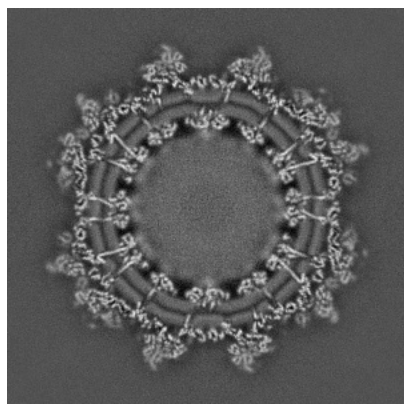


Z Index: 300

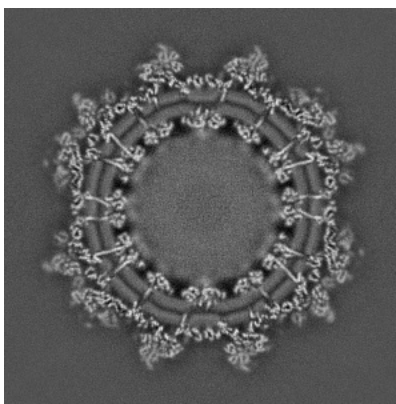
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

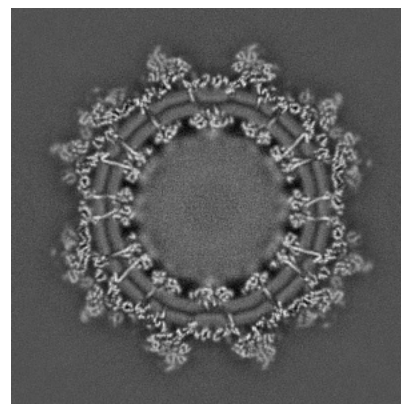
6.3.1 Primary map



X Index: 322



Y Index: 322

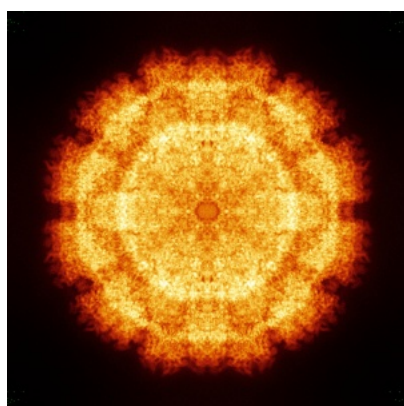


Z Index: 277

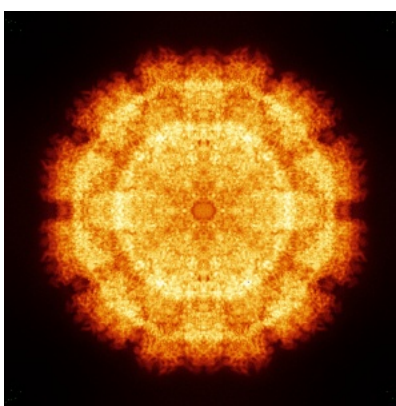
The images above show the largest variance slices of the map in three orthogonal directions.

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

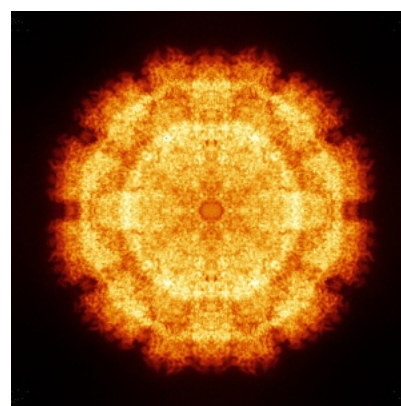
6.4.1 Primary map



X



Y

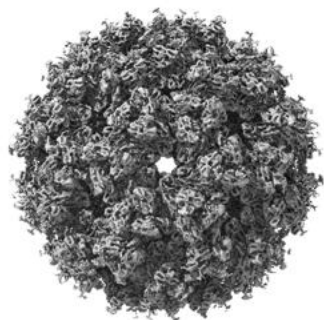


Z

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

6.5 Orthogonal surface views [i](#)

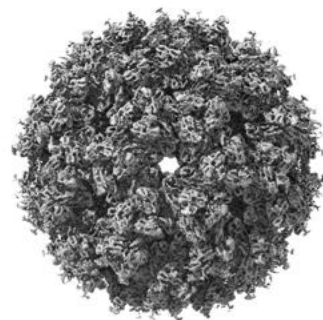
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

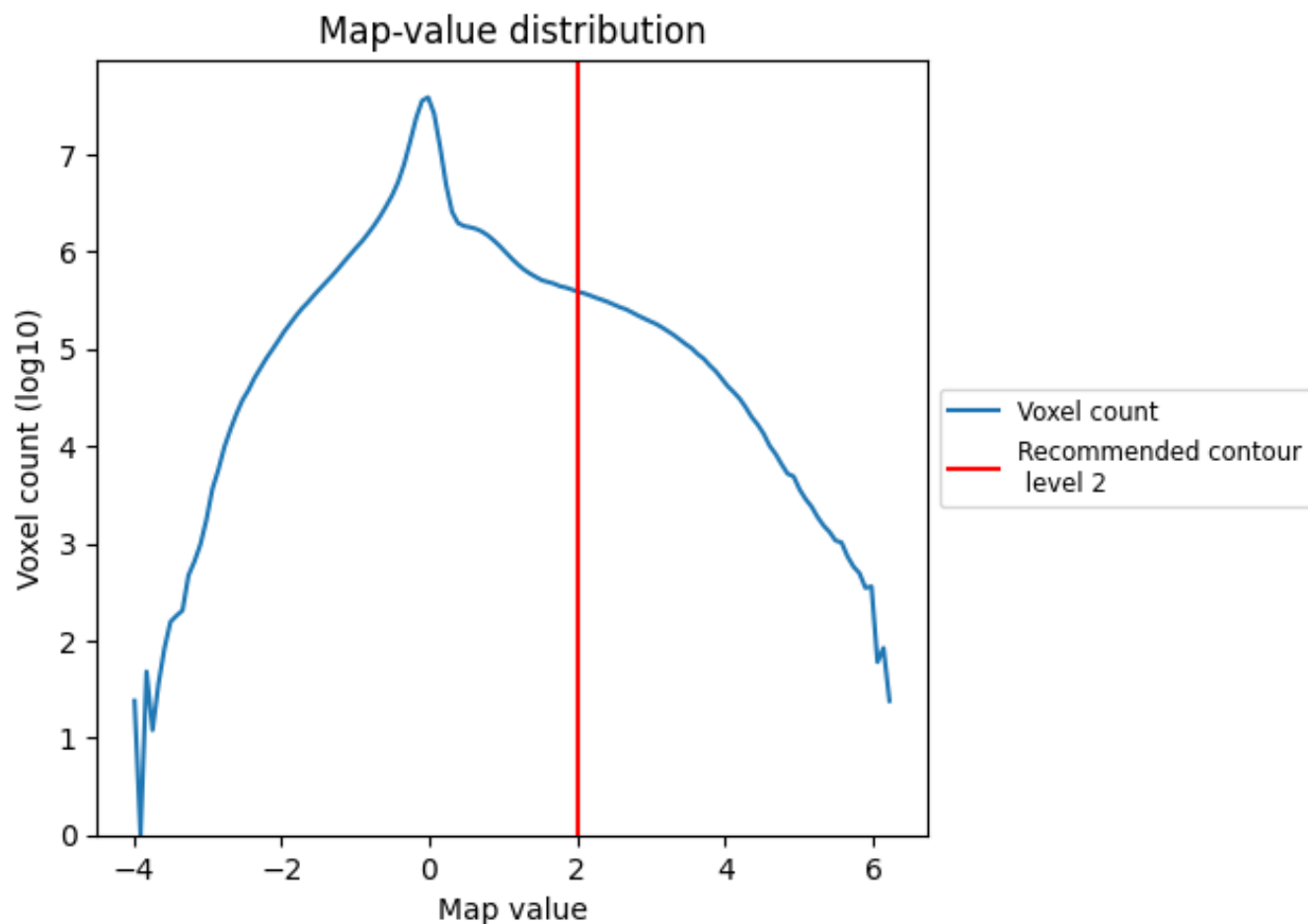
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

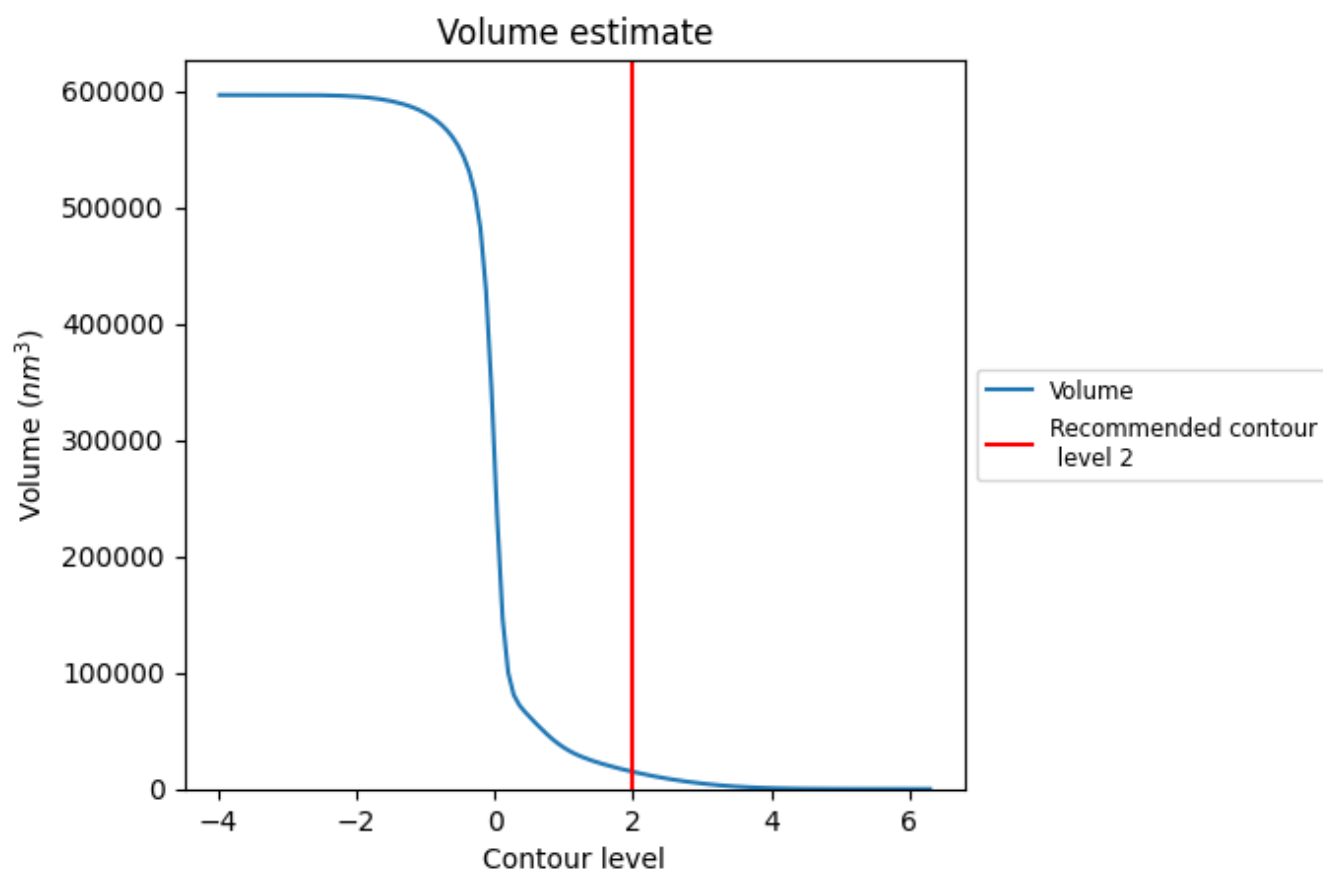
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

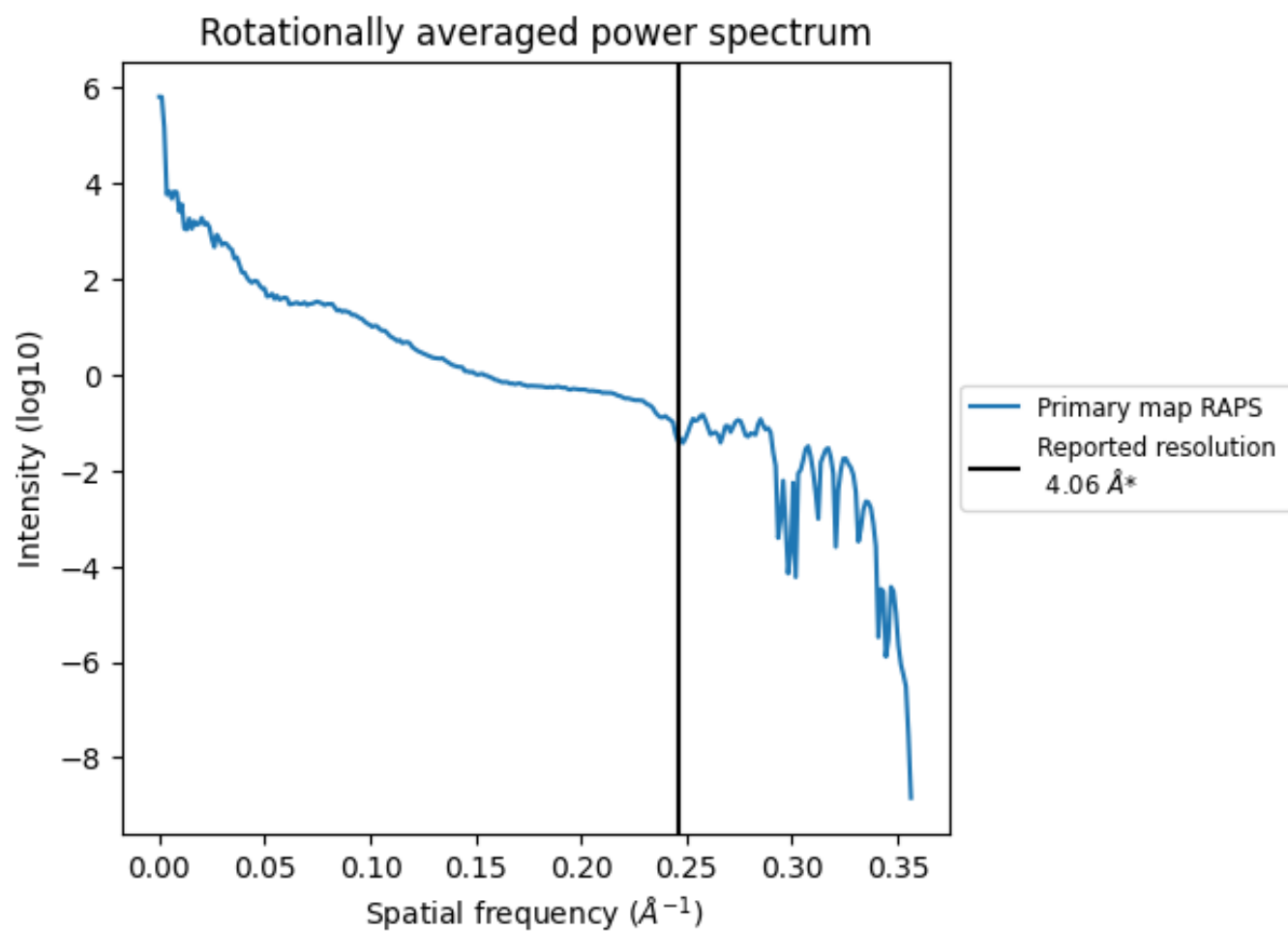
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 14765 nm³; this corresponds to an approximate mass of 13338 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 ⓘ

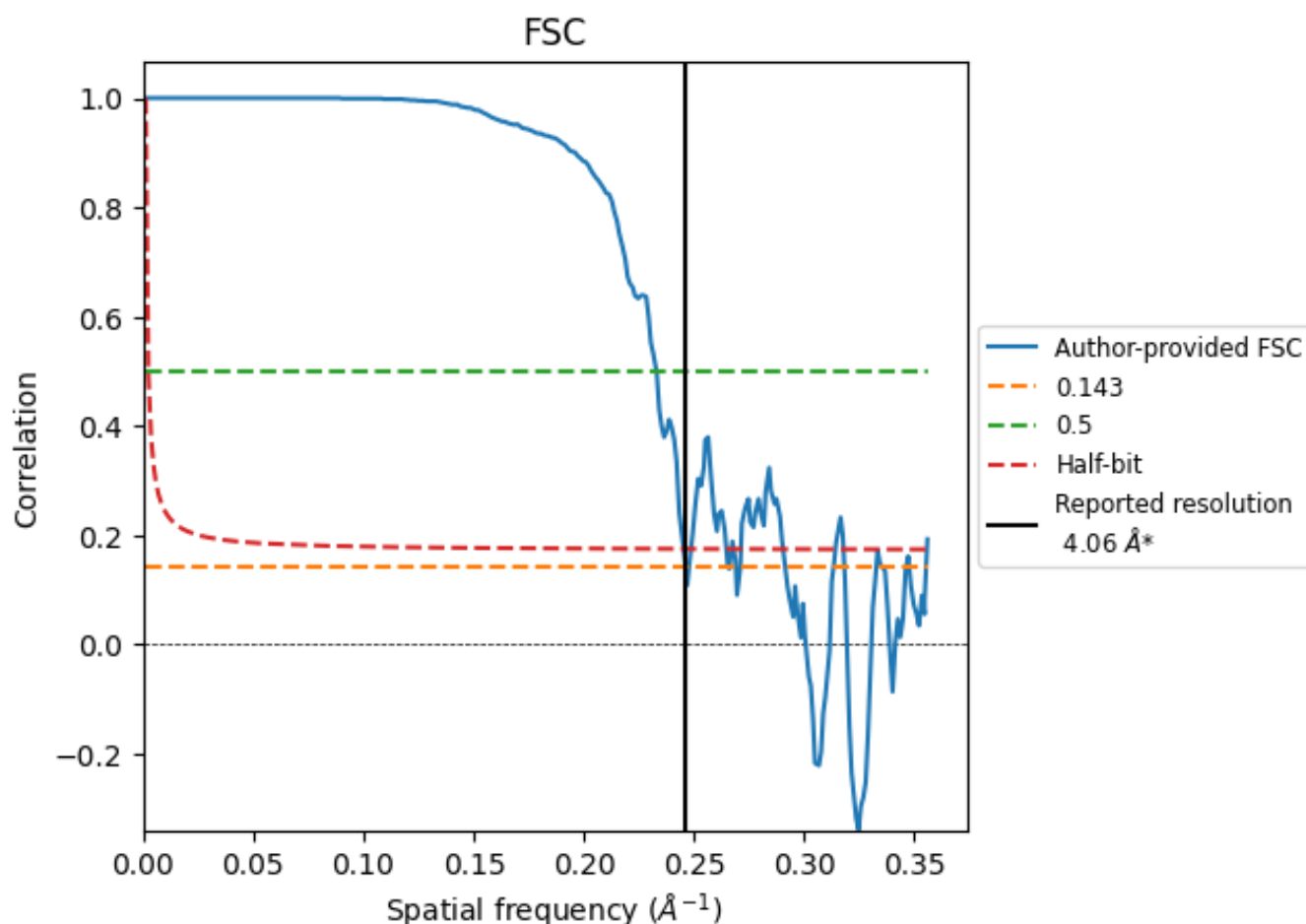


*Reported resolution corresponds to spatial frequency of 0.246 Å⁻¹

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 0.246 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.06	-	-
Author-provided FSC curve	4.06	4.29	4.08
Unmasked-calculated*	-	-	-

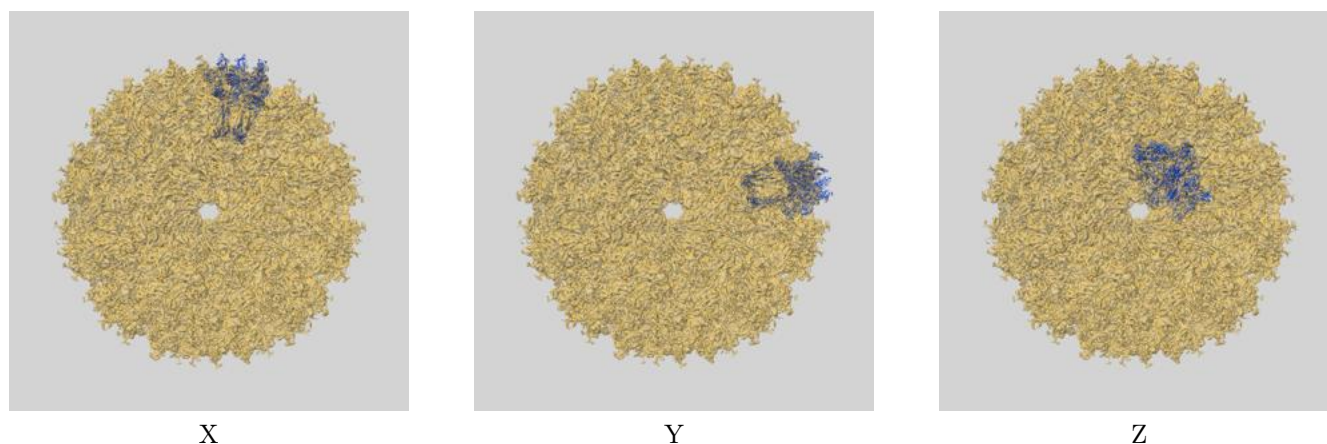
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

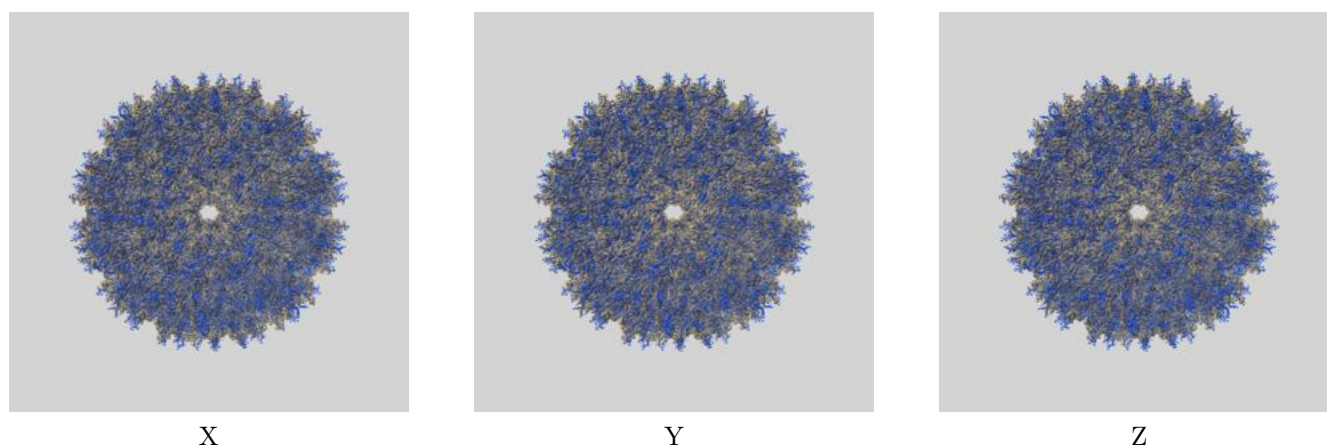
This section contains information regarding the fit between EMDB map EMD-9394 and PDB model 6NK6. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

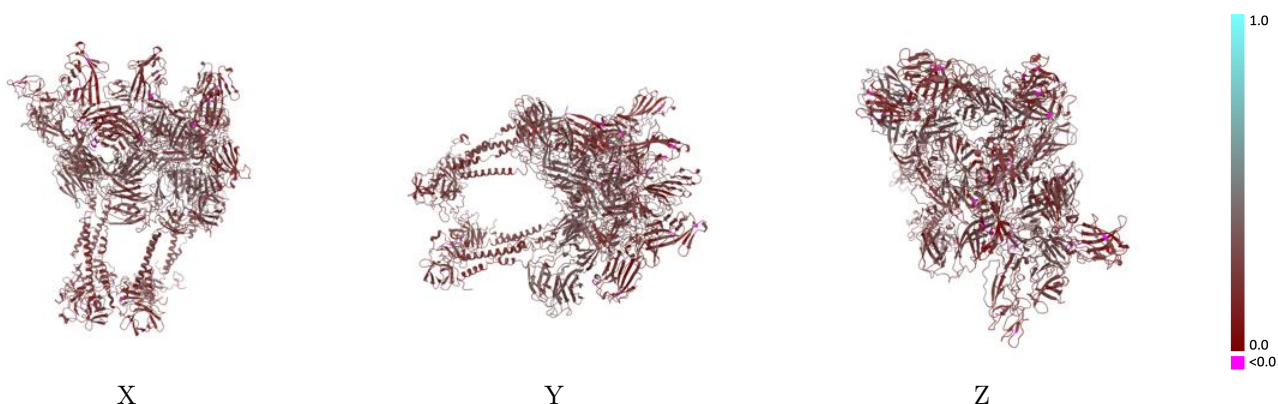


9.1.2 Map-model assembly overlay [i](#)



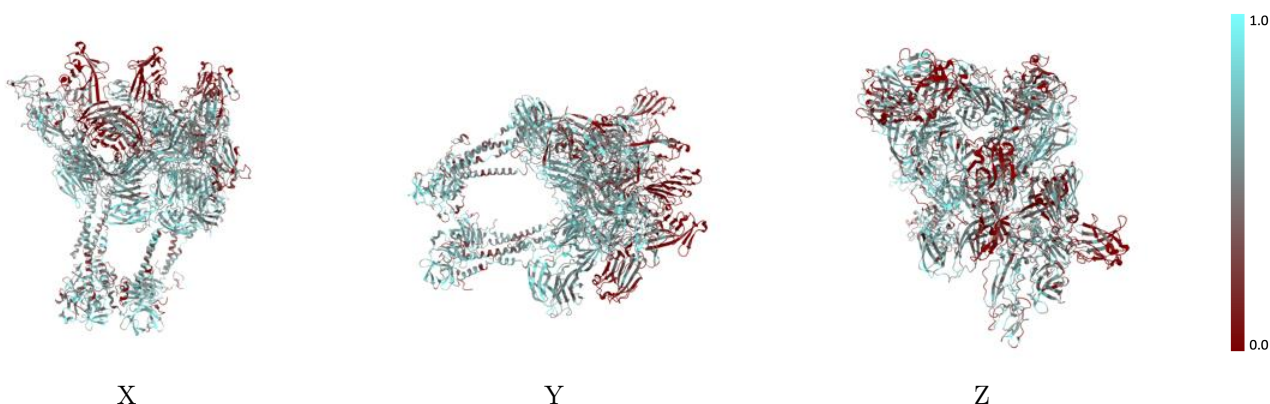
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



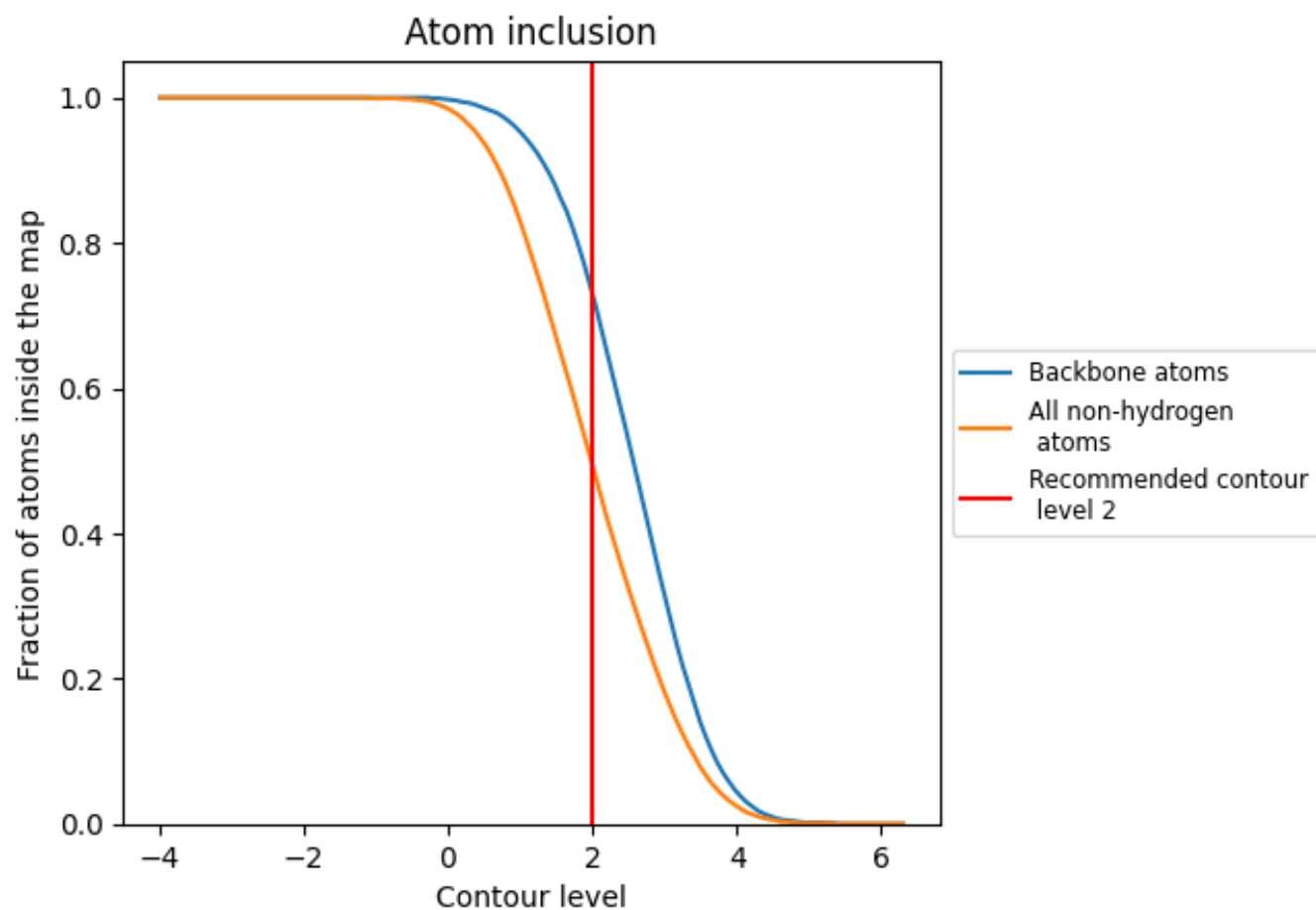
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 49% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4940	0.2660
A	0.6030	0.3090
B	0.5910	0.2950
C	0.5760	0.2960
D	0.5810	0.2910
E	0.5690	0.2840
F	0.5580	0.2860
G	0.5550	0.2840
H	0.5320	0.2800
I	0.6350	0.2470
J	0.6110	0.2390
K	0.6230	0.2420
L	0.6290	0.2470
M	0.1410	0.2060
N	0.3420	0.2110
O	0.0890	0.1910
P	0.1660	0.2080

1.0

0.0

<0.0