



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 06:51 AM EST

PDB ID : 6OGZ
EMDB ID : EMD-20060
Title : In situ structure of Rotavirus RNA-dependent RNA polymerase at transcript-elongated state
Authors : Ding, K.; Chang, T.; Shen, W.; Roy, P.; Zhou, Z.H.
Deposited on : 2019-04-03
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

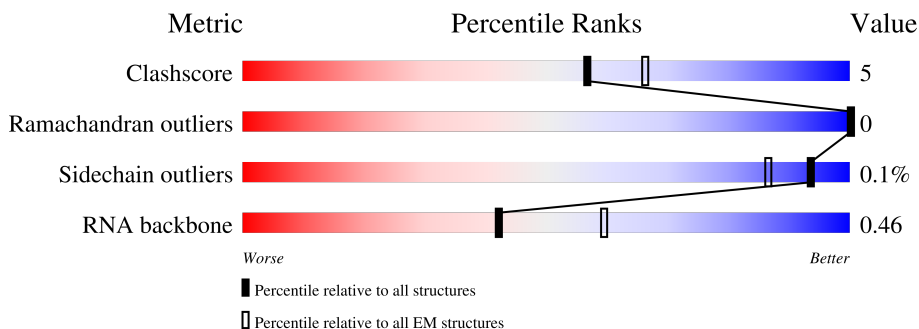
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





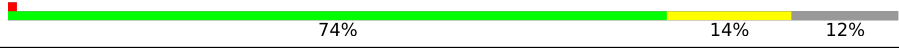



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	B	18	<div> <div>50%</div> <div>67%</div> <div>17%</div> <div>17%</div> </div>
2	C	17	<div> <div>35%</div> <div>71%</div> <div>29%</div> </div>
3	A	1088	<div> <div>5%</div> <div>86%</div> <div>13%</div> </div>
4	E	887	<div> <div>77%</div> <div>13%</div> <div>10%</div> </div>
4	F	887	<div> <div>80%</div> <div>11%</div> <div>9%</div> </div>
4	G	887	<div> <div>76%</div> <div>14%</div> <div>10%</div> </div>
4	H	887	<div> <div>78%</div> <div>13%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
4	I	887	
4	J	887	
4	K	887	
4	L	887	
4	M	887	
4	N	887	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 74962 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 RNA chain called RNA (5'-R(P*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	18	Total	C	N	O	P	0	0
			378	171	63	126	18		

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	17	Total	C	N	O	P	0	0
			358	162	61	118	17		

- Molecule 3 is a protein called RNA-dependent RNA polymerase of rotavirus A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1082	Total	C	N	O	S	0	0
			8754	5609	1450	1656	39		

- Molecule 4 is a protein called Inner capsid protein VP2.

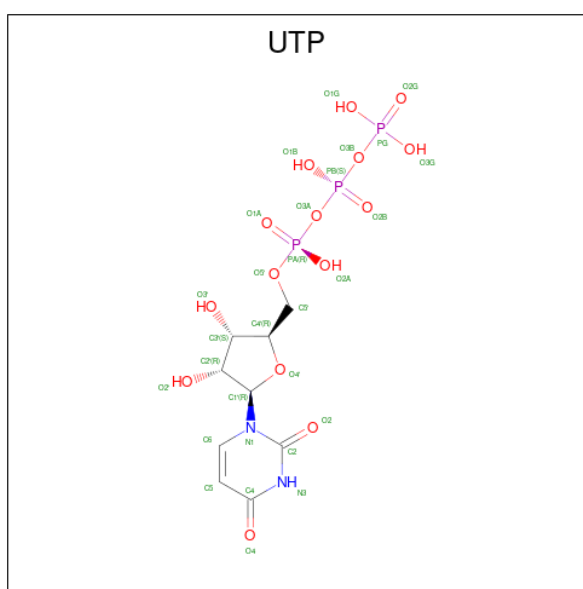
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	794	Total	C	N	O	S	0	0
			6492	4127	1117	1212	36		
4	F	803	Total	C	N	O	S	0	0
			6570	4174	1131	1229	36		
4	G	794	Total	C	N	O	S	0	0
			6487	4120	1119	1212	36		
4	I	781	Total	C	N	O	S	0	0
			6379	4052	1101	1190	36		
4	H	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		
4	J	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		

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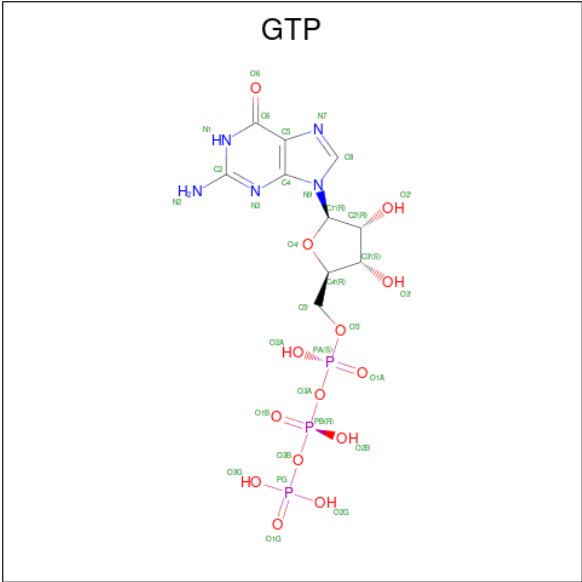
Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	781	Total	C	N	O	S	0	0
			6379	4052	1101	1190	36		
4	L	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		
4	M	826	Total	C	N	O	S	0	0
			6756	4292	1162	1266	36		
4	N	805	Total	C	N	O	S	0	0
			6587	4186	1134	1231	36		

- Molecule 5 is URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			29	9	2	15	3	

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

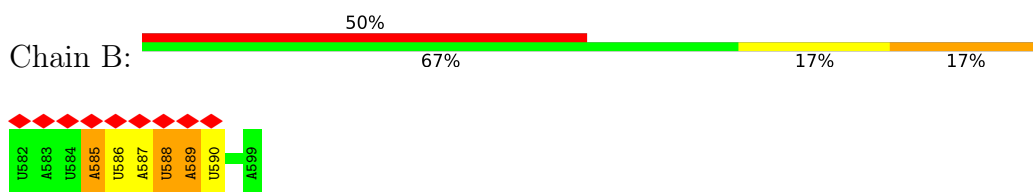


Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

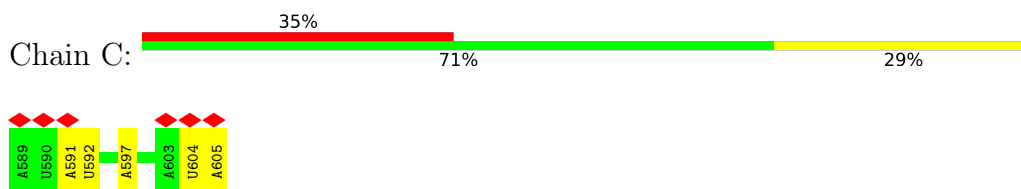
3 Residue-property plots

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.

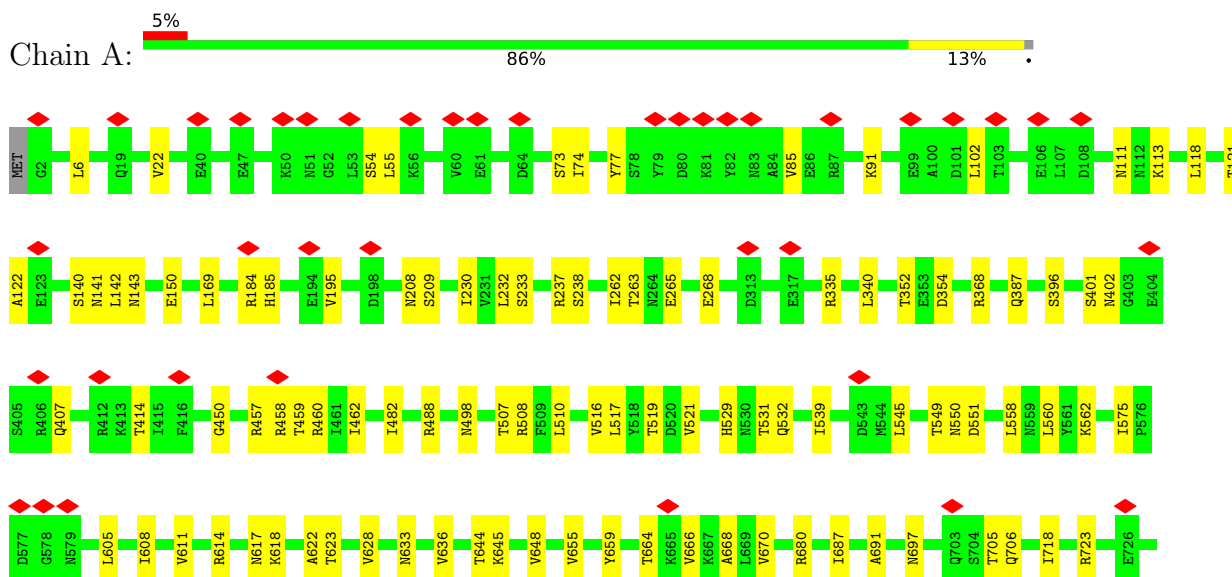
- Molecule 1: RNA (5'-R(P*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*A P*UP*A)-3')

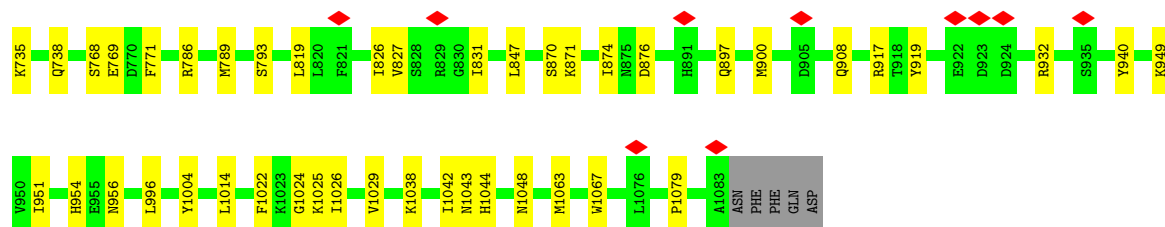


- Molecule 2: RNA (5'-R(P*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*UP*AP*U P*A)-3')



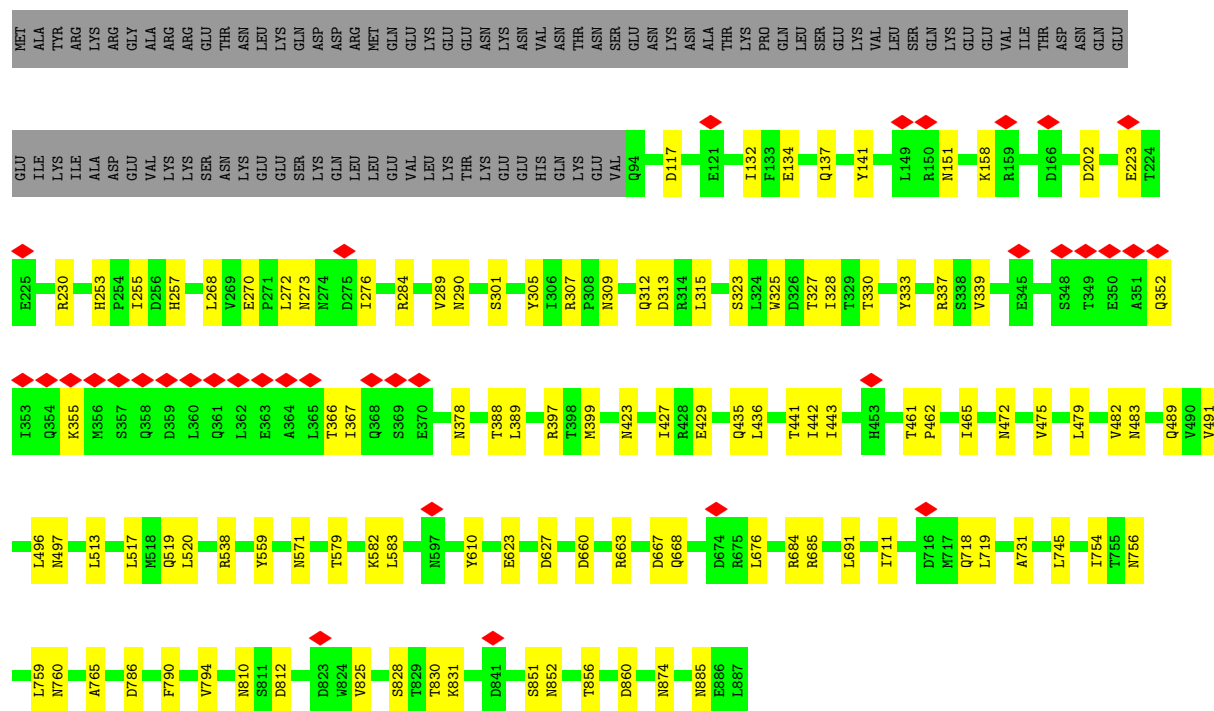
- Molecule 3: RNA-dependent RNA polymerase of rotavirus A





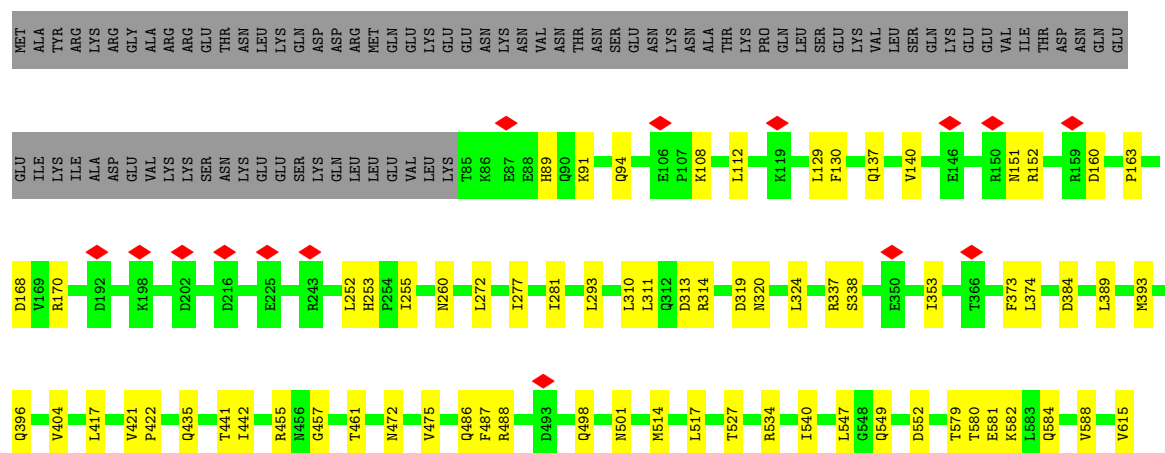
• Molecule 4: Inner capsid protein VP2

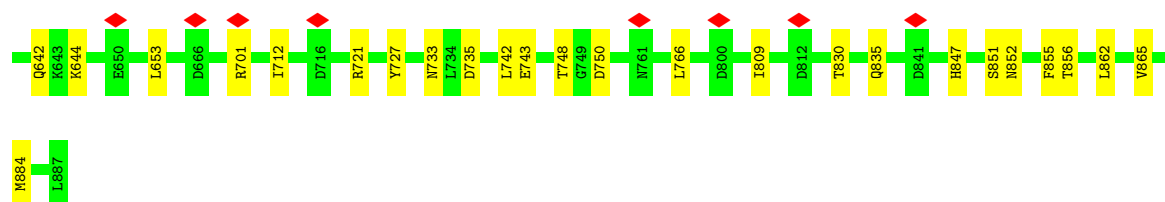
Chain E: 77% 13% 10%



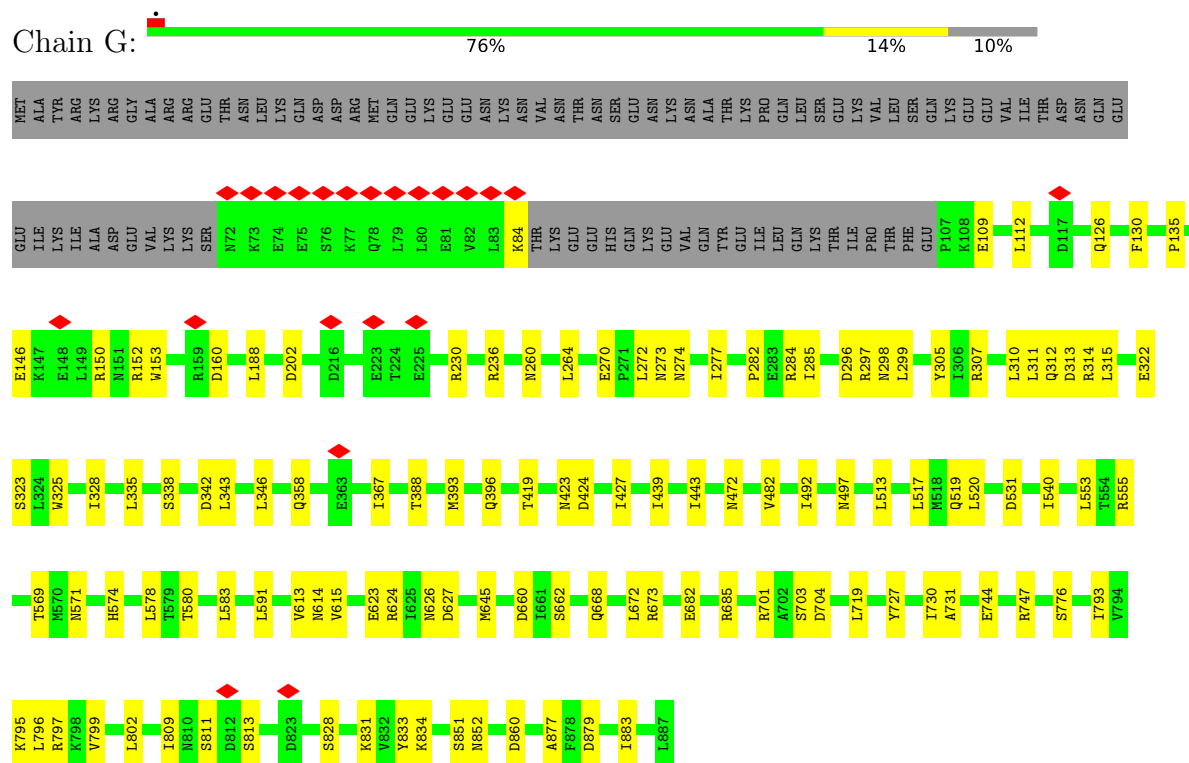
• Molecule 4: Inner capsid protein VP2

Chain F: 80% 11% 9%

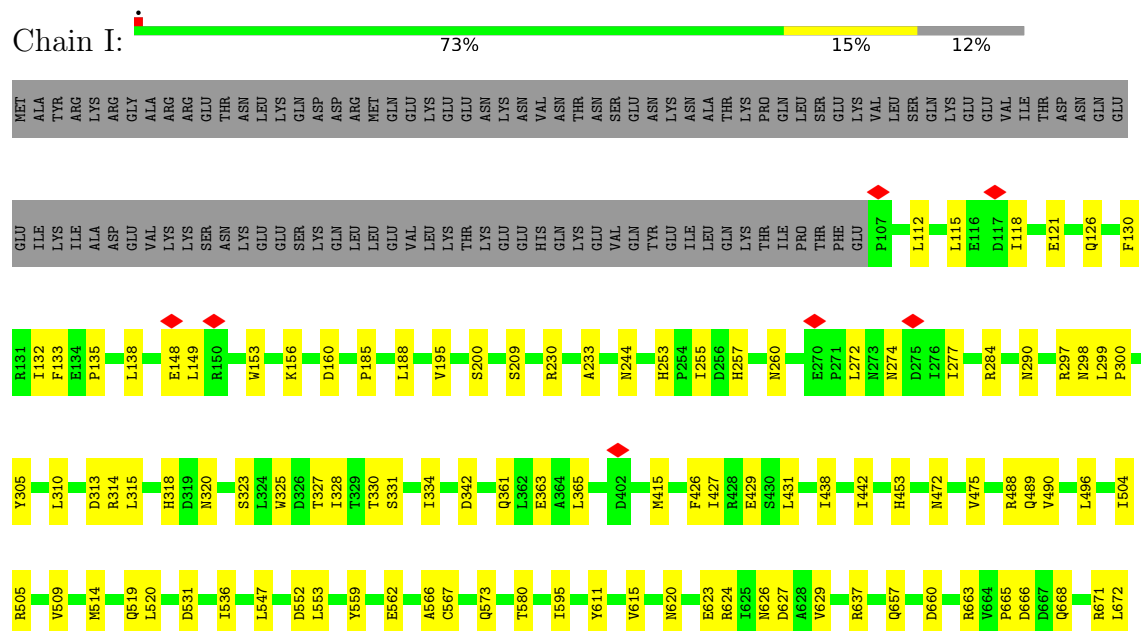


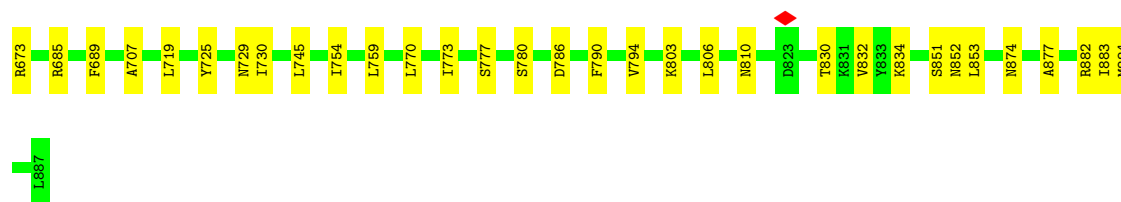


• Molecule 4: Inner capsid protein VP2



• Molecule 4: Inner capsid protein VP2





• Molecule 4: Inner capsid protein VP2

Chain H: 78% 13% 9%

MET ALA TYR ARG LYS ARG GLY ALA ARG LYS THR ASN LEU LYS GLN ASP LYS ASP ARG MET GLN VAL LYS GLU ASN LYS VAL ASN THR ASN SER GLU ASN LYS K803 L806 N810 D623 T830 K831 V832 Y833 K834 S851 N852 L853 N874 A877 R882 I883 M884

GLU ILE LYS ILE ALA ASP GLU VAL LYS SER ASN LYS GLU SER LYS GLN LEU VAL L83 K86 E87 L98 Q99 I102 E106 K113 D117 E121 Q122 K125 Q126 T127 K128 R131 L138 V140 Y141 R142 A143 N144 E148 L149 R150 N151

R152 K156 R159 D160 D192 K198 R201 V206 T211 E223 N247 L252 H253 P254 I255 D256 L264 Q267 I281 P282 E283 R284 I285 R286 N294 L299 N309 D313 N316 L317 H318 T330 R337 L343 L346 A364 L365

T366 E370 T371 Q372 I377 D384 C385 I390 L394 R397 Y408 I443 N472 V475 L479 H480 F481 V482 N483 F487 R488 Q489 D493 N497 Q498 N501 A516 L517 L520 R534 S535 I540 D552 L553 T554 R555 A566 C567 I568

L576 S587 S590 T595 N622 R637 R644 R663 D667 F689 I711 I712 A713 D716 E723 G726 Y727 A731 R732 N733 L734 D735 L742 L745 T748 G749 D750 L754 P763 V764 A765 L766 L770 P804 L805 L806 I809

N810 S811 D812 L818 V819 D823 H824 R831 V832 I836 D841 H847 T850 N851 N852 V865 V876 R882 I883 L887

• Molecule 4: Inner capsid protein VP2

Chain J: 79% 11% 9%

MET ALA TYR ARG LYS ARG GLY ALA ARG LYS THR ASN LEU LYS GLN ASP LYS ASP ARG MET GLN VAL LYS GLU ASN LYS VAL ASN THR ASN SER GLU ASN LYS I133 E134 L138 R142 A143 E146 K147 E148 L149 R150 W155 K156 L157 K158 R159 D166 R170 L188

GLU ILE LYS ILE ALA ASP GLU VAL LYS SER ASN LYS GLU SER LYS GLN LEU VAL L83 K84 T85 K86 T102 P103 T104 D117 R131 I132 F133 E134 L138 R142 A143 E146 K147 E148 L149 R150 W155 K156 L157 K158 R159 D166 R170 L188

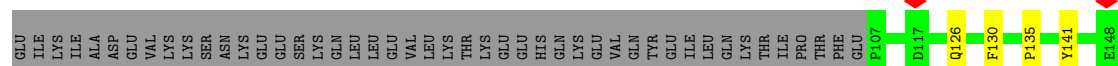
R201 T211 E223 T224 E225 R230 R238 V239 Q240 H253 D256 Q267 L272 I277 R284 I285 E322 L335 V347 Q364 K365 M366 Q367 L368 A364 Q368 S369 E370 T371 Q372 T375 Q376 L389 I390 R397 F403 T406

R407 Y408 L417 T441 I442 M449 G457 N472 L479 N483 F487 R488 N497 Q498 V499 L500 D502 N503 V509 L517 M518 Q519 R534 S535 I540 L541 L542 N545 L553 L557 Y561 L564 M565 A566 C567 T579 T580 E581 K582



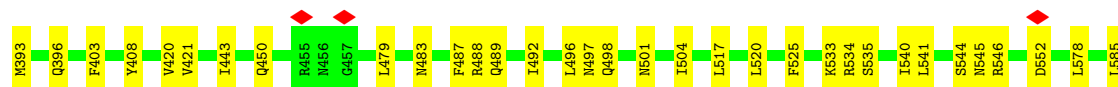
• Molecule 4: Inner capsid protein VP2

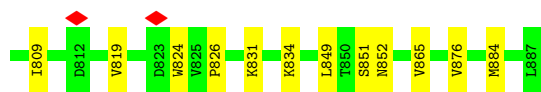
Chain K: 74% 14% 12%



• Molecule 4: Inner capsid protein VP2

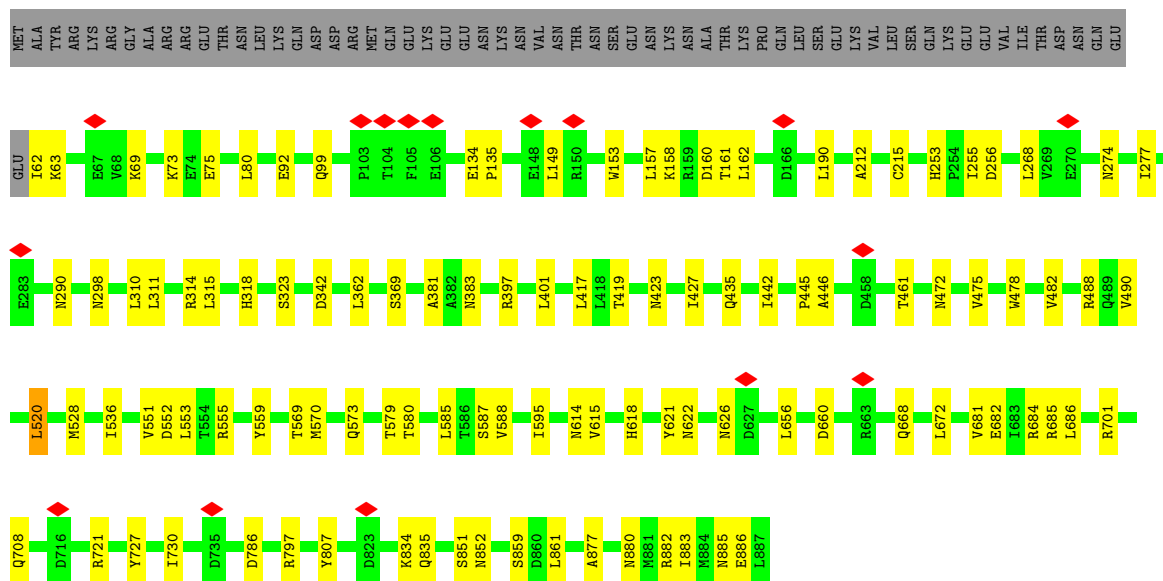
Chain L: 79% 12% 9%





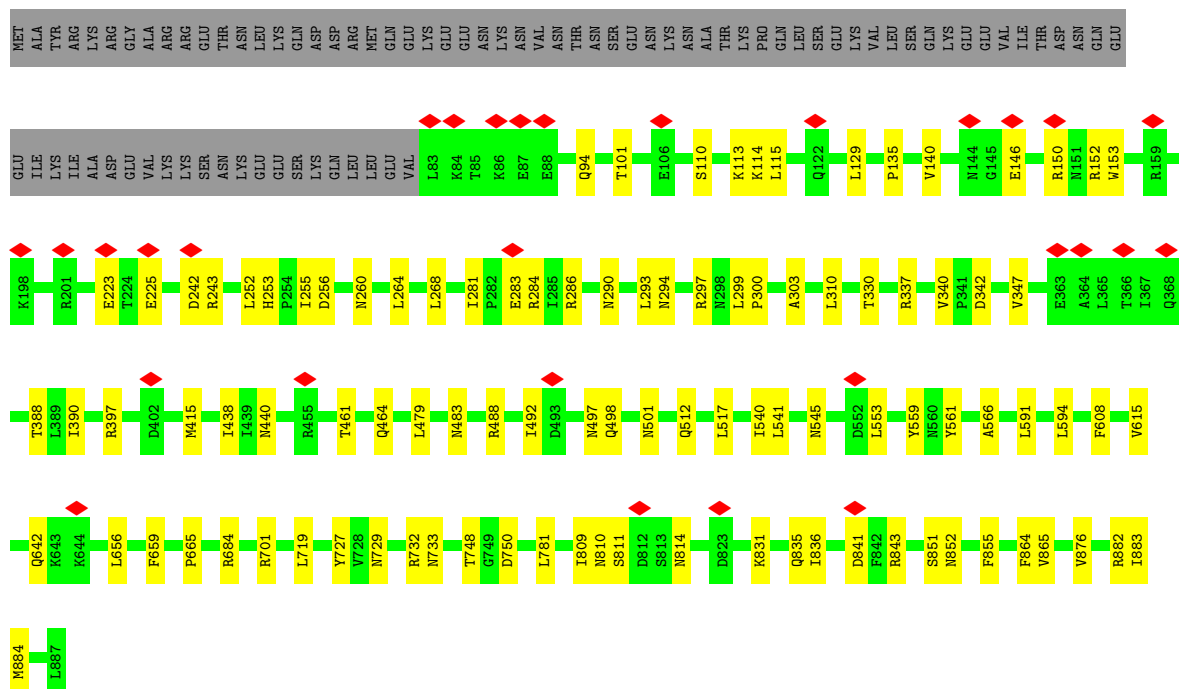
• Molecule 4: Inner capsid protein VP2

Chain M: 81% 12% 7%



• Molecule 4: Inner capsid protein VP2

Chain N: 79% 11% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	411438	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 ($e^-/\text{\AA}^2$)	18	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	0.135	Depositor
Minimum map value	-0.096	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0175	Depositor
Map size (Å)	353.76, 353.76, 353.76	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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: UTP, GTP

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	B	0.38	0/422	0.86	0/653
2	C	0.41	0/400	0.92	0/619
3	A	0.38	0/8926	0.53	0/12069
4	E	0.40	0/6611	0.58	0/8969
4	F	0.37	0/6690	0.54	0/9074
4	G	0.41	0/6602	0.58	0/8950
4	H	0.38	0/6707	0.56	0/9096
4	I	0.41	0/6495	0.58	0/8810
4	J	0.38	0/6707	0.56	0/9096
4	K	0.41	0/6495	0.58	0/8810
4	L	0.38	0/6707	0.56	0/9096
4	M	0.40	0/6876	0.57	1/9320 (0.0%)
4	N	0.38	0/6707	0.56	0/9096
All	All	0.39	0/76345	0.57	1/103658 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	M	520	LEU	CB-CG-CD1	-5.12	102.30	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	378	0	190	4	0
2	C	358	0	180	0	0
3	A	8754	0	8840	97	0
4	E	6492	0	6520	71	0
4	F	6570	0	6595	60	0
4	G	6487	0	6525	78	0
4	H	6587	0	6619	75	0
4	I	6379	0	6408	88	0
4	J	6587	0	6619	70	0
4	K	6379	0	6408	87	0
4	L	6587	0	6619	67	0
4	M	6756	0	6803	66	0
4	N	6587	0	6619	61	0
5	A	29	0	11	1	0
6	A	32	0	12	1	0
All	All	74962	0	74968	762	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 5.

All (762) 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)
4:I:148:GLU:O	4:I:149:LEU:HG	1.45	1.13
3:A:1026:ILE:HG22	3:A:1029:VAL:HG12	1.48	0.94
4:H:637:ARG:HD2	4:H:689:PHE:HE2	1.33	0.92
4:H:637:ARG:HD2	4:H:689:PHE:CE2	2.14	0.82
4:F:488:ARG:HE	4:F:501:ASN:HB3	1.52	0.75
3:A:1026:ILE:CG2	3:A:1029:VAL:HG12	2.19	0.72
4:K:322:GLU:HB3	4:K:578:LEU:HD13	1.70	0.72
4:L:488:ARG:HE	4:L:501:ASN:HB3	1.55	0.71
4:J:188:LEU:H	4:J:267:GLN:HE22	1.38	0.71
4:H:488:ARG:HE	4:H:501:ASN:HB3	1.56	0.70
4:L:420:VAL:HA	4:L:504:ILE:HD11	1.74	0.69
4:J:488:ARG:HE	4:J:501:ASN:HB3	1.58	0.69
4:H:637:ARG:CD	4:H:689:PHE:HE2	2.05	0.68
4:J:650:GLU:HG3	4:J:661:ILE:HG21	1.74	0.68
4:K:323:SER:HB3	4:K:668:GLN:HE22	1.60	0.67
4:N:140:VAL:HG11	4:N:152:ARG:HE	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:320:ASN:CG	4:K:671:ARG:NH1	2.49	0.66
4:L:188:LEU:H	4:L:267:GLN:HE22	1.44	0.65
3:A:1026:ILE:HG22	3:A:1029:VAL:CG1	2.24	0.65
4:G:343:LEU:HD23	4:G:346:LEU:HD21	1.79	0.65
3:A:517:LEU:HD11	3:A:655:VAL:HG21	1.79	0.65
3:A:819:LEU:HD11	3:A:940:TYR:HB2	1.79	0.64
3:A:184:ARG:H	3:A:195:VAL:HG21	1.63	0.64
4:L:253:HIS:HD2	4:L:255:ILE:H	1.46	0.64
4:E:323:SER:HB3	4:E:668:GLN:HE22	1.63	0.64
4:G:126:GLN:HE21	4:G:188:LEU:HD11	1.63	0.63
4:J:284:ARG:HE	4:J:566:ALA:HB2	1.63	0.63
4:K:324:LEU:HG	4:K:668:GLN:HE21	1.64	0.62
4:K:322:GLU:HA	4:K:322:GLU:OE1	2.00	0.62
4:J:389:LEU:HD23	4:J:557:LEU:HD11	1.82	0.62
4:K:320:ASN:ND2	4:L:545:ASN:OD1	2.28	0.62
4:F:517:LEU:HG	4:F:540:ILE:HG23	1.82	0.62
4:I:663:ARG:HG3	4:J:354:GLN:HE21	1.63	0.62
4:I:272:LEU:HD22	4:I:305:TYR:HB3	1.82	0.61
4:M:274:ASN:HD21	4:M:298:ASN:HA	1.64	0.61
4:N:488:ARG:HE	4:N:501:ASN:HB3	1.65	0.61
4:N:310:LEU:HD21	4:N:615:VAL:HG13	1.81	0.61
4:N:253:HIS:HD2	4:N:255:ILE:H	1.49	0.61
4:E:230:ARG:NH2	4:N:750:ASP:OD2	2.34	0.60
4:M:290:ASN:ND2	4:M:559:TYR:OH	2.34	0.60
4:H:727:TYR:HB2	4:H:809:ILE:HB	1.83	0.60
4:F:94:GLN:HE22	4:G:860:ASP:H	1.50	0.60
4:J:390:ILE:HD11	4:J:557:LEU:HG	1.83	0.60
4:M:323:SER:HB3	4:M:668:GLN:HE22	1.67	0.60
4:H:487:PHE:HB3	4:H:498:GLN:HB3	1.84	0.60
4:H:102:ILE:HD11	4:H:578:LEU:HD22	1.84	0.59
4:H:281:ILE:HD11	4:H:865:VAL:HG11	1.83	0.59
4:K:126:GLN:HE21	4:K:188:LEU:HD11	1.67	0.59
4:E:284:ARG:HH12	4:E:497:ASN:HD21	1.48	0.59
4:K:290:ASN:ND2	4:K:559:TYR:OH	2.36	0.59
4:I:130:PHE:H	4:I:260:ASN:HD21	1.50	0.59
4:I:552:ASP:OD2	4:I:884:MET:SD	2.61	0.59
4:K:320:ASN:ND2	4:K:671:ARG:NH1	2.50	0.59
4:E:429:GLU:OE1	4:F:534:ARG:NH2	2.36	0.59
4:K:253:HIS:HD2	4:K:255:ILE:H	1.51	0.59
4:J:487:PHE:HB3	4:J:498:GLN:HB3	1.85	0.58
4:I:505:ARG:NE	4:I:562:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:368:GLN:HE22	4:J:406:THR:HG21	1.68	0.58
4:M:423:ASN:ND2	4:M:482:VAL:O	2.37	0.58
4:G:272:LEU:HD22	4:G:305:TYR:HB3	1.85	0.58
4:G:311:LEU:HD11	4:G:314:ARG:HH21	1.68	0.58
4:L:94:GLN:HE22	4:M:859:SER:H	1.50	0.58
3:A:531:THR:OG1	3:A:532:GLN:N	2.36	0.58
4:N:492:ILE:HD11	4:N:497:ASN:HD21	1.68	0.58
3:A:1025:LYS:HB3	4:I:365:LEU:HD12	1.86	0.58
4:G:682:GLU:OE2	4:G:685:ARG:NH1	2.37	0.58
4:J:285:ILE:HD13	4:J:607:LEU:HD21	1.85	0.58
4:M:397:ARG:NH2	4:M:579:THR:OG1	2.37	0.58
4:J:654:LYS:HB2	4:J:661:ILE:HD11	1.86	0.58
4:K:429:GLU:OE2	4:L:534:ARG:NH2	2.36	0.58
4:N:281:ILE:HD11	4:N:865:VAL:HG11	1.84	0.58
4:I:290:ASN:ND2	4:I:559:TYR:OH	2.37	0.58
4:J:517:LEU:HG	4:J:540:ILE:HG23	1.84	0.58
4:J:819:VAL:HA	4:J:824:TRP:HE1	1.68	0.58
4:F:163:PRO:HB2	4:F:168:ASP:HB3	1.86	0.57
4:I:442:ILE:HG12	4:I:536:ILE:HD11	1.84	0.57
1:B:585:A:O2'	4:E:538:ARG:NH1	2.36	0.57
4:F:527:THR:O	4:F:527:THR:HG22	2.04	0.57
4:I:320:ASN:O	4:I:671:ARG:NH1	2.36	0.57
4:H:385:CYS:SG	4:H:587:SER:OG	2.62	0.57
4:K:320:ASN:CG	4:K:671:ARG:HH12	2.08	0.57
3:A:352:THR:HG22	3:A:354:ASP:H	1.69	0.57
4:G:793:ILE:HD12	4:G:799:VAL:HG12	1.87	0.57
4:J:564:LEU:HD23	4:J:607:LEU:HD13	1.87	0.57
4:L:517:LEU:HG	4:L:540:ILE:HG23	1.85	0.57
3:A:1026:ILE:CG2	3:A:1029:VAL:CG1	2.82	0.57
4:K:141:TYR:CE2	4:K:810:ASN:ND2	2.73	0.57
4:G:270:GLU:OE1	4:G:307:ARG:NH2	2.38	0.57
3:A:951:ILE:O	4:M:99:GLN:NE2	2.38	0.57
4:M:730:ILE:HD12	4:M:834:LYS:HB3	1.87	0.57
4:H:479:LEU:O	4:H:483:ASN:ND2	2.38	0.57
4:L:492:ILE:HD11	4:L:497:ASN:HD21	1.70	0.57
4:M:701:ARG:HD3	4:M:835:GLN:HG3	1.86	0.57
4:E:270:GLU:OE1	4:E:307:ARG:NH2	2.38	0.56
4:E:333:TYR:OH	4:E:337:ARG:NH2	2.35	0.56
4:G:472:ASN:ND2	4:G:519:GLN:OE1	2.38	0.56
4:G:310:LEU:HD11	4:G:615:VAL:HG13	1.87	0.56
3:A:1026:ILE:HD12	3:A:1063:MET:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:290:ASN:ND2	4:E:559:TYR:OH	2.38	0.56
4:F:337:ARG:NH2	4:F:384:ASP:OD1	2.36	0.56
4:K:479:LEU:O	4:K:483:ASN:ND2	2.38	0.56
4:K:553:LEU:HD12	4:K:595:ILE:HG21	1.86	0.56
4:F:579:THR:HG22	4:G:297:ARG:HE	1.69	0.56
4:I:623:GLU:O	4:I:624:ARG:NH2	2.39	0.56
4:F:170:ARG:NH2	4:F:743:GLU:OE2	2.38	0.56
4:K:343:LEU:HD23	4:K:346:LEU:HD21	1.88	0.56
4:L:131:ARG:NH2	4:L:211:THR:OG1	2.39	0.56
4:M:314:ARG:NH1	4:M:626:ASN:OD1	2.39	0.56
4:L:443:ILE:HG12	4:L:520:LEU:HD11	1.88	0.56
4:G:427:ILE:HD11	4:H:534:ARG:HH12	1.71	0.56
3:A:516:VAL:HG23	3:A:636:VAL:HG22	1.87	0.55
4:L:851:SER:OG	4:L:852:ASN:N	2.39	0.55
4:E:462:PRO:HA	4:E:465:ILE:HG22	1.88	0.55
3:A:1026:ILE:HG23	3:A:1067:TRP:HB2	1.88	0.55
4:F:472:ASN:HB3	4:F:475:VAL:HG12	1.88	0.55
4:L:337:ARG:NH2	4:L:384:ASP:OD1	2.39	0.55
3:A:1026:ILE:O	3:A:1029:VAL:HG12	2.06	0.55
4:E:230:ARG:HG3	4:N:748:THR:HB	1.89	0.55
4:G:274:ASN:HD21	4:G:298:ASN:HA	1.71	0.55
4:K:320:ASN:O	4:K:671:ARG:NH1	2.38	0.55
4:H:253:HIS:HD2	4:H:255:ILE:H	1.54	0.55
4:J:654:LYS:CA	4:J:661:ILE:HD11	2.37	0.55
4:M:381:ALA:HB1	4:M:587:SER:HB2	1.89	0.55
4:M:721:ARG:NH1	4:M:727:TYR:OH	2.40	0.55
4:E:312:GLN:HG2	4:E:571:ASN:HD22	1.72	0.54
4:H:555:ARG:HB3	4:H:883:ILE:HG22	1.88	0.54
4:K:489:GLN:HB3	4:K:496:LEU:HD11	1.89	0.54
4:F:281:ILE:HD11	4:F:865:VAL:HG11	1.90	0.54
4:L:727:TYR:HB2	4:L:809:ILE:HB	1.89	0.54
3:A:460:ARG:HH22	5:A:1101:UTP:H3'	1.72	0.54
4:J:579:THR:HG22	4:K:297:ARG:HE	1.72	0.54
4:E:397:ARG:NH2	4:E:579:THR:O	2.40	0.54
4:F:487:PHE:HB3	4:F:498:GLN:HB3	1.89	0.54
4:N:852:ASN:HD22	4:N:855:PHE:HE1	1.53	0.54
4:F:642:GLN:HG2	4:G:202:ASP:HA	1.89	0.54
4:M:69:LYS:HA	4:M:80:LEU:HD11	1.88	0.54
4:N:150:ARG:NH1	4:N:223:GLU:OE1	2.40	0.54
4:J:369:SER:HB2	4:J:372:GLN:HB2	1.90	0.54
4:L:479:LEU:O	4:L:483:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:701:ARG:HD2	4:N:835:GLN:HG3	1.90	0.54
4:F:580:THR:OG1	4:G:296:ASP:OD1	2.26	0.54
4:H:106:GLU:OE2	4:H:663:ARG:NH2	2.40	0.54
4:J:654:LYS:CB	4:J:661:ILE:HD11	2.38	0.54
4:I:553:LEU:HD12	4:I:595:ILE:HG21	1.88	0.54
4:K:504:ILE:HG12	4:K:509:VAL:HG21	1.89	0.54
4:N:719:LEU:HD11	4:N:781:LEU:HD11	1.90	0.54
4:M:445:PRO:HB3	4:M:528:MET:HG3	1.88	0.54
3:A:54:SER:OG	3:A:55:LEU:N	2.41	0.54
4:F:313:ASP:OD1	4:F:313:ASP:N	2.40	0.54
4:I:313:ASP:N	4:I:313:ASP:OD1	2.41	0.54
4:M:472:ASN:HB3	4:M:475:VAL:HG12	1.90	0.54
4:N:101:THR:HB	4:N:665:PRO:HG3	1.90	0.54
4:N:290:ASN:ND2	4:N:559:TYR:OH	2.41	0.54
4:I:427:ILE:HG23	4:J:534:ARG:HH12	1.72	0.53
4:E:272:LEU:HD22	4:E:305:TYR:HB3	1.90	0.53
4:I:274:ASN:HD21	4:I:298:ASN:HA	1.74	0.53
4:I:488:ARG:HH11	4:I:490:VAL:HG11	1.74	0.53
4:M:553:LEU:HD12	4:M:595:ILE:HG21	1.89	0.53
3:A:789:MET:SD	3:A:871:LYS:NZ	2.81	0.53
4:E:731:ALA:HB2	4:E:831:LYS:HD3	1.89	0.53
4:K:654:LYS:HB2	4:K:661:ILE:HD11	1.90	0.53
3:A:1038:LYS:NZ	4:G:367:ILE:O	2.40	0.53
4:F:281:ILE:HD13	4:F:293:LEU:HD13	1.89	0.53
4:G:150:ARG:HD2	4:G:152:ARG:HH12	1.73	0.53
4:G:314:ARG:NH1	4:G:626:ASN:OD1	2.42	0.53
4:E:309:ASN:ND2	4:E:623:GLU:OE2	2.42	0.53
4:E:479:LEU:O	4:E:483:ASN:ND2	2.41	0.53
4:G:627:ASP:OD1	4:G:685:ARG:NH2	2.42	0.53
4:I:874:ASN:OD1	4:I:882:ARG:NH1	2.41	0.53
4:K:354:GLN:HG3	4:M:75:GLU:HG3	1.90	0.53
4:L:264:LEU:HD13	4:L:849:LEU:HD12	1.91	0.53
4:L:819:VAL:HA	4:L:824:TRP:HE1	1.74	0.53
3:A:265:GLU:OE2	3:A:488:ARG:NH2	2.42	0.53
3:A:340:LEU:HA	3:A:575:ILE:HD11	1.90	0.53
4:H:732:ARG:HH11	4:H:836:ILE:HD11	1.74	0.53
4:G:701:ARG:NH1	4:G:833:TYR:OH	2.42	0.53
4:G:703:SER:OG	4:G:704:ASP:N	2.42	0.53
4:I:244:ASN:HB2	4:I:853:LEU:HB2	1.90	0.53
4:I:489:GLN:HB3	4:I:496:LEU:HD11	1.91	0.53
4:J:851:SER:OG	4:J:852:ASN:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:748:THR:HB	4:K:230:ARG:HG3	1.91	0.52
3:A:263:THR:O	3:A:508:ARG:NH1	2.40	0.52
4:F:108:LYS:NZ	4:F:581:GLU:OE2	2.42	0.52
4:H:313:ASP:OD1	4:H:313:ASP:N	2.42	0.52
4:J:355:LYS:NZ	4:J:359:ASP:OD2	2.43	0.52
4:K:327:THR:HA	4:K:330:THR:HG22	1.90	0.52
4:K:442:ILE:HD13	4:K:536:ILE:HD11	1.91	0.52
4:L:706:ILE:O	4:L:834:LYS:NZ	2.42	0.52
3:A:786:ARG:NH2	3:A:876:ASP:OD2	2.41	0.52
4:G:277:ILE:HD11	4:G:299:LEU:HD11	1.91	0.52
4:G:555:ARG:NH1	4:G:879:ASP:OD1	2.42	0.52
4:I:132:ILE:HG23	4:I:133:PHE:HD1	1.74	0.52
4:H:330:THR:OG1	4:H:397:ARG:NH2	2.42	0.52
4:G:731:ALA:HB2	4:G:831:LYS:HD3	1.91	0.52
4:I:627:ASP:OD1	4:I:685:ARG:NH1	2.40	0.52
4:H:472:ASN:HB2	4:H:475:VAL:HG22	1.90	0.52
4:H:851:SER:OG	4:H:852:ASN:N	2.43	0.52
4:E:327:THR:HA	4:E:330:THR:HG22	1.90	0.52
4:H:140:VAL:HG21	4:H:152:ARG:HH12	1.75	0.52
4:K:397:ARG:NH2	4:K:579:THR:OG1	2.42	0.52
4:L:170:ARG:NH1	4:L:639:ASN:O	2.43	0.52
4:E:756:ASN:O	4:E:760:ASN:ND2	2.42	0.52
4:I:415:MET:HG2	4:I:438:ILE:HD13	1.91	0.52
3:A:1004:TYR:OH	3:A:1043:ASN:OD1	2.24	0.52
4:E:339:VAL:HG11	4:E:610:TYR:HB2	1.91	0.52
4:H:443:ILE:HG12	4:H:520:LEU:HD11	1.92	0.52
4:M:660:ASP:OD1	4:M:660:ASP:N	2.43	0.52
4:F:253:HIS:HD2	4:F:255:ILE:H	1.57	0.52
4:N:110:SER:OG	4:N:114:LYS:NZ	2.42	0.52
4:N:883:ILE:HG22	4:N:884:MET:HG3	1.92	0.52
4:F:89:HIS:HD2	4:F:91:LYS:H	1.58	0.51
4:G:315:LEU:HD13	4:G:672:LEU:HD11	1.92	0.51
4:L:403:PHE:HB3	4:L:585:LEU:HB2	1.91	0.51
4:M:401:LEU:HD22	4:M:585:LEU:HD13	1.92	0.51
4:G:730:ILE:HD12	4:G:834:LYS:HB3	1.91	0.51
4:J:408:TYR:OH	4:J:535:SER:OG	2.28	0.51
4:K:314:ARG:NH1	4:K:626:ASN:OD1	2.42	0.51
4:K:742:LEU:HD21	4:K:766:LEU:HD23	1.92	0.51
4:H:284:ARG:HE	4:H:566:ALA:HB2	1.76	0.51
4:F:552:ASP:HB3	4:F:884:MET:HA	1.91	0.51
4:H:309:ASN:HD22	4:H:622:ASN:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:132:ILE:HG13	4:J:133:PHE:HD1	1.74	0.51
4:E:268:LEU:HD21	4:E:684:ARG:HD2	1.92	0.51
4:F:750:ASP:OD2	4:G:230:ARG:NH2	2.39	0.51
4:I:253:HIS:HD2	4:I:255:ILE:H	1.58	0.51
4:I:453:HIS:NE2	4:K:886:GLU:OE2	2.43	0.51
4:K:445:PRO:HB3	4:K:528:MET:HG3	1.93	0.51
3:A:268:GLU:HG2	3:A:919:TYR:HB3	1.92	0.51
3:A:507:THR:HG23	3:A:510:LEU:HD12	1.92	0.51
4:I:531:ASP:OD2	4:K:538:ARG:NH2	2.43	0.51
4:H:517:LEU:HG	4:H:540:ILE:HG23	1.92	0.51
4:H:553:LEU:HD12	4:H:595:ILE:HG21	1.91	0.51
4:L:450:GLN:OE1	4:M:880:ASN:ND2	2.42	0.51
4:L:487:PHE:HB3	4:L:498:GLN:HB3	1.93	0.51
3:A:73:SER:OG	3:A:74:ILE:N	2.44	0.51
4:F:748:THR:HB	4:G:230:ARG:HG3	1.93	0.51
4:G:660:ASP:N	4:G:660:ASP:OD1	2.44	0.51
4:J:131:ARG:HH22	4:J:211:THR:HB	1.76	0.51
4:K:322:GLU:HB3	4:K:578:LEU:CD1	2.40	0.51
4:N:225:GLU:OE2	4:N:843:ARG:NH1	2.43	0.51
4:I:126:GLN:HE21	4:I:188:LEU:HD11	1.76	0.51
4:L:541:LEU:O	4:L:545:ASN:ND2	2.44	0.51
1:B:587:A:H62	4:G:358:GLN:HE21	1.58	0.51
4:E:427:ILE:HD11	4:F:534:ARG:HH12	1.75	0.51
3:A:169:LEU:HD22	3:A:230:ILE:HD12	1.93	0.51
3:A:262:ILE:HD11	3:A:508:ARG:HG3	1.93	0.51
4:E:366:THR:HG23	4:E:367:ILE:HG13	1.92	0.51
3:A:22:VAL:HG12	3:A:77:TYR:HB2	1.93	0.50
4:G:146:GLU:HA	4:G:811:SER:HB2	1.93	0.50
4:K:130:PHE:H	4:K:260:ASN:HD21	1.58	0.50
4:I:300:PRO:HG3	4:H:578:LEU:HD11	1.92	0.50
4:J:479:LEU:O	4:J:483:ASN:ND2	2.44	0.50
4:F:253:HIS:CD2	4:F:255:ILE:H	2.29	0.50
4:K:321:PHE:CD1	4:K:324:LEU:HD12	2.46	0.50
4:K:472:ASN:HB3	4:K:475:VAL:HG12	1.93	0.50
3:A:614:ARG:O	3:A:617:ASN:ND2	2.45	0.50
4:H:282:PRO:HG2	4:H:285:ILE:HG12	1.94	0.50
4:H:742:LEU:HD21	4:H:766:LEU:HD23	1.93	0.50
4:J:727:TYR:HB2	4:J:809:ILE:HB	1.92	0.50
4:K:277:ILE:HG12	4:K:861:LEU:HB3	1.92	0.50
3:A:1025:LYS:HE3	4:I:363:GLU:OE1	2.12	0.50
4:H:131:ARG:NH2	4:H:211:THR:OG1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:701:ARG:HD2	4:F:835:GLN:HG3	1.93	0.50
4:G:531:ASP:OD2	4:I:361:GLN:NE2	2.45	0.50
4:I:112:LEU:HD12	4:I:334:ILE:HG22	1.94	0.50
4:I:327:THR:HA	4:I:330:THR:HG22	1.93	0.50
4:J:499:VAL:HG12	4:J:565:MET:HE1	1.93	0.50
4:M:851:SER:OG	4:M:852:ASN:N	2.44	0.50
4:N:851:SER:OG	4:N:852:ASN:N	2.44	0.50
3:A:605:LEU:HB2	3:A:628:VAL:HG11	1.93	0.50
3:A:687:ILE:HG23	3:A:900:MET:HG2	1.94	0.50
4:H:283:GLU:OE2	4:H:286:ARG:NH2	2.45	0.50
4:K:141:TYR:CZ	4:K:810:ASN:ND2	2.80	0.50
4:M:552:ASP:HA	4:M:555:ARG:HG3	1.92	0.50
4:H:337:ARG:NH2	4:H:384:ASP:OD1	2.41	0.50
4:H:734:LEU:HD12	4:H:765:ALA:HB1	1.94	0.50
4:M:682:GLU:OE1	4:M:685:ARG:NH1	2.44	0.50
4:G:424:ASP:HB3	4:G:574:HIS:HE1	1.77	0.50
4:I:314:ARG:NH1	4:I:626:ASN:OD1	2.45	0.50
4:K:270:GLU:OE2	4:K:307:ARG:NH2	2.44	0.50
4:K:320:ASN:ND2	4:K:671:ARG:HH11	2.10	0.50
4:F:137:GLN:NE2	4:F:151:ASN:O	2.45	0.49
4:H:343:LEU:HD23	4:H:346:LEU:HD21	1.94	0.49
4:K:770:LEU:HD21	4:K:802:LEU:HD22	1.93	0.49
4:E:851:SER:OG	4:E:852:ASN:N	2.45	0.49
4:G:264:LEU:HD22	4:G:851:SER:HB2	1.94	0.49
3:A:209:SER:OG	3:A:697:ASN:ND2	2.46	0.49
4:F:455:ARG:NH2	4:F:457:GLY:O	2.45	0.49
4:K:726:GLY:HA3	4:K:810:ASN:OD1	2.11	0.49
4:M:160:ASP:OD1	4:M:160:ASP:N	2.44	0.49
3:A:238:SER:HB2	3:A:335:ARG:HH11	1.78	0.49
4:F:311:LEU:HD11	4:F:314:ARG:HE	1.76	0.49
4:G:744:GLU:HG2	4:G:747:ARG:HH21	1.76	0.49
4:I:626:ASN:HA	4:I:629:VAL:HG12	1.95	0.49
4:M:315:LEU:HD13	4:M:672:LEU:HD11	1.95	0.49
3:A:85:VAL:HG22	3:A:143:ASN:HD21	1.78	0.49
4:E:790:PHE:HE2	4:E:830:THR:HG21	1.78	0.49
4:F:140:VAL:HG21	4:F:152:ARG:HE	1.77	0.49
4:G:877:ALA:HB2	4:G:883:ILE:HG23	1.94	0.49
4:K:472:ASN:ND2	4:K:519:GLN:OE1	2.35	0.49
4:L:340:VAL:HG13	4:L:387:LYS:HD3	1.95	0.49
4:E:860:ASP:O	4:N:94:GLN:NE2	2.45	0.49
4:L:290:ASN:HD21	4:L:876:VAL:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:489:GLN:HB3	4:L:496:LEU:HD11	1.95	0.49
4:N:479:LEU:O	4:N:483:ASN:ND2	2.45	0.49
3:A:827:VAL:O	3:A:831:ILE:N	2.42	0.49
4:G:797:ARG:HE	4:H:294:ASN:HD22	1.61	0.49
4:I:567:CYS:SG	4:I:611:TYR:HB2	2.52	0.49
4:F:310:LEU:HD11	4:F:615:VAL:HG13	1.95	0.49
4:I:472:ASN:HB3	4:I:475:VAL:HG12	1.94	0.49
4:L:525:PHE:H	4:L:533:LYS:HD2	1.77	0.49
4:N:876:VAL:HA	4:N:882:ARG:HA	1.93	0.49
4:E:137:GLN:HE21	4:E:151:ASN:HD22	1.60	0.48
4:F:441:THR:HG23	4:F:442:ILE:HG13	1.94	0.48
4:G:313:ASP:N	4:G:313:ASP:OD1	2.45	0.48
4:L:408:TYR:OH	4:L:535:SER:OG	2.31	0.48
3:A:608:ILE:HA	3:A:611:VAL:HG12	1.94	0.48
4:I:472:ASN:HD21	4:I:519:GLN:HG2	1.78	0.48
4:H:99:GLN:O	4:H:663:ARG:NH1	2.46	0.48
4:J:253:HIS:HB3	4:J:256:ASP:HB2	1.94	0.48
4:L:166:ASP:HB3	4:L:743:GLU:HG2	1.95	0.48
3:A:233:SER:OG	3:A:237:ARG:NH1	2.46	0.48
4:I:514:MET:HG3	4:I:547:LEU:HD13	1.94	0.48
4:J:441:THR:HG23	4:J:442:ILE:HG13	1.95	0.48
3:A:529:HIS:HD1	3:A:664:THR:HG1	1.59	0.48
3:A:622:ALA:HB2	4:F:404:VAL:HG21	1.94	0.48
4:E:435:GLN:OE1	4:E:461:THR:OG1	2.29	0.48
4:I:851:SER:OG	4:I:852:ASN:N	2.45	0.48
4:J:397:ARG:NH2	4:J:581:GLU:OE1	2.47	0.48
4:N:146:GLU:HA	4:N:811:SER:HB2	1.94	0.48
3:A:396:SER:O	3:A:396:SER:OG	2.32	0.48
4:F:851:SER:OG	4:F:852:ASN:N	2.47	0.48
4:I:673:ARG:NH2	4:J:887:LEU:OXT	2.46	0.48
4:J:238:ARG:HE	4:J:240:GLN:HE21	1.62	0.48
4:N:727:TYR:HB2	4:N:809:ILE:HB	1.95	0.48
4:I:427:ILE:HG13	4:I:580:THR:HG21	1.96	0.48
4:L:641:TYR:OH	4:L:743:GLU:OE1	2.32	0.48
4:I:504:ILE:HG13	4:I:509:VAL:HG21	1.95	0.48
4:K:718:GLN:NE2	4:K:719:LEU:O	2.47	0.48
4:E:202:ASP:HA	4:N:642:GLN:HG3	1.96	0.48
4:H:377:ILE:HA	4:H:590:SER:HB3	1.96	0.48
4:H:497:ASN:OD1	4:H:497:ASN:N	2.47	0.48
4:J:582:LYS:NZ	4:K:296:ASP:OD2	2.44	0.48
4:M:253:HIS:HD2	4:M:255:ILE:H	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:129:LEU:HD23	4:N:252:LEU:HD21	1.96	0.48
4:I:149:LEU:C	4:I:149:LEU:HD12	2.34	0.47
4:I:320:ASN:HD21	4:J:545:ASN:HD21	1.61	0.47
4:H:408:TYR:OH	4:H:535:SER:OG	2.31	0.47
4:J:655:ARG:O	4:J:657:GLN:NE2	2.47	0.47
4:K:569:THR:HG22	4:K:614:ASN:HB3	1.95	0.47
4:I:277:ILE:HD11	4:I:299:LEU:HD11	1.96	0.47
3:A:140:SER:OG	3:A:738:GLN:OE1	2.32	0.47
4:K:443:ILE:HG12	4:K:520:LEU:HD11	1.96	0.47
4:M:342:ASP:HB2	4:M:383:ASN:HD21	1.79	0.47
4:M:882:ARG:HG3	4:M:885:ASN:HB3	1.96	0.47
3:A:628:VAL:HG23	3:A:633:ASN:HB3	1.96	0.47
3:A:874:ILE:HD13	3:A:996:LEU:HG	1.96	0.47
4:K:627:ASP:OD1	4:K:685:ARG:NH2	2.42	0.47
4:N:541:LEU:O	4:N:545:ASN:ND2	2.47	0.47
4:K:202:ASP:OD1	4:K:202:ASP:N	2.38	0.47
4:F:417:LEU:HD22	4:F:588:VAL:HG21	1.97	0.47
4:L:152:ARG:NH1	4:L:723:GLU:OE1	2.47	0.47
3:A:335:ARG:O	3:A:459:THR:OG1	2.33	0.47
3:A:1079:PRO:HB3	4:M:92:GLU:HG3	1.96	0.47
4:E:472:ASN:HD21	4:E:519:GLN:HG2	1.79	0.47
4:F:721:ARG:NH1	4:F:727:TYR:OH	2.48	0.47
4:I:342:ASP:N	4:I:342:ASP:OD1	2.45	0.47
4:L:393:MET:O	4:L:396:GLN:NE2	2.48	0.47
4:L:719:LEU:HD13	4:L:826:PRO:HB2	1.97	0.47
4:M:435:GLN:OE1	4:M:461:THR:OG1	2.28	0.47
4:N:330:THR:OG1	4:N:397:ARG:NH2	2.48	0.47
3:A:826:ILE:HD11	3:A:949:LYS:HD2	1.96	0.47
3:A:1026:ILE:CD1	3:A:1063:MET:HB3	2.45	0.47
4:E:289:VAL:HG13	4:N:440:ASN:HD21	1.79	0.47
4:E:627:ASP:OD1	4:E:685:ARG:NH2	2.48	0.47
4:F:130:PHE:H	4:F:260:ASN:HD21	1.63	0.47
4:G:427:ILE:HD12	4:G:580:THR:HG21	1.96	0.47
4:I:786:ASP:OD1	4:I:786:ASP:N	2.45	0.47
4:H:818:LEU:O	4:H:824:TRP:NE1	2.47	0.47
4:J:879:ASP:OD1	4:J:879:ASP:N	2.47	0.47
4:K:272:LEU:HD22	4:K:305:TYR:HB3	1.97	0.47
3:A:141:ASN:ND2	3:A:208:ASN:OD1	2.47	0.47
4:G:719:LEU:HD23	4:G:828:SER:HB3	1.96	0.47
4:I:725:TYR:O	4:I:810:ASN:ND2	2.47	0.47
4:K:149:LEU:O	4:K:149:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:735:ASP:OD1	4:K:735:ASP:N	2.48	0.47
4:M:311:LEU:O	4:M:622:ASN:ND2	2.44	0.47
4:N:337:ARG:NH1	4:N:388:THR:OG1	2.46	0.47
4:I:806:LEU:HD12	4:I:832:VAL:HG21	1.97	0.47
4:J:503:ASN:HB3	4:J:509:VAL:HG23	1.97	0.47
4:L:740:ILE:HB	4:L:766:LEU:HD23	1.96	0.47
4:N:841:ASP:OD1	4:N:841:ASP:N	2.48	0.47
4:J:138:LEU:HD13	4:J:156:LYS:HZ1	1.79	0.46
4:K:274:ASN:HD21	4:K:298:ASN:HA	1.80	0.46
4:L:621:TYR:HD1	4:L:656:LEU:HD21	1.80	0.46
4:L:755:THR:HG22	4:L:794:VAL:HG12	1.97	0.46
4:N:461:THR:HB	4:N:464:GLN:HG3	1.97	0.46
4:E:301:SER:O	4:E:301:SER:OG	2.34	0.46
4:E:325:TRP:HA	4:E:328:ILE:HG22	1.97	0.46
4:K:253:HIS:CD2	4:K:255:ILE:H	2.32	0.46
4:M:427:ILE:HD12	4:M:580:THR:HG21	1.97	0.46
3:A:1044:HIS:CE1	3:A:1048:ASN:HD22	2.33	0.46
4:E:388:THR:HG23	4:E:583:LEU:HD12	1.97	0.46
4:H:113:LYS:HE3	4:H:117:ASP:HB2	1.97	0.46
4:L:552:ASP:HB3	4:L:884:MET:HA	1.97	0.46
3:A:545:LEU:HB3	3:A:558:LEU:HD21	1.97	0.46
4:E:874:ASN:OD1	4:E:874:ASN:N	2.49	0.46
4:G:273:ASN:N	4:G:273:ASN:OD1	2.48	0.46
4:G:388:THR:HG23	4:G:583:LEU:HD12	1.97	0.46
4:I:253:HIS:CD2	4:I:255:ILE:H	2.33	0.46
4:I:310:LEU:HD21	4:I:615:VAL:HG13	1.97	0.46
4:J:553:LEU:HD12	4:J:595:ILE:HG21	1.96	0.46
3:A:113:LYS:HB2	3:A:118:LEU:HD12	1.97	0.46
4:E:352:GLN:HA	4:E:355:LYS:HB2	1.96	0.46
4:I:660:ASP:N	4:I:660:ASP:OD1	2.48	0.46
4:J:102:ILE:HG22	4:J:104:THR:H	1.79	0.46
4:J:567:CYS:SG	4:J:607:LEU:HD11	2.55	0.46
4:L:742:LEU:HD22	4:L:799:VAL:HG21	1.97	0.46
4:E:423:ASN:HD21	4:E:482:VAL:HG12	1.81	0.46
4:H:882:ARG:HH11	4:H:887:LEU:HD11	1.80	0.46
4:N:283:GLU:OE2	4:N:286:ARG:NH2	2.48	0.46
3:A:870:SER:O	3:A:870:SER:OG	2.31	0.46
4:I:115:LEU:HD21	4:I:331:SER:HB3	1.97	0.46
4:I:230:ARG:HG3	4:H:748:THR:HB	1.98	0.46
4:I:665:PRO:HG2	4:J:355:LYS:HD2	1.97	0.46
4:H:489:GLN:NE2	4:H:498:GLN:OE1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:264:LEU:O	4:H:267:GLN:NE2	2.49	0.46
3:A:539:ILE:HG23	3:A:562:LYS:HG3	1.98	0.46
3:A:549:THR:OG1	3:A:550:ASN:N	2.48	0.46
4:I:323:SER:HB3	4:I:668:GLN:HE22	1.81	0.46
4:J:641:TYR:HB2	4:K:202:ASP:HB3	1.98	0.46
4:L:91:LYS:HD3	4:L:95:TYR:HE2	1.81	0.46
4:M:446:ALA:CB	4:M:520:LEU:CD1	2.94	0.46
3:A:91:LYS:NZ	3:A:150:GLU:OE2	2.49	0.46
4:K:665:PRO:HG3	4:L:355:LYS:HD2	1.97	0.46
3:A:1014:LEU:HD11	3:A:1042:ILE:HD11	1.98	0.45
4:F:742:LEU:HD21	4:F:766:LEU:HD22	1.97	0.45
4:I:121:GLU:OE1	4:I:624:ARG:NH1	2.50	0.45
4:N:135:PRO:HB2	4:N:153:TRP:HE3	1.81	0.45
3:A:387:GLN:NE2	3:A:551:ASP:OD2	2.47	0.45
4:I:230:ARG:NH2	4:H:750:ASP:OD2	2.46	0.45
4:H:475:VAL:HG12	4:H:516:ALA:HB1	1.98	0.45
4:G:423:ASN:ND2	4:G:482:VAL:O	2.49	0.45
4:I:118:ILE:HG12	4:I:657:GLN:HG3	1.97	0.45
4:L:253:HIS:CD2	4:L:255:ILE:H	2.31	0.45
4:M:149:LEU:O	4:M:149:LEU:HG	2.16	0.45
4:N:264:LEU:HD11	4:N:851:SER:HB2	1.98	0.45
4:G:130:PHE:N	4:G:260:ASN:OD1	2.47	0.45
4:I:325:TRP:HA	4:I:328:ILE:HG22	1.99	0.45
4:H:667:ASP:OD1	4:H:667:ASP:N	2.46	0.45
4:K:710:VAL:HG11	4:K:790:PHE:HZ	1.81	0.45
4:N:340:VAL:HG11	4:N:390:ILE:HB	1.98	0.45
4:H:394:LEU:HG	4:H:568:ILE:HD11	1.98	0.45
4:J:403:PHE:HB3	4:J:585:LEU:HB2	1.97	0.45
4:J:472:ASN:HD21	4:J:519:GLN:HG2	1.81	0.45
4:K:376:GLY:O	4:K:590:SER:OG	2.35	0.45
4:N:110:SER:HG	4:N:114:LYS:NZ	2.15	0.45
4:E:273:ASN:H	4:E:276:ILE:HG22	1.81	0.45
4:I:253:HIS:O	4:I:257:HIS:N	2.49	0.45
4:L:167:TYR:OH	4:L:641:TYR:O	2.27	0.45
4:F:393:MET:O	4:F:396:GLN:NE2	2.49	0.45
4:F:514:MET:HB2	4:F:547:LEU:HD13	1.99	0.45
4:G:325:TRP:HA	4:G:328:ILE:HG22	1.98	0.45
4:K:166:ASP:HB3	4:K:743:GLU:HB2	1.97	0.45
4:L:281:ILE:HD11	4:L:865:VAL:HG11	1.99	0.45
4:L:622:ASN:HD22	4:L:625:ILE:HD11	1.80	0.45
3:A:618:LYS:O	4:F:584:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:580:THR:OG1	4:K:296:ASP:OD1	2.33	0.45
4:K:730:ILE:HG13	4:K:834:LYS:HB3	1.98	0.45
4:M:488:ARG:HH11	4:M:490:VAL:HG11	1.82	0.45
4:E:134:GLU:HB2	4:E:158:LYS:HG3	1.98	0.45
4:E:810:ASN:OD1	4:E:810:ASN:N	2.48	0.45
4:I:877:ALA:HB2	4:I:883:ILE:HG23	1.98	0.45
4:K:701:ARG:HD3	4:K:835:GLN:HG3	1.98	0.45
4:M:419:THR:HB	4:M:478:TRP:HE1	1.82	0.45
4:N:284:ARG:HD2	4:N:566:ALA:HB2	1.97	0.45
4:F:129:LEU:HD13	4:F:252:LEU:HD11	1.99	0.44
4:H:731:ALA:HB2	4:H:831:LYS:HD2	1.99	0.44
4:K:325:TRP:HA	4:K:328:ILE:HG22	1.99	0.44
4:N:517:LEU:HG	4:N:540:ILE:HG23	1.99	0.44
4:E:443:ILE:HG12	4:E:520:LEU:HD11	1.99	0.44
4:J:375:THR:OG1	4:J:376:GLY:N	2.50	0.44
4:K:650:GLU:HG3	4:K:661:ILE:HG21	1.99	0.44
4:K:814:ASN:OD1	4:K:814:ASN:N	2.51	0.44
4:N:810:ASN:OD1	4:N:810:ASN:N	2.47	0.44
4:F:712:ILE:HA	4:F:830:THR:HG22	1.98	0.44
4:G:112:LEU:HD11	4:G:338:SER:HB3	2.00	0.44
4:G:202:ASP:OD2	4:G:236:ARG:NE	2.50	0.44
4:G:851:SER:OG	4:G:852:ASN:N	2.51	0.44
4:H:253:HIS:HB3	4:H:256:ASP:HB2	1.98	0.44
4:J:564:LEU:HD23	4:J:607:LEU:CD1	2.47	0.44
4:N:115:LEU:HD23	4:N:115:LEU:HA	1.84	0.44
4:E:489:GLN:HB3	4:E:496:LEU:HD11	1.99	0.44
4:E:667:ASP:HA	4:F:549:GLN:HE22	1.82	0.44
4:F:353:ILE:HG12	4:F:374:LEU:HD23	1.99	0.44
4:L:541:LEU:HA	4:L:544:SER:HB3	2.00	0.44
3:A:623:THR:HG21	4:F:373:PHE:HE1	1.83	0.44
3:A:900:MET:O	3:A:908:GLN:NE2	2.49	0.44
4:E:472:ASN:HB3	4:E:475:VAL:HG12	1.98	0.44
4:F:435:GLN:OE1	4:F:461:THR:OG1	2.36	0.44
4:G:284:ARG:NH1	4:G:497:ASN:HD21	2.15	0.44
4:I:284:ARG:HE	4:I:566:ALA:HB2	1.82	0.44
4:N:498:GLN:O	4:N:561:TYR:OH	2.32	0.44
4:I:135:PRO:HB2	4:I:153:TRP:HE3	1.83	0.44
4:I:475:VAL:HG21	4:I:520:LEU:HD12	1.99	0.44
4:H:138:LEU:HD11	4:H:156:LYS:HG3	2.00	0.44
4:K:731:ALA:HB2	4:K:831:LYS:HE2	2.00	0.44
4:N:293:LEU:HD11	4:N:608:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:662:SER:O	4:G:662:SER:OG	2.36	0.44
4:I:707:ALA:N	4:I:770:LEU:O	2.50	0.44
4:H:819:VAL:HA	4:H:824:TRP:HE1	1.83	0.44
4:J:417:LEU:HD22	4:J:588:VAL:HG21	2.00	0.44
4:K:390:ILE:HD12	4:K:561:TYR:HB2	2.00	0.44
3:A:705:THR:OG1	3:A:706:GLN:N	2.50	0.44
4:H:142:ARG:NH2	4:H:148:GLU:OE1	2.50	0.44
4:L:660:ASP:N	4:L:660:ASP:OD1	2.51	0.44
4:M:446:ALA:CB	4:M:520:LEU:HD11	2.47	0.44
3:A:450:GLY:O	3:A:462:ILE:N	2.50	0.44
3:A:498:ASN:HD22	3:A:917:ARG:HB3	1.83	0.44
4:E:253:HIS:CD2	4:E:255:ILE:H	2.36	0.44
4:E:441:THR:HG22	4:E:442:ILE:HG13	2.00	0.44
4:F:856:THR:O	4:F:856:THR:OG1	2.35	0.44
4:I:148:GLU:C	4:I:149:LEU:HG	2.29	0.44
4:K:419:THR:HB	4:K:478:TRP:HE1	1.83	0.44
4:K:667:ASP:OD2	4:L:546:ARG:NH1	2.50	0.44
4:M:701:ARG:HA	4:M:708:GLN:HE22	1.83	0.44
4:G:517:LEU:HD13	4:G:540:ILE:HG12	2.00	0.43
4:J:335:LEU:HD11	4:J:613:VAL:HG11	2.00	0.43
4:K:337:ARG:NH2	4:K:388:THR:OG1	2.51	0.43
4:N:297:ARG:HD3	4:N:864:PHE:HD1	1.83	0.43
3:A:847:LEU:HD23	3:A:847:LEU:HA	1.89	0.43
3:A:1026:ILE:CG2	3:A:1067:TRP:HB2	2.47	0.43
4:I:160:ASP:N	4:I:160:ASP:OD1	2.46	0.43
4:I:297:ARG:HD3	4:H:98:LEU:HD22	2.00	0.43
4:I:719:LEU:HD22	4:I:729:ASN:HB3	2.01	0.43
4:J:170:ARG:NH1	4:J:638:LEU:O	2.50	0.43
4:J:498:GLN:O	4:J:561:TYR:OH	2.30	0.43
4:L:629:VAL:HG12	4:L:681:VAL:HG12	1.99	0.43
3:A:185:HIS:H	3:A:185:HIS:CD2	2.36	0.43
3:A:232:LEU:HD23	3:A:232:LEU:HA	1.84	0.43
4:F:582:LYS:NZ	4:G:296:ASP:OD2	2.39	0.43
4:I:426:PHE:HB2	4:I:431:LEU:HB2	2.01	0.43
4:L:670:TYR:HA	4:L:673:ARG:HG2	2.00	0.43
4:E:141:TYR:OH	4:E:812:ASP:OD2	2.34	0.43
4:E:313:ASP:OD1	4:E:313:ASP:N	2.50	0.43
4:H:160:ASP:OD1	4:H:160:ASP:N	2.47	0.43
4:H:806:LEU:HD12	4:H:832:VAL:HG11	1.99	0.43
4:N:342:ASP:N	4:N:342:ASP:OD1	2.41	0.43
4:E:137:GLN:NE2	4:E:223:GLU:OE2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:491:VAL:HA	4:E:496:LEU:HA	2.01	0.43
4:F:112:LEU:HD11	4:F:338:SER:HB3	2.00	0.43
4:M:253:HIS:HB3	4:M:256:ASP:HB2	2.00	0.43
3:A:184:ARG:NH1	6:A:1102:GTP:O1G	2.51	0.43
4:G:160:ASP:OD1	4:G:160:ASP:N	2.43	0.43
4:I:185:PRO:HG3	4:I:188:LEU:HD12	2.00	0.43
4:I:637:ARG:HD2	4:I:689:PHE:HE2	1.84	0.43
4:J:873:ILE:HD12	4:J:873:ILE:HA	1.92	0.43
4:L:672:LEU:HD12	4:L:672:LEU:HA	1.84	0.43
3:A:6:LEU:HD11	4:G:84:LYS:HB2	2.01	0.43
3:A:735:LYS:HD2	3:A:735:LYS:HA	1.86	0.43
4:E:786:ASP:N	4:E:786:ASP:OD1	2.49	0.43
4:I:118:ILE:HG23	4:I:620:ASN:HD22	1.84	0.43
4:I:773:ILE:HG23	4:I:803:LYS:HD2	2.00	0.43
4:J:654:LYS:HB2	4:J:661:ILE:CD1	2.49	0.43
4:J:670:TYR:HA	4:J:673:ARG:HG2	2.01	0.43
4:L:708:GLN:H	4:L:708:GLN:HG2	1.51	0.43
4:M:318:HIS:CE1	4:M:573:GLN:HG3	2.54	0.43
4:G:323:SER:HB3	4:G:668:GLN:HE22	1.84	0.43
4:H:113:LYS:HA	4:H:113:LYS:HD2	1.91	0.43
4:H:745:LEU:HD21	4:H:754:ILE:HG21	1.99	0.43
4:L:339:VAL:HG11	4:L:610:TYR:HB2	2.00	0.43
4:L:497:ASN:OD1	4:L:497:ASN:N	2.52	0.43
1:B:588:U:H4'	3:A:932:ARG:HH22	1.83	0.43
4:I:195:VAL:HG21	4:I:209:SER:HA	2.01	0.43
4:I:759:LEU:HD21	4:I:794:VAL:HG11	2.01	0.43
4:H:253:HIS:CD2	4:H:255:ILE:H	2.35	0.43
4:M:135:PRO:HB2	4:M:153:TRP:HE3	1.84	0.43
4:M:681:VAL:HG13	4:M:686:LEU:HB2	2.01	0.43
3:A:401:SER:OG	3:A:402:ASN:N	2.52	0.43
3:A:648:VAL:HG13	3:A:670:VAL:HG23	2.01	0.43
3:A:793:SER:O	3:A:793:SER:OG	2.36	0.43
3:A:954:HIS:CD2	3:A:956:ASN:H	2.36	0.43
4:G:553:LEU:HD21	4:G:591:LEU:HG	2.00	0.43
4:J:873:ILE:HD11	4:J:887:LEU:HD11	2.01	0.43
4:E:719:LEU:HD23	4:E:828:SER:HB3	2.01	0.42
4:H:481:PHE:HZ	4:H:501:ASN:HD21	1.67	0.42
4:K:228:VAL:HB	4:K:842:PHE:HD2	1.84	0.42
4:K:453:HIS:NE2	4:M:886:GLU:OE2	2.52	0.42
3:A:519:THR:HG22	3:A:668:ALA:HA	2.01	0.42
4:F:862:LEU:HD23	4:F:862:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:876:VAL:HA	4:H:882:ARG:HA	2.00	0.42
4:M:369:SER:O	4:M:369:SER:OG	2.31	0.42
4:F:644:LYS:HB3	4:F:644:LYS:HE2	1.84	0.42
4:F:733:ASN:ND2	4:F:735:ASP:OD2	2.53	0.42
4:G:645:MET:HB2	4:G:673:ARG:HD2	2.01	0.42
4:I:427:ILE:HG22	4:I:429:GLU:HG2	2.00	0.42
4:I:790:PHE:HE2	4:I:830:THR:HG21	1.83	0.42
4:K:453:HIS:HE1	4:M:551:VAL:HG11	1.85	0.42
4:K:703:SER:O	4:K:834:LYS:NZ	2.35	0.42
4:K:830:THR:OG1	4:K:831:LYS:N	2.53	0.42
4:L:343:LEU:HB3	4:L:346:LEU:HD21	2.01	0.42
4:M:570:MET:HG3	4:M:618:HIS:CD2	2.55	0.42
4:E:378:ASN:N	4:E:378:ASN:OD1	2.52	0.42
4:E:711:ILE:HA	4:E:765:ALA:HA	2.01	0.42
4:I:244:ASN:OD1	4:I:244:ASN:N	2.51	0.42
4:L:701:ARG:HD3	4:L:708:GLN:HE22	1.85	0.42
4:M:62:ILE:HG13	4:M:63:LYS:HD3	2.00	0.42
4:F:727:TYR:HB2	4:F:809:ILE:HB	2.01	0.42
4:N:733:ASN:OD1	4:N:733:ASN:N	2.53	0.42
3:A:680:ARG:HB3	3:A:687:ILE:HD11	2.01	0.42
4:G:312:GLN:HB3	4:G:571:ASN:HB2	2.01	0.42
4:I:730:ILE:HG23	4:I:834:LYS:HB3	2.02	0.42
4:L:733:ASN:OD1	4:L:733:ASN:N	2.52	0.42
4:N:732:ARG:HH22	4:N:836:ILE:HD11	1.85	0.42
3:A:644:THR:OG1	3:A:645:LYS:N	2.53	0.42
4:E:885:ASN:OD1	4:E:885:ASN:N	2.52	0.42
4:G:135:PRO:HB2	4:G:153:TRP:HE3	1.84	0.42
4:G:443:ILE:HG12	4:G:520:LEU:HD11	2.01	0.42
4:H:316:ASN:HD22	4:H:318:HIS:CE1	2.38	0.42
4:H:390:ILE:O	4:H:394:LEU:N	2.51	0.42
4:M:253:HIS:CD2	4:M:255:ILE:H	2.37	0.42
4:M:277:ILE:HG12	4:M:861:LEU:HD12	2.02	0.42
4:M:310:LEU:HD21	4:M:615:VAL:HG22	2.02	0.42
4:N:300:PRO:HD2	4:N:303:ALA:HB2	2.01	0.42
4:N:512:GLN:O	4:N:512:GLN:NE2	2.53	0.42
3:A:521:VAL:HA	3:A:666:VAL:HG23	2.01	0.42
4:J:449:MET:H	4:J:449:MET:HG2	1.64	0.42
4:K:773:ILE:HG23	4:K:803:LYS:HE2	2.02	0.42
4:K:801:THR:O	4:K:801:THR:OG1	2.37	0.42
4:M:621:TYR:HA	4:M:656:LEU:HD21	2.02	0.42
4:N:110:SER:OG	4:N:110:SER:O	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:768:SER:OG	3:A:769:GLU:N	2.53	0.42
4:F:272:LEU:HD21	4:F:277:ILE:HD11	2.01	0.42
4:I:745:LEU:HD21	4:I:754:ILE:HG21	2.02	0.42
4:M:786:ASP:HB3	4:M:807:TYR:HE2	1.84	0.42
1:B:589:A:H61	3:A:482:ILE:HG23	1.85	0.42
4:E:132:ILE:HD12	4:E:132:ILE:HA	1.93	0.42
4:E:315:LEU:HD21	4:E:676:LEU:HD12	2.01	0.42
4:H:252:LEU:HB2	4:H:847:HIS:CE1	2.55	0.42
4:J:497:ASN:OD1	4:J:497:ASN:N	2.53	0.42
3:A:262:ILE:HG13	3:A:508:ARG:HA	2.02	0.41
4:E:691:LEU:HD23	4:E:691:LEU:HA	1.87	0.41
4:E:759:LEU:HD21	4:E:794:VAL:HG11	2.02	0.41
4:E:856:THR:O	4:E:856:THR:OG1	2.38	0.41
4:G:322:GLU:HB3	4:G:578:LEU:HD11	2.02	0.41
4:G:393:MET:O	4:G:396:GLN:NE2	2.53	0.41
4:G:439:ILE:HD13	4:G:439:ILE:HA	1.91	0.41
4:J:272:LEU:HD21	4:J:277:ILE:HD11	2.02	0.41
4:L:299:LEU:HA	4:L:300:PRO:HD3	1.94	0.41
4:M:157:LEU:HB3	4:M:160:ASP:HB3	2.02	0.41
3:A:102:LEU:O	3:A:111:ASN:ND2	2.42	0.41
3:A:633:ASN:OD1	3:A:633:ASN:N	2.53	0.41
4:F:324:LEU:HD11	4:F:653:LEU:HD21	2.02	0.41
4:G:727:TYR:HB2	4:G:809:ILE:HB	2.01	0.41
4:G:795:LYS:HG2	4:G:796:LEU:HD12	2.02	0.41
4:I:666:ASP:HB2	4:J:347:VAL:HG22	2.02	0.41
4:H:711:ILE:HA	4:H:765:ALA:HA	2.03	0.41
4:H:733:ASN:ND2	4:H:735:ASP:OD2	2.44	0.41
4:H:770:LEU:HD23	4:H:804:PRO:HD3	2.01	0.41
4:L:188:LEU:HD23	4:L:188:LEU:HA	1.93	0.41
4:L:232:ILE:HA	4:L:235:MET:HG3	2.01	0.41
4:M:569:THR:HG22	4:M:614:ASN:HB3	2.02	0.41
3:A:121:THR:OG1	3:A:122:ALA:N	2.53	0.41
4:E:389:LEU:HA	4:E:399:MET:HE1	2.02	0.41
4:E:517:LEU:HD12	4:E:517:LEU:HA	1.89	0.41
4:J:356:MET:HG3	4:J:542:LEU:HD13	2.02	0.41
4:L:504:ILE:HD13	4:L:504:ILE:HG21	1.85	0.41
4:N:268:LEU:HD22	4:N:684:ARG:HH12	1.85	0.41
3:A:1022:PHE:CZ	3:A:1024:GLY:HA2	2.54	0.41
4:E:745:LEU:HD21	4:E:754:ILE:HG21	2.02	0.41
4:H:713:ALA:HA	4:H:763:PRO:HB3	2.00	0.41
4:J:134:GLU:HG2	4:J:158:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:170:ARG:NH1	4:J:639:ASN:O	2.41	0.41
4:M:268:LEU:HD21	4:M:684:ARG:HD2	2.02	0.41
4:N:729:ASN:HD22	4:N:831:LYS:HA	1.85	0.41
4:N:814:ASN:OD1	4:N:814:ASN:N	2.50	0.41
3:A:718:ILE:HD11	3:A:771:PHE:HA	2.01	0.41
4:F:389:LEU:HD11	4:F:421:VAL:HG21	2.02	0.41
4:K:315:LEU:HD13	4:K:672:LEU:HD11	2.02	0.41
4:L:389:LEU:HD11	4:L:421:VAL:HG21	2.03	0.41
4:L:578:LEU:HD23	4:L:578:LEU:HA	1.90	0.41
4:N:113:LYS:HA	4:N:113:LYS:HD2	1.85	0.41
3:A:407:GLN:NE2	3:A:414:THR:OG1	2.54	0.41
4:I:138:LEU:HD11	4:I:156:LYS:HE2	2.02	0.41
4:K:252:LEU:HD23	4:K:256:ASP:HB3	2.02	0.41
4:L:711:ILE:HG23	4:L:831:LYS:HG3	2.02	0.41
4:M:417:LEU:HG	4:M:588:VAL:HG11	2.03	0.41
3:A:368:ARG:HH22	4:E:663:ARG:HG3	1.86	0.41
4:F:422:PRO:HB3	4:F:486:GLN:HA	2.03	0.41
4:G:282:PRO:HD2	4:G:285:ILE:HD12	2.01	0.41
4:G:419:THR:HG21	4:G:513:LEU:HD22	2.02	0.41
4:H:299:LEU:HD13	4:H:299:LEU:HA	1.94	0.41
4:H:726:GLY:HA3	4:H:810:ASN:ND2	2.35	0.41
4:L:742:LEU:HD21	4:L:766:LEU:HD22	2.03	0.41
4:N:347:VAL:HG22	4:N:594:LEU:HA	2.03	0.41
3:A:560:LEU:HD23	3:A:560:LEU:HA	1.83	0.41
4:E:253:HIS:O	4:E:257:HIS:N	2.48	0.41
4:I:777:SER:HB3	4:I:780:SER:HB3	2.02	0.41
4:H:711:ILE:HG23	4:H:831:LYS:HG3	2.02	0.41
4:J:146:GLU:HA	4:J:811:SER:HB2	2.02	0.41
4:K:135:PRO:HB2	4:K:153:TRP:HE3	1.86	0.41
4:M:157:LEU:HD12	4:M:157:LEU:HA	1.94	0.41
3:A:457:ARG:NH1	3:A:458:ARG:O	2.54	0.41
4:E:513:LEU:O	4:E:517:LEU:N	2.51	0.41
4:E:718:GLN:HE21	4:E:825:VAL:HG21	1.85	0.41
4:G:342:ASP:OD1	4:G:342:ASP:N	2.50	0.41
4:I:318:HIS:CE1	4:I:573:GLN:HG3	2.55	0.41
4:H:247:ASN:HB3	4:H:850:THR:HB	2.03	0.41
4:H:726:GLY:HA3	4:H:810:ASN:HD21	1.86	0.41
4:K:475:VAL:HG23	4:K:516:ALA:HB1	2.03	0.41
4:L:189:LEU:HD23	4:L:189:LEU:HA	1.90	0.41
4:M:134:GLU:HG2	4:M:158:LYS:HB2	2.02	0.41
4:M:212:ALA:HA	4:M:215:CYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:797:ARG:HH21	4:N:294:ASN:HB3	1.86	0.41
4:N:299:LEU:HA	4:N:300:PRO:HD3	1.91	0.41
4:N:415:MET:HG2	4:N:438:ILE:HD13	2.03	0.41
3:A:897:GLN:NE2	4:G:109:GLU:OE2	2.52	0.41
4:E:582:LYS:HE2	4:E:582:LYS:HB2	1.97	0.41
4:I:663:ARG:HD3	4:J:358:GLN:HE22	1.86	0.41
4:K:367:ILE:HD12	4:M:362:LEU:HB2	2.03	0.41
4:K:424:ASP:HB3	4:K:574:HIS:HE1	1.84	0.41
4:M:442:ILE:HA	4:M:536:ILE:HD11	2.01	0.41
4:M:877:ALA:HB2	4:M:883:ILE:HG23	2.03	0.41
4:N:553:LEU:HD11	4:N:591:LEU:HG	2.03	0.41
4:G:569:THR:OG1	4:G:614:ASN:O	2.39	0.40
4:K:181:LEU:HD11	4:K:685:ARG:HG3	2.03	0.40
4:K:836:ILE:HA	4:K:836:ILE:HD13	1.76	0.40
3:A:142:LEU:HD23	3:A:142:LEU:HA	1.94	0.40
3:A:691:ALA:HB2	3:A:723:ARG:HB3	2.03	0.40
4:E:117:ASP:OD1	4:E:117:ASP:N	2.54	0.40
4:E:436:LEU:HB2	4:E:462:PRO:HG3	2.03	0.40
4:F:319:ASP:OD1	4:F:320:ASN:N	2.54	0.40
4:G:335:LEU:HD11	4:G:613:VAL:HG11	2.03	0.40
4:G:802:LEU:HD12	4:G:802:LEU:HA	1.92	0.40
4:J:285:ILE:CD1	4:J:607:LEU:HD21	2.48	0.40
4:K:310:LEU:HD21	4:K:615:VAL:HG13	2.03	0.40
4:L:654:LYS:HB3	4:L:654:LYS:HE3	1.82	0.40
4:N:242:ASP:OD1	4:N:243:ARG:N	2.54	0.40
4:G:555:ARG:HB3	4:G:883:ILE:HG22	2.02	0.40
4:I:315:LEU:HD13	4:I:672:LEU:HD11	2.04	0.40
4:J:155:TRP:CD2	4:J:253:HIS:HD2	2.39	0.40
4:J:335:LEU:HD21	4:J:613:VAL:HG13	2.03	0.40
4:K:417:LEU:HD23	4:K:417:LEU:HA	1.91	0.40
4:L:343:LEU:HD23	4:L:346:LEU:HD21	2.03	0.40
4:M:162:LEU:HA	4:M:162:LEU:HD23	1.82	0.40
4:N:656:LEU:HD23	4:N:659:PHE:HE2	1.85	0.40
4:F:160:ASP:OD1	4:F:160:ASP:N	2.45	0.40
4:F:852:ASN:HD22	4:F:855:PHE:HE1	1.68	0.40
4:G:776:SER:HB3	4:G:813:SER:HB2	2.03	0.40
4:I:200:SER:HA	4:I:233:ALA:HA	2.02	0.40
4:H:156:LYS:HE2	4:H:156:LYS:HB3	1.88	0.40
4:J:661:ILE:O	4:J:661:ILE:HG22	2.20	0.40
4:N:256:ASP:O	4:N:260:ASN:ND2	2.55	0.40
4:E:660:ASP:OD1	4:E:660:ASP:N	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:284:ARG:HH11	4:G:492:ILE:HD12	1.87	0.40
4:G:623:GLU:O	4:G:624:ARG:NH2	2.51	0.40
4:G:624:ARG:HD3	4:G:624:ARG:HA	1.76	0.40
4:G:793:ILE:HD11	4:G:802:LEU:HD13	2.04	0.40
4:H:125:LYS:NZ	4:H:192:ASP:OD2	2.54	0.40
4:K:885:ASN:OD1	4:K:885:ASN:N	2.49	0.40
4:M:73:LYS:H	4:M:73:LYS:HG2	1.63	0.40
4:M:190:LEU:HG	4:M:851:SER:HB3	2.04	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	
3	A	1080/1088 (99%)	1025 (95%)	55 (5%)	0	100	100
4	E	792/887 (89%)	762 (96%)	30 (4%)	0	100	100
4	F	801/887 (90%)	774 (97%)	27 (3%)	0	100	100
4	G	790/887 (89%)	755 (96%)	35 (4%)	0	100	100
4	H	803/887 (90%)	769 (96%)	34 (4%)	0	100	100
4	I	779/887 (88%)	745 (96%)	34 (4%)	0	100	100
4	J	803/887 (90%)	766 (95%)	37 (5%)	0	100	100
4	K	779/887 (88%)	744 (96%)	35 (4%)	0	100	100
4	L	803/887 (90%)	771 (96%)	32 (4%)	0	100	100
4	M	824/887 (93%)	790 (96%)	34 (4%)	0	100	100
4	N	803/887 (90%)	773 (96%)	30 (4%)	0	100	100
All	All	9057/9958 (91%)	8674 (96%)	383 (4%)	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	
3	A	983/989 (99%)	982 (100%)	1 (0%)	93	98
4	E	730/818 (89%)	730 (100%)	0	100	100
4	F	739/818 (90%)	738 (100%)	1 (0%)	93	98
4	G	730/818 (89%)	730 (100%)	0	100	100
4	H	741/818 (91%)	740 (100%)	1 (0%)	93	98
4	I	717/818 (88%)	717 (100%)	0	100	100
4	J	741/818 (91%)	741 (100%)	0	100	100
4	K	717/818 (88%)	717 (100%)	0	100	100
4	L	741/818 (91%)	740 (100%)	1 (0%)	93	98
4	M	761/818 (93%)	760 (100%)	1 (0%)	93	98
4	N	741/818 (91%)	741 (100%)	0	100	100
All	All	8341/9169 (91%)	8336 (100%)	5 (0%)	93	98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	659	TYR
4	F	847	HIS
4	H	206	VAL
4	L	236	ARG
4	M	161	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	143	ASN
3	A	283	GLN
3	A	407	GLN
3	A	653	ASN
3	A	697	ASN

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Mol	Chain	Res	Type
3	A	862	GLN
3	A	912	GLN
3	A	954	HIS
3	A	1000	ASN
3	A	1044	HIS
4	E	122	GLN
4	E	151	ASN
4	E	175	ASN
4	E	247	ASN
4	E	480	HIS
4	E	497	ASN
4	E	573	GLN
4	E	574	HIS
4	E	576	GLN
4	E	668	GLN
4	E	718	GLN
4	E	760	ASN
4	F	89	HIS
4	F	94	GLN
4	F	260	ASN
4	F	352	GLN
4	F	358	GLN
4	F	396	GLN
4	F	512	GLN
4	F	573	GLN
4	F	695	ASN
4	G	126	GLN
4	G	199	ASN
4	G	265	GLN
4	G	274	ASN
4	G	358	GLN
4	G	396	GLN
4	G	480	HIS
4	G	545	ASN
4	G	574	HIS
4	G	636	ASN
4	G	708	GLN
4	G	762	GLN
4	G	852	ASN
4	I	175	ASN
4	I	260	ASN
4	I	266	HIS

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Mol	Chain	Res	Type
4	I	274	ASN
4	I	287	ASN
4	I	290	ASN
4	I	361	GLN
4	I	380	GLN
4	I	396	GLN
4	I	574	HIS
4	I	668	GLN
4	I	753	GLN
4	I	762	GLN
4	H	309	ASN
4	H	316	ASN
4	H	352	GLN
4	H	512	GLN
4	H	636	ASN
4	H	738	GLN
4	H	753	GLN
4	H	762	GLN
4	H	810	ASN
4	H	838	GLN
4	H	847	HIS
4	J	267	GLN
4	J	352	GLN
4	J	354	GLN
4	J	368	GLN
4	J	512	GLN
4	J	545	ASN
4	J	708	GLN
4	J	761	ASN
4	J	762	GLN
4	K	126	GLN
4	K	247	ASN
4	K	260	ASN
4	K	372	GLN
4	K	450	GLN
4	K	545	ASN
4	K	573	GLN
4	K	574	HIS
4	K	668	GLN
4	K	880	ASN
4	L	94	GLN
4	L	267	GLN

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Mol	Chain	Res	Type
4	L	512	GLN
4	L	622	ASN
4	L	626	ASN
4	L	636	ASN
4	M	90	GLN
4	M	260	ASN
4	M	266	HIS
4	M	274	ASN
4	M	290	ASN
4	M	396	GLN
4	M	423	ASN
4	M	574	HIS
4	M	835	GLN
4	N	220	GLN
4	N	266	HIS
4	N	287	ASN
4	N	352	GLN
4	N	368	GLN
4	N	396	GLN
4	N	695	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	17/18 (94%)	5 (29%)	0
2	C	16/17 (94%)	5 (31%)	0
All	All	33/35 (94%)	10 (30%)	0

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	585	A
1	B	586	U
1	B	588	U
1	B	589	A
1	B	590	U
2	C	591	A
2	C	592	U
2	C	597	A
2	C	604	U
2	C	605	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	UTP	A	1101	-	22,30,30	0.98	1 (4%)	27,47,47	1.09	1 (3%)
6	GTP	A	1102	-	26,34,34	1.14	2 (7%)	32,54,54	1.56	6 (18%)

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	UTP	A	1101	-	-	0/20/38/38	0/2/2/2
6	GTP	A	1102	-	-	4/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1102	GTP	C5-C6	-3.96	1.39	1.47
5	A	1101	UTP	C4-N3	3.03	1.38	1.33
6	A	1102	GTP	C2-N3	2.09	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1101	UTP	C5-C4-N3	-3.89	114.76	123.31
6	A	1102	GTP	C5-C6-N1	3.48	120.10	113.95
6	A	1102	GTP	C8-N7-C5	3.10	108.89	102.99
6	A	1102	GTP	PB-O3B-PG	-3.03	122.42	132.83
6	A	1102	GTP	C2-N1-C6	-3.00	119.57	125.10
6	A	1102	GTP	C3'-C2'-C1'	2.72	105.07	100.98
6	A	1102	GTP	PA-O3A-PB	-2.71	123.52	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

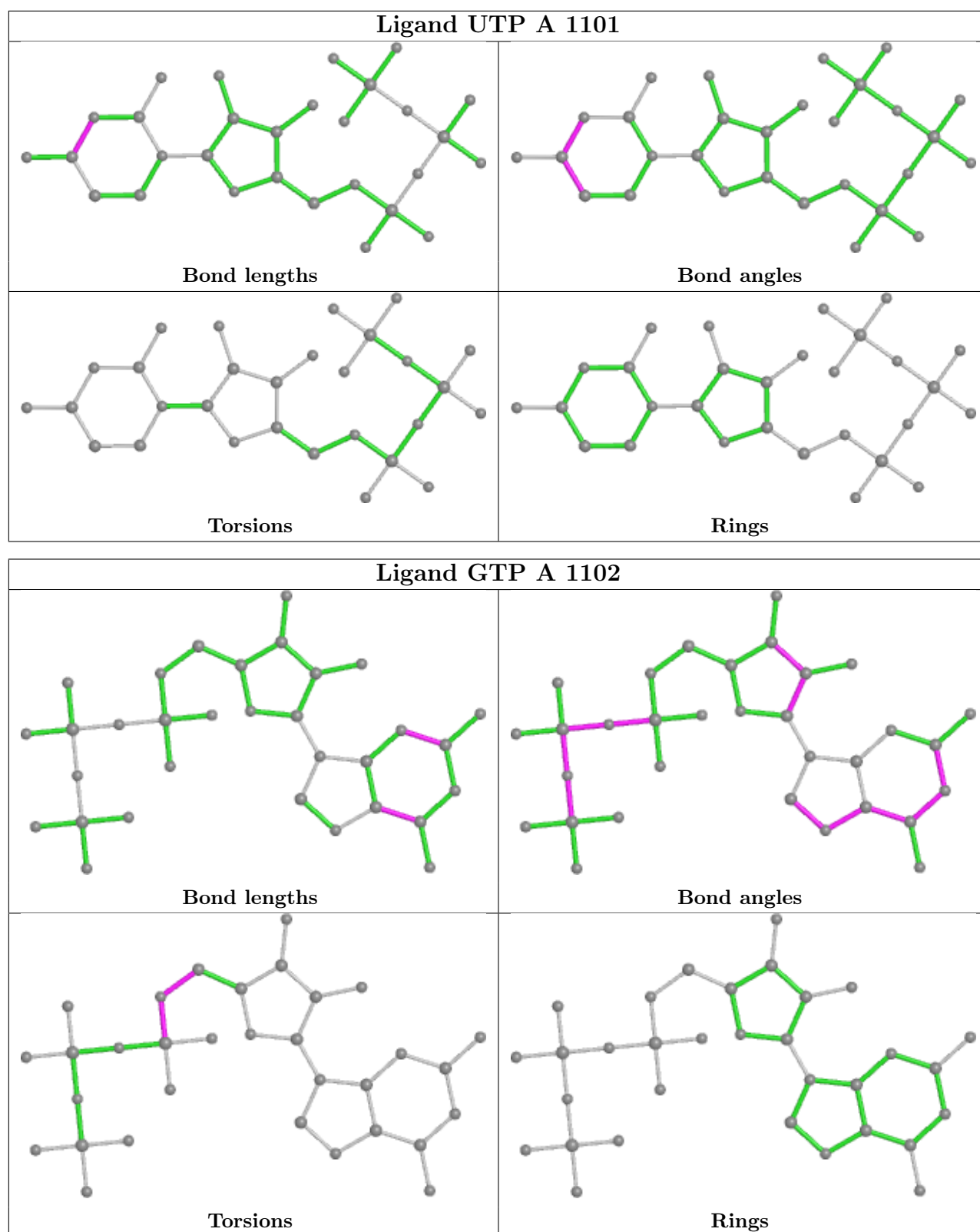
Mol	Chain	Res	Type	Atoms
6	A	1102	GTP	C5'-O5'-PA-O1A
6	A	1102	GTP	C5'-O5'-PA-O3A
6	A	1102	GTP	C4'-C5'-O5'-PA
6	A	1102	GTP	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1101	UTP	1	0
6	A	1102	GTP	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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

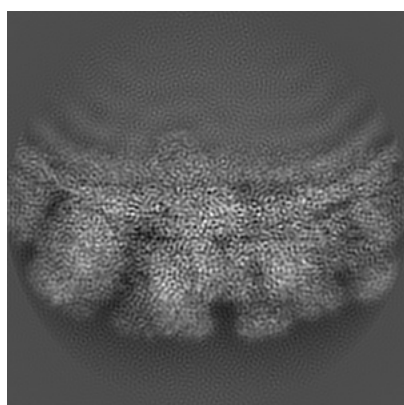
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20060. These allow visual inspection of the internal detail of the map and identification of artifacts.

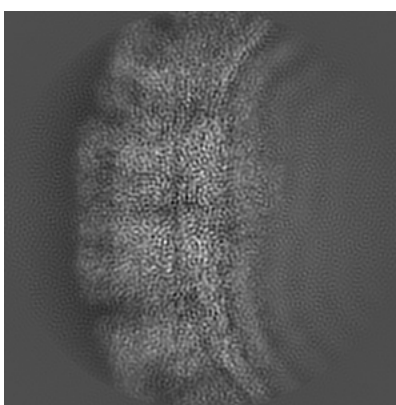
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

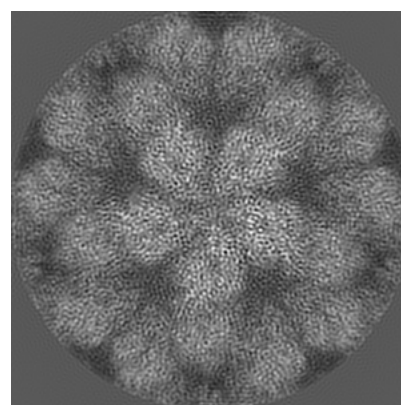
6.1.1 Primary map



X



Y

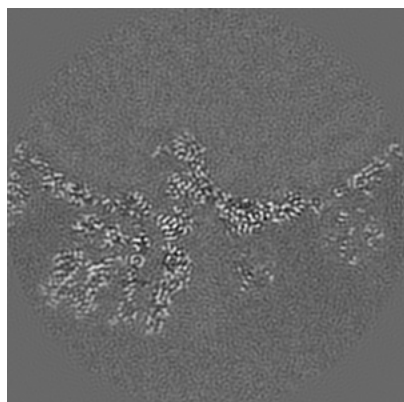


Z

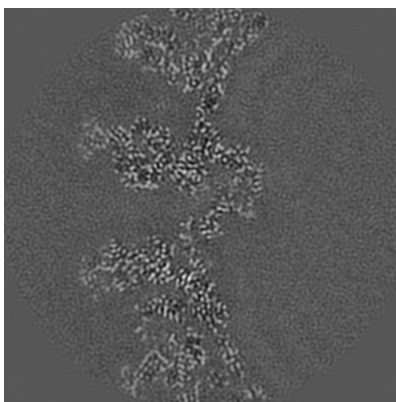
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

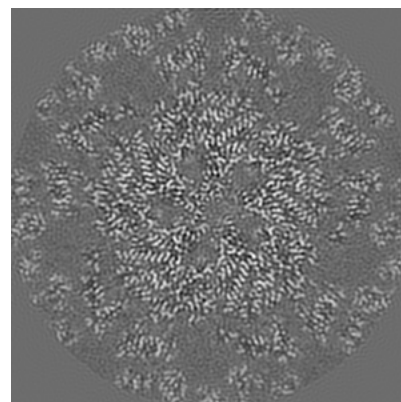
6.2.1 Primary map



X Index: 132



Y Index: 132

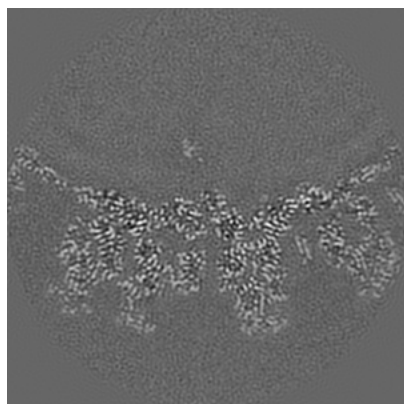


Z Index: 132

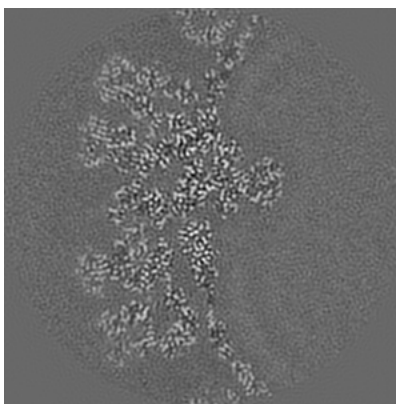
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

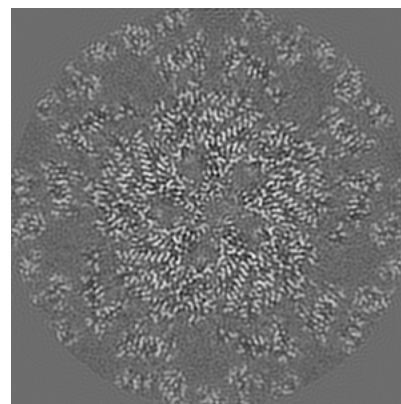
6.3.1 Primary map



X Index: 117



Y Index: 109



Z Index: 132

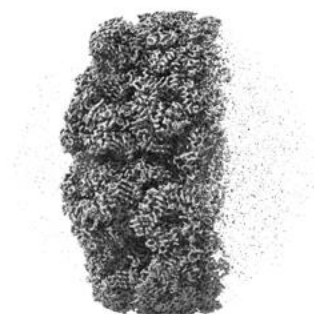
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

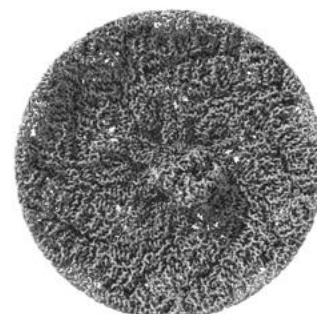
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

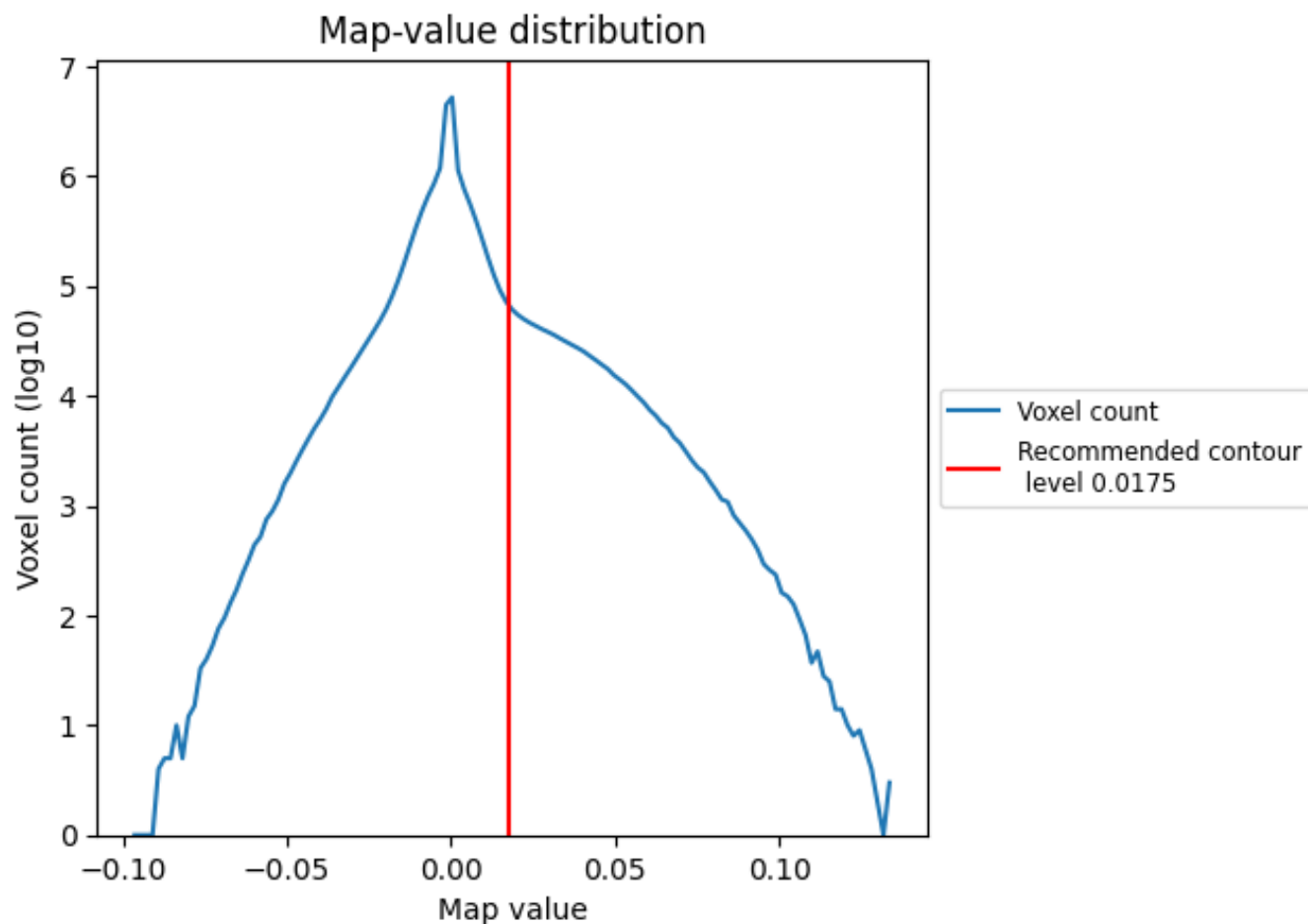
6.5 Mask visualisation

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

7 Map analysis [i](#)

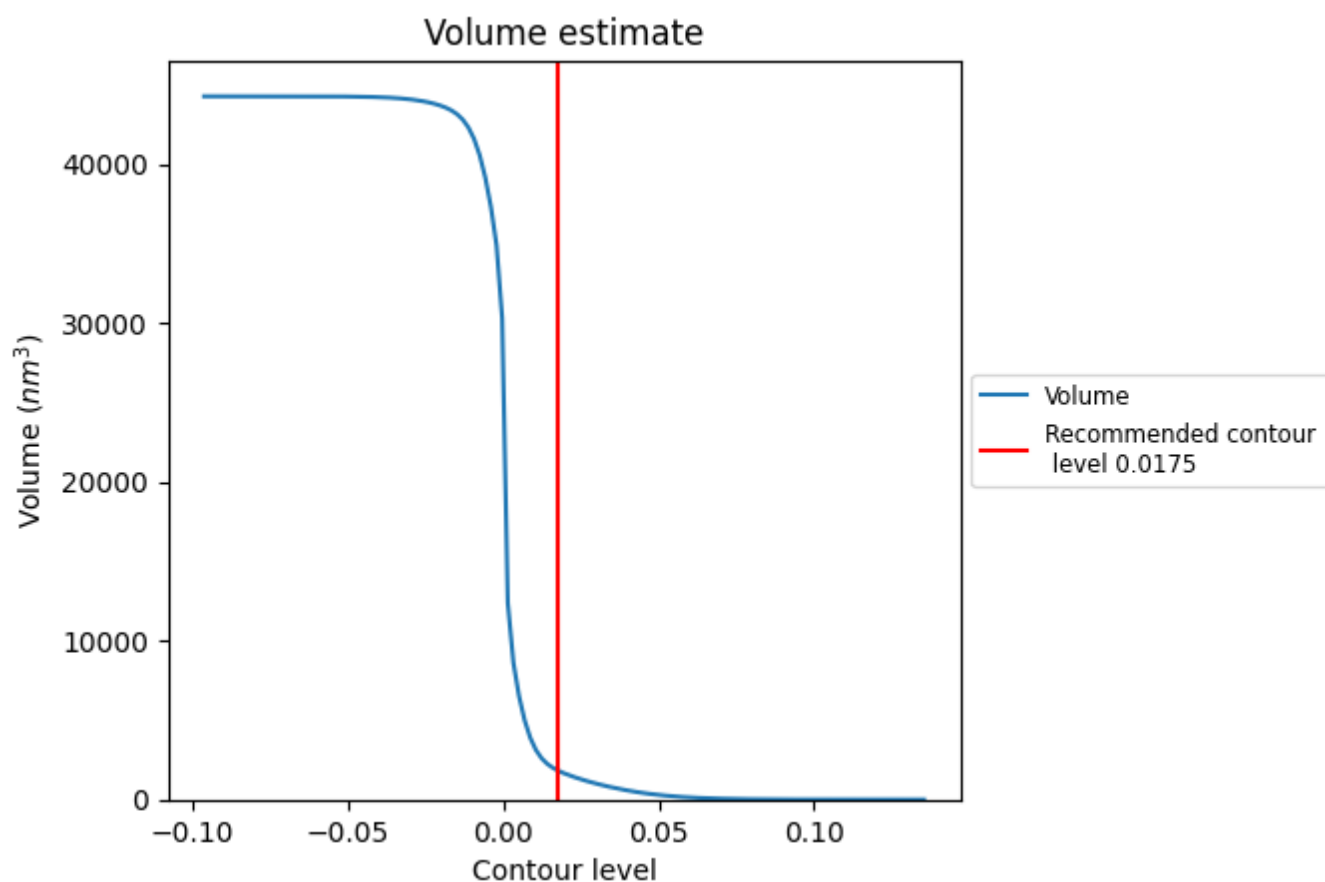
This section contains the results of statistical analysis of the map.

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.

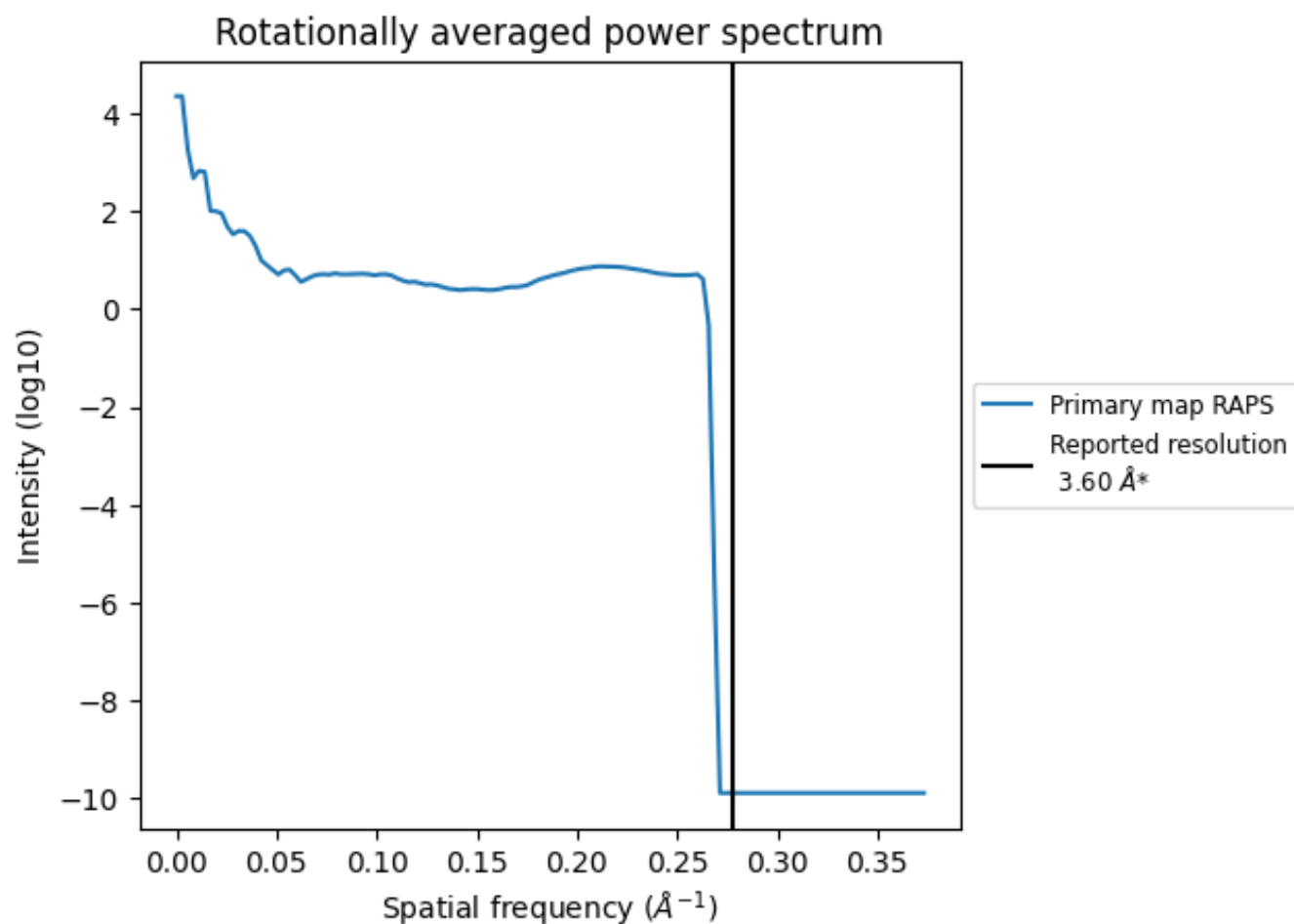
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1833 nm³; this corresponds to an approximate mass of 1656 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 0.278 Å⁻¹

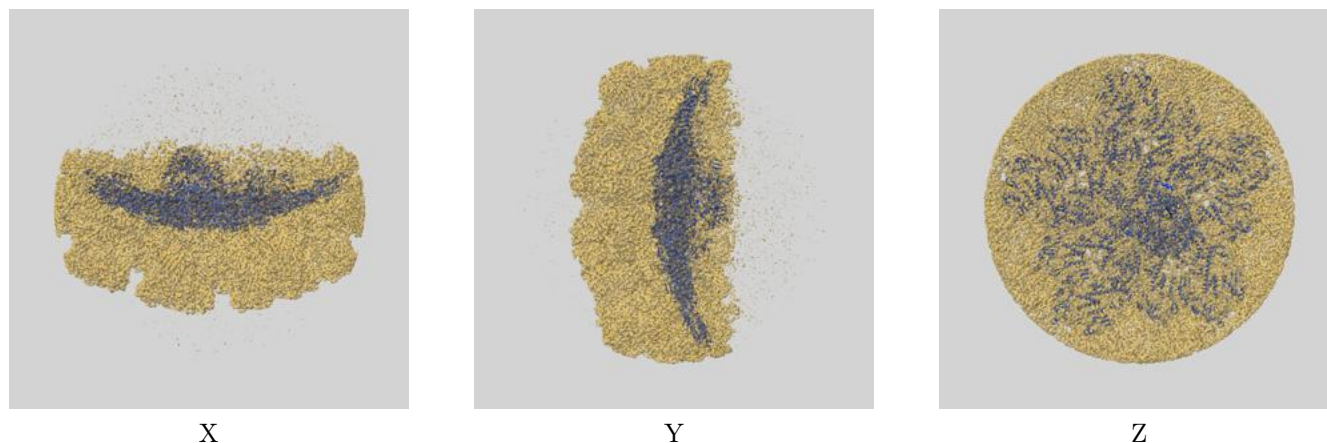
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

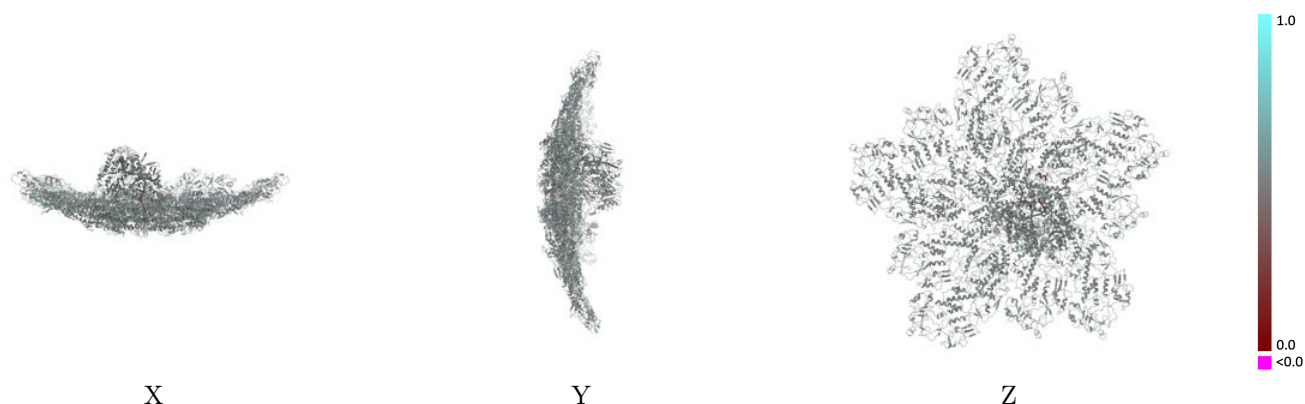
This section contains information regarding the fit between EMDB map EMD-20060 and PDB model 6OGZ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



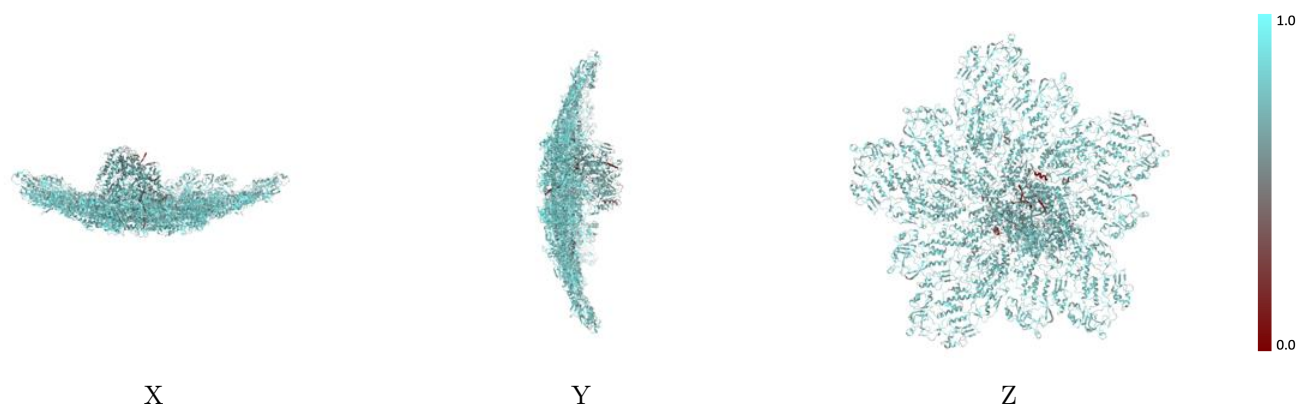
The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



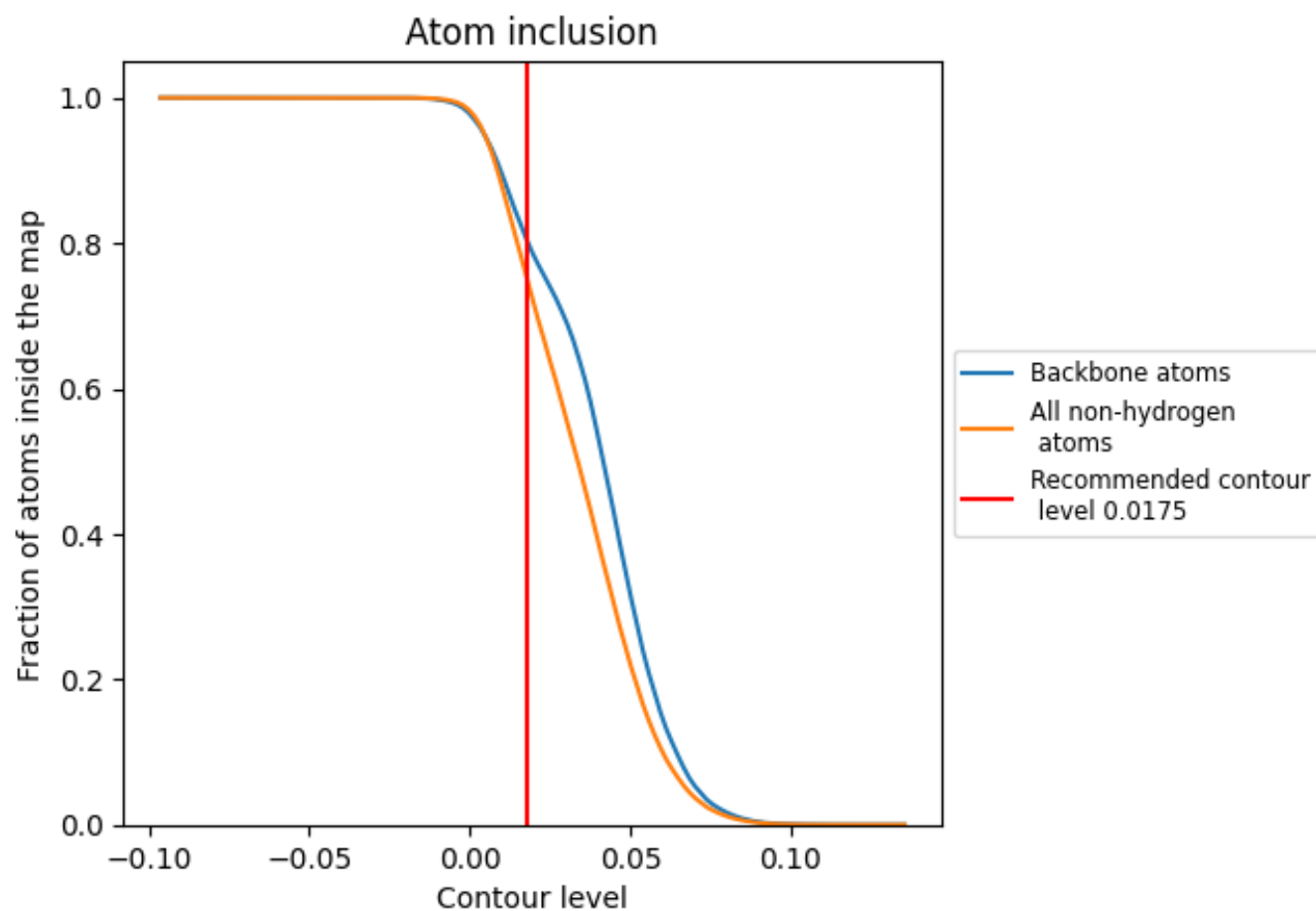
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0175).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7547	 0.5170
A	 0.7247	 0.5130
B	 0.3995	 0.3480
C	 0.4860	 0.3940
E	 0.7526	 0.5160
F	 0.7577	 0.5190
G	 0.7655	 0.5210
H	 0.7510	 0.5160
I	 0.7846	 0.5240
J	 0.7491	 0.5180
K	 0.7834	 0.5220
L	 0.7522	 0.5170
M	 0.7749	 0.5210
N	 0.7532	 0.5160

