



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 05:35 AM UTC

PDB ID : 7D73 / pdb_00007d73
EMDB ID : EMD-30600
Title : Cryo-EM structure of GMPPA/GMPPB complex bound to GTP (State I)
Authors : Zheng, L.; Liu, Z.; Wang, Y.; Yang, F.; Wang, J.; Qing, J.; Cai, X.; Mo, X.;
Gao, N.; Jia, D.
Deposited on : 2020-10-02
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

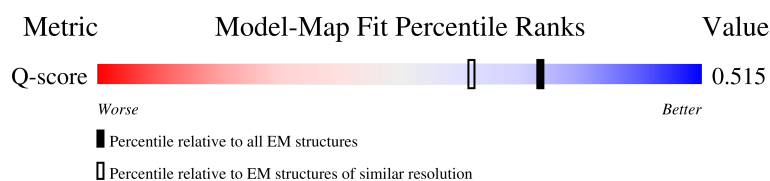
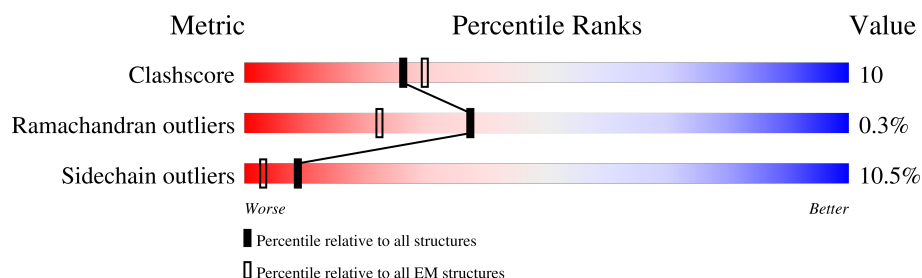
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	
1	B	420	
1	C	420	
1	D	420	

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Mol	Chain	Length	Quality of chain
2	E	360	
2	F	360	
2	G	360	
2	H	360	
2	I	360	
2	J	360	
2	K	360	
2	L	360	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	F	401	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 35292 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.

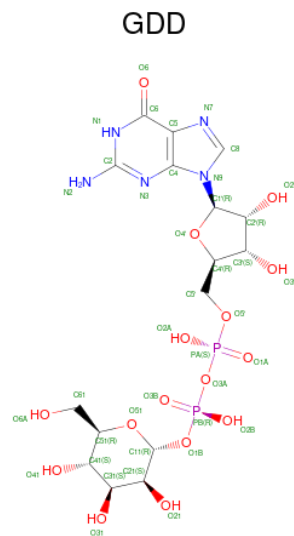
- Molecule 1 is a protein called Mannose-1-phosphate guanyltransferase alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	407	Total	C	N	O	S	0	0
			3172	2031	561	569	11		
1	B	406	Total	C	N	O	S	0	0
			3167	2028	560	568	11		
1	C	406	Total	C	N	O	S	0	0
			3167	2028	560	568	11		
1	D	406	Total	C	N	O	S	0	0
			3167	2028	560	568	11		

- Molecule 2 is a protein called Mannose-1-phosphate guanyltransferase beta.

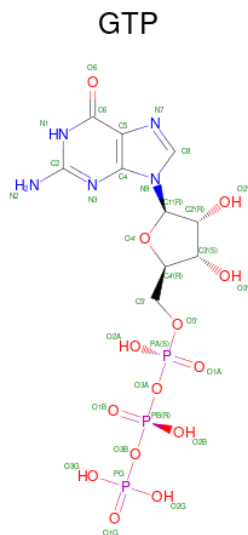
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	360	Total	C	N	O	S	0	0
			2785	1769	487	507	22		
2	F	350	Total	C	N	O	S	0	0
			2714	1728	473	492	21		
2	G	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
2	I	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
2	J	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
2	K	360	Total	C	N	O	S	0	0
			2783	1768	488	505	22		
2	L	360	Total	C	N	O	S	0	0
			2783	1768	488	505	22		
2	H	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (CCD ID: GDD) (formula: C₁₆H₂₅N₅O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 39	C 16	N 5	O 16	P 2	0
3	C	1	Total 39	C 16	N 5	O 16	P 2	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{14}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



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

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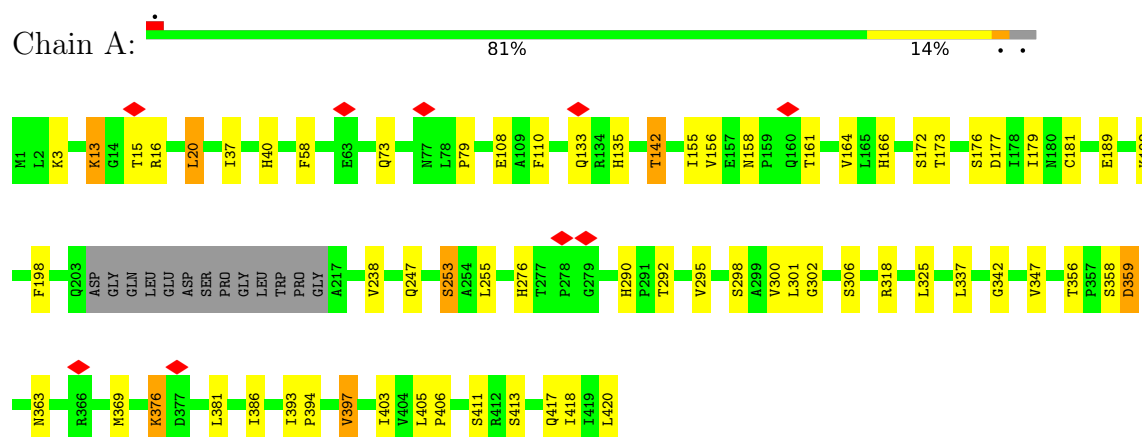
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Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total 32	C 10	N 5	O 14	P 3	0
4	D	1	Total 32	C 10	N 5	O 14	P 3	0
4	F	1	Total 32	C 10	N 5	O 14	P 3	0
4	G	1	Total 32	C 10	N 5	O 14	P 3	0
4	I	1	Total 32	C 10	N 5	O 14	P 3	0
4	J	1	Total 32	C 10	N 5	O 14	P 3	0
4	K	1	Total 32	C 10	N 5	O 14	P 3	0
4	L	1	Total 32	C 10	N 5	O 14	P 3	0
4	H	1	Total 32	C 10	N 5	O 14	P 3	0

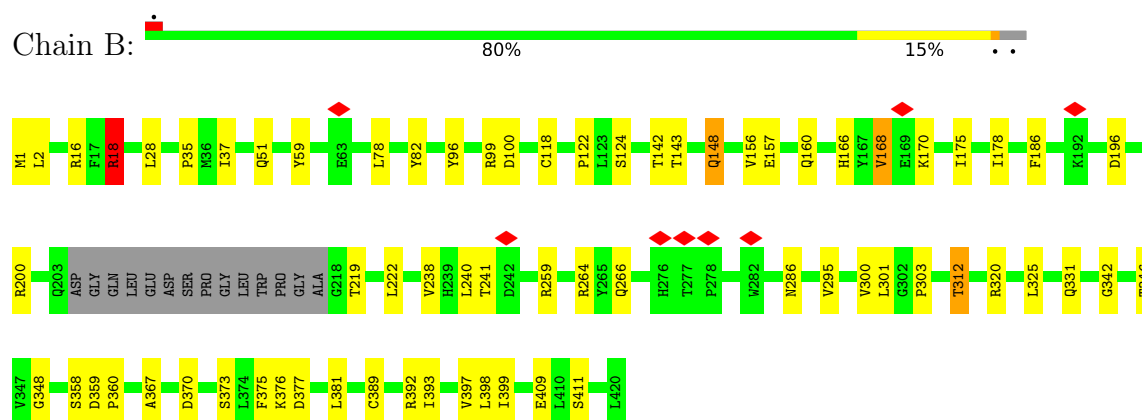
3 Residue-property plots

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.

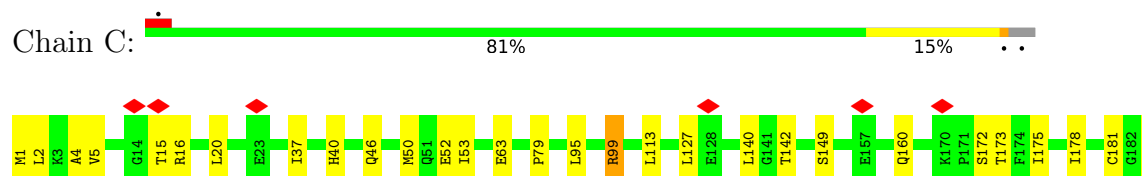
- Molecule 1: Mannose-1-phosphate guanylttransferase alpha

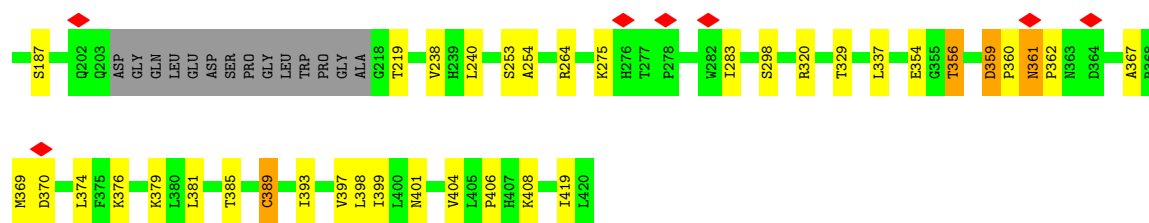


- Molecule 1: Mannose-1-phosphate guanylttransferase alpha



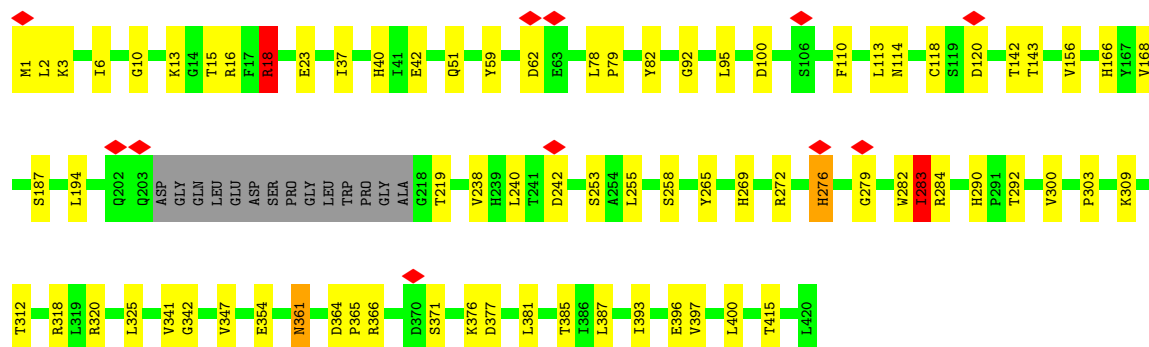
- Molecule 1: Mannose-1-phosphate guanylttransferase alpha





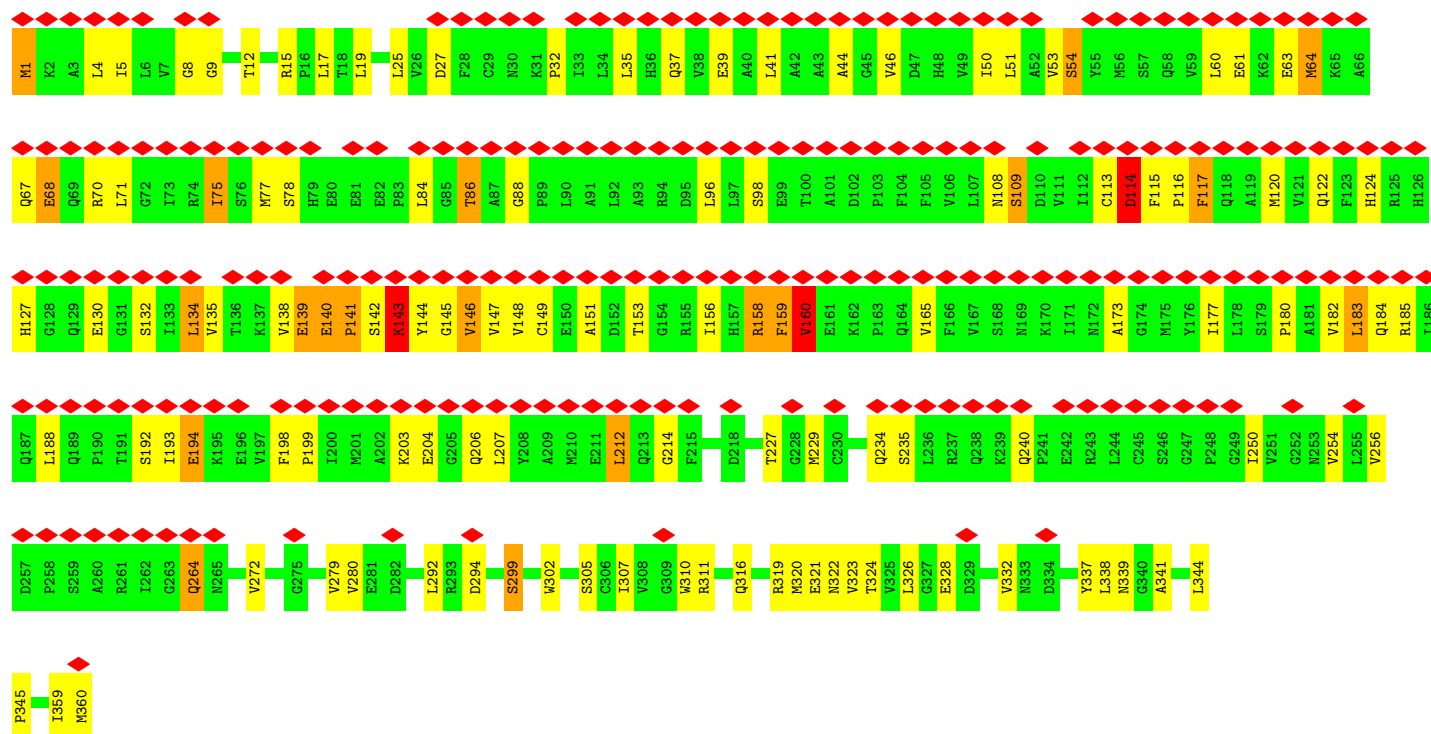
- Molecule 1: Mannose-1-phosphate guanyltransferase alpha

Chain D: 78% 17% .

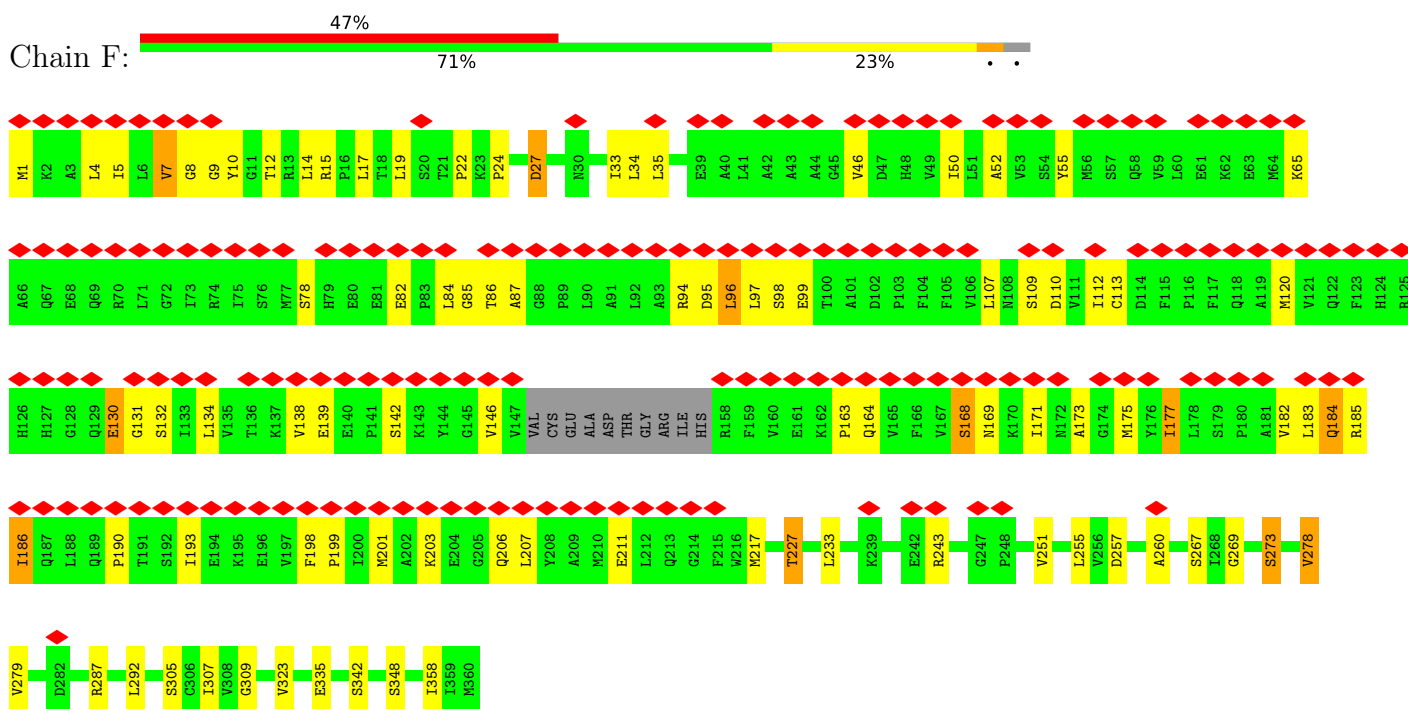


- Molecule 2: Mannose-1-phosphate guanyltransferase beta

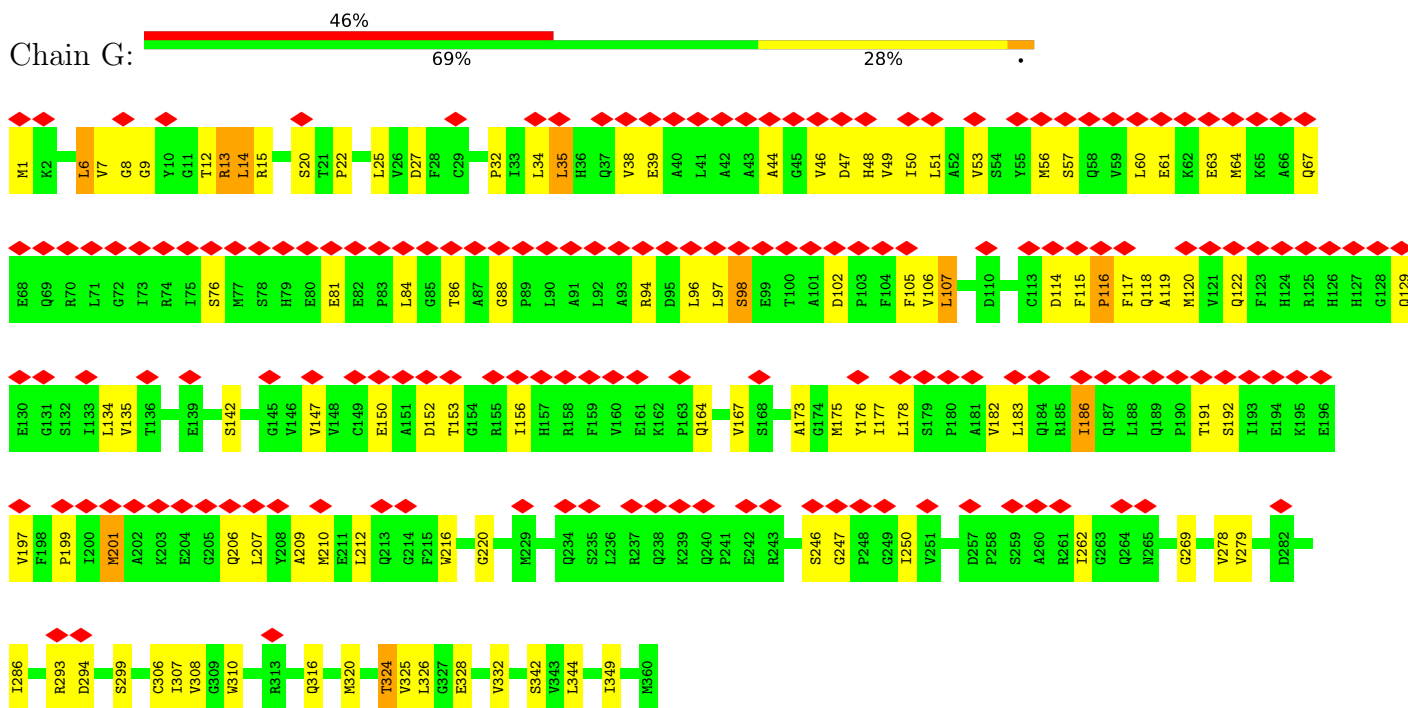
Chain E: 62% 64% 29% 6% .



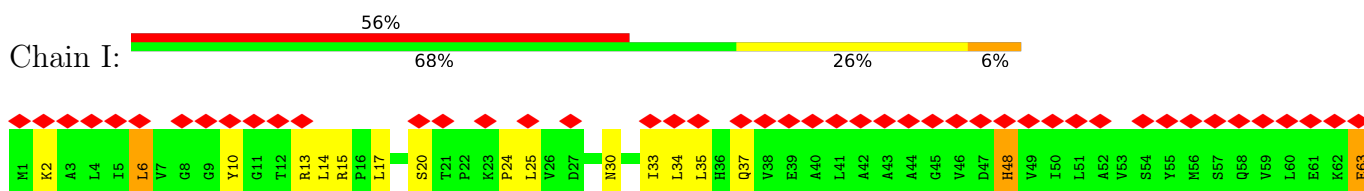
- Molecule 2: Mannose-1-phosphate guanyltransferase beta

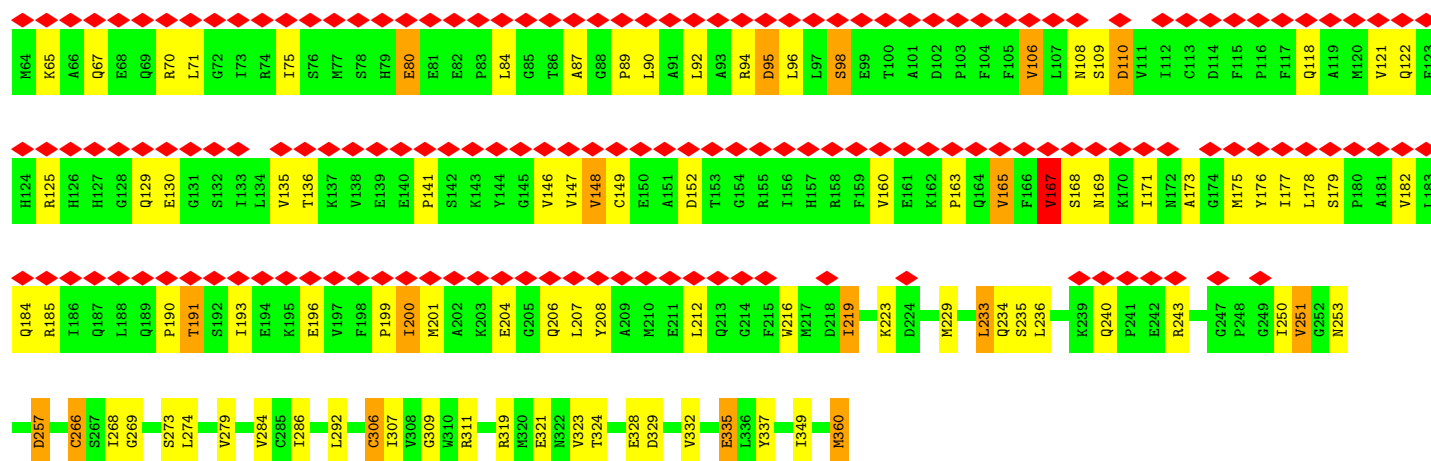


• Molecule 2: Mannose-1-phosphate guanyltrtransferase beta

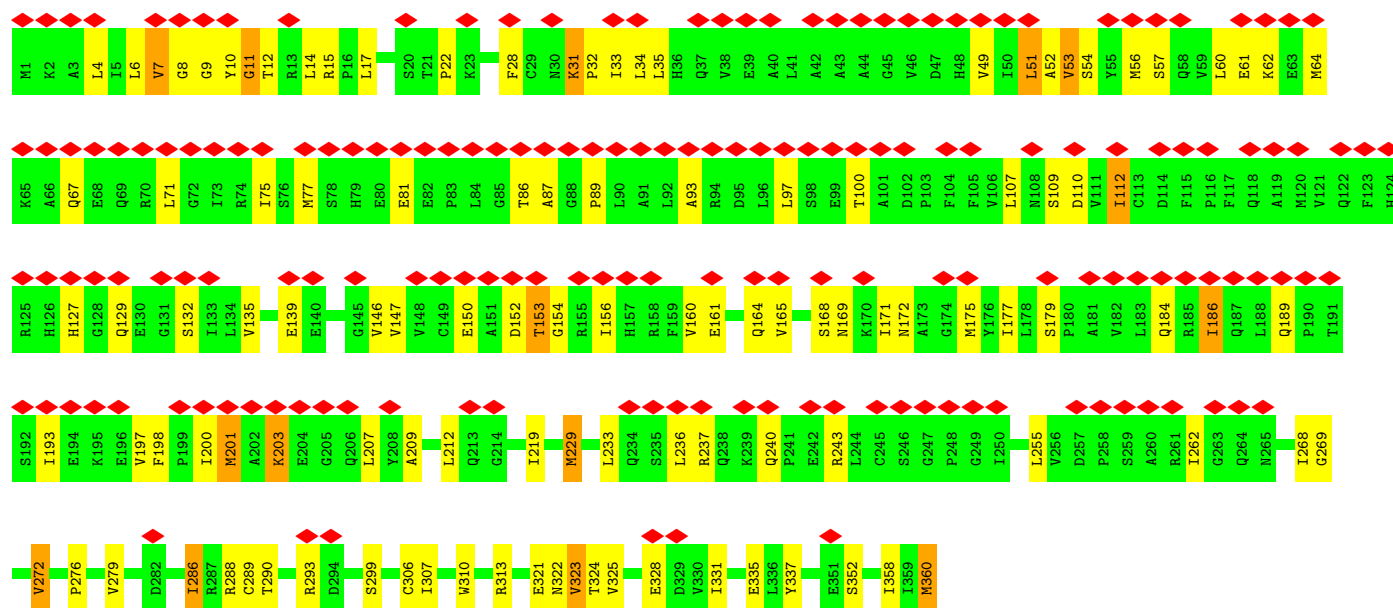


• Molecule 2: Mannose-1-phosphate guanyltrtransferase beta

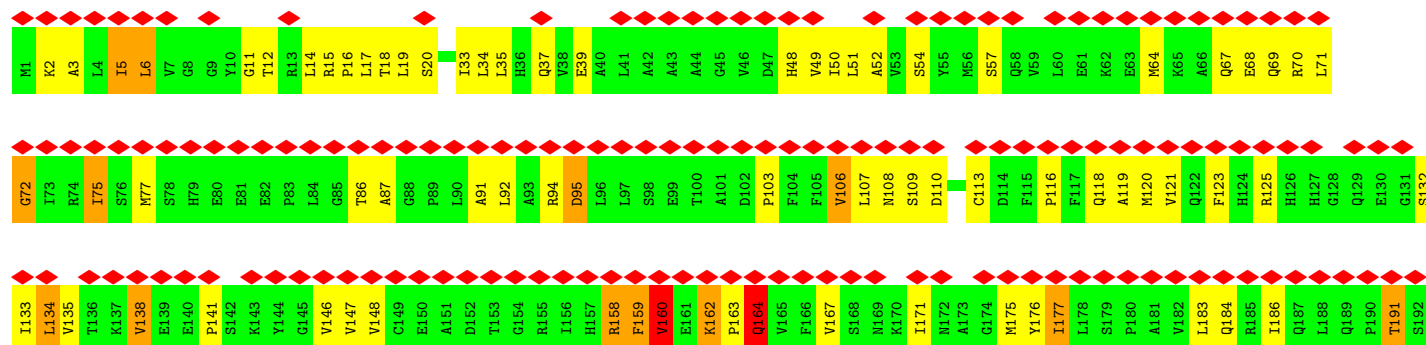


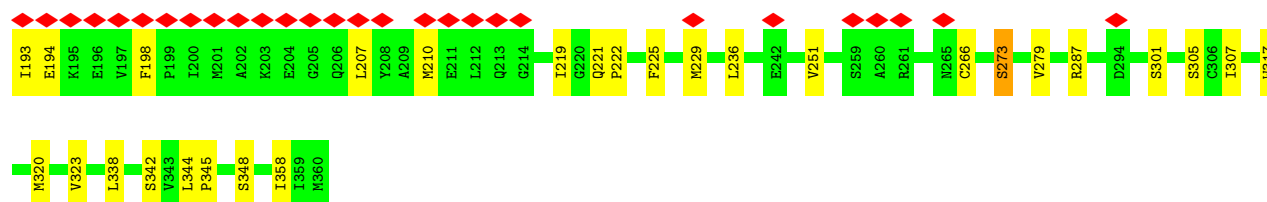


• Molecule 2: Mannose-1-phosphate guanylttransferase beta

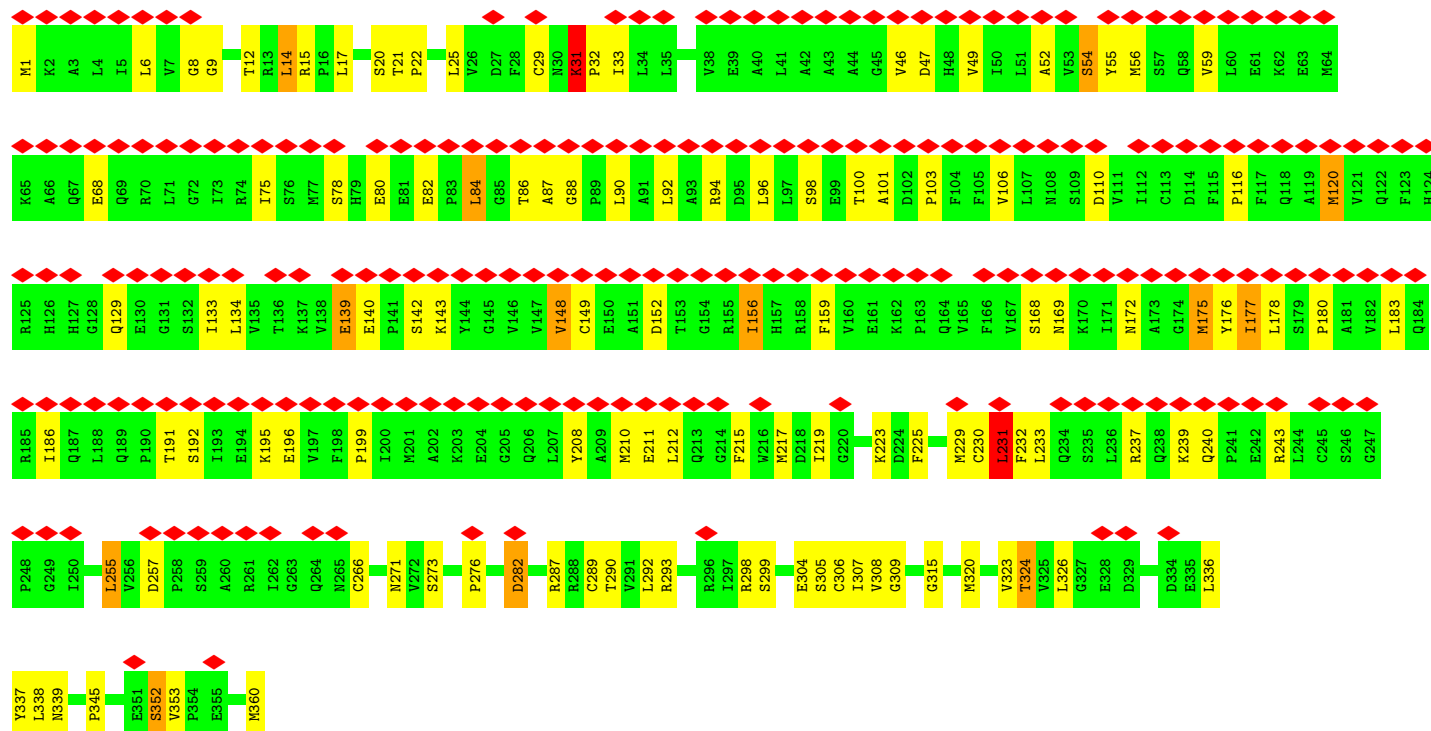


• Molecule 2: Mannose-1-phosphate guanylttransferase beta

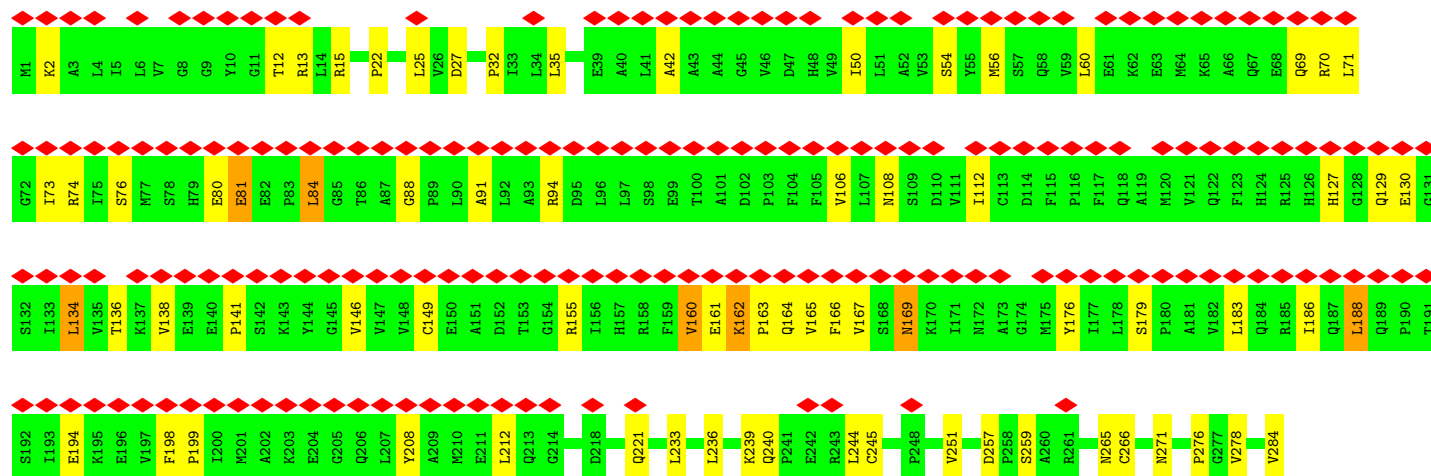
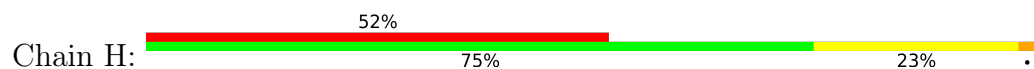




• Molecule 2: Mannose-1-phosphate guanylttransferase beta



• Molecule 2: Mannose-1-phosphate guanylttransferase beta





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	106308	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 ($e^-/\text{\AA}^2$)	64	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	0.280	Depositor
Minimum map value	-0.179	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0389	Depositor
Map size ($\text{\AA}$)	252.48001, 252.48001, 252.48001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.052, 1.052, 1.052	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: GTP, GDD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/3253	0.65	1/4427 (0.0%)
1	B	0.48	0/3248	0.65	1/4420 (0.0%)
1	C	0.49	0/3248	0.69	4/4420 (0.1%)
1	D	0.47	0/3248	0.69	4/4420 (0.1%)
2	E	0.34	0/2840	0.79	8/3850 (0.2%)
2	F	0.39	0/2767	0.67	0/3748
2	G	0.35	0/2844	0.71	5/3854 (0.1%)
2	H	0.39	0/2844	0.68	1/3854 (0.0%)
2	I	0.40	0/2844	0.71	1/3854 (0.0%)
2	J	0.33	0/2844	0.67	2/3854 (0.1%)
2	K	0.38	0/2838	0.69	4/3846 (0.1%)
2	L	0.34	0/2838	0.70	3/3846 (0.1%)
All	All	0.41	0/35656	0.69	34/48393 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	160	VAL	N-CA-C	11.87	124.50	108.84
2	L	31	LYS	CA-C-N	-11.17	108.27	119.78
2	L	31	LYS	C-N-CA	-11.17	108.27	119.78
1	C	16	ARG	N-CA-C	11.09	123.45	111.36
2	K	164	GLN	N-CA-C	-9.13	91.35	110.80
1	B	18	ARG	N-CA-C	8.86	125.74	113.16
2	E	114	ASP	N-CA-C	-8.53	94.61	108.52
2	J	203	LYS	N-CA-C	-7.43	103.12	111.14
1	C	367	ALA	N-CA-C	7.06	120.61	110.24
1	D	18	ARG	N-CA-C	7.04	123.15	113.16
1	D	283	ILE	N-CA-C	6.95	118.61	108.53
2	E	115	PHE	N-CA-C	6.91	118.35	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	322	ASN	N-CA-C	6.72	120.51	111.24
2	E	153	THR	N-CA-C	-6.69	103.98	111.28
2	G	13	ARG	N-CA-C	-6.63	100.47	110.28
2	G	114	ASP	N-CA-C	-6.57	93.94	107.67
1	D	279	GLY	N-CA-C	6.40	120.41	112.73
2	L	231	LEU	N-CA-C	-6.12	104.68	111.71
2	G	122	GLN	CB-CA-C	6.07	120.23	110.09
2	K	162	LYS	CA-C-N	5.99	127.33	119.84
2	K	162	LYS	C-N-CA	5.99	127.33	119.84
2	E	9	GLY	CA-C-N	5.94	132.89	121.54
2	E	9	GLY	C-N-CA	5.94	132.89	121.54
2	I	200	ILE	CB-CA-C	-5.73	102.97	112.26
2	E	117	PHE	N-CA-C	-5.55	105.23	111.28
1	C	359	ASP	CA-C-N	5.49	125.43	119.78
1	C	359	ASP	C-N-CA	5.49	125.43	119.78
2	E	151	ALA	CA-C-O	5.44	121.10	117.94
2	H	81	GLU	N-CA-C	5.30	117.05	111.28
2	K	72	GLY	N-CA-C	5.22	125.55	113.18
1	A	359	ASP	N-CA-C	5.17	116.34	109.93
1	D	361	ASN	N-CA-C	5.11	121.10	109.81
2	G	9	GLY	CA-C-N	5.05	131.19	121.54
2	G	9	GLY	C-N-CA	5.05	131.19	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3172	0	3188	40	0
1	B	3167	0	3184	27	0
1	C	3167	0	3184	35	0
1	D	3167	0	3184	39	0
2	E	2785	0	2828	88	0
2	F	2714	0	2769	74	0
2	G	2789	0	2840	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	2789	0	2840	55	0
2	I	2789	0	2840	71	0
2	J	2789	0	2838	70	0
2	K	2783	0	2829	82	0
2	L	2783	0	2827	84	0
3	A	39	0	22	1	0
3	C	39	0	23	0	0
4	B	32	0	12	0	0
4	D	32	0	12	1	0
4	E	32	0	12	1	0
4	F	32	0	12	16	0
4	G	32	0	10	3	0
4	H	32	0	10	1	0
4	I	32	0	12	5	0
4	J	32	0	10	2	0
4	K	32	0	10	0	0
4	L	32	0	10	5	0
All	All	35292	0	35506	716	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 (716) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:163:PRO:HG2	2:I:167:VAL:CG2	1.25	1.54
2:I:163:PRO:CG	2:I:167:VAL:HG21	1.32	1.53
1:C:406:PRO:O	1:D:18:ARG:NH1	1.66	1.26
2:G:115:PHE:CE1	2:G:175:MET:HE1	1.75	1.20
2:I:146:VAL:CG1	2:I:168:SER:O	1.88	1.20
2:J:200:ILE:HA	2:J:203:LYS:HE2	1.25	1.16
2:F:7:VAL:CG2	2:F:24:PRO:CG	2.24	1.15
2:I:80:GLU:OE2	2:I:89:PRO:HB3	1.00	1.15
2:F:7:VAL:CG2	2:F:24:PRO:HG3	1.78	1.14
2:I:146:VAL:HG11	2:I:168:SER:O	1.43	1.14
2:K:162:LYS:HG3	2:K:163:PRO:HD2	1.15	1.14
2:I:80:GLU:OE2	2:I:89:PRO:CB	1.94	1.14
2:F:8:GLY:O	2:F:55:TYR:HB3	1.45	1.13
2:G:115:PHE:CD1	2:G:175:MET:HE1	1.84	1.11
2:K:68:GLU:CA	2:K:75:ILE:HD11	1.81	1.10
1:A:16:ARG:HE	1:A:20:LEU:HD13	0.98	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:163:PRO:O	2:K:164:GLN:HG3	1.51	1.08
2:J:9:GLY:N	4:J:401:GTP:N7	1.68	1.04
2:E:320:MET:HE3	2:E:338:LEU:HD12	1.04	1.03
2:K:67:GLN:HE21	2:K:70:ARG:HD3	1.24	1.02
1:C:356:THR:HG23	1:C:401:ASN:HD21	1.24	1.02
2:F:7:VAL:CG2	2:F:24:PRO:HG2	1.90	1.00
2:G:105:PHE:CE1	2:G:117:PHE:HD1	1.79	1.00
2:E:145:GLY:HA2	2:E:160:VAL:HG23	1.39	0.99
2:K:163:PRO:O	2:K:164:GLN:CG	2.10	0.99
2:F:8:GLY:O	2:F:55:TYR:CB	2.10	0.99
2:K:68:GLU:HA	2:K:75:ILE:HD11	1.45	0.99
1:B:16:ARG:NH1	1:B:370:ASP:O	1.97	0.98
2:E:320:MET:HE3	2:E:338:LEU:CD1	1.95	0.97
2:L:29:CYS:SG	2:L:255:LEU:HD12	2.05	0.96
2:K:163:PRO:C	2:K:164:GLN:HG3	1.85	0.96
1:A:16:ARG:NE	1:A:20:LEU:HD13	1.82	0.94
1:C:356:THR:CG2	1:C:401:ASN:HD21	1.80	0.94
1:A:16:ARG:HE	1:A:20:LEU:CD1	1.80	0.94
2:K:159:PHE:CZ	2:K:198:PHE:HB3	2.04	0.92
2:I:146:VAL:HG13	2:I:168:SER:O	1.67	0.92
2:F:7:VAL:HG21	2:F:24:PRO:CG	1.99	0.92
2:F:131:GLY:O	2:F:207:LEU:HA	1.70	0.91
2:K:162:LYS:HG3	2:K:163:PRO:CD	1.99	0.91
2:F:7:VAL:HG22	2:F:24:PRO:CG	1.99	0.91
1:C:356:THR:HG23	1:C:401:ASN:ND2	1.86	0.90
2:K:68:GLU:CB	2:K:75:ILE:HD11	2.02	0.90
2:I:94:ARG:O	2:I:98:SER:HB2	1.72	0.89
2:L:29:CYS:SG	2:L:255:LEU:CD1	2.60	0.88
2:K:162:LYS:CG	2:K:163:PRO:HD2	2.03	0.88
2:G:115:PHE:HE1	2:G:175:MET:HE1	1.35	0.86
2:E:142:SER:O	2:E:144:TYR:N	2.08	0.86
2:G:119:ALA:HB1	2:G:210:MET:HE1	1.56	0.85
2:F:7:VAL:HG23	2:F:24:PRO:HG3	1.59	0.85
1:D:361:ASN:ND2	1:D:364:ASP:HB2	1.91	0.85
2:G:115:PHE:CE1	2:G:175:MET:CE	2.59	0.85
2:E:145:GLY:CA	2:E:160:VAL:HG23	2.08	0.84
1:C:359:ASP:HB3	1:C:360:PRO:HD2	1.59	0.84
2:K:159:PHE:HZ	2:K:198:PHE:HB3	1.39	0.83
2:F:7:VAL:HG22	2:F:24:PRO:HG2	1.56	0.82
1:C:359:ASP:HB3	1:C:360:PRO:CD	2.08	0.82
2:K:158:ARG:HH21	2:K:158:ARG:HG3	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:324:THR:HG23	2:E:341:ALA:O	1.80	0.81
2:H:141:PRO:HB2	2:H:164:GLN:HE22	1.45	0.81
2:G:306:CYS:HB2	2:G:324:THR:HG23	1.63	0.81
2:E:320:MET:CE	2:E:338:LEU:HD12	1.99	0.81
2:G:105:PHE:CE1	2:G:117:PHE:CD1	2.68	0.79
2:L:229:MET:HE1	2:L:271:ASN:O	1.81	0.79
2:K:68:GLU:HG3	2:K:75:ILE:HG13	1.63	0.79
2:G:115:PHE:CD1	2:G:175:MET:CE	2.65	0.78
2:L:229:MET:SD	2:L:273:SER:OG	2.40	0.78
2:F:7:VAL:HG21	2:F:24:PRO:HG2	1.59	0.78
2:L:31:LYS:HB2	2:L:31:LYS:NZ	2.00	0.77
2:E:44:ALA:HB2	2:E:117:PHE:CD2	2.20	0.76
1:D:276:HIS:CD2	1:D:283:ILE:H	2.03	0.76
2:F:7:VAL:C	4:F:401:GTP:O2'	2.29	0.76
2:E:320:MET:HE1	2:E:326:LEU:HD21	1.68	0.76
2:G:94:ARG:O	2:G:98:SER:HB2	1.86	0.75
2:F:7:VAL:HG12	2:F:52:ALA:O	1.86	0.75
2:K:68:GLU:HB2	2:K:75:ILE:HD11	1.67	0.75
2:K:68:GLU:HB2	2:K:75:ILE:CD1	2.16	0.75
2:L:230:CYS:SG	2:L:271:ASN:OD1	2.44	0.74
1:A:358:SER:O	1:A:369:MET:HE2	1.88	0.74
2:G:115:PHE:HD1	2:G:175:MET:HE1	1.52	0.74
2:L:9:GLY:HA3	4:L:401:GTP:O2B	1.88	0.74
2:H:84:LEU:HB3	2:H:88:GLY:HA3	1.68	0.73
1:C:359:ASP:CB	1:C:360:PRO:CD	2.67	0.73
2:F:120:MET:HG2	2:F:177:ILE:HD11	1.71	0.73
2:H:305:SER:O	2:H:323:VAL:HA	1.88	0.72
2:G:14:LEU:HB2	2:G:220:GLY:O	1.89	0.72
2:F:7:VAL:HA	4:F:401:GTP:O2'	1.90	0.71
2:F:12:THR:HA	2:F:15:ARG:HD3	1.72	0.71
2:J:7:VAL:CG2	2:J:53:VAL:HA	2.20	0.71
2:I:80:GLU:CD	4:I:401:GTP:HN21	1.97	0.71
2:E:41:LEU:HB3	2:E:117:PHE:CE1	2.25	0.70
2:K:68:GLU:CG	2:K:75:ILE:HG13	2.20	0.70
2:L:6:LEU:HB3	4:L:401:GTP:H1'	1.74	0.69
2:L:229:MET:SD	2:L:233:LEU:HD11	2.32	0.69
2:H:146:VAL:HB	2:H:160:VAL:HG11	1.74	0.69
2:K:107:LEU:HD23	2:K:175:MET:HE2	1.74	0.69
2:F:7:VAL:CA	4:F:401:GTP:O2'	2.40	0.69
2:E:145:GLY:HA2	2:E:160:VAL:CG2	2.19	0.68
2:F:8:GLY:N	4:F:401:GTP:O2'	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:156:ILE:HD13	2:E:159:PHE:HE2	1.59	0.67
2:I:147:VAL:O	2:I:168:SER:HB2	1.94	0.67
2:L:80:GLU:OE2	4:L:401:GTP:N1	2.26	0.67
2:J:7:VAL:HG21	2:J:53:VAL:HB	1.76	0.67
2:J:7:VAL:HG11	2:J:51:LEU:HD21	1.76	0.67
2:E:140:GLU:N	2:E:141:PRO:CD	2.58	0.66
2:G:119:ALA:CB	2:G:210:MET:HE1	2.24	0.66
1:A:20:LEU:HD12	1:A:20:LEU:H	1.60	0.66
1:B:259:ARG:NH1	1:B:359:ASP:OD2	2.28	0.66
2:E:142:SER:C	2:E:144:TYR:H	2.04	0.66
1:B:266:GLN:HE21	1:B:286:ASN:HD21	1.44	0.66
2:E:139:GLU:HB2	2:E:140:GLU:OE1	1.96	0.66
2:K:12:THR:HA	2:K:15:ARG:HD3	1.77	0.65
2:H:146:VAL:CB	2:H:160:VAL:HG11	2.26	0.65
2:G:115:PHE:HE1	2:G:175:MET:CE	2.05	0.65
2:L:140:GLU:O	2:L:140:GLU:HG2	1.97	0.64
2:H:161:GLU:HA	2:H:161:GLU:OE2	1.96	0.64
1:D:1:MET:HG2	1:D:51:GLN:HG3	1.80	0.64
2:K:163:PRO:O	2:K:164:GLN:HG2	1.96	0.64
2:I:163:PRO:CD	2:I:167:VAL:HG21	2.23	0.64
1:D:276:HIS:HD2	1:D:283:ILE:H	1.43	0.64
2:G:12:THR:HA	2:G:15:ARG:HD3	1.78	0.64
2:I:160:VAL:HG21	2:I:167:VAL:CG1	2.27	0.64
2:K:162:LYS:CG	2:K:163:PRO:CD	2.70	0.64
2:E:120:MET:HB3	2:E:177:ILE:HD11	1.77	0.64
2:E:142:SER:HB2	2:E:165:VAL:HG11	1.80	0.64
2:G:1:MET:H3	2:G:46:VAL:HA	1.63	0.64
2:J:321:GLU:OE1	2:J:337:TYR:CE1	2.51	0.64
2:K:6:LEU:HA	2:K:52:ALA:HB3	1.80	0.64
2:K:68:GLU:CB	2:K:75:ILE:CD1	2.73	0.64
2:E:63:GLU:O	2:E:67:GLN:HB2	1.98	0.63
2:E:113:CYS:SG	2:E:114:ASP:N	2.71	0.63
2:J:57:SER:O	2:J:61:GLU:HB2	1.98	0.63
2:L:229:MET:SD	2:L:233:LEU:CD1	2.87	0.63
2:K:159:PHE:HZ	2:K:198:PHE:CB	2.11	0.62
2:F:8:GLY:O	2:F:55:TYR:HB2	2.00	0.62
2:E:305:SER:O	2:E:323:VAL:HA	1.99	0.62
2:J:7:VAL:HG21	2:J:53:VAL:HA	1.81	0.62
1:A:189:GLU:O	1:A:192:LYS:HB2	1.98	0.62
2:G:119:ALA:HB1	2:G:210:MET:CE	2.28	0.62
2:L:320:MET:HE3	2:L:324:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:GLU:HB3	2:F:206:GLN:HB3	1.82	0.62
2:I:147:VAL:O	2:I:168:SER:CB	2.48	0.62
2:K:86:THR:HG23	2:K:193:ILE:H	1.64	0.62
1:D:325:LEU:HD12	1:D:342:GLY:HA2	1.82	0.62
2:J:323:VAL:HG23	2:J:323:VAL:O	2.00	0.62
2:E:75:ILE:HG22	2:E:75:ILE:O	2.00	0.62
2:L:195:LYS:HG2	2:L:196:GLU:HG3	1.81	0.62
2:F:12:THR:OG1	4:F:401:GTP:O3G	2.17	0.61
2:I:236:LEU:HD21	2:I:243:ARG:HD2	1.81	0.61
2:H:164:GLN:N	2:H:164:GLN:OE1	2.33	0.61
2:G:299:SER:HB2	2:G:316:GLN:HE21	1.64	0.61
2:E:1:MET:HB3	2:E:46:VAL:HG12	1.82	0.61
2:H:81:GLU:OE1	2:H:81:GLU:HA	2.00	0.61
2:H:323:VAL:HG23	2:H:323:VAL:O	2.00	0.61
2:E:138:VAL:HB	2:E:141:PRO:HD2	1.82	0.61
2:I:122:GLN:HA	2:I:125:ARG:HG2	1.82	0.61
2:J:7:VAL:HG22	2:J:52:ALA:O	2.01	0.60
2:L:120:MET:HE2	2:L:177:ILE:HG12	1.83	0.60
2:G:293:ARG:HB3	2:G:310:TRP:HD1	1.65	0.60
2:E:156:ILE:HG21	2:E:159:PHE:CD2	2.37	0.60
2:E:142:SER:C	2:E:144:TYR:N	2.56	0.60
2:G:13:ARG:O	2:G:14:LEU:HB3	2.01	0.60
2:L:1:MET:HB2	2:L:46:VAL:HG12	1.84	0.60
2:E:321:GLU:OE2	2:E:337:TYR:HE1	1.85	0.60
2:G:50:ILE:HA	2:G:76:SER:O	2.02	0.60
1:B:295:VAL:HG11	1:B:301:LEU:HD11	1.83	0.59
2:E:323:VAL:HG12	2:E:323:VAL:O	2.02	0.59
1:B:325:LEU:HD12	1:B:342:GLY:HA2	1.84	0.59
2:K:106:VAL:HG23	2:K:176:TYR:HB2	1.83	0.59
2:E:134:LEU:HB3	2:E:173:ALA:HB3	1.83	0.59
2:I:70:ARG:HH21	2:I:71:LEU:HD21	1.68	0.59
2:I:106:VAL:HG13	2:I:176:TYR:HB2	1.84	0.59
2:I:135:VAL:HA	2:I:171:ILE:O	2.02	0.59
2:K:68:GLU:HA	2:K:75:ILE:CD1	2.25	0.59
2:H:141:PRO:HB2	2:H:164:GLN:NE2	2.15	0.59
2:I:95:ASP:OD1	2:I:95:ASP:N	2.34	0.59
2:I:24:PRO:HB3	2:I:34:LEU:HB2	1.85	0.59
2:J:321:GLU:OE1	2:J:337:TYR:HE1	1.86	0.58
2:K:160:VAL:O	2:K:160:VAL:HG13	2.01	0.58
2:H:162:LYS:HB3	2:H:163:PRO:HD2	1.84	0.58
2:H:162:LYS:CB	2:H:163:PRO:HD2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:87:ALA:HB3	2:I:191:THR:HB	1.83	0.58
2:L:292:LEU:HD12	2:L:309:GLY:HA2	1.85	0.58
2:L:324:THR:HG22	2:L:324:THR:O	2.03	0.58
2:G:120:MET:HG2	2:G:177:ILE:HG13	1.84	0.58
2:L:31:LYS:HB2	2:L:31:LYS:HZ3	1.67	0.58
2:F:94:ARG:HE	2:F:184:GLN:HA	1.69	0.58
2:L:87:ALA:HB3	2:L:191:THR:HG23	1.85	0.58
2:J:7:VAL:O	4:J:401:GTP:O2'	2.22	0.58
2:E:50:ILE:HD11	2:E:96:LEU:HD22	1.86	0.58
2:E:156:ILE:HG21	2:E:159:PHE:CE2	2.38	0.58
2:I:30:ASN:ND2	2:I:257:ASP:OD1	2.37	0.58
2:K:17:LEU:HD11	2:K:307:ILE:HG21	1.86	0.58
2:J:127:HIS:HE2	2:J:132:SER:HB2	1.69	0.58
2:J:32:PRO:HD2	2:J:35:LEU:HD22	1.86	0.58
2:K:158:ARG:HH21	2:K:158:ARG:CG	2.14	0.57
2:L:229:MET:HE2	2:L:290:THR:OG1	2.04	0.57
2:E:64:MET:HG3	2:E:75:ILE:HG21	1.86	0.57
2:E:130:GLU:HB3	2:E:206:GLN:HB3	1.86	0.57
2:F:130:GLU:HG2	2:F:201:MET:HE1	1.86	0.57
2:G:32:PRO:HD2	2:G:35:LEU:HD22	1.87	0.57
1:A:363:ASN:ND2	2:G:142:SER:OG	2.37	0.57
2:K:49:VAL:HG12	2:K:75:ILE:HG22	1.85	0.57
2:L:240:GLN:OE1	2:L:243:ARG:NH2	2.37	0.57
2:H:80:GLU:OE2	2:H:84:LEU:HB2	2.04	0.57
2:F:8:GLY:N	4:F:401:GTP:HO2'	2.01	0.57
2:E:68:GLU:HB3	2:E:75:ILE:HB	1.85	0.57
2:I:160:VAL:HG21	2:I:167:VAL:HG11	1.85	0.57
2:E:140:GLU:H	2:E:141:PRO:CD	2.18	0.57
2:L:215:PHE:HD1	2:L:231:LEU:HD13	1.70	0.57
2:H:306:CYS:SG	2:H:307:ILE:N	2.77	0.57
2:F:9:GLY:H	4:F:401:GTP:C2'	2.16	0.57
2:H:239:LYS:HE3	2:H:240:GLN:HG3	1.85	0.57
2:H:311:ARG:NH1	2:H:329:ASP:OD1	2.38	0.57
1:A:155:ILE:HG23	1:A:164:VAL:HG13	1.87	0.56
1:D:6:ILE:HG12	1:D:113:LEU:HD12	1.86	0.56
2:F:96:LEU:HA	2:F:99:GLU:HG3	1.86	0.56
1:C:359:ASP:HA	1:C:369:MET:HE3	1.88	0.56
2:H:108:ASN:ND2	4:H:401:GTP:O2B	2.38	0.56
2:E:44:ALA:CB	2:E:117:PHE:CD2	2.87	0.56
2:F:9:GLY:HA3	4:F:401:GTP:O2B	2.05	0.56
2:I:323:VAL:HG12	2:I:323:VAL:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:94:ARG:NH2	2:K:186:ILE:O	2.38	0.56
1:B:168:VAL:HG21	1:B:175:ILE:HG13	1.86	0.56
2:J:156:ILE:HD11	2:J:209:ALA:HB2	1.87	0.56
2:K:134:LEU:HA	2:K:210:MET:O	2.05	0.56
1:C:20:LEU:H	1:C:20:LEU:HD12	1.70	0.56
2:K:273:SER:O	2:K:273:SER:OG	2.24	0.56
2:F:323:VAL:HG12	2:F:323:VAL:O	2.06	0.56
2:H:12:THR:HA	2:H:15:ARG:HD3	1.87	0.56
2:E:140:GLU:H	2:E:141:PRO:HD3	1.70	0.56
2:E:142:SER:O	2:E:143:LYS:C	2.47	0.56
2:J:7:VAL:CG2	2:J:52:ALA:O	2.54	0.56
2:I:33:ILE:HG12	2:I:219:ILE:HD11	1.88	0.56
2:E:32:PRO:HD2	2:E:35:LEU:HD22	1.88	0.55
2:K:35:LEU:O	2:K:39:GLU:HB2	2.06	0.55
1:C:356:THR:CG2	1:C:401:ASN:ND2	2.56	0.55
2:G:105:PHE:HE1	2:G:117:PHE:HD1	1.46	0.55
2:L:337:TYR:OH	2:L:339:ASN:ND2	2.40	0.55
1:C:320:ARG:NH1	2:I:335:GLU:OE1	2.39	0.55
1:C:379:LYS:NZ	1:D:377:ASP:O	2.39	0.55
2:K:305:SER:O	2:K:323:VAL:HA	2.06	0.55
1:A:158:ASN:ND2	1:A:161:THR:OG1	2.39	0.55
2:I:204:GLU:HB3	2:I:206:GLN:HG2	1.88	0.55
2:H:146:VAL:HB	2:H:160:VAL:CG1	2.36	0.55
1:B:156:VAL:HB	1:B:166:HIS:HB3	1.89	0.55
2:J:7:VAL:HG21	2:J:53:VAL:CA	2.37	0.55
2:F:87:ALA:HB2	2:F:193:ILE:HB	1.88	0.55
2:I:148:VAL:HG13	2:I:168:SER:OG	2.05	0.55
2:J:168:SER:OG	2:J:169:ASN:N	2.37	0.55
1:D:16:ARG:O	1:D:16:ARG:HG3	2.05	0.55
1:A:325:LEU:HD12	1:A:342:GLY:HA2	1.87	0.55
2:I:311:ARG:NH2	2:I:328:GLU:OE1	2.40	0.55
2:G:84:LEU:HB3	2:G:88:GLY:HA3	1.88	0.55
2:L:337:TYR:H	2:L:352:SER:HB3	1.72	0.55
2:H:94:ARG:NH2	2:H:186:ILE:O	2.38	0.55
2:G:116:PRO:HB2	2:G:119:ALA:HB3	1.89	0.55
2:F:9:GLY:HA3	4:F:401:GTP:H2'	1.88	0.54
2:F:134:LEU:HB3	2:F:173:ALA:HB3	1.89	0.54
2:H:134:LEU:HG	2:H:212:LEU:HD22	1.89	0.54
1:A:20:LEU:HD12	1:A:20:LEU:N	2.22	0.54
1:A:142:THR:HG1	1:A:181:CYS:HG	1.49	0.54
2:K:51:LEU:HD12	2:K:77:MET:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:NE2	1:B:367:ALA:O	2.40	0.54
2:I:80:GLU:CD	4:I:401:GTP:N2	2.66	0.54
1:C:20:LEU:HD23	1:C:254:ALA:HB2	1.87	0.54
2:I:141:PRO:HB3	2:I:146:VAL:HG21	1.89	0.54
2:G:34:LEU:HD21	2:G:51:LEU:HD13	1.90	0.54
2:L:192:SER:HB3	2:L:195:LYS:HE2	1.90	0.54
1:C:337:LEU:HD12	1:C:354:GLU:HG3	1.90	0.54
2:K:158:ARG:HG3	2:K:158:ARG:NH2	2.20	0.54
2:L:94:ARG:O	2:L:98:SER:HB2	2.08	0.54
1:D:276:HIS:NE2	1:D:282:TRP:HB2	2.23	0.53
2:I:6:LEU:HD22	4:I:401:GTP:H1'	1.89	0.53
2:L:308:VAL:HG13	2:L:326:LEU:HD12	1.90	0.53
1:B:96:TYR:O	1:B:99:ARG:NH1	2.41	0.53
2:I:129:GLN:HG3	2:I:208:TYR:HE2	1.73	0.53
2:G:246:SER:HA	2:G:250:ILE:HG21	1.89	0.53
2:G:156:ILE:HD11	2:G:209:ALA:HB2	1.90	0.53
2:J:146:VAL:HG12	2:J:171:ILE:HG22	1.88	0.53
2:E:12:THR:N	4:E:401:GTP:O3G	2.41	0.53
2:K:68:GLU:OE2	2:K:69:GLN:NE2	2.41	0.53
2:L:17:LEU:HD11	2:L:307:ILE:HG21	1.90	0.53
2:I:163:PRO:CG	2:I:167:VAL:CG2	2.22	0.53
2:J:7:VAL:HG11	2:J:51:LEU:CD2	2.39	0.53
2:J:10:TYR:O	2:J:11:GLY:C	2.50	0.53
1:A:290:HIS:ND1	1:A:292:THR:OG1	2.42	0.53
2:F:233:LEU:HD21	2:F:255:LEU:HB2	1.91	0.53
2:K:68:GLU:N	2:K:75:ILE:HD11	2.24	0.53
2:K:91:ALA:HB2	2:K:186:ILE:HG23	1.89	0.53
2:K:147:VAL:HA	2:K:159:PHE:HB2	1.90	0.53
2:E:299:SER:OG	2:E:316:GLN:NE2	2.41	0.53
2:L:282:ASP:OD1	2:L:282:ASP:N	2.40	0.53
2:E:84:LEU:HB3	2:E:88:GLY:HA3	1.91	0.53
2:K:87:ALA:HB3	2:K:191:THR:HB	1.90	0.53
2:L:31:LYS:HB2	2:L:31:LYS:HZ2	1.72	0.53
2:I:17:LEU:HD11	2:I:307:ILE:HG21	1.90	0.52
2:E:156:ILE:HD13	2:E:159:PHE:CE2	2.43	0.52
2:E:328:GLU:H	2:E:345:PRO:HB3	1.75	0.52
2:G:120:MET:HE3	2:G:177:ILE:HG12	1.91	0.52
2:K:94:ARG:NH2	2:K:183:LEU:O	2.43	0.52
1:D:341:VAL:HG13	1:D:387:LEU:HD12	1.91	0.52
2:K:33:ILE:HD12	2:K:219:ILE:HD11	1.92	0.52
2:H:257:ASP:OD2	2:H:259:SER:OG	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HD13	1:C:240:LEU:HD21	1.91	0.52
2:F:9:GLY:H	4:F:401:GTP:H2'	1.73	0.52
1:A:142:THR:OG1	1:A:181:CYS:SG	2.58	0.52
1:D:347:VAL:HA	1:D:393:ILE:HB	1.90	0.52
2:J:233:LEU:HD21	2:J:255:LEU:HB2	1.91	0.52
2:G:332:VAL:HG22	2:G:349:ILE:HD12	1.92	0.52
2:I:178:LEU:HD22	2:I:182:VAL:HG11	1.91	0.52
2:J:200:ILE:HA	2:J:203:LYS:CE	2.18	0.52
2:L:156:ILE:HD11	2:L:159:PHE:HA	1.90	0.52
2:E:138:VAL:HG21	2:E:141:PRO:O	2.10	0.52
1:C:356:THR:HG22	1:C:401:ASN:HD21	1.72	0.52
1:D:120:ASP:N	1:D:120:ASP:OD1	2.41	0.52
2:F:198:PHE:HA	2:F:201:MET:HB2	1.90	0.51
2:L:289:CYS:SG	2:L:306:CYS:N	2.84	0.51
2:E:180:PRO:HA	2:E:183:LEU:HB3	1.92	0.51
2:G:44:ALA:HA	2:G:118:GLN:HE22	1.75	0.51
2:G:269:GLY:N	2:G:286:ILE:O	2.43	0.51
2:L:320:MET:HE3	2:L:324:THR:HG21	1.92	0.51
2:G:107:LEU:HD23	2:G:175:MET:HG2	1.92	0.51
2:G:120:MET:HG2	2:G:177:ILE:CG1	2.39	0.51
2:J:262:ILE:HD13	2:J:268:ILE:HG13	1.92	0.51
2:L:22:PRO:HG3	2:L:56:MET:HB3	1.92	0.51
1:D:303:PRO:HD2	1:D:320:ARG:HG3	1.92	0.51
2:L:239:LYS:HD3	2:L:240:GLN:HE21	1.75	0.51
2:I:130:GLU:HB2	2:I:206:GLN:HB3	1.93	0.51
2:E:86:THR:HB	2:E:193:ILE:H	1.74	0.51
2:E:204:GLU:HB3	2:E:206:GLN:HG2	1.91	0.51
2:J:51:LEU:HD13	2:J:64:MET:HE1	1.92	0.51
2:J:153:THR:OG1	2:J:154:GLY:N	2.43	0.51
2:E:212:LEU:HD13	2:E:214:GLY:H	1.76	0.51
2:H:155:ARG:HA	2:H:208:TYR:HA	1.93	0.51
1:A:403:ILE:HD12	1:A:418:ILE:HG12	1.92	0.51
2:F:84:LEU:N	4:F:401:GTP:O6	2.44	0.51
2:G:13:ARG:O	2:G:14:LEU:CB	2.59	0.51
2:J:4:LEU:HD11	2:J:52:ALA:HB2	1.93	0.51
2:J:313:ARG:HB2	2:J:331:ILE:HD13	1.93	0.51
2:K:5:ILE:HD13	2:K:34:LEU:HD11	1.92	0.51
2:F:146:VAL:HG22	2:F:163:PRO:HG3	1.94	0.50
2:F:217:MET:HE3	2:F:227:THR:HB	1.92	0.50
1:A:295:VAL:HG11	1:A:301:LEU:HD11	1.93	0.50
2:I:160:VAL:CG2	2:I:167:VAL:HG11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:135:VAL:HG11	2:J:147:VAL:HG21	1.94	0.50
1:B:376:LYS:HB2	1:B:381:LEU:HD21	1.94	0.50
2:L:101:ALA:HA	2:L:180:PRO:HG2	1.92	0.50
2:L:148:VAL:HG22	2:L:168:SER:HB2	1.93	0.50
2:L:320:MET:HE3	2:L:324:THR:HG22	1.93	0.50
2:H:304:GLU:O	2:H:321:GLU:HA	2.11	0.50
2:I:250:ILE:HD13	2:I:268:ILE:HB	1.92	0.50
2:J:22:PRO:HG3	2:J:56:MET:HB3	1.93	0.50
1:B:59:TYR:O	1:B:82:TYR:OH	2.24	0.50
2:E:37:GLN:NE2	2:E:108:ASN:O	2.44	0.50
2:E:12:THR:HA	2:E:15:ARG:HD3	1.93	0.50
1:D:92:GLY:HA2	1:D:95:LEU:HD12	1.93	0.50
2:F:9:GLY:CA	4:F:401:GTP:H2'	2.42	0.50
2:F:9:GLY:N	4:F:401:GTP:H2'	2.26	0.50
2:F:33:ILE:HD11	2:F:112:ILE:HB	1.93	0.50
2:J:324:THR:O	2:J:324:THR:HG23	2.11	0.50
2:E:61:GLU:HA	2:E:77:MET:HE1	1.94	0.50
2:L:134:LEU:HD11	2:L:212:LEU:HG	1.94	0.50
2:L:230:CYS:SG	2:L:271:ASN:CG	2.95	0.50
1:D:3:LYS:O	1:D:110:PHE:HA	2.12	0.50
1:D:284:ARG:HH21	1:D:300:VAL:HG11	1.77	0.50
2:J:310:TRP:HE3	2:J:328:GLU:HB3	1.77	0.50
1:D:396:GLU:OE2	2:K:287:ARG:NH2	2.43	0.49
2:I:163:PRO:HB2	2:I:165:VAL:HG23	1.94	0.49
2:I:332:VAL:HG22	2:I:349:ILE:HD12	1.93	0.49
1:C:359:ASP:OD2	1:C:360:PRO:HD3	2.12	0.49
2:K:162:LYS:HD3	2:K:163:PRO:HD3	1.93	0.49
2:L:180:PRO:O	2:L:183:LEU:HB3	2.12	0.49
2:F:168:SER:OG	2:F:169:ASN:N	2.45	0.49
2:J:67:GLN:O	2:J:71:LEU:HB2	2.13	0.49
2:E:60:LEU:HG	2:E:64:MET:HE2	1.94	0.49
2:G:247:GLY:H	2:G:250:ILE:HB	1.77	0.49
2:K:116:PRO:HB2	2:K:119:ALA:HB3	1.95	0.49
2:J:7:VAL:HG21	2:J:53:VAL:CB	2.41	0.49
2:K:94:ARG:NH1	2:K:184:GLN:OE1	2.45	0.49
2:K:138:VAL:HB	2:K:141:PRO:HD2	1.94	0.49
2:L:54:SER:HB3	2:L:80:GLU:OE2	2.12	0.49
2:H:194:GLU:HA	2:H:198:PHE:HB2	1.95	0.49
2:K:95:ASP:OD1	2:K:95:ASP:N	2.46	0.49
2:I:360:MET:HB3	2:J:358:ILE:HD13	1.94	0.49
2:J:201:MET:HE2	2:J:207:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:39:GLU:OE1	2:K:70:ARG:NH2	2.41	0.49
1:A:406:PRO:O	1:B:18:ARG:NH1	2.25	0.49
2:I:146:VAL:HG11	2:I:168:SER:C	2.32	0.49
2:L:84:LEU:HB3	2:L:88:GLY:HA3	1.95	0.49
1:B:178:ILE:HD13	1:B:240:LEU:HD21	1.95	0.49
2:G:308:VAL:HG13	2:G:326:LEU:HD12	1.94	0.49
2:K:345:PRO:O	2:L:15:ARG:NH2	2.35	0.49
2:E:113:CYS:SG	2:E:114:ASP:O	2.71	0.48
2:E:138:VAL:HG11	2:E:141:PRO:HB2	1.94	0.48
2:K:15:ARG:NH2	2:L:345:PRO:O	2.32	0.48
2:H:42:ALA:HB2	2:H:73:ILE:HD13	1.95	0.48
1:A:16:ARG:HG2	1:A:20:LEU:CD1	2.43	0.48
1:B:303:PRO:HD2	1:B:320:ARG:HG3	1.94	0.48
1:B:331:GLN:HG3	1:B:348:GLY:HA2	1.94	0.48
1:D:290:HIS:CE1	1:D:309:LYS:HB3	2.47	0.48
2:K:2:LYS:HG2	2:K:48:HIS:HB3	1.94	0.48
2:L:52:ALA:O	4:L:401:GTP:N2	2.46	0.48
2:H:130:GLU:OE1	2:H:179:SER:OG	2.30	0.48
1:D:114:ASN:CG	4:D:501:GTP:H4'	2.38	0.48
2:F:22:PRO:HB2	2:F:24:PRO:HD2	1.95	0.48
2:L:116:PRO:HG3	2:L:212:LEU:HD21	1.93	0.48
1:A:417:GLN:HE22	1:B:375:PHE:H	1.60	0.48
1:B:122:PRO:HG3	1:B:241:THR:HG21	1.94	0.48
2:F:24:PRO:HB3	2:F:34:LEU:HB2	1.95	0.48
2:F:27:ASP:OD2	2:F:27:ASP:N	2.37	0.48
2:G:57:SER:O	2:G:61:GLU:HB3	2.12	0.48
2:G:115:PHE:HD1	2:G:175:MET:CE	2.17	0.48
2:I:269:GLY:N	2:I:286:ILE:O	2.41	0.48
2:G:106:VAL:HB	2:G:176:TYR:HD1	1.78	0.48
2:I:110:ASP:OD2	2:I:110:ASP:N	2.33	0.48
2:J:14:LEU:HG	2:J:17:LEU:HD12	1.96	0.48
2:J:186:ILE:HG12	2:J:197:VAL:HG21	1.94	0.48
1:B:392:ARG:HB2	1:B:409:GLU:HG2	1.96	0.48
2:F:94:ARG:O	2:F:98:SER:OG	2.31	0.48
2:E:124:HIS:HA	2:E:127:HIS:CD2	2.49	0.48
1:C:362:PRO:HB3	2:J:164:GLN:HA	1.95	0.48
1:D:364:ASP:OD2	1:D:365:PRO:N	2.47	0.48
2:J:49:VAL:HB	2:J:75:ILE:HG23	1.94	0.48
1:A:3:LYS:O	1:A:110:PHE:HA	2.12	0.48
1:C:37:ILE:HA	1:C:40:HIS:CD2	2.49	0.48
2:I:311:ARG:NH1	2:I:329:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:14:LEU:O	2:L:14:LEU:HG	2.13	0.48
2:E:37:GLN:HE22	2:E:109:SER:HA	1.79	0.48
2:L:142:SER:OG	2:L:143:LYS:N	2.44	0.48
2:H:266:CYS:HB2	2:H:284:VAL:H	1.78	0.48
2:G:201:MET:HE2	2:G:201:MET:HB2	1.70	0.47
1:A:394:PRO:HG2	1:A:397:VAL:HG21	1.95	0.47
2:G:150:GLU:OE1	2:G:153:THR:OG1	2.32	0.47
2:H:169:ASN:OD1	2:H:169:ASN:N	2.35	0.47
1:B:100:ASP:OD1	1:C:99:ARG:NH2	2.47	0.47
2:E:17:LEU:HD11	2:E:307:ILE:HG21	1.95	0.47
1:B:393:ILE:HD12	1:B:399:ILE:HG13	1.96	0.47
2:E:19:LEU:HD22	2:F:19:LEU:HD22	1.96	0.47
2:E:194:GLU:HA	2:E:198:PHE:HB2	1.96	0.47
2:F:85:GLY:O	4:F:401:GTP:C5	2.67	0.47
2:I:87:ALA:HB2	2:I:193:ILE:HB	1.95	0.47
2:E:229:MET:HE3	2:E:229:MET:HB3	1.70	0.47
2:E:321:GLU:HG3	2:E:339:ASN:HD22	1.80	0.47
2:J:193:ILE:HA	2:J:197:VAL:HB	1.97	0.47
2:L:175:MET:HB3	2:L:175:MET:HE2	1.69	0.47
1:A:133:GLN:HB3	1:A:135:HIS:CD2	2.49	0.47
2:E:311:ARG:NH2	2:E:328:GLU:OE1	2.43	0.47
2:L:106:VAL:HB	2:L:176:TYR:HD1	1.79	0.47
1:D:364:ASP:OD2	1:D:365:PRO:HD2	2.15	0.47
2:K:16:PRO:HA	2:K:19:LEU:HD12	1.96	0.47
1:C:37:ILE:HA	1:C:40:HIS:HD2	1.79	0.47
2:I:6:LEU:CD2	4:I:401:GTP:H1'	2.44	0.47
2:I:321:GLU:OE1	2:I:337:TYR:HE1	1.98	0.47
2:J:7:VAL:HG23	2:J:8:GLY:H	1.80	0.47
2:F:10:TYR:O	4:F:401:GTP:O1B	2.34	0.46
2:G:129:GLN:NE2	2:G:206:GLN:OE1	2.42	0.46
2:G:134:LEU:HB3	2:G:173:ALA:HB3	1.95	0.46
1:C:15:THR:O	1:C:15:THR:HG22	2.15	0.46
2:F:94:ARG:HG3	2:F:183:LEU:HG	1.97	0.46
2:I:37:GLN:NE2	2:I:108:ASN:O	2.49	0.46
2:I:201:MET:HE2	2:I:207:LEU:HG	1.96	0.46
2:L:276:PRO:HD2	2:L:293:ARG:HG2	1.97	0.46
2:E:160:VAL:HG13	2:E:160:VAL:O	2.14	0.46
2:K:158:ARG:CG	2:K:158:ARG:NH2	2.73	0.46
1:C:354:GLU:O	1:C:385:THR:OG1	2.30	0.46
2:L:1:MET:N	2:L:47:ASP:OD2	2.39	0.46
1:D:318:ARG:HB2	2:K:317:TRP:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:8:GLY:HA2	4:G:401:GTP:C4	2.51	0.46
2:I:201:MET:HE3	2:I:206:GLN:HB2	1.97	0.46
2:I:306:CYS:HB3	2:I:324:THR:HG23	1.97	0.46
2:J:64:MET:HA	2:J:67:GLN:HB2	1.97	0.46
2:J:87:ALA:HB1	2:J:186:ILE:HG21	1.97	0.46
2:J:110:ASP:OD2	2:J:110:ASP:N	2.39	0.46
1:A:302:GLY:N	1:A:318:ARG:HH12	2.13	0.46
2:I:292:LEU:HD12	2:I:309:GLY:HA2	1.96	0.46
2:E:302:TRP:HE3	2:E:319:ARG:HG3	1.80	0.46
2:G:310:TRP:HE3	2:G:328:GLU:HB2	1.81	0.46
2:J:7:VAL:HG23	2:J:53:VAL:HA	1.97	0.46
2:L:12:THR:HA	2:L:15:ARG:HD3	1.98	0.46
2:L:103:PRO:HA	2:L:178:LEU:O	2.16	0.46
1:C:5:VAL:HG11	1:C:95:LEU:HD21	1.98	0.45
2:I:35:LEU:HD11	2:I:67:GLN:HG2	1.98	0.45
2:K:148:VAL:N	2:K:158:ARG:O	2.46	0.45
2:E:8:GLY:HA3	2:E:54:SER:H	1.81	0.45
2:E:360:MET:HG2	2:F:358:ILE:HD13	1.97	0.45
2:G:6:LEU:O	4:G:401:GTP:O2'	2.28	0.45
2:L:180:PRO:O	2:L:183:LEU:CB	2.64	0.45
2:H:146:VAL:CB	2:H:160:VAL:CG1	2.92	0.45
1:C:393:ILE:HD12	1:C:399:ILE:HG13	1.98	0.45
2:L:133:ILE:HG22	2:L:176:TYR:HD2	1.81	0.45
2:H:162:LYS:HG3	2:H:163:PRO:HD2	1.97	0.45
2:G:35:LEU:HA	2:G:38:VAL:HG22	1.99	0.45
2:K:49:VAL:HG12	2:K:75:ILE:CG2	2.45	0.45
2:K:133:ILE:HD11	2:K:207:LEU:HD22	1.98	0.45
2:I:273:SER:O	2:I:273:SER:OG	2.34	0.45
2:J:229:MET:HB3	2:J:229:MET:HE3	1.72	0.45
2:H:321:GLU:OE1	2:H:337:TYR:HE1	1.99	0.45
1:D:13:LYS:HA	1:D:13:LYS:HD3	1.73	0.45
1:D:242:ASP:OD1	1:D:242:ASP:N	2.50	0.45
2:G:135:VAL:HG11	2:G:147:VAL:HG21	1.99	0.45
2:K:123:PHE:HB2	2:K:210:MET:HE2	1.98	0.45
2:H:91:ALA:HB1	2:H:188:LEU:HA	1.99	0.45
2:G:12:THR:HB	2:H:347:LYS:HD2	1.99	0.45
2:G:186:ILE:HG12	2:G:197:VAL:HG22	1.98	0.45
2:K:133:ILE:HG23	2:K:176:TYR:HD2	1.82	0.45
2:L:219:ILE:HB	2:L:225:PHE:HD2	1.80	0.45
2:E:148:VAL:HB	2:E:158:ARG:HB3	1.99	0.45
1:D:37:ILE:HA	1:D:40:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:MET:SD	2:F:134:LEU:HG	2.57	0.45
2:F:184:GLN:H	2:F:184:GLN:HG3	1.52	0.45
2:I:240:GLN:OE1	2:I:243:ARG:NH2	2.49	0.45
2:J:7:VAL:HG22	2:J:52:ALA:C	2.41	0.45
2:J:112:ILE:HD13	2:J:112:ILE:HA	1.83	0.45
2:K:6:LEU:H	2:K:6:LEU:HG	1.43	0.45
2:L:9:GLY:N	4:L:401:GTP:C4	2.85	0.45
2:H:127:HIS:CD2	2:H:129:GLN:H	2.35	0.45
2:K:11:GLY:O	2:K:18:THR:OG1	2.28	0.45
2:K:135:VAL:HG11	2:K:147:VAL:HG21	1.99	0.45
2:L:52:ALA:C	2:L:80:GLU:OE1	2.60	0.45
2:E:294:ASP:HB3	2:E:311:ARG:HG2	1.98	0.44
2:L:29:CYS:SG	2:L:255:LEU:HD11	2.53	0.44
2:L:68:GLU:HB3	2:L:75:ILE:HD12	1.98	0.44
2:E:27:ASP:HB3	2:E:292:LEU:HD22	2.00	0.44
2:G:25:LEU:HD11	2:G:60:LEU:HA	1.99	0.44
2:K:86:THR:HG23	2:K:193:ILE:HG22	1.99	0.44
3:A:501:GDD:H8	3:A:501:GDD:H2'	1.75	0.44
2:E:116:PRO:HG2	2:E:134:LEU:HD21	1.99	0.44
2:G:12:THR:N	4:G:401:GTP:O2G	2.46	0.44
2:G:173:ALA:O	2:G:216:TRP:NE1	2.47	0.44
2:L:229:MET:SD	2:L:233:LEU:HD12	2.58	0.44
2:E:158:ARG:HD2	2:E:158:ARG:HA	1.80	0.44
1:C:113:LEU:HD23	1:C:183:ILE:HG23	2.00	0.44
1:C:376:LYS:HB3	1:C:381:LEU:HD21	1.99	0.44
2:F:110:ASP:OD1	4:F:401:GTP:O1A	2.35	0.44
2:J:93:ALA:HB1	2:J:97:LEU:HD23	1.99	0.44
2:K:103:PRO:HB2	2:K:177:ILE:HG22	1.99	0.44
2:L:54:SER:OG	2:L:55:TYR:N	2.51	0.44
1:A:13:LYS:HB2	1:A:58:PHE:HZ	1.83	0.44
2:F:17:LEU:HD11	2:F:307:ILE:HG21	1.98	0.44
2:L:52:ALA:O	2:L:80:GLU:OE1	2.36	0.44
1:A:73:GLN:HE21	1:A:79:PRO:HA	1.82	0.44
2:E:41:LEU:HB2	2:E:46:VAL:HG22	1.99	0.44
2:E:60:LEU:O	2:E:64:MET:HB2	2.18	0.44
2:I:136:THR:HG22	2:I:212:LEU:HB3	1.99	0.44
2:H:15:ARG:HD2	2:H:15:ARG:HA	1.83	0.44
1:B:28:LEU:HA	1:B:35:PRO:HB3	2.00	0.44
2:E:134:LEU:HD12	2:E:134:LEU:HA	1.82	0.44
2:F:342:SER:O	2:F:342:SER:OG	2.36	0.44
2:I:185:ARG:HE	2:I:185:ARG:HB2	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:321:GLU:OE1	2:J:337:TYR:OH	2.33	0.44
1:A:16:ARG:HG2	1:A:20:LEU:HD12	2.00	0.44
2:E:39:GLU:HG2	2:E:71:LEU:HD21	1.98	0.44
2:E:344:LEU:HD13	2:E:360:MET:HB3	1.99	0.44
2:G:97:LEU:HB2	2:G:183:LEU:HD11	1.99	0.44
2:G:307:ILE:HD12	2:G:325:VAL:HG22	2.00	0.44
2:I:266:CYS:HB2	2:I:284:VAL:H	1.83	0.44
1:A:176:SER:OG	1:A:177:ASP:N	2.51	0.43
1:B:376:LYS:HA	1:B:376:LYS:HD3	1.74	0.43
2:G:22:PRO:HD2	2:G:25:LEU:HD12	2.00	0.43
2:E:207:LEU:HD23	2:E:207:LEU:HA	1.82	0.43
2:F:50:ILE:HD12	2:F:97:LEU:HD13	2.00	0.43
2:J:269:GLY:N	2:J:286:ILE:O	2.51	0.43
2:H:32:PRO:HD2	2:H:35:LEU:HD22	1.99	0.43
2:H:233:LEU:HD23	2:H:233:LEU:HA	1.88	0.43
1:A:156:VAL:HB	1:A:166:HIS:HB3	1.99	0.43
2:G:6:LEU:H	2:G:6:LEU:HG	1.68	0.43
2:I:13:ARG:NH2	4:I:401:GTP:O3G	2.49	0.43
2:J:243:ARG:HD2	2:J:255:LEU:HD11	2.00	0.43
1:A:20:LEU:CD1	1:A:20:LEU:H	2.28	0.43
2:F:182:VAL:HG23	2:F:185:ARG:HD2	2.00	0.43
2:G:105:PHE:CD1	2:G:117:PHE:CD1	3.04	0.43
2:J:52:ALA:HB1	2:J:89:PRO:HB3	1.99	0.43
1:A:405:LEU:HD22	1:A:420:LEU:HA	2.00	0.43
1:C:52:GLU:HG3	1:C:79:PRO:HG2	2.00	0.43
1:D:78:LEU:HD12	1:D:78:LEU:HA	1.91	0.43
2:I:251:VAL:HB	2:I:269:GLY:HA2	2.01	0.43
2:J:12:THR:HA	2:J:15:ARG:HD3	1.99	0.43
2:J:307:ILE:HB	2:J:325:VAL:HG13	2.01	0.43
2:L:172:ASN:HD21	2:L:176:TYR:HE2	1.65	0.43
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.85	0.43
1:A:376:LYS:HG3	1:A:381:LEU:HD11	2.00	0.43
2:L:52:ALA:HB1	2:L:80:GLU:OE1	2.18	0.43
2:L:215:PHE:HA	2:L:231:LEU:HD13	1.99	0.43
2:H:13:ARG:HE	2:H:221:GLN:HG2	1.83	0.43
1:D:42:GLU:OE2	1:D:269:HIS:NE2	2.51	0.43
1:D:376:LYS:HB2	1:D:381:LEU:HD21	1.99	0.43
2:H:146:VAL:CG1	2:H:160:VAL:HG11	2.49	0.43
1:D:400:LEU:HD23	1:D:415:THR:HG23	2.01	0.43
2:L:94:ARG:HE	2:L:94:ARG:HB2	1.60	0.43
1:C:140:LEU:HB3	1:C:181:CYS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:LEU:HA	2:F:190:PRO:HB3	2.01	0.43
2:G:63:GLU:HG3	2:G:67:GLN:HE21	1.84	0.43
2:J:212:LEU:HD23	2:J:212:LEU:HA	1.84	0.43
2:K:320:MET:HG2	2:K:338:LEU:HD12	2.01	0.43
2:E:54:SER:O	2:E:54:SER:OG	2.34	0.43
2:E:146:VAL:O	2:E:159:PHE:C	2.61	0.43
2:F:269:GLY:HA3	2:F:287:ARG:HG3	2.01	0.43
2:F:305:SER:O	2:F:323:VAL:HA	2.18	0.43
2:G:115:PHE:HA	2:G:116:PRO:HD3	1.69	0.43
2:J:184:GLN:H	2:J:184:GLN:HG3	1.67	0.43
1:A:347:VAL:HA	1:A:393:ILE:HB	2.00	0.42
1:D:78:LEU:HD12	1:D:79:PRO:HD2	2.00	0.42
2:K:37:GLN:NE2	2:K:108:ASN:O	2.46	0.42
2:L:287:ARG:O	2:L:304:GLU:HA	2.19	0.42
2:L:305:SER:O	2:L:323:VAL:HA	2.19	0.42
2:H:22:PRO:HD2	2:H:25:LEU:HD12	2.00	0.42
1:C:4:ALA:HB3	1:C:53:ILE:HG12	2.00	0.42
1:D:265:TYR:CE2	1:D:272:ARG:HD3	2.54	0.42
2:F:273:SER:O	2:F:273:SER:OG	2.31	0.42
2:I:233:LEU:HD22	2:I:233:LEU:HA	1.87	0.42
2:K:132:SER:O	2:K:176:TYR:HA	2.18	0.42
2:K:229:MET:HB3	2:K:229:MET:HE3	1.81	0.42
2:L:320:MET:HG2	2:L:338:LEU:HB2	2.01	0.42
2:H:165:VAL:HG23	2:H:166:PHE:H	1.84	0.42
2:E:254:VAL:HG12	2:E:272:VAL:HB	2.01	0.42
2:E:310:TRP:HB2	2:E:328:GLU:HG3	2.00	0.42
2:I:229:MET:HE3	2:I:229:MET:HB3	1.87	0.42
2:J:175:MET:HE3	2:J:175:MET:HB2	1.78	0.42
2:H:162:LYS:HD2	2:H:162:LYS:HA	1.68	0.42
1:D:354:GLU:O	1:D:385:THR:OG1	2.37	0.42
2:J:7:VAL:CG2	2:J:53:VAL:CA	2.94	0.42
2:H:162:LYS:CB	2:H:163:PRO:CD	2.97	0.42
2:G:178:LEU:HD13	2:G:182:VAL:HG11	2.01	0.42
2:I:146:VAL:CG1	2:I:168:SER:C	2.83	0.42
2:J:289:CYS:SG	2:J:306:CYS:N	2.93	0.42
2:H:74:ARG:HH21	2:H:76:SER:HB3	1.84	0.42
1:D:59:TYR:O	1:D:82:TYR:OH	2.36	0.42
2:G:105:PHE:CD1	2:G:117:PHE:HD1	2.29	0.42
2:F:5:ILE:HD13	2:F:107:LEU:HB2	2.01	0.42
1:D:15:THR:O	1:D:18:ARG:HD3	2.20	0.42
2:F:1:MET:HE3	2:F:1:MET:HB2	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:14:LEU:O	2:K:18:THR:OG1	2.37	0.42
2:L:298:ARG:HD3	2:L:315:GLY:HA2	2.02	0.42
2:I:25:LEU:HD11	2:I:63:GLU:HG3	2.02	0.42
2:J:28:PHE:N	2:J:31:LYS:O	2.47	0.42
2:H:146:VAL:HG12	2:H:160:VAL:HG11	2.02	0.42
2:E:116:PRO:O	2:E:120:MET:HB2	2.19	0.42
2:F:142:SER:HA	2:F:164:GLN:HA	2.01	0.42
2:F:267:SER:OG	2:F:287:ARG:NH1	2.53	0.42
2:G:342:SER:HB3	2:H:360:MET:HE1	2.02	0.42
1:C:389:CYS:H	1:C:406:PRO:HB3	1.84	0.41
2:F:203:LYS:HA	2:F:203:LYS:HD2	1.85	0.41
2:I:173:ALA:O	2:I:216:TRP:NE1	2.53	0.41
2:H:276:PRO:HG2	2:H:293:ARG:HB2	2.01	0.41
1:A:13:LYS:HD2	1:A:13:LYS:HA	1.78	0.41
2:E:182:VAL:HA	2:E:185:ARG:HB2	2.00	0.41
1:C:127:LEU:HD12	1:C:127:LEU:HA	1.93	0.41
2:F:14:LEU:HD22	2:F:17:LEU:HD12	2.01	0.41
2:F:15:ARG:HD2	2:F:15:ARG:HA	1.78	0.41
2:G:60:LEU:O	2:G:64:MET:HG2	2.20	0.41
2:J:276:PRO:HG2	2:J:293:ARG:HG3	2.02	0.41
2:K:110:ASP:OD2	2:K:110:ASP:N	2.43	0.41
2:L:129:GLN:HG3	2:L:208:TYR:CE2	2.55	0.41
1:A:318:ARG:HB2	2:H:317:TRP:CE2	2.56	0.41
2:E:264:GLN:H	2:E:264:GLN:HG3	1.43	0.41
1:C:404:VAL:HG22	1:C:419:ILE:HD12	2.02	0.41
2:F:292:LEU:HD12	2:F:309:GLY:HA2	2.02	0.41
2:G:320:MET:HB3	2:G:324:THR:HG21	2.02	0.41
2:I:84:LEU:H	2:I:190:PRO:HG3	1.86	0.41
2:J:237:ARG:HE	2:J:237:ARG:HB2	1.76	0.41
1:B:18:ARG:O	1:B:18:ARG:HG3	2.20	0.41
1:D:156:VAL:HB	1:D:166:HIS:HB3	2.02	0.41
2:I:2:LYS:HE2	2:I:48:HIS:HD1	1.84	0.41
1:A:247:GLN:O	1:A:253:SER:OG	2.29	0.41
2:F:97:LEU:HB3	2:F:183:LEU:HD21	2.02	0.41
2:J:335:GLU:OE1	2:L:287:ARG:NH2	2.53	0.41
2:L:231:LEU:HD23	2:L:231:LEU:HA	1.55	0.41
2:E:321:GLU:OE2	2:E:337:TYR:CE1	2.70	0.41
2:F:260:ALA:HB1	2:F:278:VAL:HG22	2.03	0.41
2:I:163:PRO:HG2	2:I:167:VAL:HG21	0.47	0.41
2:J:33:ILE:HG12	2:J:219:ILE:HD11	2.02	0.41
2:J:189:GLN:H	2:J:189:GLN:HG3	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:358:ILE:HD13	2:L:360:MET:HB2	2.02	0.41
2:L:229:MET:O	2:L:232:PHE:HB3	2.20	0.41
2:H:56:MET:HE1	2:H:81:GLU:OE1	2.21	0.41
2:H:291:VAL:HG13	2:H:308:VAL:HB	2.02	0.41
1:A:37:ILE:HA	1:A:40:HIS:CD2	2.56	0.41
1:B:196:ASP:HB3	1:B:200:ARG:HH21	1.86	0.41
1:D:364:ASP:OD2	1:D:365:PRO:CD	2.69	0.41
2:G:27:ASP:HA	2:G:32:PRO:HA	2.03	0.41
2:K:49:VAL:CG1	2:K:75:ILE:HG22	2.51	0.41
2:K:67:GLN:HA	2:K:70:ARG:HB2	2.03	0.41
2:K:221:GLN:O	2:K:225:PHE:N	2.50	0.41
2:L:223:LYS:HE3	2:L:223:LYS:HB2	1.82	0.41
2:H:27:ASP:HA	2:H:32:PRO:HA	2.02	0.41
2:F:134:LEU:HB2	2:F:175:MET:HB2	2.03	0.41
2:F:186:ILE:H	2:F:186:ILE:HG13	1.75	0.41
1:B:312:THR:O	1:B:312:THR:OG1	2.38	0.40
2:E:70:ARG:HH11	2:E:70:ARG:HD2	1.75	0.40
2:G:7:VAL:HG21	2:G:51:LEU:HD12	2.02	0.40
2:J:268:ILE:HG22	2:J:272:VAL:HG11	2.02	0.40
1:A:358:SER:O	1:A:369:MET:CE	2.65	0.40
1:A:386:ILE:HB	1:A:403:ILE:HG23	2.03	0.40
1:C:50:MET:HE2	1:C:50:MET:HB2	1.95	0.40
1:A:198:PHE:CZ	1:D:100:ASP:HB3	2.56	0.40
1:B:186:PHE:HZ	1:B:222:LEU:HD21	1.86	0.40
2:E:71:LEU:HD23	2:E:71:LEU:HA	1.89	0.40
2:E:98:SER:OG	2:E:184:GLN:OE1	2.29	0.40
1:C:361:ASN:HA	1:C:362:PRO:HD3	1.97	0.40
2:G:15:ARG:HD2	2:G:15:ARG:HA	1.89	0.40
2:H:141:PRO:CB	2:H:164:GLN:HE22	2.25	0.40
2:H:236:LEU:HB3	2:H:244:LEU:HD21	2.02	0.40
2:G:107:LEU:HD21	2:G:117:PHE:HE1	1.86	0.40
2:J:7:VAL:HG23	2:J:8:GLY:N	2.35	0.40
2:L:110:ASP:OD2	2:L:110:ASP:N	2.46	0.40
2:L:237:ARG:HD3	2:L:237:ARG:HA	1.88	0.40
2:H:70:ARG:HH11	2:H:70:ARG:HD2	1.77	0.40
1:B:170:LYS:HE3	1:B:170:LYS:HB2	1.94	0.40
1:D:10:GLY:H	1:D:13:LYS:HB2	1.86	0.40
2:F:9:GLY:O	2:F:10:TYR:C	2.65	0.40
2:I:15:ARG:HB3	2:J:360:MET:HE3	2.04	0.40
2:K:3:ALA:C	2:K:49:VAL:HG23	2.47	0.40
2:K:14:LEU:HD12	2:K:222:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:118:GLN:HA	2:K:121:VAL:HG12	2.03	0.40
2:L:25:LEU:HA	2:L:32:PRO:HB3	2.03	0.40
2:L:139:GLU:HB3	2:L:140:GLU:OE2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/420 (96%)	383 (95%)	20 (5%)	0	100	100
1	B	402/420 (96%)	381 (95%)	20 (5%)	1 (0%)	43	76
1	C	402/420 (96%)	381 (95%)	21 (5%)	0	100	100
1	D	402/420 (96%)	387 (96%)	15 (4%)	0	100	100
2	E	358/360 (99%)	325 (91%)	31 (9%)	2 (1%)	21	56
2	F	346/360 (96%)	322 (93%)	24 (7%)	0	100	100
2	G	358/360 (99%)	331 (92%)	26 (7%)	1 (0%)	36	70
2	H	358/360 (99%)	333 (93%)	24 (7%)	1 (0%)	36	70
2	I	358/360 (99%)	333 (93%)	24 (7%)	1 (0%)	36	70
2	J	358/360 (99%)	343 (96%)	14 (4%)	1 (0%)	36	70
2	K	358/360 (99%)	323 (90%)	31 (9%)	4 (1%)	11	43
2	L	358/360 (99%)	326 (91%)	31 (9%)	1 (0%)	36	70
All	All	4461/4560 (98%)	4168 (93%)	281 (6%)	12 (0%)	37	70

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	143	LYS

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Mol	Chain	Res	Type
2	G	116	PRO
2	K	72	GLY
2	K	164	GLN
2	J	11	GLY
2	K	160	VAL
1	B	360	PRO
2	I	167	VAL
2	H	162	LYS
2	K	167	VAL
2	E	141	PRO
2	L	8	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/354 (97%)	323 (94%)	21 (6%)	17	49
1	B	344/354 (97%)	317 (92%)	27 (8%)	11	39
1	C	344/354 (97%)	316 (92%)	28 (8%)	11	38
1	D	344/354 (97%)	321 (93%)	23 (7%)	15	46
2	E	310/311 (100%)	263 (85%)	47 (15%)	3	14
2	F	303/311 (97%)	270 (89%)	33 (11%)	6	26
2	G	311/311 (100%)	279 (90%)	32 (10%)	7	28
2	H	311/311 (100%)	284 (91%)	27 (9%)	9	35
2	I	311/311 (100%)	263 (85%)	48 (15%)	2	13
2	J	311/311 (100%)	269 (86%)	42 (14%)	4	18
2	K	309/311 (99%)	274 (89%)	35 (11%)	5	24
2	L	309/311 (99%)	269 (87%)	40 (13%)	4	19
All	All	3851/3904 (99%)	3448 (90%)	403 (10%)	9	27

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	15	THR
1	A	20	LEU
1	A	108	GLU
1	A	142	THR
1	A	172	SER
1	A	173	THR
1	A	179	ILE
1	A	238	VAL
1	A	253	SER
1	A	276	HIS
1	A	298	SER
1	A	300	VAL
1	A	306	SER
1	A	337	LEU
1	A	356	THR
1	A	359	ASP
1	A	376	LYS
1	A	397	VAL
1	A	411	SER
1	A	413	SER
1	B	1	MET
1	B	2	LEU
1	B	18	ARG
1	B	37	ILE
1	B	51	GLN
1	B	78	LEU
1	B	118	CYS
1	B	124	SER
1	B	142	THR
1	B	143	THR
1	B	148	GLN
1	B	157	GLU
1	B	160	GLN
1	B	168	VAL
1	B	219	THR
1	B	238	VAL
1	B	264	ARG
1	B	300	VAL
1	B	312	THR
1	B	346	THR
1	B	358	SER
1	B	373	SER

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Mol	Chain	Res	Type
1	B	377	ASP
1	B	389	CYS
1	B	397	VAL
1	B	398	LEU
1	B	411	SER
2	E	1	MET
2	E	4	LEU
2	E	5	ILE
2	E	25	LEU
2	E	51	LEU
2	E	53	VAL
2	E	54	SER
2	E	64	MET
2	E	68	GLU
2	E	75	ILE
2	E	78	SER
2	E	86	THR
2	E	109	SER
2	E	114	ASP
2	E	122	GLN
2	E	132	SER
2	E	134	LEU
2	E	135	VAL
2	E	139	GLU
2	E	140	GLU
2	E	143	LYS
2	E	146	VAL
2	E	147	VAL
2	E	149	CYS
2	E	158	ARG
2	E	159	PHE
2	E	160	VAL
2	E	183	LEU
2	E	188	LEU
2	E	192	SER
2	E	194	GLU
2	E	199	PRO
2	E	203	LYS
2	E	212	LEU
2	E	227	THR
2	E	234	GLN
2	E	235	SER

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Mol	Chain	Res	Type
2	E	240	GLN
2	E	250	ILE
2	E	256	VAL
2	E	264	GLN
2	E	279	VAL
2	E	280	VAL
2	E	299	SER
2	E	322	ASN
2	E	332	VAL
2	E	359	ILE
1	C	1	MET
1	C	2	LEU
1	C	46	GLN
1	C	63	GLU
1	C	99	ARG
1	C	142	THR
1	C	149	SER
1	C	160	GLN
1	C	172	SER
1	C	173	THR
1	C	175	ILE
1	C	187	SER
1	C	219	THR
1	C	238	VAL
1	C	253	SER
1	C	264	ARG
1	C	275	LYS
1	C	283	ILE
1	C	298	SER
1	C	329	THR
1	C	356	THR
1	C	361	ASN
1	C	370	ASP
1	C	374	LEU
1	C	389	CYS
1	C	397	VAL
1	C	398	LEU
1	C	408	LYS
1	D	2	LEU
1	D	18	ARG
1	D	23	GLU
1	D	62	ASP

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Mol	Chain	Res	Type
1	D	118	CYS
1	D	142	THR
1	D	143	THR
1	D	168	VAL
1	D	187	SER
1	D	194	LEU
1	D	219	THR
1	D	238	VAL
1	D	240	LEU
1	D	253	SER
1	D	255	LEU
1	D	258	SER
1	D	276	HIS
1	D	283	ILE
1	D	292	THR
1	D	312	THR
1	D	366	ARG
1	D	371	SER
1	D	397	VAL
2	F	4	LEU
2	F	7	VAL
2	F	27	ASP
2	F	35	LEU
2	F	46	VAL
2	F	65	LYS
2	F	78	SER
2	F	82	GLU
2	F	86	THR
2	F	95	ASP
2	F	96	LEU
2	F	109	SER
2	F	113	CYS
2	F	130	GLU
2	F	132	SER
2	F	138	VAL
2	F	139	GLU
2	F	168	SER
2	F	171	ILE
2	F	177	ILE
2	F	184	GLN
2	F	186	ILE
2	F	199	PRO

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Mol	Chain	Res	Type
2	F	211	GLU
2	F	227	THR
2	F	243	ARG
2	F	251	VAL
2	F	257	ASP
2	F	273	SER
2	F	278	VAL
2	F	279	VAL
2	F	335	GLU
2	F	348	SER
2	G	6	LEU
2	G	14	LEU
2	G	20	SER
2	G	35	LEU
2	G	39	GLU
2	G	47	ASP
2	G	48	HIS
2	G	49	VAL
2	G	53	VAL
2	G	56	MET
2	G	81	GLU
2	G	86	THR
2	G	96	LEU
2	G	98	SER
2	G	102	ASP
2	G	107	LEU
2	G	152	ASP
2	G	164	GLN
2	G	167	VAL
2	G	186	ILE
2	G	191	THR
2	G	192	SER
2	G	199	PRO
2	G	201	MET
2	G	207	LEU
2	G	212	LEU
2	G	262	ILE
2	G	278	VAL
2	G	279	VAL
2	G	294	ASP
2	G	324	THR
2	G	344	LEU

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Mol	Chain	Res	Type
2	I	6	LEU
2	I	10	TYR
2	I	14	LEU
2	I	20	SER
2	I	48	HIS
2	I	63	GLU
2	I	65	LYS
2	I	75	ILE
2	I	80	GLU
2	I	90	LEU
2	I	92	LEU
2	I	95	ASP
2	I	96	LEU
2	I	98	SER
2	I	106	VAL
2	I	109	SER
2	I	110	ASP
2	I	118	GLN
2	I	121	VAL
2	I	148	VAL
2	I	149	CYS
2	I	152	ASP
2	I	165	VAL
2	I	167	VAL
2	I	169	ASN
2	I	175	MET
2	I	177	ILE
2	I	179	SER
2	I	184	GLN
2	I	191	THR
2	I	196	GLU
2	I	199	PRO
2	I	200	ILE
2	I	219	ILE
2	I	223	LYS
2	I	233	LEU
2	I	234	GLN
2	I	235	SER
2	I	251	VAL
2	I	253	ASN
2	I	257	ASP
2	I	266	CYS

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Mol	Chain	Res	Type
2	I	274	LEU
2	I	279	VAL
2	I	306	CYS
2	I	319	ARG
2	I	335	GLU
2	I	360	MET
2	J	6	LEU
2	J	7	VAL
2	J	31	LYS
2	J	34	LEU
2	J	51	LEU
2	J	53	VAL
2	J	54	SER
2	J	60	LEU
2	J	62	LYS
2	J	77	MET
2	J	81	GLU
2	J	86	THR
2	J	100	THR
2	J	107	LEU
2	J	109	SER
2	J	112	ILE
2	J	129	GLN
2	J	139	GLU
2	J	150	GLU
2	J	152	ASP
2	J	153	THR
2	J	160	VAL
2	J	161	GLU
2	J	165	VAL
2	J	172	ASN
2	J	177	ILE
2	J	179	SER
2	J	186	ILE
2	J	198	PHE
2	J	201	MET
2	J	229	MET
2	J	236	LEU
2	J	240	GLN
2	J	272	VAL
2	J	279	VAL
2	J	286	ILE

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Mol	Chain	Res	Type
2	J	288	ARG
2	J	290	THR
2	J	299	SER
2	J	323	VAL
2	J	352	SER
2	J	360	MET
2	K	5	ILE
2	K	6	LEU
2	K	20	SER
2	K	50	ILE
2	K	54	SER
2	K	57	SER
2	K	64	MET
2	K	71	LEU
2	K	75	ILE
2	K	92	LEU
2	K	95	ASP
2	K	106	VAL
2	K	109	SER
2	K	113	CYS
2	K	120	MET
2	K	125	ARG
2	K	134	LEU
2	K	138	VAL
2	K	146	VAL
2	K	158	ARG
2	K	159	PHE
2	K	160	VAL
2	K	171	ILE
2	K	177	ILE
2	K	191	THR
2	K	194	GLU
2	K	236	LEU
2	K	251	VAL
2	K	266	CYS
2	K	273	SER
2	K	279	VAL
2	K	301	SER
2	K	342	SER
2	K	344	LEU
2	K	348	SER
2	L	14	LEU

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Mol	Chain	Res	Type
2	L	20	SER
2	L	21	THR
2	L	31	LYS
2	L	33	ILE
2	L	49	VAL
2	L	54	SER
2	L	59	VAL
2	L	78	SER
2	L	82	GLU
2	L	84	LEU
2	L	86	THR
2	L	90	LEU
2	L	92	LEU
2	L	96	LEU
2	L	100	THR
2	L	120	MET
2	L	139	GLU
2	L	148	VAL
2	L	149	CYS
2	L	152	ASP
2	L	156	ILE
2	L	169	ASN
2	L	175	MET
2	L	177	ILE
2	L	186	ILE
2	L	199	PRO
2	L	210	MET
2	L	211	GLU
2	L	217	MET
2	L	231	LEU
2	L	255	LEU
2	L	257	ASP
2	L	266	CYS
2	L	282	ASP
2	L	299	SER
2	L	324	THR
2	L	336	LEU
2	L	352	SER
2	L	353	VAL
2	H	2	LYS
2	H	50	ILE
2	H	54	SER

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Mol	Chain	Res	Type
2	H	60	LEU
2	H	69	GLN
2	H	71	LEU
2	H	84	LEU
2	H	106	VAL
2	H	112	ILE
2	H	134	LEU
2	H	136	THR
2	H	138	VAL
2	H	149	CYS
2	H	160	VAL
2	H	167	VAL
2	H	169	ASN
2	H	176	TYR
2	H	183	LEU
2	H	188	LEU
2	H	199	PRO
2	H	245	CYS
2	H	251	VAL
2	H	265	ASN
2	H	271	ASN
2	H	278	VAL
2	H	299	SER
2	H	347	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	60	GLN
1	A	73	GLN
1	A	97	HIS
1	A	135	HIS
1	A	158	ASN
1	A	201	ASN
1	A	235	GLN
1	A	286	ASN
1	A	361	ASN
1	A	363	ASN
1	A	417	GLN
1	B	12	GLN
1	B	40	HIS

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Mol	Chain	Res	Type
1	B	67	GLN
1	B	201	ASN
1	B	286	ASN
2	E	67	GLN
2	E	79	HIS
2	E	206	GLN
2	E	221	GLN
2	E	316	GLN
2	E	339	ASN
1	C	40	HIS
1	C	46	GLN
1	C	67	GLN
1	C	77	ASN
1	C	148	GLN
1	C	166	HIS
1	C	201	ASN
1	C	224	GLN
1	C	286	ASN
1	C	304	ASN
1	C	361	ASN
1	C	363	ASN
1	C	401	ASN
1	D	12	GLN
1	D	40	HIS
1	D	51	GLN
1	D	73	GLN
1	D	77	ASN
1	D	135	HIS
1	D	145	ASN
1	D	180	ASN
1	D	201	ASN
1	D	276	HIS
1	D	286	ASN
1	D	338	HIS
1	D	363	ASN
1	D	401	ASN
2	F	187	GLN
2	F	238	GLN
2	F	271	ASN
2	G	37	GLN
2	G	67	GLN
2	G	118	GLN

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Mol	Chain	Res	Type
2	G	316	GLN
2	G	346	HIS
2	I	206	GLN
2	I	221	GLN
2	I	238	GLN
2	I	346	HIS
2	J	118	GLN
2	J	169	ASN
2	J	172	ASN
2	J	187	GLN
2	J	300	HIS
2	K	48	HIS
2	K	67	GLN
2	K	122	GLN
2	K	172	ASN
2	L	48	HIS
2	L	172	ASN
2	L	322	ASN
2	L	339	ASN
2	L	346	HIS
2	H	30	ASN
2	H	122	GLN
2	H	127	HIS
2	H	221	GLN
2	H	253	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
4	GTP	K	401	-	33,34,34	0.87	1 (3%)	50,54,54	1.70	9 (18%)
4	GTP	H	401	-	33,34,34	0.87	0	50,54,54	1.72	9 (18%)
3	GDD	C	501	-	41,42,42	0.79	1 (2%)	62,65,65	1.53	13 (20%)
4	GTP	I	401	-	33,34,34	0.88	0	50,54,54	1.67	9 (18%)
4	GTP	D	501	-	33,34,34	0.94	0	50,54,54	1.63	10 (20%)
4	GTP	E	401	-	33,34,34	0.82	0	50,54,54	1.57	9 (18%)
4	GTP	B	501	-	33,34,34	0.96	1 (3%)	50,54,54	1.58	7 (14%)
4	GTP	J	401	-	33,34,34	0.85	0	50,54,54	1.90	9 (18%)
4	GTP	L	401	-	33,34,34	0.88	1 (3%)	50,54,54	1.47	8 (16%)
4	GTP	G	401	-	33,34,34	0.86	0	50,54,54	1.85	11 (22%)
3	GDD	A	501	-	41,42,42	0.80	1 (2%)	62,65,65	1.54	12 (19%)
4	GTP	F	401	-	33,34,34	0.87	1 (3%)	50,54,54	1.71	9 (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
4	GTP	K	401	-	-	5/22/38/38	0/3/3/3
4	GTP	H	401	-	-	7/22/38/38	0/3/3/3
3	GDD	C	501	-	-	10/23/59/59	0/4/4/4
4	GTP	I	401	-	-	7/22/38/38	0/3/3/3
4	GTP	D	501	-	-	8/22/38/38	0/3/3/3
4	GTP	E	401	-	-	1/22/38/38	0/3/3/3
4	GTP	B	501	-	-	3/22/38/38	0/3/3/3
4	GTP	J	401	-	-	7/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	L	401	-	-	4/22/38/38	0/3/3/3
4	GTP	G	401	-	-	6/22/38/38	0/3/3/3
3	GDD	A	501	-	-	5/23/59/59	0/4/4/4
4	GTP	F	401	-	-	5/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	401	GTP	C6-N1	-3.00	1.33	1.38
3	C	501	GDD	C6-N1	-2.13	1.34	1.38
4	F	401	GTP	C6-N1	-2.08	1.35	1.38
4	K	401	GTP	C6-N1	-2.08	1.35	1.38
4	B	501	GTP	C6-N1	-2.04	1.35	1.38
3	A	501	GDD	C6-N1	-2.04	1.35	1.38

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	401	GTP	C5-C4-N3	-6.15	118.61	128.39
4	G	401	GTP	C5-C4-N3	-5.91	118.99	128.39
4	I	401	GTP	C2-N1-C6	-5.40	115.31	125.11
4	B	501	GTP	C2-N1-C6	-5.35	115.41	125.11
4	G	401	GTP	C2-N1-C6	-5.25	115.58	125.11
4	H	401	GTP	C5-C4-N3	-5.21	120.09	128.39
4	D	501	GTP	C2-N1-C6	-5.18	115.71	125.11
4	J	401	GTP	C2-N1-C6	-5.18	115.71	125.11
4	F	401	GTP	C2-N1-C6	-5.18	115.72	125.11
4	K	401	GTP	C2-N1-C6	-5.15	115.77	125.11
4	E	401	GTP	C2-N1-C6	-5.11	115.85	125.11
4	I	401	GTP	C5-C4-N3	-5.10	120.28	128.39
4	F	401	GTP	C5-C4-N3	-5.07	120.32	128.39
4	H	401	GTP	C2-N1-C6	-5.06	115.93	125.11
4	K	401	GTP	C5-C4-N3	-5.02	120.39	128.39
4	E	401	GTP	C5-C4-N3	-4.92	120.56	128.39
3	A	501	GDD	C2-N1-C6	-4.87	116.27	125.11
4	B	501	GTP	C5-C4-N3	-4.76	120.81	128.39
4	G	401	GTP	N9-C4-N3	4.74	135.43	125.95
4	L	401	GTP	C5-C4-N3	-4.64	121.00	128.39
4	J	401	GTP	N9-C4-N3	4.58	135.12	125.95
3	C	501	GDD	C2-N1-C6	-4.42	117.09	125.11
4	D	501	GTP	C5-C4-N3	-4.26	121.62	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	401	GTP	C2-N1-C6	-4.10	117.67	125.11
4	J	401	GTP	C2-N3-C4	4.04	119.26	112.30
4	H	401	GTP	N9-C4-N3	4.03	134.02	125.95
3	A	501	GDD	C5-C4-N3	-3.99	122.04	128.39
3	C	501	GDD	C5-C4-N3	-3.83	122.29	128.39
4	G	401	GTP	C2-N3-C4	3.78	118.82	112.30
4	L	401	GTP	N9-C4-N3	3.63	133.22	125.95
4	F	401	GTP	N9-C4-N3	3.62	133.19	125.95
4	I	401	GTP	N9-C4-N3	3.60	133.15	125.95
4	K	401	GTP	N9-C4-N3	3.59	133.12	125.95
4	E	401	GTP	N9-C4-N3	3.42	132.79	125.95
4	H	401	GTP	C2-N3-C4	3.38	118.12	112.30
3	A	501	GDD	N9-C4-N3	3.38	132.71	125.95
4	J	401	GTP	C5-C6-N1	3.32	121.70	113.25
4	J	401	GTP	O6-C6-C5	-3.22	118.05	126.53
3	A	501	GDD	N9-C8-N7	-3.20	107.46	113.40
4	G	401	GTP	C5-C6-N1	3.20	121.40	113.25
4	F	401	GTP	C2-N3-C4	3.18	117.78	112.30
3	C	501	GDD	N9-C8-N7	-3.18	107.51	113.40
3	C	501	GDD	N9-C4-N3	3.16	132.28	125.95
4	K	401	GTP	C2-N3-C4	3.16	117.74	112.30
4	B	501	GTP	C2-N3-C4	3.08	117.61	112.30
4	G	401	GTP	O6-C6-C5	-3.07	118.43	126.53
4	I	401	GTP	C2-N3-C4	3.02	117.50	112.30
4	B	501	GTP	N9-C4-N3	2.99	131.94	125.95
4	F	401	GTP	C5-C6-N1	2.99	120.86	113.25
4	K	401	GTP	C5-C6-N1	2.98	120.84	113.25
4	E	401	GTP	C2-N3-C4	2.98	117.43	112.30
4	B	501	GTP	C5-C6-N1	2.94	120.73	113.25
4	H	401	GTP	C5-C6-N1	2.92	120.68	113.25
3	C	501	GDD	C2-N3-C4	2.86	117.22	112.30
4	I	401	GTP	C5-C6-N1	2.83	120.47	113.25
4	B	501	GTP	O6-C6-C5	-2.83	119.06	126.53
4	D	501	GTP	C2-N3-C4	2.83	117.17	112.30
4	D	501	GTP	C5-C6-N1	2.81	120.40	113.25
3	A	501	GDD	O6-C6-C5	-2.80	119.14	126.53
4	D	501	GTP	N9-C4-N3	2.76	131.48	125.95
4	J	401	GTP	O4'-C1'-C2'	-2.74	100.75	106.62
4	E	401	GTP	C5-C6-N1	2.74	120.22	113.25
4	L	401	GTP	C2-N3-C4	2.70	116.96	112.30
3	A	501	GDD	C5-C6-N1	2.69	120.11	113.25
4	G	401	GTP	O2'-C2'-C3'	-2.69	103.20	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	GDD	O6-C6-C5	-2.68	119.45	126.53
4	H	401	GTP	O6-C6-C5	-2.68	119.45	126.53
3	C	501	GDD	C5-C6-N1	2.68	120.06	113.25
4	D	501	GTP	O6-C6-C5	-2.66	119.50	126.53
4	I	401	GTP	O6-C6-C5	-2.66	119.51	126.53
4	F	401	GTP	C4'-O4'-C1'	-2.61	103.69	109.47
4	K	401	GTP	C4'-O4'-C1'	-2.61	103.70	109.47
3	A	501	GDD	C2-N3-C4	2.60	116.78	112.30
4	K	401	GTP	O6-C6-C5	-2.59	119.69	126.53
4	F	401	GTP	O6-C6-C5	-2.59	119.71	126.53
4	E	401	GTP	O6-C6-C5	-2.58	119.71	126.53
4	D	501	GTP	N9-C8-N7	-2.58	108.62	113.40
3	A	501	GDD	C1'-N9-C8	-2.57	119.44	126.73
4	F	401	GTP	N9-C8-N7	-2.50	108.77	113.40
4	K	401	GTP	N9-C8-N7	-2.48	108.81	113.40
3	C	501	GDD	C1'-N9-C8	-2.46	119.73	126.73
4	H	401	GTP	N9-C8-N7	-2.45	108.86	113.40
4	L	401	GTP	C5-C6-N1	2.45	119.48	113.25
4	L	401	GTP	N9-C8-N7	-2.42	108.92	113.40
4	G	401	GTP	C1'-N9-C8	-2.41	119.89	126.73
4	F	401	GTP	C8-N7-C5	2.37	108.48	104.26
4	K	401	GTP	C8-N7-C5	2.36	108.47	104.26
4	D	501	GTP	C8-N7-C5	2.36	108.47	104.26
3	C	501	GDD	C61-C51-C41	-2.33	107.30	113.02
4	I	401	GTP	N9-C8-N7	-2.32	109.10	113.40
3	A	501	GDD	N2-C2-N3	-2.31	115.16	119.67
4	I	401	GTP	N1-C2-N3	2.30	127.54	123.32
3	A	501	GDD	C8-N7-C5	2.28	108.33	104.26
3	C	501	GDD	C8-N7-C5	2.28	108.32	104.26
4	H	401	GTP	C8-N7-C5	2.24	108.25	104.26
3	A	501	GDD	C8-N9-C4	2.23	110.20	106.03
3	C	501	GDD	N2-C2-N3	-2.23	115.32	119.67
4	G	401	GTP	C8-N7-C5	2.22	108.21	104.26
4	D	501	GTP	C6-C5-N7	2.22	134.32	130.29
4	G	401	GTP	N9-C8-N7	-2.21	109.30	113.40
3	C	501	GDD	C8-N9-C4	2.20	110.16	106.03
3	A	501	GDD	O31-C31-C21	-2.20	105.20	110.38
4	L	401	GTP	O6-C6-C5	-2.16	120.82	126.53
4	I	401	GTP	C8-N7-C5	2.16	108.11	104.26
4	E	401	GTP	N9-C8-N7	-2.15	109.42	113.40
4	E	401	GTP	C8-N7-C5	2.10	108.00	104.26
4	L	401	GTP	C8-N7-C5	2.09	107.97	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	GTP	N1-C2-N3	2.08	127.12	123.32
4	J	401	GTP	C5'-C4'-C3'	-2.07	107.76	115.21
4	D	501	GTP	N1-C2-N3	2.07	127.11	123.32
3	C	501	GDD	C6-C5-N7	2.05	134.02	130.29
4	H	401	GTP	O3A-PB-O1B	-2.05	104.54	110.70
4	G	401	GTP	C5'-C4'-C3'	-2.04	107.88	115.21
4	E	401	GTP	N1-C2-N3	2.03	127.04	123.32
4	J	401	GTP	O2'-C2'-C1'	2.00	117.01	110.10

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	501	GDD	O4'-C4'-C5'-O5'
3	C	501	GDD	C5'-O5'-PA-O2A
3	C	501	GDD	C11-O1B-PB-O3A
4	B	501	GTP	O4'-C4'-C5'-O5'
4	D	501	GTP	C5'-O5'-PA-O3A
4	D	501	GTP	C5'-O5'-PA-O2A
4	G	401	GTP	PB-O3B-PG-O3G
4	G	401	GTP	C5'-O5'-PA-O3A
4	G	401	GTP	C5'-O5'-PA-O1A
4	G	401	GTP	C5'-O5'-PA-O2A
4	I	401	GTP	PB-O3A-PA-O5'
4	I	401	GTP	C5'-O5'-PA-O3A
4	I	401	GTP	C5'-O5'-PA-O1A
4	I	401	GTP	C5'-O5'-PA-O2A
4	J	401	GTP	PB-O3B-PG-O2G
4	J	401	GTP	PB-O3B-PG-O3G
4	J	401	GTP	C5'-O5'-PA-O3A
4	J	401	GTP	C5'-O5'-PA-O1A
4	J	401	GTP	C5'-O5'-PA-O2A
4	L	401	GTP	C5'-O5'-PA-O3A
4	L	401	GTP	C5'-O5'-PA-O1A
4	L	401	GTP	C5'-O5'-PA-O2A
4	H	401	GTP	C5'-O5'-PA-O1A
4	H	401	GTP	O4'-C4'-C5'-O5'
4	H	401	GTP	C3'-C4'-C5'-O5'
4	F	401	GTP	O4'-C4'-C5'-O5'
4	K	401	GTP	O4'-C4'-C5'-O5'
3	A	501	GDD	C3'-C4'-C5'-O5'
3	A	501	GDD	O4'-C4'-C5'-O5'

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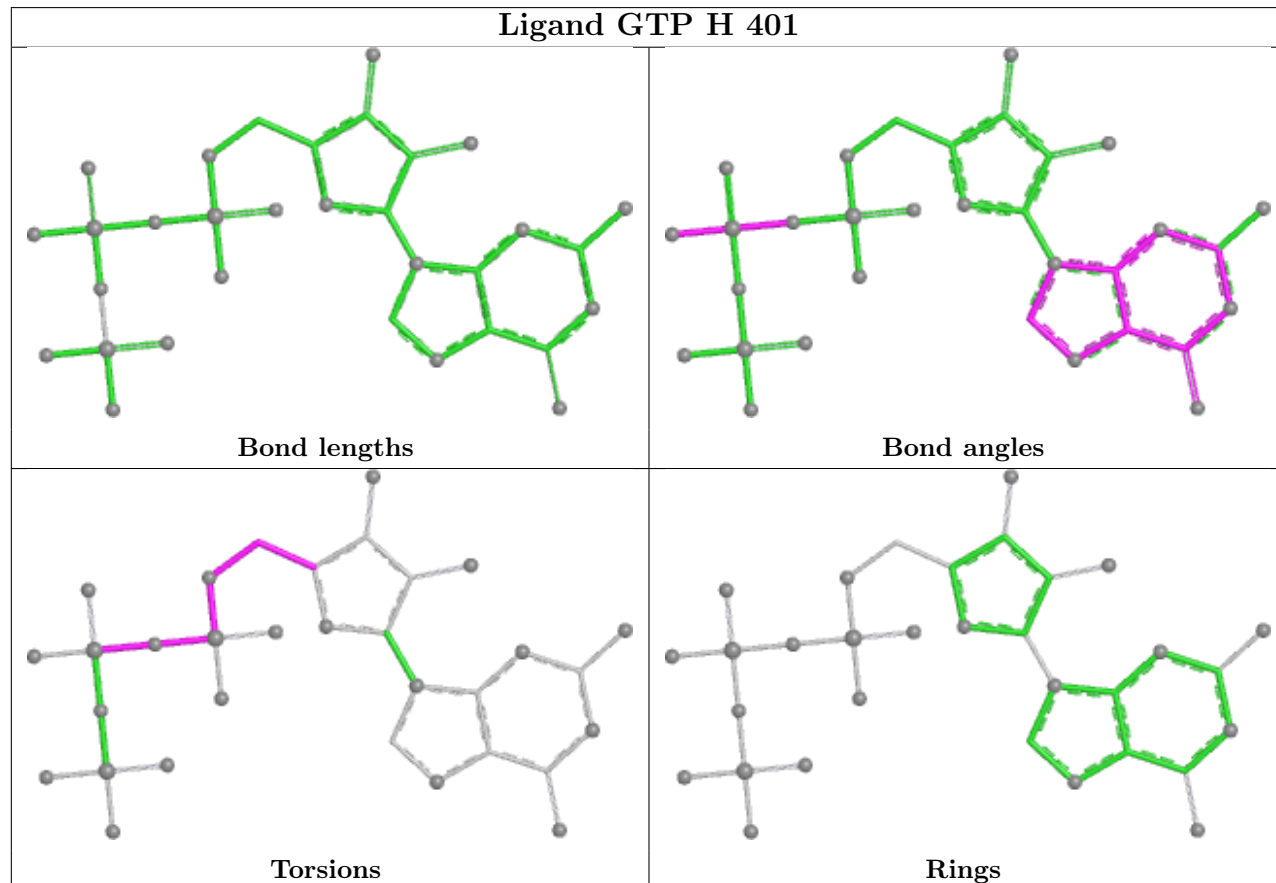
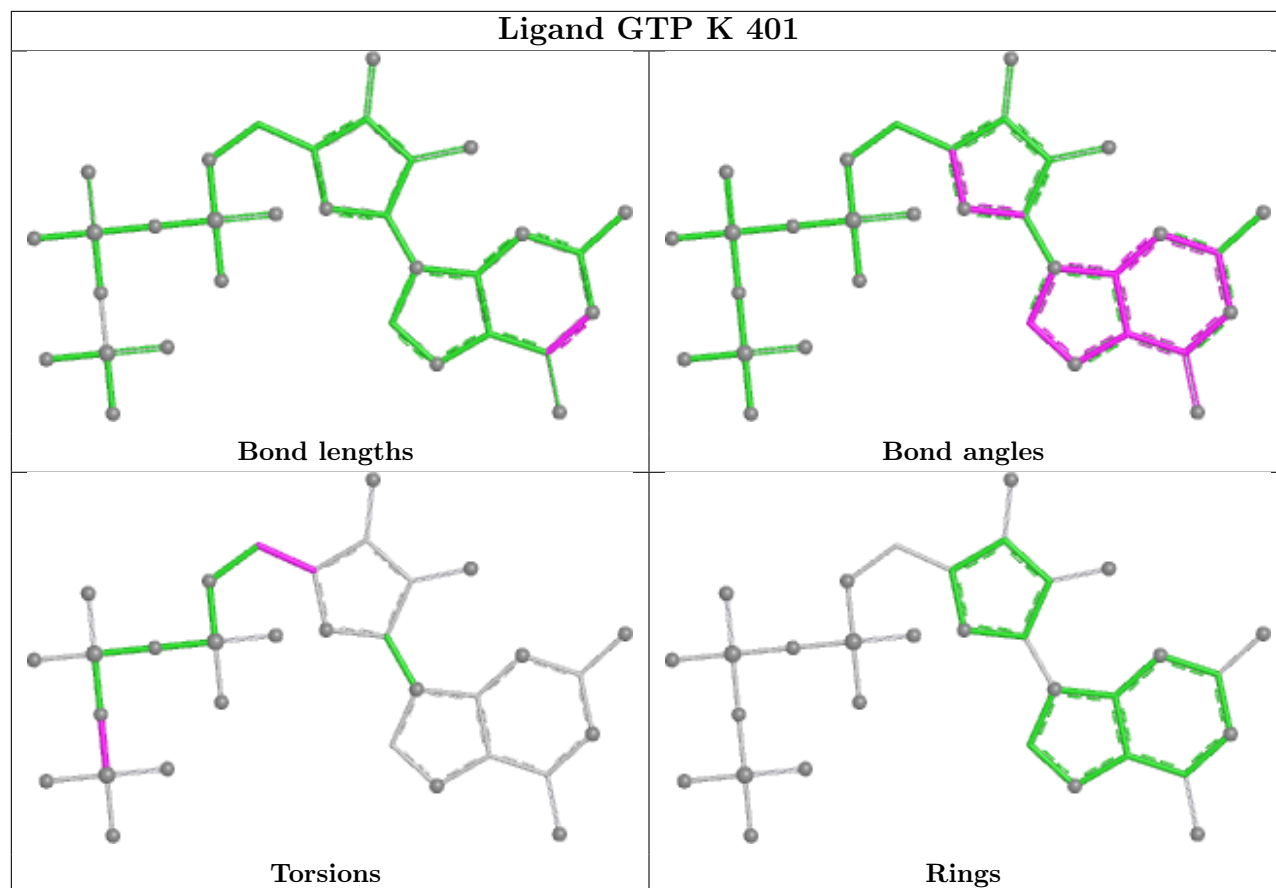
Mol	Chain	Res	Type	Atoms
4	B	501	GTP	C3'-C4'-C5'-O5'
4	I	401	GTP	O4'-C4'-C5'-O5'
4	I	401	GTP	C3'-C4'-C5'-O5'
3	C	501	GDD	C3'-C4'-C5'-O5'
3	A	501	GDD	C41-C51-C61-O6A
4	D	501	GTP	C3'-C4'-C5'-O5'
4	D	501	GTP	O4'-C4'-C5'-O5'
3	C	501	GDD	O51-C51-C61-O6A
3	A	501	GDD	O51-C51-C61-O6A
4	F	401	GTP	C3'-C4'-C5'-O5'
4	K	401	GTP	C3'-C4'-C5'-O5'
4	H	401	GTP	C4'-C5'-O5'-PA
3	A	501	GDD	PB-O3A-PA-O5'
4	H	401	GTP	PA-O3A-PB-O1B
4	E	401	GTP	O4'-C4'-C5'-O5'
3	C	501	GDD	C5'-O5'-PA-O1A
3	C	501	GDD	C5'-O5'-PA-O3A
4	J	401	GTP	C4'-C5'-O5'-PA
4	L	401	GTP	PB-O3B-PG-O1G
3	C	501	GDD	PA-O3A-PB-O2B
4	H	401	GTP	PB-O3A-PA-O1A
3	C	501	GDD	O51-C11-O1B-PB
4	D	501	GTP	PB-O3B-PG-O1G
4	F	401	GTP	PB-O3B-PG-O1G
4	K	401	GTP	PB-O3B-PG-O1G
4	J	401	GTP	PB-O3A-PA-O1A
4	G	401	GTP	PB-O3B-PG-O1G
4	B	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O2G
4	D	501	GTP	PB-O3B-PG-O3G
4	F	401	GTP	PB-O3B-PG-O2G
4	F	401	GTP	PB-O3B-PG-O3G
4	G	401	GTP	PB-O3B-PG-O2G
4	K	401	GTP	PB-O3B-PG-O2G
4	K	401	GTP	PB-O3B-PG-O3G
3	C	501	GDD	PA-O3A-PB-O3B
4	D	501	GTP	PA-O3A-PB-O1B
4	I	401	GTP	PG-O3B-PB-O2B
4	H	401	GTP	PA-O3A-PB-O2B

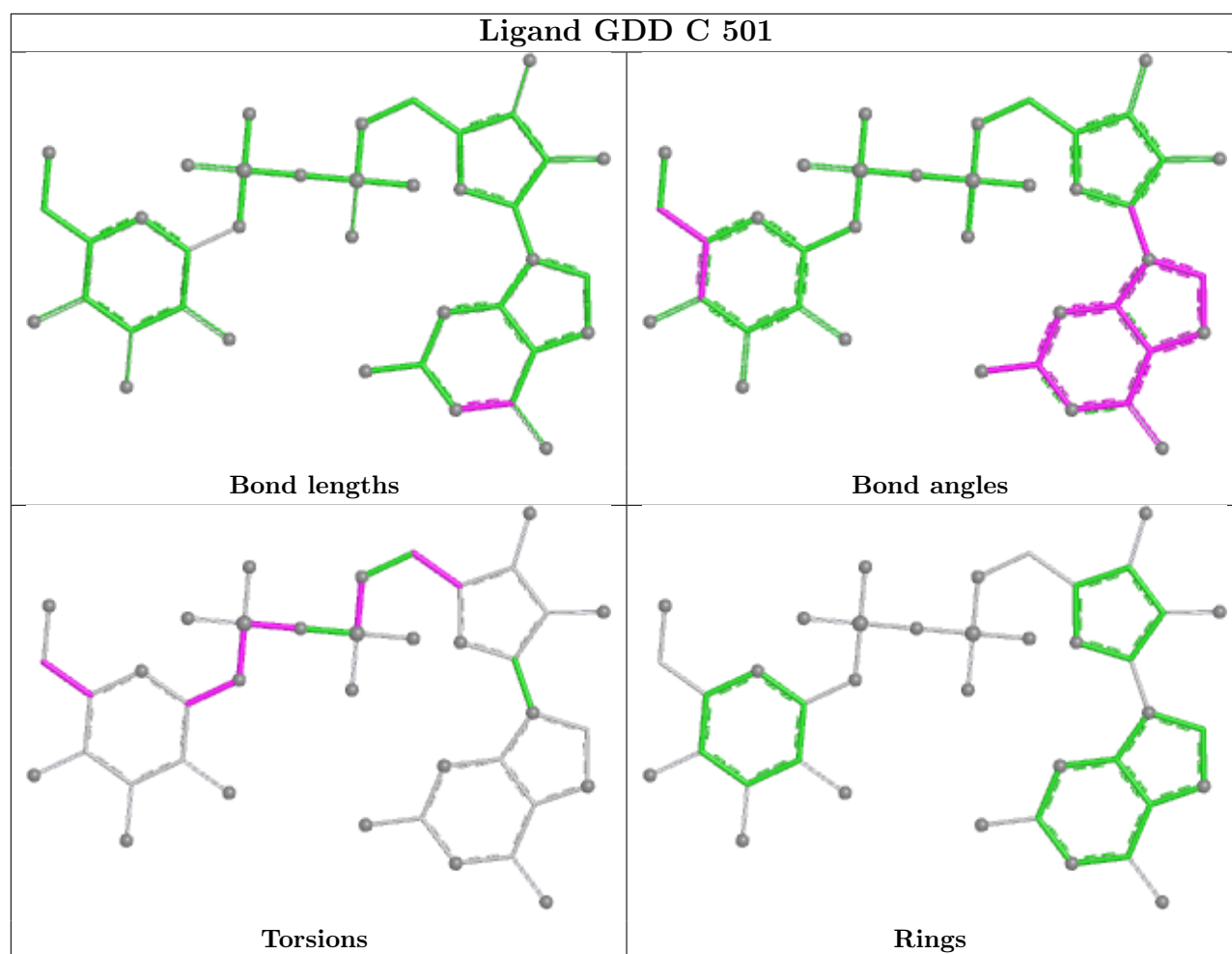
There are no ring outliers.

9 monomers are involved in 35 short contacts:

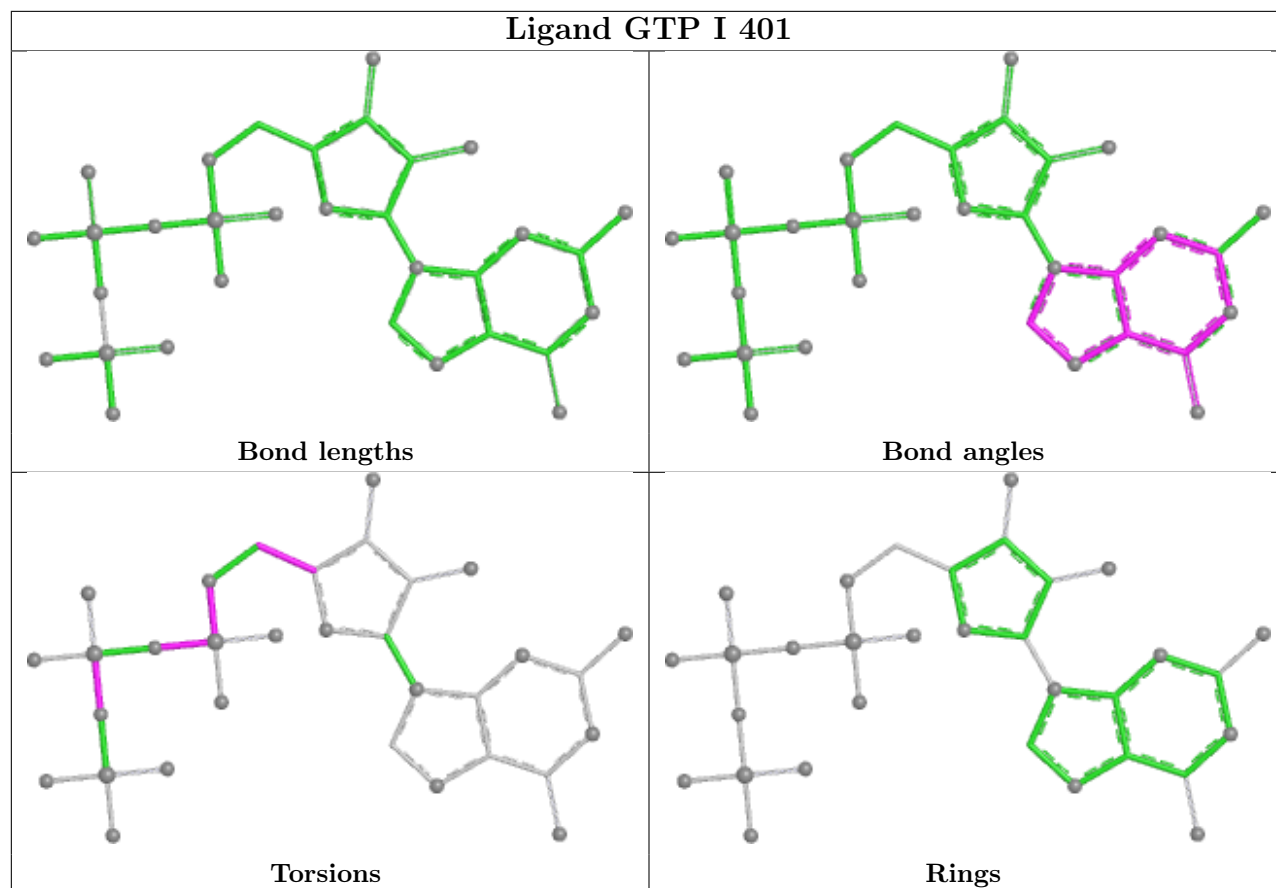
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	401	GTP	1	0
4	I	401	GTP	5	0
4	D	501	GTP	1	0
4	E	401	GTP	1	0
4	J	401	GTP	2	0
4	L	401	GTP	5	0
4	G	401	GTP	3	0
3	A	501	GDD	1	0
4	F	401	GTP	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

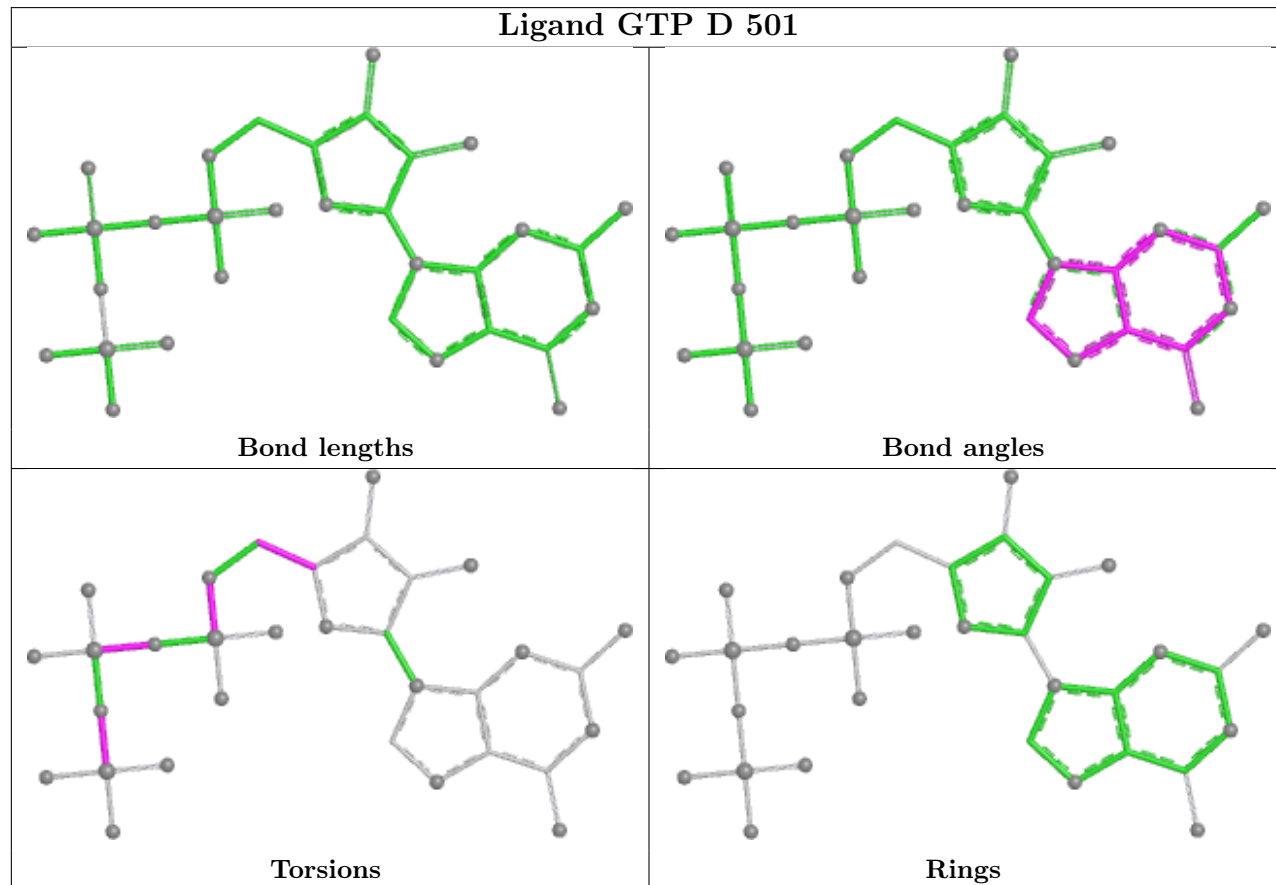




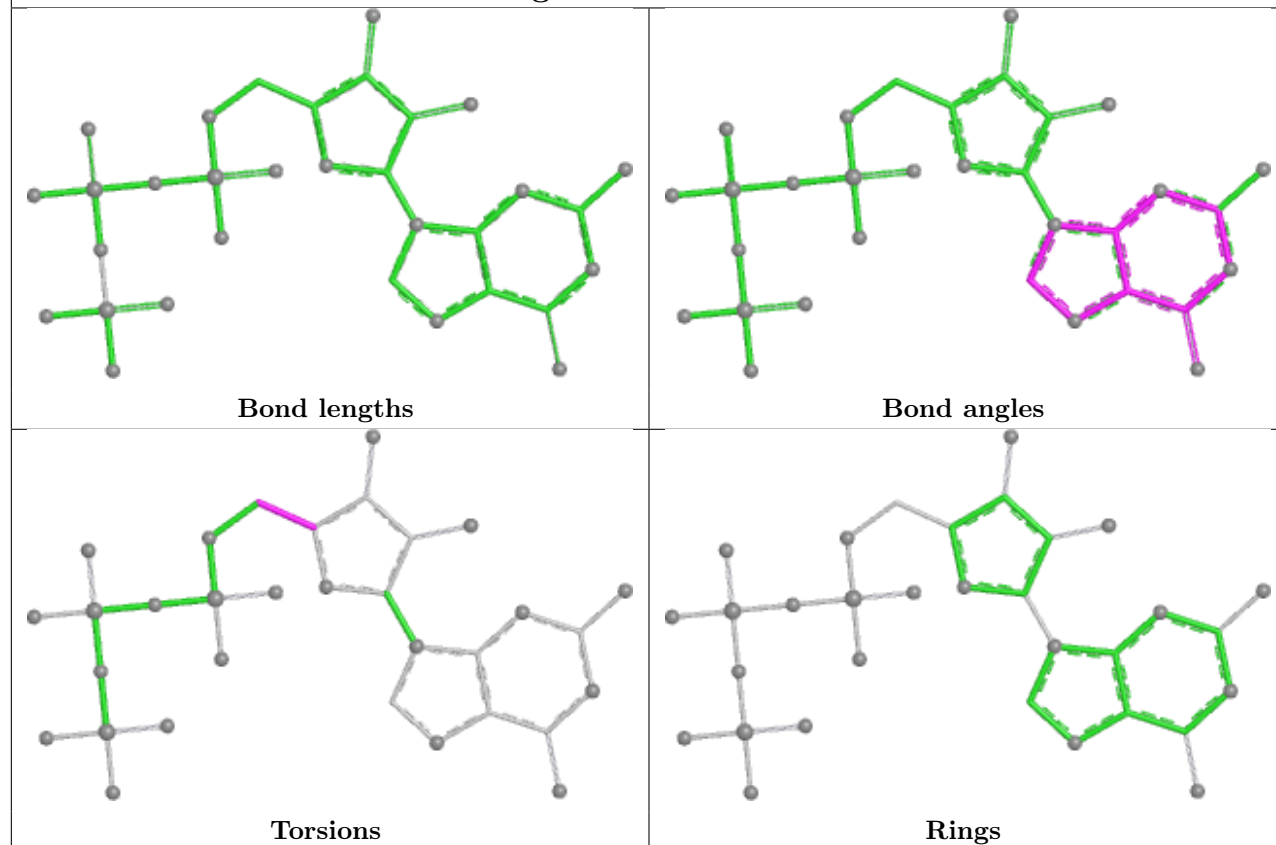
Ligand GTP I 401



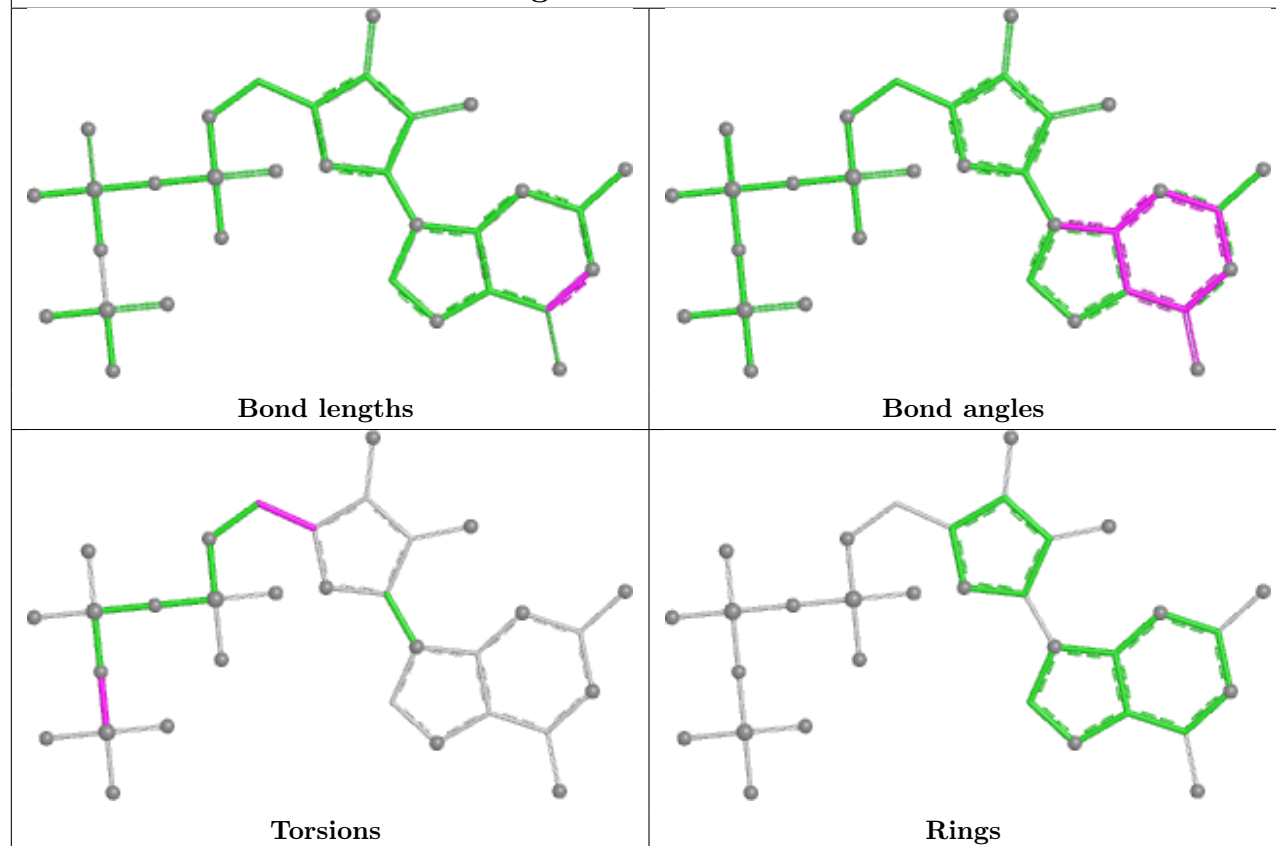
Ligand GTP D 501



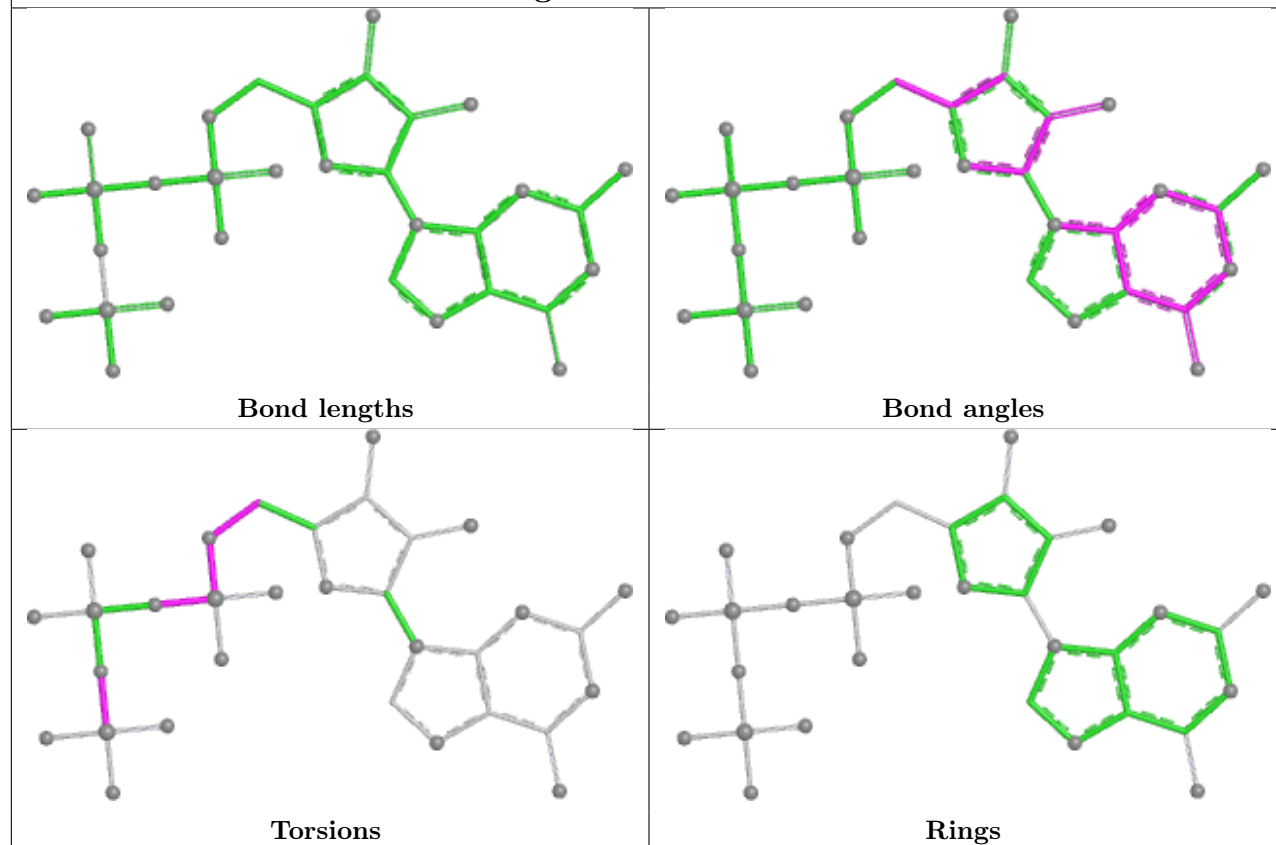
Ligand GTP E 401



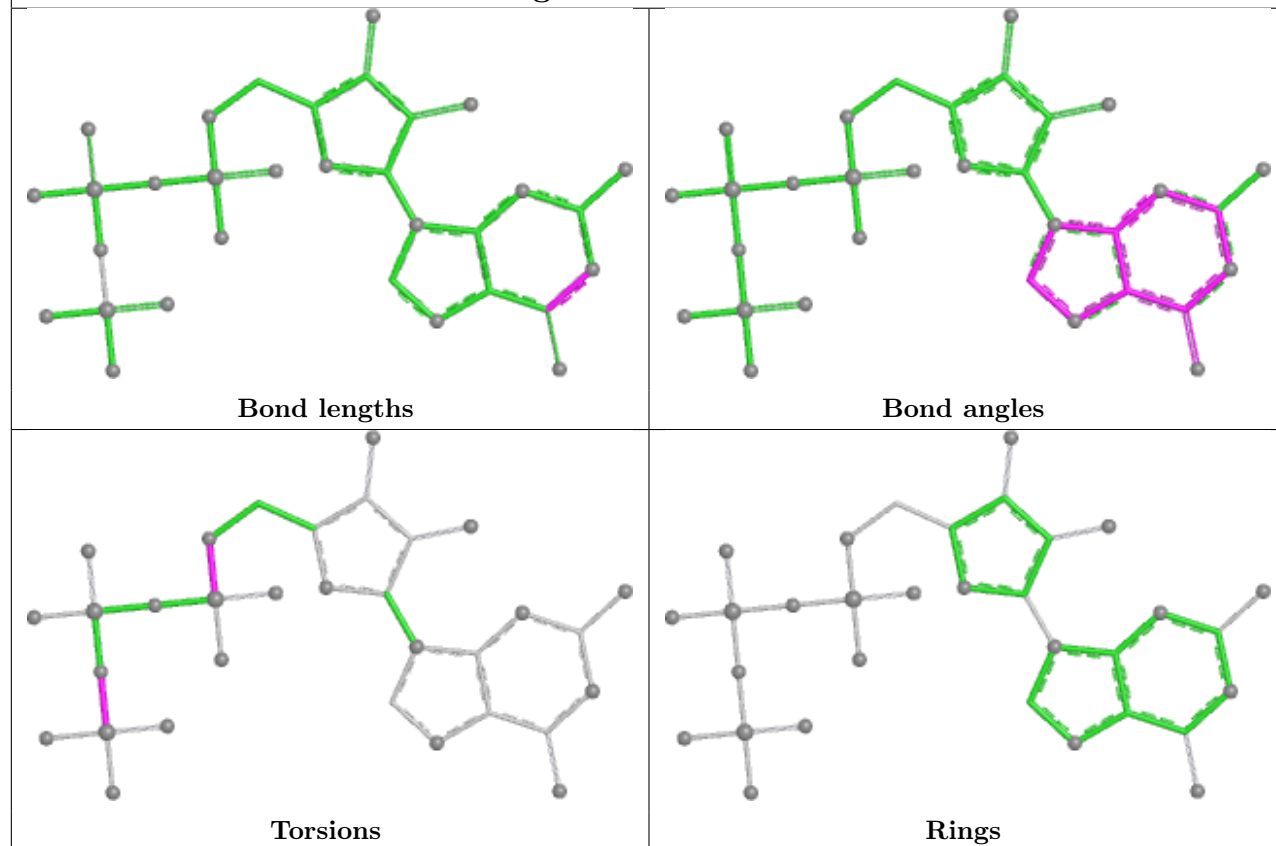
Ligand GTP B 501

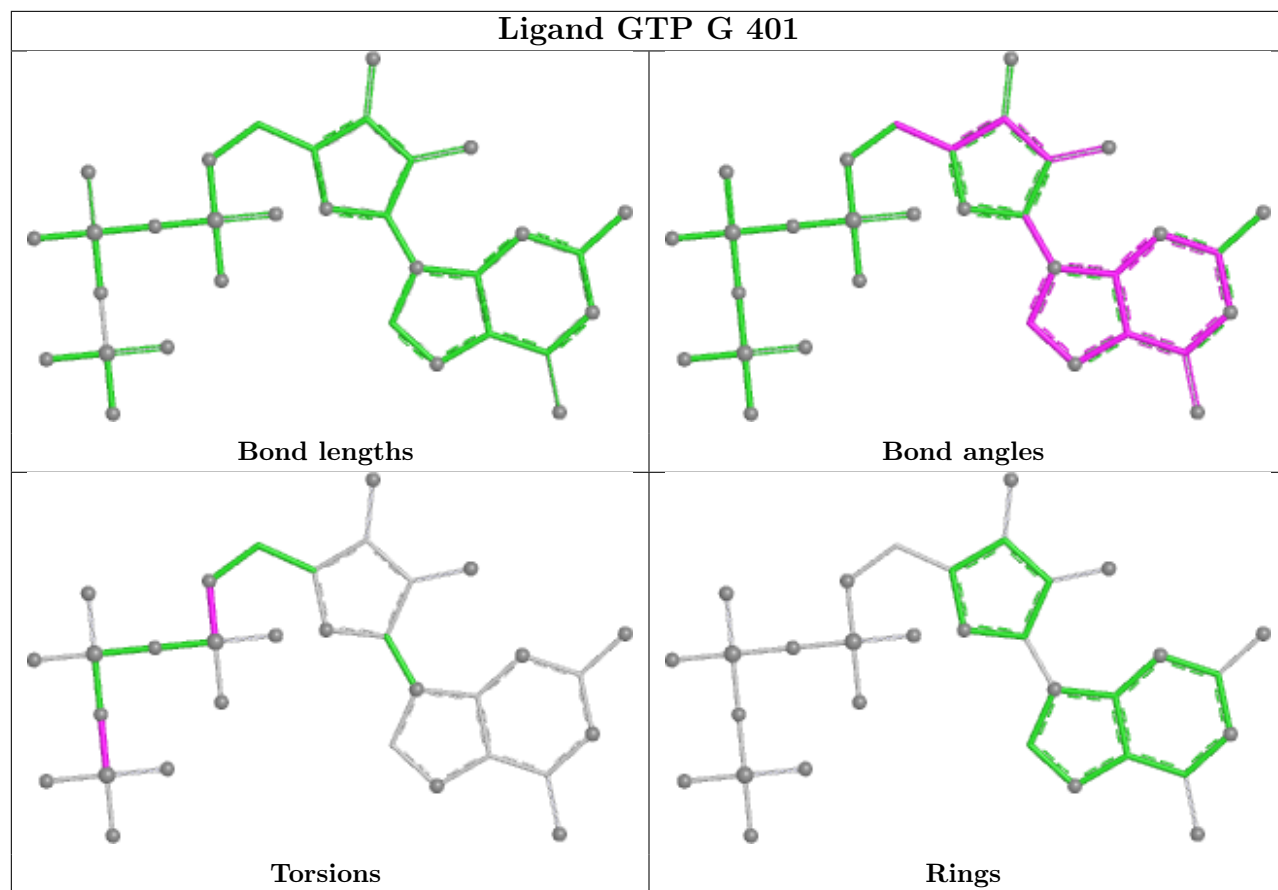


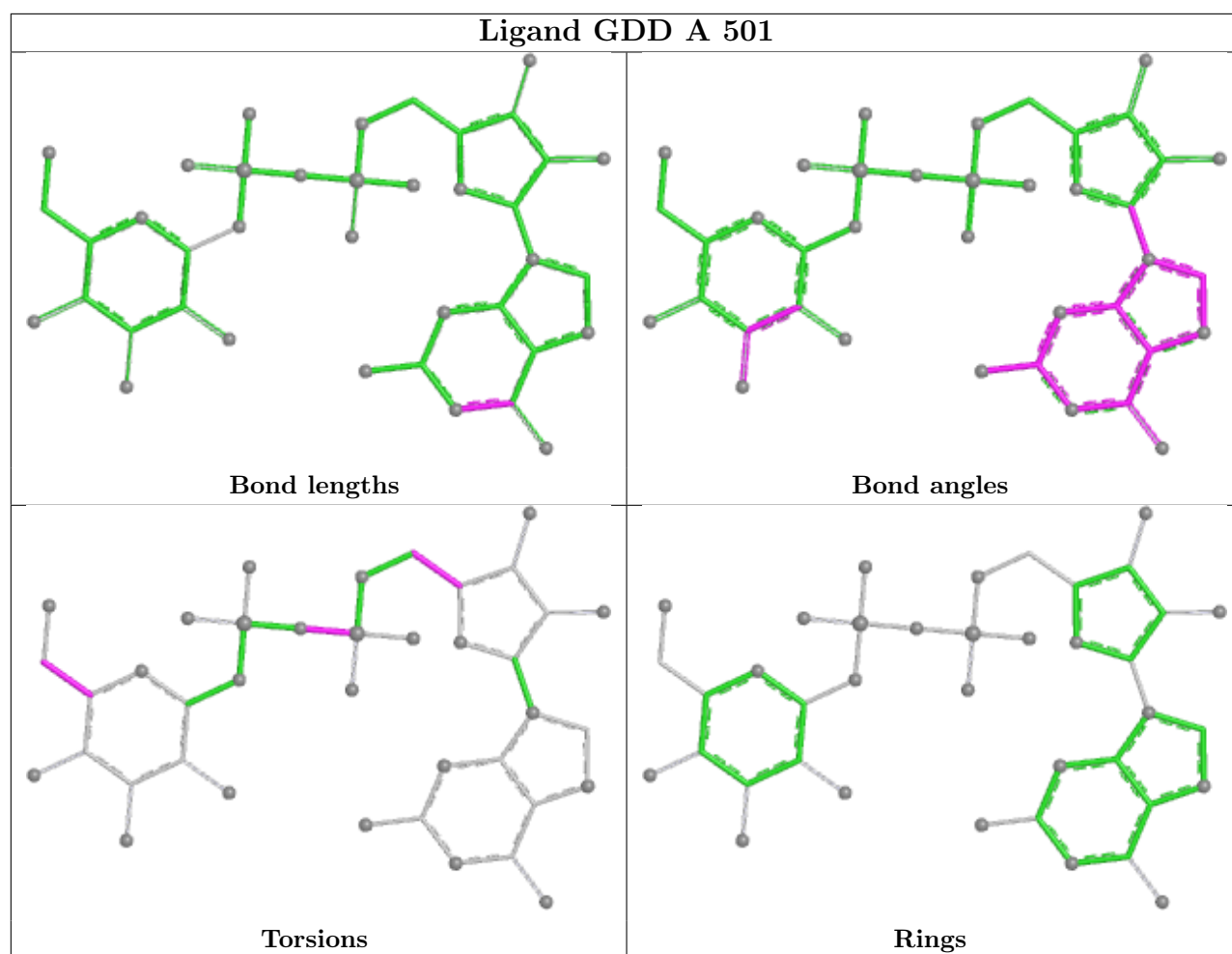
Ligand GTP J 401

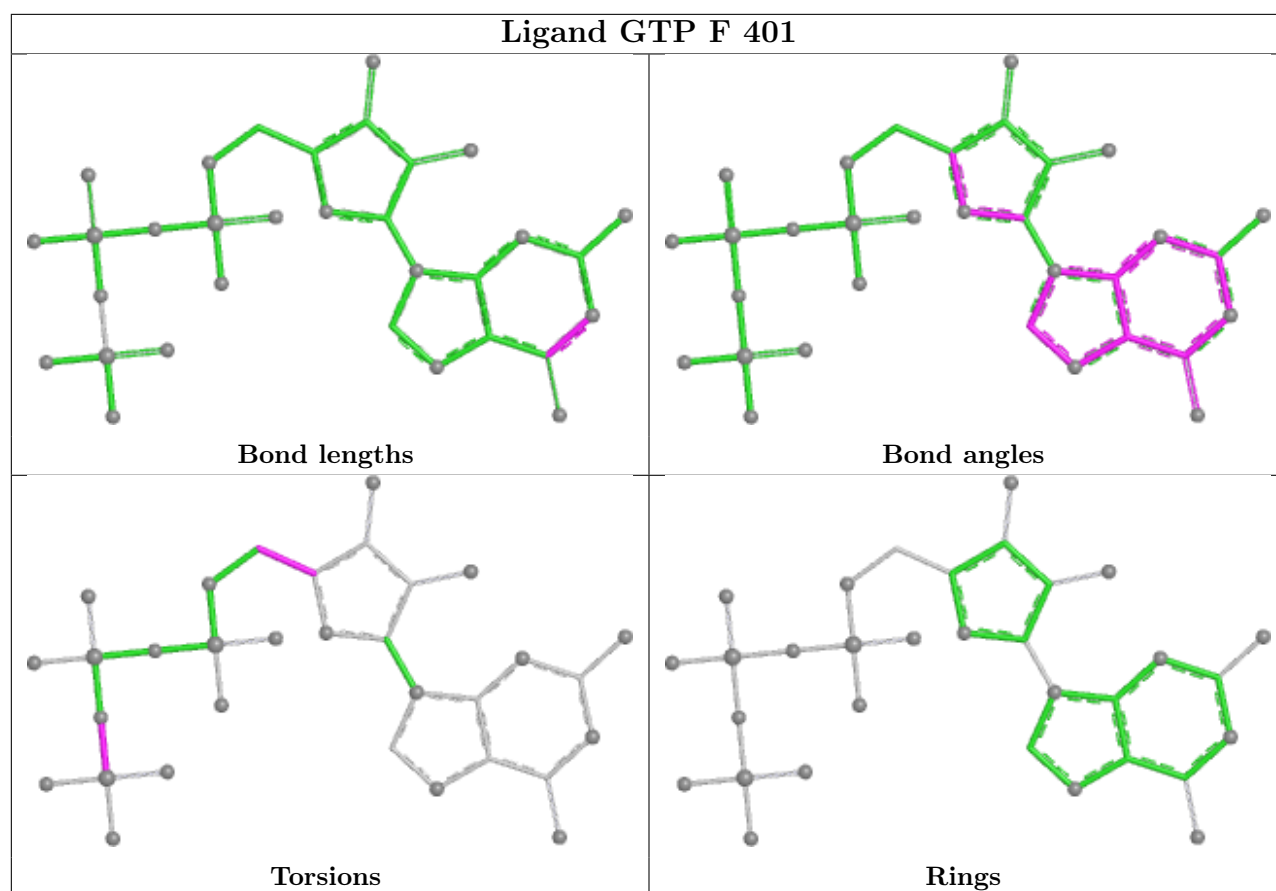


Ligand GTP L 401









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.

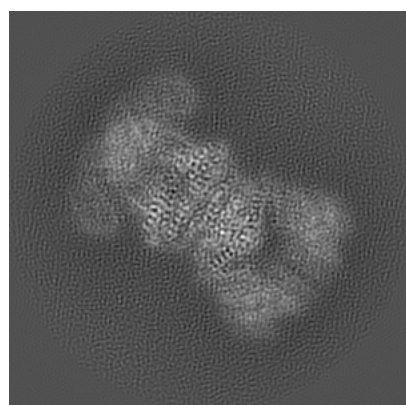
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30600. These allow visual inspection of the internal detail of the map and identification of artifacts.

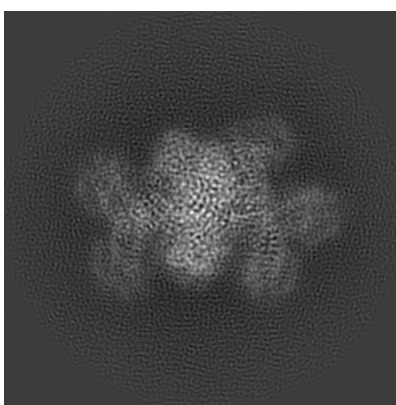
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

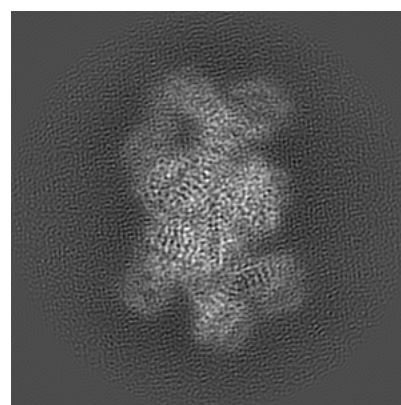
6.1.1 Primary map



X



Y

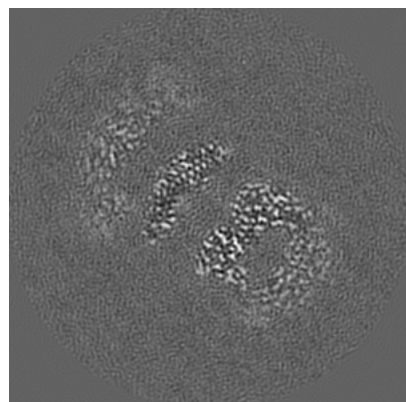


Z

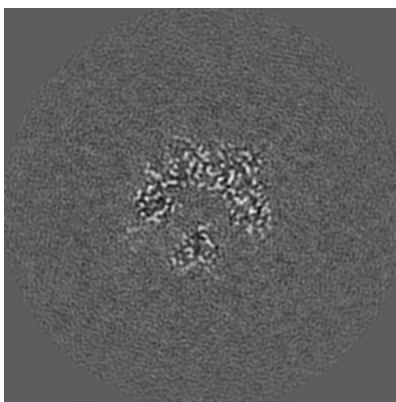
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

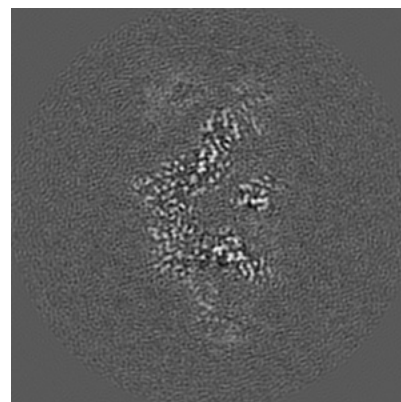
6.2.1 Primary map



X Index: 120



Y Index: 120

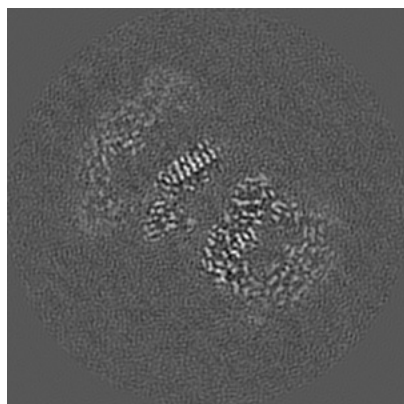


Z Index: 120

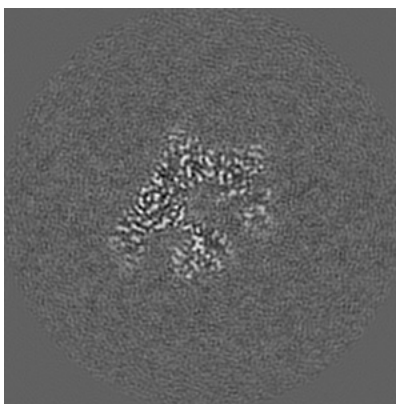
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

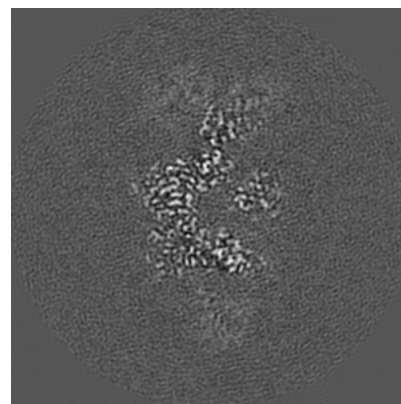
6.3.1 Primary map



X Index: 117



Y Index: 127

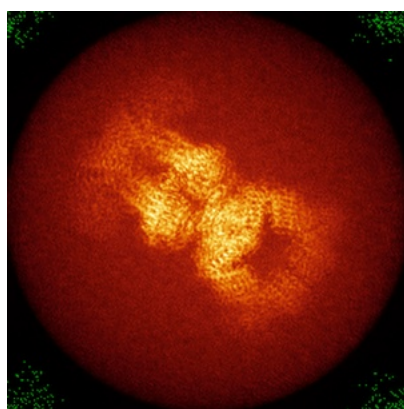


Z Index: 116

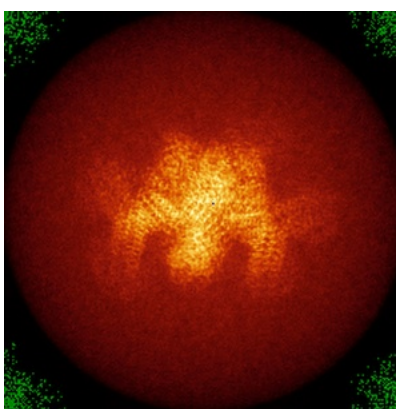
The images above show the largest variance slices of the map in three orthogonal directions.

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

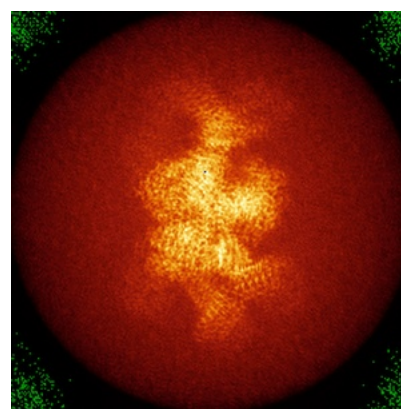
6.4.1 Primary map



X



Y

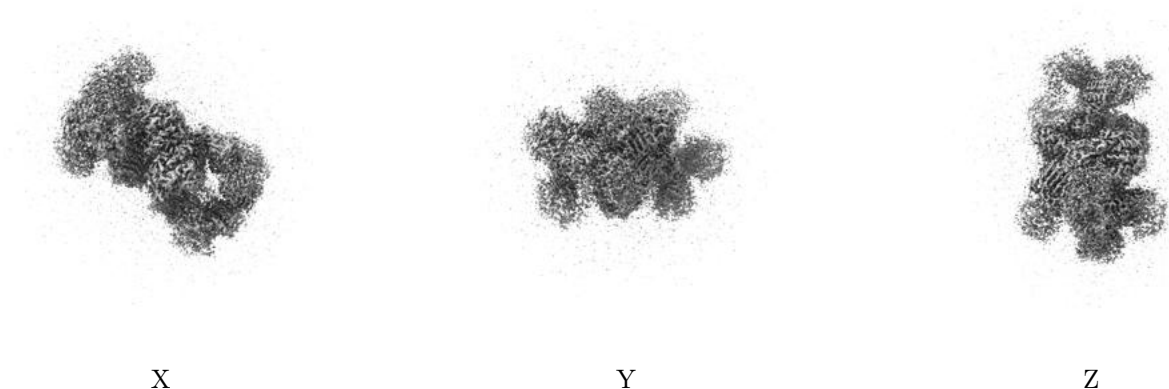


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0389. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

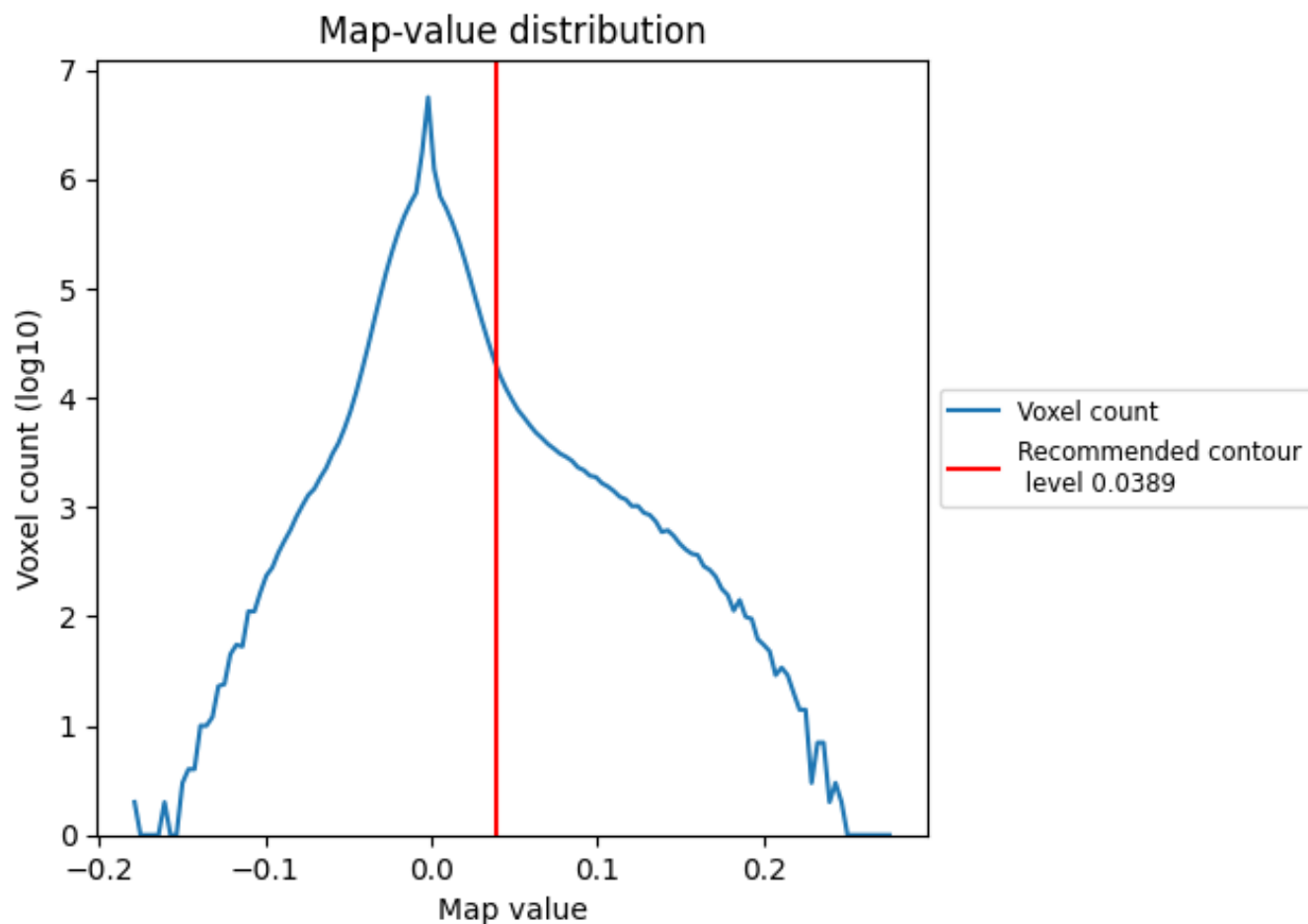
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

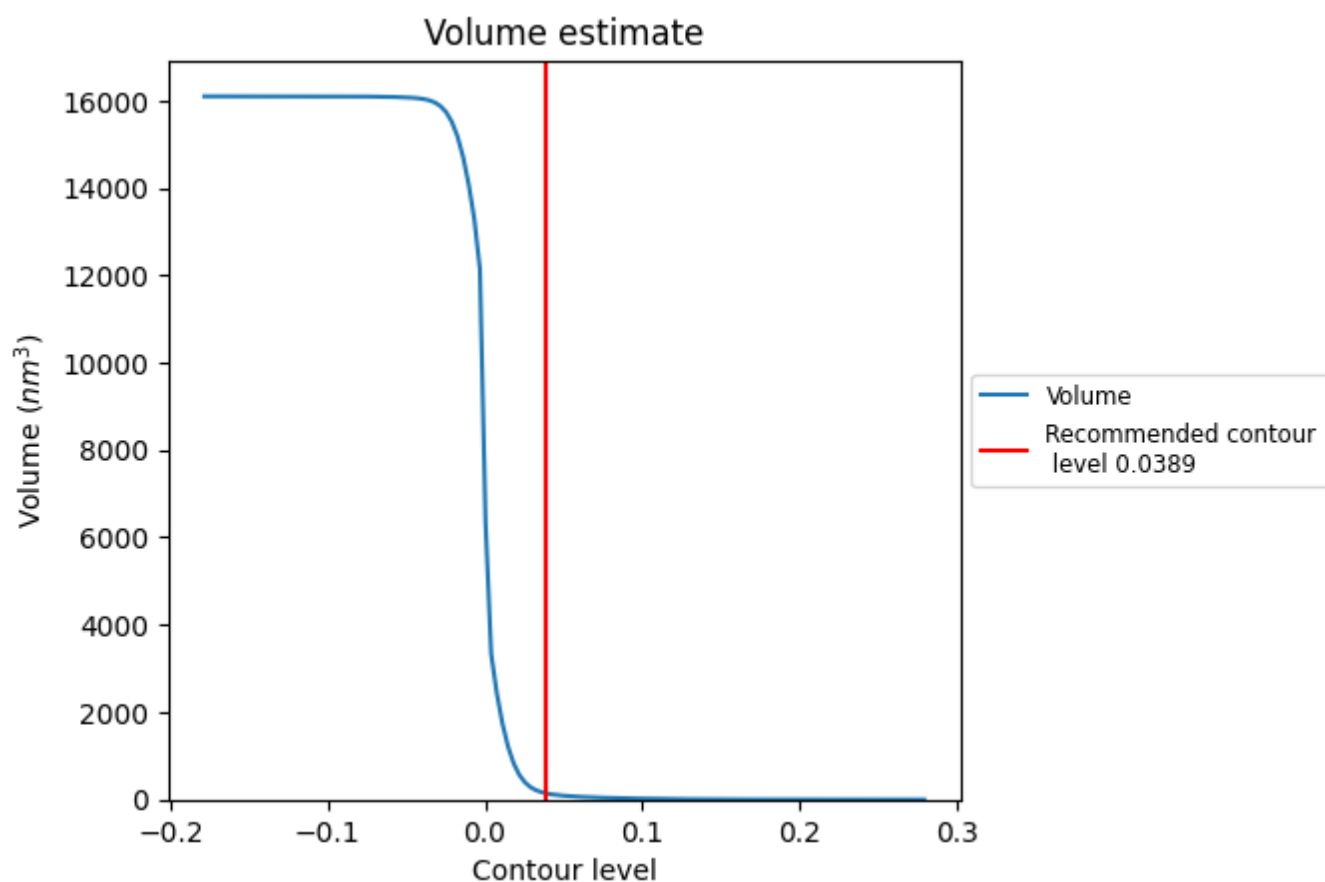
This section contains the results of statistical analysis of the map.

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.

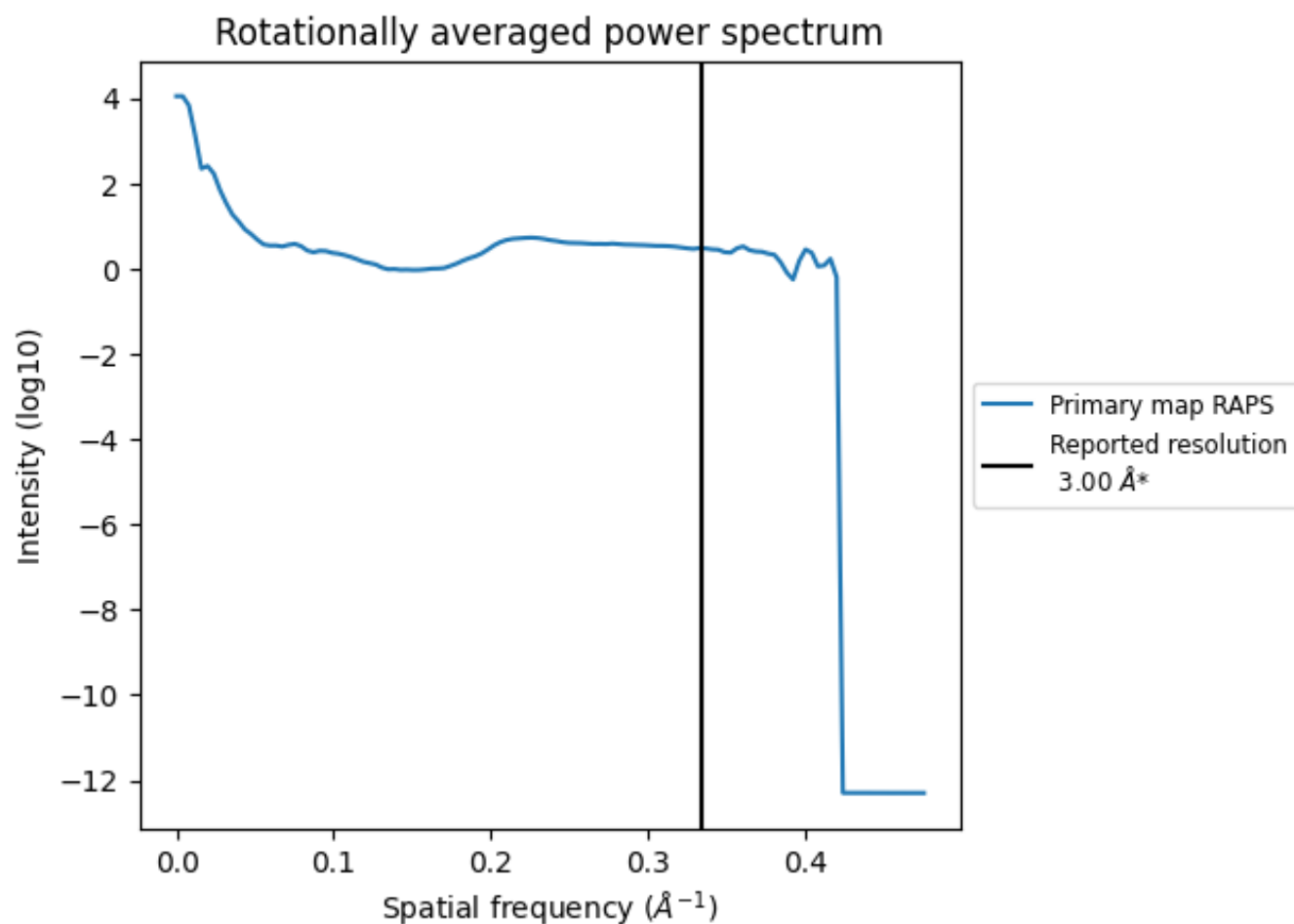
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 144 nm³; this corresponds to an approximate mass of 130 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 0.333 Å⁻¹

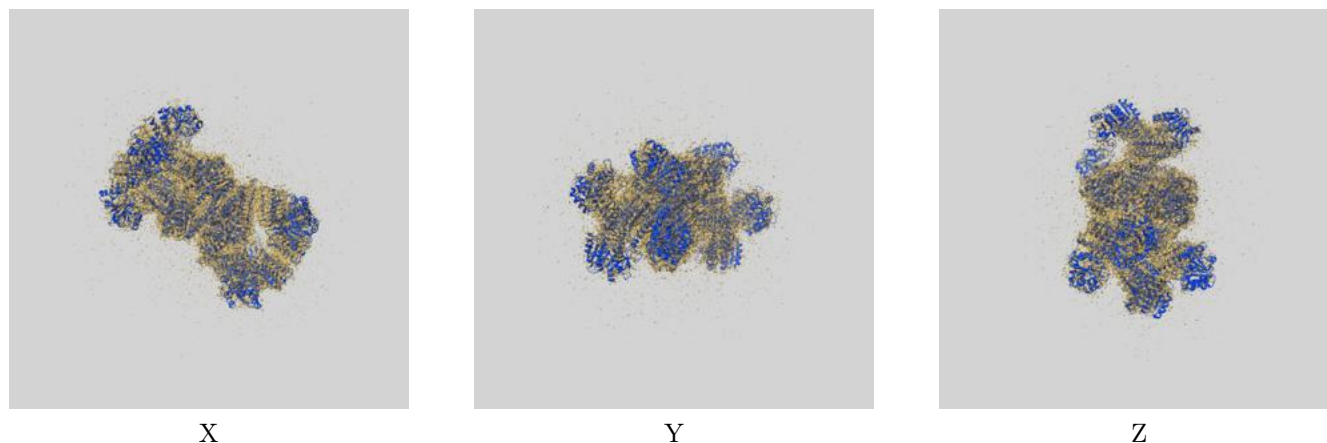
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

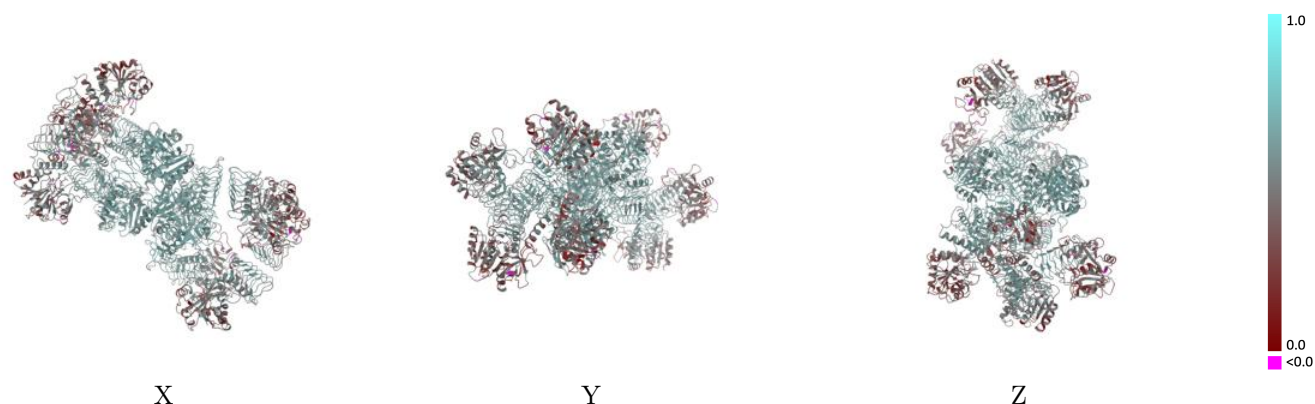
This section contains information regarding the fit between EMDB map EMD-30600 and PDB model 7D73. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



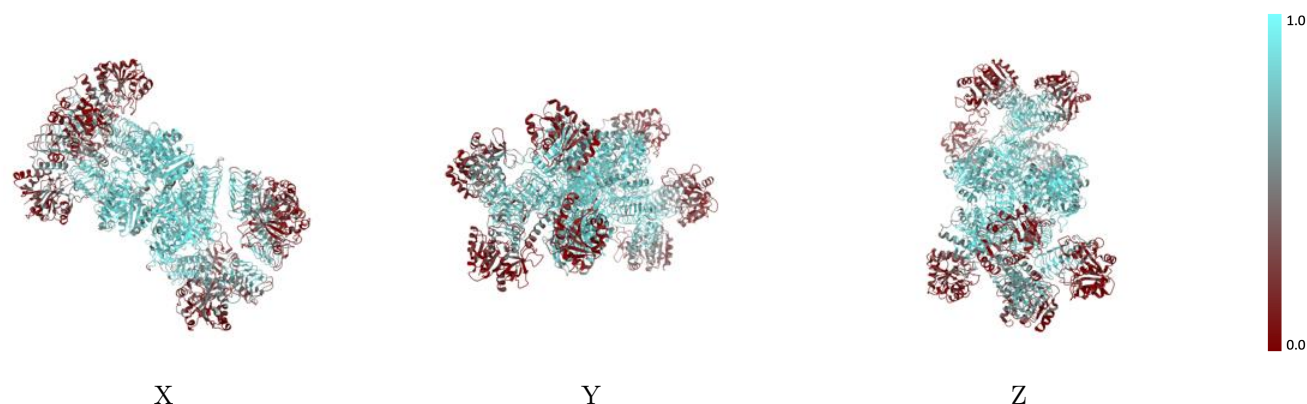
The images above show the 3D surface view of the map at the recommended contour level 0.0389 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



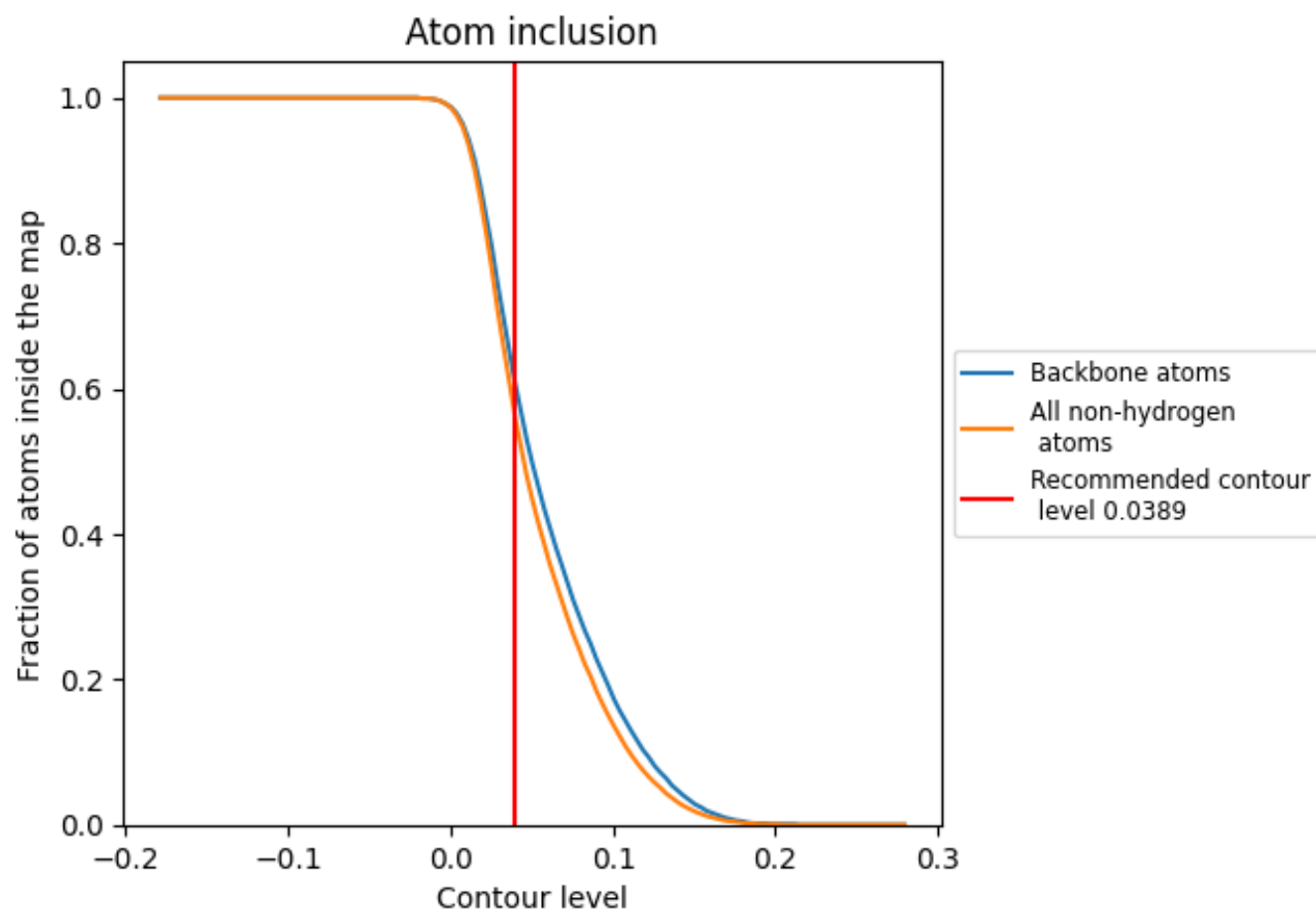
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0389).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 57% 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 (0.0389) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5720	0.5150
A	0.8620	0.6130
B	0.8510	0.6100
C	0.8400	0.6100
D	0.8430	0.6100
E	0.3490	0.4360
F	0.4650	0.4670
G	0.4350	0.4770
H	0.4230	0.4620
I	0.3870	0.4490
J	0.4250	0.4810
K	0.4630	0.4650
L	0.3640	0.4490

1.0

0.0

<0.0