



Full wwPDB EM Validation Report ⓘ

Apr 15, 2026 – 10:26 AM UTC

PDB ID : 7D72 / pdb_00007d72
EMDB ID : EMD-30599
Title : Cryo-EM structures of human GMPPA/GMPPB complex bound to GDP-Mannose
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 : 3.40 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

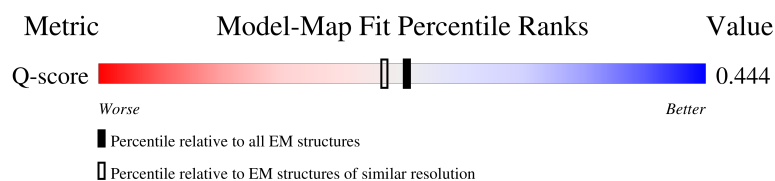
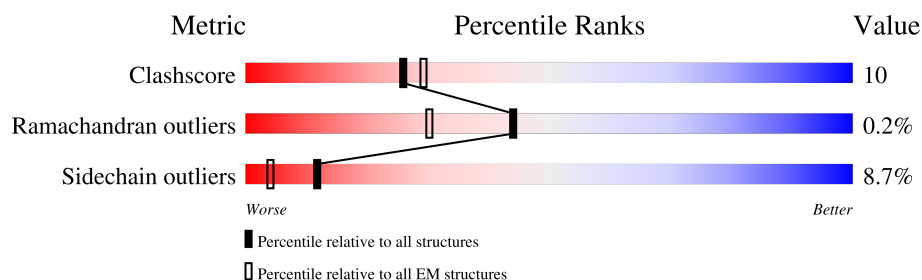
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	E	360	36% 68% 28% ..
1	F	360	28% 75% 22% .
1	G	360	19% 73% 23% .
1	H	360	37% 71% 24% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	360	47% 71% 24%
1	J	360	27% 66% 32%
1	K	360	37% 70% 26%
1	L	360	50% 71% 27%
2	A	420	76% 19%
2	B	420	80% 15%
2	C	420	81% 14%
2	D	420	79% 17%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 35458 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.

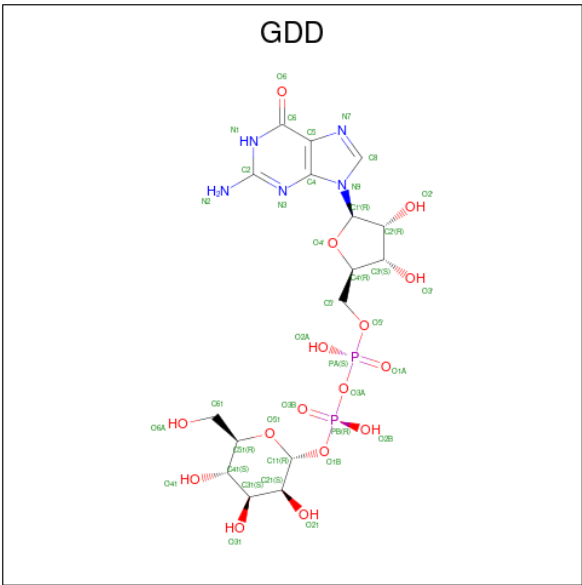
- Molecule 1 is a protein called Mannose-1-phosphate guanyltrtransferase beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	360	Total	C	N	O	S	0	0
			2787	1770	488	507	22		
1	I	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
1	E	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
1	F	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
1	G	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
1	H	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
1	J	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
1	L	360	Total	C	N	O	S	0	0
			2787	1770	488	507	22		

- Molecule 2 is a protein called Mannose-1-phosphate guanyltrtransferase alpha.

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

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (CCD ID: GDD) (formula: $C_{16}H_{25}N_5O_{16}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	G	1	Total 1	Mg 1	0

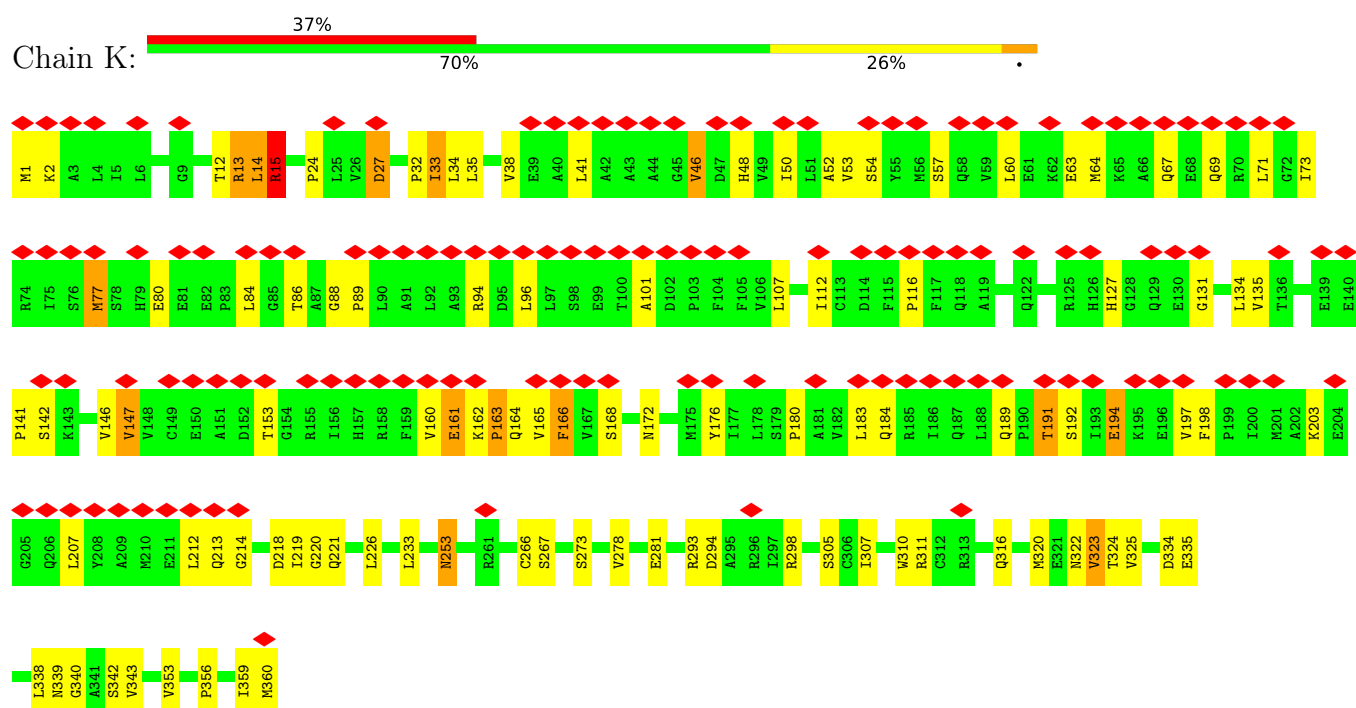
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	E	2	Total 2	O 2	0
5	F	2	Total 2	O 2	0
5	G	2	Total 2	O 2	0

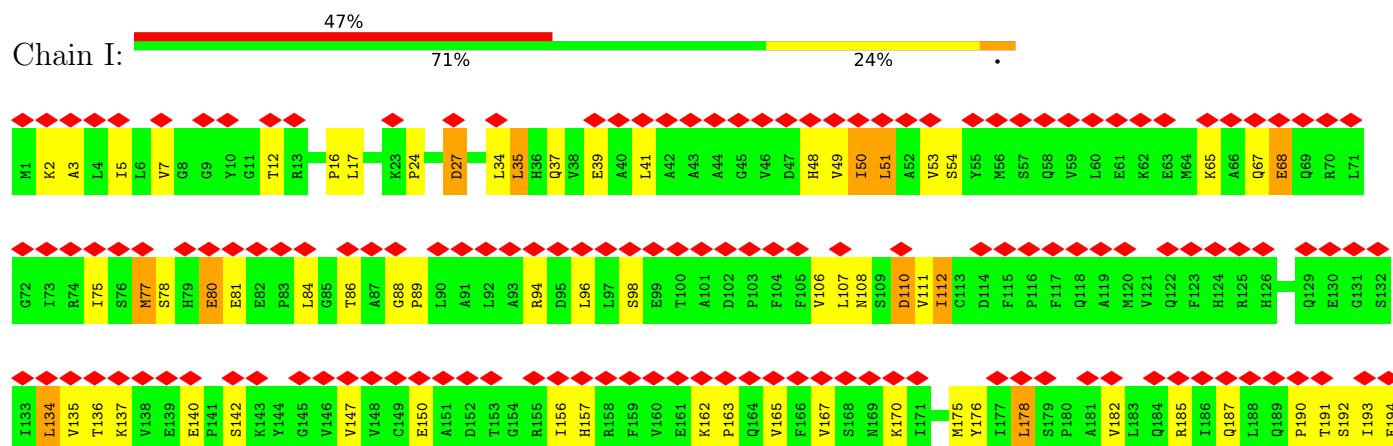
3 Residue-property plots

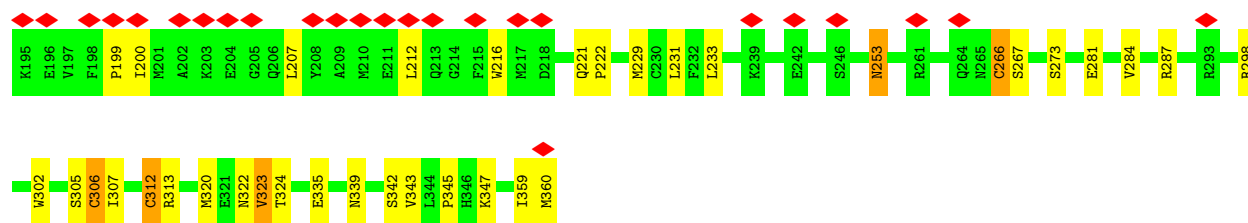
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

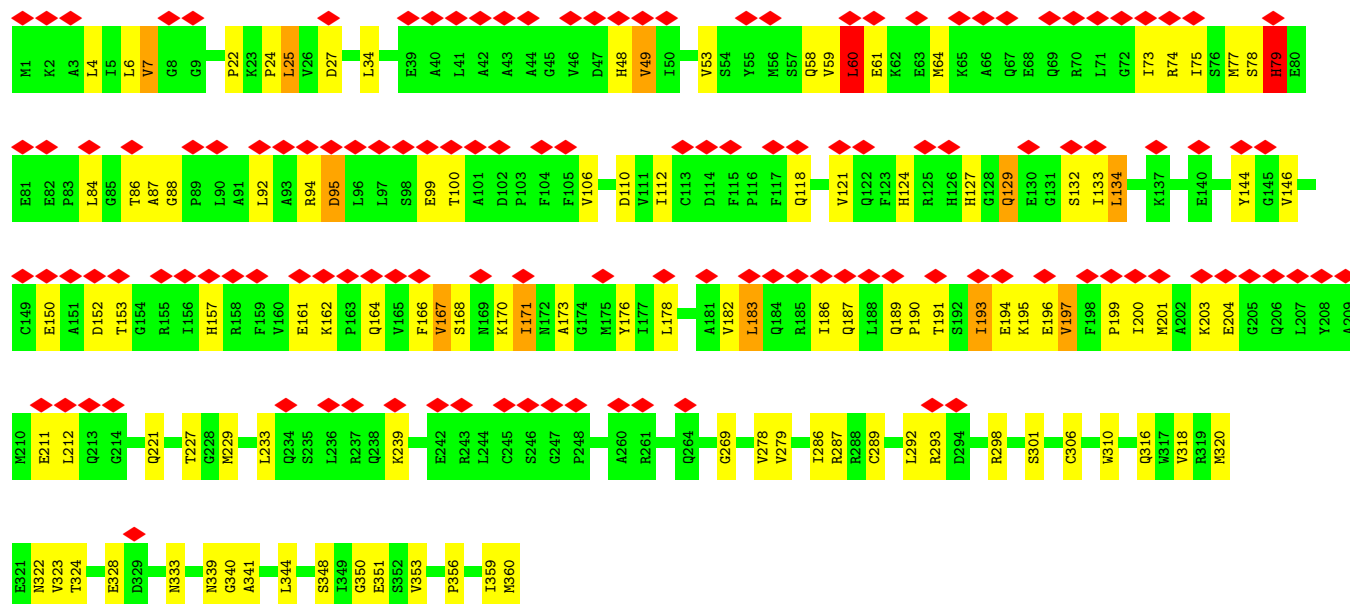


- Molecule 1: Mannose-1-phosphate guanylttransferase beta

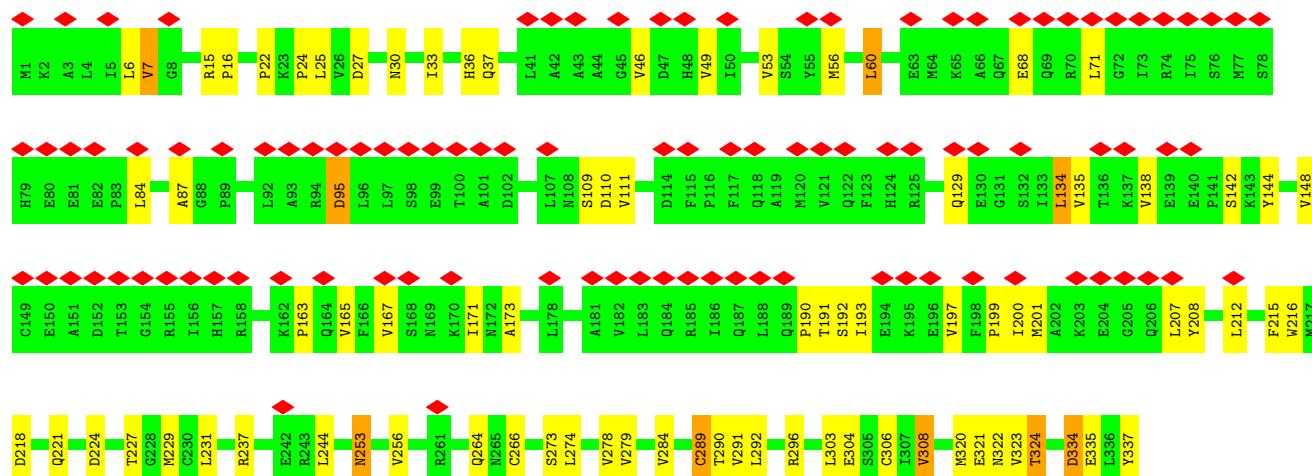
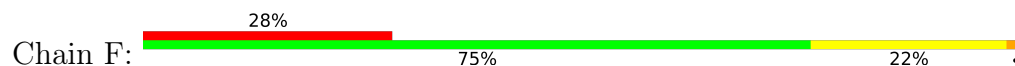


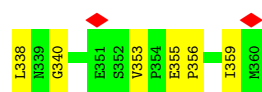


• Molecule 1: Mannose-1-phosphate guanylttransferase beta

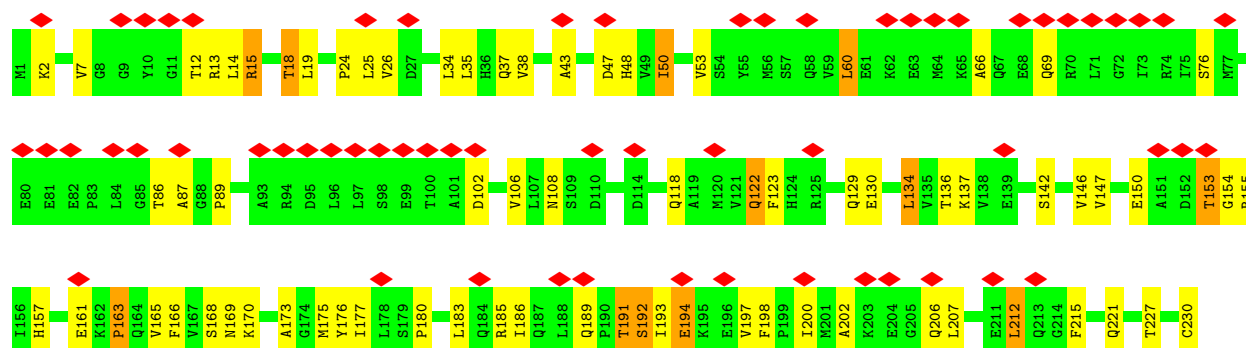
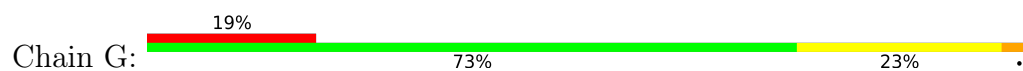


• Molecule 1: Mannose-1-phosphate guanylttransferase beta

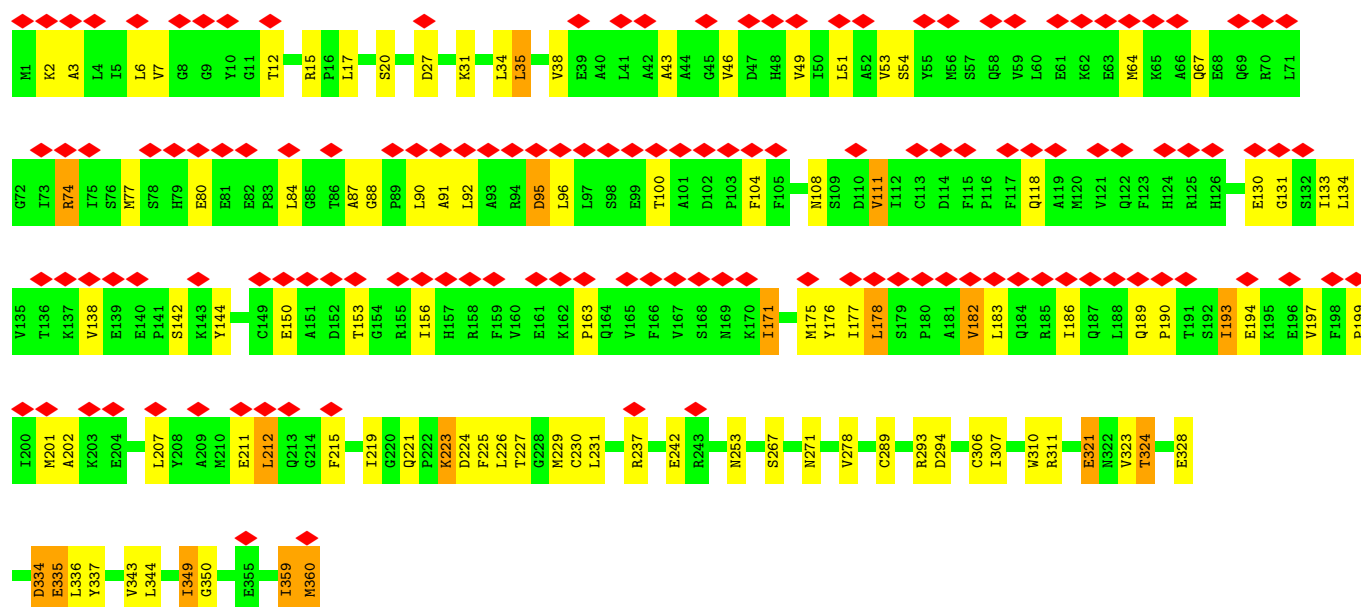




- Molecule 1: Mannose-1-phosphate guanyltrtransferase beta

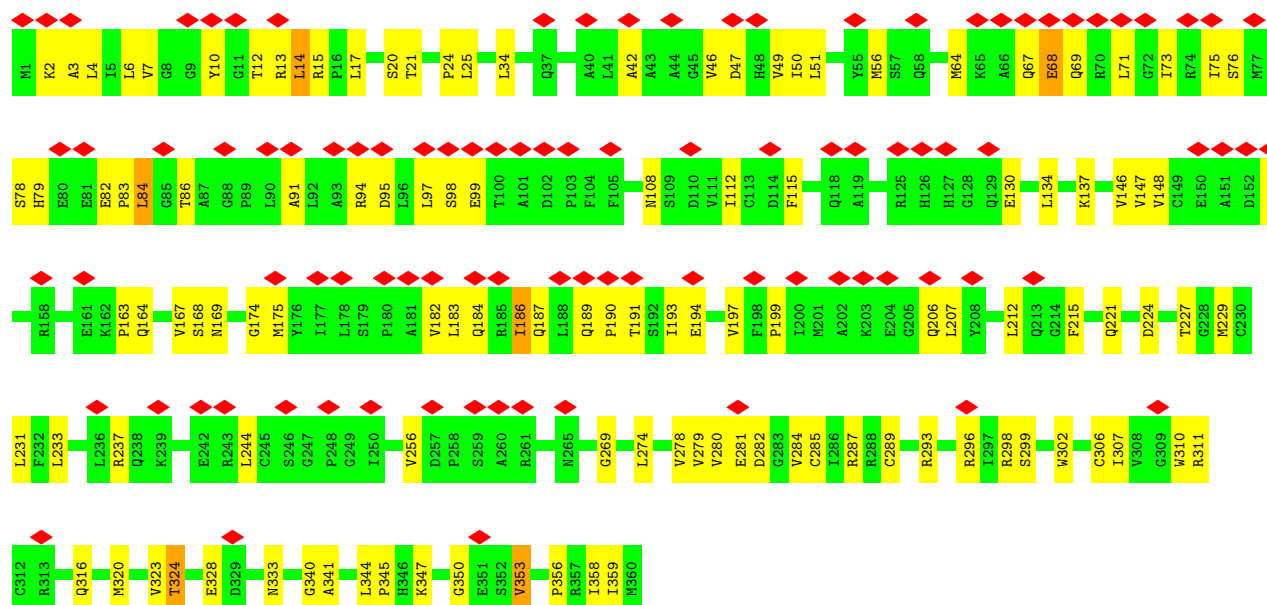


- Molecule 1: Mannose-1-phosphate guanyltrtransferase beta

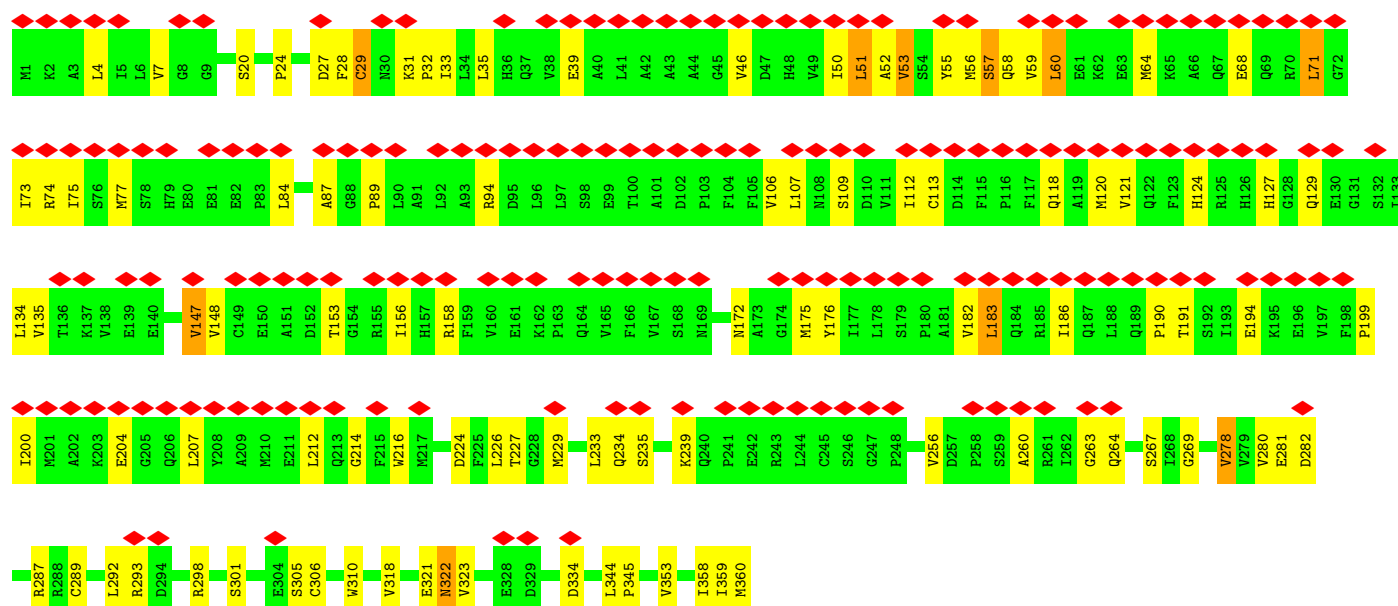


- Molecule 1: Mannose-1-phosphate guanyltrtransferase beta

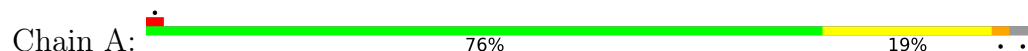


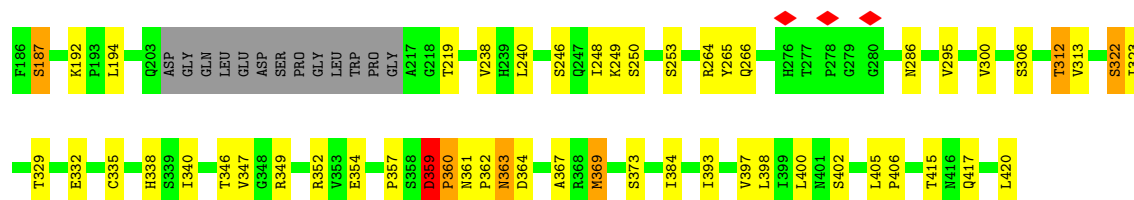


- Molecule 1: Mannose-1-phosphate guanylttransferase beta

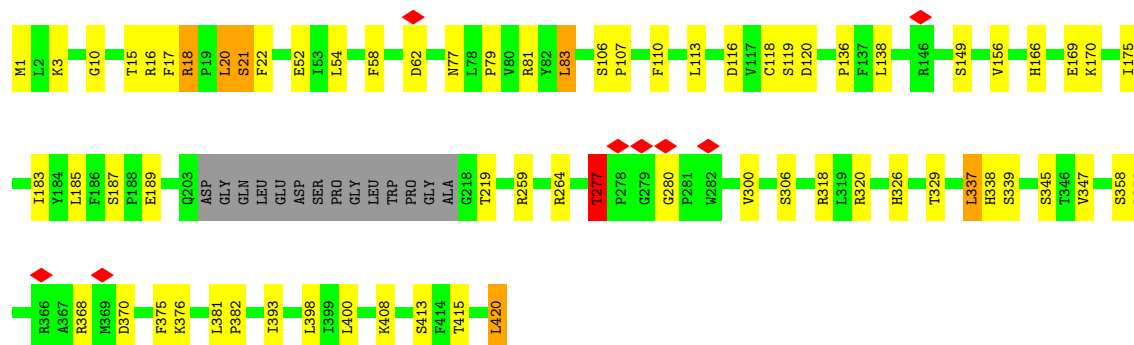
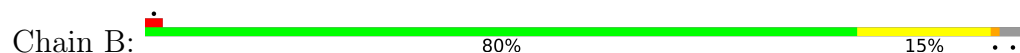


- Molecule 2: Mannose-1-phosphate guanylttransferase alpha

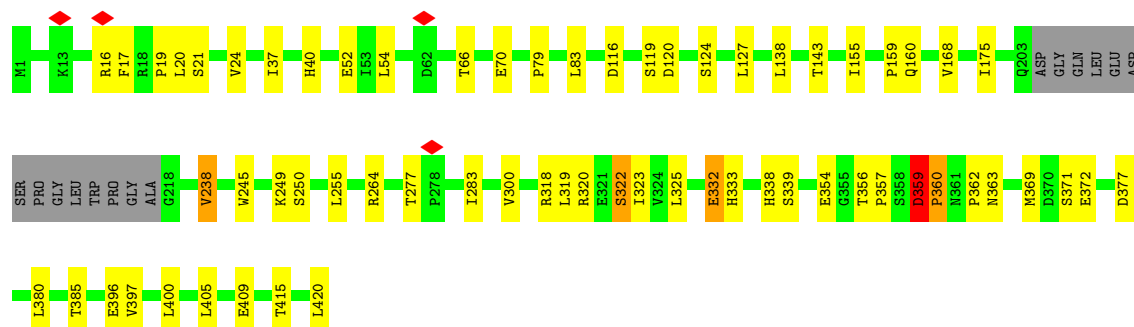
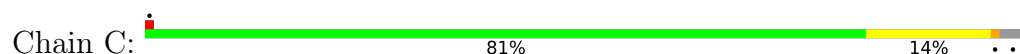




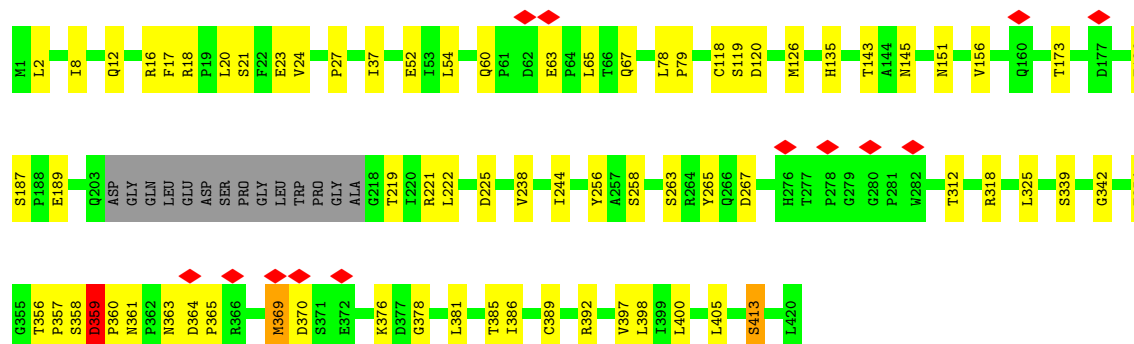
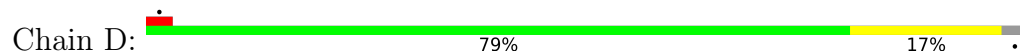
• Molecule 2: Mannose-1-phosphate guanyltransferase alpha



• Molecule 2: Mannose-1-phosphate guanyltransferase alpha



• Molecule 2: Mannose-1-phosphate guanyltransferase alpha



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57299	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	0.136	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	253.68001, 253.68001, 253.68001	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.057, 1.057, 1.057	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: GDD, MG

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	E	0.31	0/2844	0.72	5/3854 (0.1%)
1	F	0.33	0/2844	0.63	0/3854
1	G	0.30	0/2844	0.62	0/3854
1	H	0.34	0/2844	0.69	1/3854 (0.0%)
1	I	0.34	0/2844	0.72	3/3854 (0.1%)
1	J	0.30	0/2844	0.65	2/3854 (0.1%)
1	K	0.35	0/2842	0.74	7/3851 (0.2%)
1	L	0.30	0/2842	0.68	4/3851 (0.1%)
2	A	0.47	0/3253	0.60	2/4427 (0.0%)
2	B	0.44	0/3248	0.60	2/4420 (0.0%)
2	C	0.44	0/3248	0.61	2/4420 (0.0%)
2	D	0.42	0/3248	0.66	5/4420 (0.1%)
All	All	0.37	0/35745	0.66	33/48513 (0.1%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	57	SER	N-CA-C	7.86	119.85	111.28
2	D	18	ARG	N-CA-C	7.32	123.56	113.16
1	K	15	ARG	CA-C-N	-6.77	112.02	119.19
1	K	15	ARG	C-N-CA	-6.77	112.02	119.19
1	E	60	LEU	N-CA-C	-6.76	105.66	114.04
2	C	359	ASP	CA-C-N	6.68	128.19	119.84
2	C	359	ASP	C-N-CA	6.68	128.19	119.84
2	B	18	ARG	N-CA-C	6.42	122.27	113.16
1	E	78	SER	CA-C-N	-6.41	112.06	122.82
1	E	78	SER	C-N-CA	-6.41	112.06	122.82
1	E	167	VAL	N-CA-C	6.29	117.04	110.62
1	J	68	GLU	CA-C-N	-6.20	110.53	122.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	68	GLU	C-N-CA	-6.20	110.53	122.06
1	K	57	SER	CA-C-N	6.15	129.34	120.79
1	K	57	SER	C-N-CA	6.15	129.34	120.79
2	A	359	ASP	CA-C-N	6.10	127.46	119.84
2	A	359	ASP	C-N-CA	6.10	127.46	119.84
2	D	24	VAL	N-CA-C	5.70	113.86	109.19
1	L	214	GLY	CA-C-N	5.67	130.45	122.46
1	L	214	GLY	C-N-CA	5.67	130.45	122.46
1	E	79	HIS	CA-CB-CG	5.65	119.45	113.80
1	L	322	ASN	CB-CA-C	-5.36	110.38	116.54
2	D	359	ASP	CA-C-N	5.31	124.76	119.24
2	D	359	ASP	C-N-CA	5.31	124.76	119.24
1	I	67	GLN	CA-C-N	5.30	128.12	120.38
1	I	67	GLN	C-N-CA	5.30	128.12	120.38
2	B	277	THR	N-CA-C	5.21	121.32	109.81
2	D	21	SER	N-CA-C	5.12	119.15	113.01
1	K	166	PHE	N-CA-C	5.07	119.04	112.86
1	H	349	ILE	N-CA-C	5.07	115.26	108.17
1	K	214	GLY	CA-C-N	5.06	129.59	122.46
1	K	214	GLY	C-N-CA	5.06	129.59	122.46
1	I	80	GLU	CA-CB-CG	5.06	124.22	114.10

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	E	2789	0	2838	64	0
1	F	2789	0	2840	51	0
1	G	2789	0	2838	77	0
1	H	2789	0	2840	101	0
1	I	2789	0	2840	65	0
1	J	2789	0	2838	62	0
1	K	2787	0	2833	71	0
1	L	2787	0	2831	85	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3172	0	3189	64	0
2	B	3167	0	3184	39	0
2	C	3167	0	3184	39	0
2	D	3167	0	3184	41	0
3	A	39	0	23	1	0
3	B	39	0	23	1	0
3	C	39	0	23	0	0
3	D	39	0	23	0	0
3	E	39	0	23	3	0
3	F	39	0	23	2	0
3	G	39	0	23	4	0
3	H	39	0	23	6	0
3	I	39	0	23	4	0
3	J	39	0	23	1	0
3	K	39	0	23	6	0
3	L	39	0	23	2	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	E	2	0	0	1	0
5	F	2	0	0	2	0
5	G	2	0	0	1	0
All	All	35458	0	35715	727	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 (727) 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:A:359:ASP:HB3	2:A:360:PRO:CD	1.49	1.40
1:H:344:LEU:CB	1:H:360:MET:O	1.69	1.38
1:G:15:ARG:HB3	1:H:360:MET:CE	1.57	1.34
1:J:21:THR:CG2	1:J:25:LEU:HD23	1.68	1.24
1:G:134:LEU:HD21	1:G:212:LEU:CD1	1.69	1.23
2:C:359:ASP:HB3	2:C:360:PRO:CD	1.66	1.21
2:D:20:LEU:HD21	2:D:386:ILE:CG2	1.72	1.20
1:I:110:ASP:OD2	3:I:401:GDD:O3'	1.64	1.16
1:H:344:LEU:HB2	1:H:360:MET:C	1.74	1.13
1:K:142:SER:HA	1:K:163:PRO:HG2	1.20	1.13
1:L:51:LEU:HD21	1:L:77:MET:CB	1.79	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:GLU:OE2	2:D:389:CYS:SG	2.05	1.12
1:H:156:ILE:HD12	1:H:207:LEU:HD12	1.31	1.11
1:J:21:THR:HG22	1:J:25:LEU:HD23	1.19	1.09
2:A:359:ASP:HB3	2:A:360:PRO:HD2	1.33	1.09
2:D:20:LEU:HD21	2:D:386:ILE:HG23	1.24	1.09
2:D:20:LEU:CD2	2:D:386:ILE:CG2	2.31	1.09
2:A:359:ASP:HB3	2:A:360:PRO:HD3	1.28	1.08
1:L:51:LEU:HD21	1:L:77:MET:HB3	1.10	1.07
1:H:177:ILE:C	1:H:178:LEU:HD23	1.80	1.06
1:H:202:ALA:HA	1:H:207:LEU:HD21	1.35	1.06
1:G:15:ARG:HB3	1:H:360:MET:HE2	1.07	1.06
1:G:134:LEU:HD21	1:G:212:LEU:HD13	1.33	1.05
1:L:28:PHE:O	1:L:29:CYS:SG	2.13	1.05
1:K:15:ARG:NH2	1:L:345:PRO:O	1.90	1.05
2:A:359:ASP:CB	2:A:360:PRO:CD	2.36	1.04
1:L:51:LEU:HD11	1:L:64:MET:HE1	1.42	1.01
1:H:221:GLN:NE2	1:H:223:LYS:HE2	1.76	1.01
1:H:344:LEU:HB2	1:H:360:MET:O	0.83	1.00
2:C:359:ASP:HB3	2:C:360:PRO:HD2	1.41	0.97
1:G:15:ARG:CB	1:H:360:MET:CE	2.44	0.96
1:L:51:LEU:CD2	1:L:77:MET:CB	2.42	0.96
2:D:20:LEU:CD2	2:D:386:ILE:HG21	1.94	0.95
1:E:194:GLU:OE2	3:E:401:GDD:H21	1.67	0.95
1:L:51:LEU:CD2	1:L:77:MET:HB3	1.97	0.94
2:A:406:PRO:O	2:B:18:ARG:NH2	1.99	0.94
1:H:156:ILE:CD1	1:H:207:LEU:HD12	1.97	0.94
1:G:134:LEU:HD21	1:G:212:LEU:HD12	1.46	0.93
1:G:321:GLU:OE1	1:G:337:TYR:CE1	2.22	0.93
1:L:28:PHE:C	1:L:29:CYS:SG	2.52	0.92
2:C:359:ASP:CB	2:C:360:PRO:CD	2.47	0.91
1:L:28:PHE:CD2	1:L:29:CYS:SG	2.63	0.91
1:G:142:SER:HA	1:G:163:PRO:HG3	1.52	0.91
1:G:15:ARG:HB3	1:H:360:MET:HE3	1.51	0.90
1:G:108:ASN:OD1	3:G:401:GDD:H4'	1.71	0.89
2:C:359:ASP:HB3	2:C:360:PRO:HD3	1.55	0.89
2:B:17:PHE:O	2:B:21:SER:HB3	1.74	0.88
2:A:359:ASP:CB	2:A:360:PRO:HD3	1.96	0.88
1:G:321:GLU:OE1	1:G:337:TYR:HE1	1.55	0.87
1:J:21:THR:CG2	1:J:25:LEU:CD2	2.54	0.85
1:K:305:SER:O	1:K:323:VAL:HA	1.76	0.85
1:G:142:SER:HA	1:G:163:PRO:CG	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:57:SER:HA	1:L:60:LEU:HD23	1.59	0.84
1:L:51:LEU:HD11	1:L:64:MET:CE	2.07	0.84
1:F:60:LEU:HD12	1:F:60:LEU:O	1.79	0.83
1:G:15:ARG:CB	1:H:360:MET:HG3	2.09	0.83
1:L:51:LEU:HD23	1:L:51:LEU:O	1.77	0.83
1:G:15:ARG:CG	1:H:360:MET:HE3	2.09	0.82
1:H:344:LEU:CG	1:H:360:MET:O	2.27	0.82
1:H:202:ALA:CA	1:H:207:LEU:HD21	2.10	0.81
1:G:15:ARG:CB	1:H:360:MET:HE2	2.02	0.80
1:I:110:ASP:OD2	3:I:401:GDD:C3'	2.30	0.79
1:G:134:LEU:HD11	1:G:212:LEU:HD12	1.64	0.79
2:C:359:ASP:CB	2:C:360:PRO:HD3	2.11	0.79
3:E:401:GDD:O6A	5:E:501:HOH:O	2.00	0.79
1:H:80:GLU:OE2	3:H:401:GDD:N2	2.15	0.78
1:G:15:ARG:HB2	1:H:360:MET:HG3	1.65	0.77
1:G:15:ARG:CB	1:H:360:MET:HE3	2.11	0.76
2:A:359:ASP:H	2:A:369:MET:HE1	1.51	0.76
1:J:64:MET:O	1:J:68:GLU:HB3	1.86	0.75
1:H:178:LEU:HD23	1:H:178:LEU:N	2.01	0.74
1:I:51:LEU:O	1:I:77:MET:SD	2.45	0.74
2:A:361:ASN:ND2	2:A:364:ASP:OD1	2.21	0.74
1:G:134:LEU:CD2	1:G:212:LEU:HD12	2.19	0.73
2:A:359:ASP:CA	2:A:369:MET:HE3	2.18	0.73
2:D:23:GLU:CD	2:D:389:CYS:HG	1.92	0.72
1:J:328:GLU:HB3	1:J:345:PRO:HB3	1.72	0.72
1:F:306:CYS:HB2	1:F:324:THR:HG23	1.70	0.71
1:H:221:GLN:HE22	1:H:223:LYS:HE2	1.51	0.71
2:A:338:HIS:NE2	2:A:357:PRO:HG3	2.05	0.71
1:H:131:GLY:O	1:H:207:LEU:HA	1.90	0.70
1:E:146:VAL:HB	1:E:168:SER:OG	1.91	0.70
1:G:134:LEU:CD2	1:G:212:LEU:CD1	2.60	0.70
1:K:322:ASN:ND2	1:K:339:ASN:OD1	2.25	0.70
2:D:364:ASP:OD2	2:D:365:PRO:HD2	1.91	0.69
1:E:60:LEU:O	1:E:64:MET:HG3	1.93	0.69
1:J:289:CYS:SG	1:J:306:CYS:N	2.66	0.69
1:I:3:ALA:HB3	1:I:49:VAL:HG12	1.73	0.69
1:G:150:GLU:HB3	1:G:153:THR:HG23	1.73	0.69
1:F:218:ASP:OD1	5:F:501:HOH:O	2.11	0.69
1:H:344:LEU:HD22	1:H:360:MET:O	1.94	0.68
1:J:56:MET:HE2	1:J:79:HIS:HB2	1.74	0.68
1:L:4:LEU:HA	1:L:50:ILE:O	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:344:LEU:CD2	1:H:360:MET:O	2.42	0.67
2:A:359:ASP:H	2:A:369:MET:CE	2.07	0.67
1:H:34:LEU:C	1:H:34:LEU:HD12	2.19	0.67
1:F:6:LEU:HB3	3:F:401:GDD:H1'	1.75	0.67
1:E:60:LEU:O	1:E:60:LEU:HD12	1.94	0.67
1:J:94:ARG:O	1:J:98:SER:HB3	1.94	0.67
1:F:53:VAL:HG12	1:F:60:LEU:HD21	1.77	0.66
1:H:3:ALA:HB3	1:H:49:VAL:HG12	1.78	0.66
1:E:320:MET:HB3	1:E:324:THR:HG21	1.78	0.66
1:G:15:ARG:HG2	1:H:360:MET:HG3	1.77	0.66
1:I:54:SER:HA	1:I:80:GLU:HB3	1.77	0.66
2:A:359:ASP:N	2:A:369:MET:CE	2.59	0.66
1:F:60:LEU:HD12	1:F:60:LEU:C	2.21	0.66
1:L:289:CYS:SG	1:L:306:CYS:N	2.69	0.66
3:F:401:GDD:O6A	5:F:502:HOH:O	2.14	0.66
2:B:18:ARG:HG3	2:B:22:PHE:CZ	2.31	0.65
1:G:153:THR:O	1:G:155:ARG:N	2.29	0.65
1:I:178:LEU:HD12	1:I:182:VAL:HG11	1.78	0.65
1:G:289:CYS:SG	1:G:306:CYS:N	2.69	0.65
1:E:289:CYS:SG	1:E:306:CYS:N	2.69	0.65
1:I:162:LYS:HD3	1:I:163:PRO:HD2	1.78	0.65
1:L:57:SER:O	1:L:58:GLN:C	2.39	0.65
2:C:17:PHE:HB2	2:C:250:SER:HB3	1.78	0.65
2:D:364:ASP:OD2	2:D:365:PRO:CD	2.44	0.65
1:F:22:PRO:HG2	1:F:25:LEU:HD23	1.79	0.65
1:L:33:ILE:HD11	1:L:112:ILE:HB	1.79	0.65
1:K:15:ARG:HH11	1:K:15:ARG:HG3	1.62	0.65
1:K:48:HIS:HE1	1:K:96:LEU:HD21	1.61	0.65
2:D:145:ASN:HB2	2:D:363:ASN:O	1.97	0.65
1:H:202:ALA:HA	1:H:207:LEU:CD2	2.19	0.65
1:L:51:LEU:CD2	1:L:77:MET:HA	2.27	0.64
1:H:221:GLN:HE21	1:H:223:LYS:HE2	1.57	0.64
1:L:28:PHE:C	1:L:29:CYS:HG	1.96	0.64
1:I:137:LYS:HG2	1:I:170:LYS:HG2	1.79	0.64
1:K:164:GLN:HA	1:K:164:GLN:HE21	1.63	0.64
2:C:338:HIS:CD2	2:C:357:PRO:HB3	2.32	0.64
1:E:164:GLN:HB2	1:E:167:VAL:HG23	1.78	0.64
1:K:142:SER:CA	1:K:163:PRO:HG2	2.13	0.64
1:H:293:ARG:HG2	1:H:310:TRP:HD1	1.63	0.63
1:J:71:LEU:HD22	1:J:73:ILE:HB	1.81	0.63
1:G:15:ARG:CG	1:H:360:MET:HG3	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ARG:HG2	1:E:310:TRP:HD1	1.63	0.63
1:K:35:LEU:HD11	1:K:67:GLN:HG3	1.81	0.62
1:L:51:LEU:CD2	1:L:77:MET:HB2	2.30	0.62
1:K:194:GLU:OE1	3:K:401:GDD:O21	2.12	0.62
2:B:136:PRO:HA	2:B:187:SER:HB3	1.80	0.62
1:H:134:LEU:HD21	1:H:212:LEU:HD13	1.81	0.62
1:K:33:ILE:HD13	1:K:219:ILE:HD11	1.81	0.62
1:E:194:GLU:OE2	3:E:401:GDD:C21	2.46	0.62
1:H:336:LEU:HD11	1:H:350:GLY:HA2	1.82	0.62
1:I:2:LYS:HG2	1:I:48:HIS:HB3	1.80	0.62
1:K:12:THR:HA	1:K:15:ARG:CD	2.30	0.62
2:A:359:ASP:HA	2:A:369:MET:CE	2.29	0.62
1:G:321:GLU:OE1	1:G:337:TYR:CZ	2.53	0.62
1:G:134:LEU:CD1	1:G:212:LEU:HD12	2.29	0.61
1:L:56:MET:O	1:L:56:MET:HG2	1.98	0.61
2:A:363:ASN:O	1:G:166:PHE:CD1	2.53	0.61
1:L:7:VAL:HG13	1:L:24:PRO:HG3	1.82	0.61
2:A:420:LEU:O	2:B:18:ARG:NH1	2.33	0.61
1:K:116:PRO:HG3	1:K:212:LEU:HD13	1.83	0.61
2:D:20:LEU:HD23	2:D:386:ILE:HG21	1.79	0.61
1:G:323:VAL:HG23	1:G:323:VAL:O	2.01	0.61
1:I:347:LYS:HE2	1:J:12:THR:HG22	1.82	0.61
1:I:345:PRO:O	1:J:15:ARG:NH2	2.33	0.61
1:E:134:LEU:HB3	1:E:173:ALA:HB3	1.83	0.61
1:G:13:ARG:HG2	1:G:221:GLN:HG2	1.82	0.61
1:K:15:ARG:HH11	1:K:15:ARG:CG	2.14	0.61
1:H:90:LEU:HD13	1:H:193:ILE:HD13	1.82	0.61
1:L:84:LEU:HA	1:L:190:PRO:HB3	1.81	0.61
1:E:324:THR:O	1:E:324:THR:HG23	2.01	0.60
1:F:289:CYS:SG	1:F:290:THR:N	2.75	0.60
1:F:320:MET:HB3	1:F:324:THR:HG21	1.82	0.60
1:K:12:THR:HA	1:K:15:ARG:HD3	1.83	0.60
1:F:323:VAL:O	1:F:323:VAL:HG23	2.01	0.60
1:K:218:ASP:OD1	3:K:401:GDD:O6A	2.15	0.60
1:K:323:VAL:O	1:K:323:VAL:HG23	2.00	0.60
2:A:18:ARG:NH2	2:A:384:ILE:O	2.35	0.60
1:E:53:VAL:HG23	1:E:53:VAL:O	2.00	0.60
1:J:49:VAL:HB	1:J:75:ILE:HG22	1.84	0.60
2:D:325:LEU:HD12	2:D:342:GLY:HA2	1.82	0.60
1:L:51:LEU:CD2	1:L:77:MET:CA	2.80	0.60
1:K:142:SER:HA	1:K:163:PRO:CG	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:LEU:HD23	1:L:51:LEU:C	2.27	0.60
2:B:358:SER:O	2:B:358:SER:OG	2.17	0.59
1:F:53:VAL:CG1	1:F:60:LEU:HD21	2.32	0.59
1:L:323:VAL:HG12	1:L:323:VAL:O	2.02	0.59
2:D:364:ASP:OD2	2:D:365:PRO:N	2.35	0.59
1:E:323:VAL:HG23	1:E:323:VAL:O	2.03	0.59
1:J:323:VAL:HG23	1:J:323:VAL:O	2.01	0.59
1:L:120:MET:HE2	1:L:134:LEU:HD13	1.84	0.59
1:J:168:SER:OG	1:J:169:ASN:N	2.34	0.59
2:A:359:ASP:CA	2:A:369:MET:CE	2.80	0.59
2:D:256:TYR:HB2	2:D:359:ASP:HB3	1.84	0.59
1:J:94:ARG:HH21	1:J:184:GLN:HA	1.67	0.59
1:H:207:LEU:H	1:H:207:LEU:HD23	1.68	0.59
1:G:7:VAL:O	3:G:401:GDD:O2'	2.19	0.59
1:J:221:GLN:HB2	1:J:224:ASP:HB2	1.85	0.59
1:I:323:VAL:HG23	1:I:323:VAL:O	2.01	0.59
1:H:177:ILE:O	1:H:178:LEU:HD23	2.03	0.59
1:L:57:SER:O	1:L:60:LEU:N	2.31	0.58
1:I:320:MET:HE2	1:I:324:THR:CG2	2.33	0.58
2:A:417:GLN:HG2	2:B:375:PHE:HB2	1.84	0.58
1:E:87:ALA:HB1	1:E:186:ILE:HD11	1.85	0.58
1:H:323:VAL:HG23	1:H:323:VAL:O	2.03	0.58
1:I:335:GLU:OE1	2:C:320:ARG:NH1	2.36	0.58
2:A:136:PRO:HA	2:A:187:SER:HB2	1.84	0.58
1:F:27:ASP:HB2	1:F:292:LEU:HD22	1.85	0.58
1:G:321:GLU:OE1	1:G:337:TYR:OH	2.18	0.58
1:L:344:LEU:HD22	1:L:360:MET:HG2	1.84	0.58
2:A:120:ASP:OD1	2:A:264:ARG:NH2	2.36	0.58
2:D:63:GLU:O	2:D:67:GLN:HB2	2.04	0.58
1:E:84:LEU:HB3	1:E:88:GLY:HA3	1.86	0.58
1:L:147:VAL:HG12	1:L:156:ILE:HG12	1.86	0.58
1:H:108:ASN:OD1	3:H:401:GDD:H4'	2.04	0.58
1:I:24:PRO:HB2	1:I:34:LEU:HG	1.84	0.58
1:I:140:GLU:HG2	1:I:142:SER:H	1.68	0.58
2:A:359:ASP:HA	2:A:369:MET:HE3	1.86	0.58
1:F:87:ALA:HB3	1:F:191:THR:HG23	1.86	0.58
1:J:2:LYS:HE3	1:J:97:LEU:HA	1.86	0.58
1:H:221:GLN:NE2	1:H:223:LYS:CE	2.62	0.58
1:L:293:ARG:HG2	1:L:310:TRP:HD1	1.68	0.57
1:G:153:THR:C	1:G:155:ARG:H	2.12	0.57
1:K:307:ILE:HB	1:K:325:VAL:HG12	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:LEU:HB3	1:H:88:GLY:HA3	1.87	0.57
1:K:14:LEU:O	1:K:14:LEU:HD23	2.03	0.57
1:L:51:LEU:H	1:L:51:LEU:HD22	1.69	0.57
2:D:360:PRO:O	2:D:361:ASN:C	2.45	0.57
1:L:27:ASP:OD2	1:L:293:ARG:NH2	2.37	0.57
2:C:120:ASP:OD1	2:C:264:ARG:NH2	2.38	0.57
1:J:67:GLN:HE22	1:J:71:LEU:HD12	1.68	0.56
1:I:281:GLU:HG3	1:I:298:ARG:HA	1.85	0.56
2:A:108:GLU:OE1	2:A:134:ARG:NH2	2.38	0.56
2:C:168:VAL:HG11	2:C:175:ILE:HG13	1.86	0.56
1:E:94:ARG:HG3	1:E:183:LEU:HD13	1.88	0.56
1:H:193:ILE:O	1:H:197:VAL:HB	2.05	0.56
1:H:321:GLU:OE1	1:H:337:TYR:CE1	2.59	0.56
1:F:22:PRO:HD3	1:F:56:MET:HE3	1.88	0.56
1:H:34:LEU:HD12	1:H:35:LEU:N	2.20	0.56
1:I:84:LEU:HB3	1:I:88:GLY:HA3	1.88	0.56
1:I:320:MET:HB3	1:I:324:THR:HG21	1.88	0.56
1:E:269:GLY:HA3	1:E:287:ARG:HG2	1.88	0.56
1:L:77:MET:SD	1:L:77:MET:N	2.73	0.56
1:L:281:GLU:HG3	1:L:298:ARG:HA	1.87	0.56
1:L:51:LEU:CD2	1:L:51:LEU:H	2.18	0.56
1:F:110:ASP:OD2	1:F:110:ASP:N	2.39	0.56
1:G:180:PRO:O	1:G:183:LEU:HB2	2.05	0.56
1:K:212:LEU:HG	1:K:213:GLN:N	2.21	0.55
1:L:212:LEU:HD23	1:L:216:TRP:HB2	1.87	0.55
1:G:24:PRO:HB2	1:G:34:LEU:HB2	1.89	0.55
1:H:84:LEU:HA	1:H:190:PRO:HB3	1.87	0.55
1:K:146:VAL:HG21	1:K:168:SER:HB3	1.88	0.55
2:B:320:ARG:HB3	2:B:337:LEU:HD23	1.89	0.55
1:H:311:ARG:NH2	1:H:328:GLU:OE2	2.38	0.55
1:K:293:ARG:HG2	1:K:310:TRP:HD1	1.72	0.55
1:I:68:GLU:HG2	1:I:75:ILE:HG12	1.89	0.55
1:I:343:VAL:HG22	1:I:359:ILE:HD12	1.89	0.55
2:D:119:SER:OG	2:D:120:ASP:N	2.40	0.55
1:K:134:LEU:HD21	1:K:212:LEU:HB2	1.89	0.55
1:H:223:LYS:HE3	1:H:224:ASP:OD1	2.07	0.55
1:H:343:VAL:HG11	1:H:349:ILE:HD11	1.89	0.55
1:L:269:GLY:HA3	1:L:287:ARG:HG2	1.89	0.55
2:A:42:GLU:OE2	2:A:46:GLN:NE2	2.40	0.55
1:G:194:GLU:HA	1:G:198:PHE:HD2	1.71	0.55
2:D:23:GLU:CD	2:D:389:CYS:SG	2.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:ARG:O	1:I:187:GLN:NE2	2.40	0.54
2:C:322:SER:OG	2:C:323:ILE:N	2.40	0.54
1:I:306:CYS:HB2	1:I:324:THR:HG22	1.89	0.54
1:F:321:GLU:OE1	1:F:337:TYR:HE1	1.90	0.54
1:L:51:LEU:HD23	1:L:77:MET:CB	2.35	0.54
1:I:12:THR:OG1	1:J:347:LYS:NZ	2.41	0.54
1:I:17:LEU:HD11	1:I:307:ILE:HG21	1.90	0.54
1:I:266:CYS:HB2	1:I:284:VAL:H	1.72	0.54
2:A:60:GLN:OE1	2:D:60:GLN:NE2	2.40	0.54
1:H:156:ILE:HB	1:H:207:LEU:CD1	2.38	0.54
1:E:344:LEU:HD22	1:E:360:MET:HG2	1.90	0.54
1:K:52:ALA:CB	3:K:401:GDD:H2N2	2.21	0.54
1:I:110:ASP:OD2	3:I:401:GDD:H3'	2.07	0.54
1:K:320:MET:HG2	1:K:338:LEU:HB2	1.90	0.54
2:C:16:ARG:HD2	2:C:19:PRO:HA	1.88	0.54
1:E:310:TRP:HB2	1:E:328:GLU:HG3	1.89	0.54
1:G:15:ARG:HG3	1:H:360:MET:HE3	1.88	0.54
1:H:138:VAL:HG22	1:H:171:ILE:HD13	1.90	0.54
2:D:16:ARG:HH22	2:D:370:ASP:HB3	1.72	0.54
1:H:194:GLU:HG2	3:H:401:GDD:O21	2.08	0.54
1:F:321:GLU:OE1	1:F:337:TYR:CE1	2.61	0.54
1:H:130:GLU:HG2	1:H:182:VAL:HG22	1.89	0.54
1:H:237:ARG:HD2	1:H:253:ASN:HB3	1.90	0.54
2:A:352:ARG:NE	2:A:354:GLU:OE1	2.40	0.54
2:C:54:LEU:HD22	2:C:83:LEU:HD11	1.90	0.54
1:K:32:PRO:HD2	1:K:35:LEU:HD22	1.89	0.54
1:K:52:ALA:HB1	3:K:401:GDD:N2	2.23	0.54
2:A:338:HIS:CD2	2:A:357:PRO:HG3	2.43	0.54
1:G:185:ARG:HD3	1:G:200:ILE:HD11	1.90	0.54
1:H:74:ARG:HG3	1:H:74:ARG:O	2.08	0.53
1:L:94:ARG:NH1	1:L:183:LEU:O	2.41	0.53
1:G:37:GLN:NE2	1:G:108:ASN:O	2.36	0.53
1:G:360:MET:HB3	1:H:15:ARG:HG2	1.88	0.53
2:B:52:GLU:OE2	2:B:81:ARG:NE	2.41	0.53
1:K:94:ARG:HA	1:K:183:LEU:HD21	1.89	0.53
1:E:127:HIS:CD2	1:E:129:GLN:H	2.26	0.53
1:G:142:SER:HA	1:G:163:PRO:HG2	1.90	0.53
1:H:2:LYS:NZ	1:H:96:LEU:O	2.40	0.53
2:A:354:GLU:HB3	2:A:400:LEU:HD12	1.90	0.53
1:L:127:HIS:CD2	1:L:129:GLN:H	2.27	0.53
1:K:164:GLN:HA	1:K:164:GLN:NE2	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:ASN:N	1:F:253:ASN:OD1	2.42	0.53
1:J:130:GLU:HB2	1:J:206:GLN:HB3	1.90	0.53
1:K:101:ALA:HA	1:K:180:PRO:HG2	1.91	0.53
1:E:298:ARG:HB3	1:E:316:GLN:HG3	1.91	0.53
1:F:68:GLU:HA	1:F:71:LEU:HD12	1.91	0.53
2:B:15:THR:C	2:B:17:PHE:H	2.16	0.53
1:F:215:PHE:HB2	1:F:231:LEU:HG	1.89	0.53
1:H:95:ASP:OD1	1:H:95:ASP:N	2.33	0.53
1:I:84:LEU:HA	1:I:190:PRO:HB3	1.90	0.52
2:A:158:ASN:HB2	2:A:165:LEU:HD11	1.91	0.52
2:B:113:LEU:HD23	2:B:183:ILE:HG12	1.91	0.52
2:C:354:GLU:O	2:C:385:THR:OG1	2.23	0.52
1:G:168:SER:OG	1:G:169:ASN:N	2.40	0.52
1:L:224:ASP:HA	1:L:227:THR:HG22	1.91	0.52
2:A:119:SER:OG	2:A:120:ASP:N	2.42	0.52
2:D:52:GLU:HG3	2:D:79:PRO:HG2	1.90	0.52
1:E:110:ASP:OD2	1:E:110:ASP:N	2.42	0.52
1:E:200:ILE:HA	1:E:203:LYS:HG2	1.90	0.52
1:F:191:THR:OG1	1:F:192:SER:N	2.42	0.52
1:G:281:GLU:HG3	1:G:298:ARG:HA	1.90	0.52
1:J:148:VAL:HG12	1:J:168:SER:HB2	1.91	0.52
1:J:215:PHE:HB2	1:J:231:LEU:HG	1.90	0.52
1:L:113:CYS:HB3	1:L:216:TRP:HA	1.92	0.52
1:I:287:ARG:NH2	2:C:396:GLU:OE2	2.37	0.52
2:C:155:ILE:HG21	2:C:238:VAL:HG21	1.90	0.52
1:F:134:LEU:HB3	1:F:173:ALA:HB3	1.91	0.52
2:A:16:ARG:HD3	2:A:20:LEU:H	1.75	0.52
1:J:298:ARG:HD3	1:J:316:GLN:HG2	1.92	0.52
1:L:51:LEU:CD2	1:L:51:LEU:N	2.73	0.52
1:K:52:ALA:HB2	1:K:89:PRO:HB3	1.90	0.52
1:I:134:LEU:HD13	1:I:175:MET:HE3	1.90	0.52
2:C:377:ASP:N	2:C:377:ASP:OD1	2.43	0.52
1:G:87:ALA:HB1	1:G:186:ILE:HD11	1.90	0.52
1:F:212:LEU:HD23	1:F:216:TRP:HB2	1.92	0.52
1:J:134:LEU:HD21	1:J:212:LEU:HD13	1.92	0.52
1:L:235:SER:OG	1:L:239:LYS:NZ	2.43	0.52
2:D:398:LEU:H	2:D:413:SER:HB2	1.74	0.52
2:A:54:LEU:HD22	2:A:83:LEU:HD11	1.92	0.52
2:B:116:ASP:OD2	3:B:501:GDD:H3'	2.09	0.52
1:J:42:ALA:HB2	1:J:71:LEU:HD21	1.92	0.52
2:A:21:SER:OG	2:A:24:VAL:O	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:VAL:HB	2:B:166:HIS:HB3	1.92	0.51
1:G:50:ILE:HA	1:G:76:SER:O	2.10	0.51
1:K:52:ALA:HB1	3:K:401:GDD:H2N2	1.75	0.51
1:I:27:ASP:OD1	1:I:27:ASP:N	2.43	0.51
1:J:340:GLY:HA3	1:J:356:PRO:HB3	1.93	0.51
1:I:77:MET:SD	1:I:78:SER:N	2.84	0.51
2:A:359:ASP:N	2:A:369:MET:HE3	2.23	0.51
1:K:1:MET:HB3	1:K:46:VAL:HG22	1.92	0.51
1:I:37:GLN:NE2	1:I:108:ASN:O	2.39	0.51
2:A:52:GLU:OE2	2:A:81:ARG:NE	2.42	0.51
2:B:54:LEU:HD22	2:B:83:LEU:HD11	1.91	0.51
1:F:84:LEU:HA	1:F:190:PRO:HB3	1.91	0.51
1:H:221:GLN:HE21	1:H:223:LYS:CE	2.24	0.51
1:I:306:CYS:HB2	1:I:324:THR:CG2	2.39	0.51
2:C:52:GLU:HG3	2:C:79:PRO:HG2	1.93	0.51
1:I:5:ILE:HG12	1:I:107:LEU:HD12	1.91	0.51
1:G:134:LEU:HB3	1:G:175:MET:HB3	1.92	0.51
2:A:177:ASP:OD1	2:A:177:ASP:N	2.44	0.51
2:C:16:ARG:NH2	2:C:21:SER:O	2.43	0.51
1:G:215:PHE:HB2	1:G:231:LEU:HG	1.91	0.51
2:B:1:MET:HE2	2:B:107:PRO:HB3	1.93	0.51
1:E:95:ASP:N	1:E:95:ASP:OD1	2.43	0.51
1:H:293:ARG:NH1	1:H:294:ASP:OD1	2.43	0.51
1:J:3:ALA:HB3	1:J:49:VAL:HG22	1.93	0.51
1:F:256:VAL:HG22	1:F:274:LEU:HD12	1.94	0.50
1:F:334:ASP:OD1	1:F:334:ASP:N	2.42	0.50
1:J:50:ILE:HA	1:J:76:SER:O	2.11	0.50
1:L:94:ARG:HA	1:L:183:LEU:HD11	1.94	0.50
1:I:77:MET:SD	1:I:77:MET:C	2.94	0.50
1:E:7:VAL:HG12	1:E:24:PRO:HG3	1.94	0.50
1:K:212:LEU:HD12	1:K:213:GLN:H	1.77	0.50
1:I:212:LEU:HD23	1:I:216:TRP:HB2	1.92	0.50
2:C:116:ASP:OD1	2:C:249:LYS:NZ	2.41	0.50
1:E:124:HIS:HA	1:E:127:HIS:CE1	2.46	0.50
1:G:153:THR:C	1:G:155:ARG:N	2.69	0.50
1:H:230:CYS:SG	1:H:271:ASN:ND2	2.85	0.50
1:H:321:GLU:OE1	1:H:337:TYR:HE1	1.95	0.50
1:L:87:ALA:HB1	1:L:186:ILE:HD11	1.94	0.50
1:I:320:MET:HE2	1:I:324:THR:HG21	1.94	0.50
2:C:400:LEU:HD23	2:C:415:THR:HG23	1.93	0.50
1:J:24:PRO:HB2	1:J:34:LEU:HB2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:361:ASN:OD1	2:A:362:PRO:HD2	2.12	0.50
2:A:400:LEU:HD23	2:A:415:THR:HG23	1.94	0.50
1:K:298:ARG:HB3	1:K:316:GLN:HG3	1.92	0.50
1:J:187:GLN:HB2	1:J:189:GLN:HE21	1.77	0.50
1:I:156:ILE:HD12	1:I:207:LEU:HB3	1.94	0.49
1:J:293:ARG:HG2	1:J:310:TRP:HD1	1.76	0.49
2:A:19:PRO:HG3	2:B:420:LEU:HD13	1.94	0.49
2:B:18:ARG:O	2:B:22:PHE:CD2	2.65	0.49
2:C:159:PRO:HG2	2:C:160:GLN:HE21	1.78	0.49
1:E:25:LEU:CD2	1:E:60:LEU:HD13	2.42	0.49
2:C:37:ILE:HA	2:C:40:HIS:HD2	1.75	0.49
1:K:131:GLY:O	1:K:207:LEU:HA	2.13	0.49
1:K:194:GLU:O	1:K:198:PHE:HB2	2.12	0.49
1:K:343:VAL:HG22	1:K:359:ILE:HD12	1.95	0.49
1:K:353:VAL:HG21	1:K:359:ILE:HD11	1.93	0.49
2:B:106:SER:O	2:B:106:SER:OG	2.28	0.49
1:E:118:GLN:HA	1:E:121:VAL:HG12	1.93	0.49
1:K:164:GLN:HE21	1:K:164:GLN:CA	2.24	0.49
1:H:215:PHE:HB2	1:H:231:LEU:HG	1.94	0.49
2:D:20:LEU:CD2	2:D:386:ILE:HG23	2.11	0.49
1:G:122:GLN:HG2	1:G:123:PHE:N	2.27	0.49
2:A:335:CYS:SG	2:A:352:ARG:NH1	2.85	0.49
1:H:34:LEU:C	1:H:34:LEU:CD1	2.85	0.49
1:H:74:ARG:C	1:H:74:ARG:CD	2.86	0.49
2:D:376:LYS:HB2	2:D:381:LEU:HD21	1.94	0.49
2:D:356:THR:CG2	2:D:357:PRO:HD2	2.43	0.48
1:E:53:VAL:CG2	1:E:79:HIS:HB3	2.43	0.48
1:E:353:VAL:HG11	1:E:359:ILE:HD11	1.94	0.48
2:A:13:LYS:HG3	2:A:58:PHE:HZ	1.78	0.48
2:C:362:PRO:HB3	1:J:164:GLN:HA	1.96	0.48
1:H:224:ASP:HA	1:H:227:THR:HG22	1.95	0.48
1:K:53:VAL:HG21	1:K:77:MET:HE2	1.95	0.48
1:H:306:CYS:HB3	1:H:324:THR:HG23	1.95	0.48
1:J:108:ASN:ND2	1:J:174:GLY:O	2.47	0.48
1:L:71:LEU:N	1:L:71:LEU:HD23	2.27	0.48
2:C:119:SER:OG	2:C:120:ASP:N	2.47	0.48
1:E:94:ARG:NH2	1:E:183:LEU:O	2.46	0.48
2:A:405:LEU:HD11	2:B:420:LEU:HD21	1.95	0.48
2:B:119:SER:OG	2:B:120:ASP:N	2.44	0.48
1:E:178:LEU:HD12	1:E:182:VAL:HG21	1.96	0.48
1:K:335:GLU:OE2	2:D:318:ARG:NE	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:LEU:C	1:F:60:LEU:CD1	2.86	0.48
1:G:257:ASP:OD2	1:G:259:SER:N	2.47	0.48
1:H:7:VAL:HG13	1:H:53:VAL:HG12	1.96	0.48
1:L:28:PHE:HD2	1:L:29:CYS:SG	2.34	0.48
2:B:52:GLU:HG3	2:B:79:PRO:HG2	1.96	0.48
2:D:354:GLU:O	2:D:385:THR:OG1	2.31	0.48
1:E:322:ASN:ND2	1:E:322:ASN:O	2.46	0.48
2:A:62:ASP:OD1	2:A:62:ASP:N	2.44	0.48
1:H:34:LEU:CD1	1:H:35:LEU:HD22	2.44	0.48
1:L:118:GLN:HA	1:L:121:VAL:HG12	1.95	0.48
1:K:161:GLU:O	1:K:163:PRO:HD3	2.14	0.47
1:K:334:ASP:OD2	1:K:334:ASP:N	2.42	0.47
2:A:138:LEU:HB3	2:A:185:LEU:HB3	1.95	0.47
2:B:400:LEU:HD23	2:B:415:THR:HG23	1.96	0.47
1:L:107:LEU:HD21	1:L:175:MET:HE3	1.97	0.47
1:H:51:LEU:HG	1:H:77:MET:HG2	1.96	0.47
1:K:15:ARG:CG	1:K:15:ARG:NH1	2.73	0.47
1:E:84:LEU:HA	1:E:190:PRO:HB3	1.96	0.47
1:G:14:LEU:O	1:G:18:THR:OG1	2.32	0.47
1:K:33:ILE:HG22	1:K:112:ILE:HD12	1.96	0.47
2:B:20:LEU:N	2:B:20:LEU:HD13	2.29	0.47
1:H:229:MET:HE3	1:H:229:MET:HB3	1.79	0.47
2:D:126:MET:HE2	2:D:126:MET:HB3	1.81	0.47
1:L:156:ILE:HD12	1:L:207:LEU:HB3	1.97	0.47
1:F:320:MET:HE3	1:F:338:LEU:HD12	1.97	0.47
1:J:194:GLU:HG2	3:J:401:GDD:O21	2.15	0.47
1:I:322:ASN:ND2	1:I:339:ASN:OD1	2.48	0.47
1:G:134:LEU:HD23	1:G:173:ALA:HB3	1.97	0.47
1:H:359:ILE:O	1:H:360:MET:C	2.57	0.47
1:L:301:SER:OG	1:L:318:VAL:O	2.29	0.47
1:I:221:GLN:HG2	1:I:222:PRO:HD2	1.96	0.47
2:A:329:THR:HB	2:A:346:THR:HG23	1.95	0.47
1:E:144:TYR:HB2	1:E:171:ILE:HD13	1.96	0.47
1:F:340:GLY:HA3	1:F:356:PRO:HB3	1.96	0.47
1:G:180:PRO:HA	1:G:183:LEU:HD23	1.97	0.47
1:H:178:LEU:N	1:H:178:LEU:CD2	2.73	0.47
1:J:21:THR:HG23	1:J:25:LEU:HD23	1.83	0.47
2:A:359:ASP:C	2:A:369:MET:HE3	2.40	0.47
1:G:66:ALA:O	1:G:69:GLN:NE2	2.47	0.47
1:I:305:SER:O	1:I:323:VAL:HA	2.15	0.47
2:B:62:ASP:N	2:B:62:ASP:OD1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ARG:NE	1:F:335:GLU:OE2	2.48	0.47
1:E:127:HIS:HD2	1:E:129:GLN:H	1.62	0.47
1:L:135:VAL:HG12	1:L:147:VAL:HG21	1.96	0.47
2:A:362:PRO:HB2	1:G:142:SER:OG	2.14	0.46
1:E:48:HIS:CE1	1:E:74:ARG:HE	2.34	0.46
1:L:51:LEU:HD23	1:L:77:MET:HB2	1.94	0.46
1:K:84:LEU:HB3	1:K:88:GLY:HA3	1.98	0.46
1:I:7:VAL:HB	1:I:53:VAL:HG22	1.97	0.46
1:I:89:PRO:HG3	3:I:401:GDD:N2	2.30	0.46
1:G:89:PRO:HG3	3:G:401:GDD:N2	2.31	0.46
1:K:253:ASN:N	1:K:253:ASN:OD1	2.47	0.46
1:E:197:VAL:O	1:E:201:MET:HB2	2.16	0.46
1:J:94:ARG:NH2	1:J:183:LEU:O	2.47	0.46
1:J:333:ASN:HD22	1:J:350:GLY:HA2	1.80	0.46
1:J:82:GLU:HG2	1:J:83:PRO:HD2	1.97	0.46
1:L:229:MET:HB3	1:L:229:MET:HE3	1.72	0.46
1:I:150:GLU:HG3	1:I:157:HIS:CE1	2.51	0.46
1:E:61:GLU:HG2	1:E:77:MET:HG2	1.97	0.46
1:F:129:GLN:HG3	1:F:208:TYR:HE2	1.80	0.46
1:H:177:ILE:C	1:H:178:LEU:CD2	2.72	0.46
1:H:321:GLU:OE1	1:H:337:TYR:OH	2.24	0.46
2:C:380:LEU:N	2:D:378:GLY:O	2.39	0.46
2:D:369:MET:H	2:D:369:MET:HG3	1.53	0.46
1:L:57:SER:O	1:L:59:VAL:N	2.48	0.46
1:I:229:MET:HE3	1:I:229:MET:HB3	1.83	0.46
1:F:353:VAL:HG21	1:F:359:ILE:HD11	1.98	0.46
1:L:148:VAL:HB	1:L:158:ARG:O	2.16	0.46
2:A:332:GLU:OE2	2:A:349:ARG:NH1	2.49	0.46
1:J:341:ALA:HB2	1:J:353:VAL:HG21	1.97	0.46
2:A:322:SER:OG	2:A:323:ILE:N	2.46	0.46
1:E:189:GLN:H	1:E:189:GLN:HG3	1.62	0.46
1:F:237:ARG:HH21	1:F:244:LEU:HD22	1.81	0.46
1:H:108:ASN:HB2	1:H:111:VAL:HG12	1.97	0.46
2:D:8:ILE:HB	2:D:27:PRO:HG2	1.98	0.45
1:J:84:LEU:HA	1:J:190:PRO:HB3	1.98	0.45
1:J:281:GLU:OE2	1:J:296:ARG:NH2	2.50	0.45
1:K:305:SER:O	1:K:323:VAL:CA	2.55	0.45
1:E:341:ALA:HB2	1:E:353:VAL:HG21	1.97	0.45
1:F:221:GLN:HB2	1:F:224:ASP:HB2	1.98	0.45
1:G:15:ARG:HG2	1:H:360:MET:CG	2.45	0.45
1:G:259:SER:OG	1:G:277:GLY:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:THR:HG22	2:B:280:GLY:H	1.82	0.45
2:C:116:ASP:OD1	2:C:249:LYS:HE2	2.16	0.45
1:H:133:ILE:HG12	1:H:176:TYR:HD1	1.81	0.45
2:C:116:ASP:OD1	2:C:249:LYS:CE	2.64	0.45
2:D:78:LEU:HD12	2:D:78:LEU:HA	1.84	0.45
2:B:320:ARG:HH21	2:B:338:HIS:HE1	1.62	0.45
1:G:155:ARG:HH12	1:G:157:HIS:HA	1.81	0.45
2:D:186:PHE:HZ	2:D:222:LEU:HD21	1.80	0.45
1:H:156:ILE:CG2	1:H:207:LEU:HD11	2.46	0.45
1:H:226:LEU:HD23	1:H:226:LEU:HA	1.82	0.45
1:L:264:GLN:NE2	1:L:282:ASP:OD2	2.46	0.45
1:I:135:VAL:HG11	1:I:147:VAL:HG21	1.99	0.45
1:E:22:PRO:HG2	1:E:25:LEU:HB2	1.98	0.45
3:K:401:GDD:O5'	3:K:401:GDD:H8	2.17	0.45
1:I:253:ASN:N	1:I:253:ASN:OD1	2.50	0.45
1:E:360:MET:HE1	1:F:16:PRO:HG3	1.98	0.45
1:G:2:LYS:HZ2	1:G:48:HIS:HB3	1.81	0.45
1:H:35:LEU:HD11	1:H:67:GLN:HE21	1.82	0.45
1:K:166:PHE:O	1:K:166:PHE:CD1	2.70	0.45
1:F:224:ASP:HA	1:F:227:THR:HG22	1.99	0.45
1:G:35:LEU:HA	1:G:38:VAL:HG22	1.99	0.45
1:J:320:MET:HB3	1:J:324:THR:HG21	1.98	0.45
1:L:353:VAL:HG21	1:L:359:ILE:HD11	1.99	0.45
1:K:27:ASP:OD1	1:K:27:ASP:N	2.50	0.45
2:B:138:LEU:HB3	2:B:185:LEU:HB3	1.99	0.45
2:B:376:LYS:HB2	2:B:381:LEU:HD21	1.99	0.45
2:D:267:ASP:N	2:D:267:ASP:OD1	2.49	0.45
1:E:27:ASP:HB2	1:E:292:LEU:HD22	1.99	0.45
1:E:333:ASN:HD22	1:E:350:GLY:HA2	1.82	0.45
1:H:64:MET:HE3	1:H:64:MET:HB3	1.87	0.45
1:L:55:TYR:CD2	1:L:55:TYR:O	2.70	0.45
1:G:43:ALA:O	1:G:118:GLN:NE2	2.50	0.44
1:H:43:ALA:O	1:H:118:GLN:NE2	2.50	0.44
1:E:166:PHE:O	1:E:166:PHE:CD1	2.70	0.44
1:H:34:LEU:HD12	1:H:35:LEU:HD22	1.98	0.44
2:A:192:LYS:HA	2:A:192:LYS:HD2	1.84	0.44
2:B:368:ARG:NH2	2:B:382:PRO:O	2.45	0.44
1:F:229:MET:HB3	1:F:229:MET:HE3	1.73	0.44
1:G:191:THR:OG1	1:G:192:SER:N	2.51	0.44
1:L:55:TYR:O	1:L:55:TYR:CG	2.70	0.44
1:L:172:ASN:ND2	1:L:176:TYR:OH	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:VAL:HG23	1:E:75:ILE:HG23	2.00	0.44
1:F:291:VAL:HA	1:F:308:VAL:HG22	2.00	0.44
1:L:322:ASN:HB3	1:L:323:VAL:H	1.47	0.44
1:K:141:PRO:HB3	1:K:168:SER:HB2	1.99	0.44
2:A:249:LYS:HD3	2:A:249:LYS:HA	1.89	0.44
2:C:332:GLU:HB2	2:C:333:HIS:CD2	2.53	0.44
1:L:51:LEU:HD22	1:L:51:LEU:N	2.31	0.44
1:I:191:THR:OG1	1:I:192:SER:N	2.51	0.44
1:J:229:MET:HE3	1:J:229:MET:HB3	1.78	0.44
1:I:320:MET:CE	1:I:324:THR:CG2	2.96	0.44
3:H:401:GDD:O5'	3:H:401:GDD:H8	2.17	0.44
1:K:13:ARG:HB3	1:K:220:GLY:O	2.17	0.43
1:I:320:MET:CE	1:I:324:THR:HG21	2.47	0.43
1:E:162:LYS:HD2	1:E:162:LYS:HA	1.69	0.43
3:L:401:GDD:O5'	3:L:401:GDD:H8	2.18	0.43
1:K:13:ARG:HG2	1:K:221:GLN:HG2	1.99	0.43
2:D:17:PHE:CD2	2:D:17:PHE:O	2.70	0.43
2:D:359:ASP:OD2	2:D:359:ASP:N	2.51	0.43
1:G:161:GLU:OE1	1:G:161:GLU:HA	2.18	0.43
1:J:237:ARG:HH21	1:J:244:LEU:HD22	1.82	0.43
2:A:20:LEU:HD21	2:A:340:ILE:HG21	2.00	0.43
1:E:239:LYS:HA	1:E:239:LYS:HD3	1.75	0.43
1:F:142:SER:HA	1:F:163:PRO:HG2	2.01	0.43
1:G:118:GLN:H	1:G:118:GLN:HG2	1.65	0.43
1:L:175:MET:HB3	1:L:175:MET:HE2	1.66	0.43
1:K:48:HIS:CE1	1:K:96:LEU:HD21	2.48	0.43
2:A:312:THR:O	2:A:312:THR:OG1	2.35	0.43
1:L:68:GLU:HB3	1:L:75:ILE:HD12	1.99	0.43
1:L:84:LEU:HB2	1:L:89:PRO:HD3	2.00	0.43
1:K:135:VAL:HG11	1:K:147:VAL:HG21	2.01	0.43
1:I:77:MET:HE1	1:I:78:SER:O	2.18	0.43
2:A:266:GLN:HE21	2:A:286:ASN:HD21	1.66	0.43
2:D:354:GLU:HB3	2:D:400:LEU:HD12	1.99	0.43
1:K:203:LYS:HA	1:K:203:LYS:HD3	1.74	0.43
2:A:359:ASP:O	2:A:369:MET:HE3	2.19	0.43
1:E:166:PHE:O	1:E:166:PHE:CG	2.70	0.43
1:F:264:GLN:H	1:F:264:GLN:HG3	1.66	0.43
1:K:60:LEU:O	1:K:64:MET:HB2	2.19	0.43
1:K:360:MET:HB2	1:L:358:ILE:HD13	2.00	0.43
1:I:50:ILE:HD12	1:I:96:LEU:HD23	2.00	0.43
2:B:259:ARG:NH2	2:B:359:ASP:OD2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:GLN:NE2	1:F:111:VAL:O	2.52	0.43
1:F:304:GLU:O	1:F:321:GLU:HA	2.18	0.43
3:G:401:GDD:O3B	5:G:501:HOH:O	2.21	0.43
1:J:13:ARG:HA	1:J:13:ARG:HD3	1.70	0.43
1:F:266:CYS:HB2	1:F:284:VAL:H	1.84	0.43
1:K:166:PHE:O	1:K:166:PHE:HD1	2.02	0.43
1:K:212:LEU:CG	1:K:213:GLN:N	2.81	0.43
2:A:59:TYR:O	2:A:82:TYR:OH	2.33	0.43
1:F:279:VAL:HB	1:F:296:ARG:HG3	2.01	0.43
1:H:334:ASP:OD1	1:H:334:ASP:N	2.49	0.43
1:L:305:SER:O	1:L:322:ASN:O	2.37	0.43
1:K:2:LYS:HG2	1:K:48:HIS:CE1	2.54	0.43
2:A:17:PHE:HB2	2:A:250:SER:HB3	2.00	0.43
2:C:405:LEU:HD22	2:C:420:LEU:HD23	2.01	0.43
2:D:392:ARG:HE	2:D:392:ARG:HB2	1.69	0.43
1:J:91:ALA:HB2	1:J:186:ILE:HD13	2.01	0.43
1:J:282:ASP:O	1:J:299:SER:OG	2.26	0.43
1:I:81:GLU:H	1:I:81:GLU:HG3	1.68	0.42
1:E:187:GLN:HB2	1:E:189:GLN:HE21	1.82	0.42
1:F:7:VAL:HG12	1:F:24:PRO:HG3	2.01	0.42
1:L:106:VAL:HB	1:L:176:TYR:HB2	2.00	0.42
1:L:263:GLY:N	1:L:280:VAL:O	2.51	0.42
1:I:312:CYS:SG	1:I:313:ARG:N	2.92	0.42
2:B:10:GLY:HA3	2:B:58:PHE:CE2	2.54	0.42
2:B:169:GLU:HG3	2:B:170:LYS:HG2	2.01	0.42
1:G:334:ASP:OD2	1:G:334:ASP:N	2.52	0.42
1:L:52:ALA:HB2	1:L:89:PRO:HB3	2.01	0.42
1:L:226:LEU:HD23	1:L:226:LEU:HA	1.91	0.42
1:I:302:TRP:NE1	2:C:396:GLU:OE1	2.45	0.42
1:E:164:GLN:HB2	1:E:167:VAL:CG2	2.47	0.42
1:E:340:GLY:HA3	1:E:356:PRO:HB3	2.00	0.42
1:G:25:LEU:HD21	1:G:60:LEU:HB2	2.02	0.42
1:H:35:LEU:HA	1:H:38:VAL:HG22	2.00	0.42
1:J:86:THR:HG23	1:J:193:ILE:H	1.84	0.42
2:A:347:VAL:HA	2:A:393:ILE:HB	2.01	0.42
2:C:409:GLU:H	2:D:12:GLN:HE21	1.67	0.42
1:E:229:MET:HE3	1:E:229:MET:HB3	1.73	0.42
1:L:32:PRO:HB2	1:L:35:LEU:HD23	2.02	0.42
1:K:294:ASP:HB3	1:K:311:ARG:HG2	2.00	0.42
1:K:340:GLY:HA3	1:K:356:PRO:HB3	2.02	0.42
2:A:352:ARG:NH2	1:H:335:GLU:O	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:364:ASP:HB2	2:A:367:ALA:HB2	2.01	0.42
2:D:221:ARG:NH2	2:D:225:ASP:OD1	2.52	0.42
1:J:279:VAL:HB	1:J:296:ARG:HG3	2.02	0.42
1:H:175:MET:HE3	1:H:175:MET:HB2	1.88	0.42
1:J:25:LEU:O	1:J:25:LEU:HG	2.19	0.42
1:J:207:LEU:HD23	1:J:207:LEU:HA	1.87	0.42
1:K:24:PRO:HB2	1:K:34:LEU:HB2	2.00	0.42
1:K:160:VAL:HG12	1:K:162:LYS:O	2.20	0.42
2:A:8:ILE:HB	2:A:27:PRO:HG2	2.02	0.42
2:A:31:VAL:HG21	2:A:248:ILE:HD13	2.02	0.42
2:A:295:VAL:HG22	2:A:313:VAL:HB	2.01	0.42
2:B:120:ASP:OD1	2:B:264:ARG:NH2	2.53	0.42
1:F:95:ASP:OD1	1:F:95:ASP:N	2.53	0.42
1:H:91:ALA:HB2	1:H:186:ILE:HD13	2.02	0.42
1:L:94:ARG:HG3	1:L:183:LEU:HD21	2.02	0.42
2:B:3:LYS:O	2:B:110:PHE:HA	2.19	0.42
2:C:127:LEU:HD12	2:C:127:LEU:HA	1.83	0.42
2:C:119:SER:HB2	2:C:245:TRP:HD1	1.85	0.42
1:E:161:GLU:HG2	1:E:195:LYS:HB3	2.01	0.42
1:L:260:ALA:HB1	1:L:278:VAL:HG22	2.02	0.42
2:C:332:GLU:H	2:C:332:GLU:HG2	1.55	0.41
2:D:37:ILE:H	2:D:37:ILE:HG12	1.70	0.41
1:F:33:ILE:HA	1:F:36:HIS:HD2	1.85	0.41
1:G:15:ARG:HD2	1:G:15:ARG:HA	1.69	0.41
1:G:282:ASP:O	1:G:299:SER:OG	2.32	0.41
1:J:4:LEU:HD13	1:J:50:ILE:HG23	2.02	0.41
1:J:311:ARG:HE	1:J:311:ARG:HB3	1.69	0.41
1:K:71:LEU:HG	1:K:73:ILE:HB	2.02	0.41
1:I:35:LEU:O	1:I:39:GLU:HB2	2.20	0.41
1:I:94:ARG:O	1:I:98:SER:HB3	2.19	0.41
2:B:16:ARG:NH2	2:B:370:ASP:OD2	2.53	0.41
1:E:170:LYS:NZ	1:E:211:GLU:OE2	2.53	0.41
1:F:201:MET:HG2	1:F:207:LEU:HD13	2.01	0.41
1:G:130:GLU:HB2	1:G:206:GLN:HB3	2.03	0.41
1:J:14:LEU:H	1:J:14:LEU:HG	1.40	0.41
1:J:256:VAL:HG13	1:J:274:LEU:HD12	2.02	0.41
1:L:200:ILE:O	1:L:204:GLU:HG3	2.20	0.41
1:L:292:LEU:HD13	1:L:292:LEU:HA	1.89	0.41
1:I:112:ILE:HD13	1:I:112:ILE:HA	1.81	0.41
3:A:501:GDD:H8	3:A:501:GDD:H2'	1.88	0.41
1:E:4:LEU:HD22	1:E:106:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:THR:HG23	1:E:193:ILE:H	1.85	0.41
1:E:301:SER:OG	1:E:318:VAL:O	2.29	0.41
1:F:24:PRO:HG2	1:F:25:LEU:HD22	2.02	0.41
1:G:137:LYS:HE3	1:G:170:LYS:HZ2	1.85	0.41
1:G:150:GLU:HG3	1:G:157:HIS:HE1	1.84	0.41
1:H:156:ILE:HG21	1:H:207:LEU:HD11	2.02	0.41
1:L:124:HIS:HA	1:L:127:HIS:CE1	2.55	0.41
1:I:16:PRO:HG3	1:I:342:SER:HB3	2.01	0.41
2:B:15:THR:C	2:B:17:PHE:N	2.78	0.41
1:F:15:ARG:HD2	1:F:15:ARG:HA	1.80	0.41
1:H:87:ALA:HA	1:H:193:ILE:HB	2.00	0.41
1:H:142:SER:HA	1:H:163:PRO:HD2	2.01	0.41
1:J:269:GLY:HA3	1:J:287:ARG:HG2	2.03	0.41
1:J:285:CYS:HB3	1:J:302:TRP:HD1	1.84	0.41
1:L:53:VAL:HG13	1:L:57:SER:OG	2.20	0.41
2:C:138:LEU:HD12	2:C:138:LEU:HA	1.92	0.41
1:H:80:GLU:CD	3:H:401:GDD:H2N1	2.27	0.41
2:C:66:THR:O	2:C:70:GLU:HG2	2.21	0.41
1:H:219:ILE:HG22	1:H:225:PHE:HA	2.02	0.41
1:J:353:VAL:HG11	1:J:359:ILE:HD11	2.02	0.41
2:A:63:GLU:O	2:A:67:GLN:HB2	2.21	0.41
2:A:359:ASP:N	2:A:369:MET:HE1	2.21	0.41
1:E:99:GLU:H	1:E:99:GLU:HG3	1.69	0.41
1:H:104:PHE:HE2	1:H:183:LEU:HD11	1.85	0.41
1:K:172:ASN:ND2	1:K:176:TYR:OH	2.48	0.41
1:E:133:ILE:HG13	1:E:176:TYR:CD1	2.55	0.41
1:G:106:VAL:HB	1:G:176:TYR:HB2	2.02	0.41
1:H:144:TYR:HB3	3:H:401:GDD:O41	2.20	0.41
2:D:187:SER:HB3	2:D:189:GLU:HG2	2.03	0.41
1:E:221:GLN:HE21	1:E:221:GLN:HB3	1.61	0.41
1:H:27:ASP:OD1	1:H:27:ASP:N	2.53	0.41
1:J:137:LYS:HG2	1:J:169:ASN:HD22	1.84	0.41
1:L:71:LEU:O	1:L:73:ILE:HG12	2.21	0.41
1:L:109:SER:N	3:L:401:GDD:O3'	2.50	0.41
1:L:233:LEU:HA	1:L:233:LEU:HD23	1.81	0.41
1:E:150:GLU:HB3	1:E:157:HIS:CE1	2.55	0.41
1:G:202:ALA:HB2	1:G:207:LEU:HD12	2.03	0.41
1:H:189:GLN:H	1:H:189:GLN:HG3	1.57	0.41
1:E:161:GLU:H	1:E:161:GLU:HG3	1.60	0.40
1:H:17:LEU:HD11	1:H:307:ILE:HG21	2.03	0.40
1:L:51:LEU:HD23	1:L:77:MET:HA	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:226:LEU:HD23	1:K:226:LEU:HA	1.91	0.40
2:B:175:ILE:HD13	2:B:175:ILE:HA	1.92	0.40
2:C:37:ILE:HA	2:C:40:HIS:CD2	2.54	0.40
1:H:223:LYS:CE	1:H:224:ASP:OD1	2.70	0.40
1:H:226:LEU:HD12	1:H:323:VAL:HG12	2.02	0.40
1:L:267:SER:O	1:L:267:SER:OG	2.38	0.40
1:K:191:THR:OG1	1:K:192:SER:N	2.53	0.40
1:I:96:LEU:HD12	1:I:96:LEU:HA	1.97	0.40
1:I:178:LEU:HD13	1:I:178:LEU:HA	1.92	0.40
1:I:335:GLU:OE2	2:C:318:ARG:NE	2.54	0.40
1:F:6:LEU:O	1:F:109:SER:OG	2.35	0.40
1:I:324:THR:O	1:I:324:THR:HG23	2.22	0.40
1:G:129:GLN:HE21	1:G:129:GLN:HB3	1.57	0.40
1:G:136:THR:HG22	1:G:173:ALA:HB2	2.04	0.40
1:J:112:ILE:HD13	1:J:115:PHE:HZ	1.85	0.40
1:I:360:MET:SD	1:J:358:ILE:HD11	2.61	0.40
2:B:347:VAL:HA	2:B:393:ILE:HB	2.03	0.40
1:G:122:GLN:CG	1:G:123:PHE:N	2.84	0.40
1:J:17:LEU:HD11	1:J:307:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	358/360 (99%)	338 (94%)	20 (6%)	0	100	100
1	F	358/360 (99%)	343 (96%)	15 (4%)	0	100	100
1	G	358/360 (99%)	339 (95%)	16 (4%)	3 (1%)	16	44
1	H	358/360 (99%)	333 (93%)	25 (7%)	0	100	100
1	I	358/360 (99%)	344 (96%)	14 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	358/360 (99%)	333 (93%)	24 (7%)	1 (0%)	36	65
1	K	358/360 (99%)	333 (93%)	23 (6%)	2 (1%)	21	50
1	L	358/360 (99%)	342 (96%)	16 (4%)	0	100	100
2	A	403/420 (96%)	384 (95%)	17 (4%)	2 (0%)	24	54
2	B	402/420 (96%)	382 (95%)	19 (5%)	1 (0%)	43	71
2	C	402/420 (96%)	381 (95%)	19 (5%)	2 (0%)	24	54
2	D	402/420 (96%)	390 (97%)	12 (3%)	0	100	100
All	All	4473/4560 (98%)	4242 (95%)	220 (5%)	11 (0%)	44	71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	359	ASP
1	G	163	PRO
2	C	359	ASP
2	C	360	PRO
1	G	154	GLY
1	K	163	PRO
2	A	360	PRO
1	K	165	VAL
2	B	277	THR
1	J	163	PRO
1	G	165	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	311/311 (100%)	275 (88%)	36 (12%)	5	20
1	F	311/311 (100%)	283 (91%)	28 (9%)	9	30
1	G	311/311 (100%)	277 (89%)	34 (11%)	6	22
1	H	311/311 (100%)	278 (89%)	33 (11%)	6	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	311/311 (100%)	279 (90%)	32 (10%)	7	24
1	J	311/311 (100%)	280 (90%)	31 (10%)	7	26
1	K	310/311 (100%)	275 (89%)	35 (11%)	5	21
1	L	310/311 (100%)	288 (93%)	22 (7%)	13	39
2	A	344/354 (97%)	323 (94%)	21 (6%)	17	43
2	B	344/354 (97%)	324 (94%)	20 (6%)	18	45
2	C	344/354 (97%)	324 (94%)	20 (6%)	18	45
2	D	344/354 (97%)	321 (93%)	23 (7%)	15	41
All	All	3862/3904 (99%)	3527 (91%)	335 (9%)	12	32

All (335) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	13	ARG
1	K	14	LEU
1	K	15	ARG
1	K	27	ASP
1	K	33	ILE
1	K	38	VAL
1	K	41	LEU
1	K	46	VAL
1	K	50	ILE
1	K	54	SER
1	K	63	GLU
1	K	69	GLN
1	K	77	MET
1	K	80	GLU
1	K	86	THR
1	K	107	LEU
1	K	127	HIS
1	K	147	VAL
1	K	153	THR
1	K	161	GLU
1	K	184	GLN
1	K	189	GLN
1	K	191	THR
1	K	194	GLU
1	K	197	VAL
1	K	233	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	253	ASN
1	K	266	CYS
1	K	267	SER
1	K	273	SER
1	K	278	VAL
1	K	281	GLU
1	K	323	VAL
1	K	324	THR
1	K	342	SER
1	I	27	ASP
1	I	35	LEU
1	I	41	LEU
1	I	50	ILE
1	I	51	LEU
1	I	65	LYS
1	I	68	GLU
1	I	77	MET
1	I	86	THR
1	I	106	VAL
1	I	110	ASP
1	I	111	VAL
1	I	112	ILE
1	I	134	LEU
1	I	136	THR
1	I	165	VAL
1	I	167	VAL
1	I	176	TYR
1	I	178	LEU
1	I	193	ILE
1	I	194	GLU
1	I	199	PRO
1	I	200	ILE
1	I	231	LEU
1	I	233	LEU
1	I	253	ASN
1	I	266	CYS
1	I	267	SER
1	I	273	SER
1	I	306	CYS
1	I	312	CYS
1	I	323	VAL
2	A	24	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	118	CYS
2	A	177	ASP
2	A	187	SER
2	A	194	LEU
2	A	219	THR
2	A	238	VAL
2	A	240	LEU
2	A	246	SER
2	A	253	SER
2	A	265	TYR
2	A	300	VAL
2	A	306	SER
2	A	312	THR
2	A	322	SER
2	A	363	ASN
2	A	369	MET
2	A	373	SER
2	A	397	VAL
2	A	398	LEU
2	A	402	SER
2	B	20	LEU
2	B	21	SER
2	B	77	ASN
2	B	83	LEU
2	B	118	CYS
2	B	149	SER
2	B	189	GLU
2	B	219	THR
2	B	277	THR
2	B	300	VAL
2	B	306	SER
2	B	326	HIS
2	B	329	THR
2	B	337	LEU
2	B	339	SER
2	B	345	SER
2	B	398	LEU
2	B	408	LYS
2	B	413	SER
2	B	420	LEU
2	C	20	LEU
2	C	24	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	124	SER
2	C	143	THR
2	C	238	VAL
2	C	255	LEU
2	C	277	THR
2	C	283	ILE
2	C	300	VAL
2	C	319	LEU
2	C	322	SER
2	C	325	LEU
2	C	332	GLU
2	C	339	SER
2	C	356	THR
2	C	363	ASN
2	C	369	MET
2	C	371	SER
2	C	372	GLU
2	C	397	VAL
2	D	2	LEU
2	D	54	LEU
2	D	65	LEU
2	D	118	CYS
2	D	135	HIS
2	D	143	THR
2	D	151	ASN
2	D	156	VAL
2	D	173	THR
2	D	219	THR
2	D	238	VAL
2	D	244	ILE
2	D	258	SER
2	D	263	SER
2	D	265	TYR
2	D	312	THR
2	D	339	SER
2	D	358	SER
2	D	359	ASP
2	D	369	MET
2	D	397	VAL
2	D	405	LEU
2	D	413	SER
1	E	6	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	7	VAL
1	E	25	LEU
1	E	34	LEU
1	E	49	VAL
1	E	58	GLN
1	E	59	VAL
1	E	60	LEU
1	E	73	ILE
1	E	79	HIS
1	E	92	LEU
1	E	95	ASP
1	E	100	THR
1	E	112	ILE
1	E	129	GLN
1	E	132	SER
1	E	134	LEU
1	E	152	ASP
1	E	153	THR
1	E	171	ILE
1	E	183	LEU
1	E	191	THR
1	E	193	ILE
1	E	196	GLU
1	E	197	VAL
1	E	199	PRO
1	E	204	GLU
1	E	212	LEU
1	E	227	THR
1	E	233	LEU
1	E	278	VAL
1	E	279	VAL
1	E	286	ILE
1	E	339	ASN
1	E	348	SER
1	E	351	GLU
1	F	7	VAL
1	F	30	ASN
1	F	46	VAL
1	F	49	VAL
1	F	60	LEU
1	F	95	ASP
1	F	134	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	135	VAL
1	F	138	VAL
1	F	144	TYR
1	F	148	VAL
1	F	165	VAL
1	F	167	VAL
1	F	171	ILE
1	F	193	ILE
1	F	197	VAL
1	F	199	PRO
1	F	200	ILE
1	F	253	ASN
1	F	273	SER
1	F	278	VAL
1	F	289	CYS
1	F	303	LEU
1	F	308	VAL
1	F	322	ASN
1	F	324	THR
1	F	334	ASP
1	F	355	GLU
1	G	12	THR
1	G	15	ARG
1	G	18	THR
1	G	19	LEU
1	G	26	VAL
1	G	47	ASP
1	G	50	ILE
1	G	53	VAL
1	G	60	LEU
1	G	86	THR
1	G	102	ASP
1	G	122	GLN
1	G	134	LEU
1	G	146	VAL
1	G	147	VAL
1	G	153	THR
1	G	177	ILE
1	G	189	GLN
1	G	191	THR
1	G	192	SER
1	G	193	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	194	GLU
1	G	197	VAL
1	G	212	LEU
1	G	227	THR
1	G	230	CYS
1	G	257	ASP
1	G	259	SER
1	G	267	SER
1	G	318	VAL
1	G	324	THR
1	G	328	GLU
1	G	342	SER
1	G	353	VAL
1	H	6	LEU
1	H	12	THR
1	H	20	SER
1	H	31	LYS
1	H	35	LEU
1	H	46	VAL
1	H	54	SER
1	H	74	ARG
1	H	92	LEU
1	H	95	ASP
1	H	100	THR
1	H	111	VAL
1	H	150	GLU
1	H	153	THR
1	H	171	ILE
1	H	178	LEU
1	H	182	VAL
1	H	193	ILE
1	H	199	PRO
1	H	201	MET
1	H	211	GLU
1	H	212	LEU
1	H	223	LYS
1	H	242	GLU
1	H	267	SER
1	H	278	VAL
1	H	289	CYS
1	H	321	GLU
1	H	324	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	334	ASP
1	H	335	GLU
1	H	359	ILE
1	H	360	MET
1	J	6	LEU
1	J	7	VAL
1	J	10	TYR
1	J	14	LEU
1	J	20	SER
1	J	46	VAL
1	J	47	ASP
1	J	51	LEU
1	J	69	GLN
1	J	78	SER
1	J	84	LEU
1	J	95	ASP
1	J	99	GLU
1	J	146	VAL
1	J	147	VAL
1	J	153	THR
1	J	167	VAL
1	J	175	MET
1	J	182	VAL
1	J	186	ILE
1	J	191	THR
1	J	197	VAL
1	J	199	PRO
1	J	227	THR
1	J	233	LEU
1	J	278	VAL
1	J	280	VAL
1	J	284	VAL
1	J	324	THR
1	J	344	LEU
1	J	353	VAL
1	L	20	SER
1	L	29	CYS
1	L	31	LYS
1	L	39	GLU
1	L	46	VAL
1	L	51	LEU
1	L	53	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	60	LEU
1	L	71	LEU
1	L	74	ARG
1	L	147	VAL
1	L	153	THR
1	L	182	VAL
1	L	183	LEU
1	L	191	THR
1	L	194	GLU
1	L	199	PRO
1	L	234	GLN
1	L	256	VAL
1	L	278	VAL
1	L	321	GLU
1	L	334	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	30	ASN
1	K	48	HIS
1	K	164	GLN
1	K	169	ASN
1	K	172	ASN
1	K	184	GLN
1	K	240	GLN
1	I	157	HIS
1	I	187	GLN
1	I	316	GLN
1	I	322	ASN
1	I	339	ASN
2	A	40	HIS
2	A	162	HIS
2	A	199	GLN
2	A	276	HIS
2	A	286	ASN
2	A	401	ASN
2	B	40	HIS
2	B	51	GLN
2	B	199	GLN
2	B	201	ASN
2	B	235	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	331	GLN
2	B	338	HIS
2	B	363	ASN
2	B	401	ASN
2	C	38	GLN
2	C	40	HIS
2	C	160	GLN
2	C	199	GLN
2	C	201	ASN
2	C	239	HIS
2	C	286	ASN
2	C	338	HIS
2	C	363	ASN
2	C	401	ASN
2	D	12	GLN
2	D	60	GLN
2	D	133	GLN
2	D	145	ASN
2	D	199	GLN
2	D	201	ASN
2	D	304	ASN
2	D	338	HIS
2	D	401	ASN
2	D	407	HIS
1	E	48	HIS
1	E	79	HIS
1	E	127	HIS
1	E	206	GLN
1	E	221	GLN
1	E	333	ASN
1	F	108	ASN
1	F	122	GLN
1	F	206	GLN
1	F	271	ASN
1	G	30	ASN
1	G	129	GLN
1	G	157	HIS
1	G	206	GLN
1	G	265	ASN
1	H	30	ASN
1	H	36	HIS
1	H	67	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	127	HIS
1	H	271	ASN
1	J	67	GLN
1	J	127	HIS
1	J	157	HIS
1	J	169	ASN
1	J	189	GLN
1	J	206	GLN
1	J	333	ASN
1	L	127	HIS
1	L	169	ASN
1	L	316	GLN
1	L	346	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GDD	A	501	-	41,42,42	0.87	2 (4%)	62,65,65	1.76	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDD	K	401	-	41,42,42	0.71	1 (2%)	62,65,65	1.62	12 (19%)
3	GDD	L	401	-	41,42,42	0.71	2 (4%)	62,65,65	1.61	12 (19%)
3	GDD	I	401	-	41,42,42	0.73	1 (2%)	62,65,65	1.60	12 (19%)
3	GDD	G	401	-	41,42,42	0.72	1 (2%)	62,65,65	1.66	12 (19%)
3	GDD	B	501	-	41,42,42	0.86	2 (4%)	62,65,65	1.69	12 (19%)
3	GDD	J	401	-	41,42,42	0.70	1 (2%)	62,65,65	1.64	11 (17%)
3	GDD	F	401	4	41,42,42	0.69	0	62,65,65	1.64	12 (19%)
3	GDD	D	501	-	41,42,42	0.79	2 (4%)	62,65,65	1.71	10 (16%)
3	GDD	E	401	4	41,42,42	0.70	0	62,65,65	1.57	10 (16%)
3	GDD	H	401	-	41,42,42	0.71	1 (2%)	62,65,65	1.62	12 (19%)
3	GDD	C	501	-	41,42,42	0.81	2 (4%)	62,65,65	1.71	13 (20%)

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
3	GDD	A	501	-	-	9/23/59/59	0/4/4/4
3	GDD	K	401	-	-	5/23/59/59	0/4/4/4
3	GDD	L	401	-	-	5/23/59/59	0/4/4/4
3	GDD	I	401	-	-	5/23/59/59	0/4/4/4
3	GDD	G	401	-	-	6/23/59/59	0/4/4/4
3	GDD	B	501	-	-	9/23/59/59	0/4/4/4
3	GDD	J	401	-	-	4/23/59/59	0/4/4/4
3	GDD	F	401	4	-	2/23/59/59	0/4/4/4
3	GDD	D	501	-	-	7/23/59/59	0/4/4/4
3	GDD	E	401	4	-	3/23/59/59	0/4/4/4
3	GDD	H	401	-	-	5/23/59/59	0/4/4/4
3	GDD	C	501	-	-	9/23/59/59	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GDD	C6-N1	-2.71	1.33	1.38
3	B	501	GDD	C6-N1	-2.61	1.34	1.38
3	D	501	GDD	C6-N1	-2.48	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	401	GDD	C6-N1	-2.36	1.34	1.38
3	H	401	GDD	C6-N1	-2.35	1.34	1.38
3	C	501	GDD	C6-N1	-2.27	1.34	1.38
3	L	401	GDD	C6-N1	-2.23	1.34	1.38
3	C	501	GDD	C5-N7	-2.19	1.34	1.39
3	G	401	GDD	C6-N1	-2.15	1.34	1.38
3	B	501	GDD	C5-N7	-2.15	1.34	1.39
3	A	501	GDD	C5-N7	-2.12	1.34	1.39
3	D	501	GDD	C5-N7	-2.11	1.34	1.39
3	J	401	GDD	C6-N1	-2.03	1.35	1.38
3	L	401	GDD	C5-N7	-2.02	1.35	1.39
3	I	401	GDD	C6-N1	-2.02	1.35	1.38

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GDD	C2-N1-C6	-5.54	115.06	125.11
3	D	501	GDD	C2-N1-C6	-5.44	115.25	125.11
3	B	501	GDD	C2-N1-C6	-5.39	115.33	125.11
3	C	501	GDD	C2-N1-C6	-5.36	115.39	125.11
3	K	401	GDD	C2-N1-C6	-5.24	115.60	125.11
3	H	401	GDD	C2-N1-C6	-5.24	115.61	125.11
3	J	401	GDD	C2-N1-C6	-5.16	115.75	125.11
3	D	501	GDD	C5-C4-N3	-5.15	120.19	128.39
3	G	401	GDD	C2-N1-C6	-5.14	115.78	125.11
3	L	401	GDD	C2-N1-C6	-5.08	115.90	125.11
3	A	501	GDD	C5-C4-N3	-4.97	120.48	128.39
3	E	401	GDD	C2-N1-C6	-4.96	116.11	125.11
3	F	401	GDD	C2-N1-C6	-4.95	116.14	125.11
3	G	401	GDD	C5-C4-N3	-4.93	120.54	128.39
3	I	401	GDD	C2-N1-C6	-4.83	116.35	125.11
3	K	401	GDD	C5-C4-N3	-4.81	120.74	128.39
3	H	401	GDD	C5-C4-N3	-4.79	120.77	128.39
3	L	401	GDD	C5-C4-N3	-4.77	120.80	128.39
3	J	401	GDD	C5-C4-N3	-4.65	120.98	128.39
3	C	501	GDD	C5-C4-N3	-4.60	121.06	128.39
3	F	401	GDD	C5-C4-N3	-4.60	121.06	128.39
3	B	501	GDD	C5-C4-N3	-4.58	121.10	128.39
3	I	401	GDD	C5-C4-N3	-4.42	121.36	128.39
3	E	401	GDD	C5-C4-N3	-4.37	121.44	128.39
3	D	501	GDD	N9-C4-N3	4.32	134.59	125.95
3	A	501	GDD	N9-C4-N3	4.24	134.43	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	401	GDD	N9-C4-N3	4.12	134.19	125.95
3	L	401	GDD	N9-C4-N3	4.12	134.18	125.95
3	H	401	GDD	N9-C4-N3	4.11	134.17	125.95
3	G	401	GDD	N9-C4-N3	4.02	133.99	125.95
3	B	501	GDD	N9-C4-N3	3.93	133.82	125.95
3	C	501	GDD	N9-C4-N3	3.87	133.69	125.95
3	I	401	GDD	N9-C4-N3	3.85	133.66	125.95
3	F	401	GDD	N9-C4-N3	3.85	133.65	125.95
3	E	401	GDD	N9-C4-N3	3.74	133.44	125.95
3	J	401	GDD	N9-C4-N3	3.72	133.39	125.95
3	I	401	GDD	C1'-N9-C8	-3.53	116.71	126.73
3	L	401	GDD	C1'-N9-C8	-3.52	116.72	126.73
3	D	501	GDD	C1'-N9-C8	-3.50	116.79	126.73
3	G	401	GDD	C1'-N9-C8	-3.49	116.81	126.73
3	F	401	GDD	C1'-N9-C8	-3.48	116.84	126.73
3	A	501	GDD	N9-C8-N7	-3.46	106.99	113.40
3	I	401	GDD	N9-C8-N7	-3.44	107.03	113.40
3	A	501	GDD	C5-C6-N1	3.36	121.81	113.25
3	F	401	GDD	N9-C8-N7	-3.32	107.24	113.40
3	A	501	GDD	C2-N3-C4	3.31	117.99	112.30
3	K	401	GDD	C1'-N9-C8	-3.30	117.37	126.73
3	H	401	GDD	C1'-N9-C8	-3.29	117.37	126.73
3	C	501	GDD	C1'-N9-C8	-3.28	117.41	126.73
3	B	501	GDD	C1'-N9-C8	-3.27	117.43	126.73
3	E	401	GDD	N9-C8-N7	-3.25	107.38	113.40
3	J	401	GDD	N9-C8-N7	-3.24	107.39	113.40
3	G	401	GDD	N9-C8-N7	-3.21	107.45	113.40
3	F	401	GDD	C2-N3-C4	3.21	117.82	112.30
3	C	501	GDD	N9-C8-N7	-3.20	107.46	113.40
3	D	501	GDD	C2-N3-C4	3.20	117.81	112.30
3	A	501	GDD	C1'-N9-C8	-3.19	117.66	126.73
3	B	501	GDD	N9-C8-N7	-3.19	107.48	113.40
3	D	501	GDD	C5-C6-N1	3.19	121.37	113.25
3	K	401	GDD	N9-C8-N7	-3.17	107.51	113.40
3	H	401	GDD	N9-C8-N7	-3.17	107.52	113.40
3	B	501	GDD	C5-C6-N1	3.13	121.22	113.25
3	J	401	GDD	C2-N3-C4	3.13	117.68	112.30
3	E	401	GDD	C1'-N9-C8	-3.12	117.86	126.73
3	D	501	GDD	N9-C8-N7	-3.10	107.65	113.40
3	C	501	GDD	O6-C6-C5	-3.06	118.45	126.53
3	C	501	GDD	C5-C6-N1	3.04	121.00	113.25
3	J	401	GDD	C1'-N9-C8	-3.04	118.10	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	401	GDD	C5-C6-N1	3.01	120.92	113.25
3	H	401	GDD	C5-C6-N1	3.01	120.91	113.25
3	B	501	GDD	O6-C6-C5	-3.00	118.61	126.53
3	E	401	GDD	C2-N3-C4	3.00	117.46	112.30
3	G	401	GDD	C2-N3-C4	2.99	117.45	112.30
3	A	501	GDD	O6-C6-C5	-2.97	118.69	126.53
3	C	501	GDD	C2-N3-C4	2.97	117.42	112.30
3	L	401	GDD	N9-C8-N7	-2.97	107.90	113.40
3	E	401	GDD	C5-C6-N1	2.96	120.79	113.25
3	J	401	GDD	C5-C6-N1	2.91	120.65	113.25
3	D	501	GDD	O6-C6-C5	-2.88	118.93	126.53
3	I	401	GDD	C2-N3-C4	2.86	117.23	112.30
3	B	501	GDD	C2-N3-C4	2.86	117.22	112.30
3	G	401	GDD	C5-C6-N1	2.86	120.52	113.25
3	F	401	GDD	C5-C6-N1	2.80	120.38	113.25
3	K	401	GDD	C2-N3-C4	2.78	117.09	112.30
3	L	401	GDD	C5-C6-N1	2.76	120.27	113.25
3	H	401	GDD	C2-N3-C4	2.75	117.04	112.30
3	I	401	GDD	C5-C6-N1	2.74	120.24	113.25
3	G	401	GDD	O6-C6-C5	-2.73	119.32	126.53
3	E	401	GDD	O6-C6-C5	-2.68	119.45	126.53
3	L	401	GDD	O6-C6-C5	-2.65	119.54	126.53
3	G	401	GDD	C8-N7-C5	2.64	108.96	104.26
3	L	401	GDD	C2-N3-C4	2.63	116.83	112.30
3	J	401	GDD	C8-N7-C5	2.59	108.88	104.26
3	I	401	GDD	C8-N7-C5	2.58	108.85	104.26
3	F	401	GDD	O6-C6-C5	-2.57	119.76	126.53
3	F	401	GDD	C8-N7-C5	2.56	108.81	104.26
3	J	401	GDD	O6-C6-C5	-2.53	119.86	126.53
3	C	501	GDD	O2'-C2'-C3'	-2.52	103.73	111.82
3	K	401	GDD	C8-N7-C5	2.50	108.71	104.26
3	H	401	GDD	C8-N7-C5	2.50	108.70	104.26
3	I	401	GDD	O6-C6-C5	-2.47	120.02	126.53
3	J	401	GDD	C61-C51-C41	-2.45	107.00	113.02
3	I	401	GDD	C8-N9-C4	2.44	110.59	106.03
3	D	501	GDD	C8-N7-C5	2.44	108.60	104.26
3	A	501	GDD	C8-N7-C5	2.43	108.60	104.26
3	K	401	GDD	O6-C6-C5	-2.41	120.17	126.53
3	H	401	GDD	O6-C6-C5	-2.40	120.20	126.53
3	L	401	GDD	C1'-N9-C4	2.39	133.54	126.49
3	L	401	GDD	C61-C51-C41	-2.34	107.26	113.02
3	D	501	GDD	C1'-N9-C4	2.34	133.41	126.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	GDD	C8-N7-C5	2.32	108.39	104.26
3	E	401	GDD	C8-N9-C4	2.31	110.36	106.03
3	G	401	GDD	C1'-N9-C4	2.31	133.30	126.49
3	C	501	GDD	C8-N7-C5	2.30	108.35	104.26
3	L	401	GDD	C8-N7-C5	2.29	108.34	104.26
3	F	401	GDD	C61-C51-C41	-2.28	107.42	113.02
3	C	501	GDD	C5'-C4'-C3'	-2.27	107.02	115.21
3	I	401	GDD	C2'-C1'-N9	-2.24	107.00	113.25
3	A	501	GDD	O2'-C2'-C3'	-2.24	104.63	111.82
3	A	501	GDD	C8-N9-C4	2.22	110.18	106.03
3	F	401	GDD	C8-N9-C4	2.21	110.17	106.03
3	F	401	GDD	C1'-N9-C4	2.20	132.98	126.49
3	B	501	GDD	C8-N9-C4	2.18	110.11	106.03
3	B	501	GDD	C8-N7-C5	2.16	108.12	104.26
3	L	401	GDD	N1-C2-N3	2.15	127.25	123.32
3	H	401	GDD	C8-N9-C4	2.13	110.02	106.03
3	K	401	GDD	C8-N9-C4	2.12	110.00	106.03
3	C	501	GDD	C8-N9-C4	2.12	110.00	106.03
3	B	501	GDD	O31-C31-C21	-2.11	105.41	110.38
3	H	401	GDD	N1-C2-N3	2.10	127.17	123.32
3	I	401	GDD	C1'-N9-C4	2.10	132.70	126.49
3	K	401	GDD	N1-C2-N3	2.09	127.15	123.32
3	J	401	GDD	C8-N9-C4	2.09	109.94	106.03
3	K	401	GDD	C1'-N9-C4	2.08	132.62	126.49
3	H	401	GDD	C1'-N9-C4	2.07	132.61	126.49
3	G	401	GDD	C61-C51-C41	-2.07	107.94	113.02
3	C	501	GDD	C1'-N9-C4	2.06	132.58	126.49
3	G	401	GDD	C8-N9-C4	2.05	109.87	106.03
3	B	501	GDD	C1'-N9-C4	2.01	132.41	126.49

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	401	GDD	C5'-O5'-PA-O1A
3	K	401	GDD	C5'-O5'-PA-O2A
3	K	401	GDD	C5'-O5'-PA-O3A
3	K	401	GDD	C11-O1B-PB-O3A
3	I	401	GDD	C5'-O5'-PA-O2A
3	I	401	GDD	C11-O1B-PB-O3A
3	A	501	GDD	C5'-O5'-PA-O2A
3	A	501	GDD	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	501	GDD	C5'-O5'-PA-O2A
3	C	501	GDD	C5'-O5'-PA-O1A
3	C	501	GDD	C5'-O5'-PA-O2A
3	C	501	GDD	C11-O1B-PB-O3A
3	D	501	GDD	C5'-O5'-PA-O2A
3	D	501	GDD	C5'-O5'-PA-O3A
3	D	501	GDD	C11-O1B-PB-O3A
3	E	401	GDD	C11-O1B-PB-O3A
3	F	401	GDD	C11-O1B-PB-O3A
3	G	401	GDD	C5'-O5'-PA-O2A
3	G	401	GDD	C11-O1B-PB-O3A
3	H	401	GDD	C5'-O5'-PA-O1A
3	H	401	GDD	C5'-O5'-PA-O2A
3	H	401	GDD	C5'-O5'-PA-O3A
3	H	401	GDD	C11-O1B-PB-O3A
3	J	401	GDD	C5'-O5'-PA-O2A
3	J	401	GDD	C5'-O5'-PA-O3A
3	J	401	GDD	C11-O1B-PB-O3A
3	L	401	GDD	C5'-O5'-PA-O2A
3	L	401	GDD	C11-O1B-PB-O3A
3	A	501	GDD	O4'-C4'-C5'-O5'
3	B	501	GDD	O4'-C4'-C5'-O5'
3	D	501	GDD	O4'-C4'-C5'-O5'
3	A	501	GDD	O51-C51-C61-O6A
3	A	501	GDD	C41-C51-C61-O6A
3	B	501	GDD	O51-C51-C61-O6A
3	A	501	GDD	C3'-C4'-C5'-O5'
3	D	501	GDD	C3'-C4'-C5'-O5'
3	K	401	GDD	C11-O1B-PB-O3B
3	E	401	GDD	C11-O1B-PB-O3B
3	H	401	GDD	C11-O1B-PB-O3B
3	L	401	GDD	C11-O1B-PB-O3B
3	A	501	GDD	PB-O3A-PA-O2A
3	D	501	GDD	PB-O3A-PA-O2A
3	I	401	GDD	C5'-O5'-PA-O1A
3	I	401	GDD	C5'-O5'-PA-O3A
3	A	501	GDD	C11-O1B-PB-O3A
3	B	501	GDD	C5'-O5'-PA-O1A
3	B	501	GDD	C5'-O5'-PA-O3A
3	C	501	GDD	C5'-O5'-PA-O3A
3	G	401	GDD	C5'-O5'-PA-O1A
3	G	401	GDD	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L	401	GDD	C5'-O5'-PA-O1A
3	L	401	GDD	C5'-O5'-PA-O3A
3	I	401	GDD	C21-C11-O1B-PB
3	C	501	GDD	PB-O3A-PA-O2A
3	B	501	GDD	C3'-C4'-C5'-O5'
3	F	401	GDD	C21-C11-O1B-PB
3	C	501	GDD	O4'-C4'-C5'-O5'
3	A	501	GDD	C11-O1B-PB-O3B
3	C	501	GDD	C11-O1B-PB-O3B
3	D	501	GDD	C11-O1B-PB-O2B
3	G	401	GDD	C11-O1B-PB-O2B
3	J	401	GDD	C11-O1B-PB-O2B
3	B	501	GDD	PB-O3A-PA-O2A
3	C	501	GDD	PB-O3A-PA-O1A
3	B	501	GDD	C41-C51-C61-O6A
3	E	401	GDD	C21-C11-O1B-PB
3	G	401	GDD	C21-C11-O1B-PB
3	C	501	GDD	O51-C51-C61-O6A
3	B	501	GDD	PB-O3A-PA-O1A

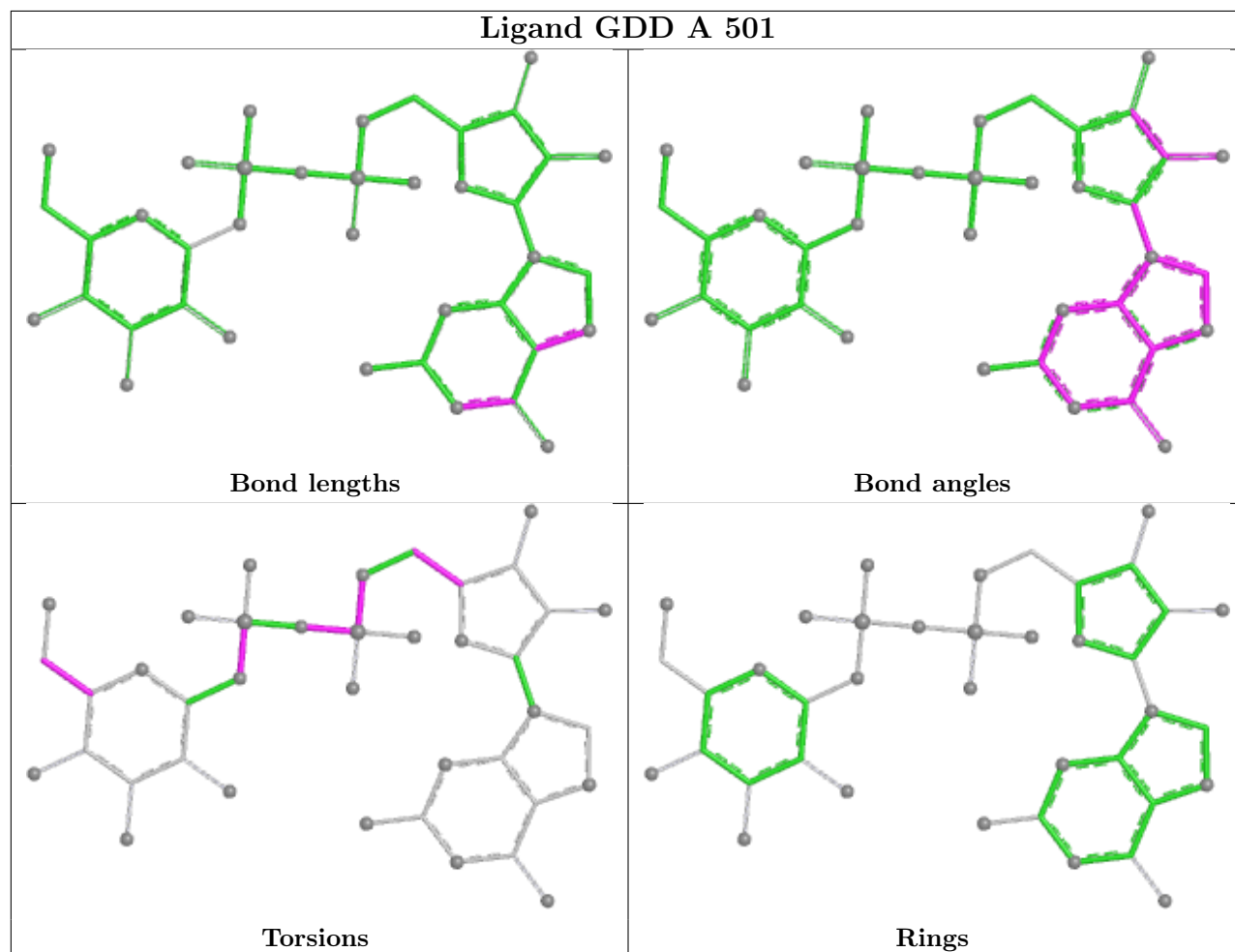
There are no ring outliers.

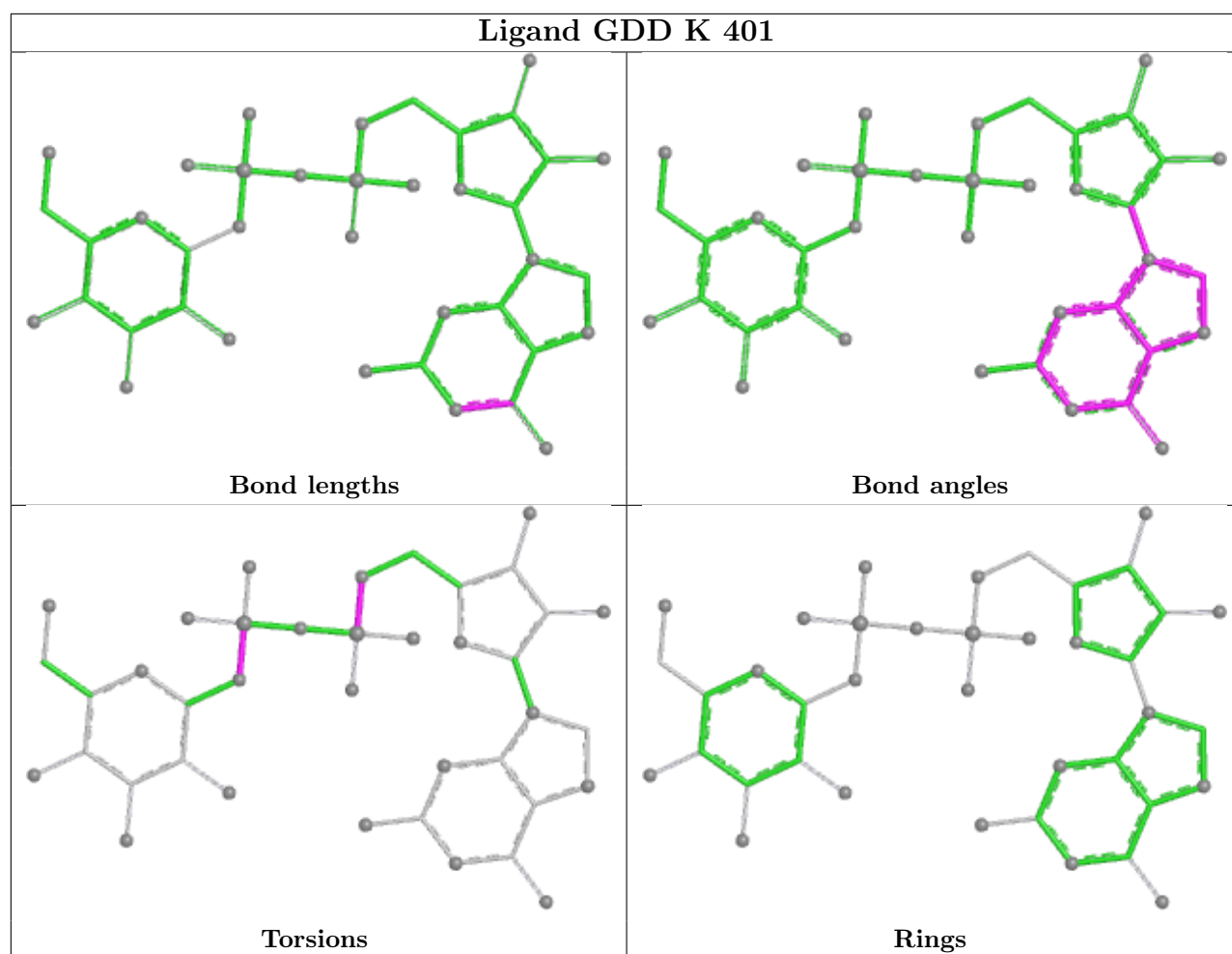
10 monomers are involved in 30 short contacts:

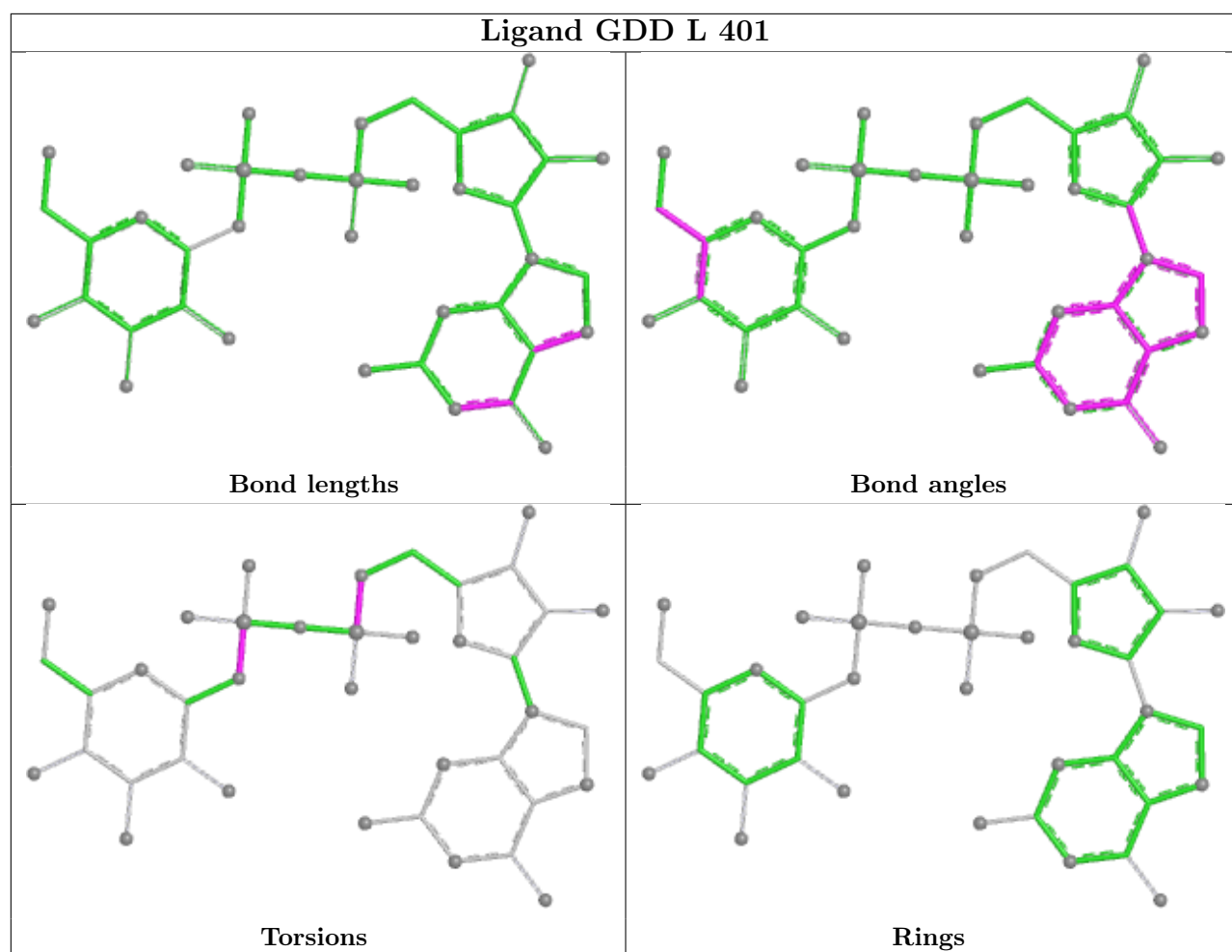
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GDD	1	0
3	K	401	GDD	6	0
3	L	401	GDD	2	0
3	I	401	GDD	4	0
3	G	401	GDD	4	0
3	B	501	GDD	1	0
3	J	401	GDD	1	0
3	F	401	GDD	2	0
3	E	401	GDD	3	0
3	H	401	GDD	6	0

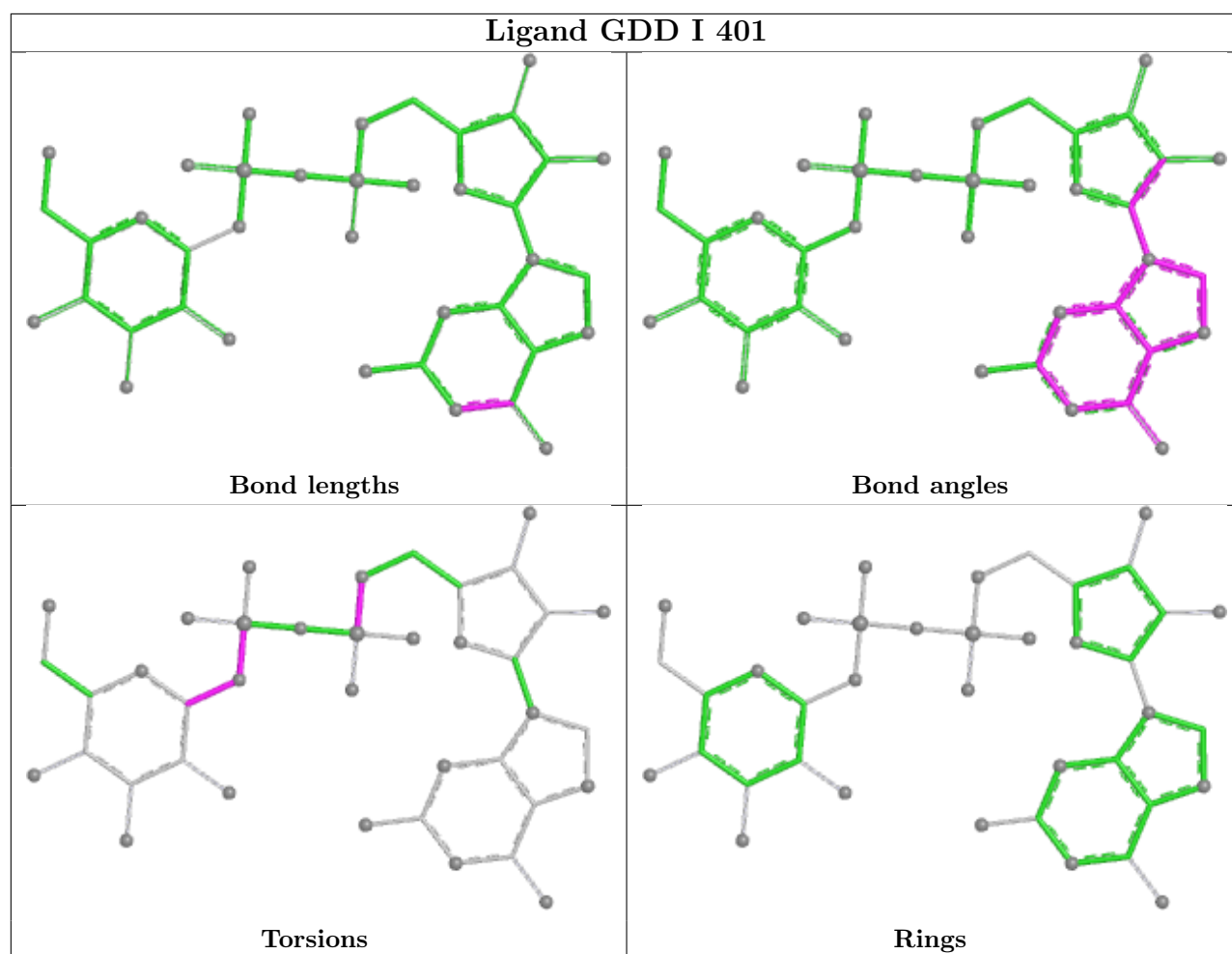
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

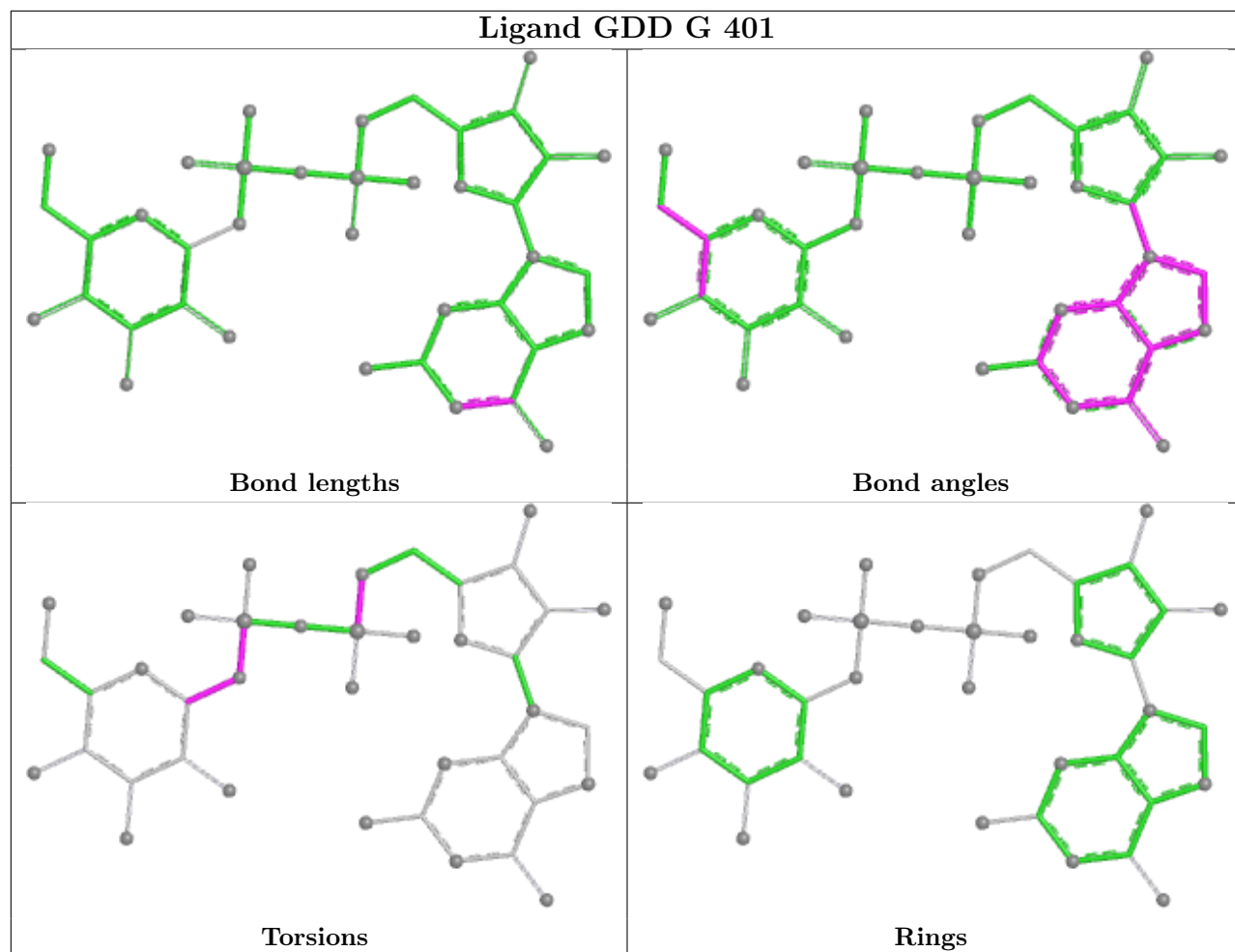
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

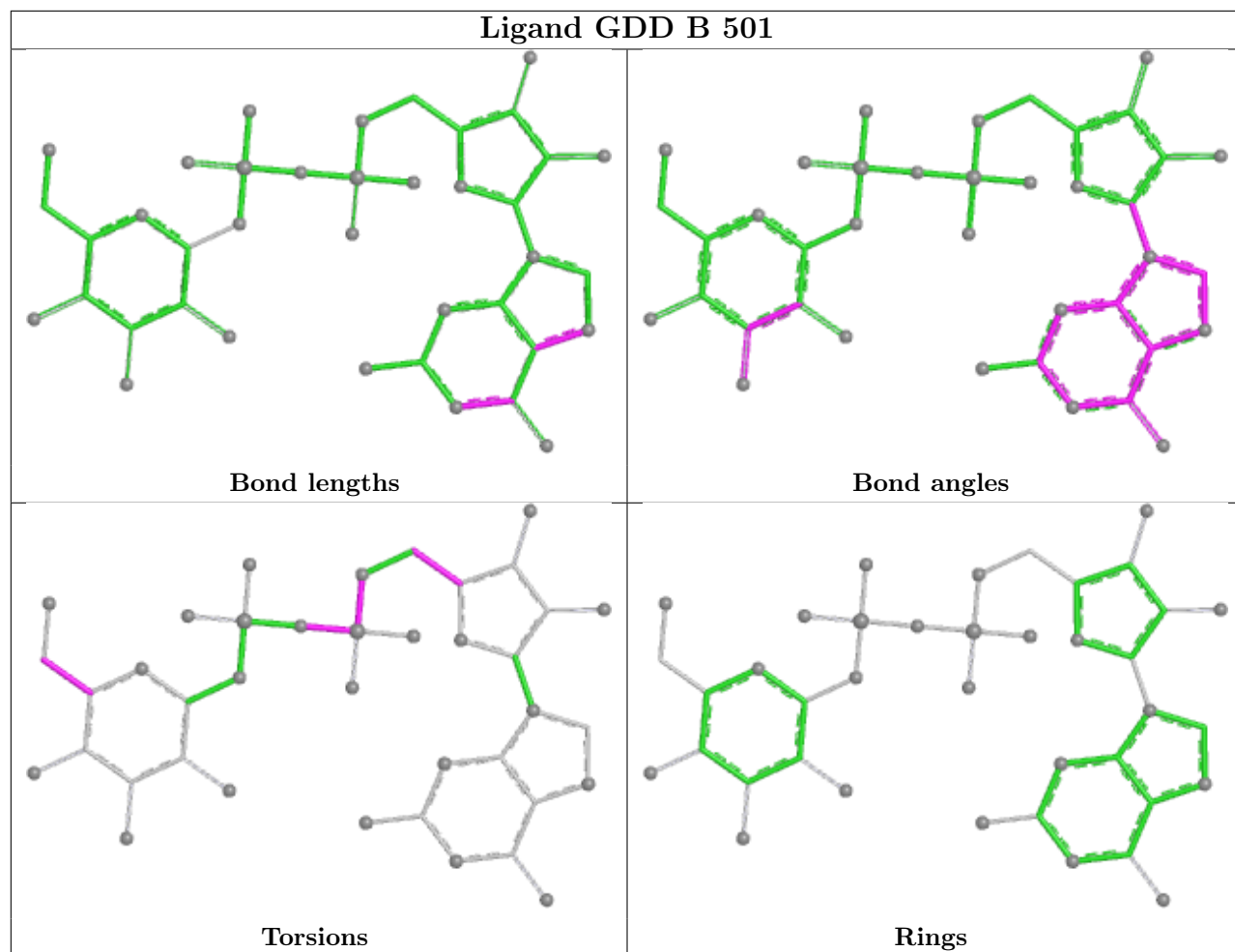


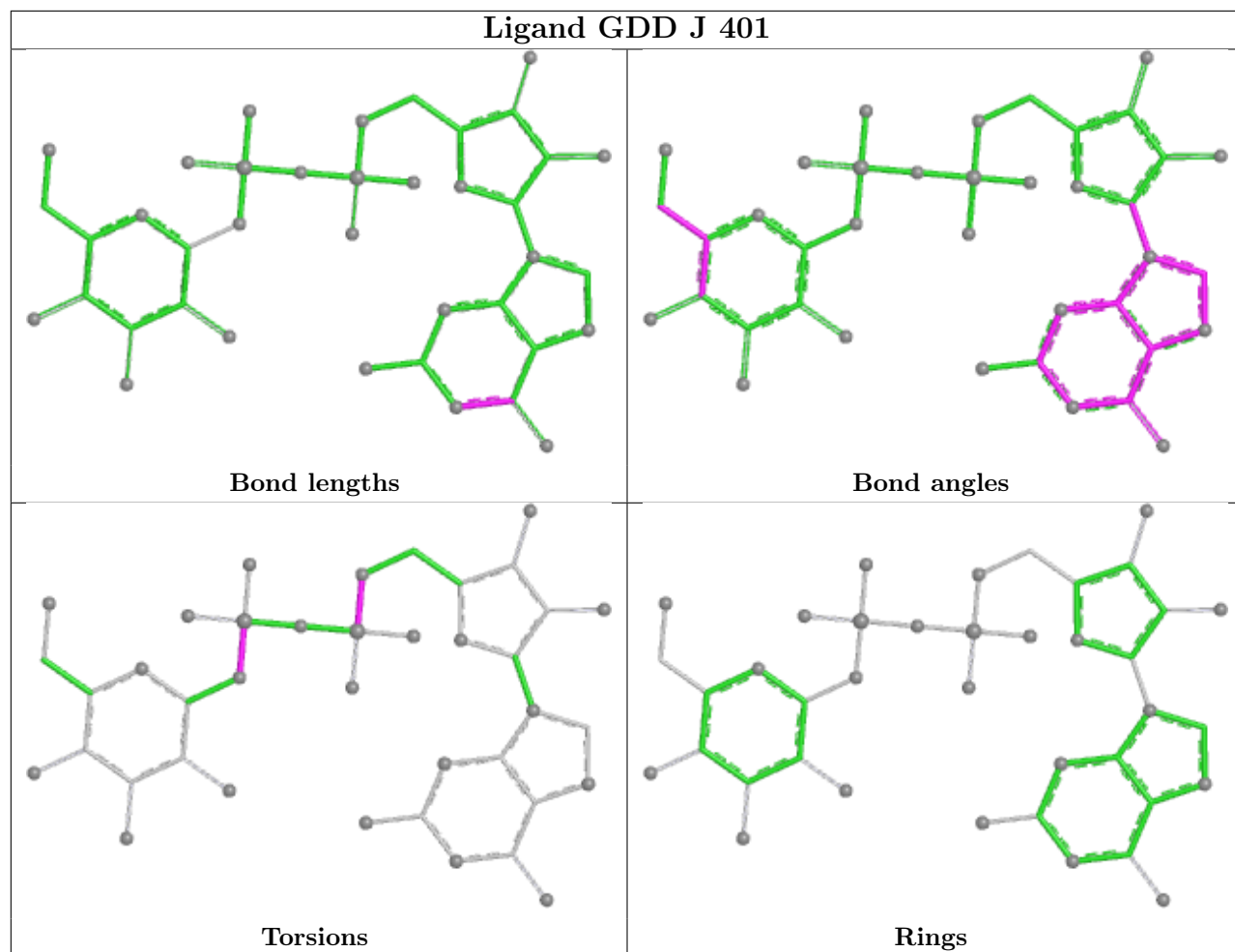


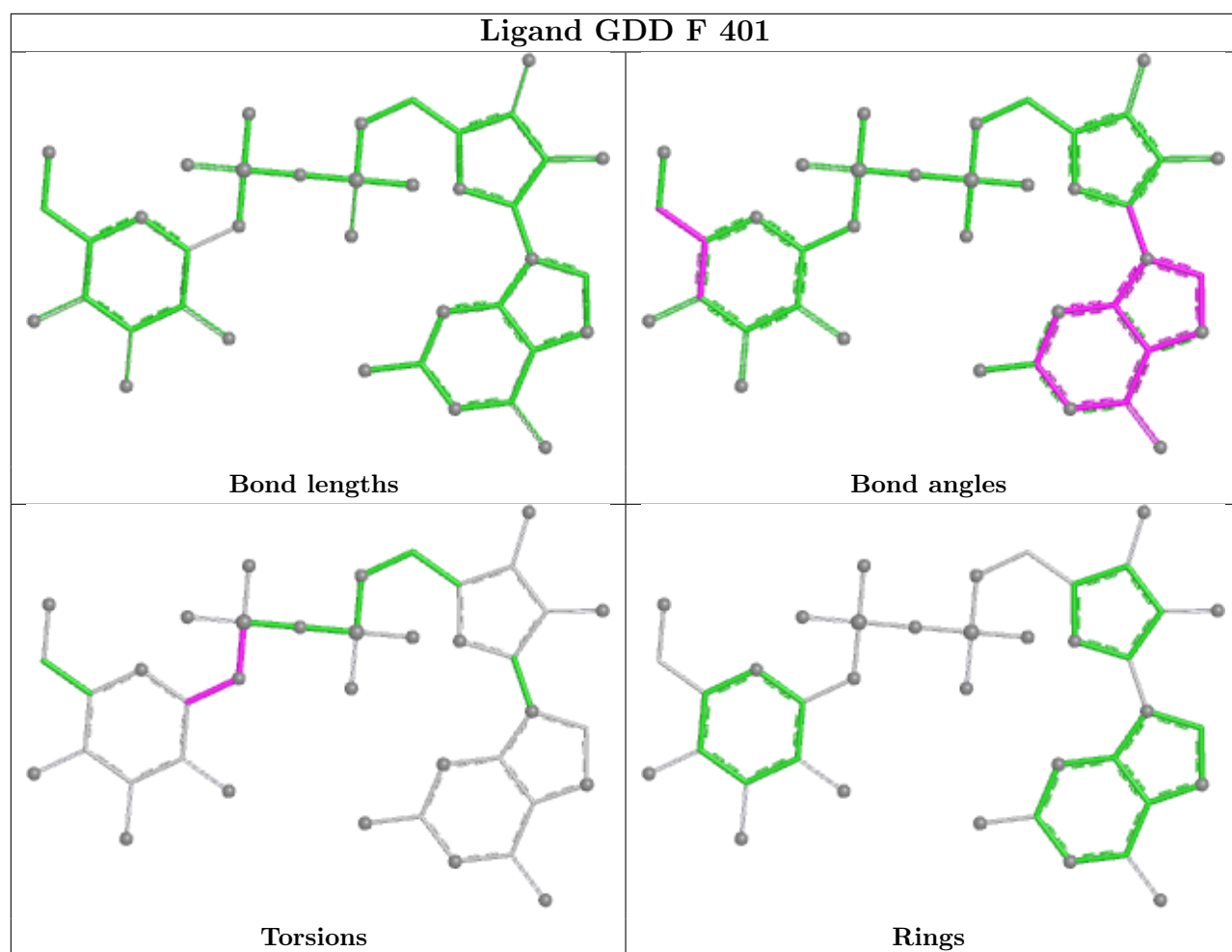


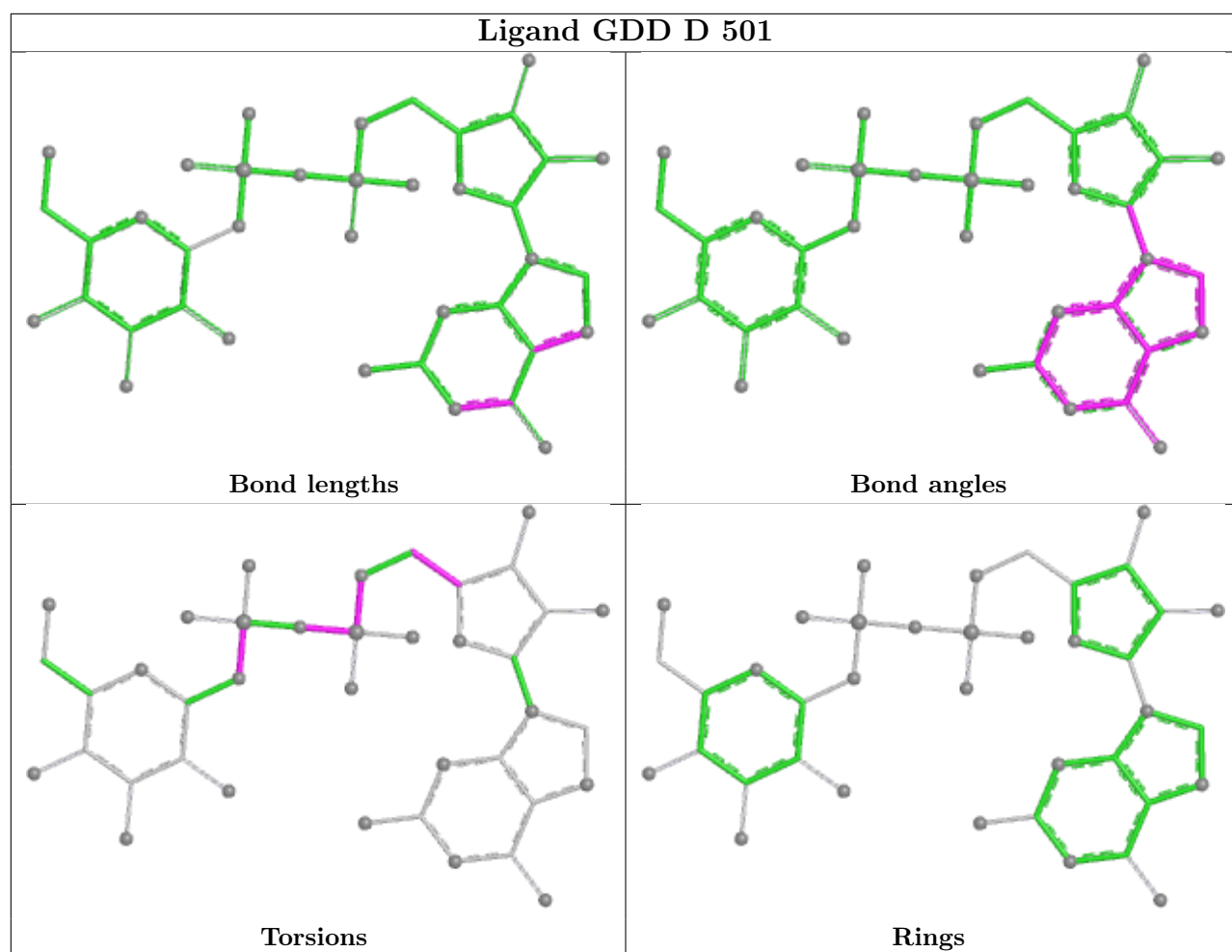


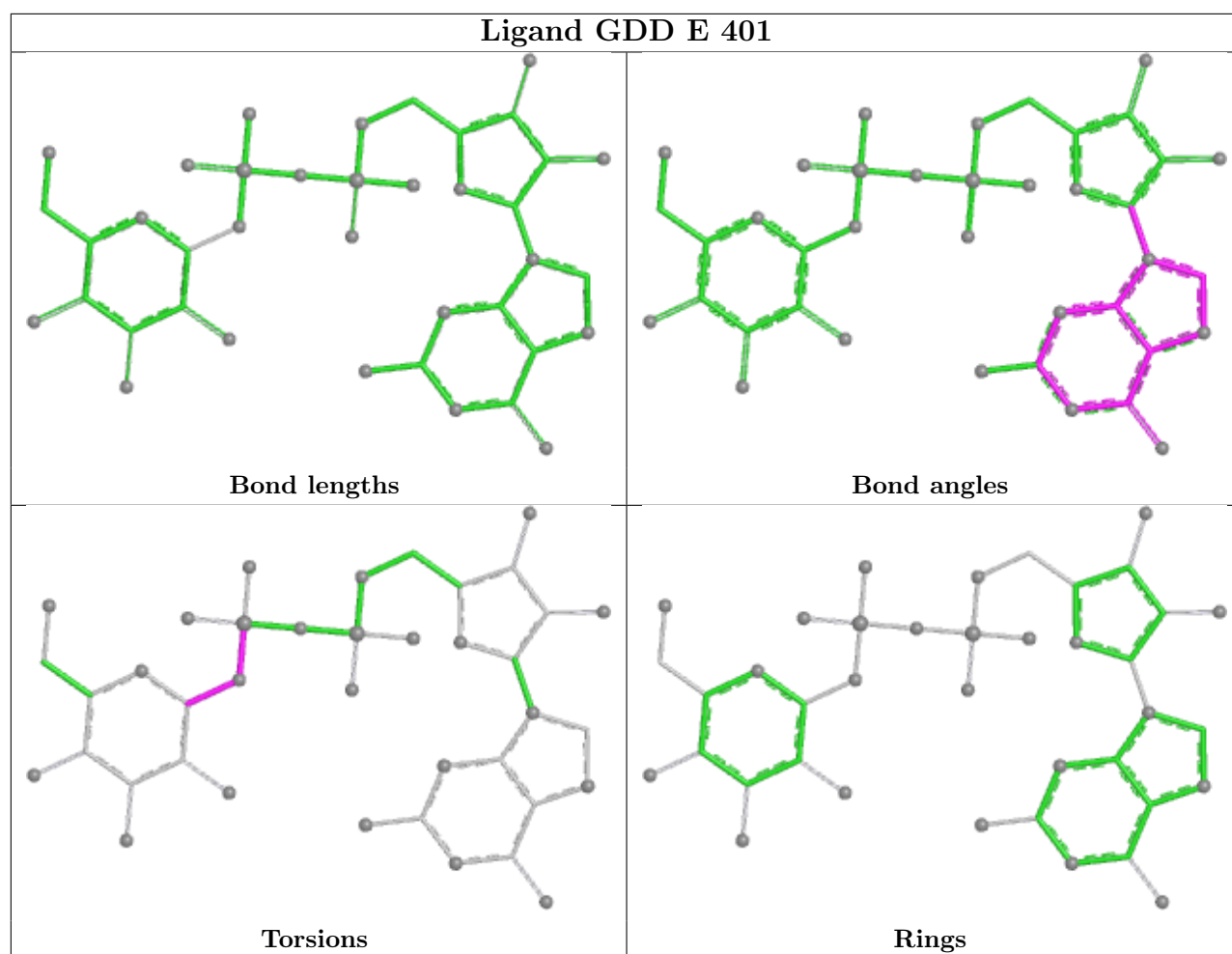


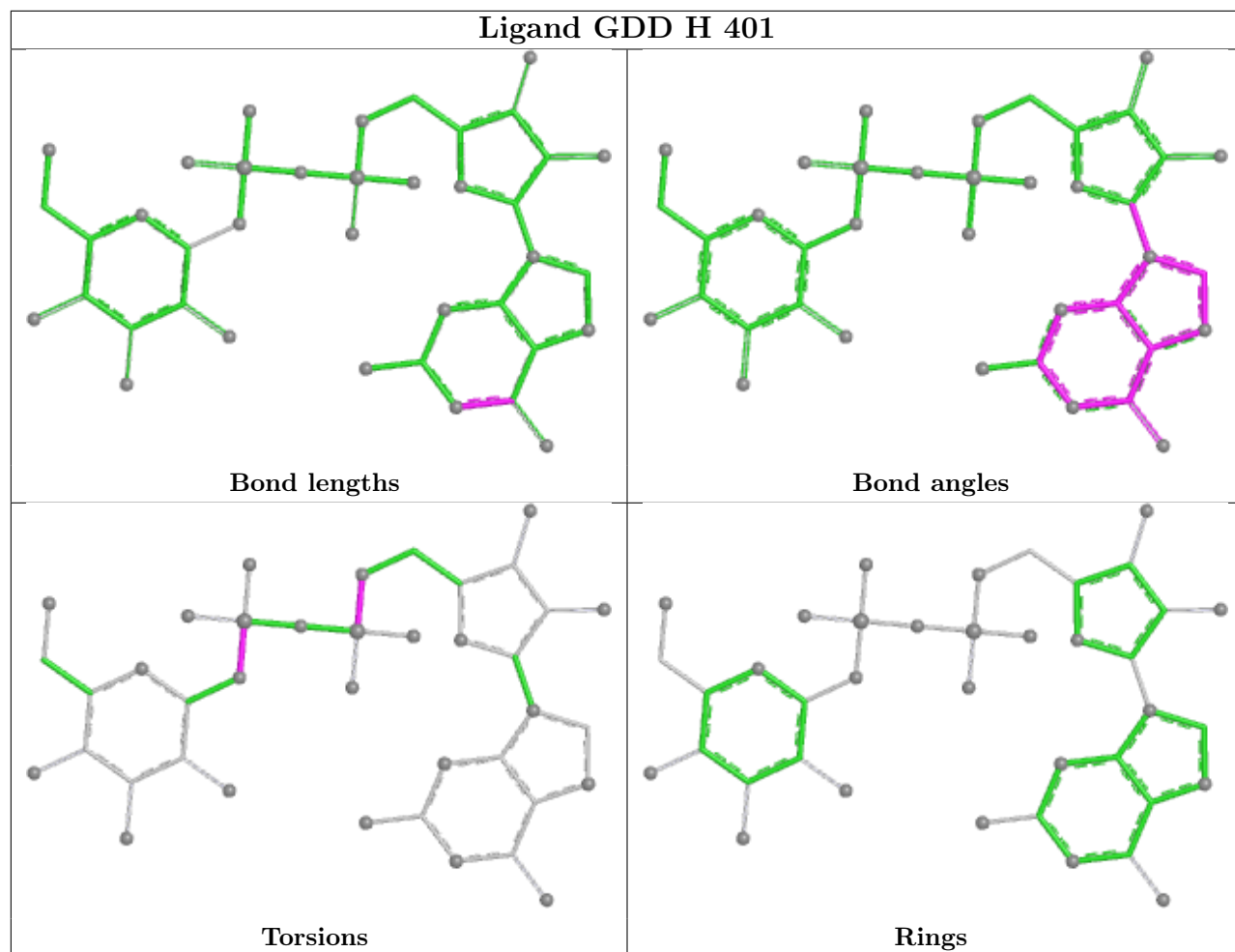


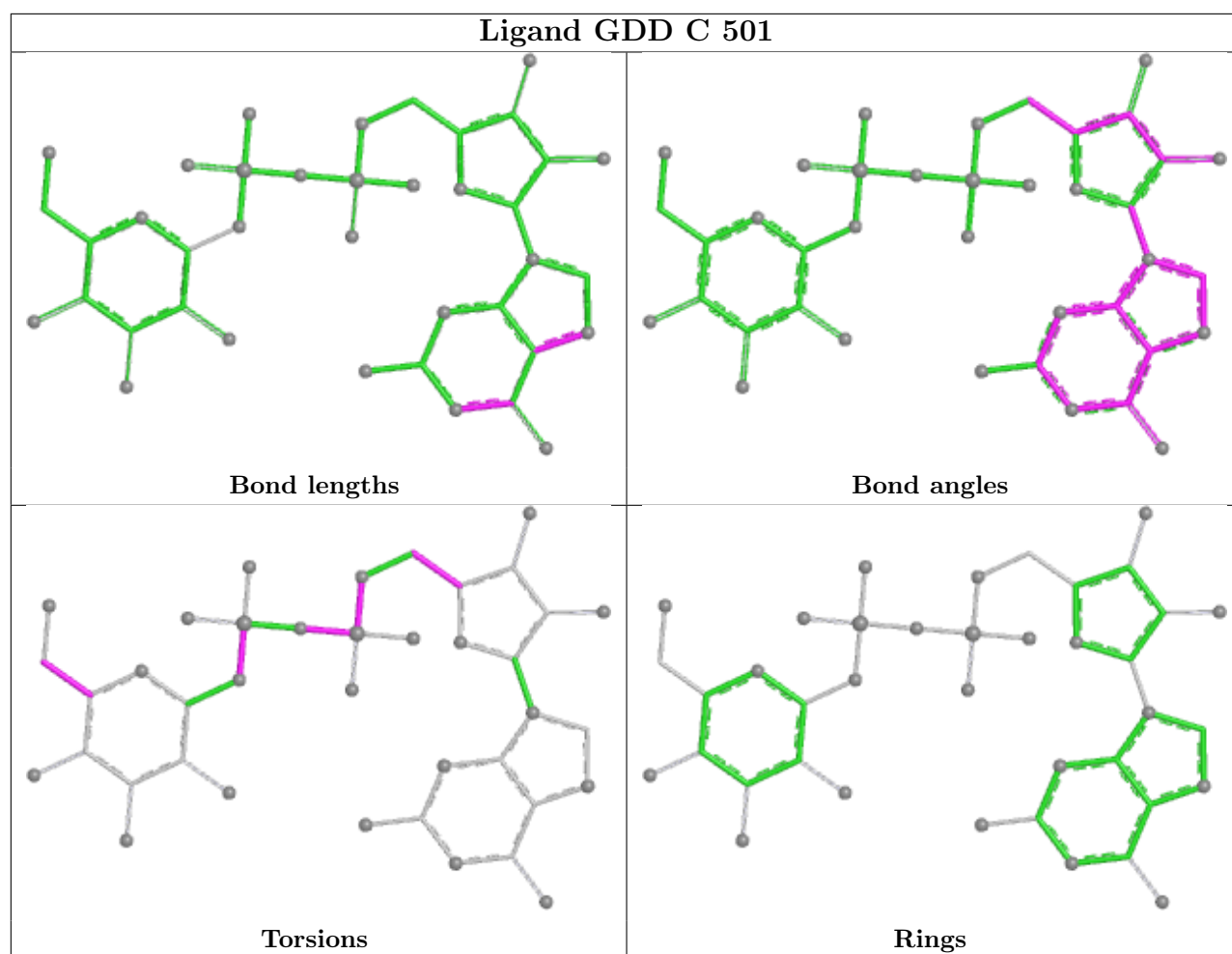












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

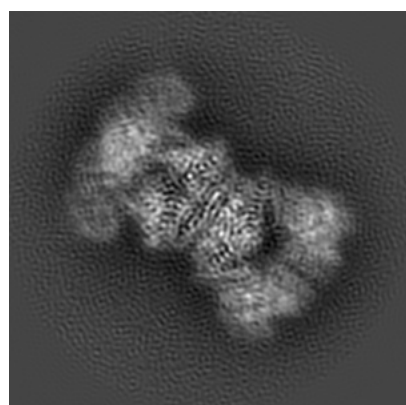
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30599. These allow visual inspection of the internal detail of the map and identification of artifacts.

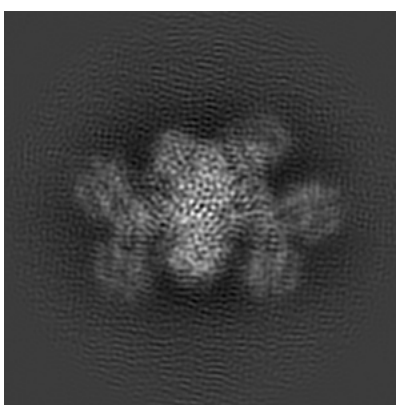
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

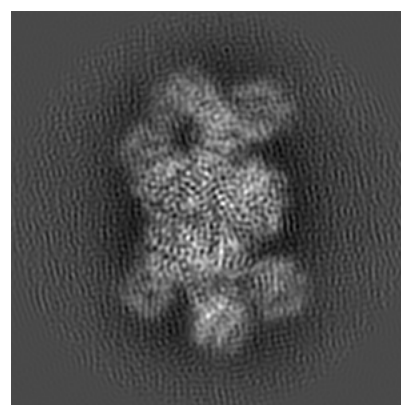
6.1.1 Primary map



X



Y

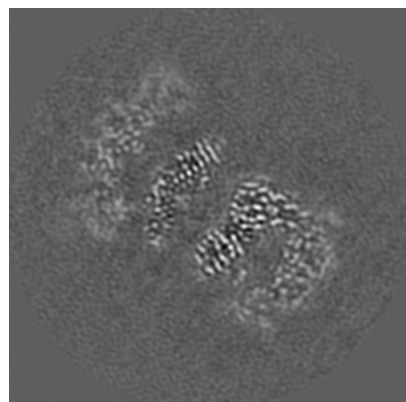


Z

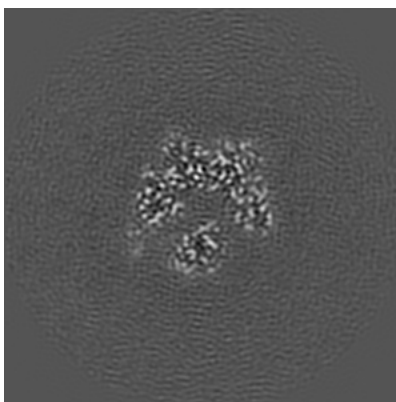
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

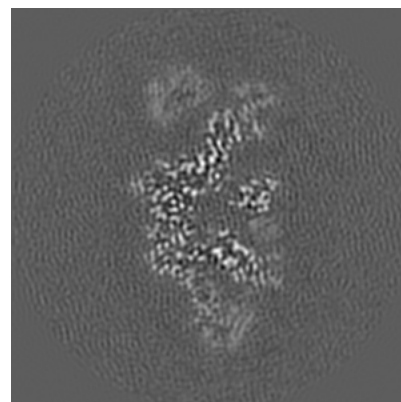
6.2.1 Primary map



X Index: 120



Y Index: 120

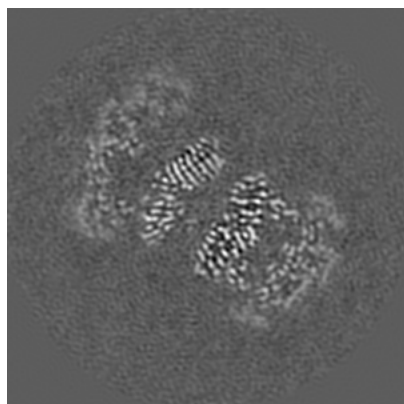


Z Index: 120

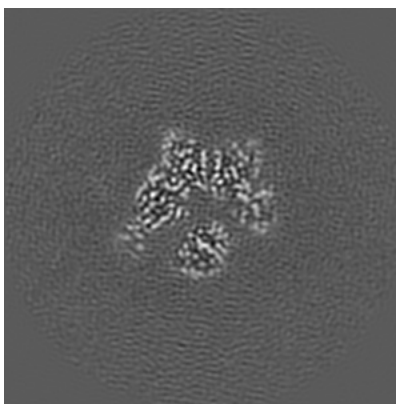
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

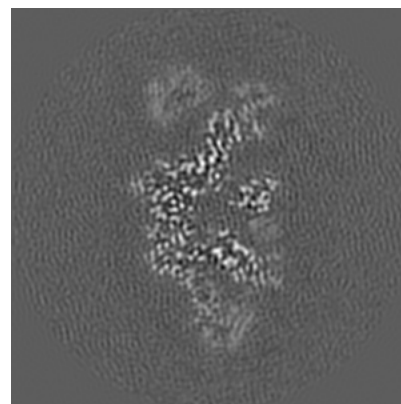
6.3.1 Primary map



X Index: 117



Y Index: 123

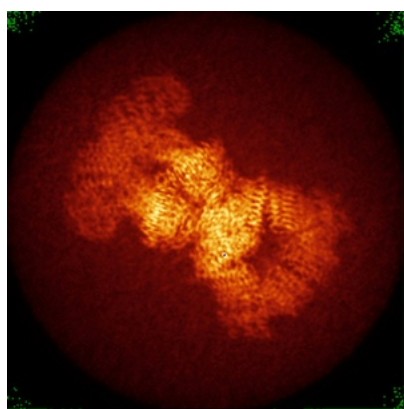


Z Index: 120

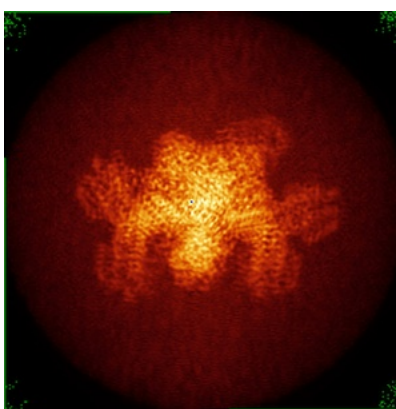
The images above show the largest variance slices of the map in three orthogonal directions.

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

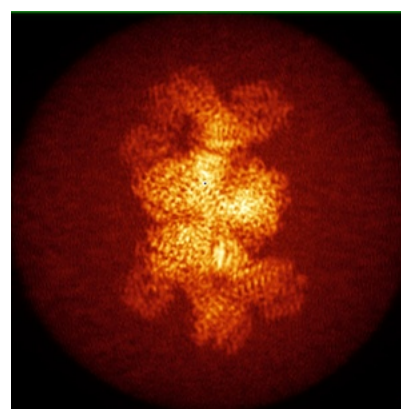
6.4.1 Primary map



X



Y

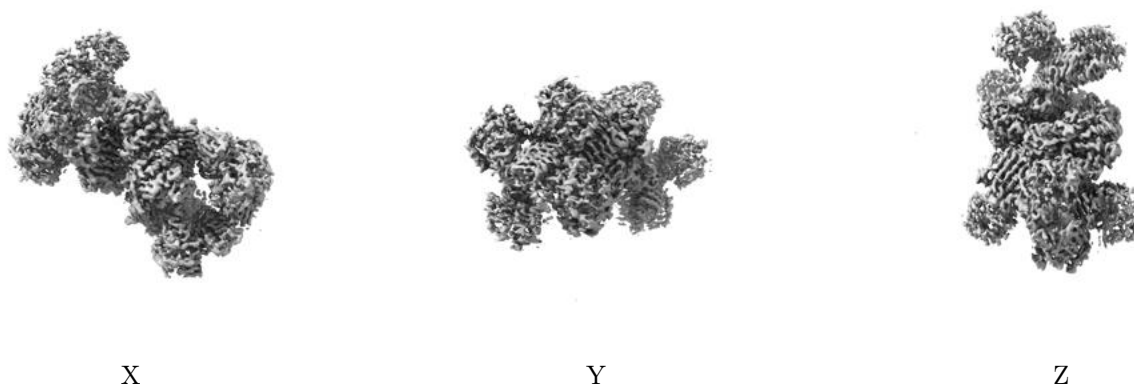


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

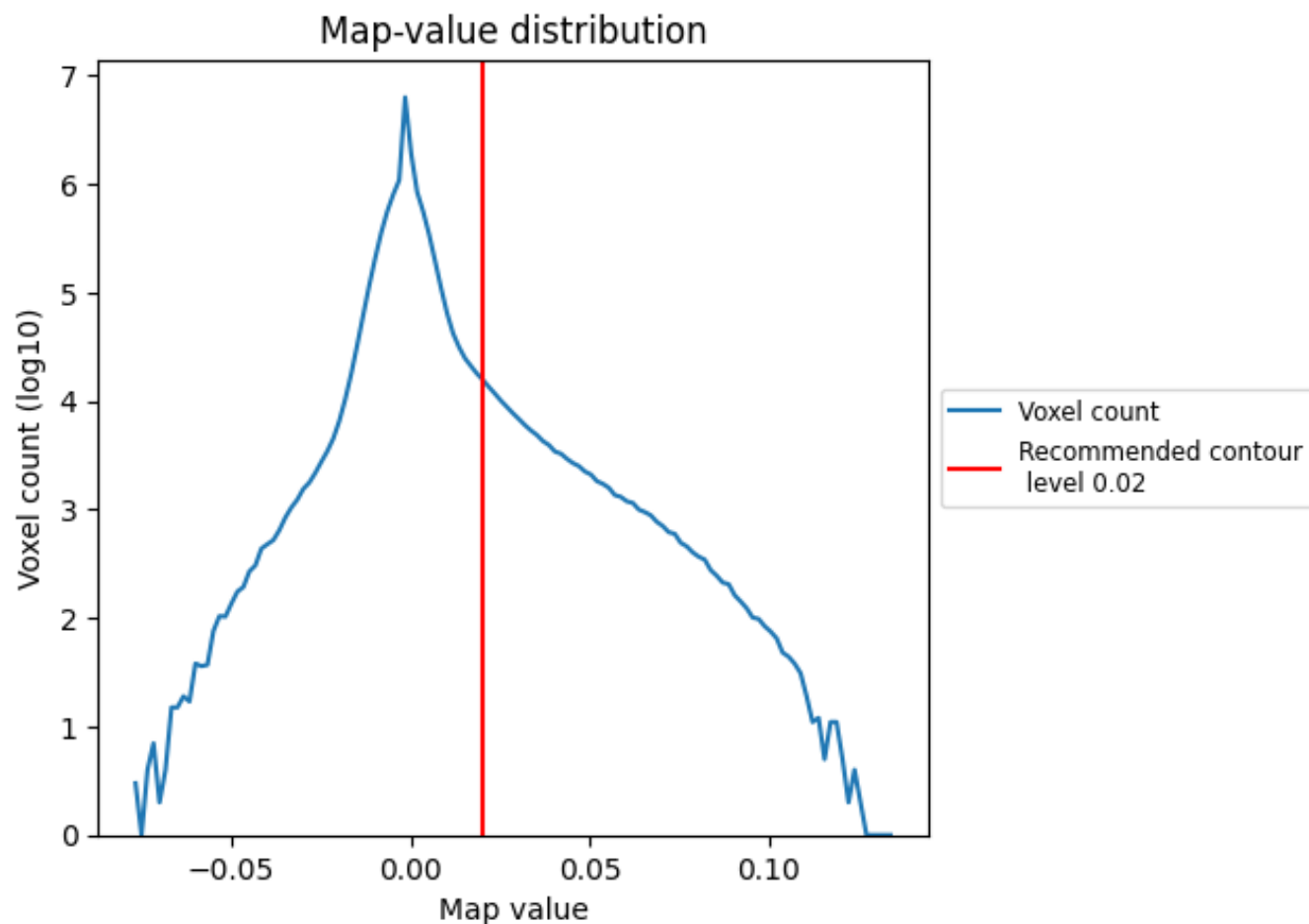
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

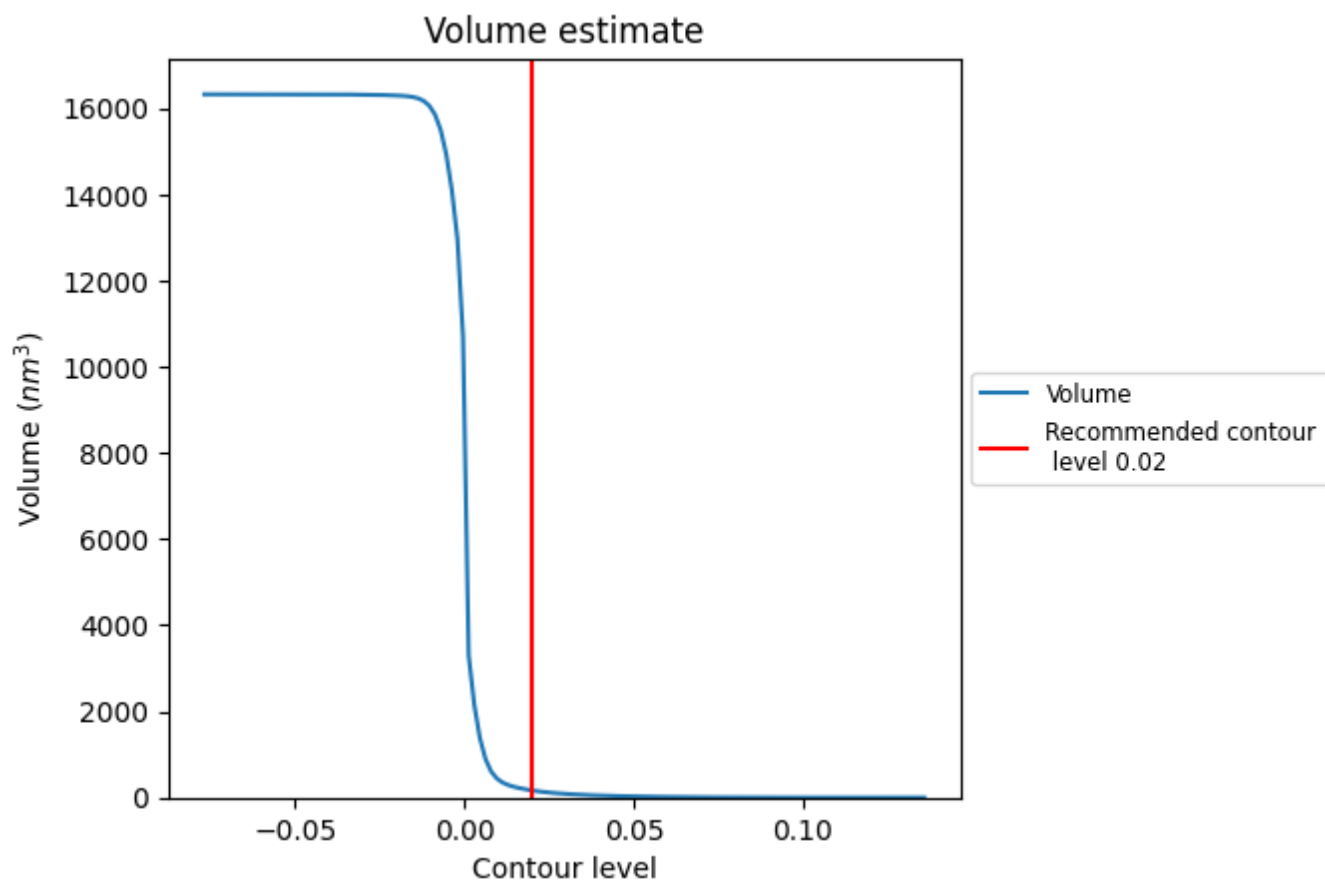
This section contains the results of statistical analysis of the map.

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.

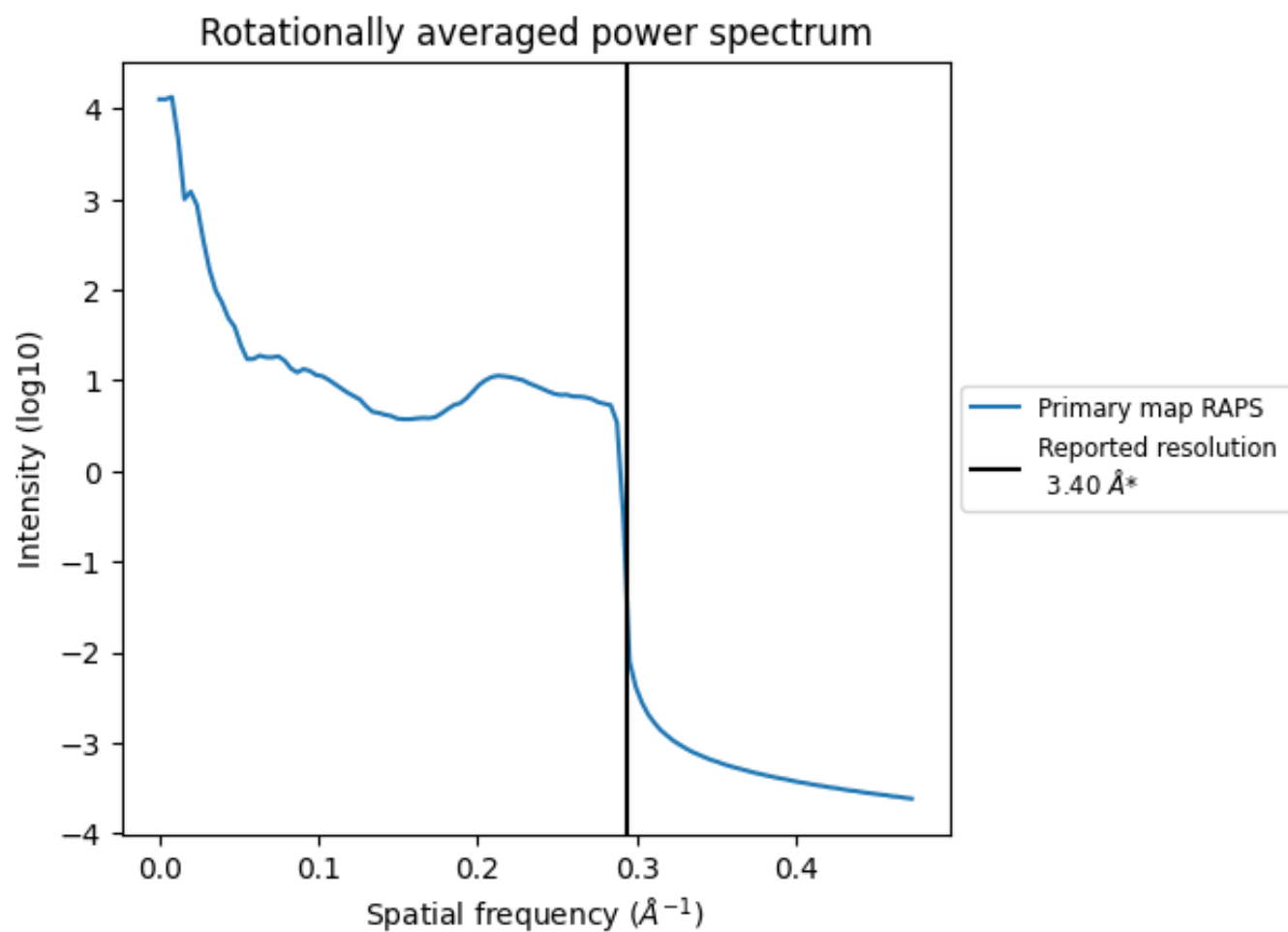
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 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 0.294 Å⁻¹

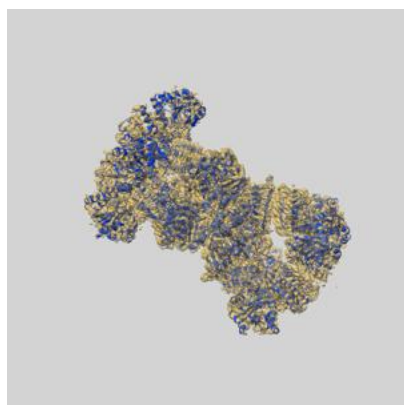
8 Fourier-Shell correlation

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

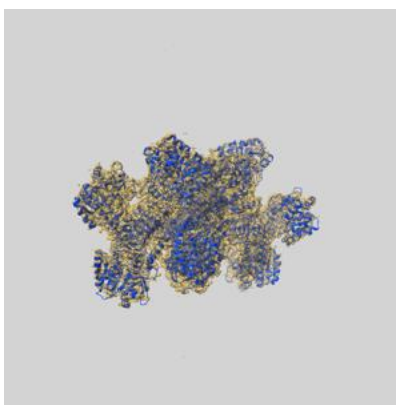
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30599 and PDB model 7D72. Per-residue inclusion information can be found in section [3](#) on page [7](#).

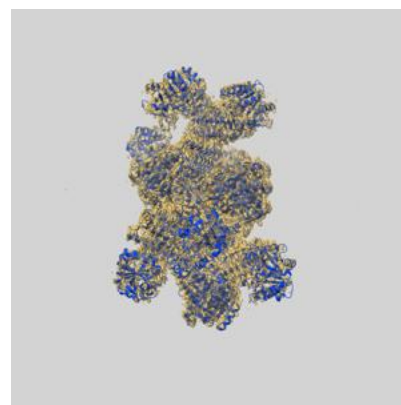
9.1 Map-model overlay [i](#)



X



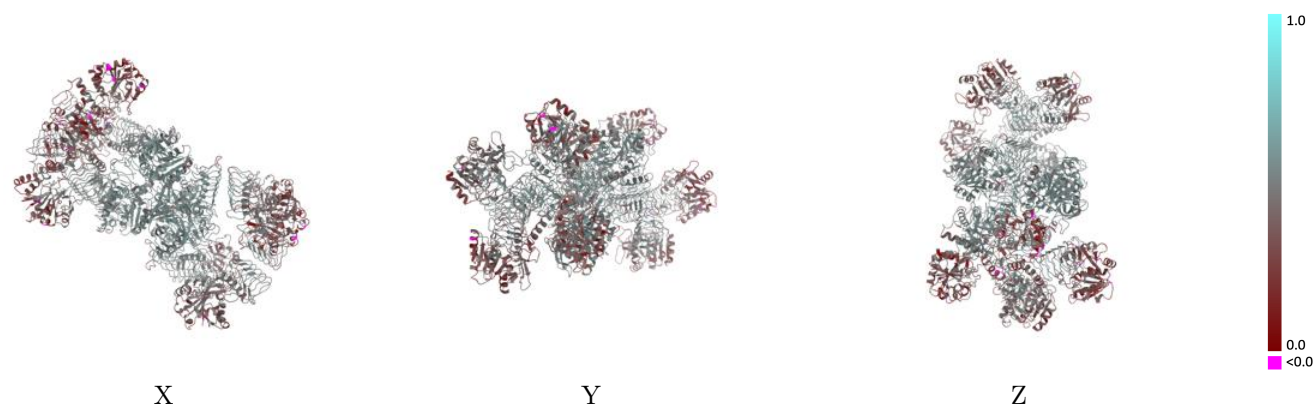
Y



Z

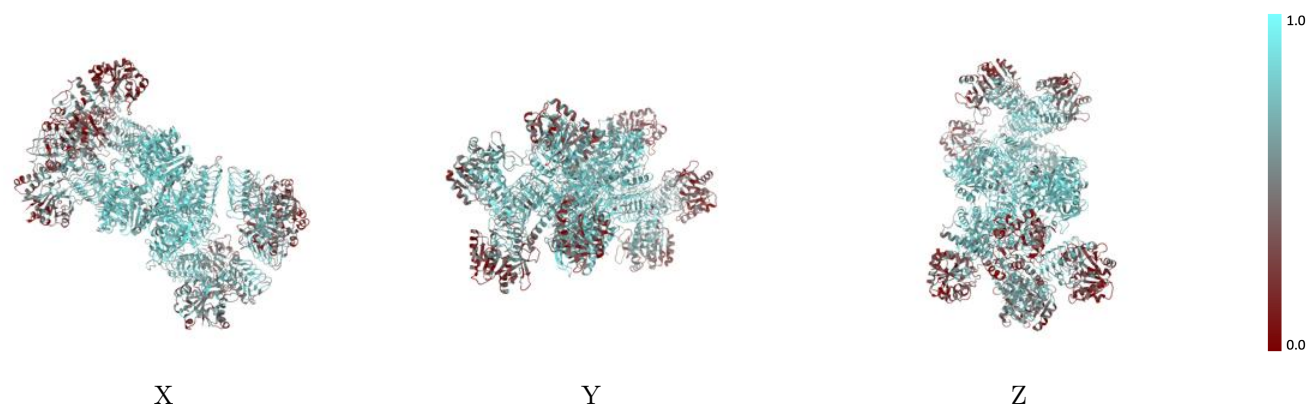
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



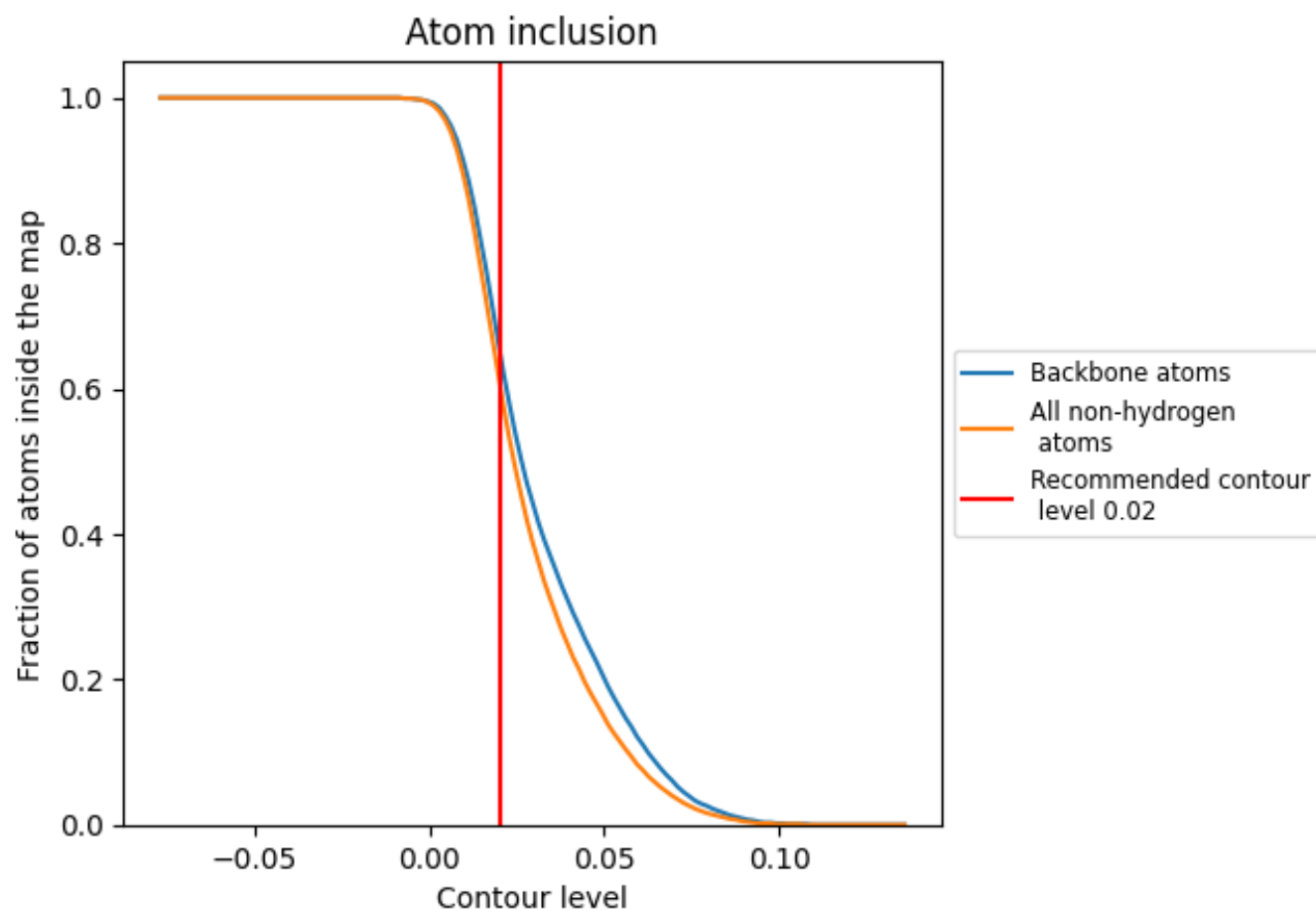
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6110	0.4440
A	0.8170	0.5330
B	0.8070	0.5250
C	0.8120	0.5300
D	0.7910	0.5230
E	0.4930	0.3940
F	0.5690	0.4140
G	0.5860	0.4310
H	0.5020	0.4040
I	0.4540	0.3770
J	0.5280	0.4030
K	0.5010	0.3940
L	0.4060	0.3580

1.0

0.0

<0.0