



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 01:19 PM UTC

PDB ID : 7D74 / pdb_00007d74
EMDB ID : EMD-30601
Title : Cryo-EM structure of GMPPA/GMPPB complex bound to GTP (state II)
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 : 3.10 Å(reported)

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

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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:

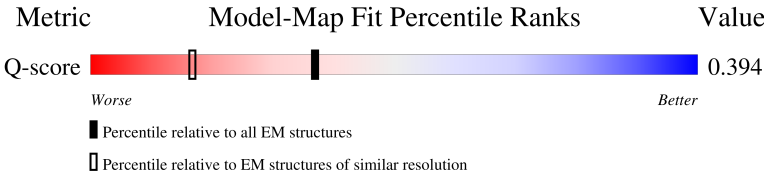
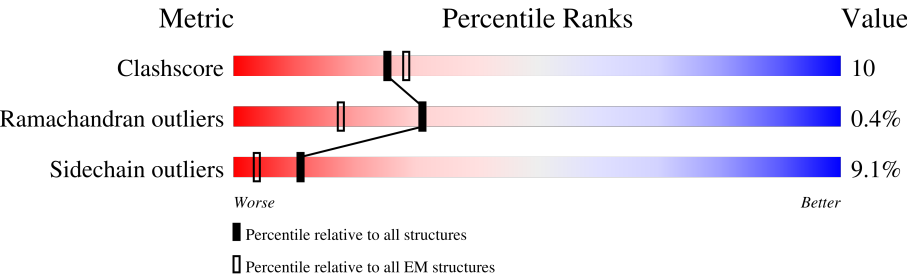
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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
3	GTP	E	401	-	-	X	-
3	GTP	F	401	-	-	X	-
3	GTP	G	401	-	-	X	-
3	GTP	H	401	-	-	X	-
3	GTP	J	401	-	-	X	-
3	GTP	K	401	-	-	X	-
3	GTP	L	401	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 35353 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	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		
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		

- 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	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		
2	G	359	Total	C	N	O	S	0	0
			2782	1767	487	506	22		
2	H	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
			2789	1772	488	507	22		
2	L	360	Total	C	N	O	S	0	0
			2789	1772	488	507	22		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

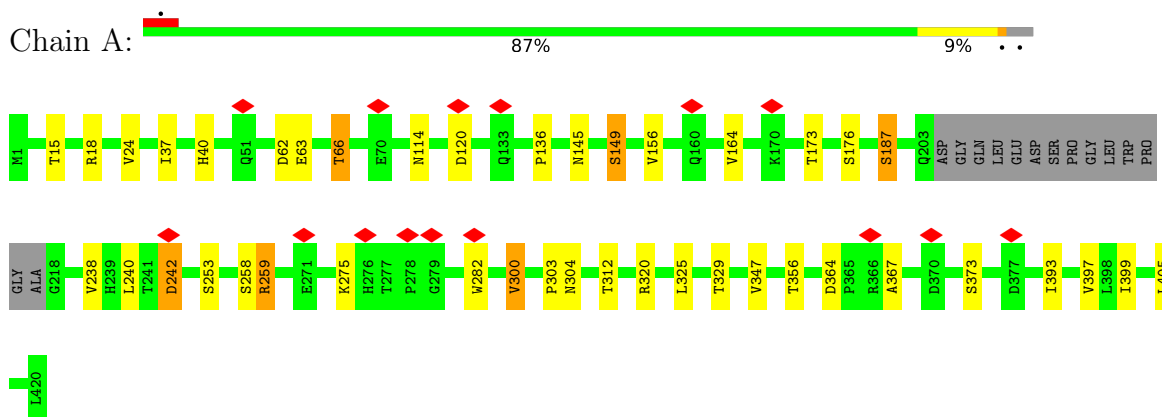


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	B	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	F	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	G	1	Total	C	N	O	P	0
			32	10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

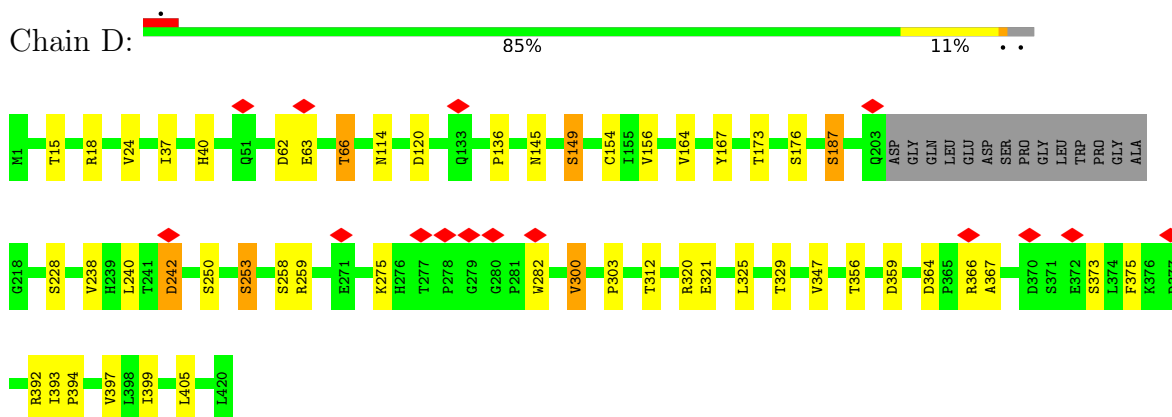
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

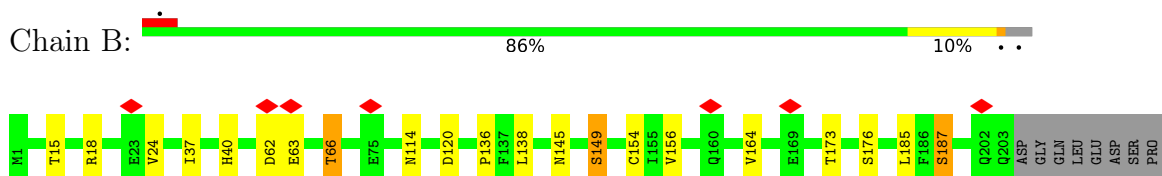
- Molecule 1: Mannose-1-phosphate guanyltransferase alpha

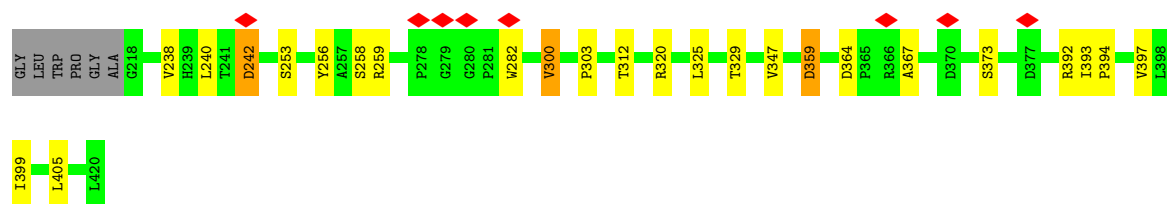


- Molecule 1: Mannose-1-phosphate guanyltransferase alpha

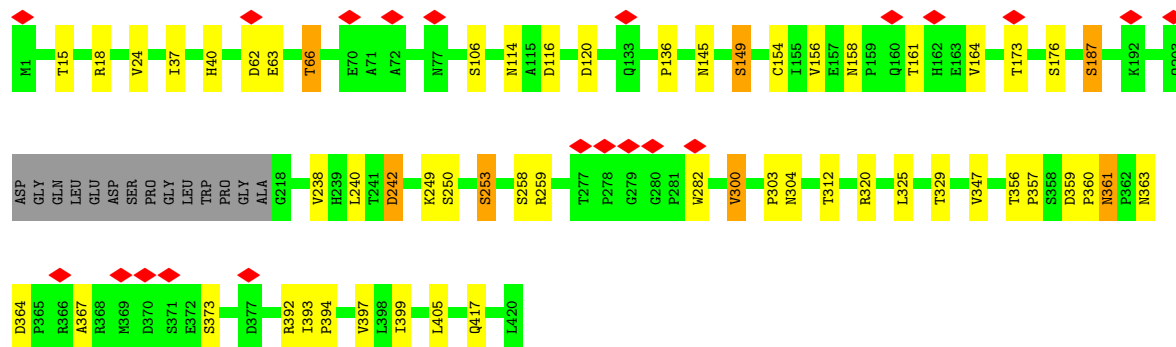
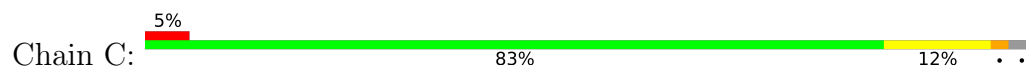


- Molecule 1: Mannose-1-phosphate guanyltransferase alpha

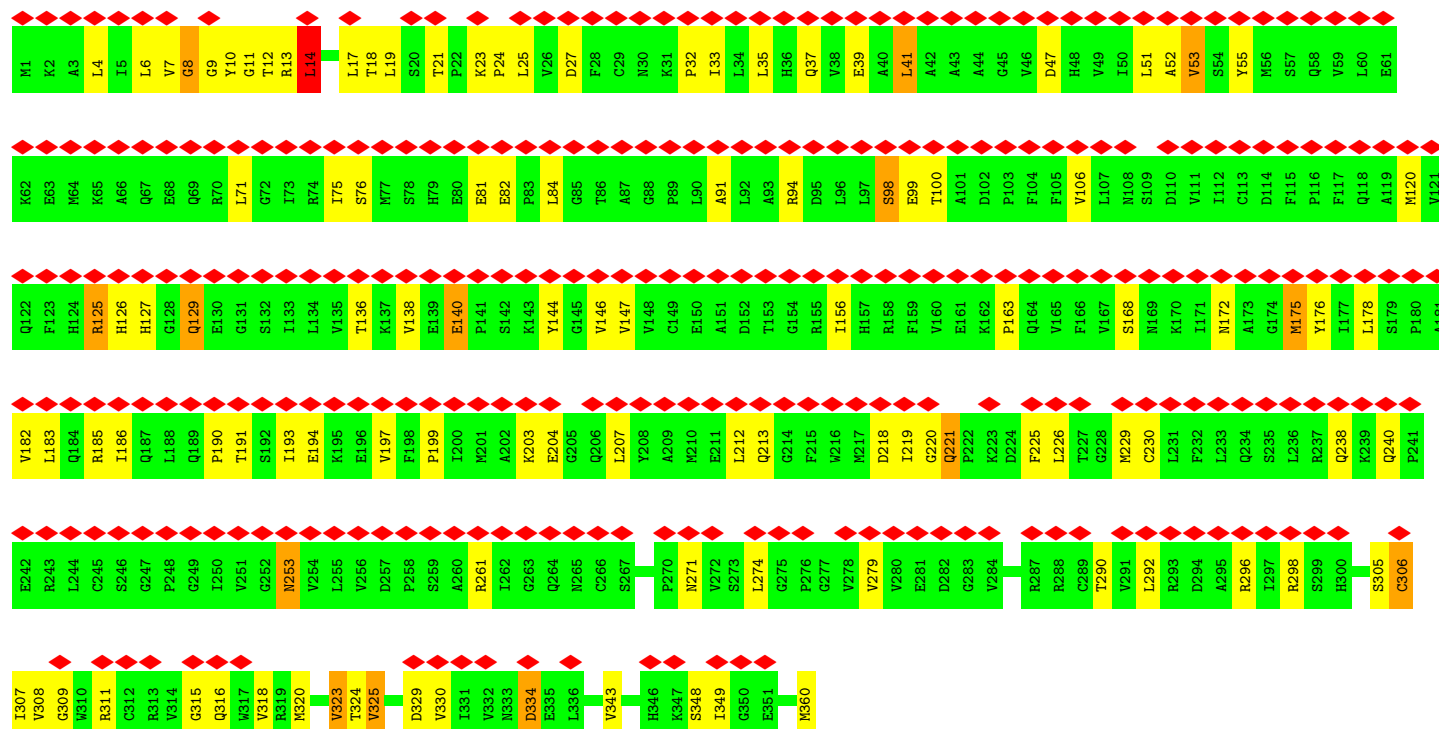
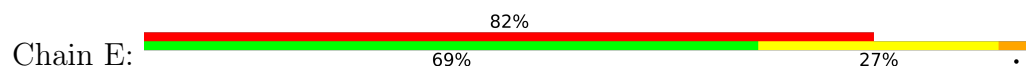




• Molecule 1: Mannose-1-phosphate guanylttransferase alpha

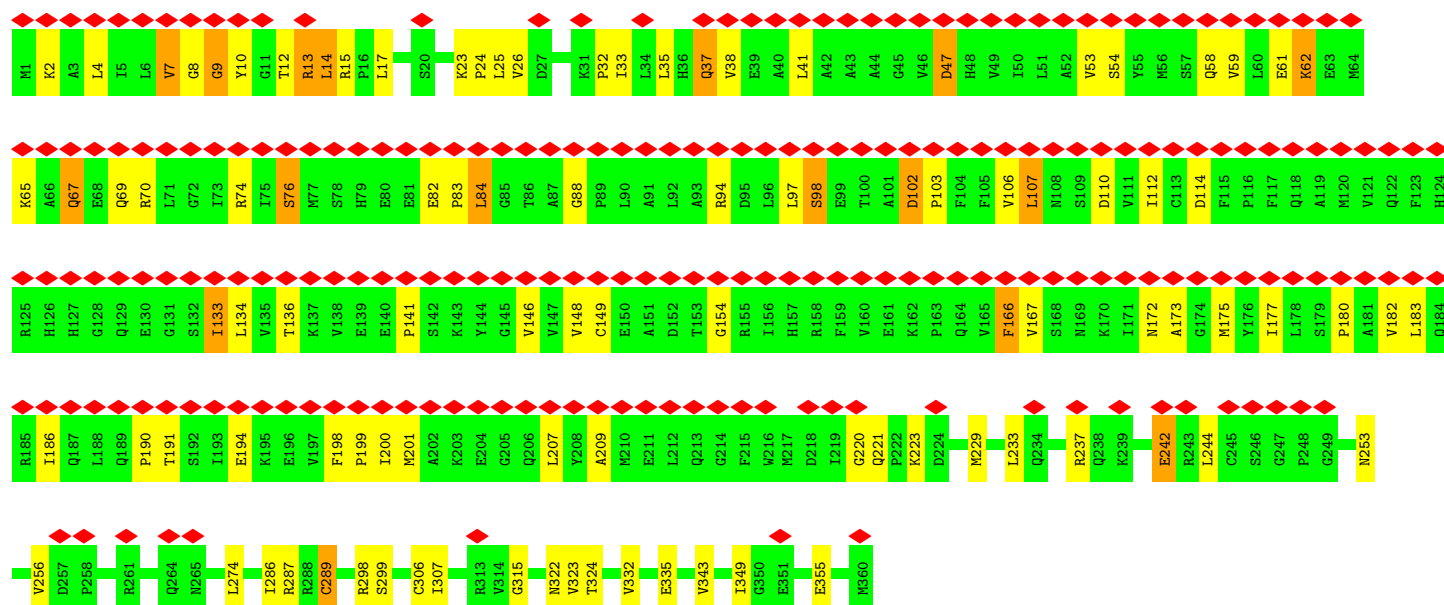


• Molecule 2: Mannose-1-phosphate guanylttransferase beta

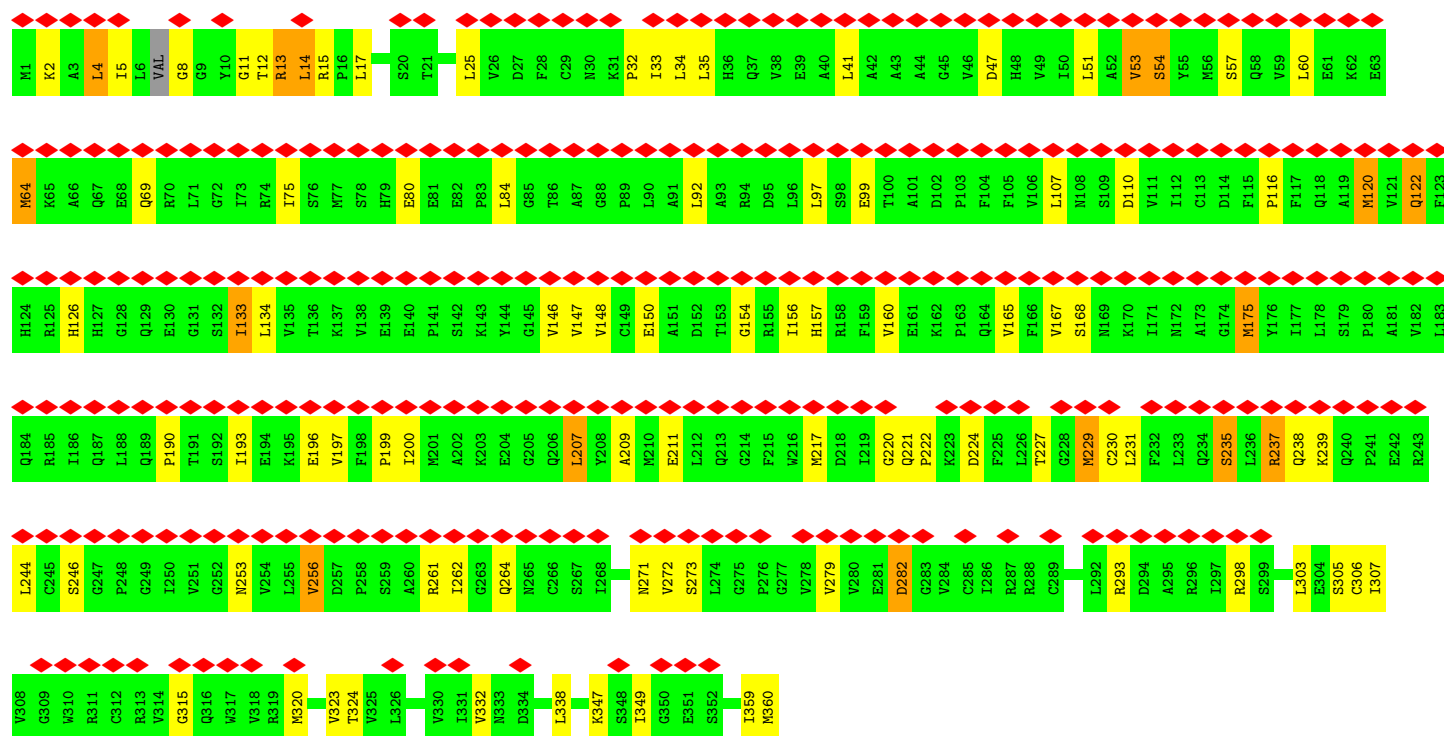
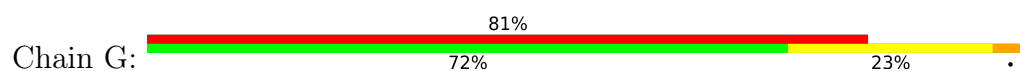


• Molecule 2: Mannose-1-phosphate guanylttransferase beta

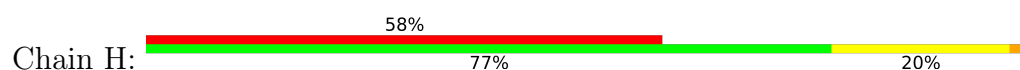


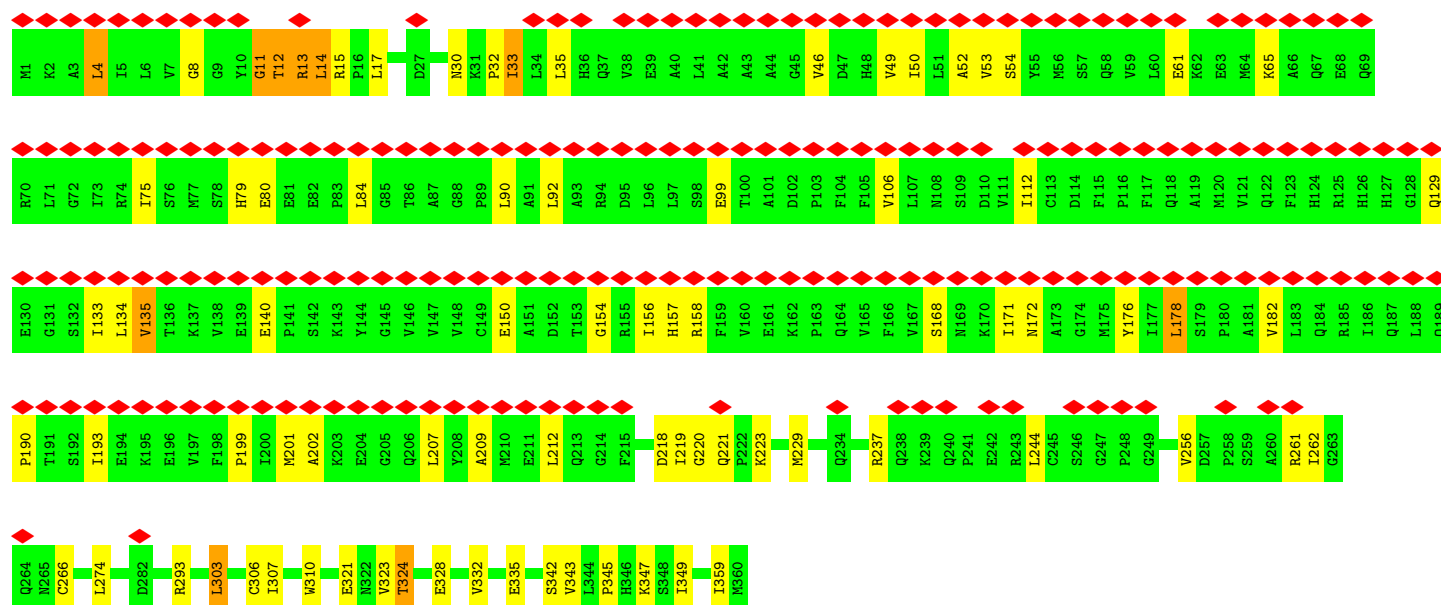


• Molecule 2: Mannose-1-phosphate guanylttransferase beta



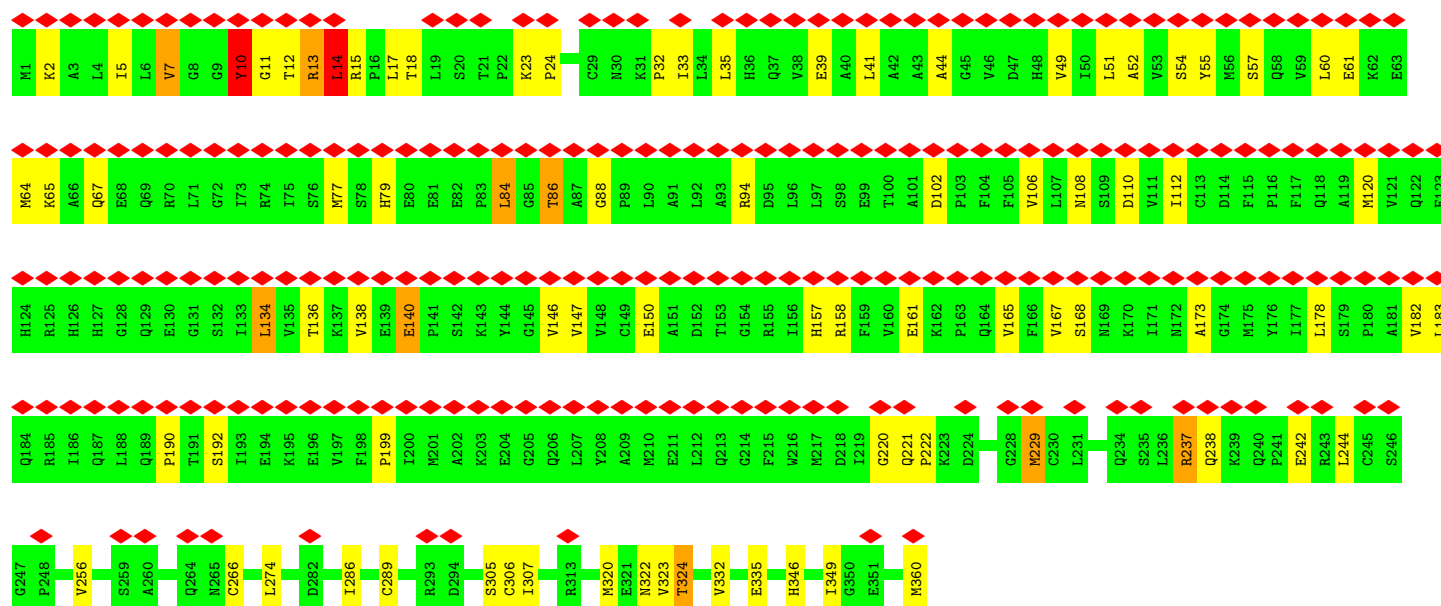
• Molecule 2: Mannose-1-phosphate guanylttransferase beta





• Molecule 2: Mannose-1-phosphate guanyltrtransferase beta

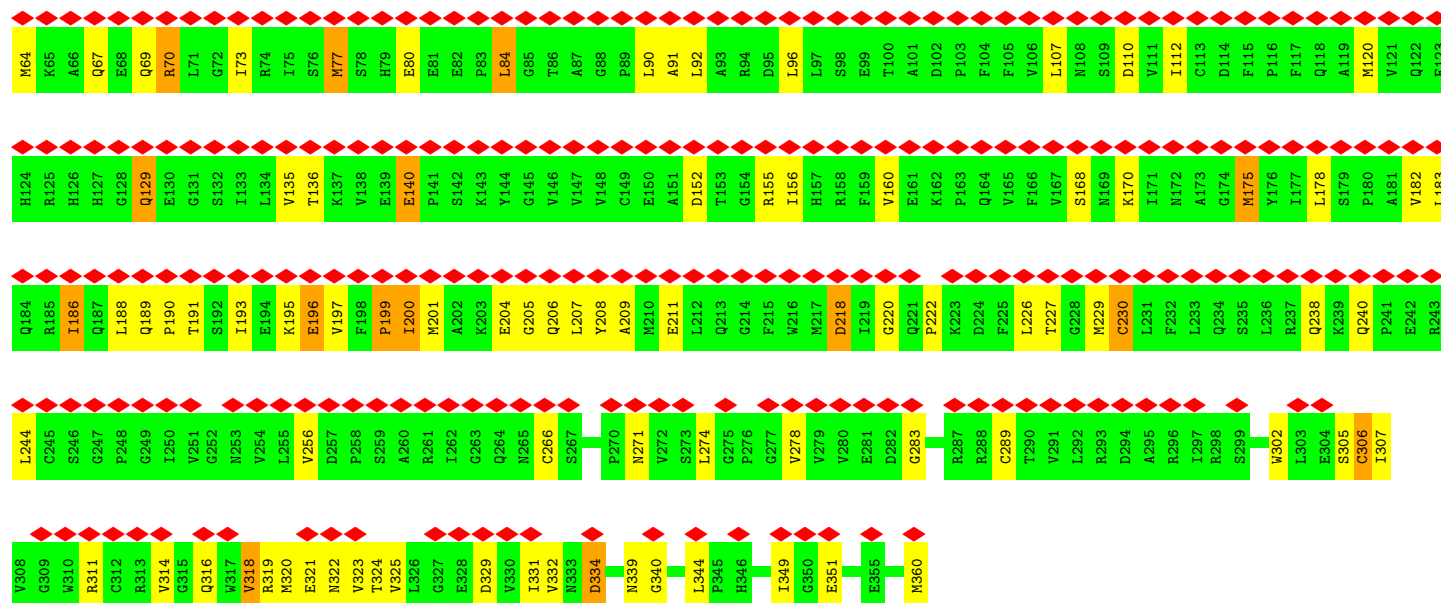
Chain I:



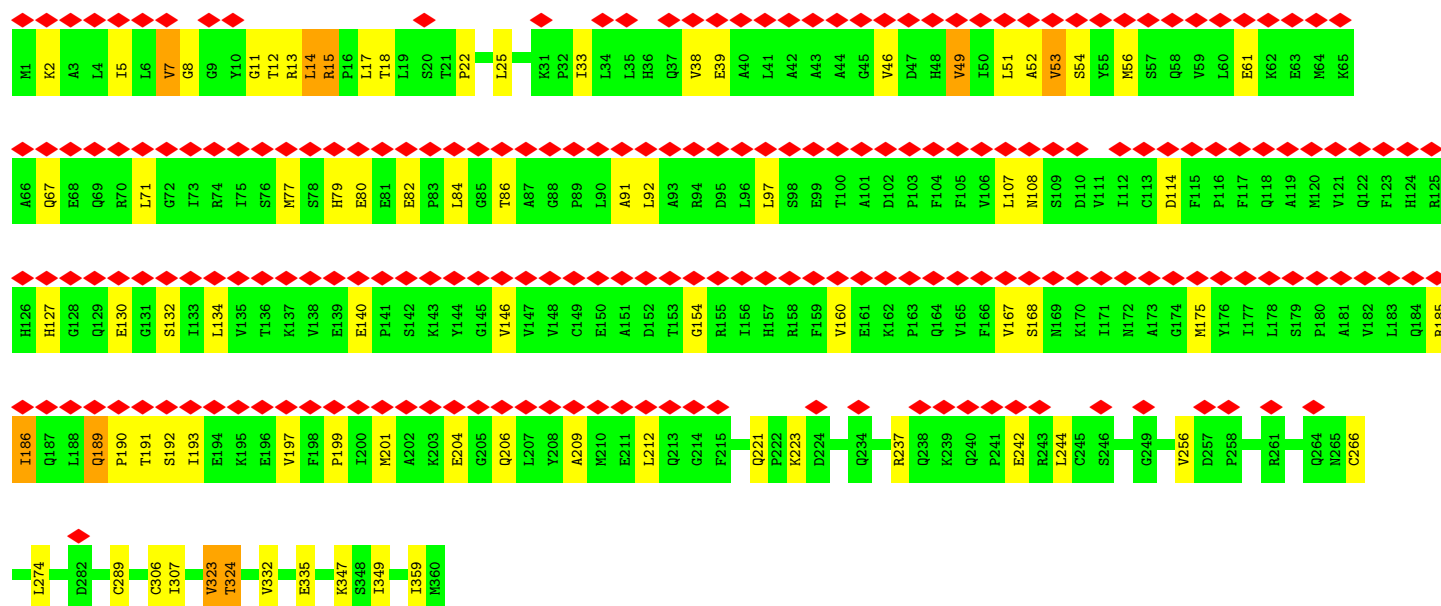
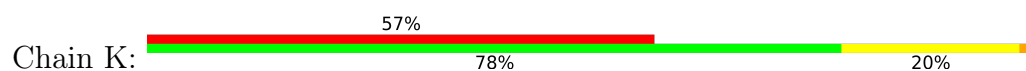
• Molecule 2: Mannose-1-phosphate guanyltrtransferase beta

Chain J:

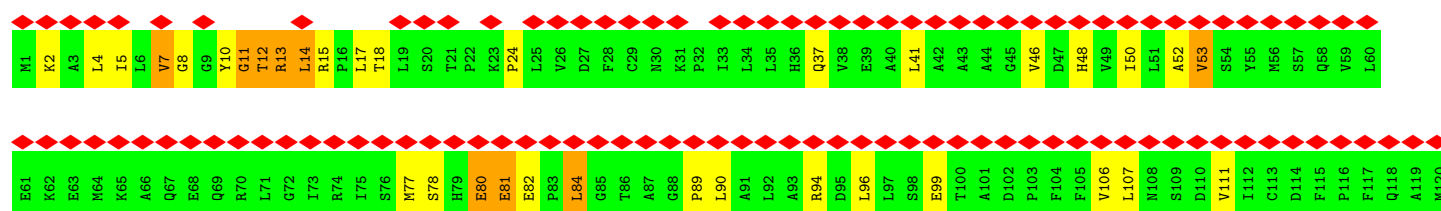
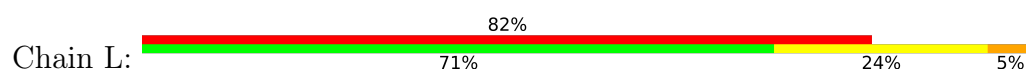




• Molecule 2: Mannose-1-phosphate guanylttransferase beta



• Molecule 2: Mannose-1-phosphate guanylttransferase beta



E304	S305	C306	I307	V308	G309	W310	R311	C312	R313	V314	G315	Q316	W317	V318	R319	M320	E321	N322	V323	T324	V330	I331	V332	N333	D334	E335	L336	Y337	G340	V343	I349	G350	E351	S352	M360																								
E242	R243	L244	C245	S246	Q247	P248	Q249	I250	V251	G252	N253	V254	L255	V256	D257	P258	S259	A260	R261	I262	G263	Q264	N265	C266	S267	I268	N271	V272	S273	L274	G275	P276	G277	V278	V279	V280	E281	D282	G283	V284	C285	I286	R287	R288	C289	L292	R293	D294	A295	R296	I297	R298	S299	H300	S301	W302	L303		
A181	V182	L183	Q184	R185	I186	Q187	L188	Q189	P190	T191	S192	I193	E194	K195	E196	V197	F198	P199	I200	M201	A202	K203	E204	G205	Q206	L207	Y208	A209	M210	E211	L212	Q213	G214	F215	W216	M217	D218	I219	G220	Q221	P222	K223	D224	F225	G228	M229	C230	L231	F232	L233	Q234	S235	L236	R237	Q238	K239	Q240	P241	
V121	Q122	F123	H124	R125	H126	H127	G128	Q129	E130	G131	S132	I133	L134	V135	T136	K137	V138	E139	E140	P141	S142	K143	Y144	G145	V146	V147	V148	C149	E150	A151	D152	T153	G154	R155	I156	H157	R158	F159	V160	E161	K162	P163	Q164	V165	F166	V167	S168	N169	K170	I171	N172	A173	G174	M175	Y176	I177	L178	S179	P180

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	115375	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	0.278	Depositor
Minimum map value	-0.170	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0365	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/3248	0.57	0/4420
1	B	0.32	0/3248	0.56	0/4420
1	C	0.33	0/3248	0.57	0/4420
1	D	0.33	0/3248	0.57	0/4420
2	E	0.42	0/2840	0.84	6/3850 (0.2%)
2	F	0.42	0/2844	0.87	4/3854 (0.1%)
2	G	0.41	0/2836	0.90	4/3841 (0.1%)
2	H	0.36	0/2844	0.79	3/3854 (0.1%)
2	I	0.41	0/2844	0.83	3/3854 (0.1%)
2	J	0.38	0/2844	0.88	6/3854 (0.2%)
2	K	0.35	0/2844	0.79	4/3854 (0.1%)
2	L	0.39	0/2844	0.88	5/3854 (0.1%)
All	All	0.37	0/35732	0.76	35/48495 (0.1%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	GLY	N-CA-C	10.19	127.47	110.56
2	L	46	VAL	CA-C-N	7.46	131.16	120.79
2	L	46	VAL	C-N-CA	7.46	131.16	120.79
2	J	9	GLY	N-CA-C	6.51	123.95	112.10
2	I	237	ARG	CA-C-N	-6.36	113.04	122.83
2	I	237	ARG	C-N-CA	-6.36	113.04	122.83
2	K	46	VAL	CA-C-N	6.24	129.46	120.79
2	K	46	VAL	C-N-CA	6.24	129.46	120.79
2	E	240	GLN	CA-CB-CG	5.94	125.99	114.10
2	G	293	ARG	CB-CG-CD	5.91	124.89	111.30
2	H	65	LYS	CA-CB-CG	5.84	125.77	114.10
2	G	237	ARG	CA-C-N	-5.78	113.05	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	237	ARG	C-N-CA	-5.78	113.05	122.65
2	J	140	GLU	CA-CB-CG	5.78	125.66	114.10
2	J	195	LYS	CA-CB-CG	5.75	125.60	114.10
2	E	240	GLN	CB-CG-CD	5.72	122.32	112.60
2	J	196	GLU	CA-CB-CG	5.72	125.53	114.10
2	K	206	GLN	CA-CB-CG	5.66	125.42	114.10
2	G	196	GLU	N-CA-CB	5.52	118.98	110.81
2	H	168	SER	CA-C-N	-5.50	114.02	122.60
2	H	168	SER	C-N-CA	-5.50	114.02	122.60
2	L	11	GLY	N-CA-C	-5.46	100.25	113.18
2	F	322	ASN	N-CA-C	5.44	117.27	110.91
2	L	158	ARG	CB-CG-CD	-5.43	98.81	111.30
2	J	170	LYS	CB-CG-CD	5.29	123.46	111.30
2	I	77	MET	CB-CG-SD	5.26	128.48	112.70
2	E	9	GLY	N-CA-C	5.24	125.59	113.18
2	J	62	LYS	CA-CB-CG	5.21	124.53	114.10
2	L	323	VAL	N-CA-C	5.16	120.08	109.34
2	E	99	GLU	CA-CB-CG	5.09	124.28	114.10
2	E	14	LEU	CA-C-N	5.07	126.10	120.06
2	E	14	LEU	C-N-CA	5.07	126.10	120.06
2	K	14	LEU	N-CA-C	-5.06	106.41	112.58
2	F	9	GLY	CA-C-N	5.03	131.15	121.54
2	F	9	GLY	C-N-CA	5.03	131.15	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	3167	0	3184	21	0
1	B	3167	0	3184	22	0
1	C	3167	0	3184	30	0
1	D	3167	0	3184	25	0
2	E	2785	0	2829	94	0
2	F	2789	0	2840	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	2782	0	2830	73	0
2	H	2789	0	2838	60	0
2	I	2789	0	2840	73	0
2	J	2789	0	2840	125	0
2	K	2789	0	2838	48	0
2	L	2789	0	2840	81	0
3	A	32	0	12	1	0
3	B	32	0	12	1	0
3	C	32	0	12	1	0
3	D	32	0	12	1	0
3	E	32	0	12	17	0
3	F	32	0	12	30	0
3	G	32	0	12	12	0
3	H	32	0	12	15	0
3	I	32	0	12	8	0
3	J	32	0	12	14	0
3	K	32	0	12	13	0
3	L	32	0	12	14	0
All	All	35353	0	35575	735	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 (735) 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:E:7:VAL:CG1	2:E:24:PRO:HG2	1.35	1.55
2:E:8:GLY:HA3	3:E:401:GTP:N3	1.22	1.51
2:F:7:VAL:CG2	2:F:24:PRO:HG3	1.43	1.49
2:F:8:GLY:HA3	3:F:401:GTP:N3	1.12	1.43
2:I:346:HIS:CG	2:J:10:TYR:CE1	2.13	1.35
2:E:8:GLY:HA3	3:E:401:GTP:C2	1.64	1.31
2:L:8:GLY:HA3	3:L:401:GTP:N3	1.45	1.30
2:J:120:MET:HE1	2:J:175:MET:SD	1.74	1.27
2:E:7:VAL:HG13	2:E:24:PRO:CG	1.67	1.25
2:E:8:GLY:CA	3:E:401:GTP:N3	1.99	1.24
2:I:346:HIS:CG	2:J:10:TYR:HE1	1.51	1.21
2:L:12:THR:N	3:L:401:GTP:O3G	1.73	1.20
2:K:306:CYS:SG	2:K:324:THR:HG23	1.83	1.19
2:L:13:ARG:NH1	3:L:401:GTP:O2G	1.75	1.17
2:F:54:SER:N	3:F:401:GTP:HN21	1.43	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:321:GLU:OE1	2:L:337:TYR:HE1	1.30	1.15
2:F:8:GLY:CA	3:F:401:GTP:N3	2.09	1.15
2:J:201:MET:HE2	2:J:207:LEU:CD2	1.78	1.14
2:J:8:GLY:HA3	3:J:401:GTP:N3	1.62	1.13
2:J:201:MET:HE2	2:J:207:LEU:HD21	1.30	1.13
2:J:107:LEU:CD2	2:J:175:MET:HG3	1.78	1.12
2:J:107:LEU:CD2	2:J:175:MET:CG	2.27	1.12
2:F:54:SER:HB2	3:F:401:GTP:HN1	1.12	1.12
2:F:7:VAL:HG22	2:F:24:PRO:HG3	1.26	1.12
2:L:8:GLY:HA3	3:L:401:GTP:C2	1.85	1.12
2:L:7:VAL:CG1	2:L:24:PRO:HG2	1.80	1.11
2:F:59:VAL:HA	2:F:62:LYS:HG3	1.25	1.09
2:L:80:GLU:OE1	2:L:84:LEU:HD22	1.52	1.09
2:E:8:GLY:CA	3:E:401:GTP:N2	2.16	1.09
2:G:306:CYS:SG	2:G:324:THR:HG22	1.93	1.09
2:J:107:LEU:HD23	2:J:175:MET:HG3	1.21	1.09
2:E:8:GLY:HA2	3:E:401:GTP:N2	1.68	1.08
2:H:14:LEU:HD13	2:H:17:LEU:HD12	1.35	1.07
2:E:7:VAL:CG1	2:E:24:PRO:CG	2.27	1.07
2:K:12:THR:N	3:K:401:GTP:O3G	1.86	1.07
2:J:12:THR:N	3:J:401:GTP:O3G	1.89	1.05
2:J:107:LEU:HD21	2:J:175:MET:CG	1.85	1.04
2:G:12:THR:N	3:G:401:GTP:O3G	1.90	1.04
2:L:8:GLY:CA	3:L:401:GTP:N3	2.20	1.04
2:E:7:VAL:HG13	2:E:24:PRO:HG2	1.06	1.04
2:F:7:VAL:CG2	2:F:24:PRO:CG	2.36	1.03
2:L:8:GLY:HA2	3:L:401:GTP:N2	1.73	1.03
2:I:12:THR:N	3:I:401:GTP:O3G	1.91	1.02
2:J:8:GLY:HA3	3:J:401:GTP:C2	1.95	1.02
1:D:259:ARG:NH1	1:D:321:GLU:OE2	1.92	1.02
2:E:8:GLY:CA	3:E:401:GTP:C2	2.38	1.01
2:E:320:MET:HE3	2:E:324:THR:HG23	1.39	1.01
2:H:13:ARG:HG2	2:H:221:GLN:HG2	1.37	1.00
2:J:52:ALA:O	3:J:401:GTP:N2	1.93	1.00
2:I:346:HIS:CB	2:J:10:TYR:CE1	2.45	0.99
2:L:7:VAL:HG13	2:L:24:PRO:HG2	1.00	0.99
2:E:320:MET:HE3	2:E:324:THR:CG2	1.91	0.99
2:J:51:LEU:HD11	2:J:64:MET:HE1	1.45	0.98
2:E:7:VAL:HG12	2:E:24:PRO:HG2	1.44	0.98
2:L:52:ALA:O	3:L:401:GTP:N2	1.96	0.98
2:H:12:THR:N	3:H:401:GTP:O3G	1.97	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:SER:N	3:F:401:GTP:N2	2.11	0.97
2:I:52:ALA:O	3:I:401:GTP:N2	1.98	0.97
2:J:305:SER:O	2:J:323:VAL:HA	1.64	0.97
1:A:259:ARG:HG3	1:A:259:ARG:HH11	1.28	0.97
2:F:7:VAL:HG21	2:F:24:PRO:HG3	1.42	0.97
2:L:7:VAL:HG13	2:L:24:PRO:CG	1.93	0.97
2:E:52:ALA:O	3:E:401:GTP:N2	1.96	0.97
2:J:306:CYS:SG	2:J:320:MET:HE2	2.05	0.97
2:F:58:GLN:O	2:F:62:LYS:HG2	1.63	0.96
2:H:52:ALA:O	3:H:401:GTP:N2	1.98	0.96
2:F:8:GLY:H	3:F:401:GTP:H1'	1.29	0.95
2:L:8:GLY:CA	3:L:401:GTP:N2	2.29	0.95
2:E:14:LEU:HD12	2:E:17:LEU:HD12	1.49	0.94
2:G:13:ARG:HG2	2:G:13:ARG:HH11	1.29	0.94
2:G:306:CYS:SG	2:G:324:THR:CG2	2.57	0.93
2:L:321:GLU:OE1	2:L:337:TYR:CE1	2.20	0.93
2:K:52:ALA:O	3:K:401:GTP:N2	2.01	0.93
2:I:13:ARG:NE	2:I:221:GLN:HG2	1.82	0.92
2:F:54:SER:CB	3:F:401:GTP:HN1	1.83	0.92
2:F:54:SER:HB2	3:F:401:GTP:N1	1.83	0.92
2:L:14:LEU:CD1	2:L:17:LEU:HD12	1.99	0.92
2:F:14:LEU:HD12	2:F:17:LEU:HD12	1.51	0.91
2:G:54:SER:HB3	3:G:401:GTP:HN1	1.33	0.91
2:J:289:CYS:SG	2:J:306:CYS:HB2	2.11	0.90
2:G:5:ILE:HB	2:G:51:LEU:HD23	1.53	0.90
2:F:8:GLY:HA3	3:F:401:GTP:C2	2.06	0.90
2:L:8:GLY:CA	3:L:401:GTP:C2	2.55	0.90
2:I:346:HIS:ND1	2:J:10:TYR:CE1	2.40	0.89
2:I:346:HIS:ND1	2:J:10:TYR:HE1	1.70	0.89
2:F:54:SER:CB	3:F:401:GTP:N1	2.36	0.89
2:J:129:GLN:HG2	2:J:206:GLN:HA	1.55	0.88
2:I:41:LEU:CD2	2:I:49:VAL:HG11	2.03	0.88
2:H:14:LEU:CD1	2:H:17:LEU:HD12	2.03	0.88
2:E:8:GLY:HA3	3:E:401:GTP:C4	2.08	0.87
2:I:346:HIS:HB3	2:J:10:TYR:CE1	2.09	0.87
2:J:226:LEU:CD1	2:J:323:VAL:HG23	2.05	0.87
2:J:155:ARG:NH2	2:J:205:GLY:HA3	1.89	0.87
2:J:201:MET:CE	2:J:207:LEU:HD21	2.05	0.86
2:I:41:LEU:HD21	2:I:49:VAL:HG11	1.56	0.85
2:J:226:LEU:HD11	2:J:323:VAL:HG23	1.57	0.85
2:E:360:MET:O	2:F:12:THR:HG23	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:102:ASP:HB2	2:F:103:PRO:CD	2.07	0.84
2:J:107:LEU:CD2	2:J:175:MET:HG2	2.07	0.84
2:G:14:LEU:HD12	2:G:17:LEU:HB2	1.60	0.83
2:G:8:GLY:HA3	3:G:401:GTP:N3	1.93	0.83
2:F:59:VAL:CA	2:F:62:LYS:HG3	2.08	0.83
2:I:13:ARG:HD2	2:I:221:GLN:HE21	1.44	0.83
2:I:41:LEU:HD21	2:I:49:VAL:CG1	2.08	0.83
2:E:12:THR:N	3:E:401:GTP:O3G	2.11	0.83
2:F:59:VAL:HA	2:F:62:LYS:CG	2.09	0.83
2:F:53:VAL:C	3:F:401:GTP:HN21	1.87	0.83
2:J:8:GLY:HA3	3:J:401:GTP:N2	1.94	0.83
2:G:8:GLY:HA3	3:G:401:GTP:C2	2.14	0.83
2:F:102:ASP:HB2	2:F:103:PRO:HD2	1.59	0.82
2:I:13:ARG:HE	2:I:221:GLN:HG2	1.41	0.82
2:J:13:ARG:HB2	2:J:220:GLY:O	1.78	0.82
2:I:7:VAL:HB	2:I:24:PRO:HG2	1.62	0.81
2:G:14:LEU:HD13	2:G:17:LEU:HD12	1.61	0.81
2:G:8:GLY:HA3	3:G:401:GTP:N2	1.96	0.80
2:K:306:CYS:SG	2:K:324:THR:CG2	2.68	0.80
2:H:14:LEU:HD12	2:H:17:LEU:HB2	1.62	0.80
2:H:8:GLY:HA3	3:H:401:GTP:N3	1.96	0.80
2:K:8:GLY:HA3	3:K:401:GTP:N2	1.97	0.79
2:K:54:SER:HB2	3:K:401:GTP:HN1	1.45	0.79
2:F:8:GLY:HA3	3:F:401:GTP:C4	2.15	0.79
2:G:14:LEU:CD1	2:G:17:LEU:HD12	2.12	0.78
2:G:14:LEU:CD1	2:G:17:LEU:HB2	2.14	0.78
2:F:13:ARG:HB3	2:F:220:GLY:O	1.83	0.78
2:F:12:THR:HA	2:F:15:ARG:HD3	1.66	0.78
2:F:8:GLY:HA2	2:F:53:VAL:HA	1.64	0.77
2:I:346:HIS:HB3	2:J:10:TYR:CZ	2.20	0.77
2:I:54:SER:HB2	3:I:401:GTP:HN1	1.49	0.77
2:J:8:GLY:CA	3:J:401:GTP:N3	2.44	0.77
2:J:8:GLY:CA	3:J:401:GTP:N2	2.47	0.77
2:I:306:CYS:SG	2:I:320:MET:HE2	2.25	0.77
2:J:107:LEU:HD23	2:J:175:MET:CG	2.00	0.77
2:L:14:LEU:HD13	2:L:17:LEU:HD12	1.67	0.76
1:A:259:ARG:HG3	1:A:259:ARG:NH1	1.98	0.76
2:G:13:ARG:HG2	2:G:13:ARG:NH1	2.00	0.76
2:J:226:LEU:HD12	2:J:323:VAL:CG2	2.15	0.76
2:J:155:ARG:NH2	2:J:205:GLY:CA	2.47	0.76
2:H:8:GLY:HA3	3:H:401:GTP:N2	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:13:ARG:O	2:K:14:LEU:HB3	1.85	0.75
2:I:346:HIS:CD2	2:J:10:TYR:HE1	2.01	0.75
2:E:8:GLY:N	3:E:401:GTP:N3	2.34	0.75
2:K:8:GLY:HA3	3:K:401:GTP:C2	2.21	0.75
2:J:60:LEU:O	2:J:64:MET:HG3	1.87	0.75
2:J:201:MET:HE2	2:J:207:LEU:HD23	1.68	0.74
1:A:259:ARG:HG2	1:A:304:ASN:CG	2.12	0.74
2:G:60:LEU:O	2:G:64:MET:HB2	1.87	0.74
2:F:7:VAL:HG23	2:F:24:PRO:HG3	1.62	0.74
2:H:8:GLY:HA3	3:H:401:GTP:C2	2.22	0.74
2:J:7:VAL:HB	2:J:24:PRO:HG2	1.70	0.73
2:H:14:LEU:CD1	2:H:17:LEU:HB2	2.17	0.73
2:G:305:SER:O	2:G:323:VAL:HA	1.88	0.73
2:F:54:SER:H	3:F:401:GTP:N2	1.84	0.73
2:F:289:CYS:HB3	2:F:306:CYS:SG	2.28	0.73
2:E:306:CYS:SG	2:E:308:VAL:HG23	2.28	0.73
2:I:13:ARG:NE	2:I:221:GLN:CG	2.52	0.73
2:F:7:VAL:HG21	2:F:24:PRO:CG	2.06	0.72
2:F:58:GLN:O	2:F:62:LYS:CG	2.36	0.72
2:F:8:GLY:CA	3:F:401:GTP:N2	2.52	0.72
2:E:7:VAL:HG11	2:E:24:PRO:HG2	1.63	0.72
2:J:322:ASN:HD22	2:J:339:ASN:CG	1.97	0.72
2:F:9:GLY:N	3:F:401:GTP:O2'	2.23	0.72
2:F:8:GLY:HA3	3:F:401:GTP:N2	2.05	0.72
2:J:8:GLY:HA2	2:J:53:VAL:HA	1.70	0.71
2:L:7:VAL:O	2:L:53:VAL:HG13	1.90	0.71
2:F:8:GLY:CA	3:F:401:GTP:HN22	2.03	0.71
2:F:8:GLY:HA2	3:F:401:GTP:HN22	1.54	0.71
2:E:13:ARG:HE	2:E:221:GLN:HG3	1.55	0.71
2:K:8:GLY:HA3	3:K:401:GTP:N3	2.06	0.71
2:E:7:VAL:HG13	2:E:24:PRO:HG3	1.66	0.71
2:J:201:MET:CE	2:J:207:LEU:CD2	2.64	0.71
2:G:13:ARG:HG2	2:G:221:GLN:HG2	1.71	0.71
2:H:11:GLY:C	3:H:401:GTP:O3G	2.34	0.71
2:F:14:LEU:CD1	2:F:17:LEU:HD12	2.21	0.70
2:L:14:LEU:HD12	2:L:17:LEU:HB2	1.73	0.70
2:I:13:ARG:HB3	2:I:220:GLY:O	1.89	0.70
2:E:94:ARG:O	2:E:98:SER:HB2	1.91	0.70
2:L:297:ILE:HG22	2:L:314:VAL:HG21	1.71	0.70
2:J:107:LEU:HD21	2:J:175:MET:HG2	1.69	0.69
2:K:289:CYS:SG	2:K:306:CYS:HB2	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:ILE:CB	2:G:51:LEU:HD23	2.21	0.69
2:J:107:LEU:HD21	2:J:175:MET:SD	2.31	0.69
2:E:8:GLY:HA2	2:E:53:VAL:HA	1.73	0.69
2:J:226:LEU:CD1	2:J:323:VAL:CG2	2.70	0.69
2:F:286:ILE:HG23	2:F:289:CYS:SG	2.33	0.69
2:J:51:LEU:HD11	2:J:64:MET:CE	2.23	0.68
2:L:8:GLY:HA3	3:L:401:GTP:C4	2.25	0.68
2:F:54:SER:HB3	3:F:401:GTP:N1	2.08	0.68
1:C:259:ARG:HD3	1:C:304:ASN:OD1	1.93	0.68
2:E:14:LEU:CD1	2:E:17:LEU:HD12	2.24	0.67
2:L:5:ILE:HG22	2:L:7:VAL:HG23	1.75	0.67
2:H:178:LEU:HD22	2:H:182:VAL:HG11	1.77	0.67
1:D:259:ARG:NH2	1:D:359:ASP:OD1	2.26	0.67
2:E:11:GLY:CA	3:E:401:GTP:O3G	2.43	0.66
2:E:185:ARG:NH1	2:E:204:GLU:OE1	2.27	0.66
2:J:155:ARG:HH22	2:J:205:GLY:HA3	1.59	0.66
2:F:4:LEU:HB3	2:F:106:VAL:HG12	1.77	0.66
2:E:320:MET:CE	2:E:324:THR:CG2	2.71	0.66
2:K:11:GLY:C	3:K:401:GTP:O3G	2.39	0.65
2:I:306:CYS:SG	2:I:324:THR:HG23	2.36	0.65
2:F:7:VAL:HA	3:F:401:GTP:O3'	1.96	0.65
2:L:14:LEU:HD12	2:L:17:LEU:HD12	1.77	0.65
2:L:8:GLY:HA2	2:L:53:VAL:HA	1.78	0.65
2:L:332:VAL:HG22	2:L:349:ILE:HD12	1.78	0.65
2:L:80:GLU:CD	2:L:84:LEU:HD22	2.21	0.65
1:A:15:THR:O	1:A:18:ARG:HB2	1.97	0.65
2:E:11:GLY:C	3:E:401:GTP:O3G	2.40	0.65
2:F:67:GLN:HA	2:F:70:ARG:HB2	1.79	0.64
2:J:11:GLY:C	3:J:401:GTP:O3G	2.39	0.64
2:I:13:ARG:HE	2:I:221:GLN:CG	2.11	0.64
1:C:15:THR:O	1:C:18:ARG:HB2	1.97	0.64
2:H:13:ARG:NH2	3:H:401:GTP:O2G	2.31	0.64
2:I:346:HIS:CD2	2:J:10:TYR:CE1	2.79	0.64
2:E:4:LEU:HB3	2:E:106:VAL:HG12	1.80	0.64
2:G:54:SER:HB3	3:G:401:GTP:N1	2.10	0.64
2:G:360:MET:O	2:H:12:THR:HG23	1.97	0.64
1:B:15:THR:O	1:B:18:ARG:HB2	1.98	0.63
2:K:289:CYS:SG	2:K:306:CYS:N	2.71	0.63
2:E:320:MET:CE	2:E:324:THR:HG23	2.23	0.63
2:J:56:MET:SD	2:J:58:GLN:NE2	2.71	0.63
1:D:15:THR:O	1:D:18:ARG:HB2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:13:ARG:HE	2:E:221:GLN:CG	2.12	0.62
2:E:226:LEU:HD12	2:E:323:VAL:HG12	1.81	0.62
2:E:11:GLY:HA2	3:E:401:GTP:O3G	1.98	0.62
2:I:306:CYS:SG	2:I:320:MET:CE	2.87	0.62
2:J:155:ARG:HH21	2:J:205:GLY:CA	2.13	0.62
2:E:320:MET:HE3	2:E:324:THR:HG21	1.79	0.62
2:G:11:GLY:C	3:G:401:GTP:O3G	2.42	0.62
2:F:58:GLN:HB2	2:F:62:LYS:NZ	2.15	0.62
2:J:17:LEU:HD11	2:J:307:ILE:HG21	1.82	0.62
2:I:13:ARG:HG2	2:I:221:GLN:HG2	1.82	0.61
2:E:14:LEU:CD2	2:E:220:GLY:O	2.48	0.61
2:I:60:LEU:O	2:I:64:MET:HB2	2.00	0.61
2:G:323:VAL:HG23	2:G:323:VAL:O	2.00	0.61
2:J:7:VAL:O	2:J:7:VAL:HG23	2.01	0.61
2:I:138:VAL:HG12	2:I:140:GLU:H	1.66	0.61
2:F:94:ARG:O	2:F:98:SER:HB2	2.01	0.61
2:F:286:ILE:CG2	2:F:289:CYS:SG	2.88	0.60
2:E:156:ILE:HD12	2:E:207:LEU:HB3	1.82	0.60
2:E:323:VAL:HG23	2:E:323:VAL:O	2.00	0.60
2:E:324:THR:HG23	2:E:324:THR:O	1.99	0.60
2:I:11:GLY:HA2	3:I:401:GTP:O3G	2.01	0.60
2:J:226:LEU:HD12	2:J:323:VAL:HG21	1.81	0.60
2:F:7:VAL:O	2:F:7:VAL:HG13	1.99	0.60
2:F:23:LYS:CE	2:F:110:ASP:HB3	2.32	0.60
2:I:306:CYS:SG	2:I:324:THR:O	2.59	0.60
2:F:53:VAL:C	3:F:401:GTP:N2	2.55	0.60
2:K:2:LYS:HE2	2:K:97:LEU:HA	1.83	0.60
2:E:334:ASP:OD2	2:E:334:ASP:N	2.29	0.60
2:J:54:SER:HB2	3:J:401:GTP:N1	2.16	0.60
2:L:324:THR:HG22	2:L:340:GLY:N	2.17	0.60
2:L:230:CYS:SG	2:L:271:ASN:ND2	2.75	0.60
2:F:7:VAL:HG22	2:F:24:PRO:CG	2.16	0.60
2:H:323:VAL:HG23	2:H:323:VAL:O	2.02	0.60
2:E:292:LEU:HD12	2:E:309:GLY:HA2	1.84	0.59
2:F:13:ARG:O	2:F:14:LEU:HD23	2.02	0.59
2:J:54:SER:HB2	3:J:401:GTP:HN1	1.67	0.59
2:K:323:VAL:O	2:K:323:VAL:HG23	2.00	0.59
2:F:8:GLY:HA2	3:F:401:GTP:N2	2.16	0.59
2:F:14:LEU:HG	2:F:14:LEU:O	2.01	0.59
2:H:33:ILE:HD12	2:H:219:ILE:HD11	1.85	0.59
2:H:14:LEU:HD12	2:H:14:LEU:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:323:VAL:HG23	2:I:323:VAL:O	2.02	0.59
2:J:11:GLY:CA	3:J:401:GTP:O3G	2.50	0.59
2:I:13:ARG:CD	2:I:221:GLN:HG2	2.33	0.59
2:H:54:SER:HB2	3:H:401:GTP:HN1	1.68	0.58
2:L:7:VAL:O	2:L:7:VAL:HG12	2.02	0.58
2:E:14:LEU:O	2:E:14:LEU:HG	2.02	0.58
2:I:146:VAL:HB	2:I:168:SER:HB2	1.85	0.58
2:J:33:ILE:HG23	2:J:112:ILE:HD11	1.85	0.58
2:F:84:LEU:HB3	2:F:88:GLY:HA3	1.84	0.58
2:F:323:VAL:O	2:F:323:VAL:HG23	2.02	0.58
2:L:323:VAL:HG23	2:L:323:VAL:O	2.04	0.58
2:E:8:GLY:CA	3:E:401:GTP:HN22	2.13	0.58
2:I:108:ASN:ND2	3:I:401:GTP:H5'	2.18	0.58
2:J:35:LEU:O	2:J:39:GLU:HB2	2.02	0.58
2:J:316:GLN:H	2:J:334:ASP:HB3	1.69	0.58
2:L:8:GLY:N	3:L:401:GTP:N3	2.52	0.58
2:E:253:ASN:OD1	2:E:253:ASN:N	2.35	0.58
2:H:321:GLU:O	2:H:324:THR:CG2	2.52	0.58
2:J:51:LEU:HD21	2:J:64:MET:SD	2.44	0.58
2:H:80:GLU:HG3	2:H:92:LEU:HD22	1.84	0.57
2:L:297:ILE:HG22	2:L:314:VAL:CG2	2.33	0.57
2:F:102:ASP:CB	2:F:103:PRO:CD	2.81	0.57
2:J:64:MET:HE3	2:J:77:MET:HE2	1.86	0.57
2:J:196:GLU:HA	2:J:199:PRO:HB2	1.86	0.57
1:B:320:ARG:NH1	2:F:335:GLU:OE1	2.38	0.57
2:J:306:CYS:SG	2:J:320:MET:CE	2.87	0.57
2:L:11:GLY:C	3:L:401:GTP:O3G	2.47	0.57
2:G:8:GLY:CA	3:G:401:GTP:N2	2.68	0.57
2:F:58:GLN:HB2	2:F:62:LYS:HZ1	1.69	0.57
2:H:54:SER:CB	3:H:401:GTP:HN1	2.18	0.57
2:E:306:CYS:SG	2:E:308:VAL:CG2	2.92	0.56
2:I:41:LEU:HD21	2:I:49:VAL:HG12	1.87	0.56
2:J:11:GLY:HA2	3:J:401:GTP:O3G	2.04	0.56
2:K:189:GLN:O	2:K:191:THR:N	2.38	0.56
2:I:86:THR:HG23	2:I:192:SER:HB2	1.87	0.56
2:L:14:LEU:CD1	2:L:17:LEU:HB2	2.34	0.56
2:E:193:ILE:HG13	2:E:197:VAL:HB	1.87	0.56
2:F:53:VAL:HA	3:F:401:GTP:HN22	1.70	0.56
2:G:306:CYS:SG	2:G:324:THR:HG23	2.46	0.56
2:J:155:ARG:HH21	2:J:205:GLY:HA3	1.68	0.56
2:G:8:GLY:CA	3:G:401:GTP:N3	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:324:THR:HG23	2:G:324:THR:O	2.06	0.56
1:C:242:ASP:OD2	1:C:242:ASP:N	2.39	0.56
2:H:11:GLY:CA	3:H:401:GTP:O3G	2.53	0.56
2:L:305:SER:O	2:L:323:VAL:HA	2.05	0.56
2:E:120:MET:HE1	2:E:175:MET:HB3	1.88	0.56
2:J:323:VAL:HG13	2:J:323:VAL:O	2.05	0.56
1:D:242:ASP:OD2	1:D:242:ASP:N	2.39	0.55
1:C:259:ARG:NH1	1:C:359:ASP:OD1	2.39	0.55
2:I:346:HIS:CE1	2:J:10:TYR:HE1	2.24	0.55
2:F:182:VAL:HG13	2:F:201:MET:HE1	1.89	0.55
2:H:150:GLU:HB2	2:H:157:HIS:HE1	1.71	0.55
1:B:242:ASP:OD2	1:B:242:ASP:N	2.39	0.55
2:E:14:LEU:HD22	2:E:220:GLY:O	2.07	0.55
2:H:11:GLY:HA2	3:H:401:GTP:O3G	2.07	0.55
2:H:332:VAL:HG22	2:H:349:ILE:HD12	1.89	0.55
2:G:13:ARG:HB3	2:G:220:GLY:O	2.06	0.55
2:J:10:TYR:N	2:J:10:TYR:CD2	2.72	0.55
2:J:156:ILE:HD11	2:J:209:ALA:HB2	1.88	0.55
2:F:134:LEU:HB3	2:F:173:ALA:HB3	1.89	0.55
2:H:13:ARG:HB3	2:H:220:GLY:O	2.06	0.54
2:F:172:ASN:ND2	2:F:194:GLU:OE1	2.41	0.54
2:H:13:ARG:HH21	3:H:401:GTP:PG	2.30	0.54
2:I:13:ARG:CD	2:I:221:GLN:HE21	2.18	0.54
2:I:17:LEU:HD11	2:I:307:ILE:HG21	1.87	0.54
2:I:332:VAL:HG22	2:I:349:ILE:HD12	1.89	0.54
2:L:297:ILE:HA	2:L:314:VAL:CG2	2.36	0.54
2:I:41:LEU:HD23	2:I:49:VAL:HG11	1.86	0.54
2:J:322:ASN:ND2	2:J:339:ASN:OD1	2.35	0.54
2:G:80:GLU:HG3	2:G:92:LEU:HD22	1.89	0.54
2:G:146:VAL:HB	2:G:168:SER:HB3	1.90	0.54
2:J:193:ILE:HG13	2:J:197:VAL:HB	1.89	0.54
2:J:14:LEU:HD12	2:J:17:LEU:HB2	1.89	0.54
1:C:356:THR:HG23	1:C:357:PRO:HD2	1.90	0.54
2:L:80:GLU:OE1	2:L:84:LEU:CD2	2.42	0.54
1:B:256:TYR:CD1	1:B:359:ASP:HB3	2.43	0.54
2:F:332:VAL:HG22	2:F:349:ILE:HD12	1.90	0.54
2:K:185:ARG:NH2	2:K:204:GLU:OE1	2.41	0.54
2:G:17:LEU:HD11	2:G:307:ILE:HG21	1.89	0.53
1:B:114:ASN:CG	3:B:501:GTP:H4'	2.33	0.53
2:E:10:TYR:HD1	2:E:55:TYR:CD1	2.26	0.53
2:J:129:GLN:HG2	2:J:206:GLN:CA	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:33:ILE:HD12	2:E:219:ILE:HD11	1.90	0.53
2:G:13:ARG:NH2	3:G:401:GTP:O2G	2.41	0.53
2:J:107:LEU:CG	2:J:175:MET:HG2	2.38	0.53
1:D:320:ARG:NH1	2:K:335:GLU:OE1	2.42	0.53
2:G:2:LYS:HE2	2:G:97:LEU:HA	1.90	0.53
2:L:17:LEU:HD11	2:L:307:ILE:HG21	1.90	0.53
1:A:242:ASP:OD2	1:A:242:ASP:N	2.39	0.53
2:F:54:SER:CB	3:F:401:GTP:C2	2.92	0.53
2:J:283:GLY:O	2:L:317:TRP:NE1	2.40	0.53
1:C:114:ASN:CG	3:C:501:GTP:H4'	2.33	0.53
2:E:32:PRO:HD2	2:E:35:LEU:HD22	1.91	0.53
1:A:114:ASN:CG	3:A:501:GTP:H4'	2.33	0.53
2:G:221:GLN:HB2	2:G:224:ASP:HB2	1.90	0.52
2:F:102:ASP:O	2:F:180:PRO:HD3	2.08	0.52
2:G:53:VAL:HG11	2:G:60:LEU:HD23	1.91	0.52
2:J:323:VAL:O	2:J:323:VAL:HG22	2.10	0.52
2:F:13:ARG:HG3	2:F:221:GLN:HG2	1.91	0.52
1:C:259:ARG:HD3	1:C:304:ASN:CG	2.35	0.52
2:E:14:LEU:HD23	2:E:220:GLY:O	2.09	0.52
2:E:316:GLN:H	2:E:334:ASP:HB3	1.74	0.52
2:G:305:SER:OG	2:G:323:VAL:HG12	2.09	0.52
2:I:346:HIS:ND1	2:J:10:TYR:CD1	2.78	0.52
2:E:37:GLN:O	2:E:41:LEU:HB2	2.09	0.52
2:L:96:LEU:HA	2:L:99:GLU:HG3	1.91	0.52
2:F:37:GLN:HG2	2:F:107:LEU:HD13	1.91	0.52
2:L:52:ALA:HA	2:L:78:SER:HB3	1.92	0.52
1:A:320:ARG:NH1	2:H:335:GLU:OE1	2.42	0.52
2:J:107:LEU:HG	2:J:175:MET:HG2	1.91	0.52
2:J:322:ASN:HD22	2:J:339:ASN:ND2	2.07	0.52
2:E:35:LEU:O	2:E:39:GLU:HB2	2.10	0.52
2:F:141:PRO:HG2	2:F:166:PHE:HE2	1.74	0.52
2:L:4:LEU:HD13	2:L:50:ILE:HG23	1.91	0.52
2:K:11:GLY:HA2	3:K:401:GTP:O3G	2.09	0.52
2:K:11:GLY:CA	3:K:401:GTP:O3G	2.58	0.52
2:I:178:LEU:HD22	2:I:182:VAL:HG11	1.92	0.51
2:K:193:ILE:HG13	2:K:197:VAL:HB	1.91	0.51
2:E:298:ARG:HD3	2:E:315:GLY:HA2	1.91	0.51
2:I:11:GLY:CA	3:I:401:GTP:O3G	2.58	0.51
2:K:80:GLU:HG3	2:K:92:LEU:HD22	1.91	0.51
2:G:8:GLY:HA2	2:G:53:VAL:HA	1.90	0.51
2:G:11:GLY:HA2	3:G:401:GTP:O3G	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:110:ASP:OD2	2:J:110:ASP:N	2.44	0.51
2:F:12:THR:N	3:F:401:GTP:O3G	2.44	0.51
2:G:150:GLU:HB2	2:G:157:HIS:HE1	1.74	0.51
2:J:11:GLY:HA3	2:J:23:LYS:HD2	1.92	0.51
2:K:256:VAL:HG22	2:K:274:LEU:HD12	1.92	0.51
1:B:282:TRP:HB2	1:B:300:VAL:HB	1.92	0.51
2:G:193:ILE:HD12	2:G:197:VAL:HB	1.91	0.51
1:A:145:ASN:O	1:A:149:SER:OG	2.29	0.51
2:F:53:VAL:HA	3:F:401:GTP:N2	2.26	0.51
2:H:134:LEU:HD21	2:H:212:LEU:HB2	1.93	0.51
2:L:185:ARG:NH2	2:L:204:GLU:OE2	2.43	0.51
2:H:172:ASN:HD21	2:H:176:TYR:HE1	1.59	0.50
2:J:8:GLY:HA2	3:J:401:GTP:N2	2.26	0.50
2:J:14:LEU:CD1	2:J:17:LEU:HD12	2.41	0.50
2:L:148:VAL:HB	2:L:168:SER:OG	2.12	0.50
2:E:138:VAL:HG13	2:E:140:GLU:H	1.76	0.50
2:F:8:GLY:N	3:F:401:GTP:H1'	2.12	0.50
2:G:320:MET:HG2	2:G:338:LEU:HB2	1.93	0.50
2:G:332:VAL:HG22	2:G:349:ILE:HD12	1.92	0.50
2:J:64:MET:O	2:J:67:GLN:N	2.45	0.50
2:J:183:LEU:HA	2:J:186:ILE:HG13	1.93	0.50
1:A:282:TRP:HB2	1:A:300:VAL:HB	1.92	0.50
2:E:230:CYS:SG	2:E:271:ASN:ND2	2.84	0.50
2:H:4:LEU:HD12	2:H:50:ILE:HB	1.93	0.50
2:J:200:ILE:O	2:J:204:GLU:HG2	2.11	0.50
2:J:311:ARG:NH1	2:J:329:ASP:OD1	2.44	0.50
2:I:13:ARG:CG	2:I:221:GLN:HG2	2.41	0.50
2:K:7:VAL:HG21	2:K:51:LEU:HD12	1.92	0.50
2:L:237:ARG:HH21	2:L:244:LEU:HD12	1.75	0.50
1:D:282:TRP:HB2	1:D:300:VAL:HB	1.92	0.50
1:C:320:ARG:NH1	2:I:335:GLU:OE1	2.44	0.50
2:E:11:GLY:H	2:E:18:THR:HG21	1.77	0.50
2:E:305:SER:O	2:E:323:VAL:HA	2.12	0.50
2:H:256:VAL:HG22	2:H:274:LEU:HD12	1.94	0.50
1:C:282:TRP:HB2	1:C:300:VAL:HB	1.92	0.50
2:F:221:GLN:OE1	2:F:223:LYS:NZ	2.44	0.50
2:G:14:LEU:HA	2:G:222:PRO:HG3	1.93	0.50
2:J:80:GLU:HG2	2:J:92:LEU:HD22	1.93	0.50
2:K:8:GLY:CA	3:K:401:GTP:N2	2.72	0.50
2:E:13:ARG:NE	2:E:221:GLN:HG3	2.24	0.49
2:J:324:THR:HG22	2:J:340:GLY:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:LYS:HE3	2:F:110:ASP:HB3	1.95	0.49
2:I:11:GLY:C	3:I:401:GTP:O3G	2.53	0.49
2:L:256:VAL:HG22	2:L:274:LEU:HD13	1.93	0.49
2:G:11:GLY:CA	3:G:401:GTP:O3G	2.60	0.49
2:J:14:LEU:HD12	2:J:17:LEU:HD12	1.95	0.49
2:J:206:GLN:O	2:J:208:TYR:HD2	1.95	0.49
1:B:145:ASN:O	1:B:149:SER:OG	2.29	0.49
2:E:178:LEU:HD22	2:E:182:VAL:HG11	1.94	0.49
2:F:38:VAL:HA	2:F:41:LEU:HB2	1.94	0.49
2:L:324:THR:HG22	2:L:340:GLY:H	1.76	0.49
1:D:114:ASN:CG	3:D:501:GTP:H4'	2.37	0.49
1:D:145:ASN:O	1:D:149:SER:OG	2.29	0.49
2:G:134:LEU:HD12	2:G:175:MET:HG2	1.95	0.49
1:C:145:ASN:O	1:C:149:SER:OG	2.29	0.49
2:J:274:LEU:HB3	2:J:278:VAL:HG21	1.94	0.49
2:E:17:LEU:HD11	2:E:307:ILE:HG21	1.95	0.49
2:F:47:ASP:OD1	2:F:47:ASP:N	2.44	0.49
2:F:133:ILE:HG22	2:F:209:ALA:HA	1.95	0.49
2:G:32:PRO:HD2	2:G:35:LEU:HD12	1.94	0.49
2:K:108:ASN:OD1	3:K:401:GTP:H5'	2.12	0.49
2:H:229:MET:HE3	2:H:229:MET:HB3	1.69	0.48
2:J:14:LEU:HA	2:J:222:PRO:HG3	1.95	0.48
2:J:135:VAL:HG23	2:J:211:GLU:HG3	1.95	0.48
2:J:218:ASP:OD2	2:J:218:ASP:N	2.42	0.48
2:H:32:PRO:HD2	2:H:35:LEU:HD22	1.95	0.48
2:K:186:ILE:HD12	2:K:197:VAL:HG11	1.94	0.48
2:E:146:VAL:HB	2:E:168:SER:HB3	1.95	0.48
2:F:84:LEU:HA	2:F:190:PRO:HB3	1.96	0.48
2:G:84:LEU:HA	2:G:190:PRO:HB3	1.95	0.48
2:I:84:LEU:HB3	2:I:88:GLY:HA3	1.94	0.48
2:J:6:LEU:C	2:J:7:VAL:CG1	2.86	0.48
2:G:133:ILE:HG22	2:G:209:ALA:HA	1.95	0.48
2:G:230:CYS:SG	2:G:271:ASN:ND2	2.87	0.48
2:J:155:ARG:NH2	2:J:205:GLY:HA2	2.26	0.48
2:K:347:LYS:HE2	2:K:359:ILE:HG22	1.95	0.48
1:C:361:ASN:OD1	1:C:364:ASP:N	2.40	0.48
2:F:33:ILE:HG23	2:F:112:ILE:HD11	1.96	0.48
2:L:297:ILE:HA	2:L:314:VAL:HG23	1.94	0.48
2:G:110:ASP:OD2	2:G:110:ASP:N	2.45	0.48
2:J:332:VAL:HG22	2:J:349:ILE:HD12	1.94	0.48
2:L:11:GLY:N	2:L:18:THR:HG21	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:ASN:ND2	2:E:176:TYR:OH	2.43	0.48
2:H:90:LEU:HD21	2:H:106:VAL:HG11	1.96	0.48
2:K:38:VAL:HG13	2:K:49:VAL:HG11	1.95	0.48
2:L:272:VAL:HG12	2:L:289:CYS:H	1.78	0.48
2:L:337:TYR:H	2:L:352:SER:HB3	1.78	0.48
1:C:136:PRO:HA	1:C:187:SER:HB3	1.96	0.48
2:F:256:VAL:HG22	2:F:274:LEU:HD12	1.95	0.48
2:H:135:VAL:HG21	2:H:209:ALA:HB1	1.95	0.48
2:I:41:LEU:O	2:I:44:ALA:HB3	2.14	0.48
2:J:4:LEU:HA	2:J:50:ILE:O	2.14	0.47
2:K:332:VAL:HG22	2:K:349:ILE:HD12	1.96	0.47
2:J:201:MET:HB3	2:J:207:LEU:HG	1.95	0.47
1:A:136:PRO:HA	1:A:187:SER:HB3	1.96	0.47
2:F:12:THR:O	2:F:15:ARG:HB2	2.13	0.47
2:F:74:ARG:HH12	2:F:76:SER:HB2	1.79	0.47
1:D:136:PRO:HA	1:D:187:SER:HB3	1.96	0.47
2:L:292:LEU:HD12	2:L:309:GLY:HA2	1.95	0.47
1:B:156:VAL:HG22	1:B:176:SER:HB2	1.97	0.47
2:H:321:GLU:O	2:H:324:THR:HG22	2.15	0.47
2:K:67:GLN:HG3	2:K:71:LEU:HD12	1.95	0.47
2:I:134:LEU:HB3	2:I:173:ALA:HB3	1.97	0.47
2:K:15:ARG:HA	2:K:18:THR:HB	1.96	0.47
1:A:37:ILE:HA	1:A:40:HIS:HD2	1.79	0.47
1:A:259:ARG:NH1	1:A:259:ARG:CG	2.72	0.47
2:E:53:VAL:HA	3:E:401:GTP:N2	2.29	0.47
2:E:84:LEU:HA	2:E:190:PRO:HB3	1.95	0.47
2:J:67:GLN:OE1	2:J:70:ARG:NH1	2.48	0.47
1:A:156:VAL:HG22	1:A:176:SER:HB2	1.97	0.47
1:A:303:PRO:HD2	1:A:320:ARG:HG3	1.97	0.47
2:E:279:VAL:HB	2:E:296:ARG:HG3	1.96	0.47
2:F:53:VAL:CA	3:F:401:GTP:N2	2.78	0.47
2:I:15:ARG:NH1	2:J:360:MET:O	2.48	0.47
2:L:298:ARG:HD3	2:L:315:GLY:HA2	1.97	0.47
1:D:156:VAL:HG22	1:D:176:SER:HB2	1.97	0.47
2:F:17:LEU:HD11	2:F:307:ILE:HG21	1.97	0.47
2:G:282:ASP:OD2	2:G:282:ASP:N	2.48	0.47
2:K:134:LEU:HD21	2:K:212:LEU:HG	1.97	0.47
2:L:280:VAL:HG22	2:L:297:ILE:HD11	1.97	0.47
1:D:37:ILE:HA	1:D:40:HIS:HD2	1.80	0.46
1:D:303:PRO:HD2	1:D:320:ARG:HG3	1.97	0.46
1:B:136:PRO:HA	1:B:187:SER:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:193:ILE:HG13	2:L:197:VAL:HB	1.96	0.46
1:B:37:ILE:HA	1:B:40:HIS:HD2	1.80	0.46
2:E:125:ARG:HB3	2:E:125:ARG:NH1	2.30	0.46
2:I:61:GLU:OE2	2:I:79:HIS:NE2	2.44	0.46
2:I:256:VAL:HG22	2:I:274:LEU:HD12	1.97	0.46
2:E:7:VAL:HG12	2:E:7:VAL:O	2.15	0.46
1:B:303:PRO:HD2	1:B:320:ARG:HG3	1.97	0.46
2:E:11:GLY:N	2:E:18:THR:HG21	2.30	0.46
1:D:366:ARG:NH2	2:L:164:GLN:OE1	2.48	0.46
2:I:32:PRO:HD2	2:I:35:LEU:HD22	1.97	0.46
2:I:229:MET:HE3	2:I:229:MET:HB3	1.70	0.46
1:B:256:TYR:CG	1:B:359:ASP:HB3	2.50	0.46
2:G:47:ASP:OD2	2:G:47:ASP:N	2.47	0.46
2:J:230:CYS:SG	2:J:271:ASN:ND2	2.89	0.46
2:G:303:LEU:HD23	2:G:320:MET:HB2	1.97	0.46
2:J:302:TRP:HE3	2:J:319:ARG:HG3	1.81	0.46
2:J:201:MET:CE	2:J:207:LEU:HD23	2.42	0.46
2:J:314:VAL:HG12	2:J:318:VAL:HG21	1.98	0.46
2:L:94:ARG:HA	2:L:183:LEU:HD11	1.98	0.46
2:G:5:ILE:HG13	2:G:51:LEU:CD2	2.46	0.46
2:J:324:THR:HG22	2:J:340:GLY:N	2.31	0.46
1:C:303:PRO:HD2	1:C:320:ARG:HG3	1.97	0.45
2:F:298:ARG:HD3	2:F:315:GLY:HA2	1.98	0.45
2:G:156:ILE:HD12	2:G:207:LEU:HD23	1.97	0.45
2:G:154:GLY:O	2:G:209:ALA:N	2.44	0.45
2:G:34:LEU:HD11	2:G:51:LEU:CD2	2.45	0.45
1:C:37:ILE:HA	1:C:40:HIS:HD2	1.80	0.45
2:E:226:LEU:CD1	2:E:323:VAL:HG12	2.46	0.45
2:L:14:LEU:O	2:L:14:LEU:HG	2.15	0.45
2:L:81:GLU:H	2:L:81:GLU:HG2	1.51	0.45
2:J:5:ILE:HG22	2:J:7:VAL:HG12	1.98	0.45
2:L:127:HIS:CD2	2:L:129:GLN:H	2.34	0.45
1:C:156:VAL:HG22	1:C:176:SER:HB2	1.97	0.45
2:I:10:TYR:HD1	2:I:55:TYR:CD1	2.35	0.45
2:I:94:ARG:HA	2:I:183:LEU:HD11	1.99	0.45
2:E:261:ARG:HE	2:E:279:VAL:HG13	1.81	0.45
2:H:343:VAL:HG11	2:H:349:ILE:HD11	1.99	0.45
2:K:107:LEU:HD22	2:K:175:MET:HG2	1.97	0.45
2:K:154:GLY:O	2:K:209:ALA:N	2.46	0.45
1:C:361:ASN:HD21	1:C:363:ASN:HB2	1.82	0.45
2:F:287:ARG:O	2:F:289:CYS:SG	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:ILE:HD12	2:H:207:LEU:HB3	1.98	0.45
1:A:275:LYS:HB3	1:A:275:LYS:HE3	1.73	0.45
1:C:106:SER:O	1:C:106:SER:OG	2.33	0.45
2:E:53:VAL:CA	3:E:401:GTP:HN21	2.29	0.45
2:I:346:HIS:CB	2:J:10:TYR:CD1	2.98	0.45
2:F:54:SER:HB3	3:F:401:GTP:C2	2.51	0.45
2:E:203:LYS:HE2	2:E:203:LYS:HB3	1.77	0.44
2:K:22:PRO:HD2	2:K:25:LEU:HD12	1.99	0.44
2:K:54:SER:CB	3:K:401:GTP:HN1	2.23	0.44
1:B:37:ILE:HA	1:B:40:HIS:CD2	2.53	0.44
2:E:91:ALA:HB2	2:E:186:ILE:HG22	1.98	0.44
2:G:14:LEU:HD12	2:G:17:LEU:CB	2.39	0.44
2:I:11:GLY:HA3	2:I:23:LYS:HD2	1.98	0.44
2:L:229:MET:SD	2:L:273:SER:OG	2.73	0.44
1:D:37:ILE:HA	1:D:40:HIS:CD2	2.53	0.44
1:C:364:ASP:HB3	1:C:367:ALA:HB2	2.00	0.44
2:I:305:SER:O	2:I:323:VAL:HA	2.17	0.44
1:C:37:ILE:HA	1:C:40:HIS:CD2	2.53	0.44
2:E:10:TYR:O	2:E:10:TYR:CD2	2.70	0.44
2:E:311:ARG:NH1	2:E:329:ASP:OD2	2.50	0.44
2:H:17:LEU:HD11	2:H:307:ILE:HG21	1.98	0.44
2:F:26:VAL:O	2:F:32:PRO:HA	2.18	0.44
2:H:33:ILE:HG13	2:H:112:ILE:HD11	2.00	0.44
2:H:84:LEU:HA	2:H:190:PRO:HB3	1.98	0.44
2:K:8:GLY:CA	3:K:401:GTP:N3	2.80	0.44
2:G:41:LEU:HD23	2:G:41:LEU:HA	1.88	0.44
2:K:13:ARG:O	2:K:14:LEU:CB	2.60	0.44
2:K:17:LEU:HD11	2:K:307:ILE:HG21	2.00	0.44
2:F:61:GLU:O	2:F:65:LYS:HB2	2.18	0.44
2:G:14:LEU:HD11	2:G:17:LEU:HB2	1.95	0.44
2:G:256:VAL:HG21	2:G:262:ILE:HD11	2.00	0.44
2:L:13:ARG:HD3	3:L:401:GTP:O2G	2.18	0.44
1:D:62:ASP:O	1:D:66:THR:OG1	2.36	0.43
1:B:62:ASP:O	1:B:66:THR:OG1	2.36	0.43
2:E:13:ARG:HB3	2:E:221:GLN:HG3	2.00	0.43
2:G:235:SER:O	2:G:239:LYS:HB2	2.18	0.43
2:G:298:ARG:HD3	2:G:315:GLY:HA2	1.99	0.43
2:J:324:THR:O	2:J:324:THR:OG1	2.29	0.43
1:A:364:ASP:HB3	1:A:367:ALA:HB2	2.00	0.43
1:B:259:ARG:NH2	1:B:359:ASP:OD1	2.51	0.43
2:I:14:LEU:HD12	2:I:14:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:221:GLN:OE1	2:K:223:LYS:NZ	2.48	0.43
2:L:233:LEU:HD23	2:L:233:LEU:HA	1.90	0.43
1:C:393:ILE:HD12	1:C:399:ILE:HG13	2.01	0.43
2:F:15:ARG:HD2	2:F:15:ARG:HA	1.87	0.43
2:H:237:ARG:HD3	2:H:244:LEU:HD12	2.00	0.43
2:I:150:GLU:HB3	2:I:157:HIS:HE1	1.84	0.43
2:L:52:ALA:C	3:L:401:GTP:N2	2.74	0.43
1:A:37:ILE:HA	1:A:40:HIS:CD2	2.53	0.43
1:A:393:ILE:HD12	1:A:399:ILE:HG13	2.01	0.43
2:G:122:GLN:O	2:G:126:HIS:ND1	2.51	0.43
2:J:178:LEU:HD22	2:J:182:VAL:HG11	1.99	0.43
2:K:127:HIS:HE1	2:K:132:SER:HB2	1.84	0.43
2:H:30:ASN:ND2	2:H:274:LEU:O	2.51	0.43
2:J:91:ALA:HB1	2:J:188:LEU:HD23	2.01	0.43
2:L:147:VAL:O	2:L:168:SER:CB	2.66	0.43
1:B:364:ASP:HB3	1:B:367:ALA:HB2	2.00	0.43
2:J:42:ALA:HB2	2:J:73:ILE:HD13	2.01	0.43
2:L:154:GLY:O	2:L:209:ALA:N	2.40	0.43
1:D:364:ASP:HB3	1:D:367:ALA:HB2	2.00	0.43
2:F:237:ARG:HD3	2:F:244:LEU:HD12	2.01	0.43
2:G:237:ARG:HD3	2:G:244:LEU:HD12	2.00	0.43
2:I:10:TYR:CD1	2:I:55:TYR:CD1	3.06	0.43
2:K:8:GLY:HA2	2:K:53:VAL:HA	1.99	0.43
2:G:14:LEU:HD12	2:G:14:LEU:O	2.18	0.43
2:H:154:GLY:O	2:H:209:ALA:N	2.44	0.43
2:I:84:LEU:HA	2:I:190:PRO:HB3	1.99	0.43
2:J:67:GLN:HA	2:J:70:ARG:HB2	2.00	0.43
1:C:359:ASP:HA	1:C:360:PRO:HD3	1.89	0.43
2:E:225:PHE:HE1	2:E:290:THR:HG21	1.83	0.43
2:F:175:MET:HE3	2:F:175:MET:HB2	1.78	0.43
2:I:237:ARG:HD3	2:I:244:LEU:HD12	2.00	0.43
2:J:307:ILE:HB	2:J:325:VAL:HG13	2.01	0.43
2:F:286:ILE:HG22	2:F:289:CYS:SG	2.59	0.42
2:H:202:ALA:HB2	2:H:207:LEU:HD12	2.00	0.42
2:I:14:LEU:HA	2:I:222:PRO:HG3	2.01	0.42
2:K:61:GLU:OE2	2:K:79:HIS:NE2	2.52	0.42
2:L:343:VAL:HG11	2:L:349:ILE:HD11	2.00	0.42
1:A:259:ARG:HH11	1:A:259:ARG:CG	2.11	0.42
2:L:84:LEU:HA	2:L:190:PRO:HB3	2.02	0.42
1:D:275:LYS:HE3	1:D:275:LYS:HB3	1.73	0.42
2:L:2:LYS:HB3	2:L:48:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:303:LEU:HD23	2:L:306:CYS:SG	2.59	0.42
1:A:62:ASP:O	1:A:66:THR:OG1	2.36	0.42
2:H:8:GLY:CA	3:H:401:GTP:N3	2.74	0.42
2:J:84:LEU:HA	2:J:190:PRO:HB3	2.01	0.42
2:E:13:ARG:NH1	2:E:13:ARG:HA	2.34	0.42
2:L:13:ARG:HG2	2:L:221:GLN:HG2	2.01	0.42
2:E:94:ARG:HA	2:E:183:LEU:HD21	2.02	0.42
2:F:94:ARG:HA	2:F:183:LEU:HD11	2.02	0.42
2:F:229:MET:HB3	2:F:229:MET:HE3	1.70	0.42
2:I:13:ARG:HG2	2:I:221:GLN:HA	2.02	0.42
2:E:320:MET:HB3	2:E:324:THR:HG21	2.02	0.42
2:G:261:ARG:HD2	2:G:279:VAL:HG13	2.01	0.42
1:B:393:ILE:HD12	1:B:399:ILE:HG13	2.01	0.42
1:C:253:SER:HB3	1:C:360:PRO:HG3	2.01	0.42
1:C:347:VAL:HA	1:C:393:ILE:HB	2.02	0.42
2:F:32:PRO:HD2	2:F:35:LEU:HD22	2.02	0.42
2:H:303:LEU:HD23	2:H:306:CYS:SG	2.60	0.42
2:K:91:ALA:HB2	2:K:186:ILE:HG23	2.02	0.42
2:K:130:GLU:HG2	2:K:201:MET:HE3	2.01	0.42
1:C:62:ASP:O	1:C:66:THR:OG1	2.36	0.42
2:E:307:ILE:HB	2:E:325:VAL:HG13	2.01	0.42
2:J:8:GLY:N	3:J:401:GTP:N3	2.68	0.42
2:L:50:ILE:HD13	2:L:50:ILE:HG21	1.88	0.42
2:L:106:VAL:HG21	2:L:178:LEU:HD12	2.01	0.42
1:B:347:VAL:HA	1:B:393:ILE:HB	2.02	0.42
2:E:14:LEU:HD12	2:E:17:LEU:CD1	2.35	0.42
2:I:110:ASP:OD1	2:I:110:ASP:N	2.53	0.42
2:J:7:VAL:HB	2:J:24:PRO:CG	2.44	0.42
1:B:154:CYS:HB3	1:B:176:SER:HB3	2.02	0.41
2:F:23:LYS:NZ	2:F:110:ASP:HB3	2.35	0.41
2:L:14:LEU:HA	2:L:222:PRO:HG3	2.02	0.41
2:L:37:GLN:O	2:L:41:LEU:HB2	2.20	0.41
1:D:18:ARG:HD2	1:D:18:ARG:HA	1.90	0.41
2:I:35:LEU:HG	2:I:67:GLN:NE2	2.35	0.41
1:D:154:CYS:HB3	1:D:176:SER:HB3	2.02	0.41
1:C:154:CYS:HB3	1:C:176:SER:HB3	2.02	0.41
2:H:328:GLU:HG2	2:H:345:PRO:HB3	2.03	0.41
2:J:206:GLN:O	2:J:208:TYR:CD2	2.73	0.41
2:G:116:PRO:O	2:G:120:MET:HB2	2.21	0.41
2:G:347:LYS:HE2	2:G:359:ILE:HG22	2.02	0.41
2:I:106:VAL:HG21	2:I:178:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:SER:O	1:D:253:SER:OG	2.39	0.41
1:D:393:ILE:HD12	1:D:399:ILE:HG13	2.01	0.41
1:B:392:ARG:HH11	1:B:394:PRO:HB3	1.86	0.41
2:E:47:ASP:OD2	2:E:47:ASP:N	2.54	0.41
2:E:229:MET:HE3	2:E:229:MET:HB3	1.73	0.41
2:H:15:ARG:HA	2:H:15:ARG:HD2	1.93	0.41
2:I:54:SER:CB	3:I:401:GTP:HN1	2.27	0.41
2:L:133:ILE:HD11	2:L:172:ASN:ND2	2.36	0.41
1:A:347:VAL:HA	1:A:393:ILE:HB	2.02	0.41
1:D:347:VAL:HA	1:D:393:ILE:HB	2.02	0.41
1:C:116:ASP:OD2	1:C:249:LYS:NZ	2.49	0.41
2:F:177:ILE:HD13	2:F:177:ILE:HG21	1.85	0.41
2:G:229:MET:HB3	2:G:229:MET:HE3	1.69	0.41
2:J:6:LEU:C	2:J:7:VAL:HG12	2.46	0.41
2:K:80:GLU:HG2	2:K:84:LEU:HD22	2.02	0.41
2:F:13:ARG:HD3	2:F:13:ARG:HA	1.72	0.41
2:H:54:SER:HB3	3:H:401:GTP:N1	2.36	0.41
2:H:106:VAL:HG22	2:H:176:TYR:HB2	2.03	0.41
2:I:11:GLY:O	2:I:18:THR:HG21	2.21	0.41
2:I:286:ILE:CG2	2:I:289:CYS:HB2	2.50	0.41
2:K:237:ARG:HH21	2:K:244:LEU:HD12	1.86	0.41
2:F:83:PRO:HA	3:F:401:GTP:O6	2.20	0.41
2:F:242:GLU:H	2:F:242:GLU:HG3	1.71	0.41
2:G:15:ARG:HD2	2:G:15:ARG:HA	1.90	0.41
2:L:4:LEU:HD23	2:L:90:LEU:HG	2.03	0.41
1:D:392:ARG:HH11	1:D:394:PRO:HB3	1.86	0.41
1:C:158:ASN:ND2	1:C:161:THR:OG1	2.53	0.41
2:E:19:LEU:HD23	2:E:19:LEU:HA	1.94	0.41
2:E:27:ASP:HB2	2:E:292:LEU:HD22	2.02	0.41
2:E:127:HIS:CD2	2:E:129:GLN:H	2.39	0.41
2:E:194:GLU:H	2:E:194:GLU:HG3	1.72	0.41
2:H:221:GLN:OE1	2:H:223:LYS:NZ	2.42	0.41
2:J:120:MET:CE	2:J:175:MET:SD	2.70	0.41
2:K:146:VAL:HB	2:K:168:SER:HB3	2.03	0.41
2:L:84:LEU:HB3	2:L:89:PRO:HD3	2.02	0.41
2:F:25:LEU:HD23	2:F:25:LEU:HA	1.73	0.41
2:F:154:GLY:O	2:F:209:ALA:N	2.50	0.41
2:G:4:LEU:HD23	2:G:97:LEU:HD11	2.03	0.41
2:G:13:ARG:NH1	2:G:13:ARG:CG	2.73	0.41
2:L:254:VAL:HG13	2:L:272:VAL:HG23	2.03	0.41
1:C:392:ARG:HH11	1:C:394:PRO:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:SER:HB3	2:G:60:LEU:HB3	2.02	0.40
2:H:8:GLY:HA2	2:H:53:VAL:HA	2.02	0.40
2:H:293:ARG:HG2	2:H:310:TRP:HD1	1.86	0.40
2:H:347:LYS:HE2	2:H:359:ILE:HG22	2.02	0.40
1:D:167:TYR:HB3	1:D:228:SER:HA	2.03	0.40
2:E:23:LYS:NZ	3:E:401:GTP:O1G	2.52	0.40
2:F:233:LEU:HD23	2:F:233:LEU:HA	1.90	0.40
2:H:150:GLU:HB2	2:H:157:HIS:CE1	2.54	0.40
2:H:261:ARG:HE	2:H:262:ILE:H	1.68	0.40
2:J:229:MET:HE3	2:J:229:MET:HB3	1.77	0.40
2:J:302:TRP:CE3	2:J:319:ARG:HG3	2.56	0.40
2:L:15:ARG:HD2	2:L:15:ARG:HA	1.83	0.40
2:L:302:TRP:HE3	2:L:319:ARG:HG3	1.87	0.40
2:F:343:VAL:HG11	2:F:349:ILE:HD11	2.02	0.40
2:J:11:GLY:N	2:J:18:THR:HG21	2.37	0.40
1:B:138:LEU:HB3	1:B:185:LEU:HB3	2.03	0.40
2:E:343:VAL:HG11	2:E:349:ILE:HD11	2.03	0.40
2:F:198:PHE:HD1	2:F:207:LEU:HD21	1.87	0.40
2:H:158:ARG:HE	2:H:158:ARG:HB3	1.74	0.40
1:D:375:PHE:HB2	1:C:417:GLN:HG2	2.04	0.40
1:B:18:ARG:HD2	1:B:18:ARG:HA	1.90	0.40
1:C:250:SER:O	1:C:253:SER:OG	2.39	0.40
2:H:8:GLY:CA	3:H:401:GTP:N2	2.78	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	402/420 (96%)	391 (97%)	11 (3%)	0	100	100
1	B	402/420 (96%)	392 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	402/420 (96%)	392 (98%)	10 (2%)	0	100	100
1	D	402/420 (96%)	392 (98%)	10 (2%)	0	100	100
2	E	358/360 (99%)	334 (93%)	21 (6%)	3 (1%)	16	47
2	F	358/360 (99%)	332 (93%)	23 (6%)	3 (1%)	16	47
2	G	355/360 (99%)	331 (93%)	24 (7%)	0	100	100
2	H	358/360 (99%)	336 (94%)	21 (6%)	1 (0%)	36	67
2	I	358/360 (99%)	336 (94%)	20 (6%)	2 (1%)	21	52
2	J	358/360 (99%)	333 (93%)	22 (6%)	3 (1%)	16	47
2	K	358/360 (99%)	335 (94%)	22 (6%)	1 (0%)	36	67
2	L	358/360 (99%)	333 (93%)	22 (6%)	3 (1%)	16	47
All	All	4469/4560 (98%)	4237 (95%)	216 (5%)	16 (0%)	31	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	8	GLY
2	F	10	TYR
2	I	10	TYR
2	J	8	GLY
2	L	10	TYR
2	F	7	VAL
2	E	323	VAL
2	I	14	LEU
2	K	190	PRO
2	E	163	PRO
2	J	10	TYR
2	J	7	VAL
2	H	11	GLY
2	F	102	ASP
2	L	7	VAL
2	L	323	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	A	344/354 (97%)	322 (94%)	22 (6%)	16	44
1	B	344/354 (97%)	323 (94%)	21 (6%)	17	46
1	C	344/354 (97%)	323 (94%)	21 (6%)	17	46
1	D	344/354 (97%)	323 (94%)	21 (6%)	17	46
2	E	310/311 (100%)	273 (88%)	37 (12%)	5	21
2	F	311/311 (100%)	279 (90%)	32 (10%)	7	27
2	G	310/311 (100%)	272 (88%)	38 (12%)	4	20
2	H	311/311 (100%)	286 (92%)	25 (8%)	11	37
2	I	311/311 (100%)	279 (90%)	32 (10%)	7	27
2	J	311/311 (100%)	269 (86%)	42 (14%)	4	16
2	K	311/311 (100%)	288 (93%)	23 (7%)	13	40
2	L	311/311 (100%)	274 (88%)	37 (12%)	5	21
All	All	3862/3904 (99%)	3511 (91%)	351 (9%)	11	32

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	63	GLU
1	A	66	THR
1	A	120	ASP
1	A	149	SER
1	A	164	VAL
1	A	173	THR
1	A	187	SER
1	A	238	VAL
1	A	240	LEU
1	A	242	ASP
1	A	253	SER
1	A	258	SER
1	A	259	ARG
1	A	300	VAL
1	A	312	THR
1	A	325	LEU
1	A	329	THR
1	A	356	THR
1	A	373	SER

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Mol	Chain	Res	Type
1	A	397	VAL
1	A	405	LEU
1	D	24	VAL
1	D	63	GLU
1	D	66	THR
1	D	120	ASP
1	D	149	SER
1	D	164	VAL
1	D	173	THR
1	D	187	SER
1	D	238	VAL
1	D	240	LEU
1	D	242	ASP
1	D	253	SER
1	D	258	SER
1	D	300	VAL
1	D	312	THR
1	D	325	LEU
1	D	329	THR
1	D	356	THR
1	D	373	SER
1	D	397	VAL
1	D	405	LEU
1	B	24	VAL
1	B	63	GLU
1	B	66	THR
1	B	120	ASP
1	B	149	SER
1	B	164	VAL
1	B	173	THR
1	B	187	SER
1	B	238	VAL
1	B	240	LEU
1	B	242	ASP
1	B	253	SER
1	B	258	SER
1	B	300	VAL
1	B	312	THR
1	B	325	LEU
1	B	329	THR
1	B	359	ASP
1	B	373	SER

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Mol	Chain	Res	Type
1	B	397	VAL
1	B	405	LEU
1	C	24	VAL
1	C	63	GLU
1	C	66	THR
1	C	120	ASP
1	C	149	SER
1	C	164	VAL
1	C	173	THR
1	C	187	SER
1	C	238	VAL
1	C	240	LEU
1	C	242	ASP
1	C	253	SER
1	C	258	SER
1	C	300	VAL
1	C	312	THR
1	C	325	LEU
1	C	329	THR
1	C	361	ASN
1	C	373	SER
1	C	397	VAL
1	C	405	LEU
2	E	6	LEU
2	E	14	LEU
2	E	21	THR
2	E	25	LEU
2	E	41	LEU
2	E	51	LEU
2	E	53	VAL
2	E	71	LEU
2	E	75	ILE
2	E	76	SER
2	E	81	GLU
2	E	82	GLU
2	E	98	SER
2	E	100	THR
2	E	125	ARG
2	E	126	HIS
2	E	129	GLN
2	E	136	THR
2	E	140	GLU

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Mol	Chain	Res	Type
2	E	144	TYR
2	E	147	VAL
2	E	175	MET
2	E	191	THR
2	E	199	PRO
2	E	212	LEU
2	E	213	GLN
2	E	218	ASP
2	E	221	GLN
2	E	238	GLN
2	E	253	ASN
2	E	274	LEU
2	E	306	CYS
2	E	318	VAL
2	E	325	VAL
2	E	330	VAL
2	E	334	ASP
2	E	348	SER
2	F	2	LYS
2	F	13	ARG
2	F	14	LEU
2	F	37	GLN
2	F	47	ASP
2	F	62	LYS
2	F	67	GLN
2	F	69	GLN
2	F	76	SER
2	F	82	GLU
2	F	84	LEU
2	F	97	LEU
2	F	98	SER
2	F	107	LEU
2	F	114	ASP
2	F	133	ILE
2	F	136	THR
2	F	146	VAL
2	F	148	VAL
2	F	149	CYS
2	F	166	PHE
2	F	167	VAL
2	F	186	ILE
2	F	191	THR

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Mol	Chain	Res	Type
2	F	199	PRO
2	F	200	ILE
2	F	242	GLU
2	F	253	ASN
2	F	289	CYS
2	F	299	SER
2	F	324	THR
2	F	355	GLU
2	G	4	LEU
2	G	13	ARG
2	G	14	LEU
2	G	25	LEU
2	G	33	ILE
2	G	53	VAL
2	G	54	SER
2	G	64	MET
2	G	69	GLN
2	G	75	ILE
2	G	99	GLU
2	G	107	LEU
2	G	120	MET
2	G	122	GLN
2	G	133	ILE
2	G	147	VAL
2	G	148	VAL
2	G	160	VAL
2	G	165	VAL
2	G	167	VAL
2	G	175	MET
2	G	199	PRO
2	G	200	ILE
2	G	207	LEU
2	G	211	GLU
2	G	217	MET
2	G	227	THR
2	G	229	MET
2	G	231	LEU
2	G	235	SER
2	G	238	GLN
2	G	246	SER
2	G	253	ASN
2	G	256	VAL

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Mol	Chain	Res	Type
2	G	264	GLN
2	G	272	VAL
2	G	273	SER
2	G	282	ASP
2	H	4	LEU
2	H	12	THR
2	H	13	ARG
2	H	14	LEU
2	H	33	ILE
2	H	46	VAL
2	H	49	VAL
2	H	61	GLU
2	H	75	ILE
2	H	79	HIS
2	H	99	GLU
2	H	129	GLN
2	H	133	ILE
2	H	135	VAL
2	H	140	GLU
2	H	171	ILE
2	H	178	LEU
2	H	193	ILE
2	H	199	PRO
2	H	201	MET
2	H	218	ASP
2	H	266	CYS
2	H	303	LEU
2	H	324	THR
2	H	342	SER
2	I	2	LYS
2	I	5	ILE
2	I	7	VAL
2	I	10	TYR
2	I	13	ARG
2	I	14	LEU
2	I	33	ILE
2	I	39	GLU
2	I	51	LEU
2	I	57	SER
2	I	65	LYS
2	I	84	LEU
2	I	86	THR

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Mol	Chain	Res	Type
2	I	102	ASP
2	I	112	ILE
2	I	120	MET
2	I	134	LEU
2	I	136	THR
2	I	140	GLU
2	I	147	VAL
2	I	158	ARG
2	I	161	GLU
2	I	165	VAL
2	I	167	VAL
2	I	199	PRO
2	I	229	MET
2	I	238	GLN
2	I	242	GLU
2	I	266	CYS
2	I	322	ASN
2	I	324	THR
2	I	360	MET
2	J	7	VAL
2	J	10	TYR
2	J	14	LEU
2	J	49	VAL
2	J	53	VAL
2	J	54	SER
2	J	56	MET
2	J	57	SER
2	J	61	GLU
2	J	69	GLN
2	J	70	ARG
2	J	77	MET
2	J	84	LEU
2	J	90	LEU
2	J	96	LEU
2	J	129	GLN
2	J	136	THR
2	J	140	GLU
2	J	152	ASP
2	J	160	VAL
2	J	168	SER
2	J	175	MET
2	J	186	ILE

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Mol	Chain	Res	Type
2	J	189	GLN
2	J	191	THR
2	J	199	PRO
2	J	200	ILE
2	J	218	ASP
2	J	227	THR
2	J	230	CYS
2	J	238	GLN
2	J	240	GLN
2	J	244	LEU
2	J	256	VAL
2	J	266	CYS
2	J	306	CYS
2	J	318	VAL
2	J	321	GLU
2	J	331	ILE
2	J	334	ASP
2	J	344	LEU
2	J	351	GLU
2	K	5	ILE
2	K	7	VAL
2	K	15	ARG
2	K	33	ILE
2	K	39	GLU
2	K	49	VAL
2	K	53	VAL
2	K	56	MET
2	K	77	MET
2	K	82	GLU
2	K	86	THR
2	K	114	ASP
2	K	140	GLU
2	K	160	VAL
2	K	167	VAL
2	K	186	ILE
2	K	189	GLN
2	K	192	SER
2	K	199	PRO
2	K	242	GLU
2	K	266	CYS
2	K	323	VAL
2	K	324	THR

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Mol	Chain	Res	Type
2	L	12	THR
2	L	13	ARG
2	L	14	LEU
2	L	53	VAL
2	L	77	MET
2	L	80	GLU
2	L	81	GLU
2	L	82	GLU
2	L	84	LEU
2	L	107	LEU
2	L	111	VAL
2	L	122	GLN
2	L	129	GLN
2	L	147	VAL
2	L	148	VAL
2	L	149	CYS
2	L	157	HIS
2	L	158	ARG
2	L	161	GLU
2	L	162	LYS
2	L	168	SER
2	L	183	LEU
2	L	191	THR
2	L	192	SER
2	L	196	GLU
2	L	199	PRO
2	L	200	ILE
2	L	204	GLU
2	L	218	ASP
2	L	236	LEU
2	L	246	SER
2	L	253	ASN
2	L	257	ASP
2	L	273	SER
2	L	297	ILE
2	L	299	SER
2	L	352	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN

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Mol	Chain	Res	Type
1	A	40	HIS
1	A	51	GLN
1	A	145	ASN
1	A	158	ASN
1	A	266	GLN
1	A	401	ASN
1	A	407	HIS
1	D	12	GLN
1	D	40	HIS
1	D	51	GLN
1	D	145	ASN
1	D	158	ASN
1	D	180	ASN
1	D	247	GLN
1	D	266	GLN
1	D	401	ASN
1	D	407	HIS
1	B	12	GLN
1	B	40	HIS
1	B	51	GLN
1	B	145	ASN
1	B	158	ASN
1	B	266	GLN
1	B	401	ASN
1	B	407	HIS
1	C	40	HIS
1	C	51	GLN
1	C	145	ASN
1	C	158	ASN
1	C	266	GLN
1	C	401	ASN
1	C	407	HIS
2	E	48	HIS
2	E	124	HIS
2	E	127	HIS
2	E	206	GLN
2	E	271	ASN
2	E	316	GLN
2	F	124	HIS
2	F	157	HIS
2	F	206	GLN
2	F	240	GLN

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Mol	Chain	Res	Type
2	G	48	HIS
2	G	271	ASN
2	H	48	HIS
2	H	157	HIS
2	H	172	ASN
2	H	206	GLN
2	H	253	ASN
2	H	265	ASN
2	H	339	ASN
2	I	48	HIS
2	I	67	GLN
2	I	122	GLN
2	I	157	HIS
2	I	206	GLN
2	J	48	HIS
2	J	79	HIS
2	J	271	ASN
2	J	322	ASN
2	K	69	GLN
2	K	127	HIS
2	K	189	GLN
2	K	213	GLN
2	K	339	ASN
2	L	37	GLN
2	L	206	GLN
2	L	240	GLN
2	L	271	ASN
2	L	339	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
3	GTP	A	501	-	33,34,34	1.02	1 (3%)	50,54,54	1.64	10 (20%)
3	GTP	F	401	-	33,34,34	0.85	1 (3%)	50,54,54	2.83	14 (28%)
3	GTP	J	401	-	33,34,34	0.85	2 (6%)	50,54,54	2.83	14 (28%)
3	GTP	L	401	-	33,34,34	0.85	2 (6%)	50,54,54	2.83	14 (28%)
3	GTP	D	501	-	33,34,34	1.01	1 (3%)	50,54,54	1.64	10 (20%)
3	GTP	G	401	-	33,34,34	0.85	2 (6%)	50,54,54	2.83	14 (28%)
3	GTP	H	401	-	33,34,34	0.85	2 (6%)	50,54,54	2.84	14 (28%)
3	GTP	K	401	-	33,34,34	0.85	2 (6%)	50,54,54	2.83	14 (28%)
3	GTP	E	401	-	33,34,34	0.85	2 (6%)	50,54,54	2.83	14 (28%)
3	GTP	I	401	-	33,34,34	0.85	2 (6%)	50,54,54	2.84	14 (28%)
3	GTP	C	501	-	33,34,34	1.01	1 (3%)	50,54,54	1.64	10 (20%)
3	GTP	B	501	-	33,34,34	1.01	1 (3%)	50,54,54	1.64	10 (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	GTP	A	501	-	-	5/22/38/38	0/3/3/3
3	GTP	F	401	-	-	2/22/38/38	0/3/3/3
3	GTP	J	401	-	-	2/22/38/38	0/3/3/3
3	GTP	L	401	-	-	2/22/38/38	0/3/3/3
3	GTP	D	501	-	-	6/22/38/38	0/3/3/3
3	GTP	G	401	-	-	2/22/38/38	0/3/3/3
3	GTP	H	401	-	-	2/22/38/38	0/3/3/3
3	GTP	K	401	-	-	2/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	E	401	-	-	2/22/38/38	0/3/3/3
3	GTP	I	401	-	-	2/22/38/38	0/3/3/3
3	GTP	C	501	-	-	6/22/38/38	0/3/3/3
3	GTP	B	501	-	-	6/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	GTP	C6-N1	-3.08	1.33	1.38
3	C	501	GTP	C6-N1	-3.06	1.33	1.38
3	B	501	GTP	C6-N1	-3.04	1.33	1.38
3	D	501	GTP	C6-N1	-3.01	1.33	1.38
3	G	401	GTP	PG-O2G	2.07	1.62	1.54
3	H	401	GTP	PG-O2G	2.07	1.62	1.54
3	G	401	GTP	C6-N1	-2.07	1.35	1.38
3	F	401	GTP	PG-O2G	2.07	1.62	1.54
3	K	401	GTP	PG-O2G	2.06	1.62	1.54
3	E	401	GTP	PG-O2G	2.05	1.62	1.54
3	L	401	GTP	PG-O2G	2.05	1.62	1.54
3	I	401	GTP	PG-O2G	2.05	1.62	1.54
3	E	401	GTP	C6-N1	-2.04	1.35	1.38
3	J	401	GTP	PG-O2G	2.04	1.62	1.54
3	I	401	GTP	C6-N1	-2.04	1.35	1.38
3	H	401	GTP	C6-N1	-2.02	1.35	1.38
3	L	401	GTP	C6-N1	-2.02	1.35	1.38
3	J	401	GTP	C6-N1	-2.02	1.35	1.38
3	K	401	GTP	C6-N1	-2.01	1.35	1.38

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	GTP	N2-C2-N3	-11.96	96.32	119.67
3	E	401	GTP	N2-C2-N3	-11.95	96.35	119.67
3	I	401	GTP	N2-C2-N3	-11.94	96.36	119.67
3	J	401	GTP	N2-C2-N3	-11.93	96.37	119.67
3	G	401	GTP	N2-C2-N3	-11.93	96.38	119.67
3	H	401	GTP	N2-C2-N3	-11.93	96.39	119.67
3	K	401	GTP	N2-C2-N3	-11.92	96.40	119.67
3	L	401	GTP	N2-C2-N3	-11.92	96.41	119.67
3	K	401	GTP	C2-N1-C6	-8.32	110.01	125.11
3	I	401	GTP	C2-N1-C6	-8.31	110.03	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	401	GTP	C2-N1-C6	-8.31	110.04	125.11
3	H	401	GTP	C2-N1-C6	-8.31	110.04	125.11
3	J	401	GTP	C2-N1-C6	-8.30	110.05	125.11
3	E	401	GTP	C2-N1-C6	-8.29	110.07	125.11
3	F	401	GTP	C2-N1-C6	-8.27	110.10	125.11
3	G	401	GTP	C2-N1-C6	-8.27	110.11	125.11
3	H	401	GTP	C5-C4-N3	-6.20	118.52	128.39
3	I	401	GTP	C5-C4-N3	-6.20	118.53	128.39
3	G	401	GTP	C5-C4-N3	-6.20	118.53	128.39
3	F	401	GTP	C5-C4-N3	-6.19	118.54	128.39
3	L	401	GTP	C5-C4-N3	-6.19	118.54	128.39
3	J	401	GTP	C5-C4-N3	-6.19	118.54	128.39
3	K	401	GTP	C5-C4-N3	-6.16	118.58	128.39
3	E	401	GTP	C5-C4-N3	-6.14	118.61	128.39
3	G	401	GTP	N2-C2-N1	6.02	129.47	116.76
3	F	401	GTP	N2-C2-N1	6.01	129.46	116.76
3	E	401	GTP	N2-C2-N1	6.00	129.42	116.76
3	H	401	GTP	N2-C2-N1	5.99	129.41	116.76
3	I	401	GTP	N2-C2-N1	5.99	129.41	116.76
3	J	401	GTP	N2-C2-N1	5.99	129.40	116.76
3	L	401	GTP	N2-C2-N1	5.98	129.38	116.76
3	K	401	GTP	N2-C2-N1	5.98	129.38	116.76
3	D	501	GTP	C2-N1-C6	-5.09	115.87	125.11
3	A	501	GTP	C2-N1-C6	-5.08	115.90	125.11
3	C	501	GTP	C2-N1-C6	-5.06	115.93	125.11
3	B	501	GTP	C2-N1-C6	-5.04	115.97	125.11
3	C	501	GTP	C5-C4-N3	-4.81	120.74	128.39
3	B	501	GTP	C5-C4-N3	-4.78	120.78	128.39
3	A	501	GTP	C5-C4-N3	-4.78	120.78	128.39
3	D	501	GTP	C5-C4-N3	-4.76	120.81	128.39
3	I	401	GTP	N9-C4-N3	4.02	133.99	125.95
3	F	401	GTP	N9-C4-N3	4.01	133.97	125.95
3	H	401	GTP	N9-C4-N3	4.00	133.96	125.95
3	L	401	GTP	N9-C4-N3	4.00	133.96	125.95
3	J	401	GTP	N9-C4-N3	4.00	133.95	125.95
3	G	401	GTP	N9-C4-N3	4.00	133.95	125.95
3	K	401	GTP	N9-C4-N3	3.99	133.92	125.95
3	E	401	GTP	N9-C4-N3	3.96	133.87	125.95
3	H	401	GTP	C5-C6-N1	3.91	123.20	113.25
3	I	401	GTP	C5-C6-N1	3.91	123.20	113.25
3	L	401	GTP	C5-C6-N1	3.91	123.20	113.25
3	K	401	GTP	C5-C6-N1	3.90	123.19	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	401	GTP	N1-C2-N3	3.90	130.46	123.32
3	G	401	GTP	C5-C6-N1	3.90	123.17	113.25
3	K	401	GTP	N1-C2-N3	3.89	130.44	123.32
3	E	401	GTP	C5-C6-N1	3.89	123.15	113.25
3	J	401	GTP	C5-C6-N1	3.89	123.15	113.25
3	I	401	GTP	N1-C2-N3	3.89	130.44	123.32
3	E	401	GTP	N1-C2-N3	3.89	130.44	123.32
3	F	401	GTP	N1-C2-N3	3.88	130.43	123.32
3	H	401	GTP	N1-C2-N3	3.88	130.42	123.32
3	L	401	GTP	N1-C2-N3	3.87	130.40	123.32
3	F	401	GTP	C5-C6-N1	3.87	123.09	113.25
3	G	401	GTP	N1-C2-N3	3.85	130.36	123.32
3	I	401	GTP	O6-C6-C5	-3.43	117.47	126.53
3	G	401	GTP	O6-C6-C5	-3.43	117.48	126.53
3	H	401	GTP	O6-C6-C5	-3.42	117.49	126.53
3	K	401	GTP	O6-C6-C5	-3.42	117.52	126.53
3	L	401	GTP	O6-C6-C5	-3.41	117.52	126.53
3	E	401	GTP	O6-C6-C5	-3.41	117.52	126.53
3	F	401	GTP	O6-C6-C5	-3.41	117.53	126.53
3	J	401	GTP	O6-C6-C5	-3.41	117.54	126.53
3	C	501	GTP	N9-C4-N3	3.40	132.75	125.95
3	B	501	GTP	N9-C4-N3	3.39	132.73	125.95
3	A	501	GTP	N9-C4-N3	3.37	132.69	125.95
3	D	501	GTP	N9-C4-N3	3.36	132.68	125.95
3	A	501	GTP	C5-C6-N1	2.99	120.86	113.25
3	D	501	GTP	C5-C6-N1	2.98	120.84	113.25
3	C	501	GTP	C5-C6-N1	2.98	120.84	113.25
3	B	501	GTP	C5-C6-N1	2.98	120.83	113.25
3	C	501	GTP	C2-N3-C4	2.82	117.15	112.30
3	C	501	GTP	O6-C6-C5	-2.81	119.12	126.53
3	B	501	GTP	C2-N3-C4	2.81	117.13	112.30
3	A	501	GTP	O6-C6-C5	-2.80	119.13	126.53
3	B	501	GTP	O6-C6-C5	-2.80	119.13	126.53
3	D	501	GTP	O6-C6-C5	-2.80	119.15	126.53
3	D	501	GTP	C2-N3-C4	2.78	117.09	112.30
3	A	501	GTP	C2-N3-C4	2.77	117.06	112.30
3	B	501	GTP	O3A-PB-O1B	-2.66	102.69	110.70
3	A	501	GTP	O3A-PB-O1B	-2.66	102.70	110.70
3	C	501	GTP	O3A-PB-O1B	-2.66	102.72	110.70
3	D	501	GTP	O3A-PB-O1B	-2.65	102.72	110.70
3	J	401	GTP	O2G-PG-O3B	2.63	113.46	104.64
3	K	401	GTP	O2G-PG-O3B	2.62	113.42	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	401	GTP	O2G-PG-O3B	2.62	113.41	104.64
3	H	401	GTP	O2G-PG-O3B	2.61	113.40	104.64
3	G	401	GTP	O2G-PG-O3B	2.61	113.39	104.64
3	I	401	GTP	O2G-PG-O3B	2.61	113.39	104.64
3	E	401	GTP	O2G-PG-O3B	2.61	113.38	104.64
3	F	401	GTP	O2G-PG-O3B	2.61	113.38	104.64
3	B	501	GTP	N9-C8-N7	-2.56	108.65	113.40
3	C	501	GTP	N9-C8-N7	-2.56	108.66	113.40
3	D	501	GTP	N9-C8-N7	-2.55	108.67	113.40
3	A	501	GTP	N9-C8-N7	-2.53	108.70	113.40
3	G	401	GTP	C8-N7-C5	2.53	108.77	104.26
3	E	401	GTP	C8-N7-C5	2.53	108.76	104.26
3	G	401	GTP	O3A-PB-O1B	-2.52	103.12	110.70
3	E	401	GTP	O3A-PB-O1B	-2.52	103.14	110.70
3	I	401	GTP	C8-N7-C5	2.51	108.74	104.26
3	K	401	GTP	O3A-PB-O1B	-2.51	103.15	110.70
3	J	401	GTP	C8-N7-C5	2.51	108.73	104.26
3	L	401	GTP	C8-N7-C5	2.51	108.72	104.26
3	L	401	GTP	O3A-PB-O1B	-2.50	103.17	110.70
3	I	401	GTP	O3A-PB-O1B	-2.50	103.17	110.70
3	F	401	GTP	N9-C8-N7	-2.50	108.76	113.40
3	H	401	GTP	C8-N7-C5	2.50	108.72	104.26
3	J	401	GTP	O3A-PB-O1B	-2.50	103.17	110.70
3	H	401	GTP	O3A-PB-O1B	-2.50	103.19	110.70
3	E	401	GTP	N9-C8-N7	-2.50	108.77	113.40
3	K	401	GTP	C8-N7-C5	2.50	108.71	104.26
3	G	401	GTP	N9-C8-N7	-2.49	108.78	113.40
3	H	401	GTP	N9-C8-N7	-2.49	108.78	113.40
3	F	401	GTP	O3A-PB-O1B	-2.49	103.22	110.70
3	J	401	GTP	N9-C8-N7	-2.49	108.79	113.40
3	K	401	GTP	N9-C8-N7	-2.49	108.79	113.40
3	I	401	GTP	N9-C8-N7	-2.48	108.80	113.40
3	L	401	GTP	N9-C8-N7	-2.48	108.81	113.40
3	F	401	GTP	C8-N7-C5	2.47	108.66	104.26
3	H	401	GTP	C2-N3-C4	2.43	116.49	112.30
3	G	401	GTP	C2-N3-C4	2.43	116.48	112.30
3	L	401	GTP	C2-N3-C4	2.43	116.48	112.30
3	I	401	GTP	C2-N3-C4	2.42	116.47	112.30
3	F	401	GTP	C2-N3-C4	2.41	116.45	112.30
3	K	401	GTP	C2-N3-C4	2.41	116.45	112.30
3	J	401	GTP	C2-N3-C4	2.41	116.45	112.30
3	E	401	GTP	C2-N3-C4	2.36	116.36	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	GTP	C8-N7-C5	2.26	108.30	104.26
3	C	501	GTP	C8-N7-C5	2.26	108.29	104.26
3	B	501	GTP	C8-N7-C5	2.25	108.28	104.26
3	A	501	GTP	C8-N7-C5	2.23	108.24	104.26
3	G	401	GTP	C4-C5-N7	-2.13	107.30	110.67
3	E	401	GTP	C4-C5-N7	-2.10	107.35	110.67
3	I	401	GTP	C4-C5-N7	-2.09	107.35	110.67
3	H	401	GTP	C4-C5-N7	-2.09	107.35	110.67
3	J	401	GTP	C4-C5-N7	-2.09	107.36	110.67
3	L	401	GTP	C4-C5-N7	-2.09	107.36	110.67
3	K	401	GTP	C4-C5-N7	-2.08	107.37	110.67
3	A	501	GTP	N1-C2-N3	2.06	127.08	123.32
3	F	401	GTP	C4-C5-N7	-2.05	107.42	110.67
3	D	501	GTP	N1-C2-N3	2.05	127.07	123.32
3	C	501	GTP	N1-C2-N3	2.02	127.02	123.32
3	B	501	GTP	N1-C2-N3	2.02	127.01	123.32

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	GTP	C5'-O5'-PA-O2A
3	D	501	GTP	C5'-O5'-PA-O2A
3	B	501	GTP	C5'-O5'-PA-O2A
3	C	501	GTP	C5'-O5'-PA-O2A
3	A	501	GTP	PB-O3A-PA-O1A
3	D	501	GTP	PB-O3A-PA-O1A
3	B	501	GTP	PB-O3A-PA-O1A
3	C	501	GTP	PB-O3A-PA-O1A
3	A	501	GTP	C5'-O5'-PA-O3A
3	A	501	GTP	C5'-O5'-PA-O1A
3	D	501	GTP	C5'-O5'-PA-O3A
3	D	501	GTP	C5'-O5'-PA-O1A
3	B	501	GTP	C5'-O5'-PA-O3A
3	B	501	GTP	C5'-O5'-PA-O1A
3	C	501	GTP	C5'-O5'-PA-O3A
3	C	501	GTP	C5'-O5'-PA-O1A
3	E	401	GTP	O4'-C4'-C5'-O5'
3	F	401	GTP	O4'-C4'-C5'-O5'
3	G	401	GTP	O4'-C4'-C5'-O5'
3	H	401	GTP	O4'-C4'-C5'-O5'
3	I	401	GTP	O4'-C4'-C5'-O5'

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

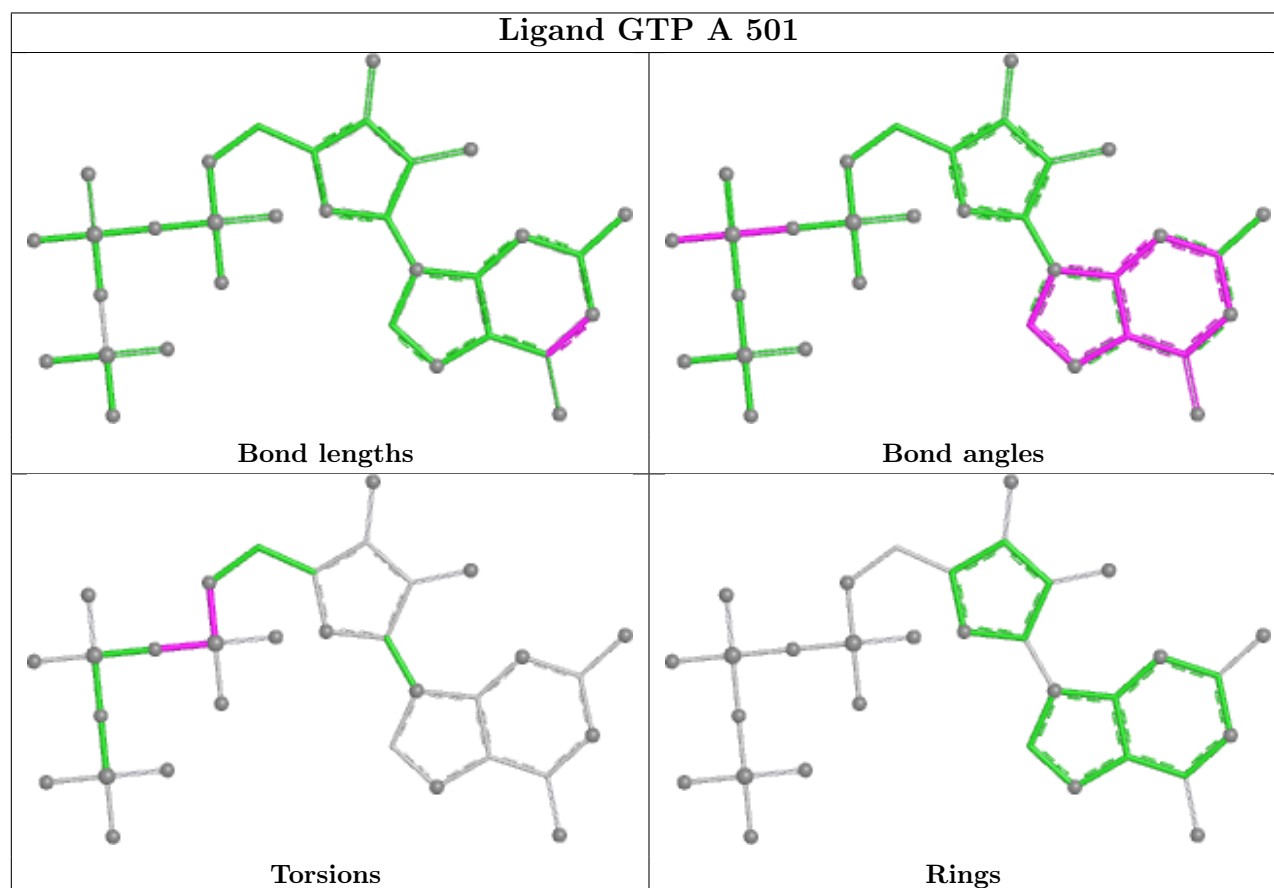
There are no ring outliers.

12 monomers are involved in 127 short contacts:

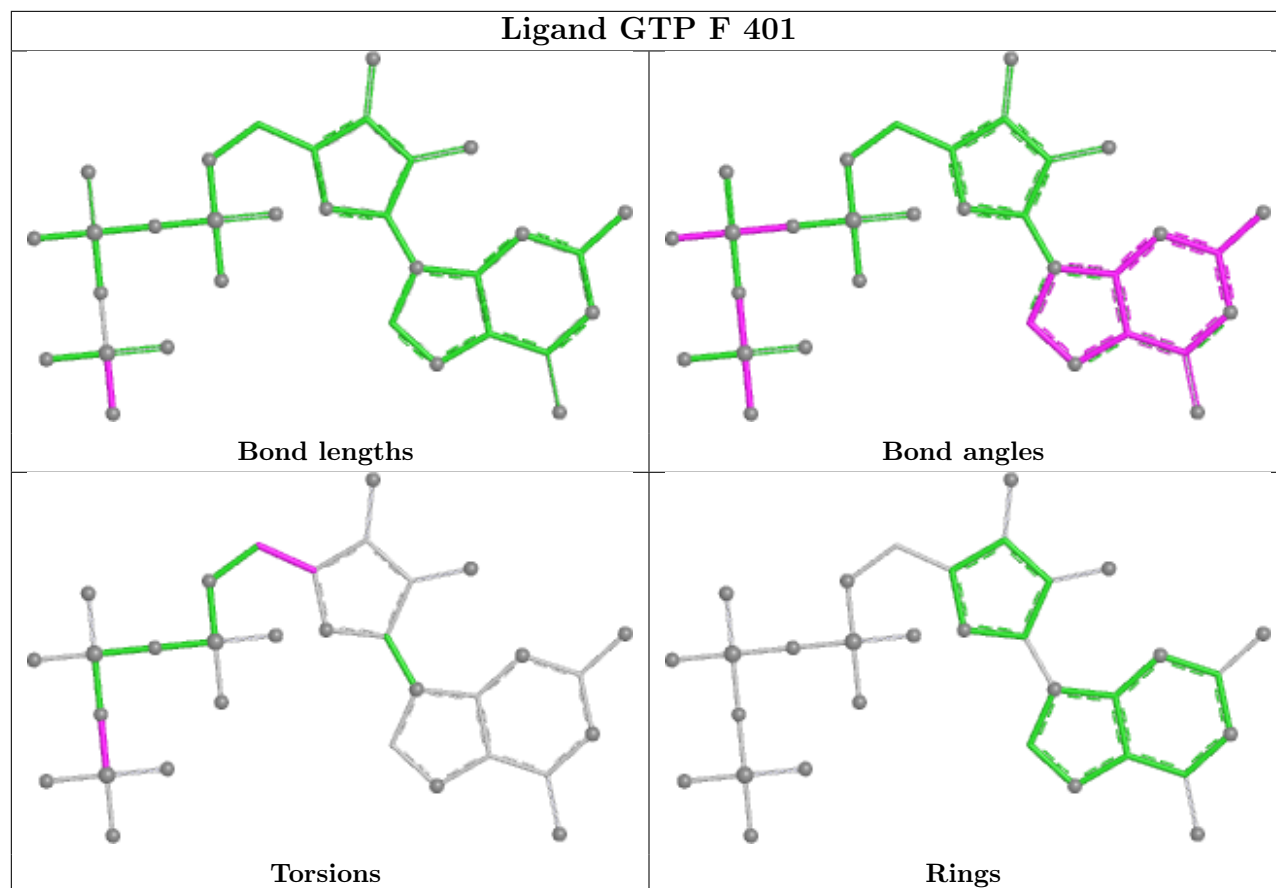
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GTP	1	0
3	F	401	GTP	30	0
3	J	401	GTP	14	0
3	L	401	GTP	14	0
3	D	501	GTP	1	0
3	G	401	GTP	12	0
3	H	401	GTP	15	0
3	K	401	GTP	13	0
3	E	401	GTP	17	0
3	I	401	GTP	8	0
3	C	501	GTP	1	0
3	B	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

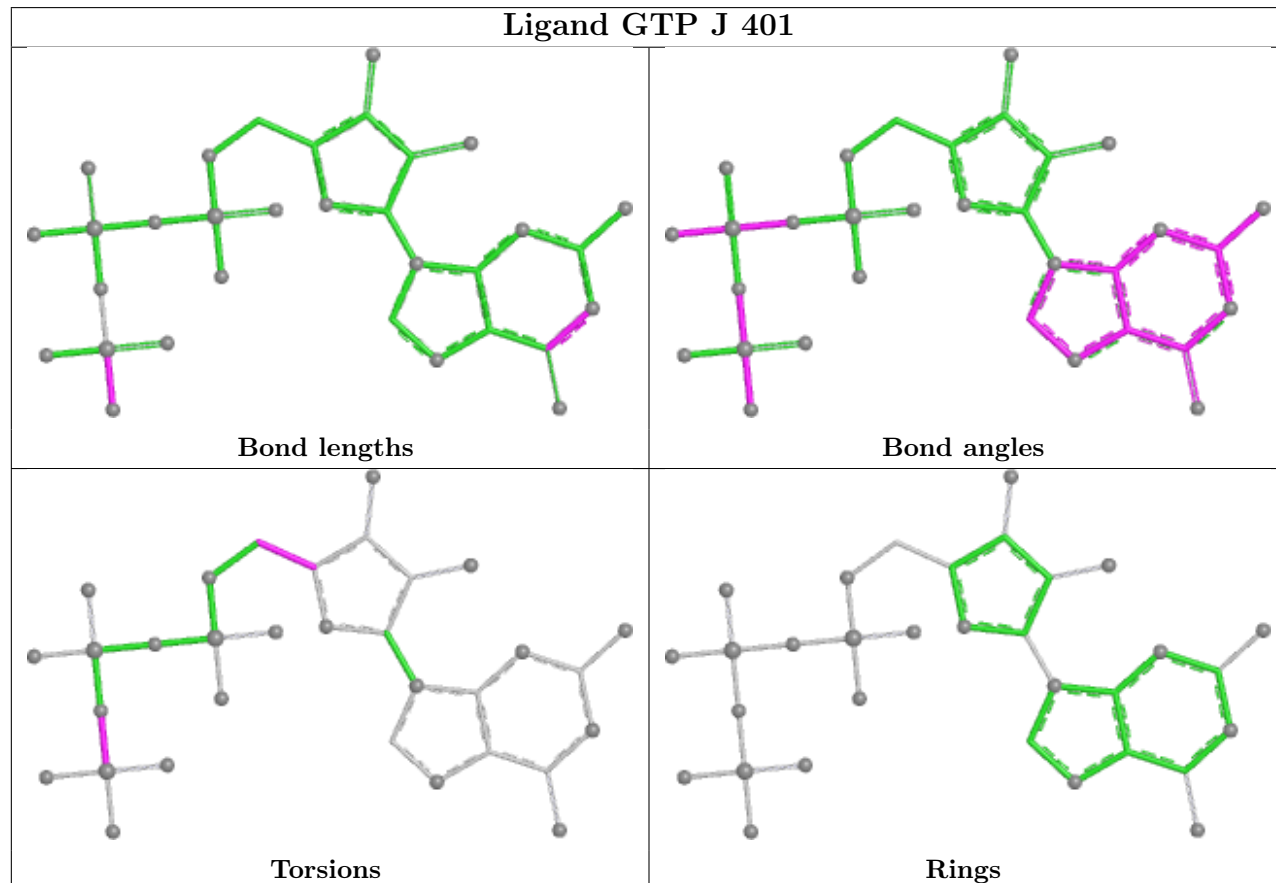
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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



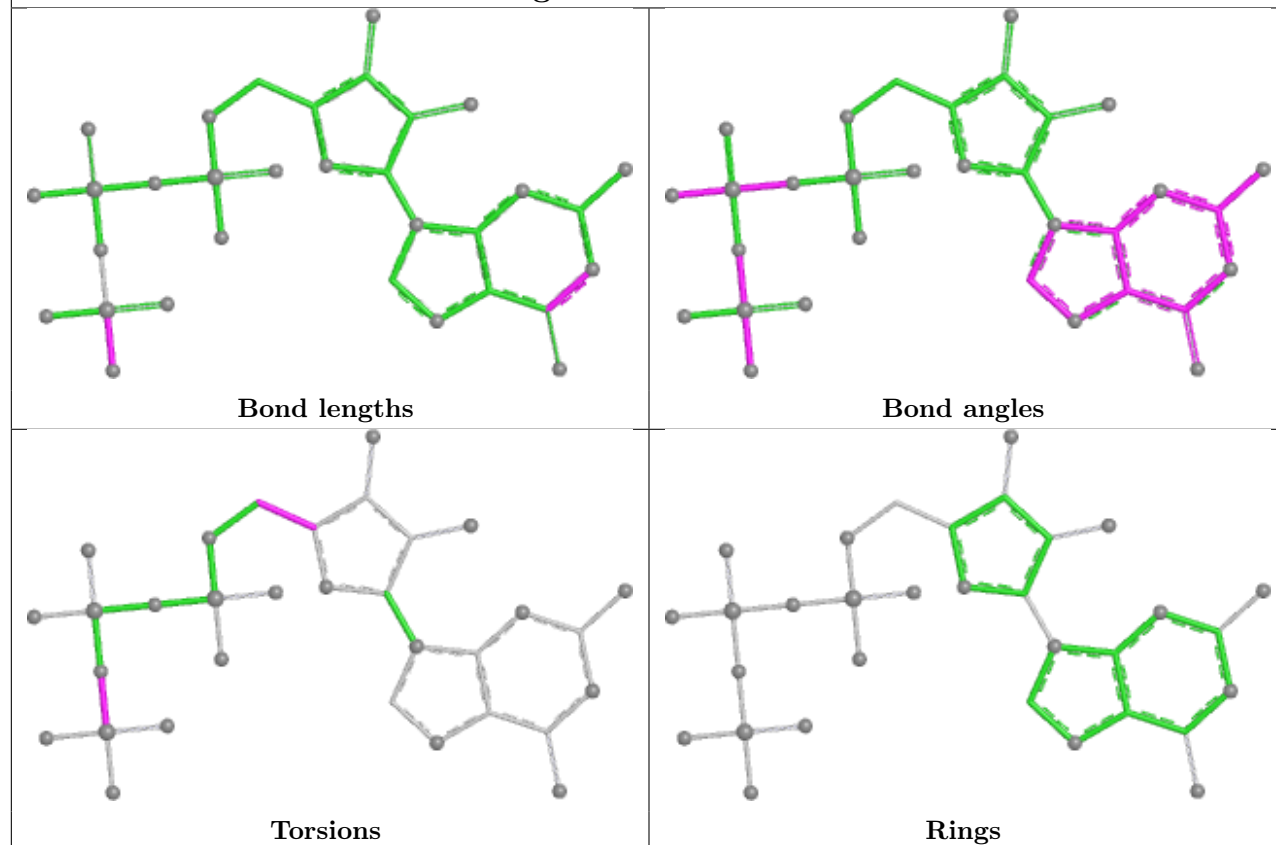
Ligand GTP F 401



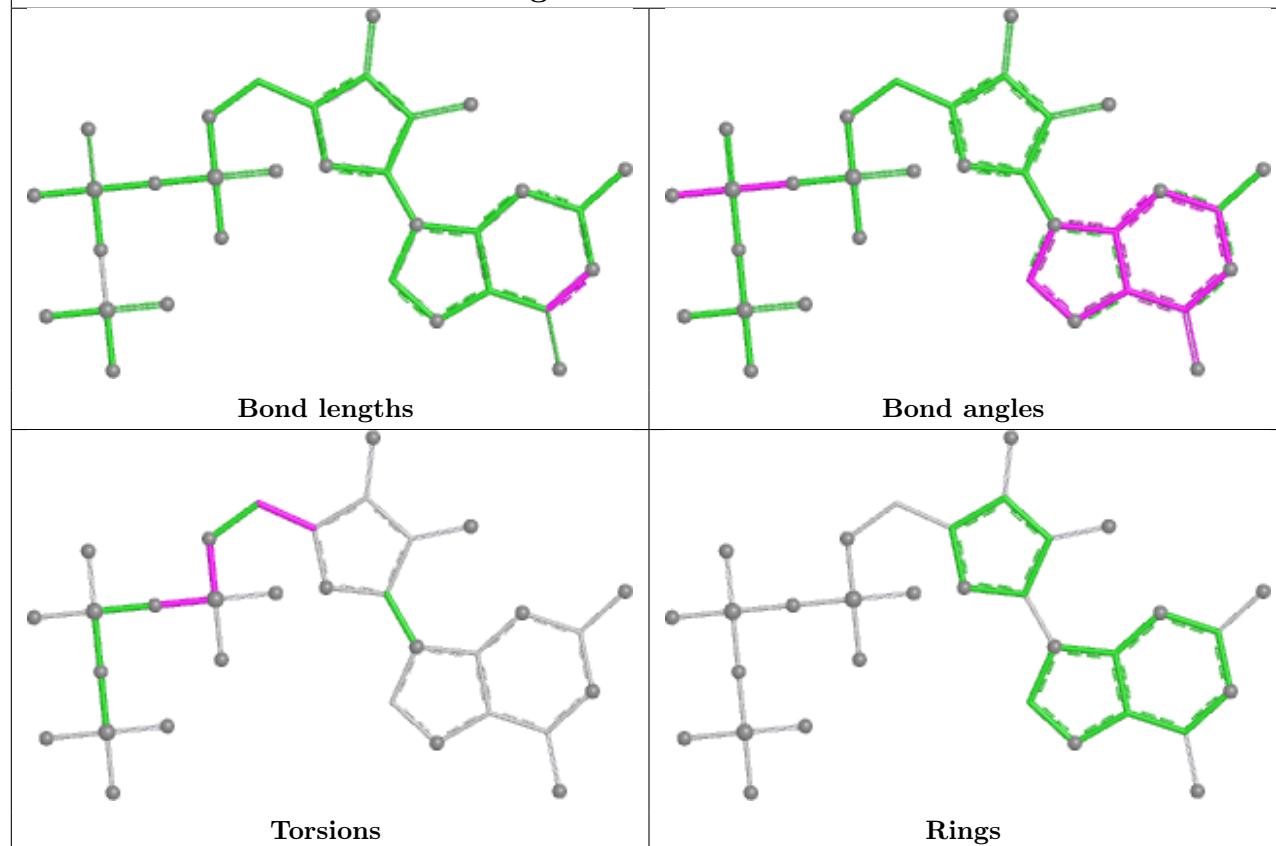
Ligand GTP J 401

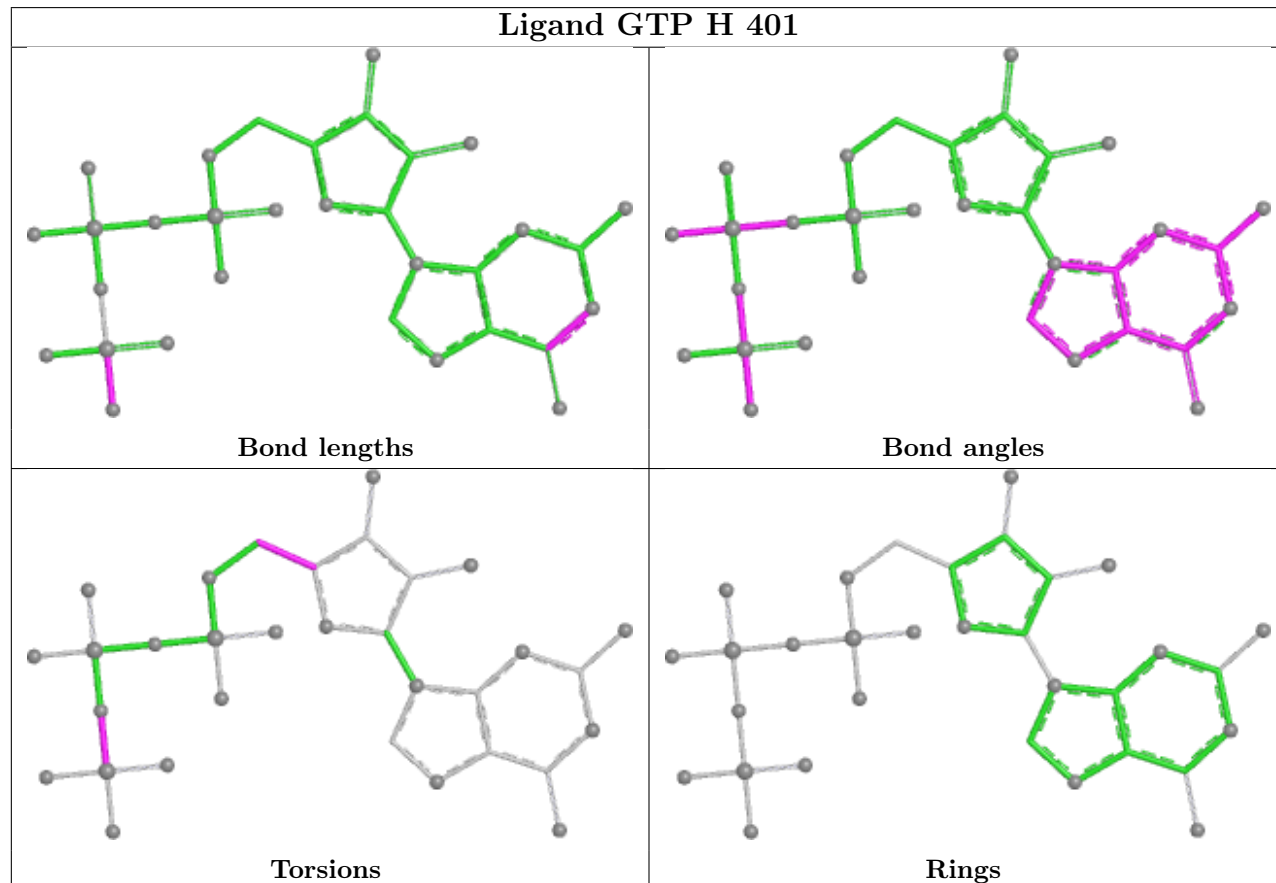
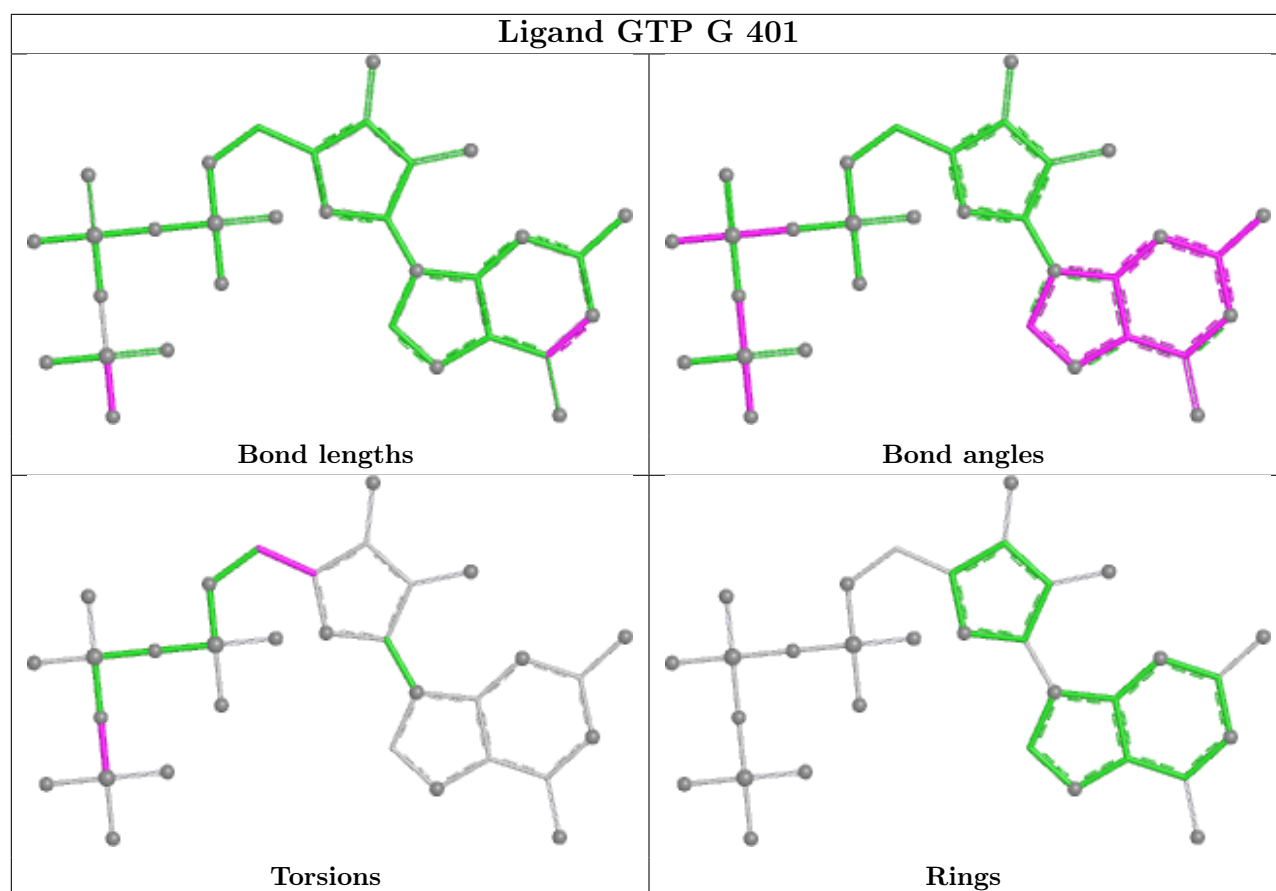


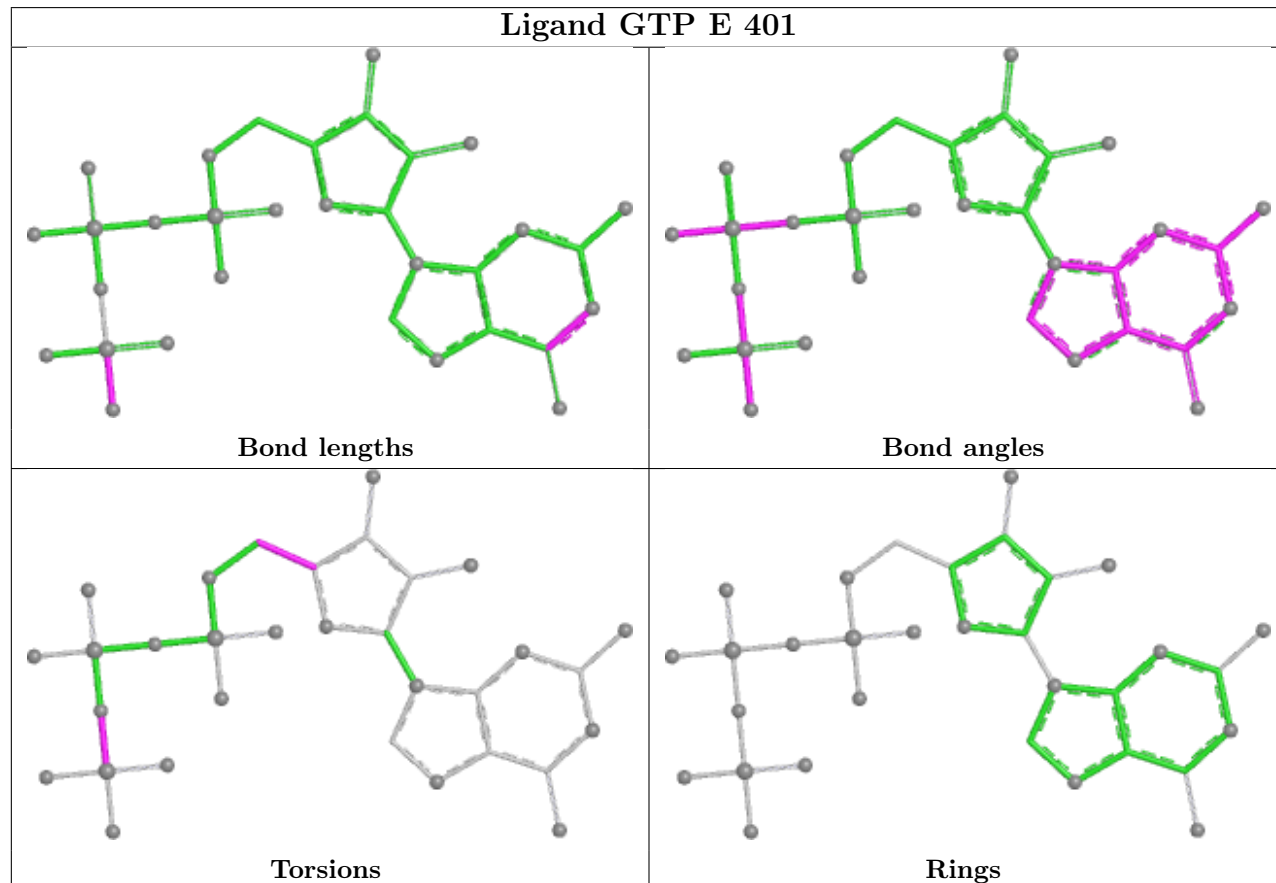
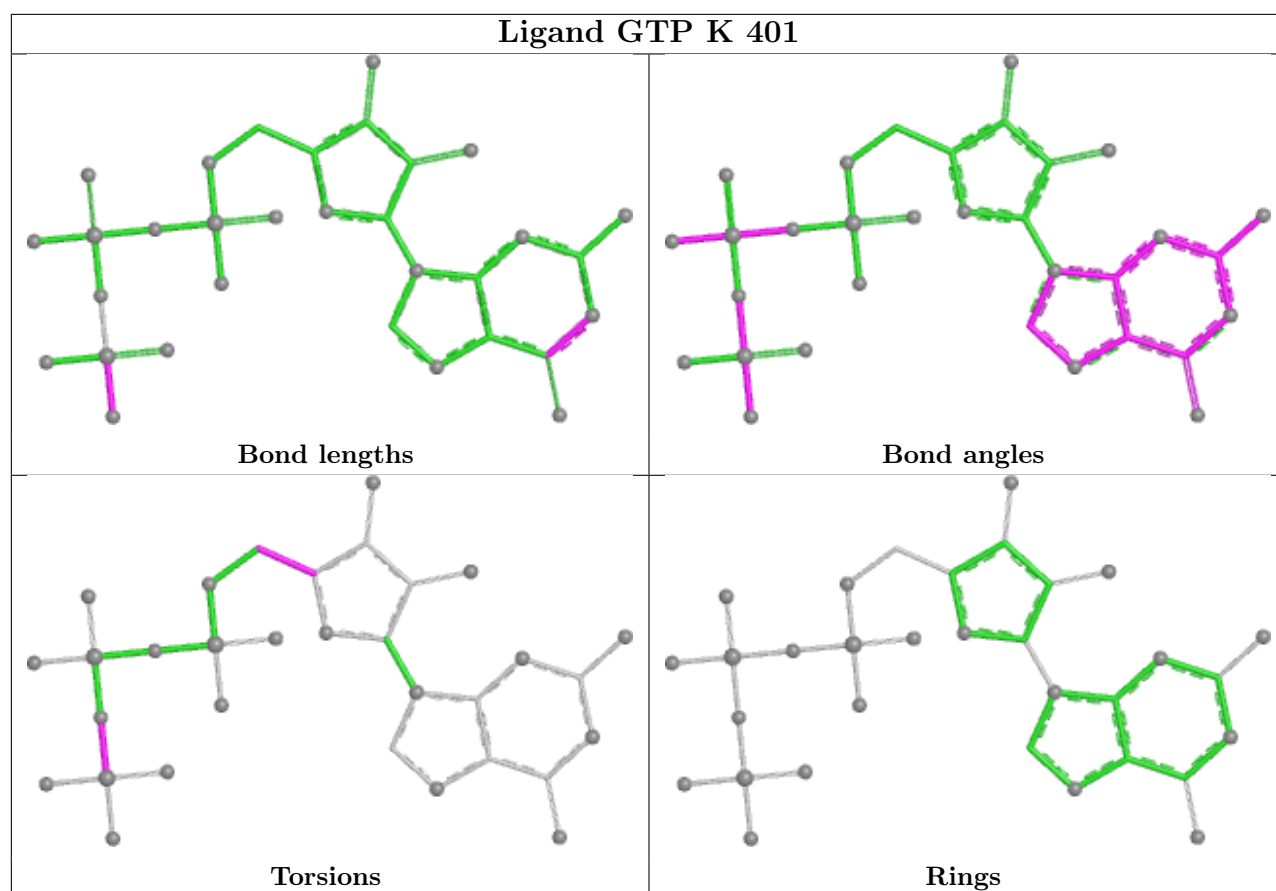
Ligand GTP L 401



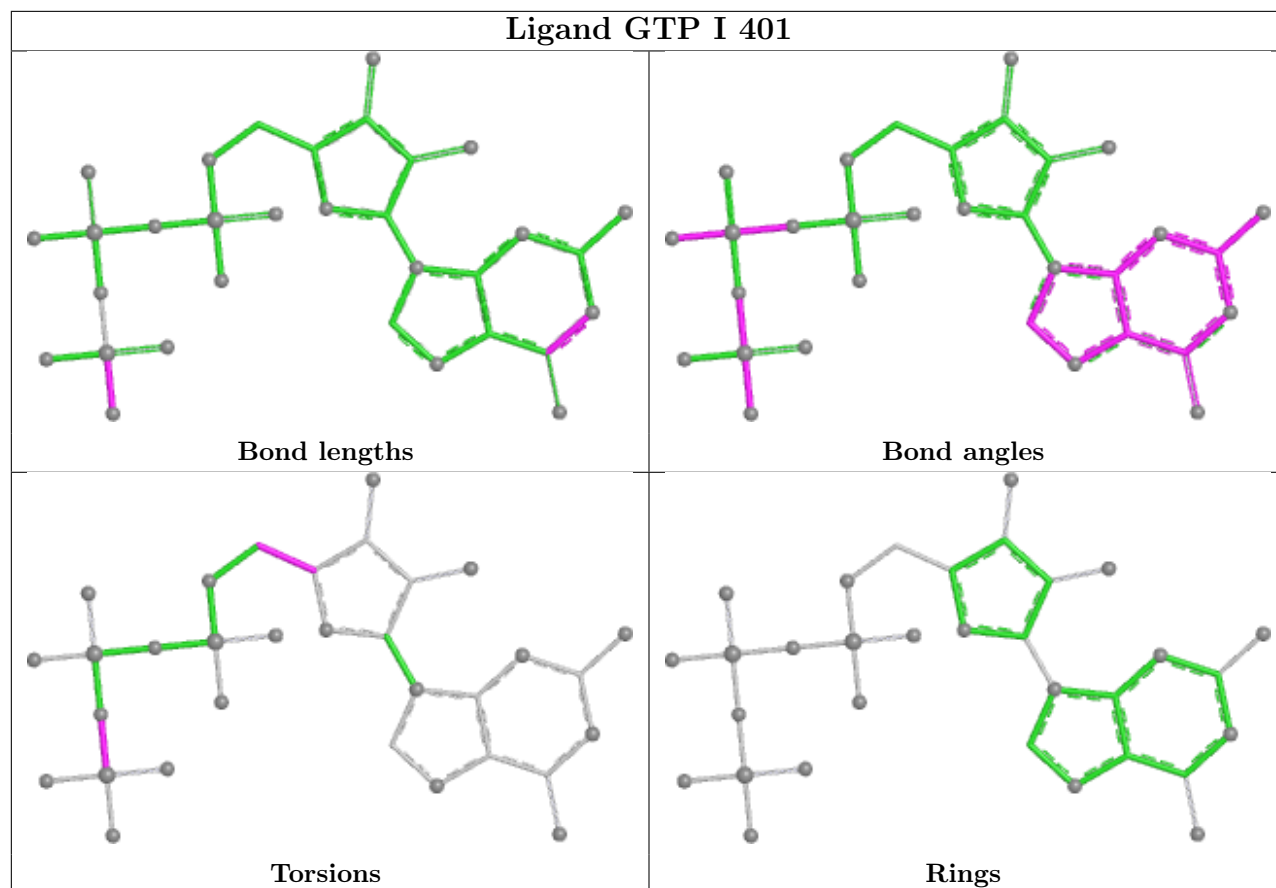
Ligand GTP D 501



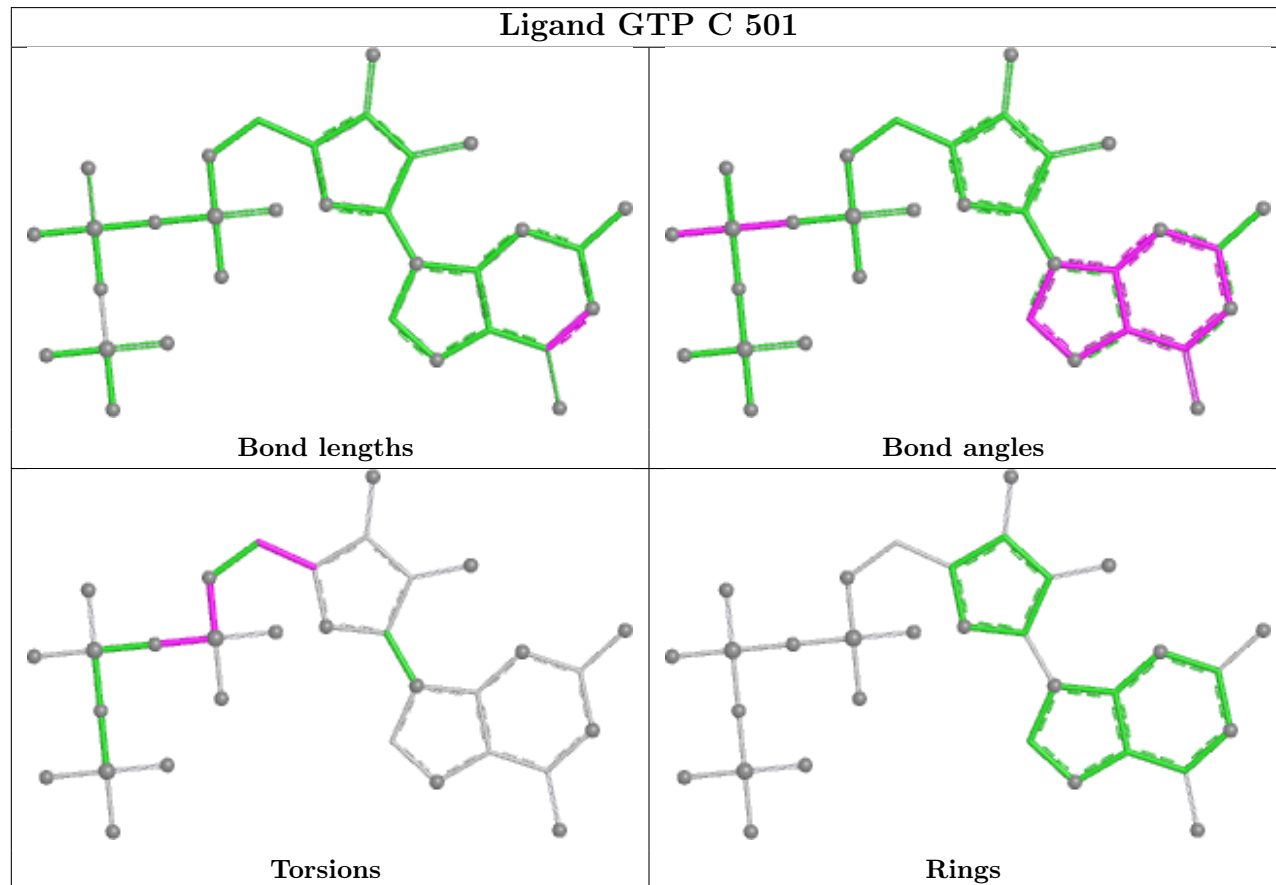


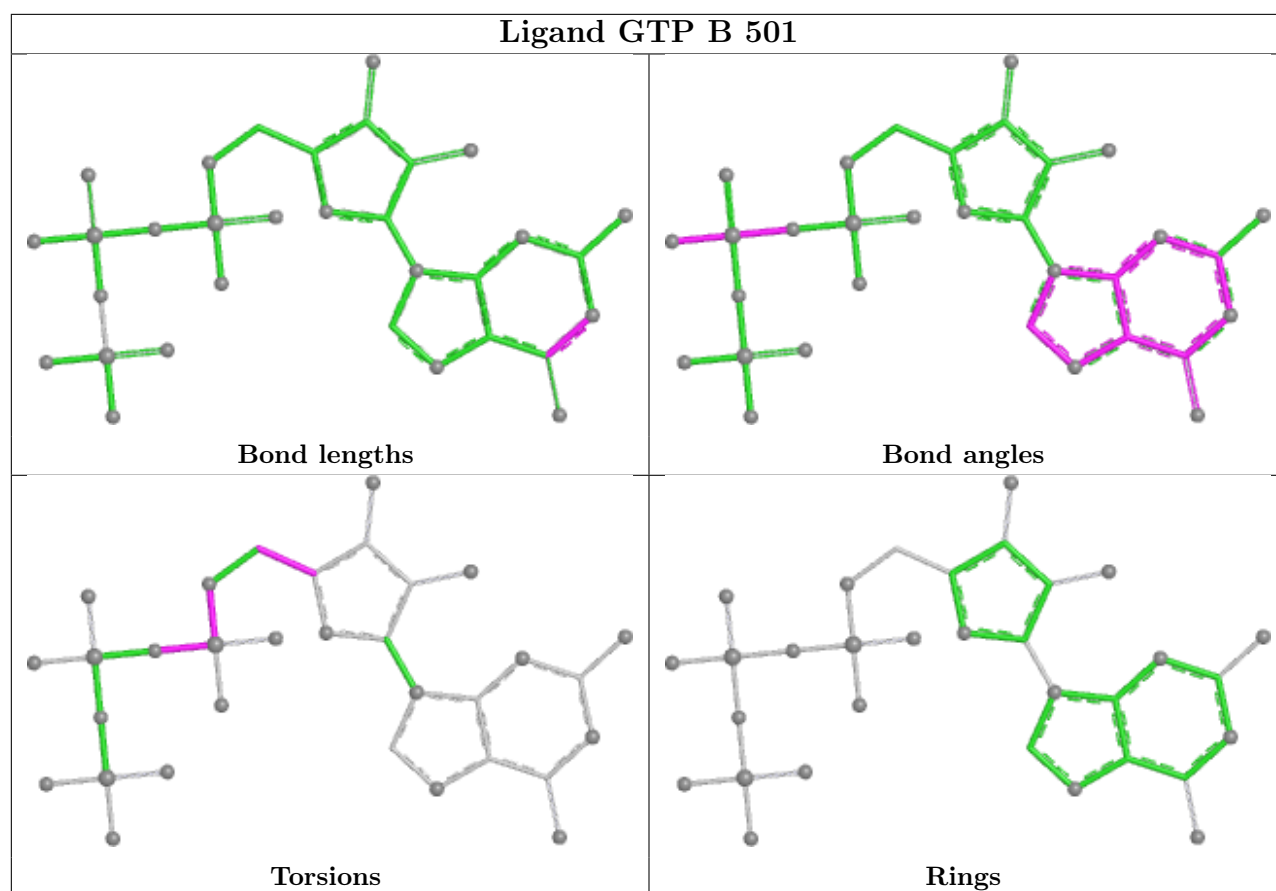


Ligand GTP I 401



Ligand GTP C 501





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.

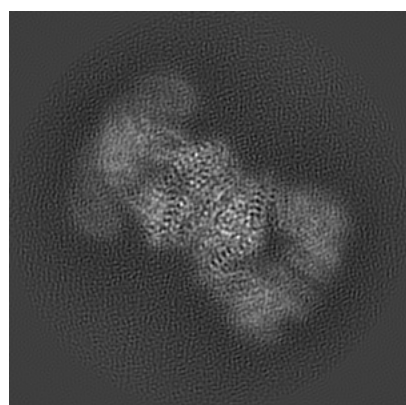
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30601. These allow visual inspection of the internal detail of the map and identification of artifacts.

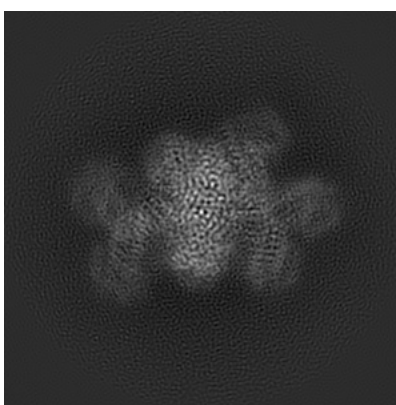
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

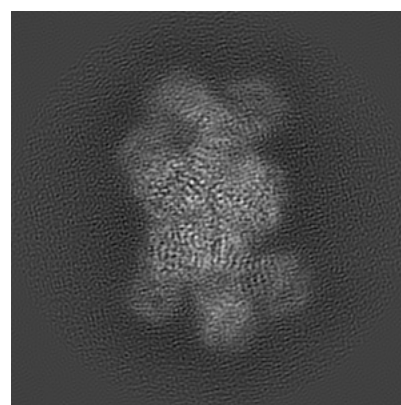
6.1.1 Primary map



X



Y

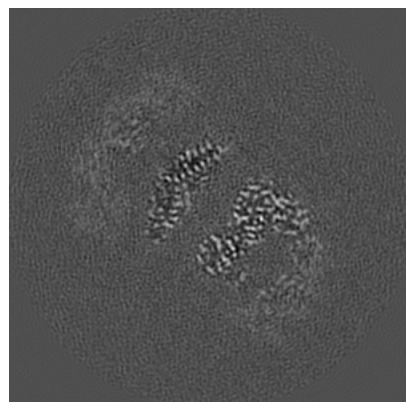


Z

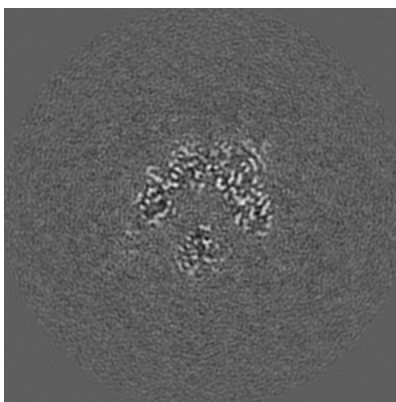
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

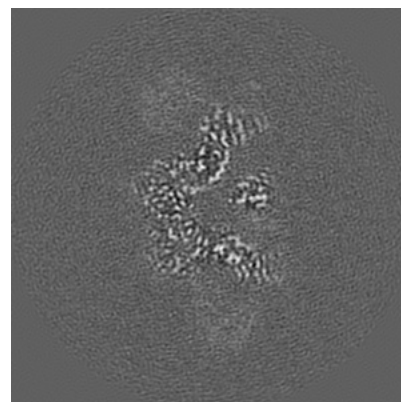
6.2.1 Primary map



X Index: 120



Y Index: 120

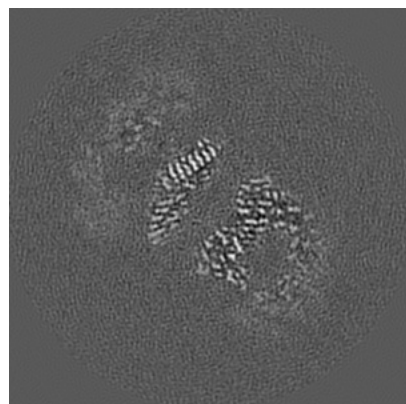


Z Index: 120

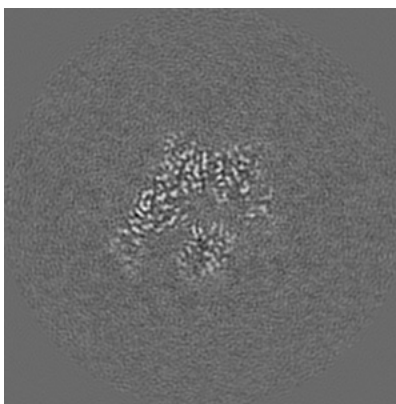
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

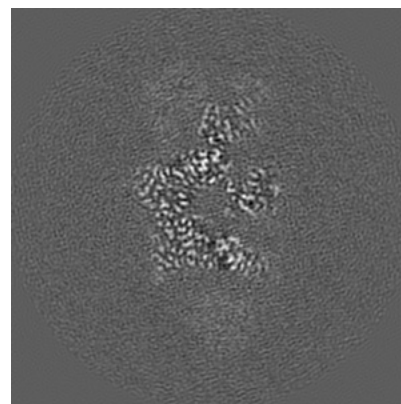
6.3.1 Primary map



X Index: 118



Y Index: 126

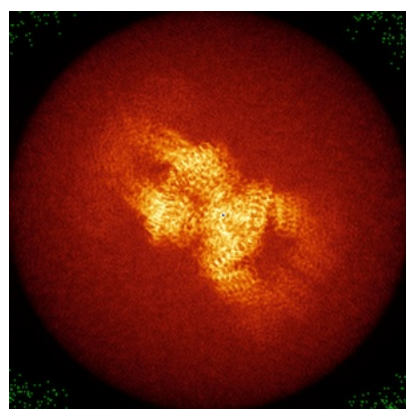


Z Index: 115

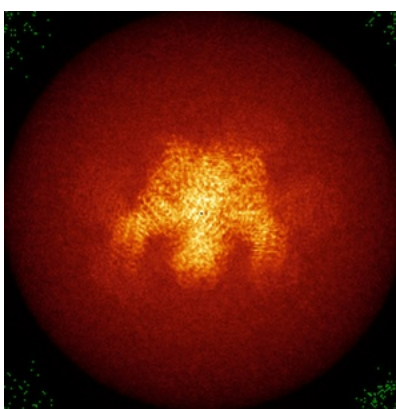
The images above show the largest variance slices of the map in three orthogonal directions.

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

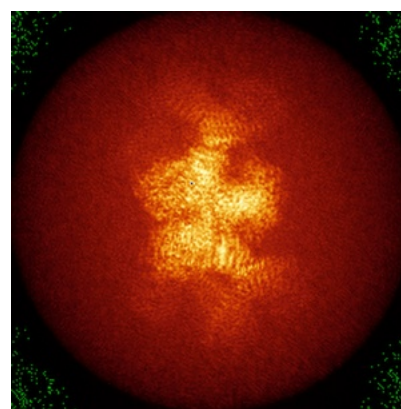
6.4.1 Primary map



X



Y

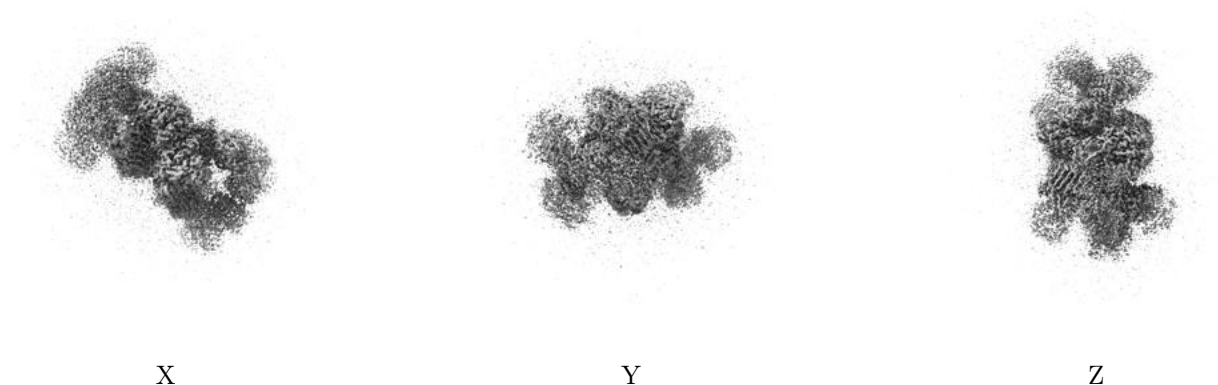


Z

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 0.0365. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

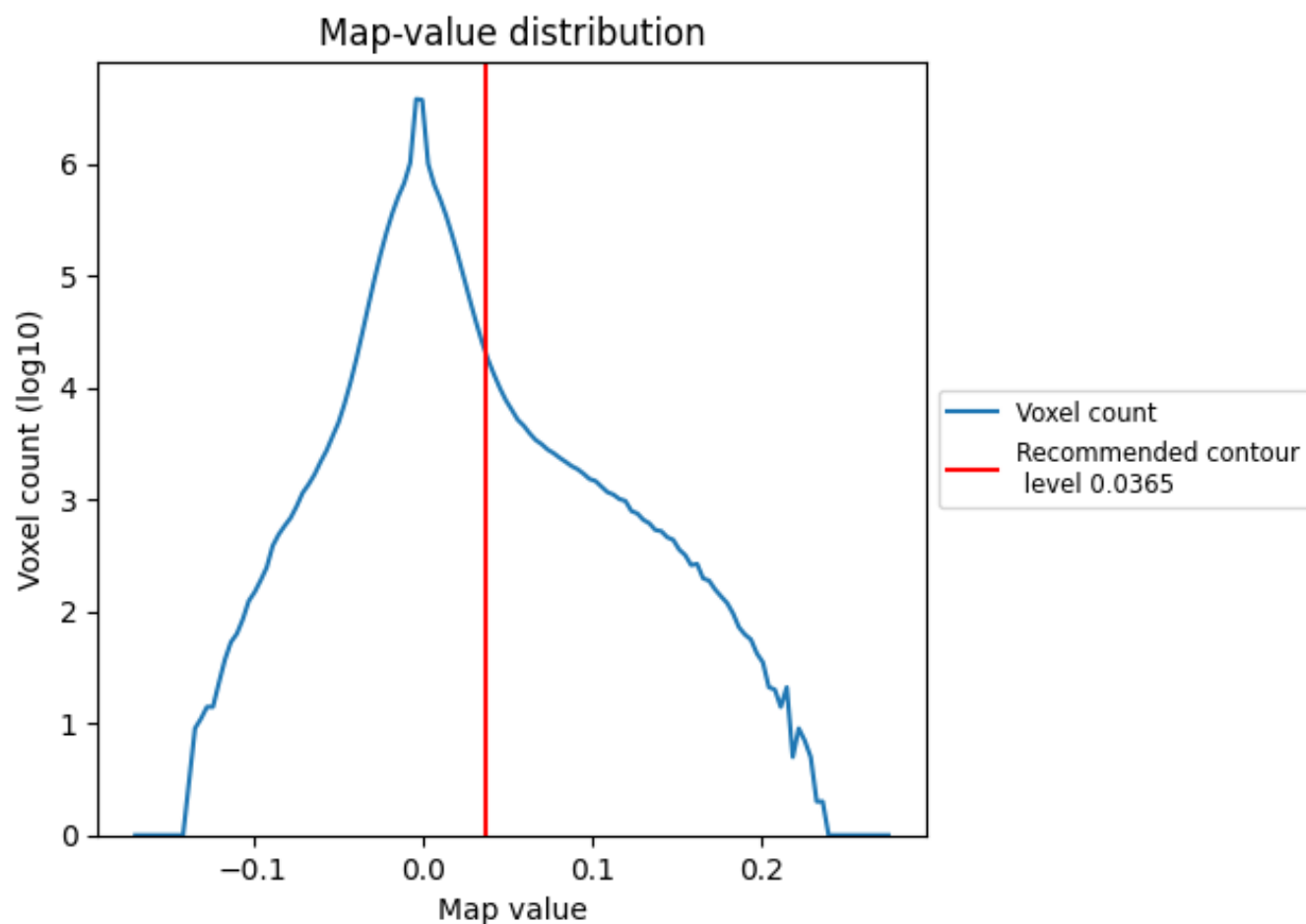
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

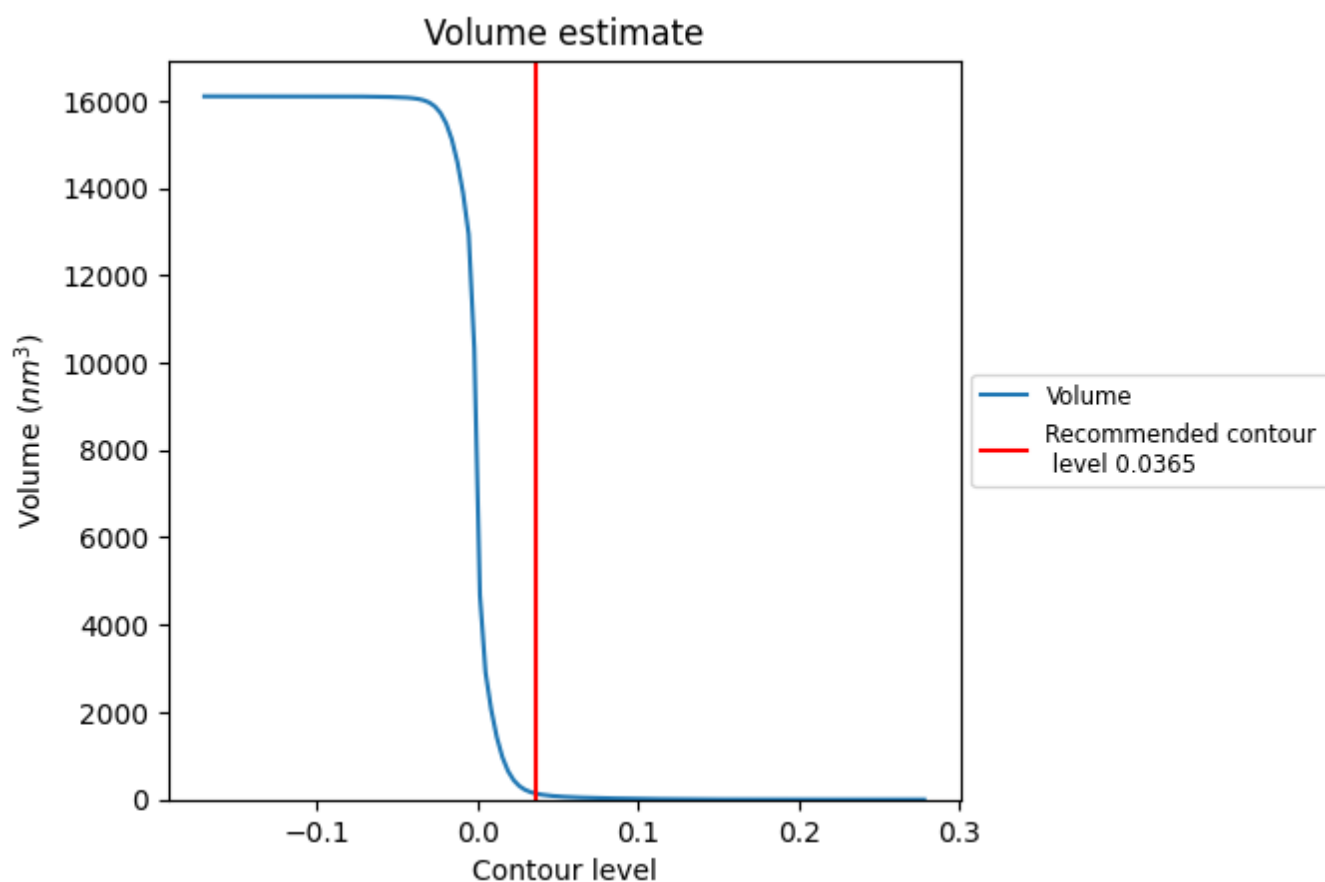
This section contains the results of statistical analysis of the map.

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.

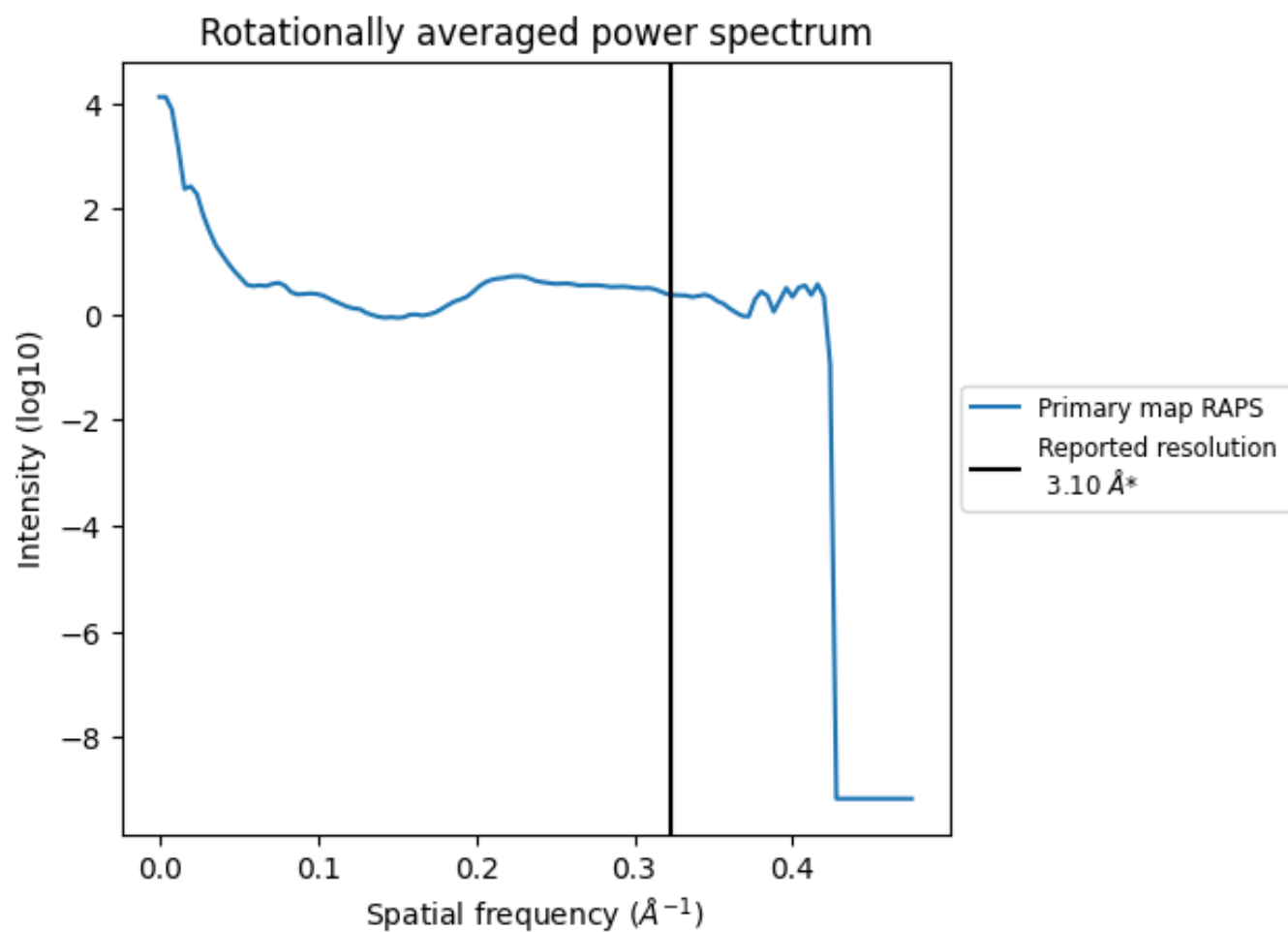
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 125 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 0.323 Å⁻¹

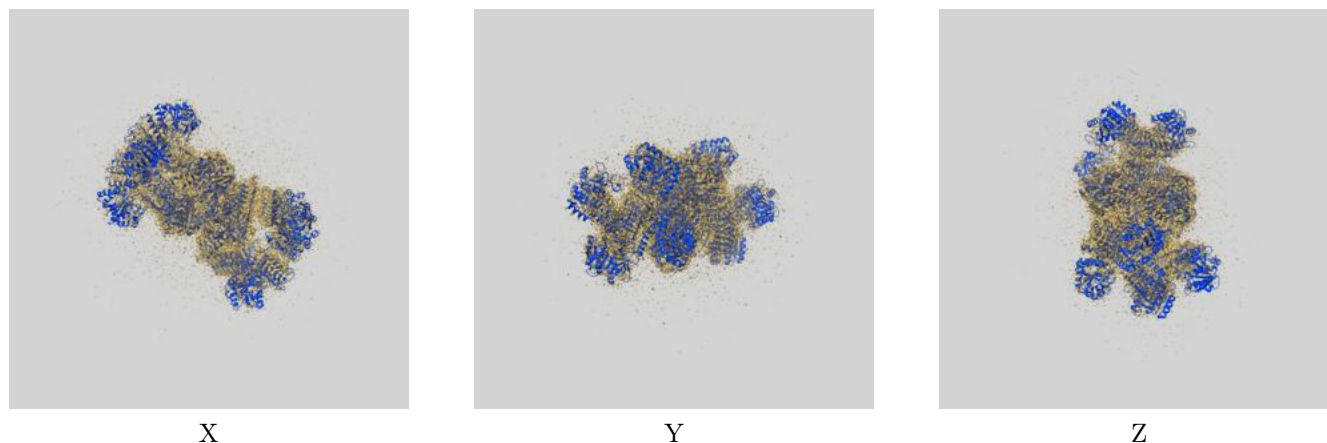
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

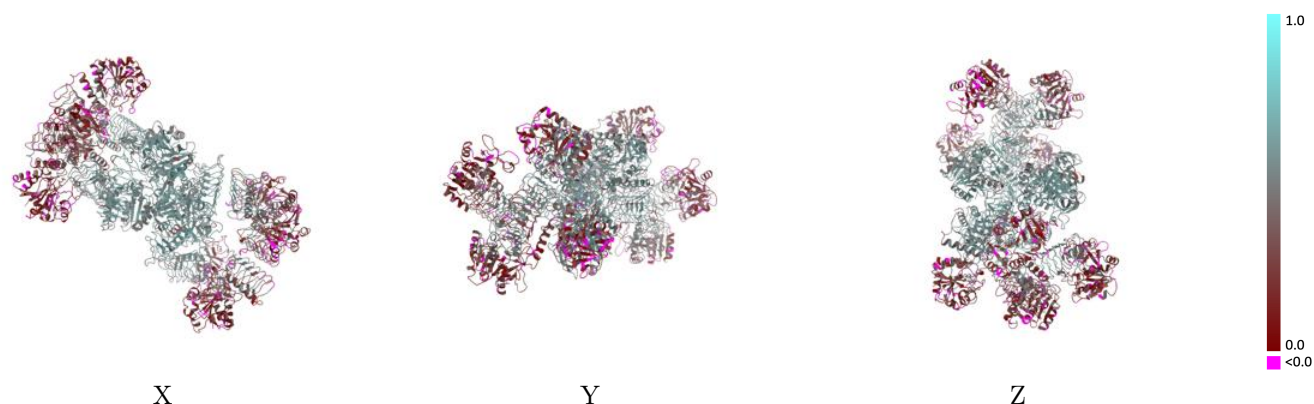
This section contains information regarding the fit between EMDB map EMD-30601 and PDB model 7D74. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



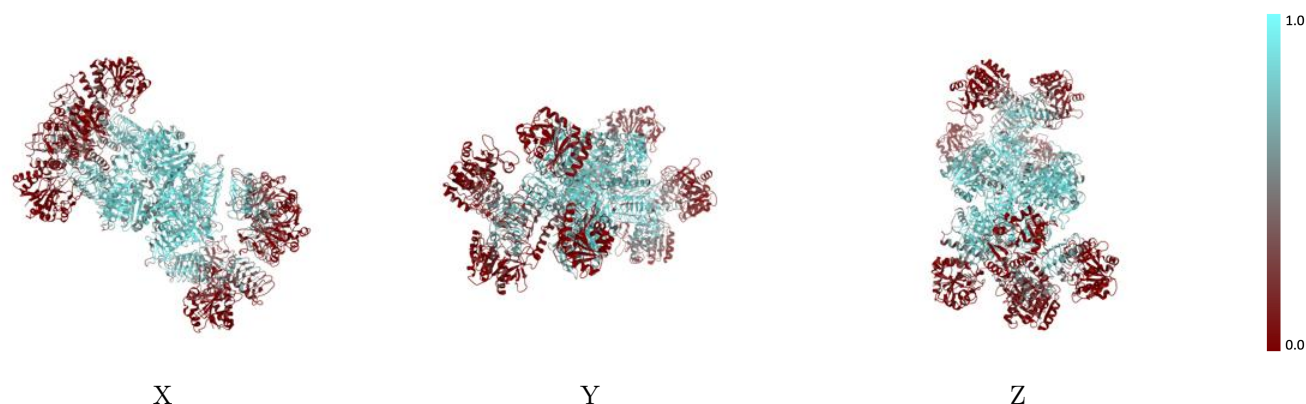
The images above show the 3D surface view of the map at the recommended contour level 0.0365 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



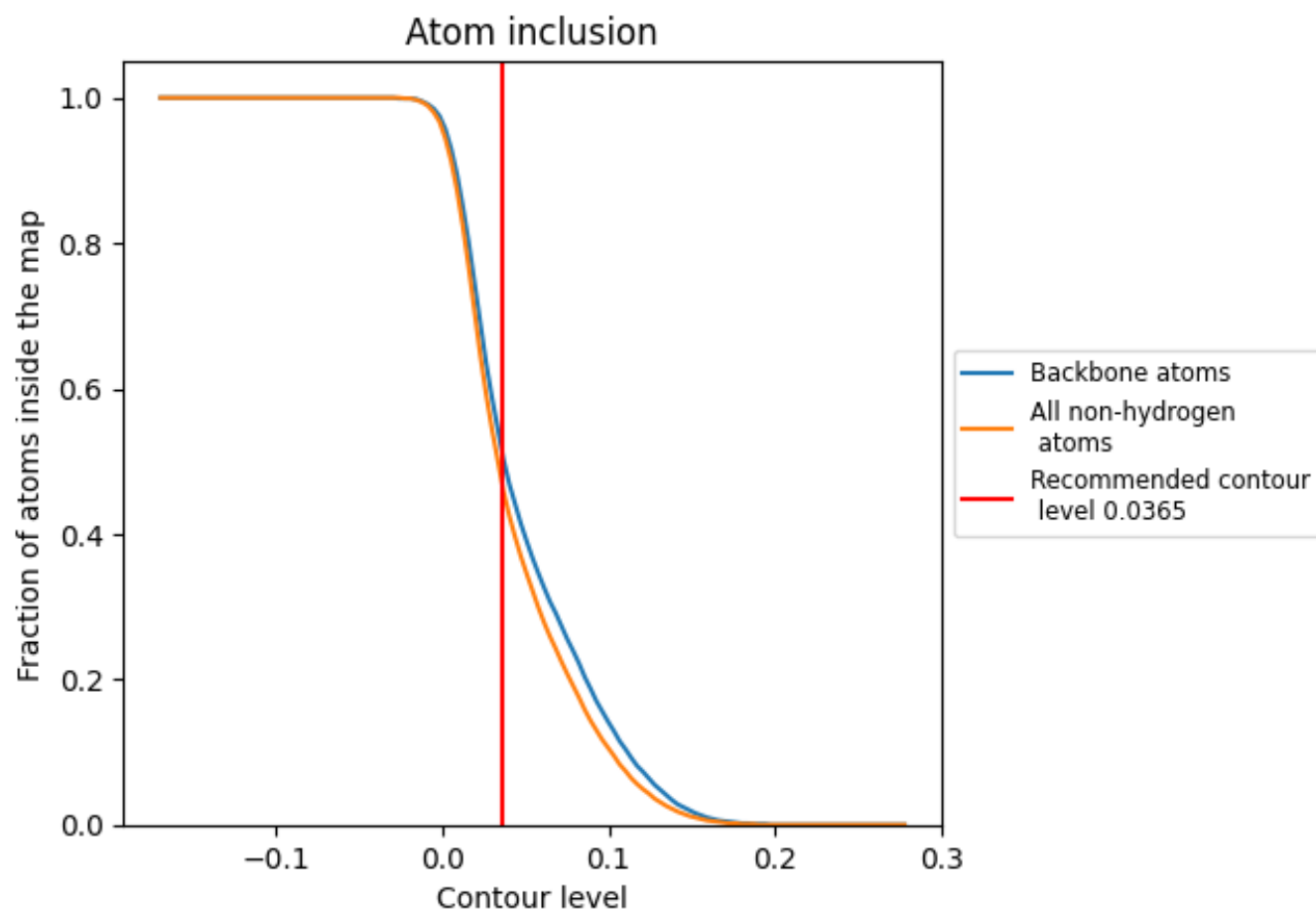
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0365).

9.4 Atom inclusion [i](#)



At the recommended contour level, 51% of all backbone atoms, 46% 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 (0.0365) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4620	0.3940
A	0.8190	0.5710
B	0.8130	0.5660
C	0.8020	0.5640
D	0.8120	0.5620
E	0.1640	0.2230
F	0.3460	0.3490
G	0.1850	0.2680
H	0.3850	0.3680
I	0.3060	0.3230
J	0.1560	0.2210
K	0.3760	0.3540
L	0.1870	0.2730

