



Full wwPDB EM Validation Report ⓘ

Sep 10, 2026 – 03:29 PM EDT

PDB ID : 9ZN9 / pdb_00009zn9
EMDB ID : EMD-74439
Title : Structure of rabbit RyR1 complexed with FKBP12.6, calmodulin, ATP, 4-chloro-m-cresol, and caffeine
Authors : Kim, K.; Clarke, O.B.
Deposited on : 2025-12-12
Resolution : 2.77 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.dev133
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) : 2.50

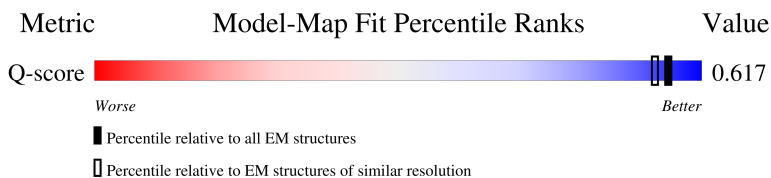
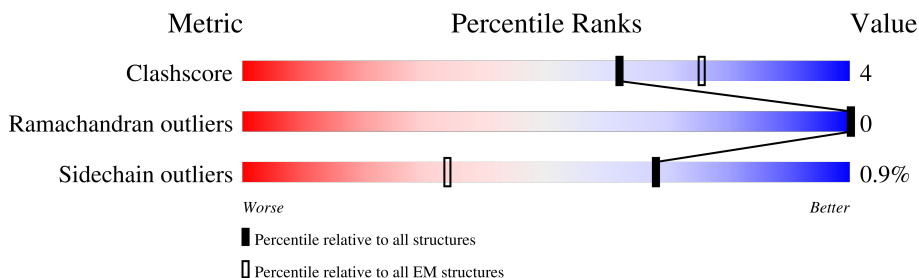
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.77 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	10695 (2.27 - 3.27)

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	107	
1	F	107	
1	G	107	
1	H	107	

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Mol	Chain	Length	Quality of chain
2	I	148	35% 85% 15%
2	J	148	36% 84% 16%
2	K	148	32% 84% 16%
2	L	148	34% 86% 14%
3	A	5037	7% 75% 9% 16%
3	B	5037	7% 75% 9% 16%
3	C	5037	7% 75% 9% 16%
3	D	5037	7% 75% 10% 16%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 146239 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	F	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	J	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	K	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		
2	L	148	Total	C	N	O	S	0	0
			1017	624	174	213	6		

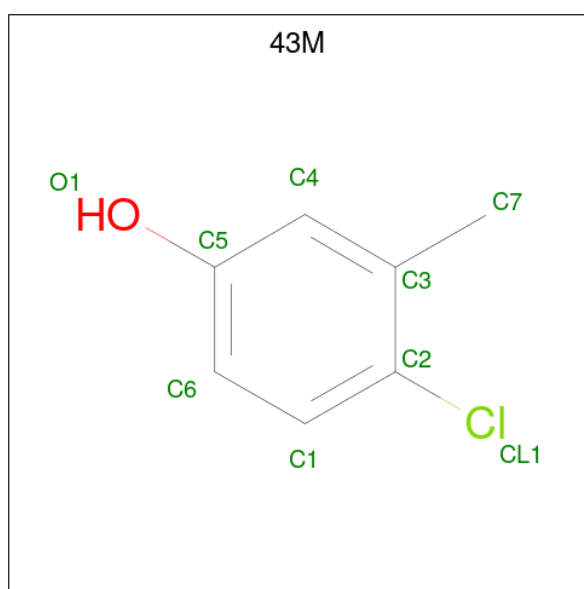
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	HIS	-	expression tag	UNP P0DP23
J	-1	HIS	-	expression tag	UNP P0DP23
K	-1	HIS	-	expression tag	UNP P0DP23
L	-1	HIS	-	expression tag	UNP P0DP23

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	C	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	D	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		
3	B	4249	Total	C	N	O	S	1	0
			33879	21584	5829	6232	234		

- Molecule 4 is 4-CHLORO-3-METHYLPHENOL (CCD ID: 43M) (formula: C₇H₇ClO) (labeled as "Ligand of Interest" by depositor).



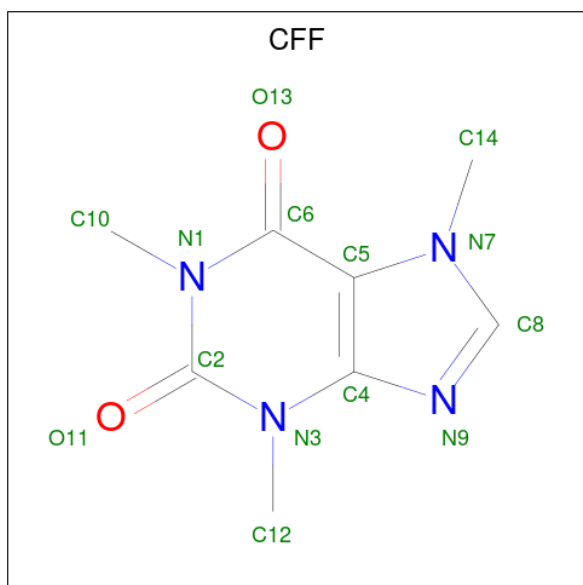
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	A	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	
4	C	1	Total	C	Cl	O	0
			9	7	1	1	

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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	Cl	O	0
			9	7	1	1	
4	D	1	Total	C	Cl	O	0
			9	7	1	1	
4	D	1	Total	C	Cl	O	0
			9	7	1	1	
4	D	1	Total	C	Cl	O	0
			9	7	1	1	
4	D	1	Total	C	Cl	O	0
			9	7	1	1	
4	B	1	Total	C	Cl	O	0
			9	7	1	1	
4	B	1	Total	C	Cl	O	0
			9	7	1	1	
4	B	1	Total	C	Cl	O	0
			9	7	1	1	
4	B	1	Total	C	Cl	O	0
			9	7	1	1	

- Molecule 5 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	4	2	
5	C	1	Total	C	N	O	0
			14	8	4	2	

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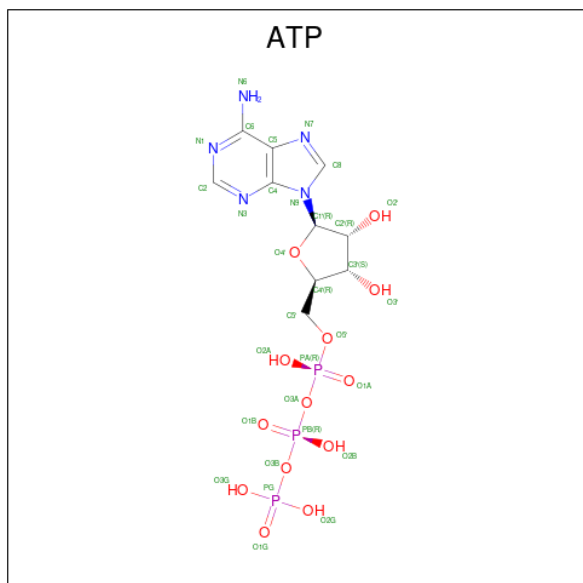
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Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			14	8	4	2	
5	B	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	Zn	0
			1	1	
8	C	1	Total	Zn	0
			1	1	
8	D	1	Total	Zn	0
			1	1	
8	B	1	Total	Zn	0
			1	1	

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	E	14	Total	O	0
			14	14	
9	F	15	Total	O	0
			15	15	
9	G	15	Total	O	0
			15	15	
9	H	15	Total	O	0
			15	15	
9	I	30	Total	O	0
			30	30	
9	J	30	Total	O	0
			30	30	
9	K	30	Total	O	0
			30	30	

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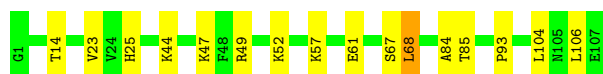
Mol	Chain	Residues	Atoms		AltConf
9	L	33	Total 33	O 33	0
9	A	704	Total 704	O 704	0
9	C	673	Total 673	O 673	0
9	D	692	Total 692	O 692	0
9	B	672	Total 672	O 672	0

3 Residue-property plots [i](#)

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: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



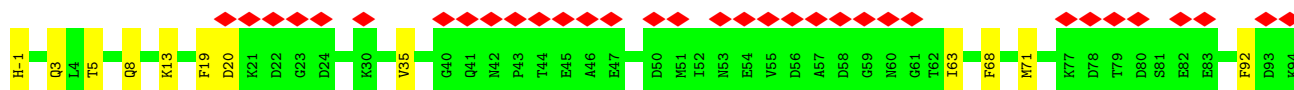
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

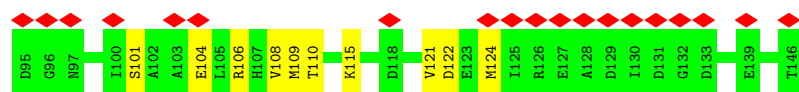
Chain H: 



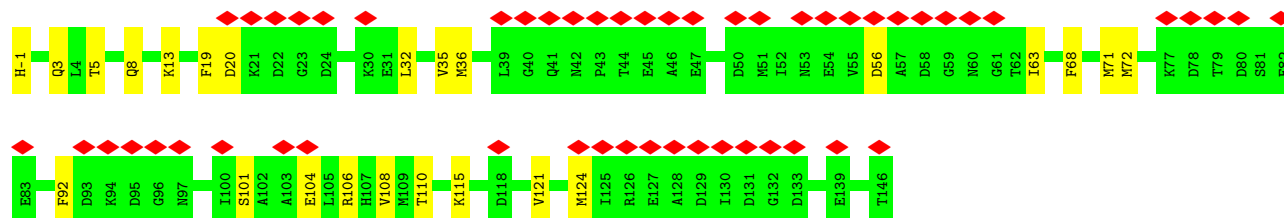
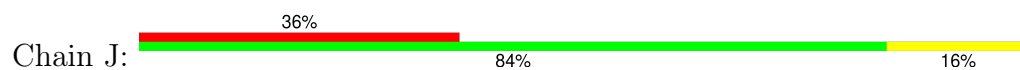
- Molecule 2: Calmodulin-1

Chain I: 

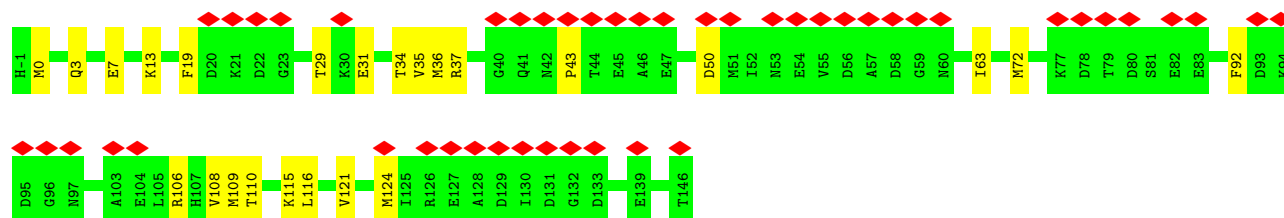
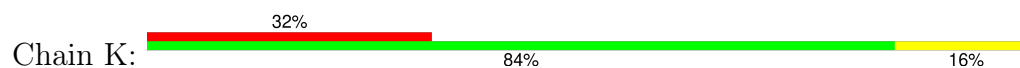




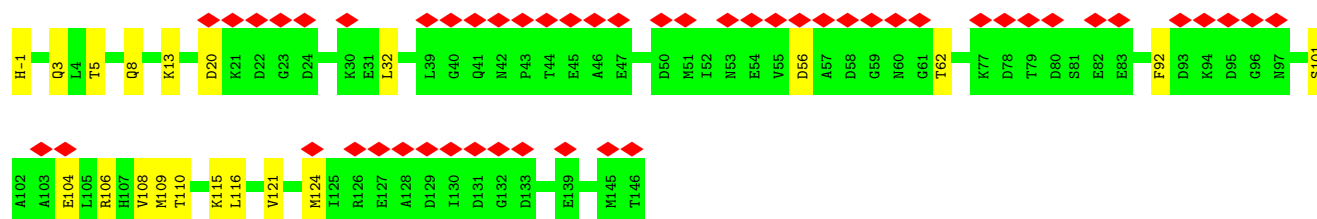
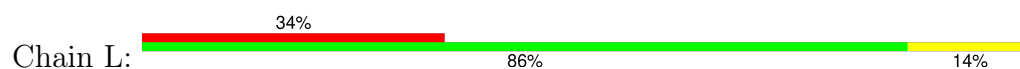
• Molecule 2: Calmodulin-1



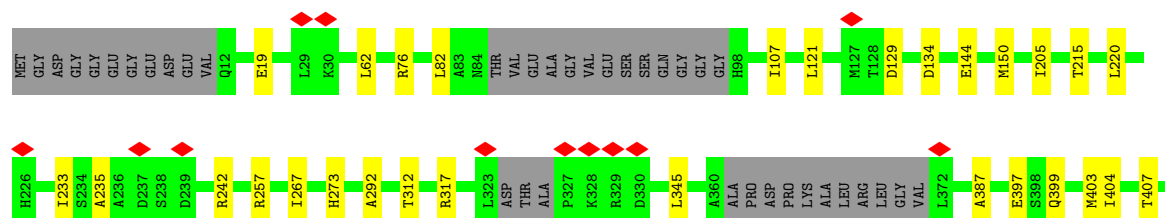
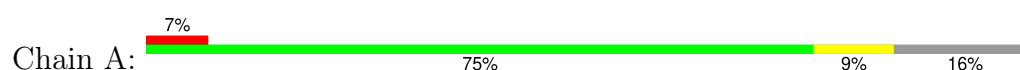
• Molecule 2: Calmodulin-1

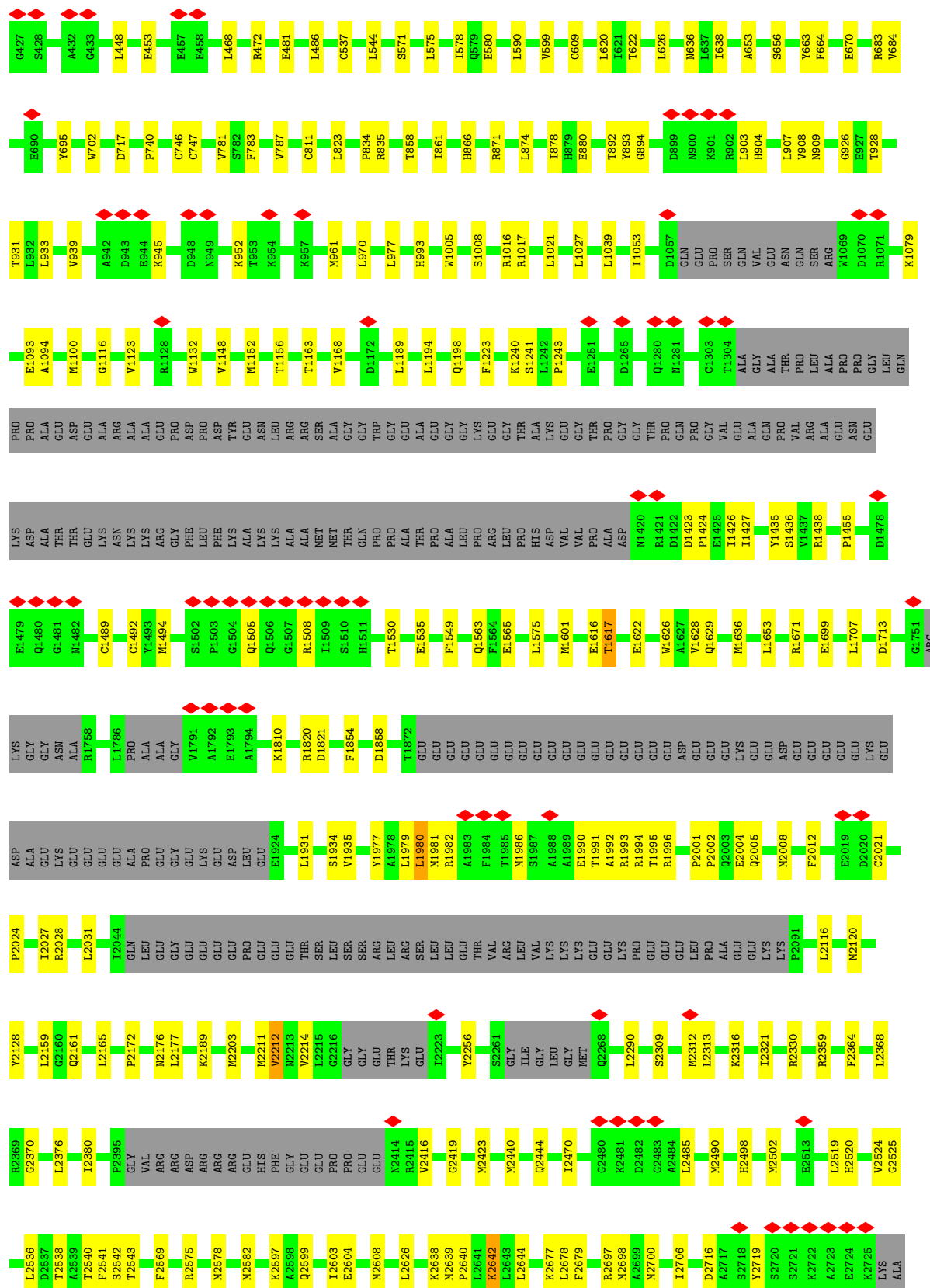


• Molecule 2: Calmodulin-1

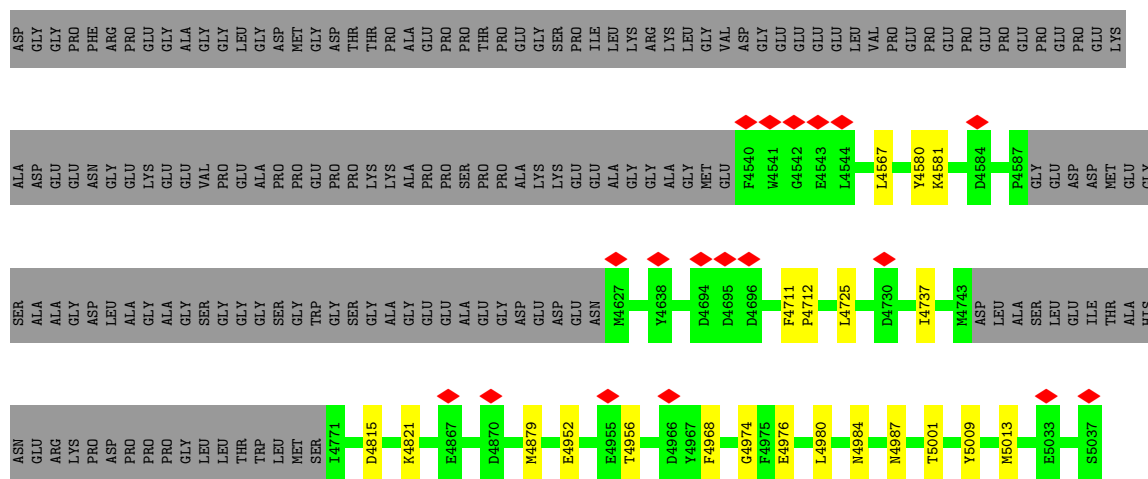


• Molecule 3: Ryanodine receptor 1

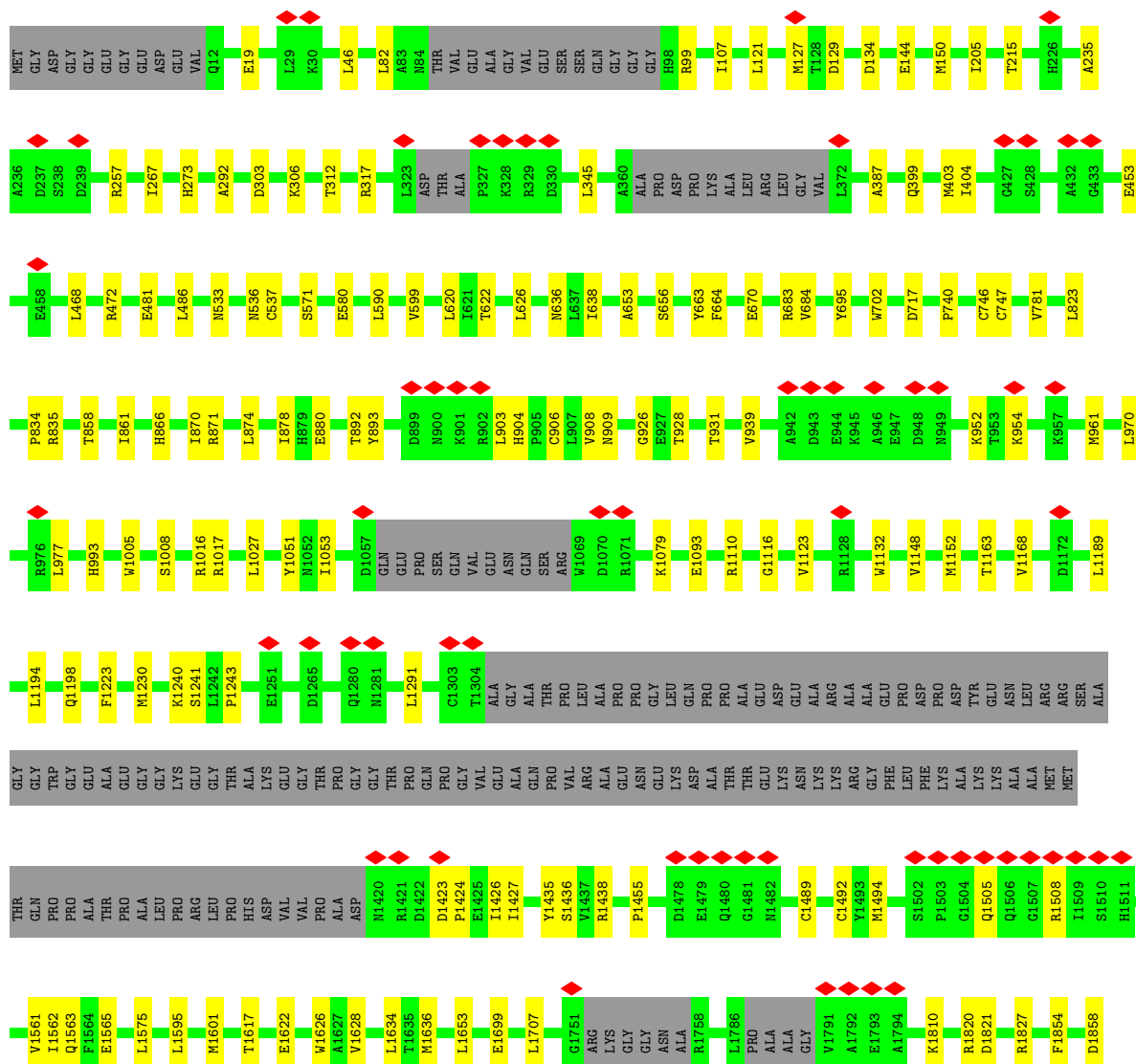
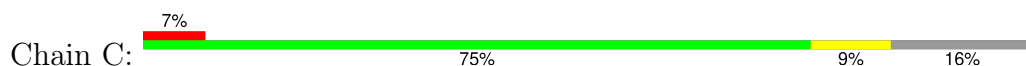








• Molecule 3: Ryanodine receptor 1





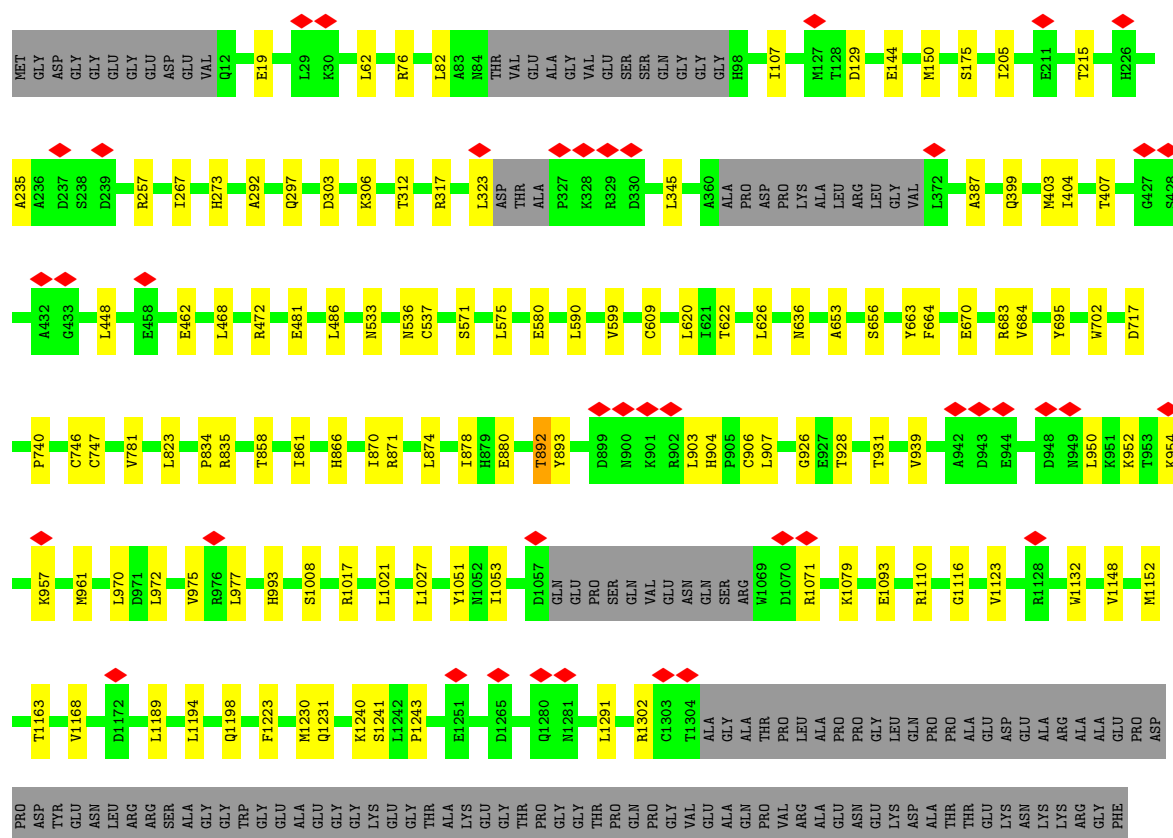
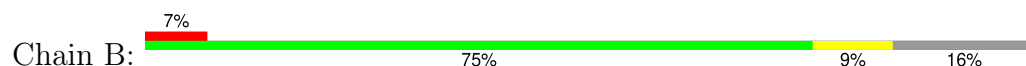


Amino Acid	Percentage (%)	Category	Marked
MET	~1.5	Standard	No
GLY	~2.5	Standard	No
ASP	~3.5	Standard	No
GLY	~4.5	Standard	No
GLY	~5.5	Standard	No
GLU	~6.5	Standard	No
GLY	~7.5	Standard	No
GLU	~8.5	Standard	No
ASP	~9.5	Standard	No
GLU	~10.5	Standard	No
VAL	~11.5	Standard	No
GLI2	~12.5	Modified	No
E19	~13.5	Modified	No
L29	~14.5	Standard	Yes
K30	~15.5	Standard	Yes
L62	~16.5	Standard	No
L73	~17.5	Standard	No
R76	~18.5	Standard	No
Q79	~19.5	Standard	No
L82	~20.5	Standard	No
A83	~21.5	Standard	No
M84	~22.5	Modified	No
THR	~23.5	Standard	No
VAL	~24.5	Standard	No
GLU	~25.5	Standard	No
ALA	~26.5	Standard	No
GLY	~27.5	Standard	No
VAL	~28.5	Standard	No
GLU	~29.5	Standard	No
SER	~30.5	Standard	No
SER	~31.5	Standard	No
GLN	~32.5	Standard	No
GLY	~33.5	Standard	No
GLY	~34.5	Standard	No
H98	~35.5	Modified	No
R99	~36.5	Modified	No
M127	~37.5	Standard	Yes
T128	~38.5	Standard	No
D129	~39.5	Standard	No
E144	~40.5	Standard	No
I206	~41.5	Standard	No
T215	~42.5	Standard	No
H226	~43.5	Standard	Yes
A235	~44.5	Standard	No
A236	~45.5	Standard	No



WORLDWIDE
PDB
PROTEIN DATA BANK

- Molecule 3: Ryanodine receptor 1







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	259362	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	71.2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	9.289	Depositor
Minimum map value	0.000	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.142	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	542.72, 542.72, 542.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: 43M, CA, ZN, CFF, ATP

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	0.12	0/835	0.28	0/1123
1	F	0.11	0/835	0.27	0/1123
1	G	0.11	0/835	0.27	0/1123
1	H	0.11	0/835	0.28	0/1123
2	I	0.10	0/1026	0.29	0/1386
2	J	0.10	0/1026	0.30	0/1386
2	K	0.11	0/1026	0.32	0/1386
2	L	0.10	0/1026	0.30	0/1386
3	A	0.12	0/34640	0.29	0/46902
3	B	0.12	0/34640	0.28	0/46902
3	C	0.12	0/34640	0.29	0/46902
3	D	0.12	0/34640	0.29	0/46902
All	All	0.12	0/146004	0.29	0/197644

There are no bond length outliers.

There are no bond angle outliers.

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	819	0	824	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	819	0	824	6	0
1	G	819	0	824	8	0
1	H	819	0	824	9	0
2	I	1017	0	841	12	0
2	J	1017	0	841	15	0
2	K	1017	0	841	16	0
2	L	1017	0	841	12	0
3	A	33879	0	33511	277	0
3	B	33879	0	33511	283	0
3	C	33879	0	33511	287	0
3	D	33879	0	33511	294	0
4	A	36	0	24	0	0
4	B	36	0	24	0	0
4	C	36	0	24	0	0
4	D	36	0	24	0	0
5	A	14	0	10	0	0
5	B	14	0	10	0	0
5	C	14	0	10	0	0
5	D	14	0	10	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	62	0	24	0	0
7	B	62	0	24	0	0
7	C	62	0	24	0	0
7	D	62	0	24	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	704	0	0	1	0
9	B	672	0	0	0	0
9	C	673	0	0	1	0
9	D	692	0	0	1	0
9	E	14	0	0	0	0
9	F	15	0	0	0	0
9	G	15	0	0	0	0
9	H	15	0	0	0	0
9	I	30	0	0	0	0
9	J	30	0	0	0	0
9	K	30	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	L	33	0	0	0	0
All	All	146239	0	140936	1215	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 4.

All (1215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4090:LYS:HG3	3:D:4121:GLU:HB3	1.64	0.80
3:B:2801:ASP:HA	3:B:2804:ILE:HG12	1.66	0.78
3:D:2801:ASP:HA	3:D:2804:ILE:HG12	1.66	0.77
3:D:2208:MET:HE2	3:D:2250:MET:HE1	1.68	0.76
3:C:2801:ASP:HA	3:C:2804:ILE:HG12	1.66	0.76
3:C:127:MET:HE3	3:C:127:MET:H	1.52	0.74
3:B:4034:ASN:HD21	3:B:4041:ALA:HB2	1.53	0.74
3:A:2801:ASP:HA	3:A:2804:ILE:HG12	1.69	0.73
3:D:4034:ASN:HD21	3:D:4041:ALA:HB2	1.54	0.72
3:C:1990:GLU:HA	3:C:1993:ARG:HB3	1.72	0.72
3:D:1990:GLU:HA	3:D:1993:ARG:HB3	1.71	0.71
3:B:1990:GLU:HA	3:B:1993:ARG:HB3	1.71	0.71
3:C:2159:LEU:HD13	3:C:2203:MET:HG2	1.73	0.70
3:B:2159:LEU:HD13	3:B:2203:MET:HG2	1.73	0.70
3:D:2159:LEU:HD13	3:D:2203:MET:HG2	1.73	0.70
3:C:4034:ASN:HD21	3:C:4041:ALA:HB2	1.56	0.69
3:D:2865:VAL:HB	3:D:2928:LYS:HE2	1.74	0.69
3:C:874:LEU:O	3:C:878:ILE:HG12	1.92	0.69
3:D:874:LEU:O	3:D:878:ILE:HG12	1.92	0.69
3:A:1990:GLU:HA	3:A:1993:ARG:HB3	1.72	0.69
3:A:2865:VAL:HB	3:A:2928:LYS:HE2	1.75	0.69
3:A:4034:ASN:HD21	3:A:4041:ALA:HB2	1.57	0.68
3:A:2159:LEU:HD13	3:A:2203:MET:HG2	1.74	0.68
3:B:874:LEU:O	3:B:878:ILE:HG12	1.92	0.68
3:C:2597:LYS:HE2	3:C:2597:LYS:HA	1.74	0.68
3:D:823:LEU:HD11	3:D:1626:TRP:HB3	1.76	0.67
3:A:399:GLN:O	3:A:403:MET:HG3	1.94	0.67
3:C:399:GLN:O	3:C:403:MET:HG3	1.95	0.67
3:A:874:LEU:O	3:A:878:ILE:HG12	1.94	0.67
3:C:2767:ALA:O	3:C:2771:ILE:HG23	1.94	0.66
3:D:399:GLN:O	3:D:403:MET:HG3	1.94	0.66
3:A:1699:GLU:HG3	3:A:1810:LYS:HE3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:823:LEU:HD11	3:B:1626:TRP:HB3	1.77	0.66
3:B:399:GLN:O	3:B:403:MET:HG3	1.95	0.66
3:A:3758:MET:HE3	3:A:3758:MET:HA	1.77	0.65
3:D:3989:VAL:HG13	3:D:4023:MET:HE3	1.77	0.65
3:B:2767:ALA:O	3:B:2771:ILE:HG23	1.95	0.65
3:C:2519:LEU:HD22	3:C:2578:MET:HE1	1.77	0.65
3:C:3758:MET:HE3	3:C:3758:MET:HA	1.77	0.65
3:C:3329:ILE:HD11	3:C:3332:ALA:HB2	1.77	0.65
3:B:2519:LEU:HD22	3:B:2578:MET:HE1	1.79	0.65
3:C:823:LEU:HD11	3:C:1626:TRP:HB3	1.78	0.64
2:L:110:THR:HG22	2:L:121:VAL:HG21	1.78	0.64
3:B:2116:LEU:O	3:B:2120:MET:HG3	1.97	0.64
3:A:1424:PRO:HA	3:A:1427:ILE:HG22	1.79	0.64
3:A:3329:ILE:HD11	3:A:3332:ALA:HB2	1.79	0.64
2:I:115:LYS:HB2	3:A:3858:MET:HE1	1.80	0.64
2:K:110:THR:HG22	2:K:121:VAL:HG21	1.80	0.63
3:C:4151:SER:HB2	3:C:4164:LEU:HD11	1.81	0.63
2:J:110:THR:HG22	2:J:121:VAL:HG21	1.79	0.63
3:A:1979:LEU:HD12	3:A:1982:ARG:HH12	1.62	0.63
3:A:1423:ASP:HB2	3:A:1426:ILE:HD12	1.81	0.62
3:A:823:LEU:HD11	3:A:1626:TRP:HB3	1.81	0.62
3:C:2930:LEU:HD23	3:C:2937:VAL:HG11	1.82	0.62
3:B:1622:GLU:CD	3:B:1622:GLU:H	2.08	0.62
3:B:2930:LEU:HD23	3:B:2937:VAL:HG11	1.82	0.62
3:B:3589:PRO:O	3:B:3593:VAL:HG23	1.99	0.62
3:C:1622:GLU:H	3:C:1622:GLU:CD	2.08	0.62
3:C:4976:GLU:O	3:C:4980:LEU:HG	2.00	0.62
3:D:3589:PRO:O	3:D:3593:VAL:HG23	2.00	0.62
3:C:1699:GLU:HG3	3:C:1810:LYS:HE3	1.81	0.62
3:B:404:ILE:HG21	3:B:481:GLU:HG3	1.81	0.62
3:A:3540:TYR:HB3	3:A:3604:TYR:CD2	2.33	0.62
3:D:1622:GLU:CD	3:D:1622:GLU:H	2.08	0.62
3:B:4976:GLU:O	3:B:4980:LEU:HG	2.00	0.61
3:A:3648:ARG:O	3:A:3652:MET:HG3	2.00	0.61
3:B:1699:GLU:HG3	3:B:1810:LYS:HE3	1.81	0.61
3:B:2004:GLU:O	3:B:2008:MET:HG3	2.00	0.61
3:D:3540:TYR:HB3	3:D:3604:TYR:CD1	2.36	0.61
3:D:2116:LEU:O	3:D:2120:MET:HG3	1.99	0.61
3:B:3648:ARG:O	3:B:3652:MET:HG3	2.01	0.61
2:I:110:THR:HG22	2:I:121:VAL:HG21	1.80	0.61
3:B:462:GLU:H	3:B:462:GLU:CD	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3540:TYR:HB3	3:C:3604:TYR:CD1	2.35	0.61
3:B:2161:GLN:HE21	3:B:2177:LEU:HD11	1.64	0.61
3:D:3648:ARG:O	3:D:3652:MET:HG3	2.00	0.61
3:D:4976:GLU:O	3:D:4980:LEU:HG	2.01	0.61
3:B:2872:GLN:O	3:B:2876:GLU:HG2	2.01	0.61
3:D:2161:GLN:HE21	3:D:2177:LEU:HD11	1.65	0.60
3:C:303:ASP:HB2	3:C:306:LYS:HE3	1.83	0.60
3:A:858:THR:HA	3:A:861:ILE:HD12	1.84	0.60
3:C:2004:GLU:O	3:C:2008:MET:HG3	2.01	0.60
3:D:1699:GLU:HG3	3:D:1810:LYS:HE3	1.81	0.60
3:D:2004:GLU:O	3:D:2008:MET:HG3	2.01	0.60
3:D:3553:LEU:HB2	3:D:3593:VAL:HG13	1.83	0.60
3:A:2004:GLU:O	3:A:2008:MET:HG3	2.01	0.60
3:B:858:THR:HA	3:B:861:ILE:HD12	1.84	0.60
3:C:404:ILE:HG21	3:C:481:GLU:HG3	1.81	0.60
3:B:3540:TYR:HB3	3:B:3604:TYR:CD2	2.35	0.60
3:C:3106:MET:HE2	3:C:3132:THR:HB	1.84	0.60
3:D:404:ILE:HG21	3:D:481:GLU:HG3	1.81	0.60
3:A:2904:LEU:HD21	3:A:2915:GLU:HG3	1.83	0.60
3:A:2810:LYS:O	3:A:2814:LYS:HG2	2.02	0.60
3:A:1163:THR:HG22	3:A:1168:VAL:HA	1.83	0.60
3:A:2970:SER:HA	3:A:2973:PHE:CE2	2.37	0.60
3:C:3709:ALA:HB2	3:C:3782:MET:HE2	1.84	0.60
3:A:2758:PHE:HD2	3:A:2809:ILE:HG12	1.67	0.59
3:C:2970:SER:HA	3:C:2973:PHE:CE2	2.37	0.59
3:A:4976:GLU:O	3:A:4980:LEU:HG	2.01	0.59
3:D:858:THR:HA	3:D:861:ILE:HD12	1.83	0.59
3:B:3553:LEU:HB2	3:B:3593:VAL:HG13	1.83	0.59
3:D:3709:ALA:HB2	3:D:3782:MET:HE2	1.84	0.59
2:I:106:ARG:O	2:I:110:THR:HG23	2.01	0.59
3:C:858:THR:HA	3:C:861:ILE:HD12	1.84	0.59
3:B:2970:SER:HA	3:B:2973:PHE:CE2	2.37	0.59
3:C:580:GLU:HG3	3:C:620:LEU:HD22	1.85	0.59
2:J:106:ARG:O	2:J:110:THR:HG23	2.02	0.59
3:B:3178:THR:C	3:B:3179:LYS:HD2	2.28	0.59
3:A:404:ILE:HG21	3:A:481:GLU:HG3	1.83	0.59
3:A:670:GLU:HA	3:A:740:PRO:HG3	1.84	0.59
3:D:4062:PHE:HB3	3:D:4170:ILE:HD13	1.85	0.59
2:K:106:ARG:O	2:K:110:THR:HG23	2.03	0.59
3:B:2879:ALA:HB1	3:B:2919:ASP:HB3	1.84	0.58
3:D:2930:LEU:HD23	3:D:2937:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:106:ARG:O	2:L:110:THR:HG23	2.02	0.58
3:C:3589:PRO:O	3:C:3593:VAL:HG23	2.04	0.58
3:B:670:GLU:HA	3:B:740:PRO:HG3	1.84	0.58
3:A:4062:PHE:HB3	3:A:4170:ILE:HD13	1.84	0.58
3:C:3535:LEU:HD11	3:C:3559:LEU:HD12	1.86	0.58
3:D:2738:ARG:HD3	3:D:2738:ARG:N	2.19	0.58
3:D:3535:LEU:HD11	3:D:3559:LEU:HD12	1.86	0.58
3:D:580:GLU:HG3	3:D:620:LEU:HD22	1.85	0.58
3:C:670:GLU:HA	3:C:740:PRO:HG3	1.85	0.58
3:B:1820:ARG:HH21	3:B:1821:ASP:HB3	1.69	0.58
3:D:670:GLU:HA	3:D:740:PRO:HG3	1.85	0.58
3:B:3535:LEU:HD11	3:B:3559:LEU:HD12	1.86	0.58
3:A:2874:MET:HE1	3:A:2941:LEU:HB3	1.85	0.58
3:A:1116:GLY:HA3	3:A:1132:TRP:HB3	1.86	0.58
3:D:1163:THR:HG22	3:D:1168:VAL:HA	1.86	0.58
3:D:2970:SER:HA	3:D:2973:PHE:CE2	2.38	0.58
3:C:2172:PRO:O	3:C:2176:ASN:ND2	2.35	0.57
3:C:3553:LEU:HB2	3:C:3593:VAL:HG13	1.85	0.57
3:B:2519:LEU:HD13	3:B:2575:ARG:HG3	1.86	0.57
3:A:1622:GLU:H	3:A:1622:GLU:CD	2.11	0.57
3:C:1163:THR:HG22	3:C:1168:VAL:HA	1.87	0.57
3:A:3553:LEU:HB2	3:A:3593:VAL:HG13	1.85	0.57
3:B:1116:GLY:HA3	3:B:1132:TRP:HB3	1.87	0.57
3:B:2738:ARG:HD3	3:B:2738:ARG:N	2.19	0.57
3:B:3758:MET:HE2	3:B:3758:MET:HA	1.87	0.57
3:C:2904:LEU:HD21	3:C:2915:GLU:HG3	1.87	0.57
3:C:3834:ALA:O	3:C:3838:THR:HG23	2.04	0.57
3:B:3329:ILE:HD11	3:B:3332:ALA:HB2	1.85	0.57
3:B:3709:ALA:HB2	3:B:3782:MET:HE2	1.85	0.57
3:D:1116:GLY:HA3	3:D:1132:TRP:HB3	1.86	0.57
3:D:2250:MET:HE2	3:D:2250:MET:HA	1.85	0.57
3:D:2519:LEU:HD13	3:D:2575:ARG:HG3	1.87	0.57
3:D:3536:ALA:HB2	3:D:3553:LEU:HD21	1.87	0.57
3:A:893:TYR:H	3:A:961:MET:HE3	1.68	0.57
3:C:2420:HIS:HA	3:C:2423:MET:HE2	1.86	0.57
3:C:3379:LEU:HD11	3:C:3387:ALA:O	2.04	0.57
3:D:1820:ARG:HH21	3:D:1821:ASP:HB3	1.68	0.57
3:D:2172:PRO:O	3:D:2176:ASN:ND2	2.36	0.57
3:D:2810:LYS:O	3:D:2814:LYS:HG2	2.05	0.57
3:B:2419:GLY:O	3:B:2423:MET:HG3	2.05	0.57
1:G:4:ILE:HD11	1:G:62:GLY:HA2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3081:MET:HE1	3:B:3089:LYS:HA	1.87	0.57
3:C:2519:LEU:HD13	3:C:2575:ARG:HG3	1.87	0.57
3:C:3536:ALA:HB2	3:C:3553:LEU:HD21	1.87	0.57
3:B:3906:GLN:H	3:B:3912:THR:HG23	1.70	0.57
3:C:4648:LEU:HD23	3:C:4803:HIS:HE1	1.70	0.56
3:D:3729:MET:HE3	3:D:3770:LEU:HD22	1.87	0.56
3:B:580:GLU:HG3	3:B:620:LEU:HD22	1.85	0.56
3:A:2781:VAL:HG12	3:A:2789:PRO:HD3	1.86	0.56
3:A:3906:GLN:H	3:A:3912:THR:HG23	1.70	0.56
3:C:1820:ARG:HH21	3:C:1821:ASP:HB3	1.71	0.56
3:C:2116:LEU:O	3:C:2120:MET:HG3	2.05	0.56
3:B:1163:THR:HG22	3:B:1168:VAL:HA	1.86	0.56
3:A:2419:GLY:O	3:A:2423:MET:HG3	2.05	0.56
3:A:3626:LYS:HD2	3:A:3626:LYS:C	2.31	0.56
3:C:1116:GLY:HA3	3:C:1132:TRP:HB3	1.86	0.56
3:D:4648:LEU:HD23	3:D:4803:HIS:HE1	1.70	0.56
3:B:3563:VAL:HA	3:B:3569:LEU:HD22	1.87	0.56
3:C:2865:VAL:HB	3:C:2928:LYS:HE2	1.86	0.56
3:C:3626:LYS:HD2	3:C:3626:LYS:C	2.31	0.56
3:C:2810:LYS:O	3:C:2814:LYS:HG2	2.05	0.56
3:A:3702:VAL:HG13	3:A:3778:MET:HE3	1.87	0.56
3:B:2865:VAL:HB	3:B:2928:LYS:HE2	1.87	0.56
3:A:2519:LEU:HD13	3:A:2575:ARG:HG3	1.88	0.56
3:C:3107:VAL:HG22	3:C:3175:LEU:HD21	1.88	0.56
3:C:3648:ARG:O	3:C:3652:MET:HG3	2.06	0.56
3:C:3906:GLN:H	3:C:3912:THR:HG23	1.70	0.56
3:B:892:THR:HA	3:B:961:MET:HE1	1.88	0.56
3:C:1977:TYR:CZ	3:C:1981:MET:HE2	2.41	0.56
3:D:892:THR:HA	3:D:961:MET:HE1	1.88	0.56
3:B:3729:MET:HE3	3:B:3770:LEU:HD22	1.87	0.56
3:C:3250:MET:HE2	3:C:3250:MET:HA	1.88	0.55
3:D:3906:GLN:H	3:D:3912:THR:HG23	1.71	0.55
1:F:4:ILE:HD11	1:F:62:GLY:HA2	1.88	0.55
3:A:2519:LEU:HD22	3:A:2578:MET:HE1	1.88	0.55
3:D:3329:ILE:HD11	3:D:3332:ALA:HB2	1.89	0.55
3:B:4090:LYS:HE2	3:B:4112:LEU:HD22	1.89	0.55
3:C:2879:ALA:HB1	3:C:2919:ASP:HB3	1.88	0.55
3:D:3384:LYS:H	3:D:3387:ALA:HB3	1.71	0.55
3:D:2758:PHE:HD2	3:D:2809:ILE:HG12	1.70	0.55
3:A:2165:LEU:HD21	3:A:2177:LEU:HD23	1.88	0.55
3:A:3081:MET:HE1	3:A:3089:LYS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:622:THR:HG23	3:C:626:LEU:HD22	1.89	0.55
3:B:303:ASP:HB2	3:B:306:LYS:HE3	1.89	0.55
3:A:2644:LEU:HD13	3:A:2678:LEU:HD21	1.89	0.55
3:A:3536:ALA:HB2	3:A:3553:LEU:HD21	1.89	0.55
3:D:2644:LEU:HD13	3:D:2678:LEU:HD21	1.89	0.55
3:B:2974:ILE:HD12	3:B:3056:LEU:HD21	1.89	0.55
3:B:3250:MET:HA	3:B:3250:MET:HE2	1.89	0.55
3:B:2810:LYS:O	3:B:2814:LYS:HG2	2.05	0.55
3:B:3536:ALA:HB2	3:B:3553:LEU:HD21	1.88	0.55
3:A:2116:LEU:O	3:A:2120:MET:HG3	2.06	0.55
3:A:3729:MET:HE3	3:A:3770:LEU:HD22	1.89	0.55
3:C:2738:ARG:HD3	3:C:2738:ARG:N	2.21	0.55
3:C:3989:VAL:HG13	3:C:4023:MET:HE3	1.89	0.55
2:L:116:LEU:HD13	2:L:124:MET:HE1	1.89	0.55
3:D:622:THR:HG23	3:D:626:LEU:HD22	1.89	0.55
3:A:3535:LEU:HD11	3:A:3559:LEU:HD12	1.89	0.55
3:D:2974:ILE:HD12	3:D:3056:LEU:HD21	1.89	0.55
3:B:2172:PRO:O	3:B:2176:ASN:ND2	2.37	0.55
3:C:2644:LEU:HD13	3:C:2678:LEU:HD21	1.89	0.54
3:A:3589:PRO:O	3:A:3593:VAL:HG23	2.06	0.54
3:B:3384:LYS:H	3:B:3387:ALA:HB3	1.72	0.54
3:B:4090:LYS:HG2	3:B:4123:ILE:HD11	1.89	0.54
3:B:622:THR:HG23	3:B:626:LEU:HD22	1.89	0.54
3:D:303:ASP:HB2	3:D:306:LYS:HE3	1.89	0.54
3:B:2644:LEU:HD13	3:B:2678:LEU:HD21	1.89	0.54
3:C:3729:MET:HE3	3:C:3770:LEU:HD22	1.88	0.54
3:C:2974:ILE:HD12	3:C:3056:LEU:HD21	1.89	0.54
3:D:73:LEU:HD23	3:D:99:ARG:HH12	1.73	0.54
3:D:3081:MET:HE1	3:D:3089:LYS:HA	1.88	0.54
3:D:3379:LEU:HD11	3:D:3387:ALA:O	2.07	0.54
3:B:3107:VAL:HG22	3:B:3175:LEU:HD21	1.89	0.54
1:E:68:LEU:HD23	1:E:106:LEU:HG	1.89	0.54
2:J:115:LYS:HB2	3:B:3858:MET:HE1	1.89	0.54
3:A:235:ALA:HA	3:A:257:ARG:HD3	1.88	0.54
3:A:1980:LEU:HD11	3:A:1994:ARG:HD2	1.89	0.54
3:A:2800:LYS:O	3:A:2804:ILE:HG23	2.08	0.54
3:B:2904:LEU:HD21	3:B:2915:GLU:HG3	1.90	0.54
3:B:2758:PHE:HD2	3:B:2809:ILE:HG12	1.71	0.54
3:B:3725:TYR:O	3:B:3729:MET:HG3	2.08	0.54
1:H:4:ILE:HD11	1:H:62:GLY:HA2	1.89	0.54
3:A:580:GLU:HG3	3:A:620:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3178:THR:C	3:A:3179:LYS:HD2	2.32	0.54
3:C:2758:PHE:HD2	3:C:2809:ILE:HG12	1.71	0.54
3:C:3178:THR:C	3:C:3179:LYS:HD2	2.32	0.54
3:C:2800:LYS:O	3:C:2804:ILE:HG23	2.08	0.54
3:D:2874:MET:HE1	3:D:2941:LEU:HB3	1.89	0.54
3:B:1505:GLN:HG3	3:B:1508:ARG:HH21	1.73	0.54
3:B:3847:PHE:HE1	3:B:3946:GLN:HE21	1.55	0.54
3:C:2351:ASN:HB3	3:C:2355:ARG:HH21	1.73	0.53
3:B:3132:THR:HA	3:B:3136:LEU:HB3	1.90	0.53
3:A:3132:THR:HA	3:A:3136:LEU:HB3	1.90	0.53
3:C:3384:LYS:H	3:C:3387:ALA:HB3	1.72	0.53
3:C:4719:PHE:HA	3:C:4722:ARG:HE	1.72	0.53
3:D:3107:VAL:HG22	3:D:3175:LEU:HD21	1.90	0.53
3:D:3132:THR:HA	3:D:3136:LEU:HB3	1.90	0.53
3:B:3757:GLU:O	3:B:3761:GLN:HG2	2.09	0.53
3:C:4091:LYS:O	3:C:4095:LYS:HG2	2.09	0.53
3:B:462:GLU:HG3	3:B:3710:LEU:HD13	1.89	0.53
3:B:3034:LYS:HE3	3:B:3038:MET:HE2	1.91	0.53
3:A:904:HIS:HB3	3:A:907:LEU:HD13	1.90	0.53
3:A:3384:LYS:H	3:A:3387:ALA:HB3	1.73	0.53
3:C:127:MET:H	3:C:127:MET:CE	2.20	0.53
3:D:3725:TYR:O	3:D:3729:MET:HG3	2.09	0.53
2:L:115:LYS:HG2	3:D:3858:MET:HE1	1.90	0.53
3:A:1820:ARG:HH21	3:A:1821:ASP:HB3	1.72	0.53
3:A:5009:TYR:CZ	3:A:5013:MET:HE3	2.44	0.53
3:C:3132:THR:HA	3:C:3136:LEU:HB3	1.91	0.53
3:A:1977:TYR:CZ	3:A:1981:MET:HE2	2.43	0.53
3:C:3184:GLU:HG2	3:C:3187:ARG:HH12	1.74	0.53
3:D:1505:GLN:HG3	3:D:1508:ARG:HH21	1.73	0.53
3:D:3178:THR:C	3:D:3179:LYS:HD2	2.33	0.53
3:B:2800:LYS:O	3:B:2804:ILE:HG23	2.09	0.53
2:L:-1:HIS:O	2:L:3:GLN:HG3	2.08	0.53
2:I:-1:HIS:O	2:I:3:GLN:HG3	2.08	0.53
3:A:2697:ARG:HG2	3:A:2697:ARG:HH11	1.74	0.53
3:A:3989:VAL:HG13	3:A:4023:MET:HE3	1.91	0.53
3:C:1505:GLN:HG3	3:C:1508:ARG:HH21	1.74	0.53
3:D:2165:LEU:HD21	3:D:2177:LEU:HD23	1.91	0.53
3:D:2879:ALA:HB1	3:D:2919:ASP:HB3	1.90	0.53
3:D:1123:VAL:HG23	3:D:1132:TRP:HB2	1.91	0.53
3:B:235:ALA:HA	3:B:257:ARG:HD3	1.91	0.53
3:A:2172:PRO:O	3:A:2176:ASN:ND2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2498:HIS:O	3:A:2502:MET:HG2	2.10	0.52
3:A:3250:MET:HE2	3:A:3250:MET:HA	1.91	0.52
3:D:2608:MET:HE1	3:D:2642:LYS:HB3	1.90	0.52
2:L:101:SER:HB2	2:L:104:GLU:HG3	1.91	0.52
3:C:235:ALA:HA	3:C:257:ARG:HD3	1.91	0.52
3:C:1123:VAL:HG23	3:C:1132:TRP:HB2	1.91	0.52
3:D:4719:PHE:HA	3:D:4722:ARG:HE	1.75	0.52
3:B:2165:LEU:HD21	3:B:2177:LEU:HD23	1.91	0.52
3:B:3379:LEU:HD11	3:B:3387:ALA:O	2.10	0.52
3:A:823:LEU:HB2	3:A:1617:THR:HG21	1.92	0.52
3:A:928:THR:HA	3:A:931:THR:HG22	1.92	0.52
3:D:3250:MET:HA	3:D:3250:MET:HE2	1.90	0.52
3:D:5009:TYR:CZ	3:D:5013:MET:HE3	2.45	0.52
3:B:2351:ASN:HB3	3:B:2355:ARG:HH21	1.75	0.52
3:B:5009:TYR:CZ	3:B:5013:MET:HE3	2.45	0.52
2:J:-1:HIS:O	2:J:3:GLN:HG3	2.09	0.52
3:C:1992:ALA:HA	3:C:1995:THR:HG22	1.92	0.52
3:A:3725:TYR:O	3:A:3729:MET:HG3	2.10	0.52
3:D:928:THR:HA	3:D:931:THR:HG22	1.92	0.52
3:D:1492:CYS:SG	3:D:1494:MET:HG3	2.49	0.52
3:B:2608:MET:HE1	3:B:2642:LYS:HB3	1.92	0.52
3:B:3179:LYS:HD2	3:B:3179:LYS:N	2.24	0.52
3:A:622:THR:HG23	3:A:626:LEU:HD22	1.90	0.52
3:A:1992:ALA:HA	3:A:1995:THR:HG22	1.92	0.52
3:A:2921:GLU:O	3:A:2925:GLU:HG2	2.10	0.52
3:C:3569:LEU:O	3:C:3573:MET:HG2	2.09	0.52
3:B:3035:GLU:HA	3:B:3038:MET:HE3	1.91	0.52
3:C:1492:CYS:SG	3:C:1494:MET:HG3	2.49	0.52
3:C:2753:SER:HA	3:C:2756:ASN:HD21	1.75	0.52
3:B:4056:GLU:HG2	3:B:4166:LEU:HD13	1.92	0.52
3:A:292:ALA:HB2	3:A:312:THR:HG22	1.92	0.52
3:A:2608:MET:HE1	3:A:2642:LYS:HB3	1.91	0.52
3:A:2738:ARG:HD3	3:A:2738:ARG:N	2.25	0.52
3:D:2800:LYS:O	3:D:2804:ILE:HG23	2.10	0.52
3:C:823:LEU:HD13	3:C:1628:VAL:HG22	1.92	0.51
3:D:1980:LEU:HD11	3:D:1994:ARG:HD2	1.92	0.51
3:D:2522:LEU:HD13	3:D:2582:MET:HE2	1.92	0.51
3:B:1492:CYS:SG	3:B:1494:MET:HG3	2.49	0.51
2:K:31:GLU:O	2:K:35:VAL:HG22	2.10	0.51
3:C:684:VAL:HG22	3:C:781:VAL:HG12	1.93	0.51
3:A:1505:GLN:HG3	3:A:1508:ARG:HH21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4056:GLU:HG2	3:A:4166:LEU:HD13	1.91	0.51
3:D:1992:ALA:HA	3:D:1995:THR:HG22	1.93	0.51
3:D:2626:LEU:HD22	3:D:2640:PRO:HB3	1.93	0.51
3:B:2753:SER:HA	3:B:2756:ASN:HD21	1.75	0.51
3:A:3709:ALA:HB2	3:A:3782:MET:HE2	1.93	0.51
3:C:2758:PHE:CD2	3:C:2809:ILE:HG12	2.45	0.51
3:D:2608:MET:HE2	3:D:2639:MET:HG2	1.91	0.51
3:B:1123:VAL:HG23	3:B:1132:TRP:HB2	1.91	0.51
3:A:2753:SER:HA	3:A:2756:ASN:HD21	1.76	0.51
3:D:2753:SER:HA	3:D:2756:ASN:HD21	1.75	0.51
3:D:2904:LEU:HD21	3:D:2915:GLU:HG3	1.93	0.51
3:B:2753:SER:HA	3:B:2756:ASN:ND2	2.26	0.51
3:B:3989:VAL:HG13	3:B:4023:MET:HE3	1.93	0.51
3:D:2498:HIS:O	3:D:2502:MET:HG2	2.11	0.51
3:A:2747:ILE:HD11	3:A:2751:LEU:HD11	1.92	0.51
3:C:2608:MET:HE1	3:C:2642:LYS:HB3	1.92	0.51
3:C:2890:LYS:HA	3:C:2893:GLU:OE2	2.11	0.51
3:D:235:ALA:HA	3:D:257:ARG:HD3	1.91	0.51
3:D:823:LEU:HD13	3:D:1628:VAL:HG22	1.92	0.51
3:D:4097:MET:HG3	3:D:4103:PHE:HD2	1.75	0.51
3:B:1992:ALA:HA	3:B:1995:THR:HG22	1.93	0.51
3:C:4090:LYS:HG3	3:C:4121:GLU:HG2	1.91	0.51
3:D:684:VAL:HG22	3:D:781:VAL:HG12	1.93	0.51
3:D:3184:GLU:HG2	3:D:3187:ARG:HH12	1.75	0.51
3:B:684:VAL:HG22	3:B:781:VAL:HG12	1.92	0.51
3:B:928:THR:HA	3:B:931:THR:HG22	1.92	0.51
3:A:945:LYS:HD2	3:A:945:LYS:C	2.36	0.51
3:C:3379:LEU:HD21	3:C:3390:GLY:HA3	1.93	0.51
3:D:3847:PHE:HE1	3:D:3946:GLN:HE21	1.57	0.51
3:B:2758:PHE:CD2	3:B:2809:ILE:HG12	2.45	0.51
3:C:292:ALA:HB2	3:C:312:THR:HG22	1.93	0.51
3:C:1980:LEU:HD11	3:C:1994:ARG:HD2	1.91	0.51
3:C:3563:VAL:HA	3:C:3569:LEU:HD22	1.92	0.51
3:C:3725:TYR:O	3:C:3729:MET:HG3	2.10	0.51
3:D:2747:ILE:HD11	3:D:2751:LEU:HD11	1.93	0.51
3:D:3339:ALA:O	3:D:3343:GLN:HG2	2.11	0.51
3:A:575:LEU:HD22	3:A:609:CYS:HB2	1.93	0.50
3:A:1492:CYS:SG	3:A:1494:MET:HG3	2.51	0.50
3:A:2753:SER:HA	3:A:2756:ASN:ND2	2.27	0.50
3:A:2758:PHE:CD2	3:A:2809:ILE:HG12	2.46	0.50
3:C:928:THR:HA	3:C:931:THR:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1977:TYR:CZ	3:B:1981:MET:HE2	2.46	0.50
1:F:49:ARG:HH21	1:F:52:LYS:HE2	1.77	0.50
3:D:2351:ASN:HB3	3:D:2355:ARG:HH21	1.76	0.50
3:D:3563:VAL:HA	3:D:3569:LEU:HD22	1.93	0.50
3:D:4151:SER:HB2	3:D:4164:LEU:HD11	1.93	0.50
1:E:57:LYS:HG3	1:E:61:GLU:OE2	2.11	0.50
3:D:2753:SER:HA	3:D:2756:ASN:ND2	2.26	0.50
3:C:893:TYR:H	3:C:961:MET:HE1	1.76	0.50
3:C:2753:SER:HA	3:C:2756:ASN:ND2	2.26	0.50
3:D:2313:LEU:HD21	3:D:2416:VAL:HG11	1.93	0.50
3:B:468:LEU:O	3:B:472:ARG:HG2	2.12	0.50
3:B:823:LEU:HD13	3:B:1628:VAL:HG22	1.92	0.50
3:A:993:HIS:CE1	3:A:1027:LEU:HD11	2.47	0.50
3:A:1854:PHE:HD1	3:A:1858:ASP:HB3	1.77	0.50
3:C:468:LEU:O	3:C:472:ARG:HG2	2.12	0.50
3:C:3757:GLU:O	3:C:3761:GLN:HG2	2.12	0.50
3:D:1424:PRO:HA	3:D:1427:ILE:HG22	1.93	0.50
3:A:3705:PHE:HB2	3:A:3778:MET:HE2	1.94	0.50
3:D:468:LEU:O	3:D:472:ARG:HG2	2.12	0.50
3:D:1854:PHE:HD1	3:D:1858:ASP:HB3	1.77	0.50
3:A:3563:VAL:HA	3:A:3569:LEU:HD22	1.93	0.50
3:C:892:THR:HA	3:C:961:MET:HE1	1.94	0.50
3:C:3339:ALA:O	3:C:3343:GLN:HG2	2.11	0.50
3:C:3564:GLU:HA	3:C:3570:ARG:HH22	1.77	0.50
3:D:993:HIS:CE1	3:D:1027:LEU:HD11	2.47	0.50
3:B:1854:PHE:HD1	3:B:1858:ASP:HB3	1.77	0.50
3:B:1980:LEU:HD11	3:B:1994:ARG:HD2	1.93	0.50
3:C:1854:PHE:HD1	3:C:1858:ASP:HB3	1.77	0.50
3:D:3564:GLU:HA	3:D:3570:ARG:HH22	1.77	0.50
3:B:292:ALA:HB2	3:B:312:THR:HG22	1.94	0.50
3:B:1424:PRO:HA	3:B:1427:ILE:HG22	1.93	0.50
3:D:2005:GLN:HA	3:D:2008:MET:HE3	1.94	0.50
3:B:2890:LYS:HA	3:B:2893:GLU:OE2	2.12	0.50
3:B:2626:LEU:HD22	3:B:2640:PRO:HB3	1.93	0.49
3:D:292:ALA:HB2	3:D:312:THR:HG22	1.94	0.49
3:B:3550:ARG:HH11	3:B:3594:ARG:HH22	1.58	0.49
2:L:13:LYS:HG2	3:D:2189:LYS:HB3	1.94	0.49
3:A:4097:MET:HG3	3:A:4103:PHE:HD2	1.77	0.49
3:C:2626:LEU:HD22	3:C:2640:PRO:HB3	1.94	0.49
3:C:3312:LEU:HD22	3:C:3348:ARG:HG3	1.93	0.49
3:C:3528:THR:HG23	3:C:3573:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:952:LYS:HD3	3:D:970:LEU:HD23	1.95	0.49
3:D:2758:PHE:CD2	3:D:2809:ILE:HG12	2.47	0.49
3:B:4097:MET:HG3	3:B:4103:PHE:HD2	1.76	0.49
3:A:684:VAL:HG22	3:A:781:VAL:HG12	1.94	0.49
3:A:1094:ALA:HB1	3:A:1100:MET:HE1	1.94	0.49
3:B:4151:SER:HB2	3:B:4164:LEU:HD21	1.95	0.49
3:C:2747:ILE:HD11	3:C:2751:LEU:HD11	1.95	0.49
2:K:115:LYS:HB2	3:C:3858:MET:HE1	1.94	0.49
3:A:2884:ASN:O	3:A:2888:ARG:HD2	2.12	0.49
3:A:3107:VAL:HG22	3:A:3175:LEU:HD21	1.94	0.49
3:C:1993:ARG:O	3:C:1996:ARG:HG2	2.11	0.49
3:B:2161:GLN:HE21	3:B:2177:LEU:CD1	2.26	0.49
3:B:2908:TYR:HE2	3:B:2920:ARG:HH12	1.59	0.49
3:A:1123:VAL:HG23	3:A:1132:TRP:HB2	1.93	0.49
3:C:3327:LEU:HD21	3:C:3408:LEU:HD11	1.94	0.49
3:A:468:LEU:O	3:A:472:ARG:HG2	2.12	0.49
3:C:1424:PRO:HA	3:C:1427:ILE:HG22	1.93	0.49
3:B:993:HIS:CE1	3:B:1027:LEU:HD11	2.47	0.49
3:D:2921:GLU:O	3:D:2925:GLU:HG2	2.13	0.49
3:A:4567:LEU:HD13	3:A:4815:ASP:HB3	1.94	0.49
3:C:2946:LEU:HD23	3:C:2946:LEU:H	1.77	0.49
3:D:2538:THR:O	3:D:2542:SER:HB3	2.13	0.49
3:B:2520:HIS:O	3:B:2524:VAL:HG22	2.13	0.49
3:A:3312:LEU:HD22	3:A:3348:ARG:HG3	1.94	0.48
3:C:2538:THR:O	3:C:2542:SER:HB3	2.13	0.48
3:B:952:LYS:HD3	3:B:970:LEU:HD23	1.94	0.48
2:K:7:GLU:CD	2:K:7:GLU:H	2.21	0.48
3:A:82:LEU:HD13	3:A:144:GLU:HG2	1.94	0.48
3:A:2626:LEU:HD22	3:A:2640:PRO:HB3	1.95	0.48
3:C:1291:LEU:HD13	3:C:1595:LEU:HD11	1.95	0.48
3:C:3719:ASP:HB3	3:C:3722:TYR:HB3	1.95	0.48
3:C:3847:PHE:HE1	3:C:3946:GLN:HE21	1.59	0.48
3:B:2765:LYS:HA	3:B:2765:LYS:HD3	1.58	0.48
3:C:993:HIS:CE1	3:C:1027:LEU:HD11	2.48	0.48
3:D:3379:LEU:HD21	3:D:3390:GLY:HA3	1.95	0.48
3:D:5009:TYR:CE1	3:D:5013:MET:HE3	2.49	0.48
3:B:2608:MET:HE2	3:B:2639:MET:HG2	1.94	0.48
3:A:2608:MET:HE2	3:A:2639:MET:HG2	1.94	0.48
3:A:3414:ARG:HA	3:A:3414:ARG:HD3	1.64	0.48
3:A:4158:PRO:HA	3:A:4161:ARG:HG3	1.94	0.48
3:D:3768:SER:HA	3:D:3771:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3169:LEU:HD12	3:B:3194:LEU:HD11	1.94	0.48
3:A:3169:LEU:HD12	3:A:3194:LEU:HD11	1.95	0.48
3:C:4097:MET:HG3	3:C:4103:PHE:HD2	1.78	0.48
3:D:3169:LEU:HD12	3:D:3194:LEU:HD11	1.94	0.48
3:D:3534:MET:HE3	3:D:3534:MET:HA	1.96	0.48
3:D:3550:ARG:HH11	3:D:3594:ARG:HH22	1.61	0.48
3:B:82:LEU:HD13	3:B:144:GLU:HG2	1.94	0.48
2:K:92:PHE:HE2	2:K:108:VAL:HB	1.79	0.48
3:B:2498:HIS:O	3:B:2502:MET:HG2	2.13	0.48
1:G:49:ARG:HB3	1:G:52:LYS:HG3	1.96	0.48
2:I:13:LYS:HG2	3:A:2189:LYS:HB3	1.95	0.48
3:C:2921:GLU:O	3:C:2925:GLU:HG2	2.13	0.48
3:D:2312:MET:HE3	3:D:2316:LYS:HD2	1.95	0.48
3:B:2747:ILE:HD11	3:B:2751:LEU:HD11	1.95	0.48
2:J:36:MET:SD	2:J:72:MET:HE1	2.54	0.48
3:A:215:THR:HG22	3:A:273:HIS:HA	1.96	0.48
3:A:2021:CYS:HB3	3:A:2028:ARG:HH21	1.79	0.48
3:C:952:LYS:HD3	3:C:970:LEU:HD23	1.95	0.48
3:C:3035:GLU:HA	3:C:3038:MET:HE3	1.94	0.48
3:C:3534:MET:HE3	3:C:3534:MET:HA	1.96	0.48
3:C:3568:SER:O	3:C:3572:GLN:HG3	2.14	0.48
3:D:82:LEU:HD13	3:D:144:GLU:HG2	1.94	0.48
3:D:1423:ASP:HB2	3:D:1426:ILE:HD12	1.95	0.48
3:D:2782:ASP:HB3	3:D:2785:LEU:HG	1.96	0.48
3:D:3327:LEU:HD21	3:D:3408:LEU:HD11	1.96	0.48
3:B:1291:LEU:HD13	3:B:1595:LEU:HD11	1.96	0.48
3:B:4014:LYS:HG2	3:B:4135:PRO:HB3	1.96	0.48
3:A:2359:ARG:HA	3:A:2359:ARG:HD3	1.72	0.48
3:C:82:LEU:HD13	3:C:144:GLU:HG2	1.94	0.48
3:D:3604:TYR:O	3:D:3607:GLU:HG2	2.14	0.48
3:B:2538:THR:O	3:B:2542:SER:HB3	2.13	0.48
3:A:1008:SER:HB3	3:A:1017:ARG:HB3	1.96	0.47
3:A:2912:THR:HG21	3:A:2914:LYS:HE3	1.96	0.47
3:A:3755:GLU:O	3:A:3759:GLU:HG3	2.14	0.47
2:J:13:LYS:HG2	3:B:2189:LYS:HB3	1.96	0.47
3:A:952:LYS:HD3	3:A:970:LEU:HD23	1.96	0.47
3:A:3720:TYR:HA	3:A:3723:MET:HE2	1.97	0.47
3:A:3768:SER:HA	3:A:3771:HIS:ND1	2.29	0.47
3:D:2716:ASP:HB3	3:D:2719:TYR:HB2	1.97	0.47
3:D:3965:LEU:O	3:D:3969:ILE:HG12	2.15	0.47
3:A:908:VAL:HG22	3:A:909:ASN:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1505:GLN:HA	3:A:1508:ARG:HH21	1.79	0.47
3:A:3965:LEU:O	3:A:3969:ILE:HG12	2.14	0.47
3:D:1079:LYS:HA	3:D:1189:LEU:HD11	1.95	0.47
3:D:4567:LEU:HD13	3:D:4815:ASP:HB3	1.96	0.47
3:B:1993:ARG:O	3:B:1996:ARG:HG2	2.13	0.47
3:B:3339:ALA:O	3:B:3343:GLN:HG2	2.15	0.47
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.95	0.47
2:I:101:SER:HB2	2:I:104:GLU:HG3	1.97	0.47
2:J:101:SER:HB2	2:J:104:GLU:HG3	1.96	0.47
3:A:3035:GLU:HA	3:A:3038:MET:HE3	1.96	0.47
3:C:3169:LEU:HD12	3:C:3194:LEU:HD11	1.94	0.47
3:B:3768:SER:HA	3:B:3771:HIS:ND1	2.29	0.47
3:A:3081:MET:HE3	3:A:3092:LEU:HD23	1.96	0.47
3:C:1079:LYS:HA	3:C:1189:LEU:HD11	1.96	0.47
3:C:2470:ILE:HG22	3:C:2525:GLY:HA3	1.96	0.47
3:D:2519:LEU:HD22	3:D:2578:MET:HE1	1.95	0.47
3:D:2946:LEU:H	3:D:2946:LEU:HD23	1.79	0.47
3:D:4014:LYS:HG2	3:D:4135:PRO:HB3	1.96	0.47
3:D:4183:ILE:HG12	3:D:4193:ILE:HD13	1.97	0.47
3:B:1079:LYS:HA	3:B:1189:LEU:HD11	1.95	0.47
3:B:1152:MET:HB3	3:B:1223:PHE:CE2	2.50	0.47
3:B:2921:GLU:O	3:B:2925:GLU:HG2	2.13	0.47
3:A:1194:LEU:HB3	3:A:1198:GLN:HB2	1.97	0.47
3:A:2538:THR:O	3:A:2542:SER:HB3	2.13	0.47
3:A:2890:LYS:HA	3:A:2893:GLU:OE2	2.13	0.47
3:A:3184:GLU:HG2	3:A:3187:ARG:HH12	1.80	0.47
3:D:2677:LYS:HE3	3:D:2677:LYS:HB3	1.48	0.47
3:D:2765:LYS:HA	3:D:2765:LYS:HD3	1.58	0.47
3:B:3719:ASP:HB3	3:B:3722:TYR:HB3	1.97	0.47
3:A:2002:PRO:HG2	3:A:3652:MET:HE1	1.97	0.47
3:C:2498:HIS:O	3:C:2502:MET:HG2	2.13	0.47
3:C:3361:THR:HG21	3:C:3408:LEU:HD22	1.97	0.47
3:D:1194:LEU:HB3	3:D:1198:GLN:HB2	1.97	0.47
3:D:1505:GLN:HA	3:D:1508:ARG:HH21	1.80	0.47
3:D:1977:TYR:CZ	3:D:1981:MET:HE2	2.49	0.47
3:D:3414:ARG:HD3	3:D:3414:ARG:HA	1.64	0.47
3:D:4864:ASN:HD21	3:D:4872:PRO:HB3	1.80	0.47
3:B:2470:ILE:HG22	3:B:2525:GLY:HA3	1.95	0.47
3:A:3624:LEU:HD23	3:A:3628:ARG:HG2	1.96	0.47
3:C:1110:ARG:HG2	3:C:1110:ARG:HH11	1.80	0.47
3:C:2697:ARG:HH11	3:C:2697:ARG:HG2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2781:VAL:HG12	3:C:2789:PRO:HD3	1.96	0.47
3:C:4056:GLU:HG2	3:C:4166:LEU:HD13	1.96	0.47
3:D:893:TYR:H	3:D:961:MET:HE1	1.80	0.47
3:D:2470:ILE:HG22	3:D:2525:GLY:HA3	1.96	0.47
3:D:3588:ASP:OD1	3:D:3589:PRO:HD2	2.15	0.47
3:B:2599:GLN:O	3:B:2603:ILE:HG13	2.15	0.47
1:H:49:ARG:HH21	1:H:52:LYS:HE2	1.79	0.47
3:A:3548:GLU:O	3:A:3551:GLU:HG2	2.15	0.47
3:A:4218:ILE:O	3:A:4222:VAL:HG23	2.15	0.47
3:D:2599:GLN:O	3:D:2603:ILE:HG13	2.15	0.47
3:D:4056:GLU:HG2	3:D:4166:LEU:HD13	1.97	0.47
3:B:3568:SER:O	3:B:3572:GLN:HG3	2.15	0.47
3:A:2440:MET:O	3:A:2444:GLN:HG3	2.15	0.47
3:A:3545:THR:OG1	3:A:3548:GLU:HG3	2.15	0.47
3:C:1152:MET:HB3	3:C:1223:PHE:CE2	2.50	0.47
3:C:1986:MET:HE2	3:C:1991:THR:OG1	2.15	0.47
3:D:4984:ASN:HB3	3:D:4987:ASN:HB2	1.97	0.47
1:E:23:VAL:HG22	1:E:47:LYS:HG2	1.97	0.46
1:G:23:VAL:HG22	1:G:47:LYS:HG2	1.96	0.46
3:C:2599:GLN:O	3:C:2603:ILE:HG13	2.15	0.46
3:C:3768:SER:HA	3:C:3771:HIS:ND1	2.29	0.46
3:C:4678:ALA:HB1	3:C:4720:VAL:HG21	1.97	0.46
3:C:4984:ASN:HB3	3:C:4987:ASN:HB2	1.97	0.46
3:D:4678:ALA:HB1	3:D:4720:VAL:HG21	1.96	0.46
3:B:2312:MET:O	3:B:2316:LYS:HG2	2.15	0.46
3:B:2777:TYR:HB2	3:B:2791:LEU:HB3	1.97	0.46
3:A:1079:LYS:HA	3:A:1189:LEU:HD11	1.97	0.46
3:A:1993:ARG:O	3:A:1996:ARG:HG2	2.15	0.46
3:C:4218:ILE:O	3:C:4222:VAL:HG23	2.15	0.46
3:D:1110:ARG:HG2	3:D:1110:ARG:HH11	1.81	0.46
3:D:1152:MET:HB3	3:D:1223:PHE:CE2	2.50	0.46
3:D:4547:GLN:O	3:D:4550:LYS:HG3	2.15	0.46
3:B:893:TYR:H	3:B:961:MET:HE1	1.80	0.46
3:B:2700:MET:HE3	3:B:2700:MET:HB3	1.80	0.46
3:C:1505:GLN:HA	3:C:1508:ARG:HH21	1.80	0.46
3:A:2790:MET:HE3	3:A:2801:ASP:HB3	1.97	0.46
3:D:834:PRO:O	3:D:835:ARG:HG2	2.16	0.46
3:D:1093:GLU:HG3	3:D:1148:VAL:HG22	1.98	0.46
3:D:2359:ARG:HA	3:D:2359:ARG:HD3	1.72	0.46
3:B:3327:LEU:HD21	3:B:3408:LEU:HD11	1.97	0.46
3:A:2677:LYS:HB3	3:A:2677:LYS:HE3	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4156:HIS:HA	3:C:4161:ARG:HH22	1.79	0.46
3:D:1993:ARG:O	3:D:1996:ARG:HG2	2.15	0.46
3:B:1230:MET:HE3	3:B:1827:ARG:HB2	1.98	0.46
3:B:2697:ARG:HG2	3:B:2697:ARG:HH11	1.80	0.46
3:B:3548:GLU:O	3:B:3551:GLU:HG2	2.16	0.46
2:J:72:MET:HA	2:J:72:MET:HE2	1.97	0.46
3:A:2470:ILE:HG22	3:A:2525:GLY:HA3	1.97	0.46
3:A:2599:GLN:O	3:A:2603:ILE:HG13	2.15	0.46
3:D:1230:MET:HE3	3:D:1827:ARG:HB2	1.98	0.46
3:D:2161:GLN:HE21	3:D:2177:LEU:CD1	2.27	0.46
3:D:3035:GLU:HA	3:D:3038:MET:HE3	1.96	0.46
3:D:3568:SER:O	3:D:3572:GLN:HG3	2.15	0.46
2:K:13:LYS:HG2	3:C:2189:LYS:HB3	1.96	0.46
3:A:1152:MET:HB3	3:A:1223:PHE:CE2	2.50	0.46
3:A:3568:SER:O	3:A:3572:GLN:HG3	2.15	0.46
3:C:2890:LYS:HA	3:C:2890:LYS:HD2	1.78	0.46
3:D:3629:ARG:H	3:D:3629:ARG:HG2	1.63	0.46
3:B:1438:ARG:HB3	3:B:1563:GLN:HG2	1.98	0.46
3:B:2440:MET:O	3:B:2444:GLN:HG3	2.15	0.46
3:A:2777:TYR:HB2	3:A:2791:LEU:HB3	1.97	0.46
3:A:3179:LYS:NZ	3:A:3187:ARG:HH21	2.13	0.46
3:C:2165:LEU:HD21	3:C:2177:LEU:HD23	1.98	0.46
3:C:3082:LYS:HA	3:C:3082:LYS:HD3	1.73	0.46
3:D:2440:MET:O	3:D:2444:GLN:HG3	2.15	0.46
3:D:3361:THR:HG21	3:D:3408:LEU:HD22	1.98	0.46
3:D:3548:GLU:O	3:D:3551:GLU:HG2	2.16	0.46
3:A:3528:THR:HG23	3:A:3573:MET:SD	2.56	0.46
3:A:4014:LYS:HG2	3:A:4135:PRO:HB3	1.97	0.46
2:I:109:MET:HE3	2:I:109:MET:HB3	1.80	0.46
3:A:834:PRO:O	3:A:835:ARG:HG2	2.16	0.46
3:A:893:TYR:N	3:A:961:MET:HE3	2.31	0.46
3:A:2312:MET:O	3:A:2316:LYS:HG2	2.16	0.46
3:C:3626:LYS:HD2	3:C:3626:LYS:O	2.15	0.46
3:C:3965:LEU:O	3:C:3969:ILE:HG12	2.15	0.46
3:C:3974:THR:O	3:C:3978:GLN:HG2	2.16	0.46
3:D:1291:LEU:HD13	3:D:1595:LEU:HD11	1.97	0.46
3:B:3965:LEU:O	3:B:3969:ILE:HG12	2.15	0.46
3:B:4218:ILE:O	3:B:4222:VAL:HG23	2.15	0.46
3:C:834:PRO:O	3:C:835:ARG:HG2	2.16	0.45
3:C:1230:MET:HE3	3:C:1827:ARG:HB2	1.98	0.45
3:C:2440:MET:O	3:C:2444:GLN:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1505:GLN:HA	3:B:1508:ARG:HH21	1.80	0.45
3:A:345:LEU:HB3	3:A:387:ALA:HB1	1.97	0.45
3:A:2885:THR:HA	3:A:2888:ARG:CD	2.46	0.45
3:A:4047:MET:HE3	3:A:4047:MET:HB3	1.87	0.45
3:C:2128:TYR:CG	3:C:3673:MET:HE3	2.51	0.45
3:C:3980:LEU:HD13	3:C:3985:LEU:HD22	1.98	0.45
3:D:1986:MET:HE2	3:D:1991:THR:OG1	2.16	0.45
3:A:2886:TRP:CZ3	3:A:2904:LEU:HD12	2.52	0.45
3:C:4161:ARG:HA	3:C:4164:LEU:HD12	1.97	0.45
3:D:2885:THR:HA	3:D:2888:ARG:HD2	1.97	0.45
3:D:3362:ILE:HB	3:D:3437:MET:HE3	1.99	0.45
3:D:3719:ASP:HB3	3:D:3722:TYR:HB3	1.98	0.45
3:A:2012:PHE:CZ	3:A:2031:LEU:HD23	2.52	0.45
3:C:939:VAL:HG22	3:C:1053:ILE:HG12	1.99	0.45
3:C:3548:GLU:O	3:C:3551:GLU:HG2	2.16	0.45
3:D:2912:THR:HG21	3:D:2914:LYS:HE3	1.99	0.45
3:D:3081:MET:HE3	3:D:3092:LEU:HD23	1.99	0.45
3:B:1110:ARG:HG2	3:B:1110:ARG:HH11	1.81	0.45
3:B:2781:VAL:HG12	3:B:2789:PRO:HD3	1.97	0.45
1:F:84:ALA:O	1:F:93:PRO:HB3	2.17	0.45
2:K:36:MET:SD	2:K:72:MET:HE1	2.56	0.45
3:A:1986:MET:HE2	3:A:1991:THR:OG1	2.17	0.45
3:A:2604:GLU:HG2	3:A:2639:MET:HG3	1.99	0.45
3:D:3104:GLU:OE1	3:D:3167:ARG:HB3	2.16	0.45
3:D:3509:LEU:HD23	3:D:3509:LEU:HA	1.82	0.45
3:B:1243:PRO:HA	3:B:1601:MET:O	2.17	0.45
3:B:5009:TYR:CE1	3:B:5013:MET:HE3	2.52	0.45
1:G:49:ARG:HH21	1:G:52:LYS:HE2	1.80	0.45
3:A:2313:LEU:HD21	3:A:2416:VAL:HG11	1.99	0.45
3:A:2942:LYS:HG2	3:A:2943:ASP:N	2.32	0.45
3:C:215:THR:HG22	3:C:273:HIS:HA	1.98	0.45
3:C:1194:LEU:HB3	3:C:1198:GLN:HB2	1.98	0.45
3:C:1438:ARG:HB3	3:C:1563:GLN:HG2	1.98	0.45
3:C:2608:MET:HE2	3:C:2639:MET:HG2	1.98	0.45
3:B:2012:PHE:CZ	3:B:2031:LEU:HD23	2.52	0.45
3:B:2638:LYS:HD2	3:B:2698:MET:HG3	1.99	0.45
3:C:2604:GLU:HG2	3:C:2639:MET:HG3	1.98	0.45
3:C:4014:LYS:HG2	3:C:4135:PRO:HB3	1.98	0.45
3:D:2012:PHE:CZ	3:D:2031:LEU:HD23	2.52	0.45
3:D:2569:PHE:CE1	3:D:2582:MET:HE1	2.52	0.45
3:D:2928:LYS:O	3:D:2932:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3528:THR:HG23	3:D:3573:MET:SD	2.56	0.45
3:B:2128:TYR:CG	3:B:3673:MET:HE3	2.52	0.45
3:B:2885:THR:HA	3:B:2888:ARG:CD	2.47	0.45
3:A:3569:LEU:O	3:A:3573:MET:HG2	2.17	0.45
3:C:3604:TYR:O	3:C:3607:GLU:HG2	2.17	0.45
3:C:4047:MET:HE3	3:C:4047:MET:HB3	1.91	0.45
3:D:2128:TYR:CG	3:D:3673:MET:HE3	2.51	0.45
3:B:3312:LEU:HD22	3:B:3348:ARG:HG3	1.98	0.45
3:A:866:HIS:CD2	3:A:866:HIS:H	2.35	0.45
3:C:1980:LEU:HD21	3:C:1994:ARG:HG3	1.98	0.45
3:C:3223:SER:OG	3:C:3225:ARG:HG2	2.16	0.45
3:D:892:THR:HG23	3:D:903:LEU:HD23	1.98	0.45
3:D:2240:CYS:SG	3:D:2250:MET:HG3	2.57	0.45
3:D:3625:SER:O	3:D:3629:ARG:HG2	2.17	0.45
3:A:1435:TYR:HB3	3:A:1575:LEU:HG	1.99	0.45
3:A:2161:GLN:HE21	3:A:2177:LEU:HD11	1.81	0.45
3:A:2765:LYS:HA	3:A:2765:LYS:HD3	1.61	0.45
3:A:3223:SER:OG	3:A:3225:ARG:HG2	2.17	0.45
3:A:3626:LYS:HD2	3:A:3626:LYS:O	2.16	0.45
3:C:2012:PHE:CZ	3:C:2031:LEU:HD23	2.52	0.45
3:C:2716:ASP:HB3	3:C:2719:TYR:HB2	1.99	0.45
3:C:4567:LEU:HD13	3:C:4815:ASP:HB3	1.99	0.45
3:D:1438:ARG:HB3	3:D:1563:GLN:HG2	1.99	0.45
3:B:1653:LEU:HD23	3:B:1707:LEU:HD11	1.98	0.45
3:C:1243:PRO:HA	3:C:1601:MET:O	2.16	0.44
3:C:1561:VAL:HG12	3:C:1562:ILE:HG23	1.98	0.44
3:D:1435:TYR:HB3	3:D:1575:LEU:HG	1.99	0.44
3:D:1653:LEU:HD23	3:D:1707:LEU:HD11	1.99	0.44
3:D:2661:TRP:CD1	3:D:2662:ALA:H	2.35	0.44
3:B:1194:LEU:HB3	3:B:1198:GLN:HB2	1.99	0.44
3:B:1435:TYR:HB3	3:B:1575:LEU:HG	1.99	0.44
3:B:2679:PHE:HB2	3:B:2706:ILE:HG21	1.99	0.44
3:B:4161:ARG:O	3:B:4165:GLU:HG3	2.17	0.44
1:E:25:HIS:CD2	1:E:104:LEU:HD11	2.52	0.44
1:E:84:ALA:O	1:E:93:PRO:HB3	2.17	0.44
3:A:1653:LEU:HD23	3:A:1707:LEU:HD11	1.99	0.44
3:A:3557:LEU:HD23	3:A:3557:LEU:HA	1.87	0.44
3:C:3604:TYR:HE2	3:C:3608:GLN:NE2	2.15	0.44
3:C:3629:ARG:H	3:C:3629:ARG:HG2	1.65	0.44
3:C:3776:ALA:HB1	3:C:3816:MET:HG3	1.99	0.44
3:D:954:LYS:HA	3:D:954:LYS:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4968:PHE:O	3:D:4974:GLY:HA3	2.17	0.44
1:G:84:ALA:O	1:G:93:PRO:HB3	2.17	0.44
3:A:3951:PHE:O	3:A:3955:MET:HG3	2.17	0.44
3:A:4091:LYS:O	3:A:4095:LYS:HG2	2.17	0.44
3:C:2886:TRP:CZ3	3:C:2904:LEU:HD12	2.53	0.44
3:C:2942:LYS:HG2	3:C:2943:ASP:N	2.33	0.44
3:D:636:ASN:HB2	3:D:702:TRP:CZ3	2.53	0.44
3:D:3285:TRP:CE2	3:D:3348:ARG:HD2	2.52	0.44
3:D:4157:ASP:O	3:D:4161:ARG:HG2	2.17	0.44
3:B:892:THR:HG23	3:B:903:LEU:HD23	1.98	0.44
3:B:2716:ASP:HB3	3:B:2719:TYR:HB2	1.99	0.44
3:B:3361:THR:HG21	3:B:3408:LEU:HD22	2.00	0.44
3:B:3414:ARG:HA	3:B:3414:ARG:HD3	1.63	0.44
3:B:3588:ASP:OD2	3:B:3589:PRO:HD2	2.17	0.44
3:B:3980:LEU:HD13	3:B:3985:LEU:HD22	1.99	0.44
3:A:636:ASN:HB2	3:A:702:TRP:CZ3	2.52	0.44
3:A:1243:PRO:HA	3:A:1601:MET:O	2.17	0.44
3:A:1438:ARG:HB3	3:A:1563:GLN:HG2	1.98	0.44
3:A:4968:PHE:O	3:A:4974:GLY:HA3	2.17	0.44
3:C:636:ASN:HB2	3:C:702:TRP:CZ3	2.53	0.44
3:C:866:HIS:CD2	3:C:866:HIS:H	2.35	0.44
3:C:2485:LEU:HD23	3:C:2485:LEU:HA	1.76	0.44
3:C:3588:ASP:O	3:C:3592:ILE:HG13	2.18	0.44
3:B:834:PRO:O	3:B:835:ARG:HG2	2.16	0.44
3:B:1093:GLU:HG3	3:B:1148:VAL:HG22	1.99	0.44
3:B:1986:MET:HE2	3:B:1991:THR:OG1	2.16	0.44
3:B:2677:LYS:HB3	3:B:2677:LYS:HE3	1.49	0.44
3:B:3081:MET:HE3	3:B:3092:LEU:HD23	2.00	0.44
3:B:3223:SER:OG	3:B:3225:ARG:HG2	2.17	0.44
3:B:3569:LEU:O	3:B:3573:MET:HG2	2.17	0.44
3:B:4156:HIS:HA	3:B:4161:ARG:HH22	1.81	0.44
3:B:4567:LEU:HD13	3:B:4815:ASP:HB3	1.99	0.44
3:B:4984:ASN:HB3	3:B:4987:ASN:HB2	1.99	0.44
1:F:44:LYS:HB3	1:F:44:LYS:HE3	1.70	0.44
1:H:25:HIS:CD2	1:H:104:LEU:HD11	2.52	0.44
2:I:92:PHE:HE2	2:I:108:VAL:HB	1.83	0.44
3:A:2128:TYR:CG	3:A:3673:MET:HE3	2.53	0.44
3:A:2485:LEU:HA	3:A:2485:LEU:HD23	1.79	0.44
3:A:2520:HIS:O	3:A:2524:VAL:HG22	2.17	0.44
3:C:1435:TYR:HB3	3:C:1575:LEU:HG	1.99	0.44
3:C:2312:MET:O	3:C:2316:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2912:THR:HG21	3:C:2914:LYS:HE3	1.99	0.44
3:C:4581:LYS:HD2	3:C:4633:GLU:HB2	1.99	0.44
3:D:2520:HIS:O	3:D:2524:VAL:HG22	2.17	0.44
3:D:2700:MET:SD	3:D:3004:PRO:HB2	2.57	0.44
3:B:2024:PRO:HD2	3:B:2027:ILE:HD12	1.99	0.44
3:C:638:ILE:HD11	3:C:1636:MET:HE2	2.00	0.44
3:D:2942:LYS:HG2	3:D:2943:ASP:N	2.33	0.44
3:B:3528:THR:HG23	3:B:3573:MET:SD	2.57	0.44
3:A:537:CYS:HB3	3:A:571:SER:HB2	1.99	0.44
3:A:2024:PRO:HD2	3:A:2027:ILE:HD12	1.99	0.44
3:C:3362:ILE:HB	3:C:3437:MET:HE3	1.99	0.44
3:D:486:LEU:HD12	3:D:486:LEU:HA	1.87	0.44
3:D:939:VAL:HG22	3:D:1053:ILE:HG12	1.99	0.44
3:D:3630:ARG:HH12	3:D:3860:ASN:HA	1.83	0.44
3:D:3980:LEU:HD13	3:D:3985:LEU:HD22	2.00	0.44
3:B:2942:LYS:HG2	3:B:2943:ASP:N	2.33	0.44
3:B:4678:ALA:HB1	3:B:4720:VAL:HG21	1.99	0.44
3:A:3003:LEU:HB2	3:A:3004:PRO:HD3	2.00	0.44
3:A:3034:LYS:HE3	3:A:3034:LYS:HB3	1.63	0.44
3:C:2677:LYS:HB3	3:C:2677:LYS:HE3	1.50	0.44
3:D:1243:PRO:HA	3:D:1601:MET:O	2.17	0.44
3:D:3569:LEU:O	3:D:3573:MET:HG2	2.16	0.44
3:B:215:THR:HG22	3:B:273:HIS:HA	2.00	0.44
3:B:4879:MET:HE3	3:B:4879:MET:HB3	1.89	0.44
1:E:44:LYS:HB3	1:E:44:LYS:HE3	1.75	0.44
1:E:52:LYS:HB3	1:E:52:LYS:HE3	1.77	0.44
2:J:92:PHE:HE2	2:J:108:VAL:HB	1.83	0.44
2:L:109:MET:HE3	2:L:109:MET:HB3	1.78	0.44
3:A:1436:SER:OG	3:A:1565:GLU:HB2	2.18	0.44
3:A:1530:THR:HG22	3:A:1535:GLU:HA	2.00	0.44
3:A:5009:TYR:CE1	3:A:5013:MET:HE3	2.53	0.44
3:C:2370:GLY:O	3:D:129:ASP:HA	2.18	0.44
3:C:2679:PHE:HB2	3:C:2706:ILE:HG21	1.99	0.44
3:D:2604:GLU:HG2	3:D:2639:MET:HG3	2.00	0.44
3:B:537:CYS:HB3	3:B:571:SER:HB2	2.00	0.44
3:B:939:VAL:HG22	3:B:1053:ILE:HG12	2.00	0.44
2:K:109:MET:HE3	2:K:109:MET:HB3	1.83	0.43
3:A:2700:MET:SD	3:A:3004:PRO:HB2	2.58	0.43
3:A:4984:ASN:HB3	3:A:4987:ASN:HB2	2.00	0.43
3:C:893:TYR:N	3:C:961:MET:HE1	2.33	0.43
3:C:4968:PHE:O	3:C:4974:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:19:GLU:HB3	3:D:205:ILE:HB	2.00	0.43
3:D:345:LEU:HB3	3:D:387:ALA:HB1	2.00	0.43
3:D:2781:VAL:HG12	3:D:2789:PRO:HD3	2.00	0.43
3:D:3223:SER:OG	3:D:3225:ARG:HG2	2.18	0.43
3:D:3368:ARG:HG2	3:D:3401:LEU:HD13	2.00	0.43
3:D:4156:HIS:HA	3:D:4161:ARG:NH2	2.32	0.43
3:B:2912:THR:HG21	3:B:2914:LYS:HE3	1.99	0.43
2:K:37:ARG:HH21	2:K:43:PRO:HB3	1.83	0.43
2:K:72:MET:HE2	2:K:72:MET:HA	1.99	0.43
3:A:2908:TYR:CE2	3:A:2916:LYS:HD3	2.52	0.43
3:C:1653:LEU:HD23	3:C:1707:LEU:HD11	1.99	0.43
3:D:4218:ILE:O	3:D:4222:VAL:HG23	2.18	0.43
3:B:2661:TRP:CD1	3:B:2662:ALA:H	2.37	0.43
3:B:3184:GLU:HG2	3:B:3187:ARG:HH12	1.82	0.43
3:B:3629:ARG:H	3:B:3629:ARG:HG2	1.61	0.43
3:A:121:LEU:HD12	3:A:134:ASP:HB3	2.00	0.43
3:A:2638:LYS:HD3	3:A:2638:LYS:HA	1.75	0.43
3:A:3331:GLU:OE1	3:A:3331:GLU:N	2.51	0.43
3:A:4821:LYS:HE2	3:A:4821:LYS:HB3	1.86	0.43
3:D:904:HIS:HB3	3:D:907:LEU:HD13	1.99	0.43
3:D:3023:LYS:HB2	3:D:3023:LYS:HE2	1.91	0.43
3:D:4026:MET:HE2	3:D:4026:MET:HB3	1.83	0.43
3:D:4952:GLU:O	3:D:4956:THR:HG23	2.18	0.43
3:B:2364:PHE:HB3	3:B:2368:LEU:HB2	2.00	0.43
3:B:3362:ILE:HB	3:B:3437:MET:HE3	1.99	0.43
3:B:4989:MET:HE3	3:B:4993:MET:HE2	1.99	0.43
3:A:933:LEU:HD23	3:A:933:LEU:HA	1.84	0.43
3:A:2001:PRO:O	3:A:2005:GLN:HG3	2.18	0.43
3:A:2370:GLY:O	3:B:129:ASP:HA	2.18	0.43
3:C:908:VAL:HG22	3:C:909:ASN:H	1.83	0.43
3:C:2024:PRO:HD2	3:C:2027:ILE:HD12	1.99	0.43
3:C:2765:LYS:HA	3:C:2765:LYS:HD3	1.58	0.43
3:C:4952:GLU:O	3:C:4956:THR:HG23	2.18	0.43
3:D:663:TYR:HD1	3:D:747:CYS:SG	2.41	0.43
3:D:2024:PRO:HD2	3:D:2027:ILE:HD12	2.00	0.43
3:D:2530:MET:HB3	3:D:2585:THR:HG21	2.01	0.43
3:D:2679:PHE:HB2	3:D:2706:ILE:HG21	2.00	0.43
3:D:4007:SER:C	3:D:4009:GLN:H	2.25	0.43
3:B:1423:ASP:HB2	3:B:1426:ILE:HD12	2.00	0.43
2:J:5:THR:OG1	2:J:8:GLN:HG3	2.19	0.43
3:A:107:ILE:HG23	3:A:150:MET:HE2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4952:GLU:O	3:A:4956:THR:HG23	2.18	0.43
3:C:1436:SER:OG	3:C:1565:GLU:HB2	2.19	0.43
3:C:3414:ARG:HA	3:C:3414:ARG:HD3	1.64	0.43
3:D:951:LYS:HB2	3:D:951:LYS:HE3	1.69	0.43
3:D:2766:TRP:CZ3	3:D:2790:MET:HG2	2.53	0.43
3:D:2872:GLN:O	3:D:2876:GLU:HG2	2.19	0.43
3:B:866:HIS:CD2	3:B:866:HIS:H	2.35	0.43
3:B:2170:MET:HE2	3:B:2174:GLU:HB3	2.00	0.43
3:B:4968:PHE:O	3:B:4974:GLY:HA3	2.18	0.43
1:H:14:THR:HG22	1:H:106:LEU:HD12	2.01	0.43
1:H:84:ALA:O	1:H:93:PRO:HB3	2.18	0.43
2:I:5:THR:OG1	2:I:8:GLN:HG3	2.19	0.43
3:A:2536:LEU:HD22	3:A:2541:PHE:HB3	2.00	0.43
3:C:486:LEU:HD12	3:C:486:LEU:HA	1.87	0.43
3:C:2515:GLN:O	3:C:2519:LEU:HG	2.19	0.43
3:C:4091:LYS:HE2	3:C:4091:LYS:HB2	1.77	0.43
3:C:5013:MET:HE2	3:C:5018:CYS:HB3	2.00	0.43
3:D:1617:THR:HG22	3:D:1628:VAL:HG13	2.01	0.43
3:D:4648:LEU:HD23	3:D:4803:HIS:CE1	2.51	0.43
3:B:2212:VAL:HG21	3:B:2256:TYR:CZ	2.52	0.43
3:B:3104:GLU:OE1	3:B:3167:ARG:HB3	2.18	0.43
2:K:31:GLU:HA	2:K:34:THR:HG22	2.00	0.43
3:A:2597:LYS:H	3:A:2597:LYS:HD3	1.84	0.43
3:C:1423:ASP:HB2	3:C:1426:ILE:HD12	2.00	0.43
3:C:2874:MET:HE3	3:C:2874:MET:HB2	1.95	0.43
3:C:3034:LYS:HA	3:C:3034:LYS:HD2	1.81	0.43
3:D:866:HIS:H	3:D:866:HIS:CD2	2.35	0.43
3:D:2214:VAL:HG21	3:D:2228:MET:SD	2.59	0.43
3:B:636:ASN:HB2	3:B:702:TRP:CZ3	2.53	0.43
3:B:3003:LEU:HB2	3:B:3004:PRO:HD3	2.01	0.43
3:C:653:ALA:HB3	3:C:656:SER:HB2	2.00	0.43
3:C:2885:THR:HA	3:C:2888:ARG:CD	2.49	0.43
3:C:3546:ASP:HB3	3:C:3550:ARG:HH21	1.84	0.43
3:C:4218:ILE:HD13	3:C:4218:ILE:HA	1.92	0.43
3:D:2885:THR:HA	3:D:2888:ARG:CD	2.48	0.43
3:B:663:TYR:HD1	3:B:747:CYS:SG	2.41	0.43
3:B:2700:MET:SD	3:B:3004:PRO:HB2	2.59	0.43
3:B:2782:ASP:HB3	3:B:2785:LEU:HG	2.01	0.43
3:B:3082:LYS:HD3	3:B:3082:LYS:HA	1.57	0.43
3:B:3720:TYR:HA	3:B:3723:MET:HE2	2.01	0.43
3:A:653:ALA:HB3	3:A:656:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:LEU:HD12	3:C:134:ASP:HB3	2.00	0.43
3:C:1634:LEU:HD23	3:C:1634:LEU:HA	1.93	0.43
3:C:2520:HIS:O	3:C:2524:VAL:HG22	2.19	0.43
3:C:2661:TRP:CD1	3:C:2662:ALA:H	2.36	0.43
3:D:638:ILE:HD11	3:D:1636:MET:HE2	2.00	0.43
3:B:407:THR:HG21	3:B:448:LEU:HD11	2.01	0.43
3:B:1617:THR:HG22	3:B:1628:VAL:HG13	2.01	0.43
3:B:2111:VAL:HG21	3:B:2120:MET:HE1	2.00	0.43
3:B:3082:LYS:HE2	3:B:3155:ASP:HB3	2.01	0.43
3:B:4242:ILE:HG13	3:B:4989:MET:HE1	1.99	0.43
3:B:4952:GLU:O	3:B:4956:THR:HG23	2.18	0.43
3:A:3092:LEU:HD12	3:A:3092:LEU:HA	1.89	0.43
3:C:107:ILE:HG23	3:C:150:MET:HE2	2.01	0.43
3:C:345:LEU:HB3	3:C:387:ALA:HB1	2.00	0.43
3:C:904:HIS:CE1	3:C:906:CYS:HB2	2.54	0.43
3:C:1093:GLU:HG3	3:C:1148:VAL:HG22	1.99	0.43
3:C:2697:ARG:HG2	3:C:2697:ARG:NH1	2.33	0.43
3:C:3179:LYS:NZ	3:C:3187:ARG:HH21	2.17	0.43
3:D:695:TYR:CD2	3:D:1240:LYS:HD2	2.54	0.43
3:D:1986:MET:HG2	3:D:1990:GLU:OE2	2.19	0.43
3:D:2364:PHE:HB3	3:D:2368:LEU:HB2	2.01	0.43
3:D:2965:ARG:NH1	3:D:2969:ILE:HD11	2.34	0.43
3:B:3354:LEU:HB2	3:B:3415:TYR:HE2	1.83	0.43
1:E:14:THR:HG22	1:E:106:LEU:HD12	2.01	0.42
1:F:25:HIS:CD2	1:F:104:LEU:HD11	2.53	0.42
2:I:20:ASP:OD2	2:I:20:ASP:C	2.62	0.42
2:L:20:ASP:OD2	2:L:20:ASP:C	2.62	0.42
3:A:129:ASP:HA	3:D:2370:GLY:O	2.19	0.42
3:A:663:TYR:HD1	3:A:747:CYS:SG	2.42	0.42
3:A:908:VAL:HG22	3:A:909:ASN:N	2.34	0.42
3:A:1821:ASP:OD2	3:A:1821:ASP:C	2.62	0.42
3:A:2782:ASP:HB3	3:A:2785:LEU:HG	2.00	0.42
3:A:3368:ARG:HG2	3:A:3401:LEU:HD13	2.01	0.42
3:C:537:CYS:HB3	3:C:571:SER:HB2	2.01	0.42
3:C:1997:GLU:HA	3:C:2008:MET:HE1	2.00	0.42
3:D:3545:THR:OG1	3:D:3548:GLU:HG3	2.19	0.42
3:B:19:GLU:HB3	3:B:205:ILE:HB	2.01	0.42
3:B:957:LYS:HB2	3:B:957:LYS:HE3	1.77	0.42
3:B:3546:ASP:HB3	3:B:3550:ARG:HH21	1.84	0.42
3:B:4547:GLN:O	3:B:4550:LYS:HG3	2.19	0.42
1:G:68:LEU:HD23	1:G:106:LEU:HG	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1005:TRP:HA	3:A:1016:ARG:HB3	2.01	0.42
3:A:1455:PRO:HG3	3:A:1549:PHE:HE1	1.84	0.42
3:A:2716:ASP:HB3	3:A:2719:TYR:HB2	2.01	0.42
3:A:3362:ILE:HB	3:A:3437:MET:HE3	2.01	0.42
3:A:3719:ASP:HB3	3:A:3722:TYR:HB3	2.01	0.42
3:C:2782:ASP:HB3	3:C:2785:LEU:HG	2.01	0.42
3:C:2891:LYS:NZ	3:C:2905:LEU:HD23	2.34	0.42
3:C:3023:LYS:HB2	3:C:3023:LYS:HE2	1.91	0.42
3:C:4648:LEU:HD23	3:C:4803:HIS:CE1	2.51	0.42
3:D:950:LEU:HD23	3:D:950:LEU:HA	1.91	0.42
3:D:3546:ASP:HB3	3:D:3550:ARG:HH21	1.84	0.42
3:D:4689:THR:HG22	3:D:4732:PHE:CZ	2.54	0.42
3:B:107:ILE:HG23	3:B:150:MET:HE2	2.01	0.42
3:B:2638:LYS:HD3	3:B:2638:LYS:HA	1.75	0.42
1:G:25:HIS:CD2	1:G:104:LEU:HD11	2.53	0.42
3:A:638:ILE:HD11	3:A:1636:MET:HE2	2.00	0.42
3:C:695:TYR:CD2	3:C:1240:LYS:HD2	2.54	0.42
3:C:2872:GLN:O	3:C:2876:GLU:HG2	2.19	0.42
3:C:3003:LEU:HB2	3:C:3004:PRO:HD3	2.01	0.42
3:C:3550:ARG:HH11	3:C:3594:ARG:HH22	1.67	0.42
3:D:1455:PRO:HG3	3:D:1549:PHE:HE1	1.84	0.42
3:D:2208:MET:HE1	3:D:2253:HIS:ND1	2.34	0.42
3:D:3354:LEU:HB2	3:D:3415:TYR:HE2	1.83	0.42
3:D:3626:LYS:NZ	3:D:3630:ARG:HB2	2.35	0.42
3:B:345:LEU:HB3	3:B:387:ALA:HB1	2.00	0.42
3:B:653:ALA:HB3	3:B:656:SER:HB2	2.01	0.42
3:B:904:HIS:HB3	3:B:907:LEU:HD13	2.00	0.42
3:B:1008:SER:HB3	3:B:1017:ARG:HB3	2.02	0.42
3:B:2697:ARG:HG2	3:B:2697:ARG:NH1	2.33	0.42
3:A:2128:TYR:CD1	3:A:3673:MET:HE3	2.54	0.42
3:A:2776:SER:OG	3:A:2787:THR:HG22	2.18	0.42
3:A:2785:LEU:HD12	3:A:2787:THR:H	1.84	0.42
3:A:3354:LEU:HB2	3:A:3415:TYR:HE2	1.84	0.42
3:C:19:GLU:HB3	3:C:205:ILE:HB	2.00	0.42
3:C:892:THR:HG23	3:C:903:LEU:HD23	1.99	0.42
3:C:2001:PRO:O	3:C:2005:GLN:HG3	2.19	0.42
3:C:2536:LEU:HD22	3:C:2541:PHE:HB3	2.02	0.42
3:C:3104:GLU:OE1	3:C:3167:ARG:HB3	2.20	0.42
3:D:215:THR:HG22	3:D:273:HIS:HA	2.01	0.42
3:D:537:CYS:HB3	3:D:571:SER:HB2	2.00	0.42
3:D:3626:LYS:HZ3	3:D:3630:ARG:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2766:TRP:CZ3	3:B:2790:MET:HG2	2.54	0.42
3:B:3092:LEU:HD12	3:B:3092:LEU:HA	1.91	0.42
3:B:3723:MET:HE2	3:B:3723:MET:HB2	1.85	0.42
3:A:486:LEU:HD12	3:A:486:LEU:HA	1.87	0.42
3:A:695:TYR:CD2	3:A:1240:LYS:HD2	2.54	0.42
3:A:2869:ARG:HA	3:A:2869:ARG:HD3	1.78	0.42
3:A:4157:ASP:O	3:A:4161:ARG:HG2	2.20	0.42
9:A:5201:HOH:O	3:B:76:ARG:HD2	2.20	0.42
3:C:590:LEU:HD13	3:C:599:VAL:HB	2.01	0.42
3:C:663:TYR:HD1	3:C:747:CYS:SG	2.41	0.42
3:D:3179:LYS:NZ	3:D:3187:ARG:HH21	2.18	0.42
3:D:3720:TYR:HA	3:D:3723:MET:HE2	2.01	0.42
3:B:1436:SER:OG	3:B:1565:GLU:HB2	2.19	0.42
3:B:2536:LEU:HD22	3:B:2541:PHE:HB3	2.02	0.42
3:B:2604:GLU:HG2	3:B:2639:MET:HG3	2.02	0.42
3:A:407:THR:HG21	3:A:448:LEU:HD11	2.02	0.42
3:A:2212:VAL:HG11	3:A:2256:TYR:OH	2.19	0.42
3:A:3564:GLU:HA	3:A:3570:ARG:HH22	1.85	0.42
3:A:3575:LEU:HD23	3:A:3575:LEU:HA	1.91	0.42
3:C:683:ARG:HG2	3:C:717:ASP:HB3	2.01	0.42
3:C:2330:ARG:H	3:C:2330:ARG:HG2	1.65	0.42
3:C:2766:TRP:CZ3	3:C:2790:MET:HG2	2.55	0.42
3:D:683:ARG:HG2	3:D:717:ASP:HB3	2.02	0.42
3:D:3003:LEU:HB2	3:D:3004:PRO:HD3	2.01	0.42
3:D:3588:ASP:O	3:D:3592:ILE:HG13	2.20	0.42
3:B:664:PHE:CE1	3:B:746:CYS:HB2	2.55	0.42
3:B:695:TYR:CD2	3:B:1240:LYS:HD2	2.54	0.42
3:B:4188:ARG:HA	3:B:4188:ARG:HD2	1.88	0.42
1:F:52:LYS:HB3	1:F:52:LYS:HE3	1.78	0.42
2:I:19:PHE:CD2	2:I:35:VAL:HG22	2.54	0.42
2:J:63:ILE:HD12	2:J:68:PHE:HB2	2.02	0.42
3:A:1093:GLU:HG3	3:A:1148:VAL:HG22	2.01	0.42
3:A:2490:MET:HE3	3:A:2490:MET:HB3	1.84	0.42
3:A:4879:MET:HE3	3:A:4879:MET:HB3	1.84	0.42
3:C:2700:MET:HE3	3:C:2700:MET:HB3	1.80	0.42
3:C:2700:MET:SD	3:C:3004:PRO:HB2	2.59	0.42
3:D:590:LEU:HD13	3:D:599:VAL:HB	2.01	0.42
3:D:664:PHE:CE1	3:D:746:CYS:HB2	2.55	0.42
3:D:3092:LEU:HD12	3:D:3092:LEU:HA	1.91	0.42
3:B:590:LEU:HD13	3:B:599:VAL:HB	2.01	0.42
3:B:2886:TRP:CZ3	3:B:2904:LEU:HD12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3034:LYS:HE3	3:B:3034:LYS:HB3	1.70	0.42
1:E:49:ARG:HH21	1:E:52:LYS:HE2	1.85	0.42
3:A:823:LEU:HD12	3:A:1617:THR:HG23	2.02	0.42
3:A:871:ARG:NH2	3:A:926:GLY:HA3	2.35	0.42
3:A:3588:ASP:O	3:A:3592:ILE:HG13	2.19	0.42
3:A:4017:LEU:HD22	3:A:4139:ILE:HG21	2.00	0.42
3:A:4160:LEU:HD12	3:A:4160:LEU:HA	1.90	0.42
3:C:664:PHE:CE1	3:C:746:CYS:HB2	2.55	0.42
3:C:4156:HIS:HA	3:C:4161:ARG:NH2	2.35	0.42
3:D:2801:ASP:HB2	3:D:2805:TYR:CE2	2.55	0.42
3:B:1071:ARG:HA	3:B:1071:ARG:HD2	1.84	0.42
3:B:2804:ILE:HG13	3:B:2805:TYR:N	2.35	0.42
3:B:4725:LEU:HA	3:B:4737:ILE:HG21	2.02	0.42
1:H:66:MET:HE1	1:H:101:VAL:HB	2.02	0.42
2:J:20:ASP:OD2	2:J:20:ASP:C	2.62	0.42
3:A:664:PHE:CE1	3:A:746:CYS:HB2	2.55	0.42
3:C:1821:ASP:OD2	3:C:1821:ASP:C	2.62	0.42
3:C:2965:ARG:NH1	3:C:2969:ILE:HD11	2.35	0.42
3:C:4547:GLN:O	3:C:4550:LYS:HG3	2.19	0.42
3:D:1436:SER:OG	3:D:1565:GLU:HB2	2.19	0.42
3:D:2208:MET:HE1	3:D:2253:HIS:CG	2.54	0.42
3:D:4242:ILE:HG13	3:D:4989:MET:HE1	2.01	0.42
3:B:2001:PRO:O	3:B:2005:GLN:HG3	2.19	0.42
3:A:19:GLU:HB3	3:A:205:ILE:HB	2.02	0.42
3:A:823:LEU:HD13	3:A:1628:VAL:HG22	2.01	0.42
3:A:2290:LEU:HD12	3:A:2290:LEU:HA	1.87	0.42
3:A:2679:PHE:HB2	3:A:2706:ILE:HG21	2.01	0.42
3:A:2739:PRO:HA	3:A:2888:ARG:NH2	2.35	0.42
3:A:3625:SER:O	3:A:3629:ARG:HG2	2.20	0.42
3:C:3625:SER:O	3:C:3629:ARG:HG2	2.20	0.42
3:C:3720:TYR:HA	3:C:3723:MET:HE2	2.01	0.42
3:C:3793:MET:HB3	3:C:3793:MET:HE3	1.78	0.42
3:D:3405:LEU:O	3:D:3409:TYR:HB2	2.19	0.42
3:D:3793:MET:HE3	3:D:3793:MET:HB3	1.85	0.42
3:B:533:ASN:HB3	3:B:536:ASN:HB2	2.02	0.42
3:B:1997:GLU:HA	3:B:2008:MET:HE1	2.02	0.42
3:B:2884:ASN:O	3:B:2888:ARG:HD2	2.20	0.42
3:B:2891:LYS:NZ	3:B:2905:LEU:HD23	2.35	0.42
2:J:19:PHE:CD1	2:J:35:VAL:HG22	2.55	0.41
3:A:683:ARG:HG2	3:A:717:ASP:HB3	2.02	0.41
3:A:2161:GLN:NE2	3:A:2177:LEU:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2891:LYS:NZ	3:A:2905:LEU:HD23	2.35	0.41
3:C:129:ASP:HA	3:B:2370:GLY:O	2.20	0.41
3:C:1617:THR:HG22	3:C:1628:VAL:HG13	2.02	0.41
3:C:2359:ARG:HA	3:C:2359:ARG:HD3	1.71	0.41
3:D:1021:LEU:HD12	3:D:1021:LEU:HA	1.82	0.41
3:D:2485:LEU:HD23	3:D:2485:LEU:HA	1.77	0.41
3:D:2578:MET:HE2	3:D:2578:MET:HB3	1.94	0.41
3:B:2890:LYS:HD2	3:B:2893:GLU:OE2	2.20	0.41
3:B:4026:MET:HB3	3:B:4026:MET:HE2	1.79	0.41
1:H:52:LYS:HE3	1:H:52:LYS:HB3	1.77	0.41
2:L:92:PHE:HE2	2:L:108:VAL:HB	1.85	0.41
3:A:2890:LYS:HA	3:A:2890:LYS:HD2	1.75	0.41
3:C:1005:TRP:HA	3:C:1016:ARG:HB3	2.02	0.41
3:C:3324:VAL:HA	3:C:3327:LEU:HG	2.01	0.41
3:C:3756:LYS:O	3:C:3759:GLU:HG2	2.20	0.41
3:D:1005:TRP:HA	3:D:1016:ARG:HB3	2.02	0.41
3:D:2614:ILE:HG23	3:D:2618:MET:HE3	2.01	0.41
3:B:486:LEU:HD12	3:B:486:LEU:HA	1.87	0.41
3:B:1455:PRO:HG3	3:B:1549:PHE:HE1	1.84	0.41
3:B:2330:ARG:H	3:B:2330:ARG:HG2	1.68	0.41
3:B:3625:SER:O	3:B:3629:ARG:HG2	2.19	0.41
3:B:3793:MET:HB3	3:B:3793:MET:HE3	1.85	0.41
2:L:32:LEU:HD12	2:L:32:LEU:O	2.21	0.41
3:A:2211:MET:HE2	3:A:2211:MET:HB3	1.95	0.41
3:A:3361:THR:HG21	3:A:3408:LEU:HD22	2.02	0.41
3:C:3951:PHE:O	3:C:3955:MET:HG3	2.21	0.41
3:C:4989:MET:HE3	3:C:4993:MET:HE2	2.02	0.41
3:D:394:GLN:HB2	3:D:397:GLU:HG2	2.02	0.41
3:D:2001:PRO:O	3:D:2005:GLN:HG3	2.20	0.41
3:D:3082:LYS:HE2	3:D:3155:ASP:HB3	2.02	0.41
3:D:3564:GLU:HA	3:D:3570:ARG:NH2	2.35	0.41
3:B:904:HIS:CE1	3:B:906:CYS:HB2	2.56	0.41
3:B:3509:LEU:HD23	3:B:3509:LEU:HA	1.82	0.41
3:B:4564:PHE:CD1	3:B:4564:PHE:C	2.98	0.41
1:G:52:LYS:HB2	1:G:54:GLU:HG3	2.02	0.41
2:I:63:ILE:HD12	2:I:68:PHE:HB2	2.02	0.41
2:K:50:ASP:OD2	2:K:50:ASP:C	2.63	0.41
2:L:5:THR:OG1	2:L:8:GLN:HG3	2.20	0.41
3:A:892:THR:O	3:A:903:LEU:HA	2.20	0.41
3:A:1575:LEU:HD23	3:A:1575:LEU:HA	1.90	0.41
3:A:4105:GLY:O	3:A:4109:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2752:ASP:HA	3:C:2755:ILE:HG12	2.03	0.41
3:C:3545:THR:OG1	3:C:3548:GLU:HG3	2.19	0.41
3:D:306:LYS:H	3:D:306:LYS:HG2	1.67	0.41
3:D:2212:VAL:HG21	3:D:2256:TYR:CZ	2.55	0.41
3:D:2536:LEU:HD22	3:D:2541:PHE:HB3	2.02	0.41
3:B:575:LEU:HD22	3:B:609:CYS:HB2	2.02	0.41
3:B:2752:ASP:HA	3:B:2755:ILE:HG12	2.02	0.41
3:B:4156:HIS:HA	3:B:4161:ARG:NH2	2.35	0.41
3:A:1021:LEU:HD12	3:A:1021:LEU:HA	1.82	0.41
3:A:2364:PHE:HB3	3:A:2368:LEU:HB2	2.03	0.41
3:A:3250:MET:HE3	3:A:3277:LEU:HD13	2.02	0.41
3:C:46:LEU:HD23	3:C:46:LEU:HA	1.90	0.41
3:C:2614:ILE:HG23	3:C:2618:MET:HE3	2.03	0.41
3:D:1008:SER:HB3	3:D:1017:ARG:HB3	2.01	0.41
3:D:2935:TYR:HB2	3:D:2939:ARG:HH12	1.86	0.41
3:B:954:LYS:HA	3:B:954:LYS:HD2	1.83	0.41
3:A:2918:ARG:O	3:A:2921:GLU:HG3	2.20	0.41
3:A:4581:LYS:HE3	3:A:4581:LYS:HB2	1.71	0.41
3:A:4711:PHE:HA	3:A:4712:PRO:HA	1.91	0.41
3:C:1008:SER:HB3	3:C:1017:ARG:HB3	2.02	0.41
3:C:2364:PHE:HB3	3:C:2368:LEU:HB2	2.02	0.41
3:D:1447:CYS:HB3	3:D:1555:LEU:HB3	2.03	0.41
3:D:2876:GLU:OE1	3:D:2876:GLU:HA	2.20	0.41
3:D:3277:LEU:HD23	3:D:3277:LEU:HA	1.85	0.41
3:B:323:LEU:HD23	3:B:323:LEU:HA	1.94	0.41
3:B:683:ARG:HG2	3:B:717:ASP:HB3	2.02	0.41
3:B:2128:TYR:CD1	3:B:3673:MET:HE3	2.56	0.41
3:B:2211:MET:HE2	3:B:2211:MET:HB3	1.98	0.41
3:B:2874:MET:HE3	3:B:2874:MET:HB2	1.96	0.41
2:K:0:MET:HE3	2:K:0:MET:HB2	1.93	0.41
3:A:76:ARG:HD2	9:D:5201:HOH:O	2.20	0.41
3:A:783:PHE:HB2	3:A:787:VAL:HG21	2.03	0.41
3:A:2798:SER:HB2	3:A:2801:ASP:OD1	2.21	0.41
3:A:2801:ASP:HB2	3:A:2805:TYR:CZ	2.56	0.41
3:A:2890:LYS:HD2	3:A:2893:GLU:OE2	2.21	0.41
3:C:1455:PRO:HG3	3:C:1549:PHE:HE1	1.85	0.41
3:C:2804:ILE:HG13	3:C:2805:TYR:N	2.35	0.41
3:C:2890:LYS:O	3:C:2894:LEU:HG	2.21	0.41
3:C:4242:ILE:HG13	3:C:4989:MET:HE1	2.02	0.41
3:C:4581:LYS:HE2	3:C:4581:LYS:HB2	1.70	0.41
3:D:2128:TYR:CD1	3:D:3673:MET:HE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2376:LEU:O	3:D:2380:ILE:HG12	2.21	0.41
3:D:2891:LYS:HZ2	3:D:2905:LEU:HD23	1.85	0.41
3:B:1021:LEU:HD12	3:B:1021:LEU:HA	1.82	0.41
3:B:2485:LEU:HD23	3:B:2485:LEU:HA	1.80	0.41
3:B:2614:ILE:HG23	3:B:2618:MET:HE3	2.03	0.41
1:H:68:LEU:HD23	1:H:106:LEU:HG	2.03	0.41
2:J:32:LEU:HD12	2:J:32:LEU:O	2.21	0.41
2:K:63:ILE:HG12	9:K:201:HOH:O	2.21	0.41
2:K:116:LEU:HD13	2:K:124:MET:HE1	2.01	0.41
3:A:1931:LEU:HD22	3:A:1935:VAL:HG11	2.02	0.41
3:A:4725:LEU:HA	3:A:4737:ILE:HG21	2.03	0.41
3:C:3104:GLU:HG3	3:C:3171:SER:OG	2.21	0.41
3:C:4790:LEU:HD23	3:C:4790:LEU:HA	1.95	0.41
3:A:939:VAL:HG12	3:A:1053:ILE:HG12	2.02	0.41
3:A:1616:GLU:HB3	3:A:1629:GLN:HG2	2.02	0.41
3:A:1671:ARG:HD3	3:A:1713:ASP:HB3	2.03	0.41
3:A:3568:SER:HA	3:A:3571:TRP:CD1	2.56	0.41
3:A:3702:VAL:HA	3:A:3778:MET:CE	2.51	0.41
3:C:2530:MET:HB3	3:C:2585:THR:HG21	2.03	0.41
3:C:4929:LEU:HD23	3:C:4929:LEU:HA	1.95	0.41
3:D:871:ARG:NH2	3:D:926:GLY:HA3	2.36	0.41
3:D:2869:ARG:HA	3:D:2869:ARG:HD3	1.76	0.41
3:D:2891:LYS:NZ	3:D:2905:LEU:HD23	2.36	0.41
3:D:3557:LEU:HD23	3:D:3557:LEU:HA	1.86	0.41
3:D:4218:ILE:HD13	3:D:4218:ILE:HA	1.93	0.41
3:B:144:GLU:HB2	3:B:175:SER:HB3	2.02	0.41
3:B:2359:ARG:HA	3:B:2359:ARG:HD3	1.72	0.41
3:B:2530:MET:HB3	3:B:2585:THR:HG21	2.03	0.41
3:B:2869:ARG:HA	3:B:2869:ARG:HD3	1.86	0.41
3:B:2890:LYS:HA	3:B:2890:LYS:HD2	1.76	0.41
3:B:2918:ARG:O	3:B:2921:GLU:HG3	2.21	0.41
3:B:3324:VAL:HA	3:B:3327:LEU:HG	2.02	0.41
3:B:4091:LYS:O	3:B:4095:LYS:HG2	2.21	0.41
3:B:4864:ASN:HD21	3:B:4872:PRO:HB3	1.86	0.41
3:A:2638:LYS:HD2	3:A:2698:MET:HG3	2.02	0.41
3:C:2476:ILE:HG23	3:C:2536:LEU:HD21	2.03	0.41
3:C:2890:LYS:HD2	3:C:2893:GLU:OE2	2.21	0.41
3:C:4060:LYS:HG3	3:C:4064:MET:SD	2.61	0.41
9:C:5201:HOH:O	3:D:76:ARG:HD2	2.21	0.41
3:D:407:THR:HG21	3:D:448:LEU:HD11	2.03	0.41
3:D:904:HIS:CE1	3:D:906:CYS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1071:ARG:HA	3:D:1071:ARG:HD2	1.84	0.41
3:D:2889:LYS:HB3	3:D:2889:LYS:HE3	1.86	0.41
3:D:4060:LYS:O	3:D:4064:MET:HG3	2.21	0.41
3:B:972:LEU:O	3:B:975:VAL:HG22	2.21	0.41
2:J:115:LYS:H	3:B:3858:MET:HE1	1.86	0.40
3:A:233:ILE:HD12	3:A:242:ARG:HB3	2.02	0.40
3:A:590:LEU:HD13	3:A:599:VAL:HB	2.02	0.40
3:A:1039:LEU:HD13	3:A:1039:LEU:HA	1.97	0.40
3:A:2376:LEU:O	3:A:2380:ILE:HG12	2.21	0.40
3:A:2569:PHE:CZ	3:A:2582:MET:HE1	2.56	0.40
3:A:4026:MET:HE2	3:A:4026:MET:HB3	1.83	0.40
3:C:533:ASN:HB3	3:C:536:ASN:HB2	2.03	0.40
3:C:871:ARG:NH2	3:C:926:GLY:HA3	2.36	0.40
3:C:3557:LEU:HD23	3:C:3557:LEU:HA	1.87	0.40
3:C:4564:PHE:CD1	3:C:4564:PHE:C	2.99	0.40
3:D:2752:ASP:HA	3:D:2755:ILE:HG12	2.03	0.40
3:D:2996:LYS:HA	3:D:2996:LYS:HD3	1.85	0.40
3:D:3568:SER:HA	3:D:3571:TRP:CD1	2.56	0.40
3:D:3630:ARG:HH22	3:D:3861:GLU:H	1.68	0.40
3:B:1545:ASN:HD22	3:B:1545:ASN:HA	1.59	0.40
3:B:2637:ALA:C	3:B:2640:PRO:HD2	2.46	0.40
3:A:2309:SER:HB2	3:A:2321:ILE:O	2.21	0.40
3:A:2597:LYS:HD3	3:A:2597:LYS:N	2.35	0.40
3:A:2959:PHE:HZ	3:A:3005:LEU:HG	1.86	0.40
3:C:2801:ASP:HB2	3:C:2805:TYR:CE2	2.56	0.40
3:C:2942:LYS:HG2	3:C:2943:ASP:H	1.86	0.40
3:C:4181:ILE:HD12	3:C:4183:ILE:HG23	2.04	0.40
3:C:4879:MET:HE3	3:C:4879:MET:HB3	1.89	0.40
3:D:402:ARG:HA	3:D:402:ARG:HD2	1.91	0.40
3:D:2636:PHE:HD1	3:D:2636:PHE:HA	1.77	0.40
3:D:3104:GLU:HG3	3:D:3171:SER:OG	2.21	0.40
3:B:2476:ILE:HG23	3:B:2536:LEU:HD21	2.03	0.40
3:B:3544:ASP:OD2	3:B:3548:GLU:HB2	2.20	0.40
3:B:3550:ARG:NH1	3:B:3594:ARG:HH22	2.18	0.40
3:A:894:GLY:HA3	3:A:903:LEU:HB3	2.02	0.40
3:A:2801:ASP:HB2	3:A:2805:TYR:CE2	2.56	0.40
3:A:3509:LEU:HA	3:A:3509:LEU:HD23	1.81	0.40
3:A:4156:HIS:HA	3:A:4161:ARG:NH2	2.37	0.40
3:C:306:LYS:H	3:C:306:LYS:HG2	1.63	0.40
3:C:870:ILE:HD13	3:C:1051:TYR:HE1	1.86	0.40
3:C:954:LYS:HA	3:C:954:LYS:HD2	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2885:THR:HA	3:C:2888:ARG:HD2	2.03	0.40
3:C:4204:GLN:HB3	3:C:4245:MET:HG2	2.04	0.40
3:C:4801:LEU:HD23	3:C:4801:LEU:HA	1.92	0.40
3:D:1561:VAL:HG12	3:D:1562:ILE:HG23	2.04	0.40
3:D:2637:ALA:C	3:D:2640:PRO:HD2	2.46	0.40
3:D:3432:GLU:HG2	3:D:3524:MET:SD	2.62	0.40
3:D:3951:PHE:CE2	3:D:3999:MET:HE2	2.56	0.40
3:D:3971:GLY:N	3:D:3972:PRO:HA	2.37	0.40
3:B:950:LEU:HD23	3:B:950:LEU:HA	1.91	0.40
3:A:544:LEU:HD21	3:A:578:ILE:HD13	2.04	0.40
3:A:2882:TYR:HB2	3:A:2919:ASP:OD1	2.21	0.40
3:A:3082:LYS:HD3	3:A:3082:LYS:HA	1.71	0.40
3:A:4188:ARG:HA	3:A:4188:ARG:HD2	1.88	0.40
3:C:2307:LEU:HD23	3:C:2307:LEU:HA	1.90	0.40
3:C:3405:LEU:O	3:C:3409:TYR:HB2	2.21	0.40
3:C:4725:LEU:HA	3:C:4737:ILE:HG21	2.03	0.40
3:D:2490:MET:HE3	3:D:2490:MET:HB3	1.95	0.40
3:D:2804:ILE:HG13	3:D:2805:TYR:N	2.36	0.40
3:D:3034:LYS:HA	3:D:3034:LYS:HD2	1.80	0.40
3:D:4003:LEU:HD22	3:D:4009:GLN:HB3	2.04	0.40
3:B:3409:TYR:HD1	3:B:3409:TYR:HA	1.77	0.40
3:B:3534:MET:HE3	3:B:3534:MET:HA	2.04	0.40
3:B:4057:MET:HE3	3:B:4057:MET:HB2	1.91	0.40
3:A:3194:LEU:HD12	3:A:3194:LEU:HA	1.98	0.40
3:C:3723:MET:HE2	3:C:3723:MET:HB2	1.84	0.40
3:C:4093:PHE:CZ	3:C:4097:MET:HE3	2.56	0.40
3:D:533:ASN:HB3	3:D:536:ASN:HB2	2.03	0.40
3:D:2211:MET:HE2	3:D:2211:MET:HB3	1.97	0.40
3:D:2908:TYR:CE2	3:D:2916:LYS:HD3	2.57	0.40
3:B:870:ILE:HD13	3:B:1051:TYR:HE1	1.87	0.40
3:B:871:ARG:NH2	3:B:926:GLY:HA3	2.36	0.40
3:B:1447:CYS:HB3	3:B:1555:LEU:HB3	2.03	0.40
3:B:2801:ASP:HB2	3:B:2805:TYR:CE2	2.56	0.40
3:B:3104:GLU:HG3	3:B:3171:SER:OG	2.21	0.40
3:B:3412:LEU:HD11	3:B:3434:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
1	F	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
1	G	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	H	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
2	I	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
2	J	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
2	K	146/148 (99%)	142 (97%)	4 (3%)	0	100	100
2	L	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
3	A	4198/5037 (83%)	4124 (98%)	74 (2%)	0	100	100
3	B	4198/5037 (83%)	4118 (98%)	80 (2%)	0	100	100
3	C	4198/5037 (83%)	4119 (98%)	79 (2%)	0	100	100
3	D	4198/5037 (83%)	4120 (98%)	78 (2%)	0	100	100
All	All	17796/21168 (84%)	17455 (98%)	341 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	88/88 (100%)	85 (97%)	3 (3%)	32	65
1	F	88/88 (100%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	87 (99%)	1 (1%)	65	85
2	I	82/127 (65%)	79 (96%)	3 (4%)	30	62
2	J	82/127 (65%)	79 (96%)	3 (4%)	30	62
2	K	82/127 (65%)	79 (96%)	3 (4%)	30	62
2	L	82/127 (65%)	80 (98%)	2 (2%)	43	74
3	A	3696/4276 (86%)	3658 (99%)	38 (1%)	68	86
3	B	3696/4276 (86%)	3668 (99%)	28 (1%)	73	89
3	C	3696/4276 (86%)	3668 (99%)	28 (1%)	73	89
3	D	3696/4276 (86%)	3664 (99%)	32 (1%)	70	87
All	All	15464/17964 (86%)	15323 (99%)	141 (1%)	68	87

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	67	SER
1	E	68	LEU
1	E	85	THR
1	H	85	THR
2	I	71	MET
2	I	122	ASP
2	I	124	MET
2	J	56	ASP
2	J	71	MET
2	J	124	MET
2	K	3	GLN
2	K	19	PHE
2	K	29	THR
2	L	56	ASP
2	L	62	THR
3	A	62	LEU
3	A	220	LEU
3	A	267	ILE
3	A	317	ARG
3	A	397	GLU
3	A	453	GLU
3	A	811	CYS
3	A	880	GLU

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Mol	Chain	Res	Type
3	A	977	LEU
3	A	1156	THR
3	A	1241	SER
3	A	1489	CYS
3	A	1617	THR
3	A	1934	SER
3	A	1980	LEU
3	A	2212	VAL
3	A	2214	VAL
3	A	2330	ARG
3	A	2540	THR
3	A	2543	THR
3	A	2642	LYS
3	A	2791	LEU
3	A	2792	ARG
3	A	2801	ASP
3	A	2806	ARG
3	A	2893	GLU
3	A	2904	LEU
3	A	3169	LEU
3	A	3367	LYS
3	A	3409	TYR
3	A	3420	ARG
3	A	3453	ARG
3	A	3608	GLN
3	A	3790	THR
3	A	3899	PHE
3	A	4094	GLN
3	A	4580	TYR
3	A	5001	THR
3	C	99	ARG
3	C	267	ILE
3	C	317	ARG
3	C	453	GLU
3	C	880	GLU
3	C	977	LEU
3	C	1241	SER
3	C	1489	CYS
3	C	1934	SER
3	C	2161	GLN
3	C	2786	LYS
3	C	2801	ASP

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Mol	Chain	Res	Type
3	C	2806	ARG
3	C	2893	GLU
3	C	2904	LEU
3	C	3169	LEU
3	C	3409	TYR
3	C	3420	ARG
3	C	3453	ARG
3	C	3715	LYS
3	C	3778	MET
3	C	3854	GLU
3	C	3899	PHE
3	C	4094	GLN
3	C	4151	SER
3	C	4229	GLU
3	C	4676	GLU
3	C	5013	MET
3	D	62	LEU
3	D	79	GLN
3	D	267	ILE
3	D	297	GLN
3	D	317	ARG
3	D	453	GLU
3	D	811	CYS
3	D	892	THR
3	D	977	LEU
3	D	1241	SER
3	D	1527	MET
3	D	1536	SER
3	D	1934	SER
3	D	1980	LEU
3	D	2636	PHE
3	D	2642	LYS
3	D	2771	ILE
3	D	2786	LYS
3	D	2796	THR
3	D	2801	ASP
3	D	2806	ARG
3	D	2904	LEU
3	D	3059	THR
3	D	3169	LEU
3	D	3343	GLN
3	D	3409	TYR

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Mol	Chain	Res	Type
3	D	3420	ARG
3	D	3453	ARG
3	D	3790	THR
3	D	3899	PHE
3	D	4229	GLU
3	D	4544	LEU
3	B	62	LEU
3	B	267	ILE
3	B	297	GLN
3	B	317	ARG
3	B	880	GLU
3	B	892	THR
3	B	977	LEU
3	B	1231	GLN
3	B	1241	SER
3	B	1302	ARG
3	B	1934	SER
3	B	2208	MET
3	B	2540	THR
3	B	2786	LYS
3	B	2801	ASP
3	B	2806	ARG
3	B	2874	MET
3	B	2893	GLU
3	B	2904	LEU
3	B	3169	LEU
3	B	3409	TYR
3	B	3453	ARG
3	B	3608	GLN
3	B	3754	GLU
3	B	3790	THR
3	B	3899	PHE
3	B	3924	LEU
3	B	4089	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	GLN
1	E	43	ASN
1	F	20	GLN
1	F	43	ASN

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Mol	Chain	Res	Type
1	G	20	GLN
1	G	43	ASN
1	H	43	ASN
2	J	3	GLN
2	K	3	GLN
3	A	113	HIS
3	A	395	GLN
3	A	465	GLN
3	A	489	ASN
3	A	678	GLN
3	A	765	GLN
3	A	1300	HIS
3	A	1460	HIS
3	A	1590	GLN
3	A	1598	GLN
3	A	1660	GLN
3	A	1691	GLN
3	A	2011	HIS
3	A	2100	HIS
3	A	2161	GLN
3	A	2194	HIS
3	A	2283	ASN
3	A	2514	ASN
3	A	2599	GLN
3	A	2856	ASN
3	A	2858	GLN
3	A	2961	GLN
3	A	2991	HIS
3	A	3069	HIS
3	A	3127	GLN
3	A	3418	ASN
3	A	3771	HIS
3	A	3882	GLN
3	A	3914	ASN
3	A	3970	GLN
3	A	4034	ASN
3	A	4558	ASN
3	A	4728	HIS
3	A	4984	ASN
3	A	5035	GLN
3	C	181	HIS
3	C	241	GLN

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Mol	Chain	Res	Type
3	C	395	GLN
3	C	465	GLN
3	C	489	ASN
3	C	658	GLN
3	C	678	GLN
3	C	765	GLN
3	C	1035	ASN
3	C	1133	HIS
3	C	1460	HIS
3	C	1660	GLN
3	C	1691	GLN
3	C	2011	HIS
3	C	2100	HIS
3	C	2173	GLN
3	C	2194	HIS
3	C	2515	GLN
3	C	2599	GLN
3	C	2744	ASN
3	C	2856	ASN
3	C	2858	GLN
3	C	2877	GLN
3	C	3127	GLN
3	C	3418	ASN
3	C	3465	ASN
3	C	3556	ASN
3	C	3605	HIS
3	C	3608	GLN
3	C	3771	HIS
3	C	3882	GLN
3	C	3896	ASN
3	C	3914	ASN
3	C	3994	HIS
3	C	4034	ASN
3	C	4094	GLN
3	C	4558	ASN
3	C	4728	HIS
3	D	380	GLN
3	D	395	GLN
3	D	489	ASN
3	D	765	GLN
3	D	877	ASN
3	D	1035	ASN

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Mol	Chain	Res	Type
3	D	1133	HIS
3	D	1460	HIS
3	D	1590	GLN
3	D	1660	GLN
3	D	2011	HIS
3	D	2100	HIS
3	D	2161	GLN
3	D	2194	HIS
3	D	2283	ASN
3	D	2284	ASN
3	D	2342	ASN
3	D	2515	GLN
3	D	2599	GLN
3	D	2856	ASN
3	D	2858	GLN
3	D	2877	GLN
3	D	2931	GLN
3	D	3127	GLN
3	D	3418	ASN
3	D	3465	ASN
3	D	3605	HIS
3	D	3771	HIS
3	D	3882	GLN
3	D	3914	ASN
3	D	3994	HIS
3	D	3998	HIS
3	D	4034	ASN
3	D	4558	ASN
3	D	4833	ASN
3	D	5015	GLN
3	B	241	GLN
3	B	489	ASN
3	B	678	GLN
3	B	765	GLN
3	B	1133	HIS
3	B	1231	GLN
3	B	1460	HIS
3	B	1660	GLN
3	B	1691	GLN
3	B	2011	HIS
3	B	2161	GLN
3	B	2194	HIS

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Mol	Chain	Res	Type
3	B	2253	HIS
3	B	2342	ASN
3	B	2515	GLN
3	B	2599	GLN
3	B	2856	ASN
3	B	2858	GLN
3	B	3127	GLN
3	B	3343	GLN
3	B	3418	ASN
3	B	3465	ASN
3	B	3605	HIS
3	B	3771	HIS
3	B	3814	GLN
3	B	3882	GLN
3	B	3914	ASN
3	B	3994	HIS
3	B	3998	HIS
3	B	4034	ASN
3	B	4558	ASN
3	B	4728	HIS
3	B	5015	GLN
3	B	5035	GLN

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 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 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	$\# Z > 2$
4	43M	C	5101	-	9,9,9	0.39	0	12,12,12	0.52	0
4	43M	C	5102	-	9,9,9	0.40	0	12,12,12	0.53	0
4	43M	B	5101	-	9,9,9	0.40	0	12,12,12	0.53	0
4	43M	A	5101	-	9,9,9	0.39	0	12,12,12	0.54	0
4	43M	A	5102	-	9,9,9	0.38	0	12,12,12	0.52	0
4	43M	D	5105	-	9,9,9	0.37	0	12,12,12	0.56	0
5	CFF	A	5103	-	15,15,15	0.59	0	23,23,23	0.72	1 (4%)
4	43M	D	5102	-	9,9,9	0.38	0	12,12,12	0.53	0
4	43M	A	5107	-	9,9,9	0.38	0	12,12,12	0.53	0
4	43M	D	5107	-	9,9,9	0.37	0	12,12,12	0.52	0
7	ATP	B	5108	-	32,33,33	0.29	0	48,52,52	0.38	0
7	ATP	A	5106	-	32,33,33	0.28	0	48,52,52	0.36	0
7	ATP	C	5108	-	32,33,33	0.28	0	48,52,52	0.38	0
7	ATP	C	5106	-	32,33,33	0.28	0	48,52,52	0.36	0
7	ATP	D	5106	-	32,33,33	0.29	0	48,52,52	0.36	0
4	43M	B	5105	-	9,9,9	0.38	0	12,12,12	0.55	0
4	43M	C	5105	-	9,9,9	0.36	0	12,12,12	0.55	0
7	ATP	D	5108	-	32,33,33	0.29	0	48,52,52	0.38	0
5	CFF	C	5103	-	15,15,15	0.58	0	23,23,23	0.74	1 (4%)
4	43M	D	5101	-	9,9,9	0.39	0	12,12,12	0.54	0
7	ATP	A	5108	-	32,33,33	0.29	0	48,52,52	0.38	0
4	43M	B	5102	-	9,9,9	0.38	0	12,12,12	0.53	0
5	CFF	B	5103	-	15,15,15	0.59	0	23,23,23	0.73	1 (4%)
4	43M	A	5105	-	9,9,9	0.35	0	12,12,12	0.55	0
5	CFF	D	5103	-	15,15,15	0.59	0	23,23,23	0.73	1 (4%)
4	43M	C	5107	-	9,9,9	0.39	0	12,12,12	0.53	0
4	43M	B	5107	-	9,9,9	0.38	0	12,12,12	0.52	0
7	ATP	B	5106	-	32,33,33	0.28	0	48,52,52	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	43M	C	5101	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	43M	C	5102	-	-	-	0/1/1/1
4	43M	A	5101	-	-	-	0/1/1/1
4	43M	B	5101	-	-	-	0/1/1/1
4	43M	A	5102	-	-	-	0/1/1/1
4	43M	D	5105	-	-	-	0/1/1/1
5	CFF	A	5103	-	-	-	0/2/2/2
4	43M	D	5102	-	-	-	0/1/1/1
4	43M	A	5107	-	-	-	0/1/1/1
4	43M	D	5107	-	-	-	0/1/1/1
7	ATP	B	5108	-	-	5/22/38/38	0/3/3/3
7	ATP	A	5106	-	-	7/22/38/38	0/3/3/3
7	ATP	C	5108	-	-	5/22/38/38	0/3/3/3
7	ATP	C	5106	-	-	5/22/38/38	0/3/3/3
7	ATP	D	5106	-	-	5/22/38/38	0/3/3/3
4	43M	B	5105	-	-	-	0/1/1/1
4	43M	C	5105	-	-	-	0/1/1/1
7	ATP	D	5108	-	-	6/22/38/38	0/3/3/3
5	CFF	C	5103	-	-	-	0/2/2/2
4	43M	D	5101	-	-	-	0/1/1/1
7	ATP	A	5108	-	-	7/22/38/38	0/3/3/3
4	43M	B	5102	-	-	-	0/1/1/1
5	CFF	B	5103	-	-	-	0/2/2/2
4	43M	A	5105	-	-	-	0/1/1/1
5	CFF	D	5103	-	-	-	0/2/2/2
4	43M	C	5107	-	-	-	0/1/1/1
4	43M	B	5107	-	-	-	0/1/1/1
7	ATP	B	5106	-	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5103	CFF	C12-N3-C2	2.39	121.50	117.33
5	D	5103	CFF	C12-N3-C2	2.39	121.50	117.33
5	B	5103	CFF	C12-N3-C2	2.37	121.46	117.33
5	A	5103	CFF	C12-N3-C2	2.34	121.41	117.33

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	5106	ATP	C5'-O5'-PA-O2A
7	A	5106	ATP	C5'-O5'-PA-O3A
7	A	5108	ATP	PB-O3B-PG-O2G
7	C	5106	ATP	C5'-O5'-PA-O2A
7	C	5106	ATP	C5'-O5'-PA-O3A
7	C	5108	ATP	PB-O3B-PG-O2G
7	D	5106	ATP	C5'-O5'-PA-O2A
7	D	5106	ATP	C5'-O5'-PA-O3A
7	D	5108	ATP	PB-O3B-PG-O2G
7	B	5106	ATP	C5'-O5'-PA-O2A
7	B	5106	ATP	C5'-O5'-PA-O3A
7	B	5108	ATP	PB-O3B-PG-O2G
7	B	5108	ATP	O4'-C4'-C5'-O5'
7	A	5108	ATP	O4'-C4'-C5'-O5'
7	C	5108	ATP	O4'-C4'-C5'-O5'
7	D	5108	ATP	O4'-C4'-C5'-O5'
7	C	5106	ATP	PG-O3B-PB-O3A
7	D	5106	ATP	PG-O3B-PB-O3A
7	B	5106	ATP	PG-O3B-PB-O3A
7	A	5108	ATP	PB-O3A-PA-O5'
7	C	5108	ATP	PB-O3A-PA-O5'
7	D	5108	ATP	PB-O3A-PA-O5'
7	B	5108	ATP	PB-O3A-PA-O5'
7	A	5106	ATP	PG-O3B-PB-O3A
7	A	5106	ATP	PB-O3A-PA-O2A
7	C	5106	ATP	PB-O3A-PA-O2A
7	D	5106	ATP	PB-O3A-PA-O2A
7	B	5106	ATP	PB-O3A-PA-O2A
7	A	5108	ATP	PB-O3B-PG-O3G
7	C	5108	ATP	PB-O3B-PG-O3G
7	D	5108	ATP	PB-O3B-PG-O3G
7	B	5108	ATP	PB-O3B-PG-O3G
7	A	5106	ATP	PG-O3B-PB-O1B
7	A	5106	ATP	PB-O3A-PA-O1A
7	A	5108	ATP	PG-O3B-PB-O2B
7	C	5106	ATP	PB-O3A-PA-O1A
7	D	5106	ATP	PB-O3A-PA-O1A
7	B	5106	ATP	PB-O3A-PA-O1A
7	A	5108	ATP	O4'-C1'-N9-C8
7	A	5108	ATP	PB-O3B-PG-O1G
7	C	5108	ATP	O4'-C1'-N9-C8
7	D	5108	ATP	O4'-C1'-N9-C8
7	B	5108	ATP	O4'-C1'-N9-C8

Continued on next page...

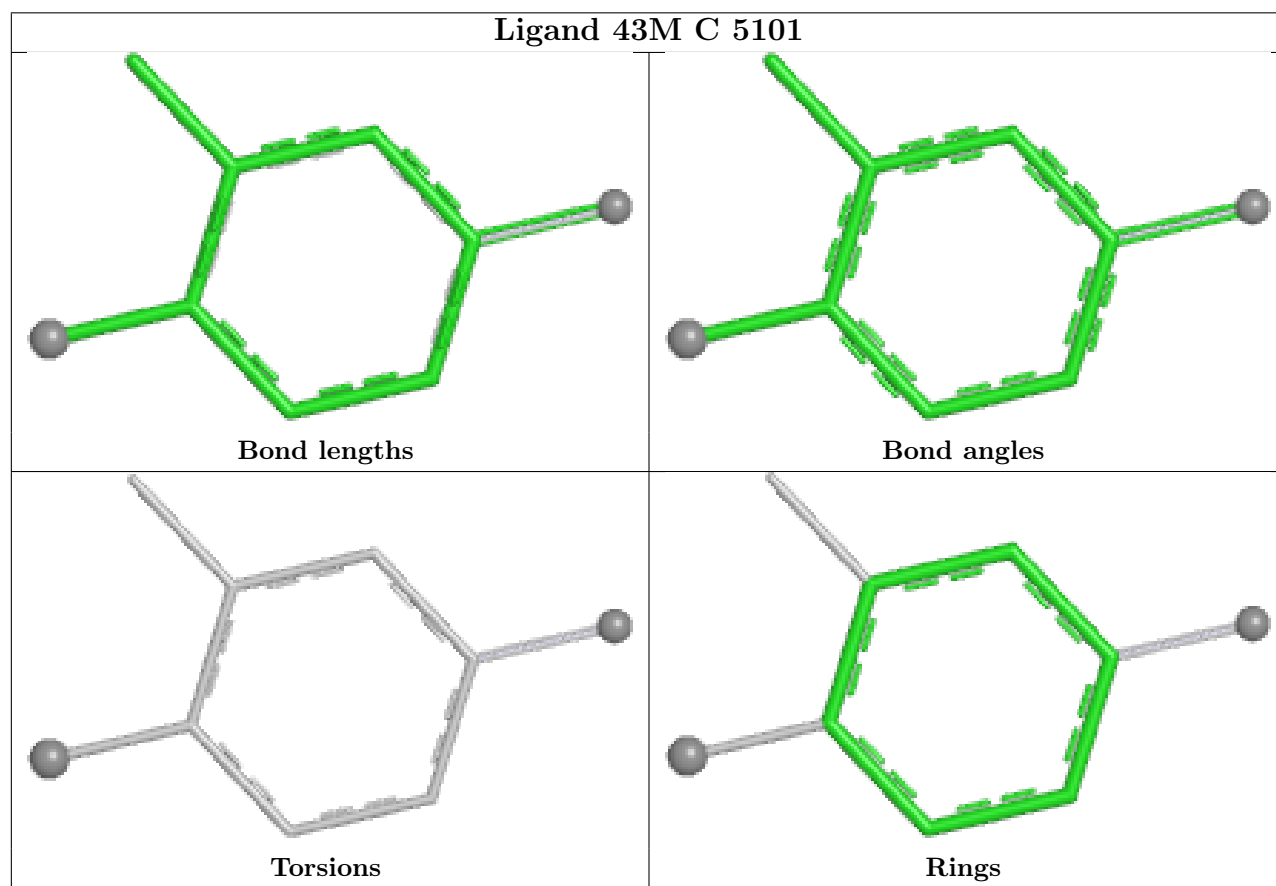
Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	5106	ATP	PG-O3B-PB-O2B
7	D	5108	ATP	PB-O3A-PA-O2A

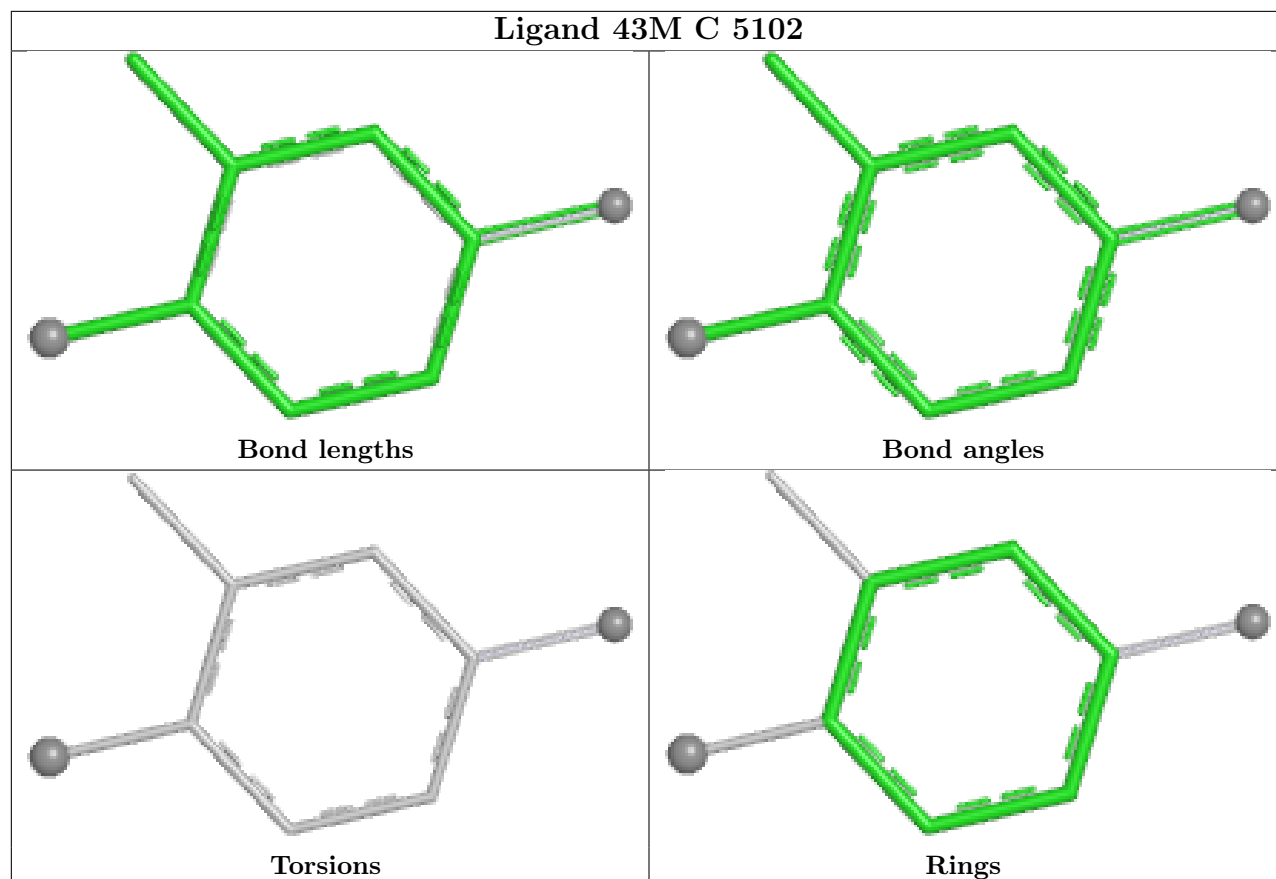
There are no ring outliers.

No monomer is involved in short contacts.

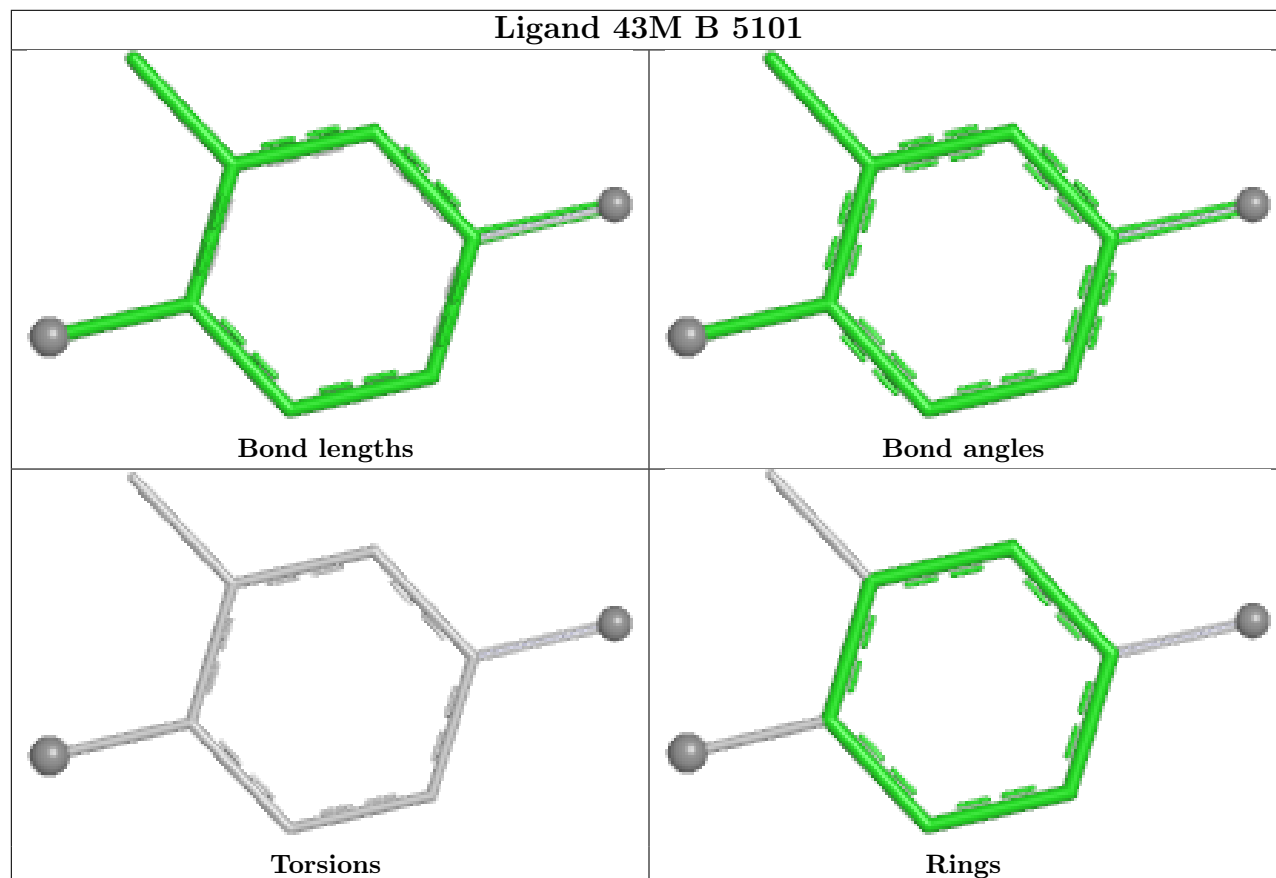
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



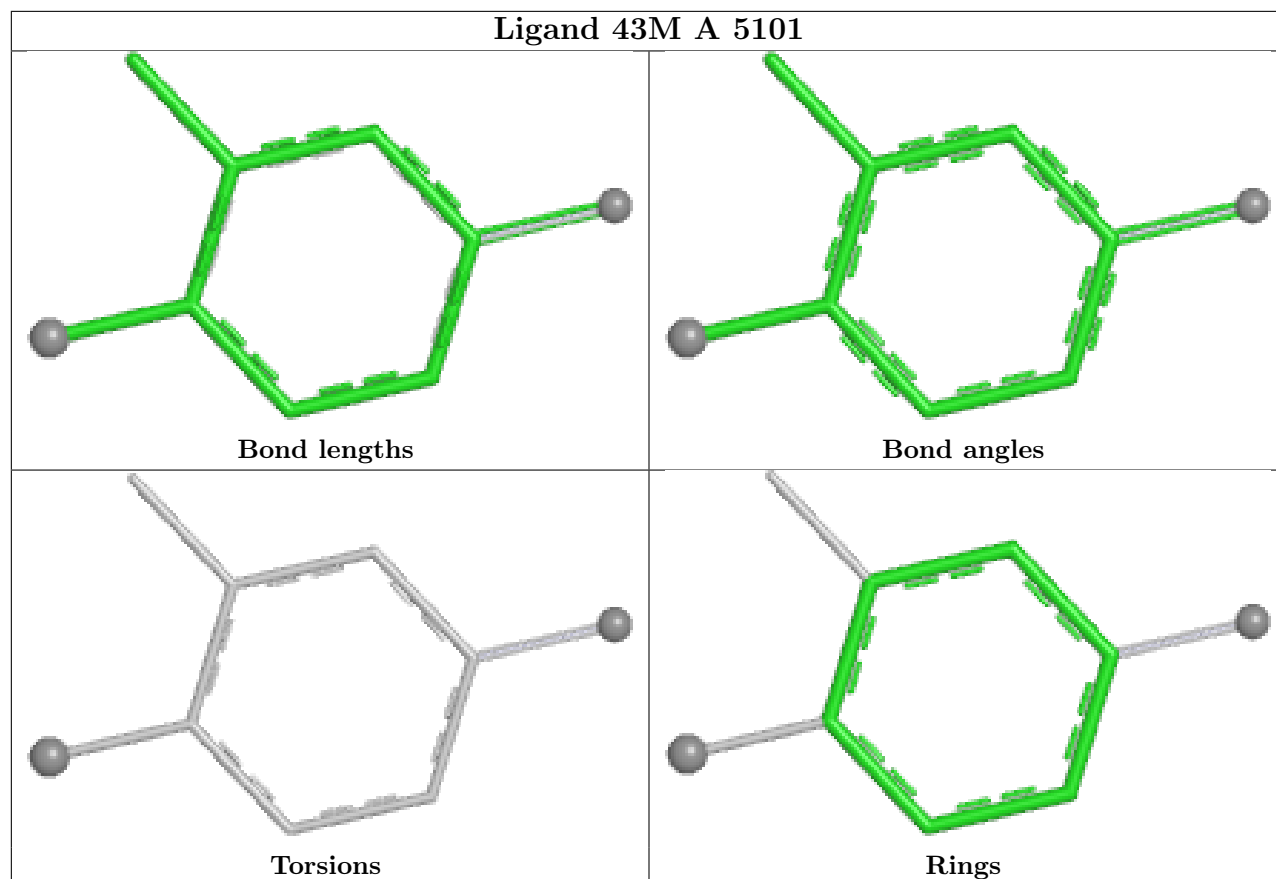
Ligand 43M C 5102



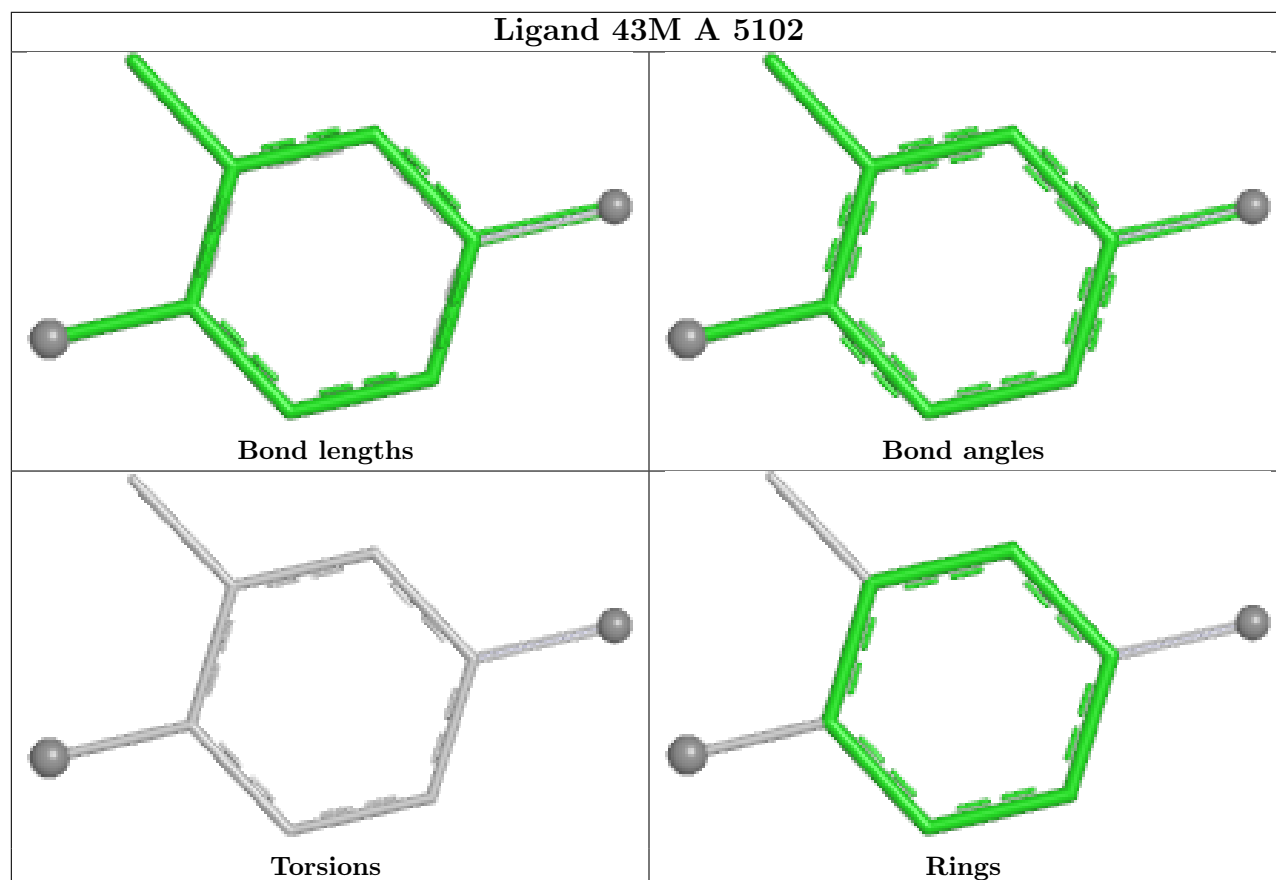
Ligand 43M B 5101

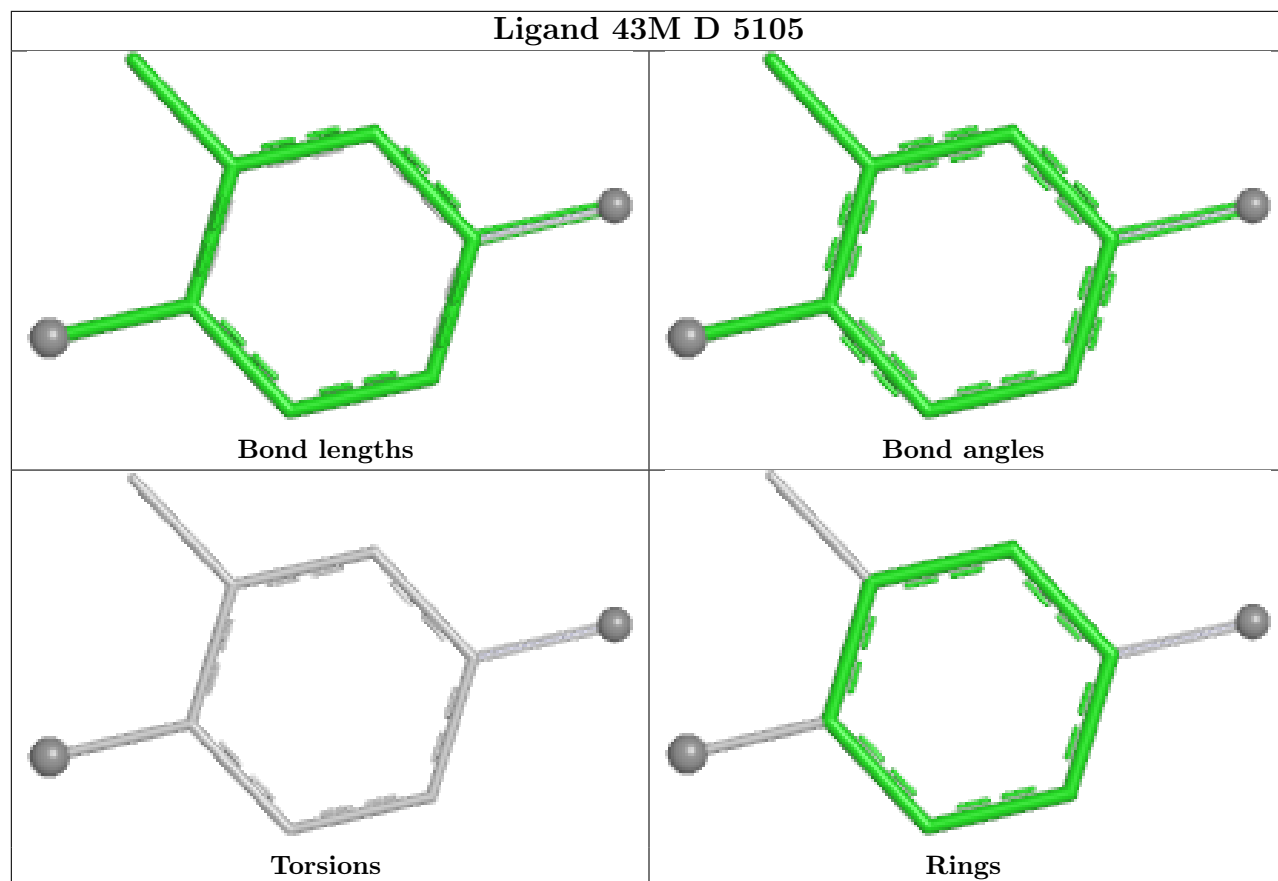


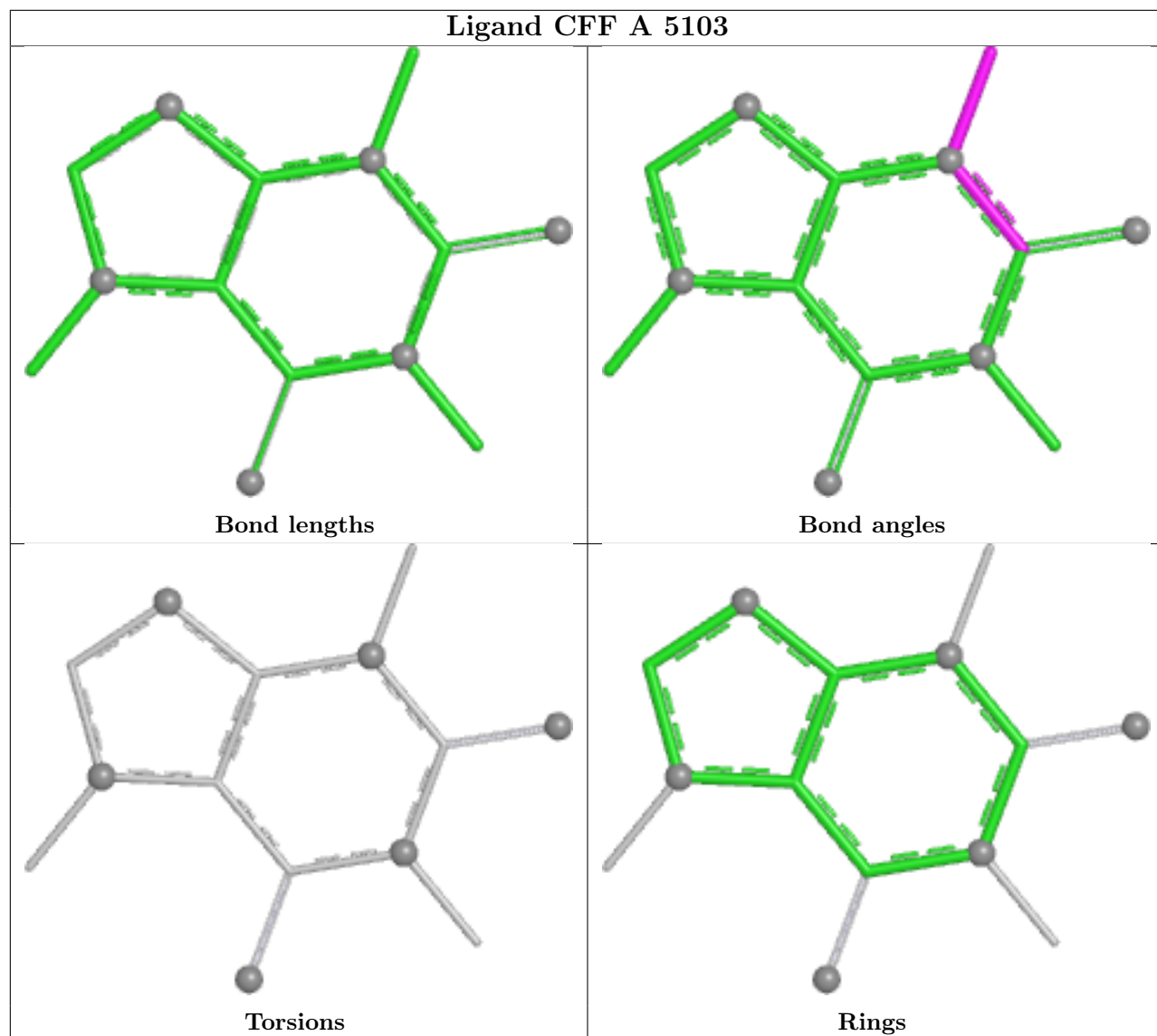
Ligand 43M A 5101



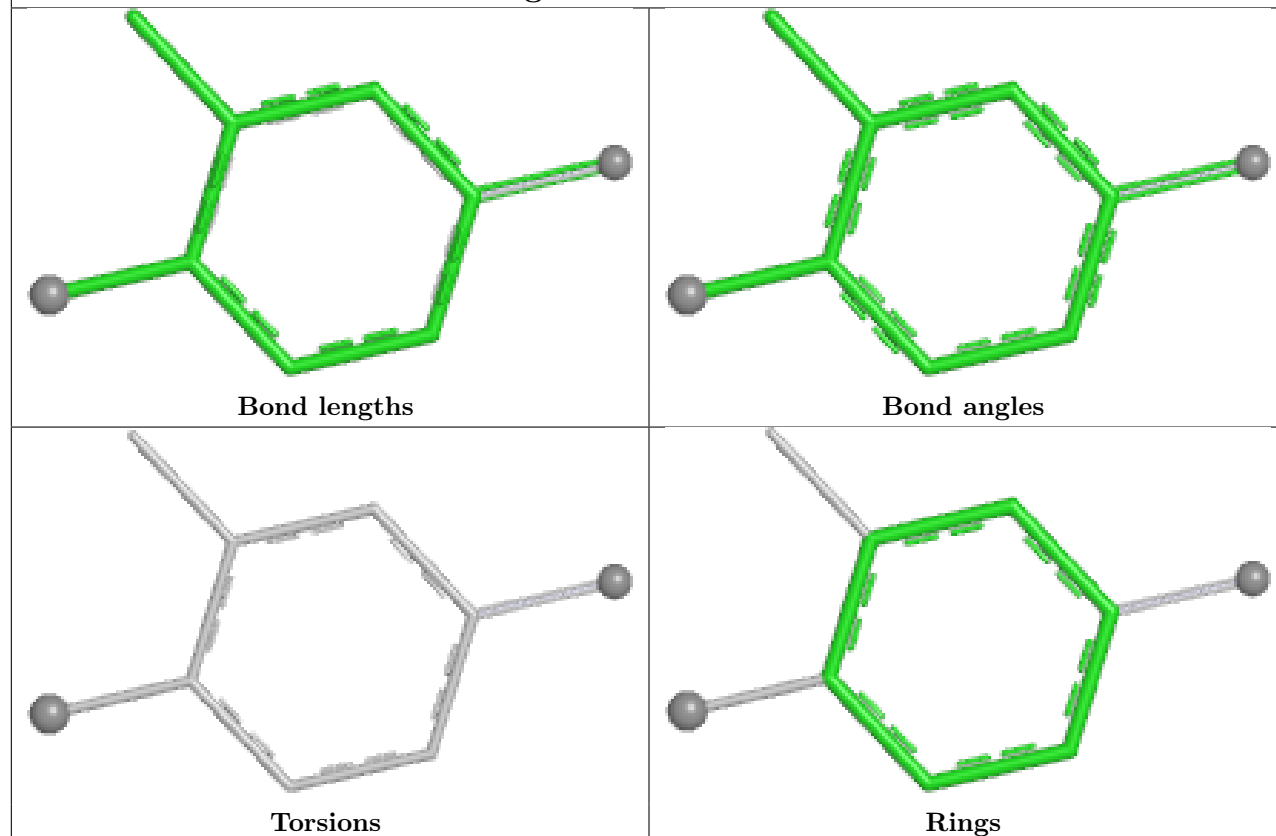
Ligand 43M A 5102



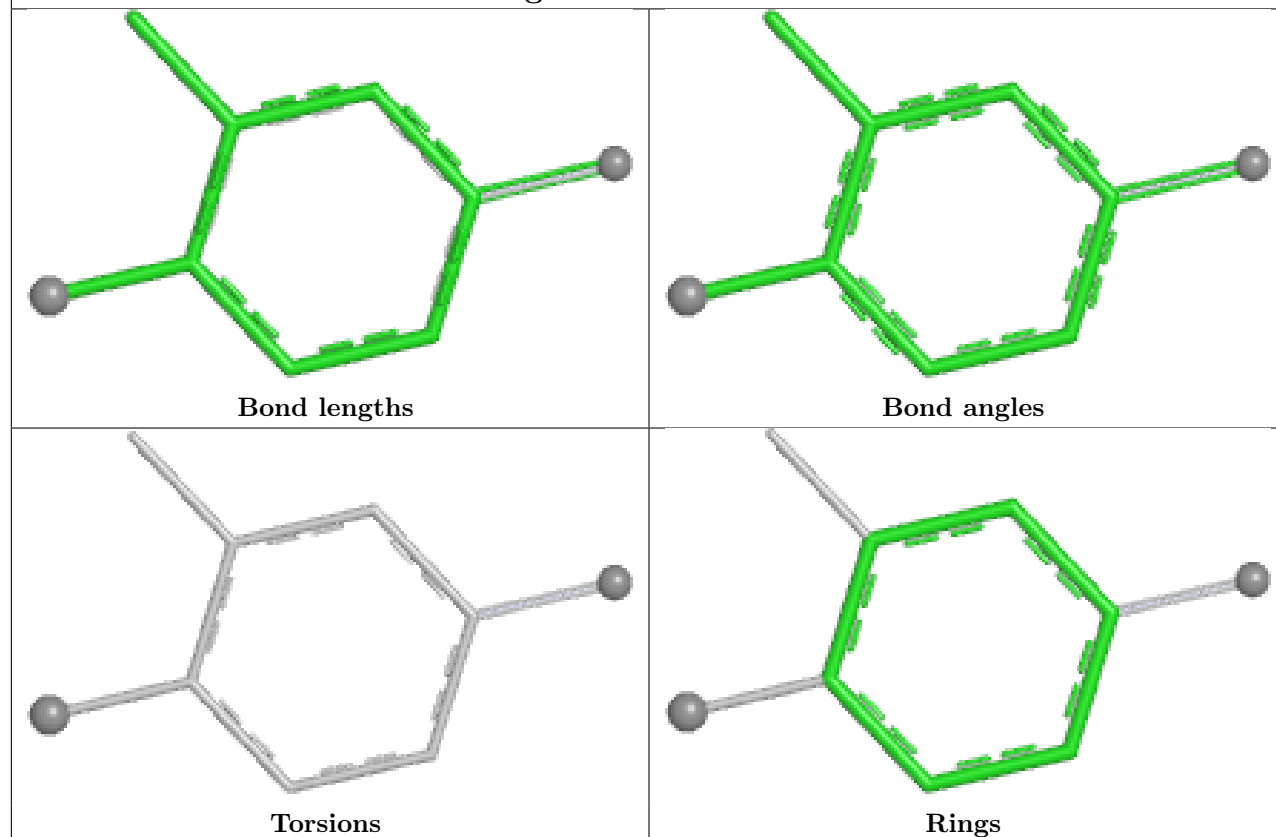


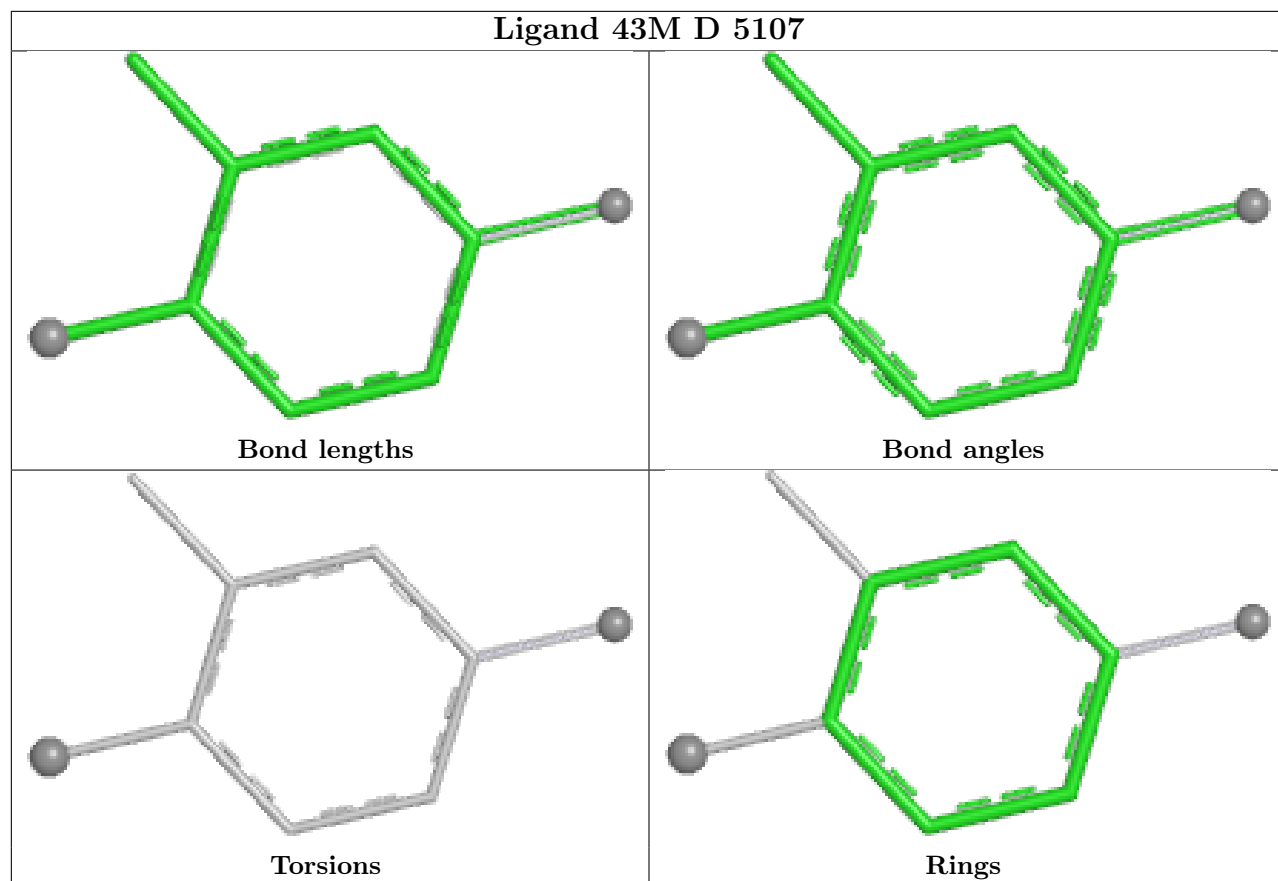


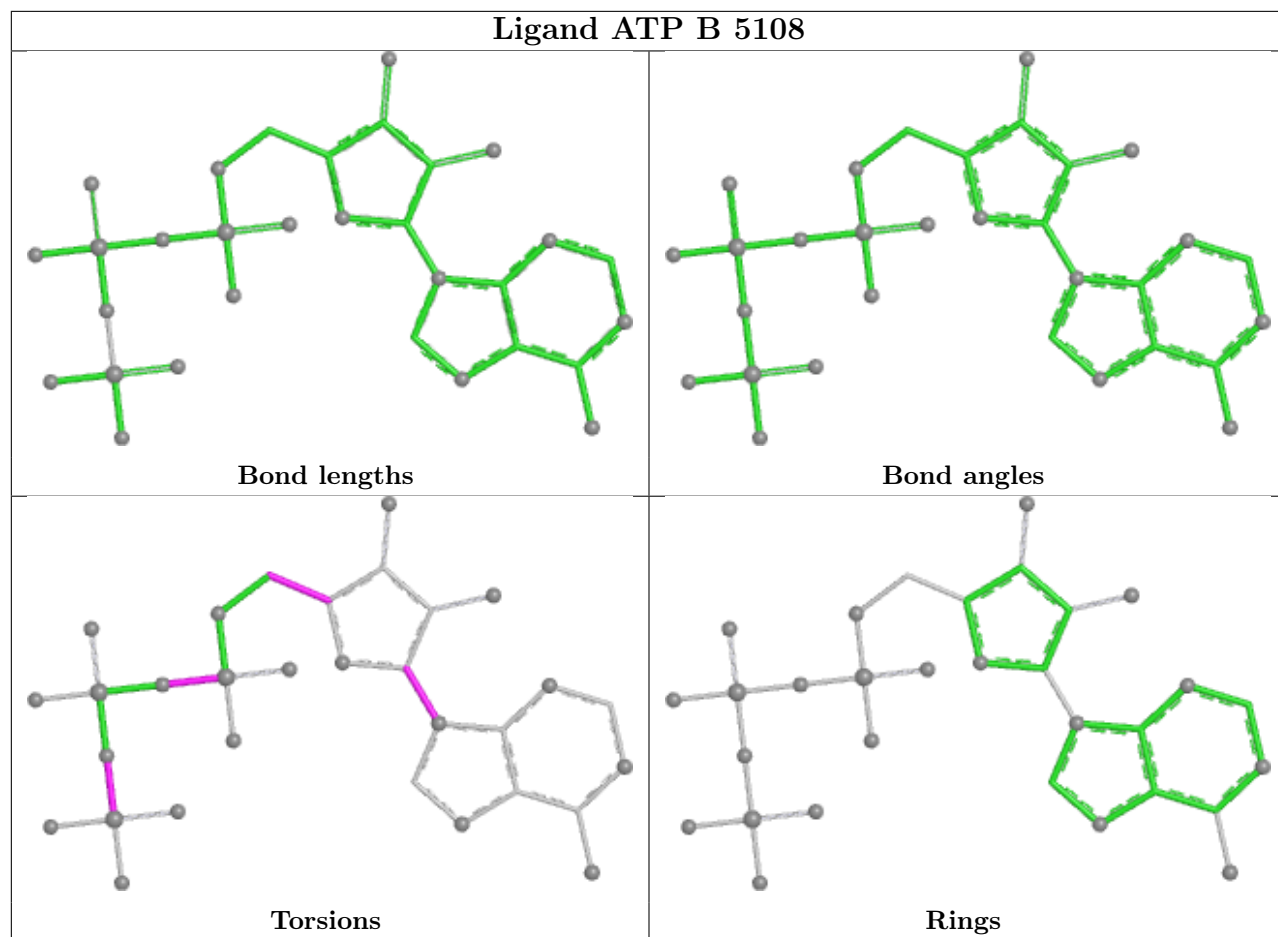
Ligand 43M D 5102

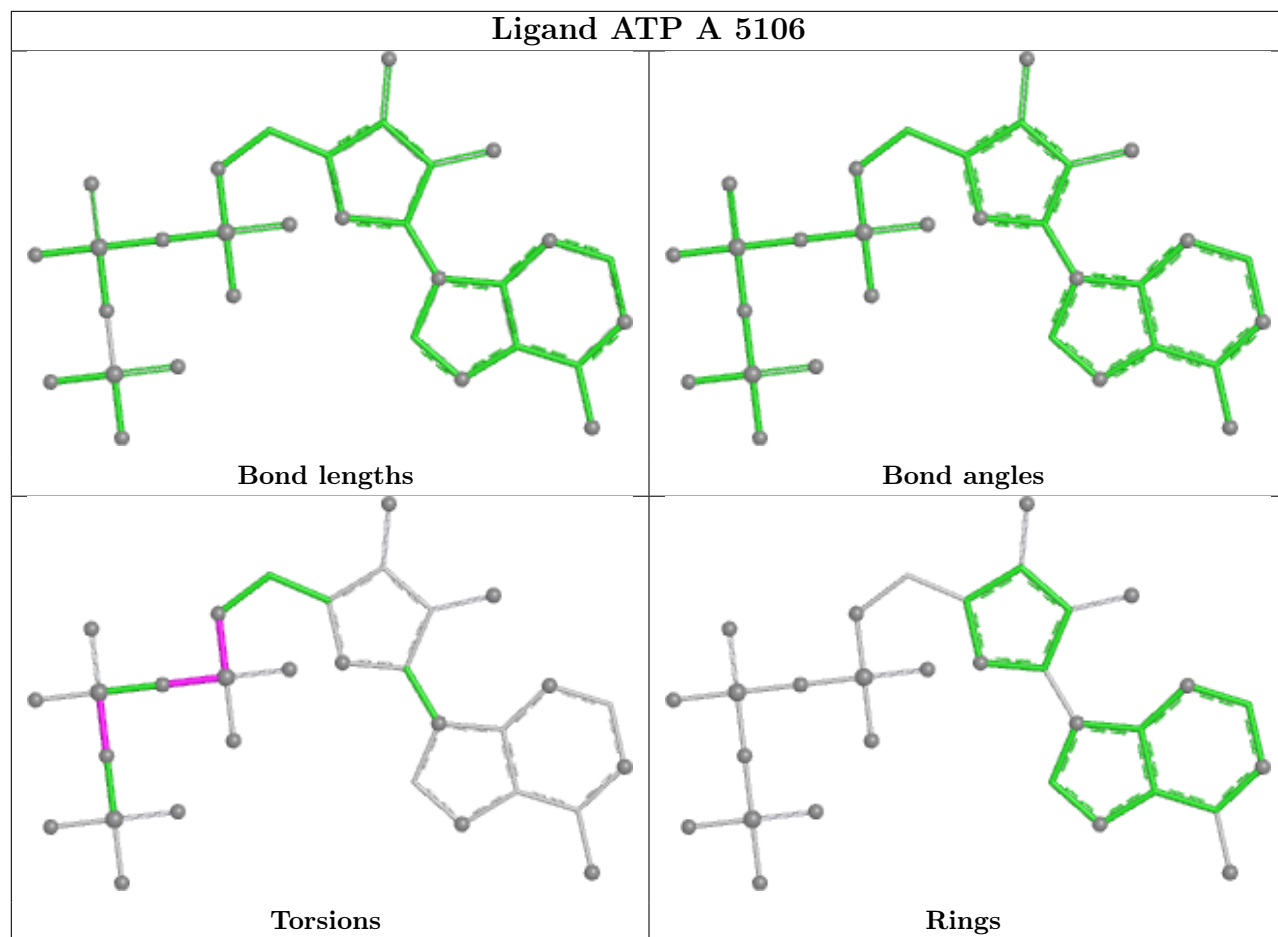


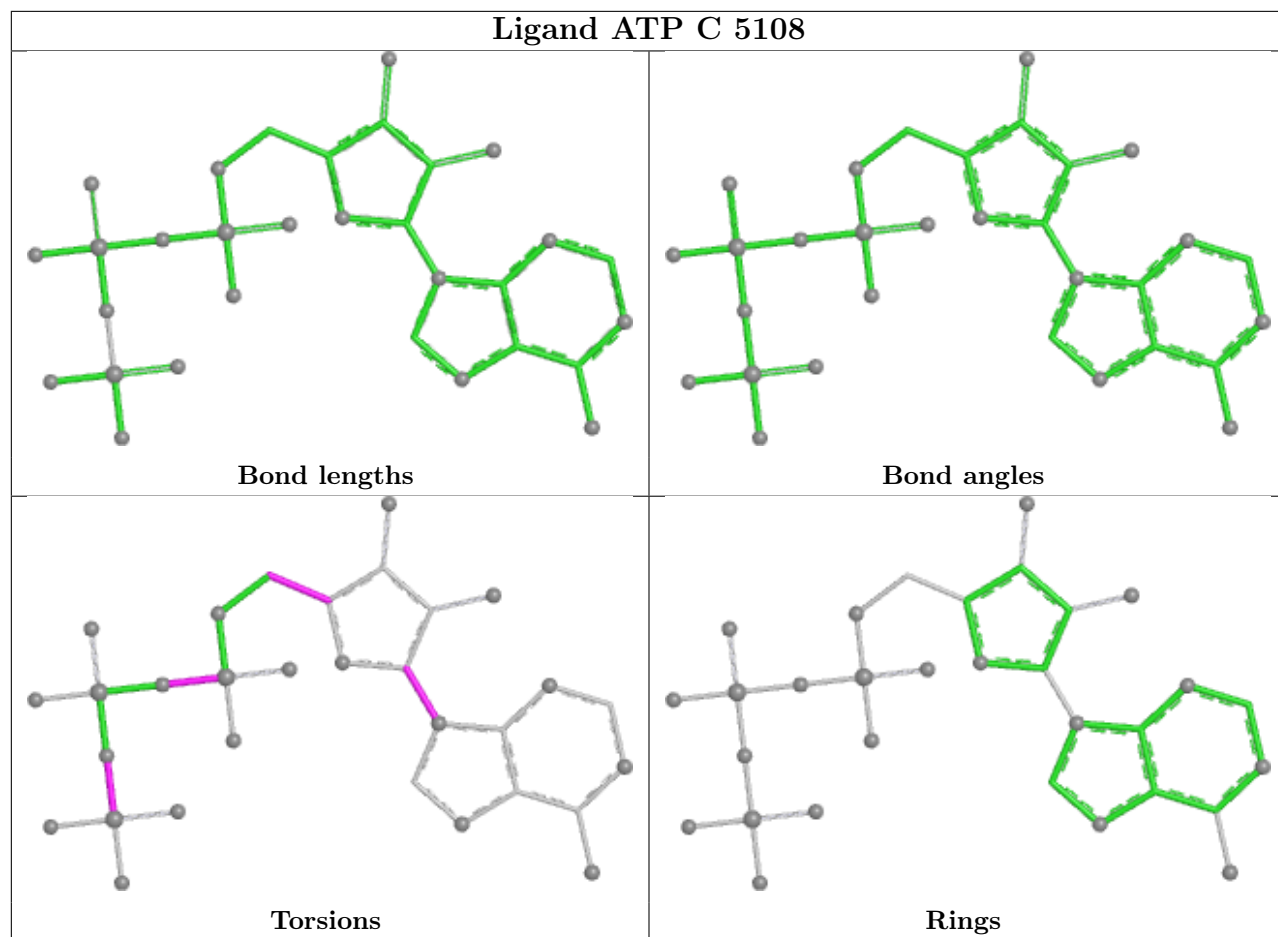
Ligand 43M A 5107

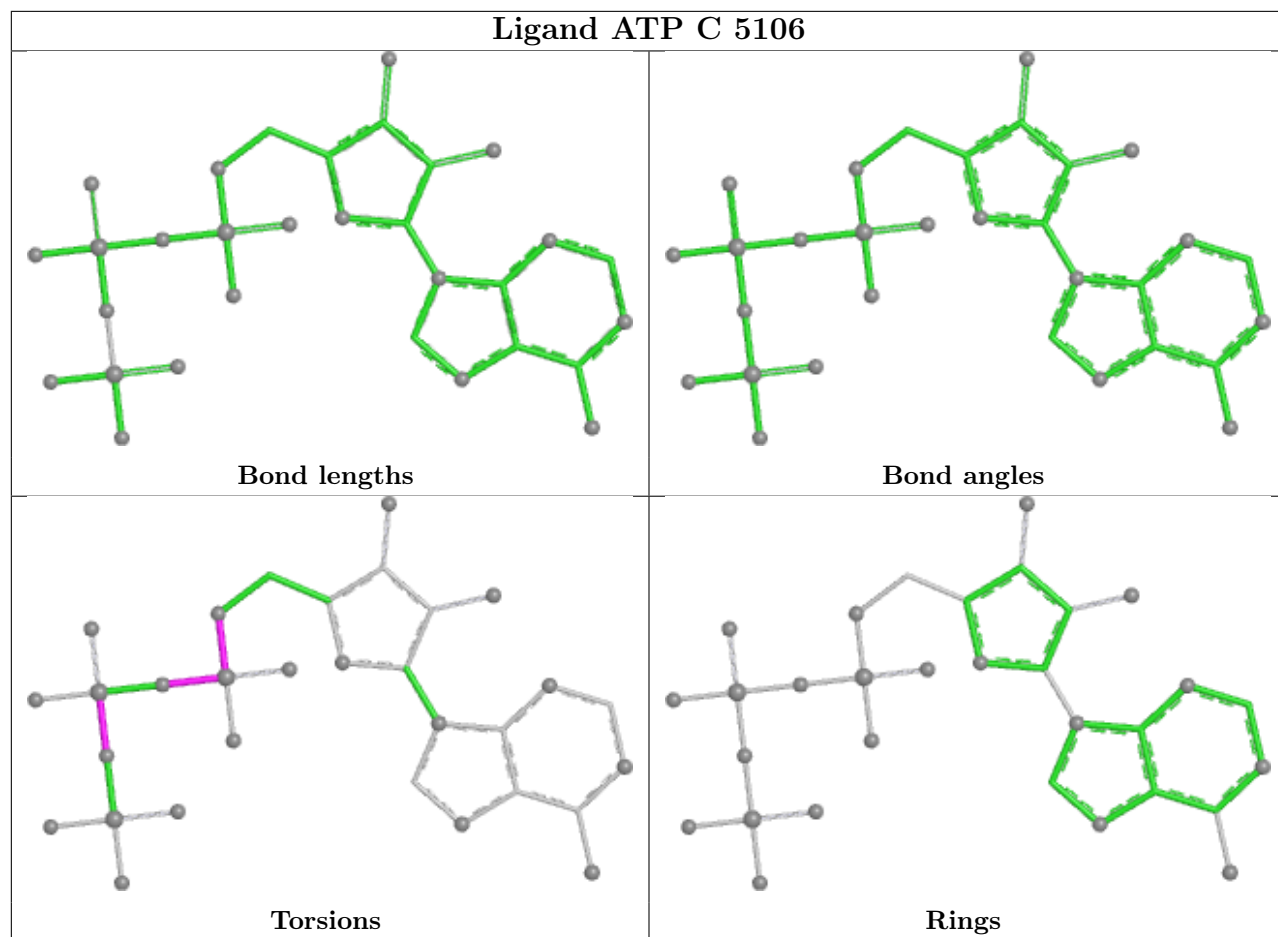


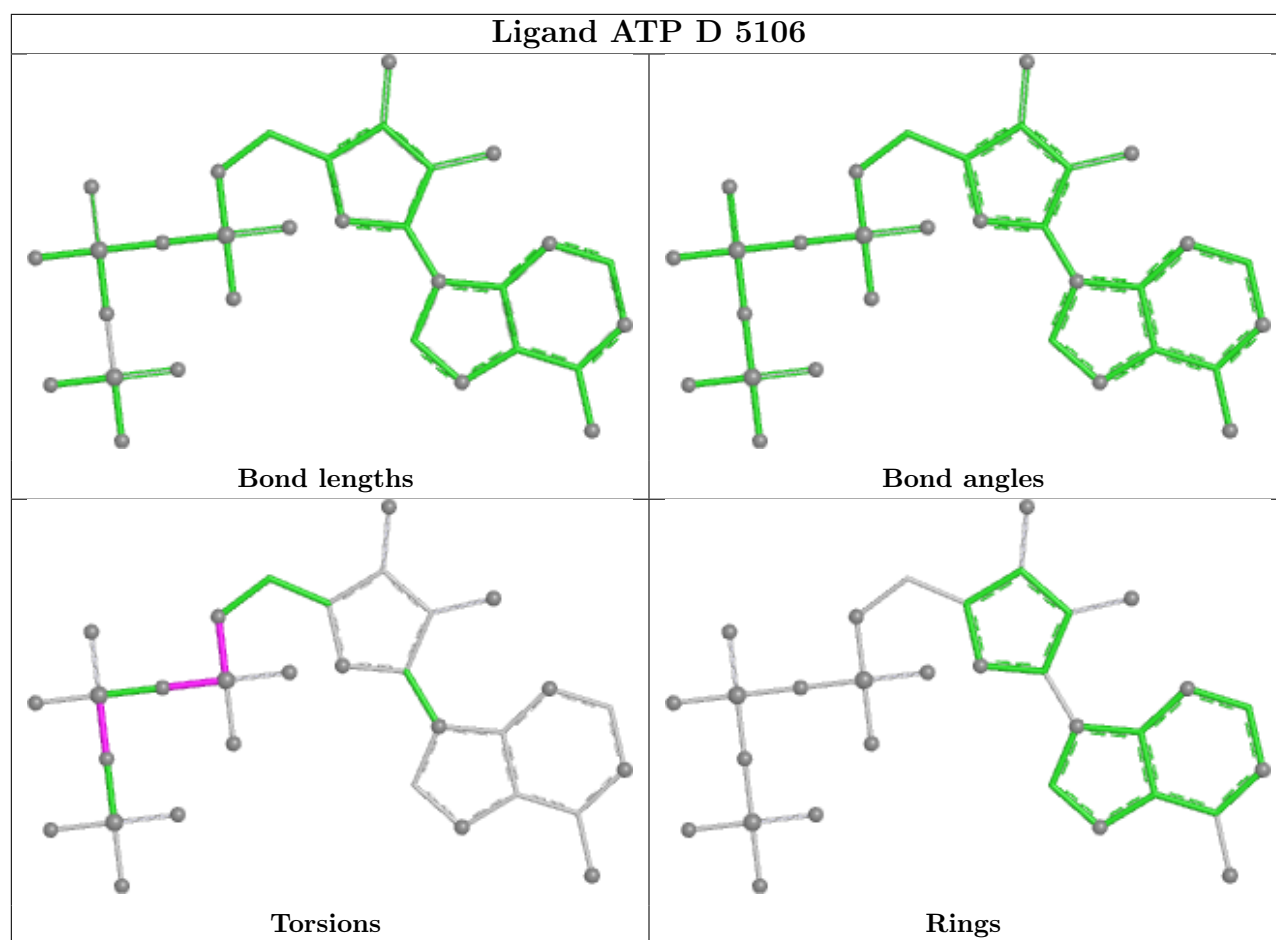




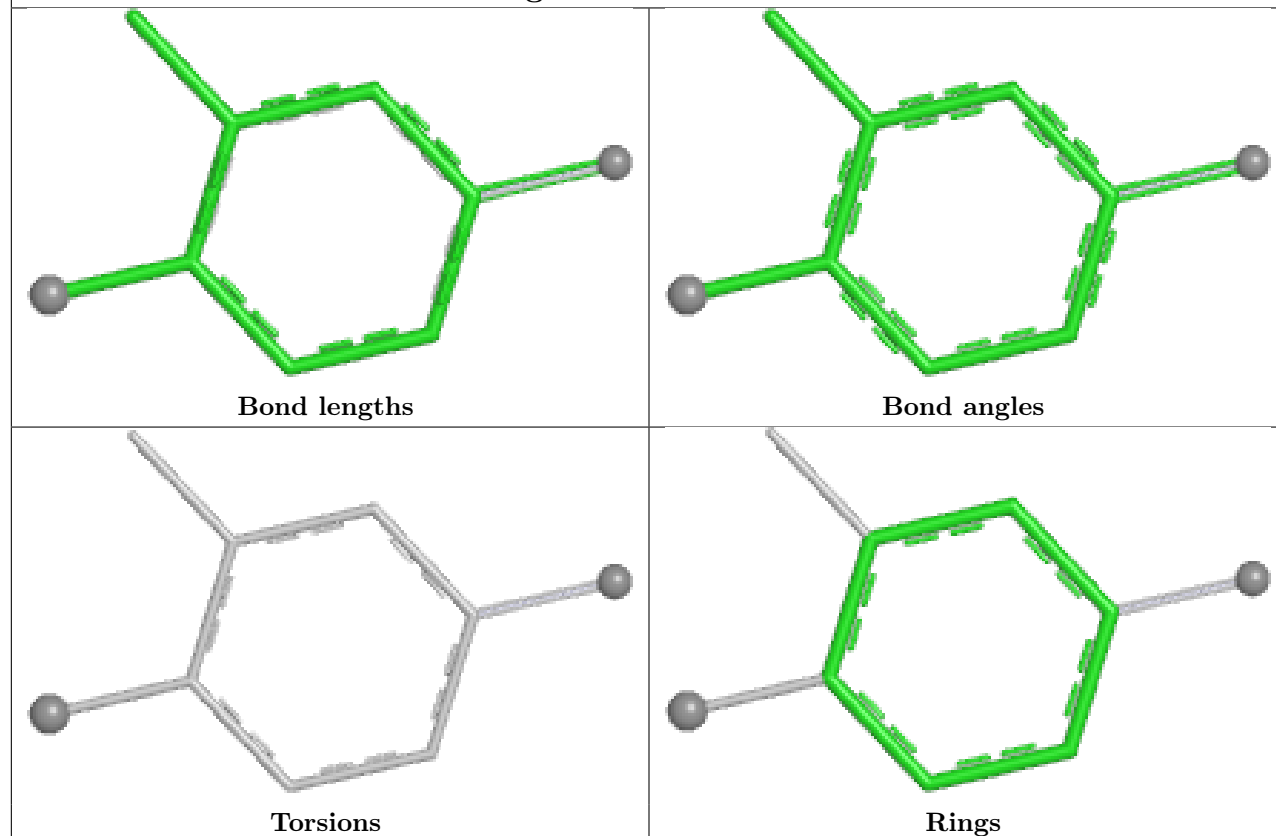




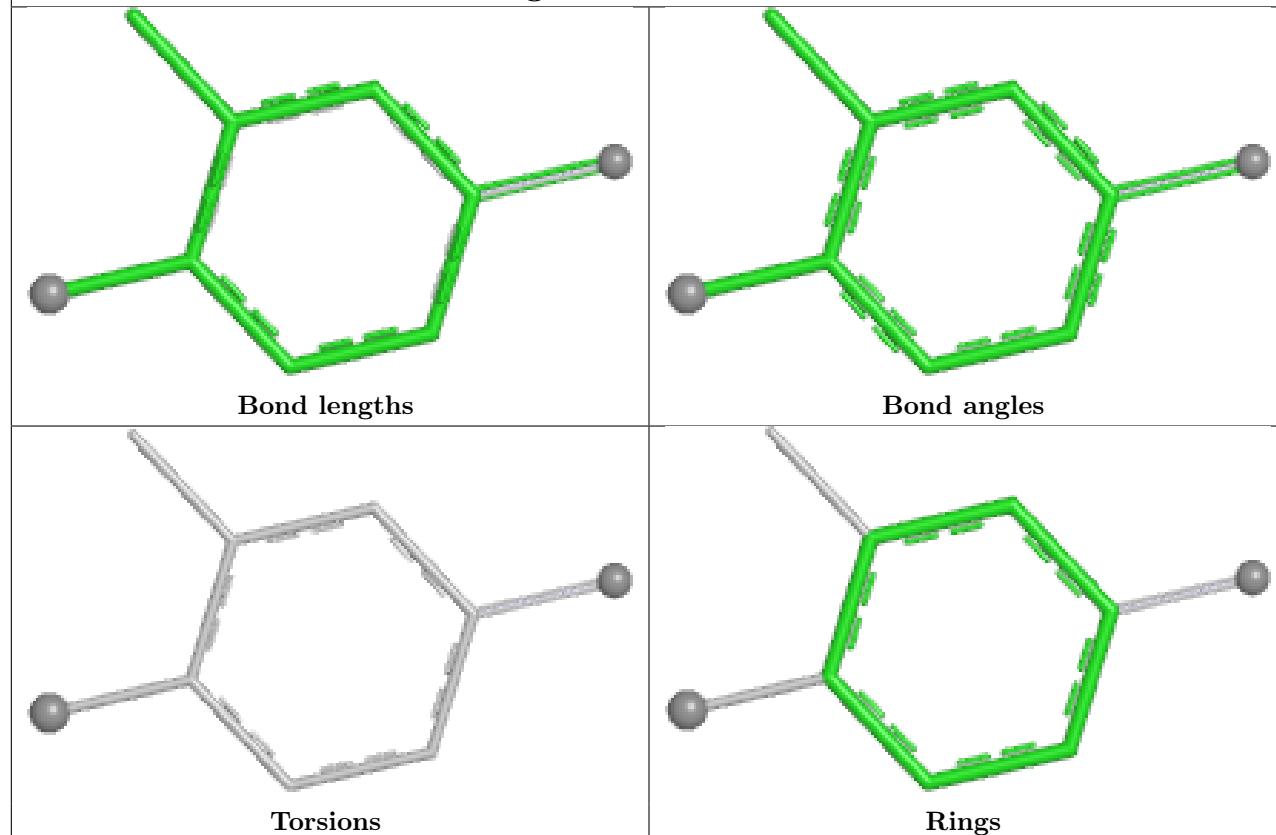


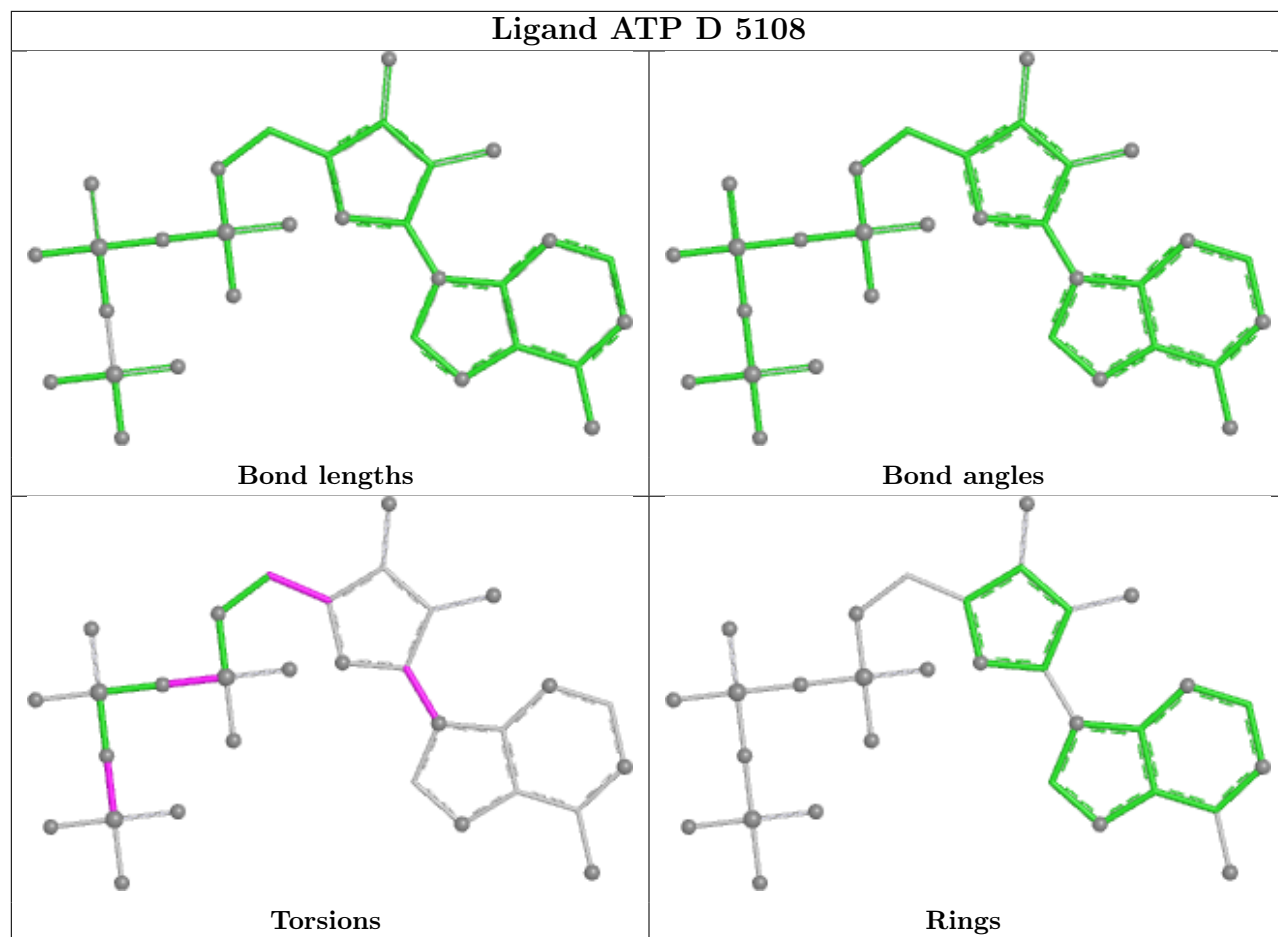


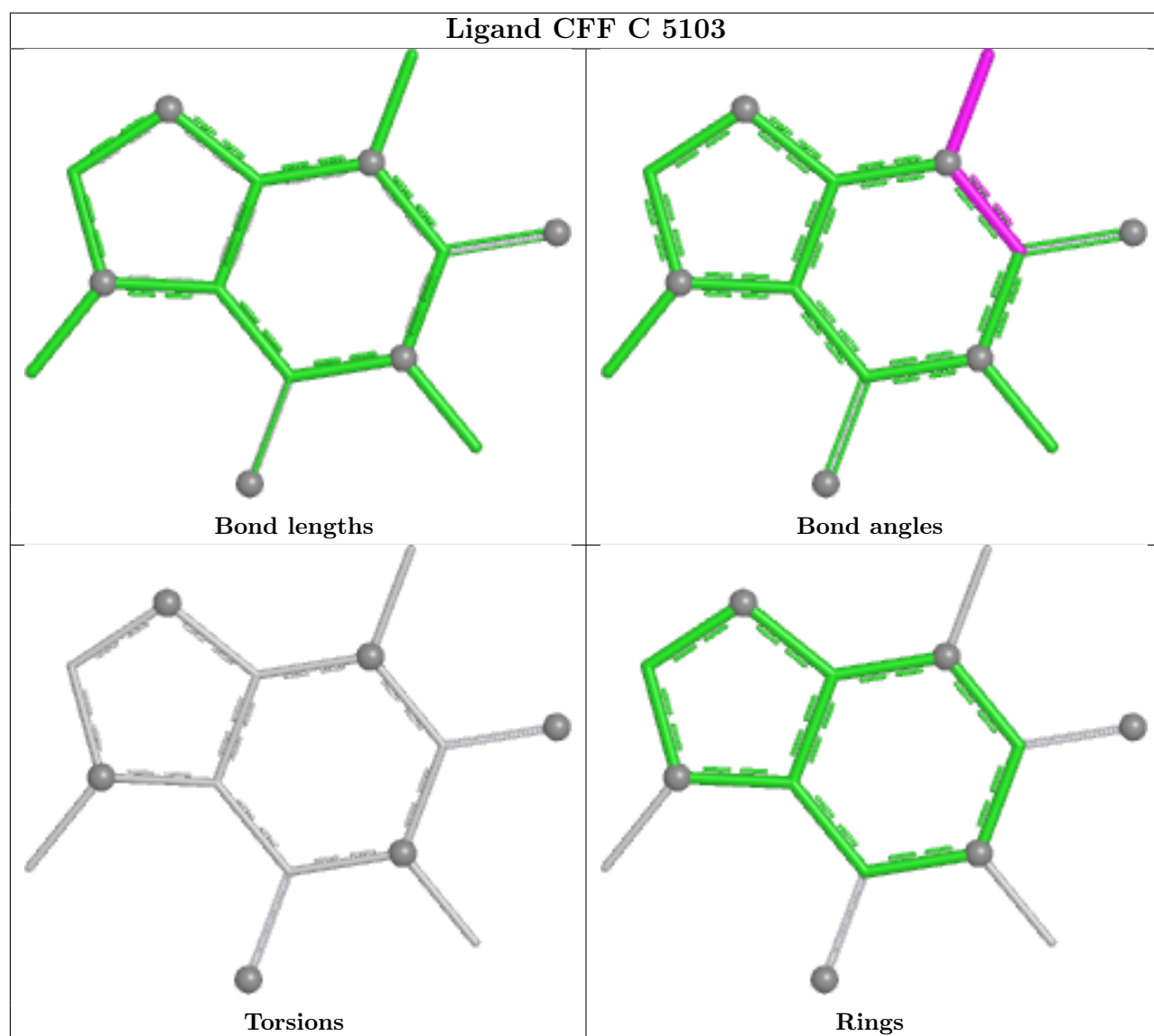
Ligand 43M B 5105

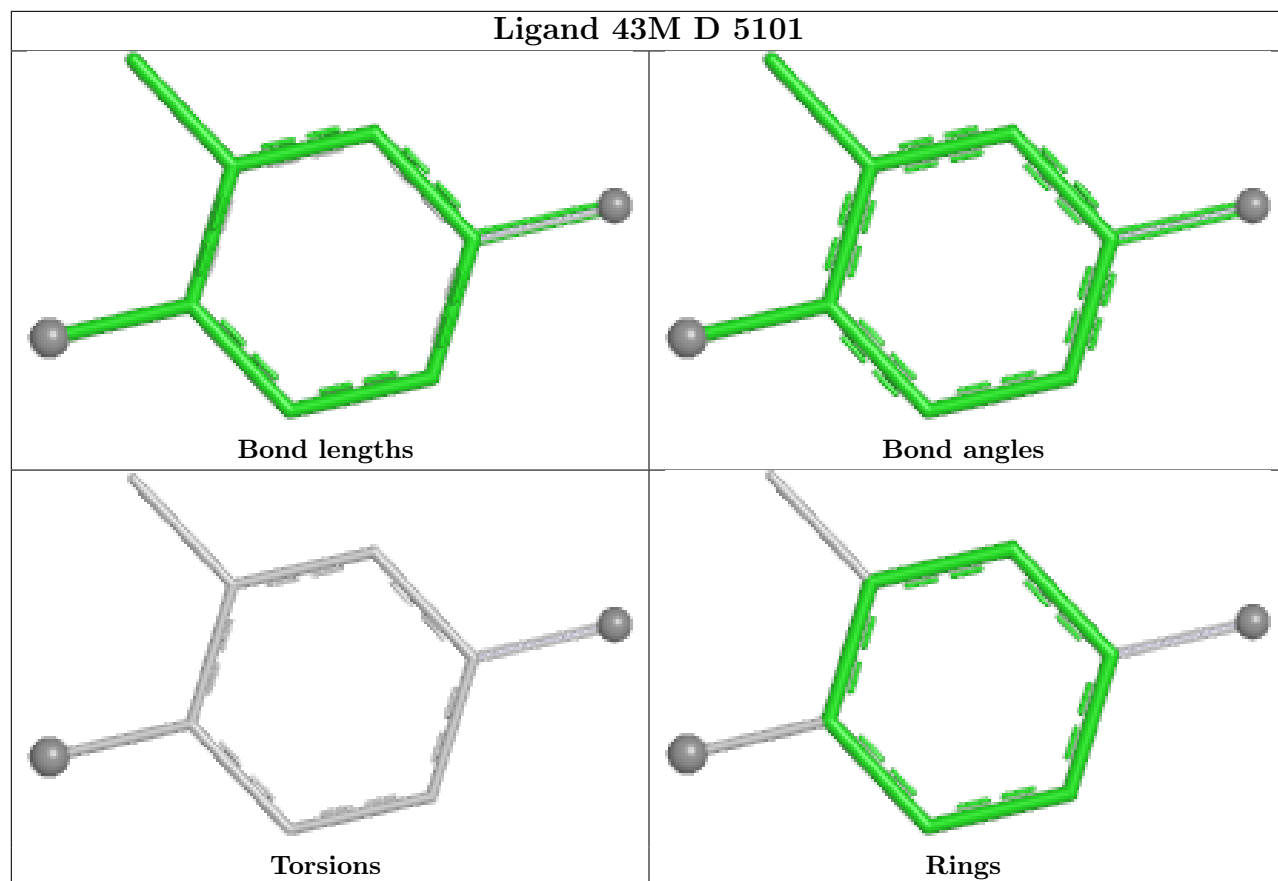


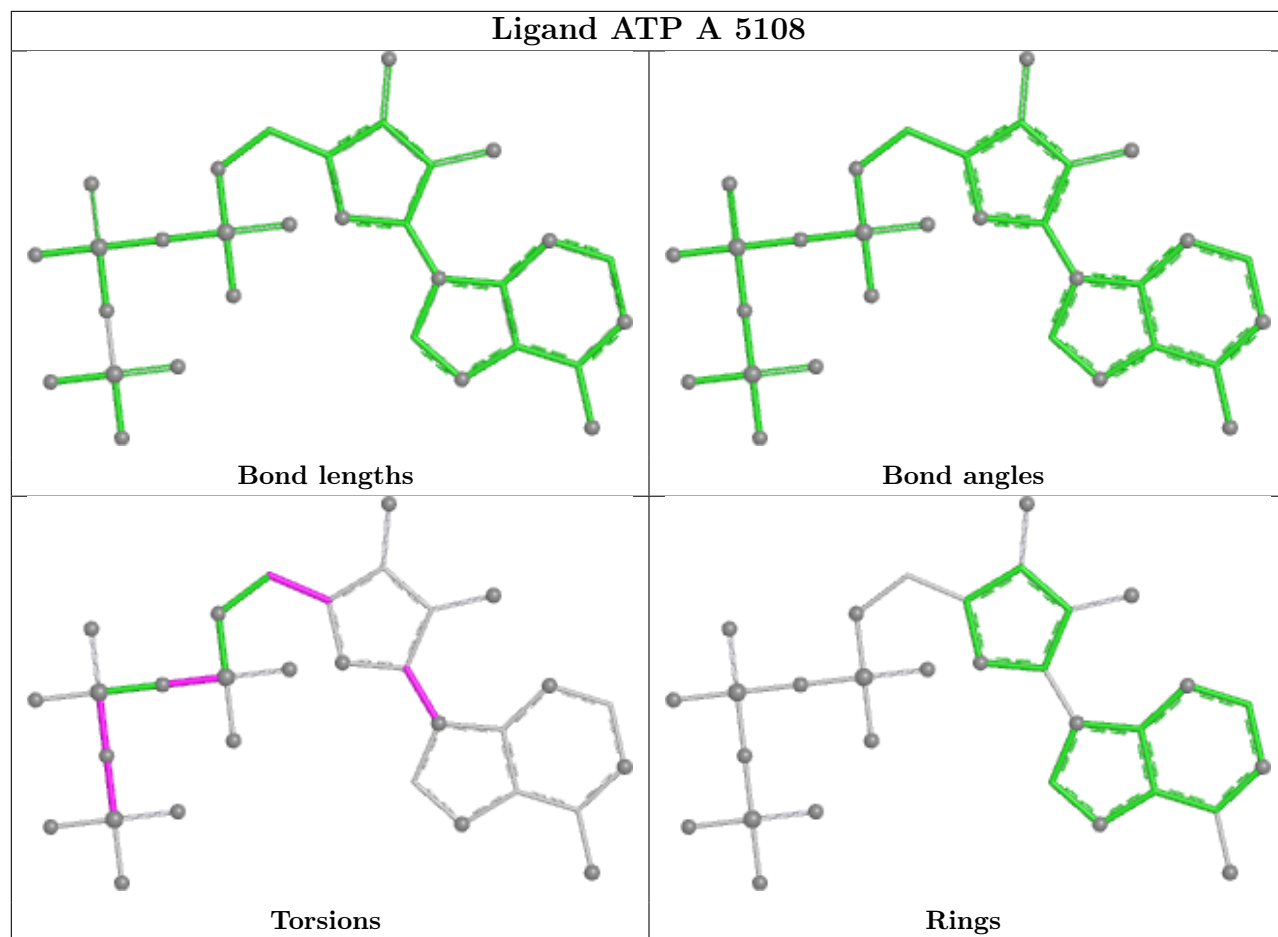
Ligand 43M C 5105

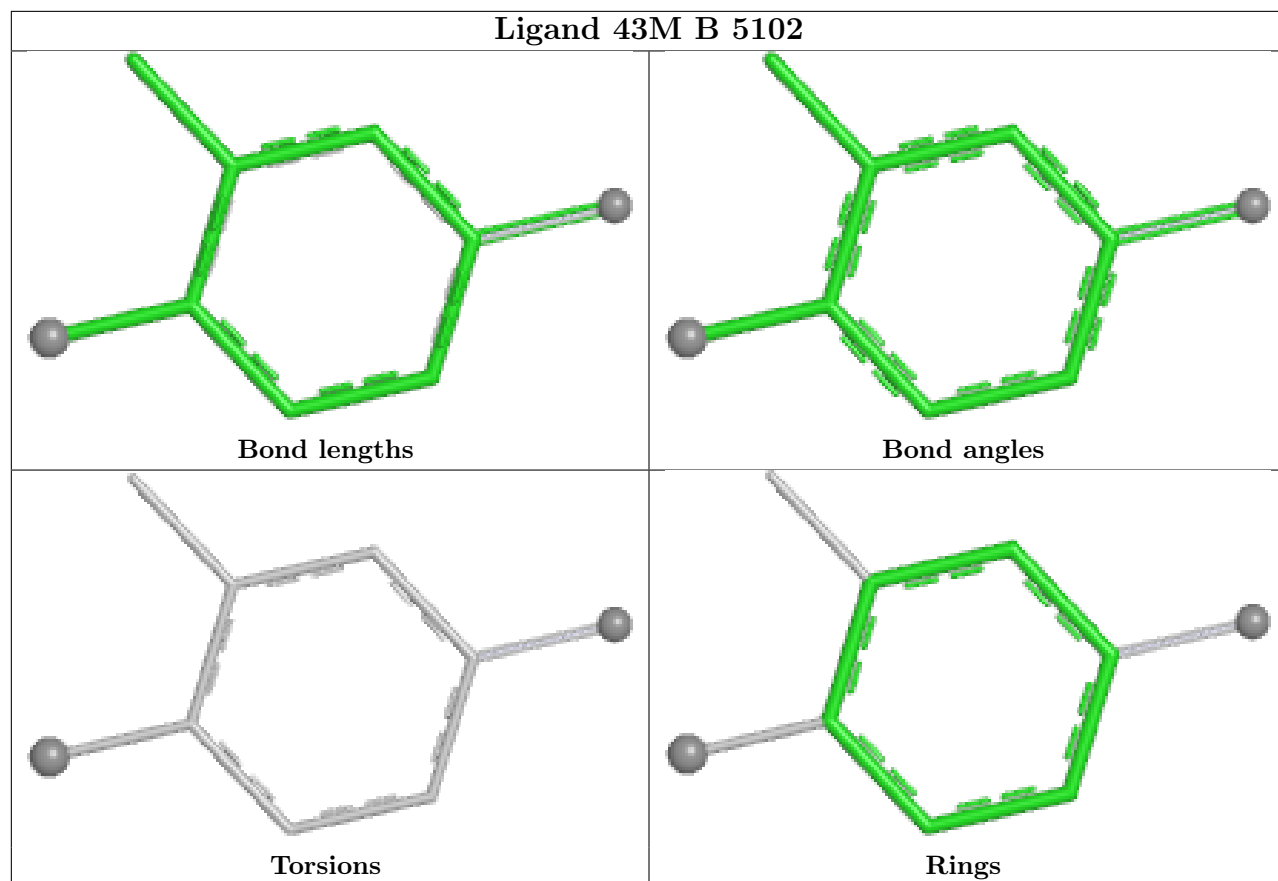


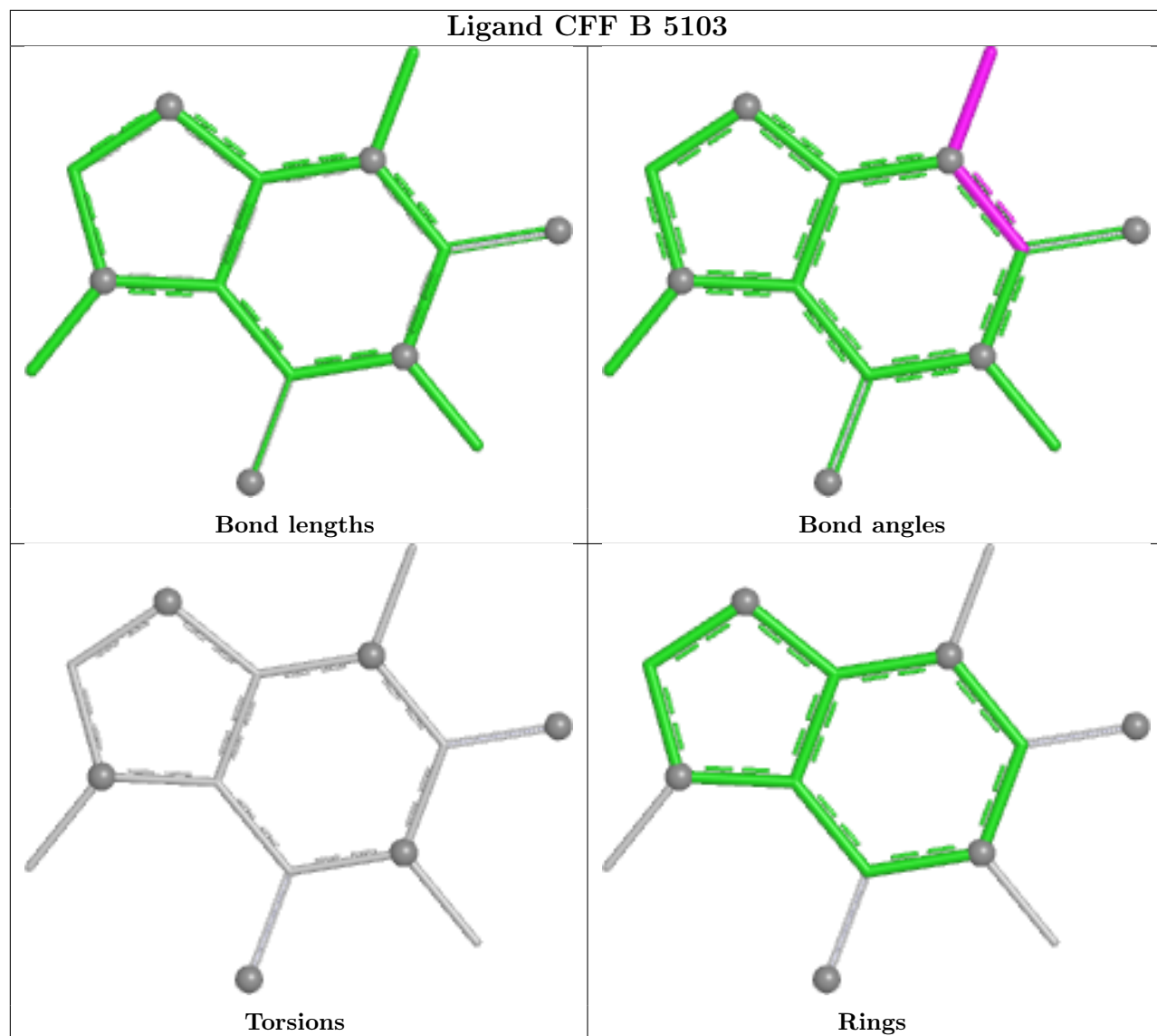


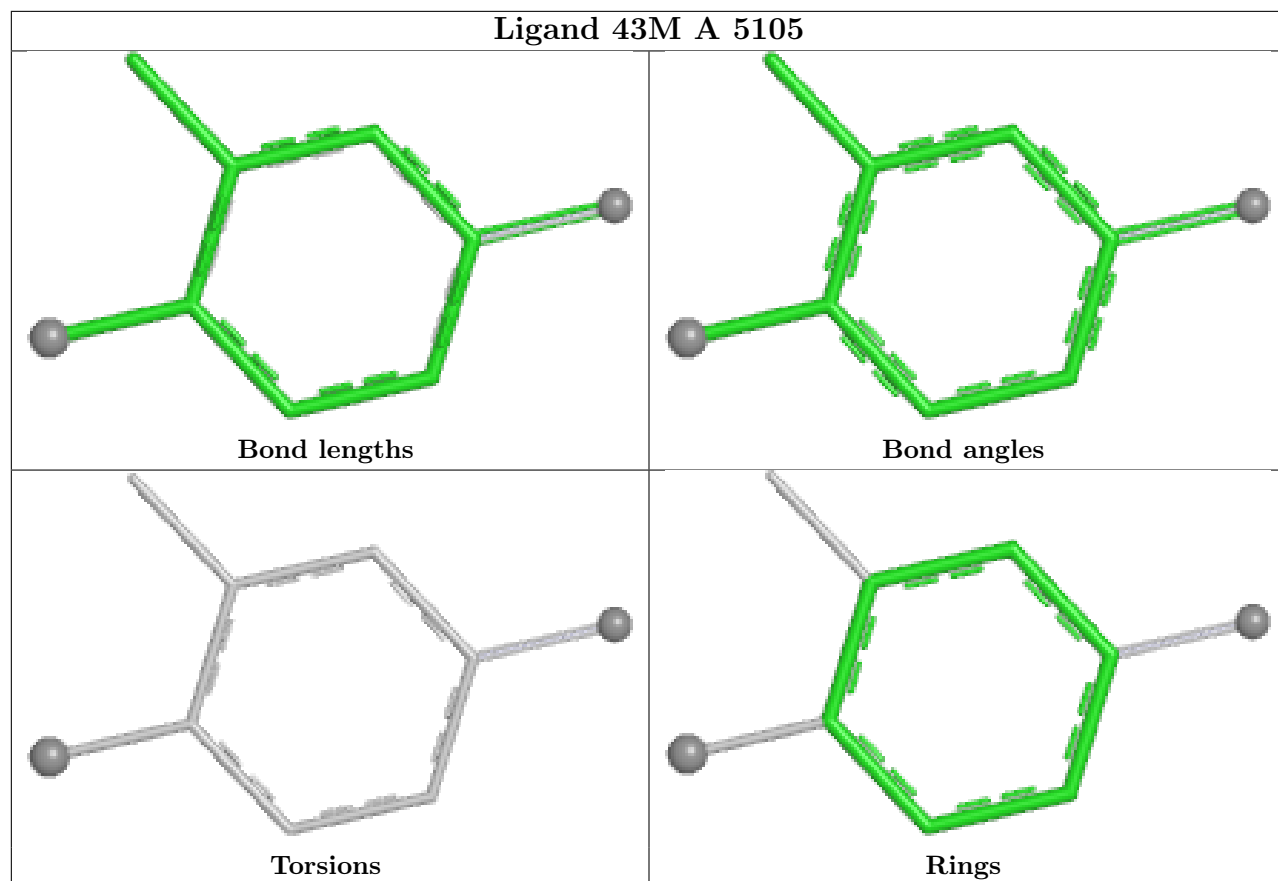


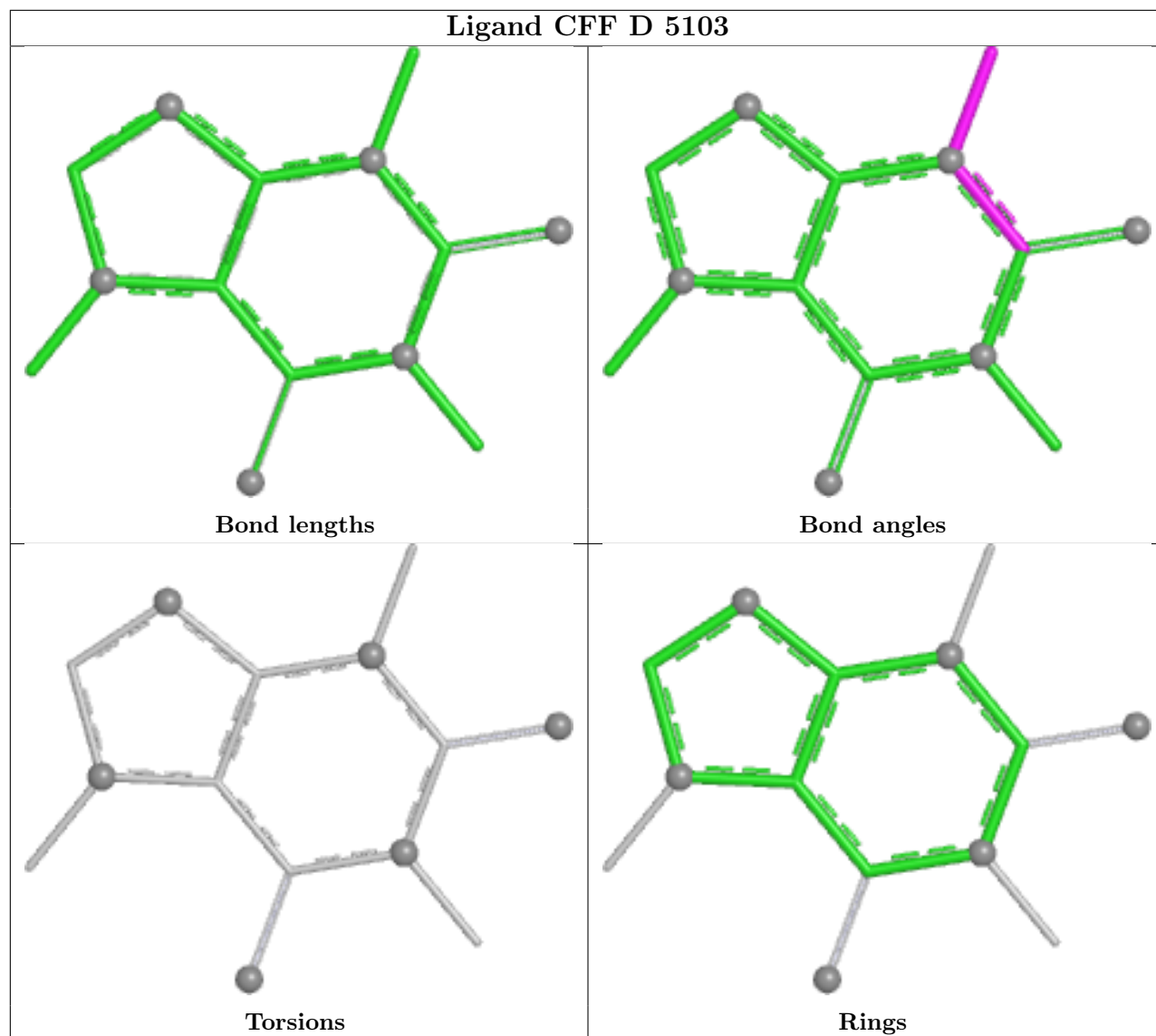




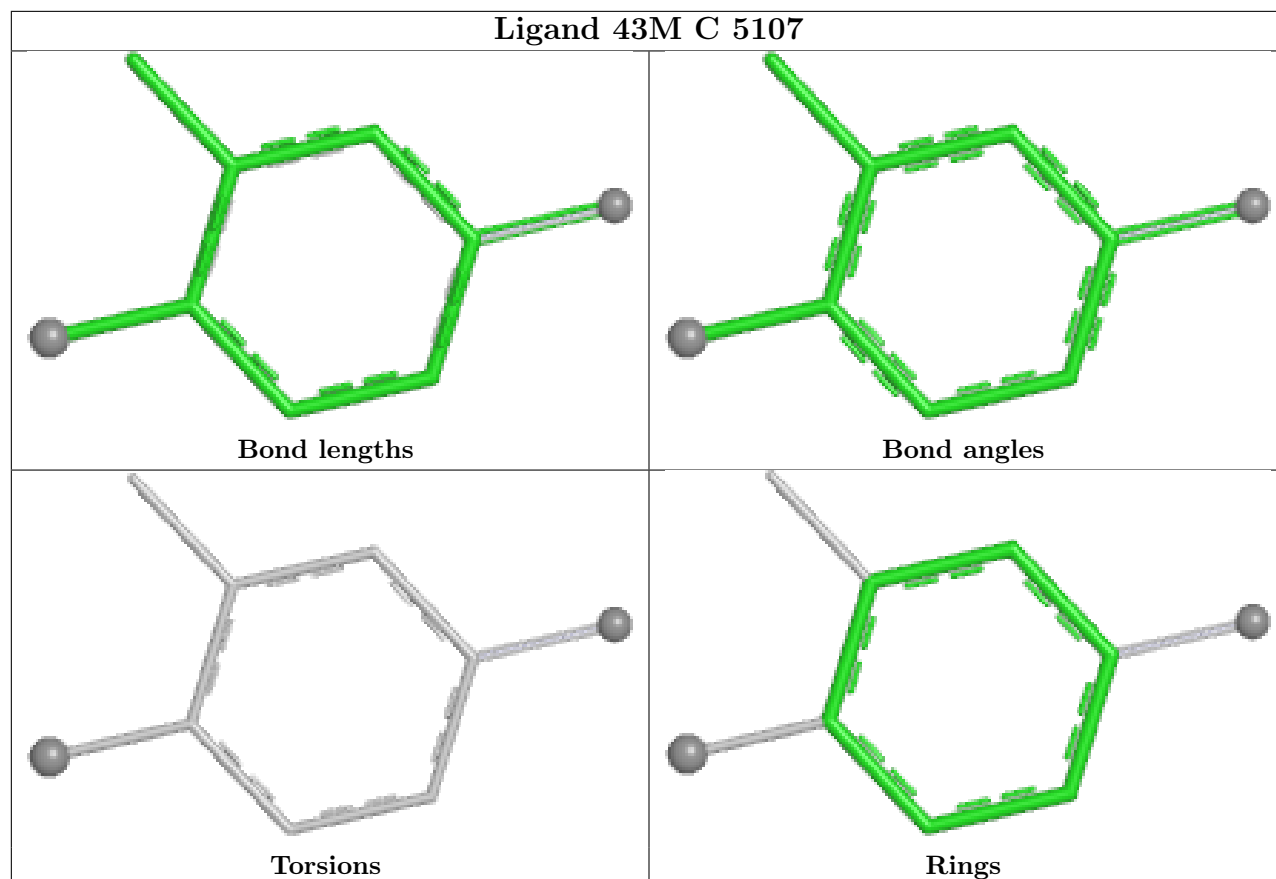




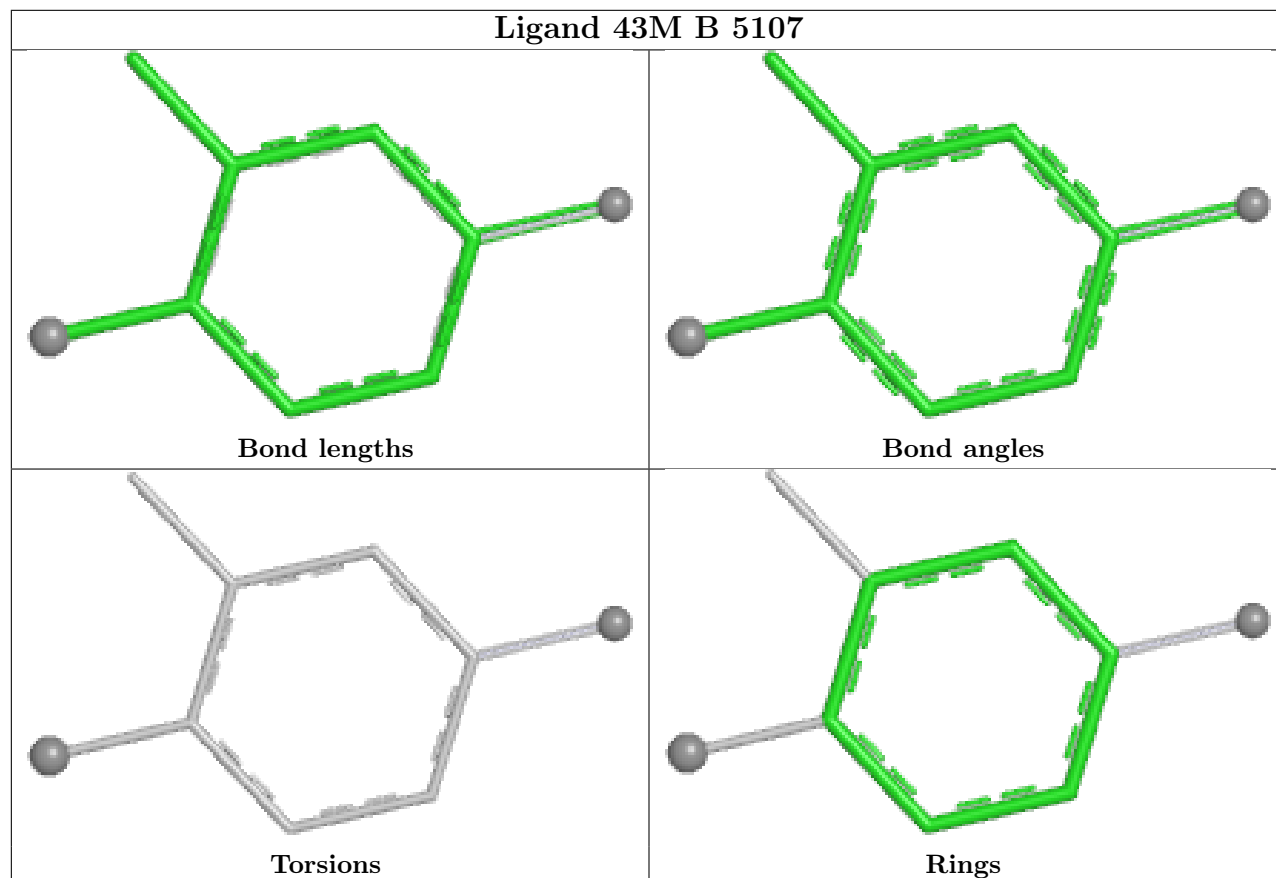


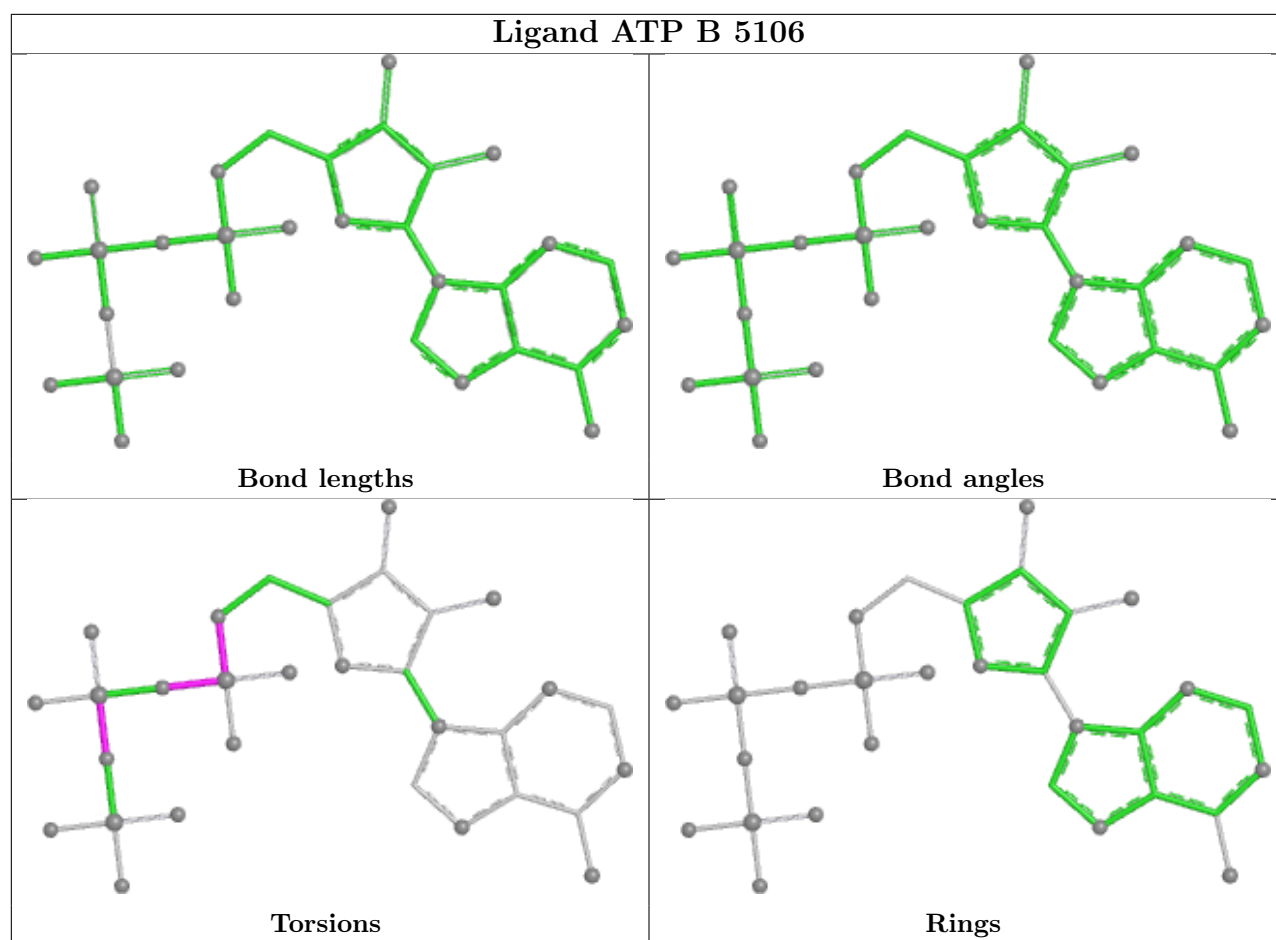


Ligand 43M C 5107



Ligand 43M B 5107





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.

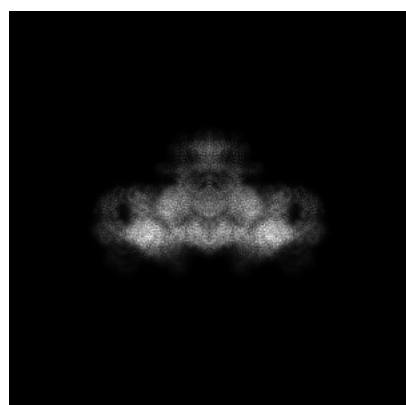
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74439. These allow visual inspection of the internal detail of the map and identification of artifacts.

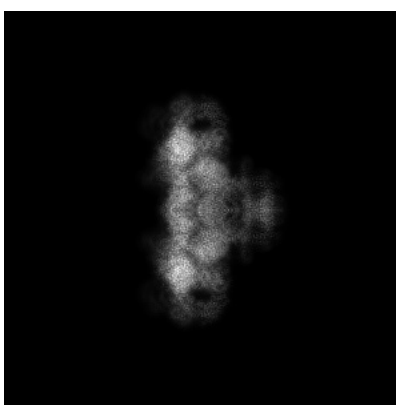
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

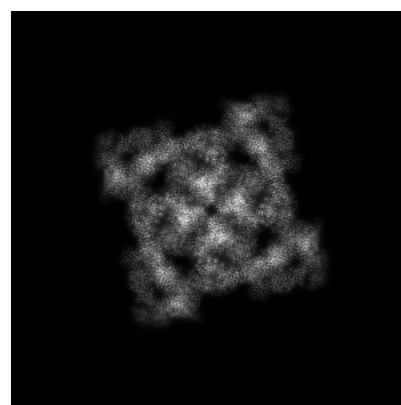
6.1.1 Primary map



X



Y

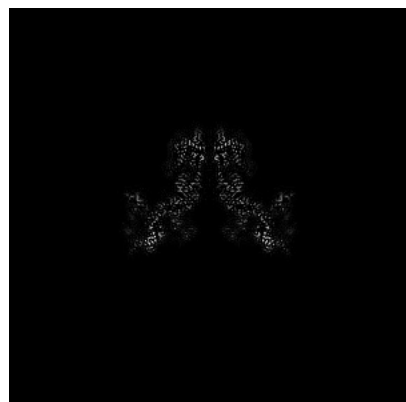


Z

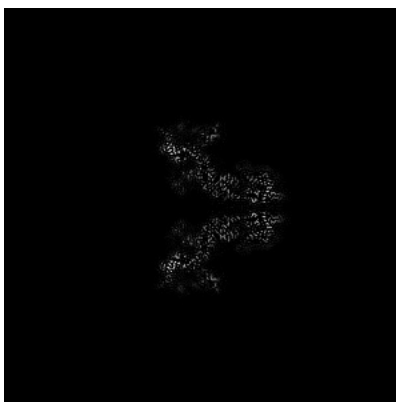
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

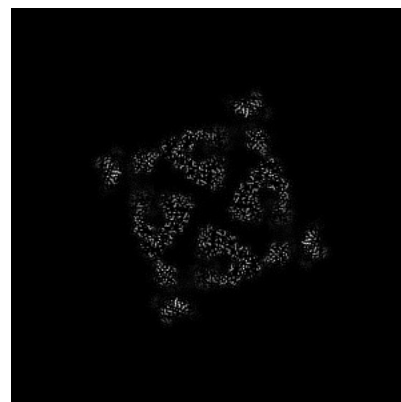
6.2.1 Primary map



X Index: 256



Y Index: 256

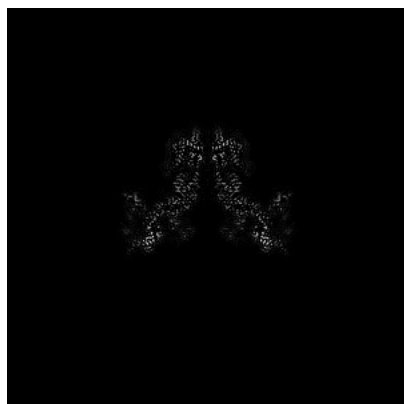


Z Index: 256

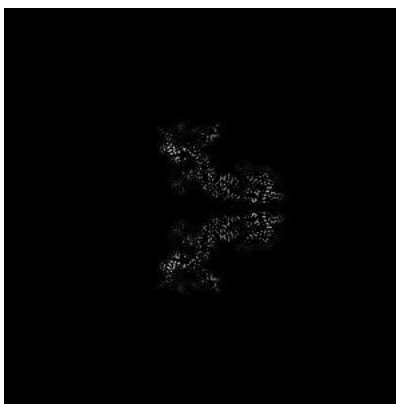
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

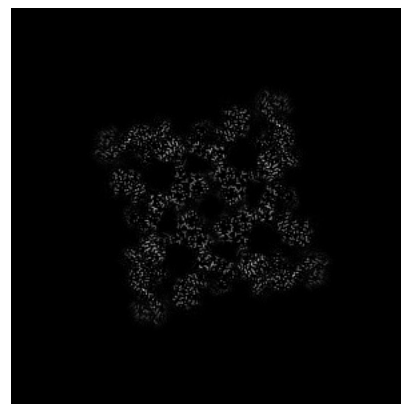
6.3.1 Primary map



X Index: 256



Y Index: 256

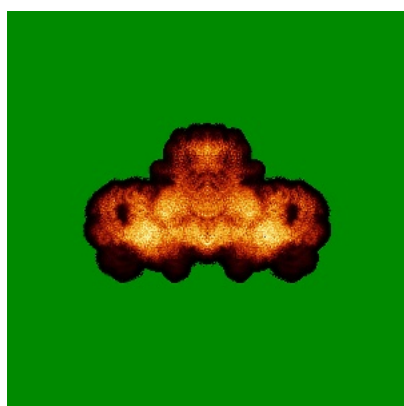


Z Index: 230

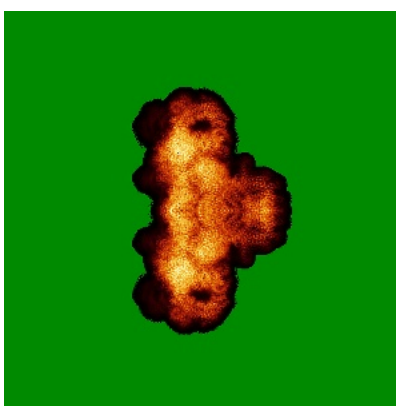
The images above show the largest variance slices of the map in three orthogonal directions.

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

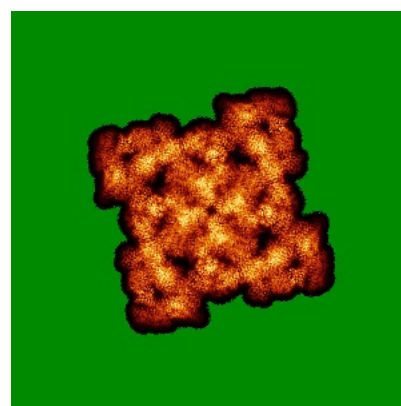
6.4.1 Primary map



X



Y

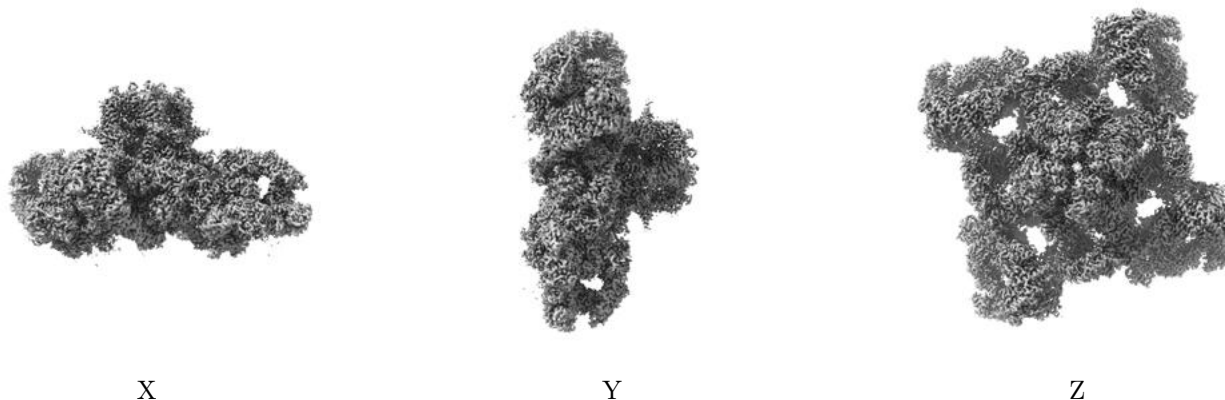


Z

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

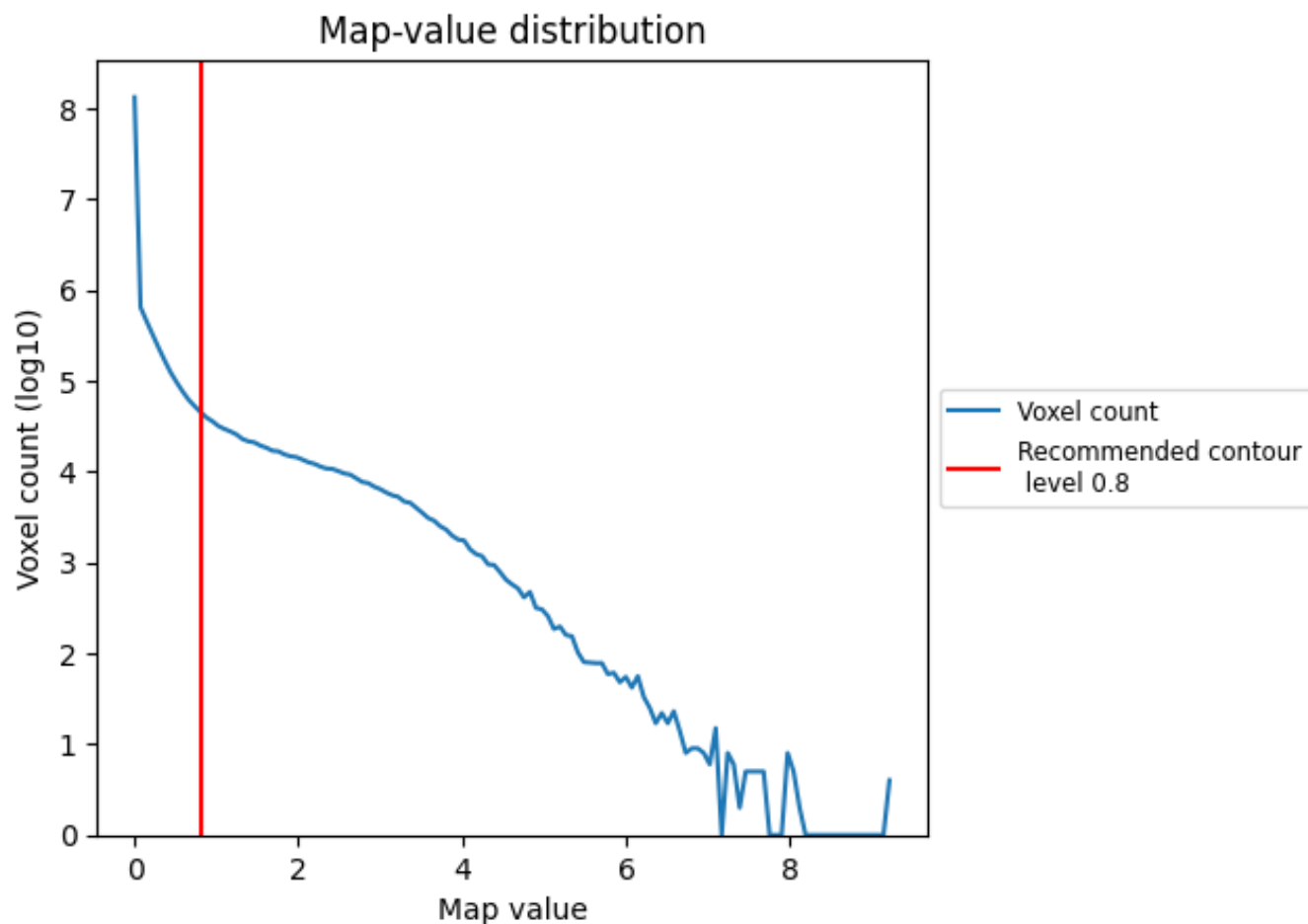
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

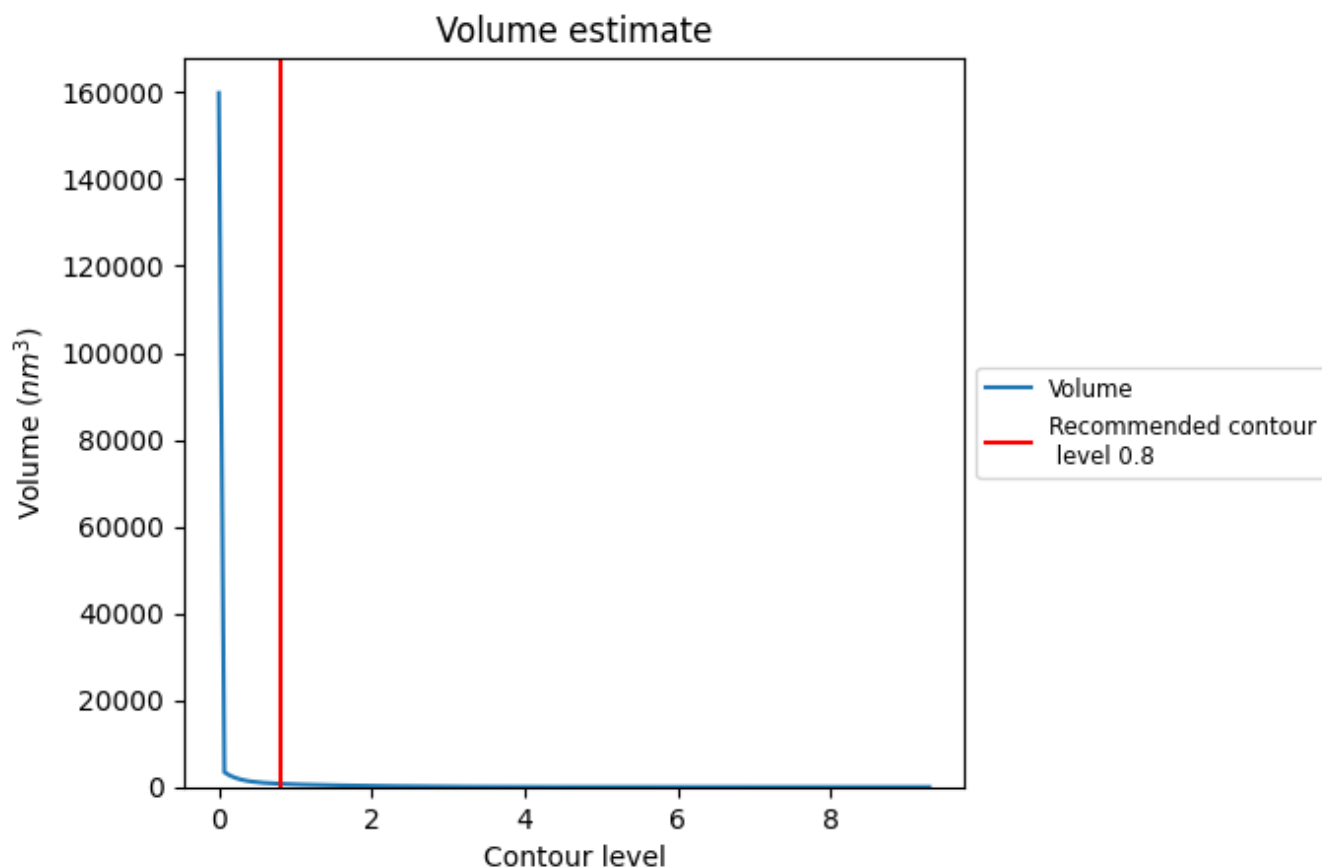
This section contains the results of statistical analysis of the map.

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.

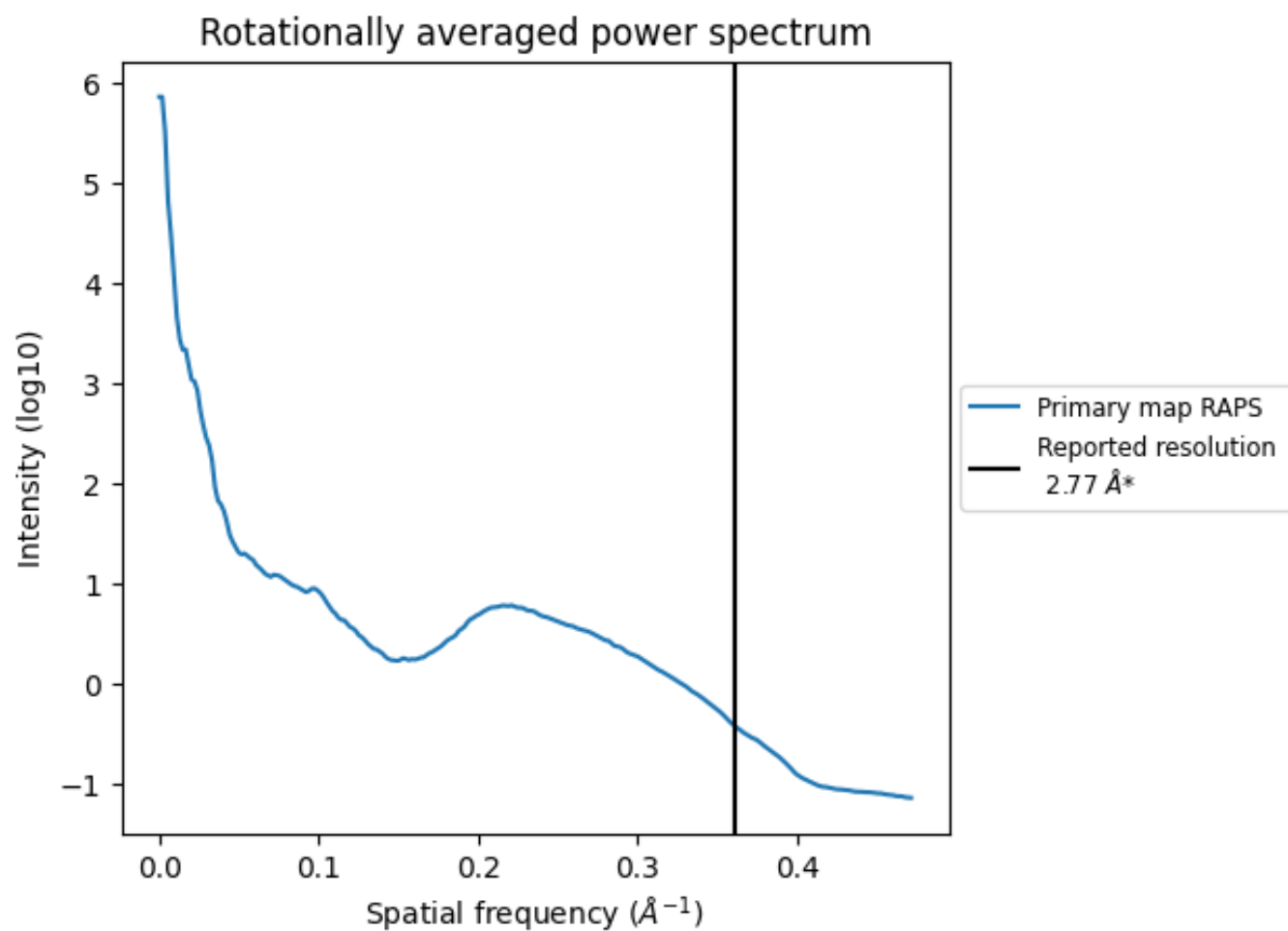
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 735 nm^3 ; this corresponds to an approximate mass of 664 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 0.361 Å⁻¹

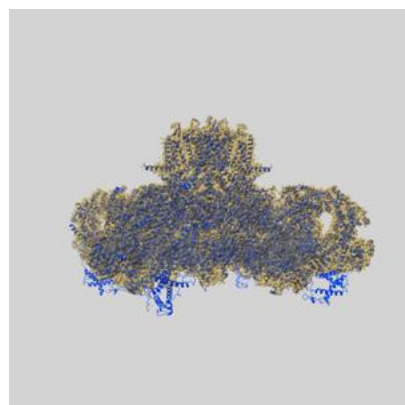
8 Fourier-Shell correlation ⓘ

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

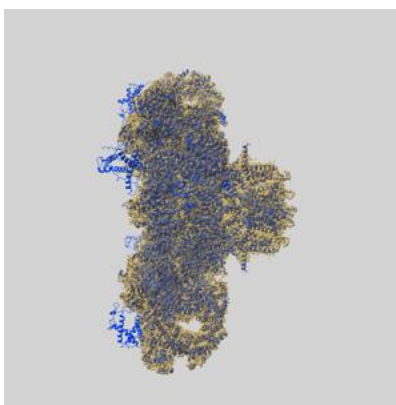
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74439 and PDB model 9ZN9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

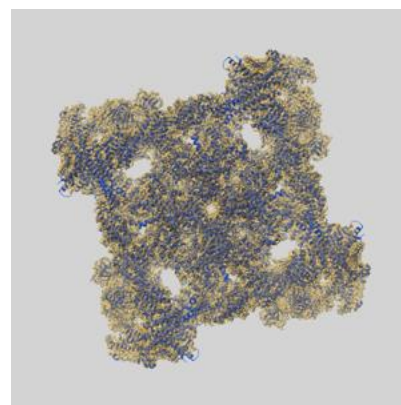
9.1 Map-model overlay [i](#)



X



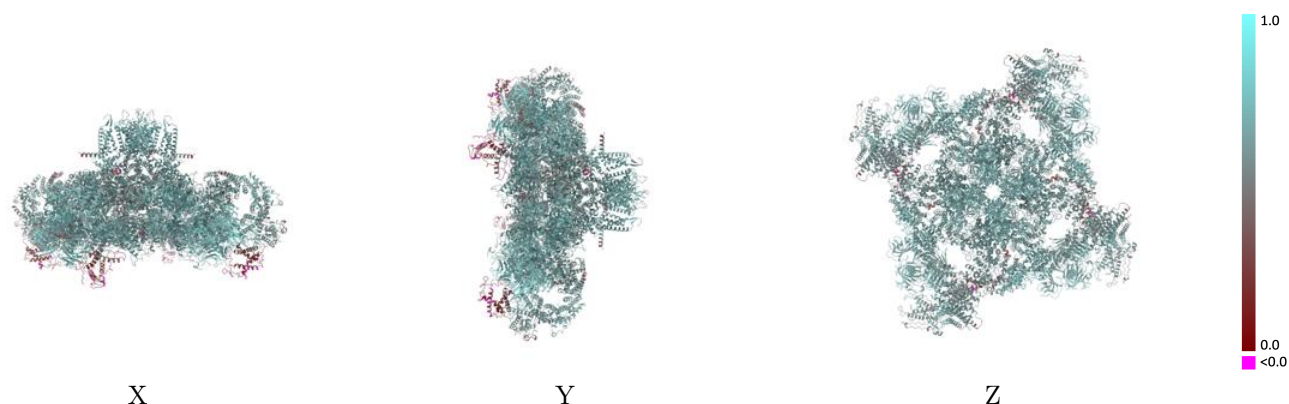
Y



Z

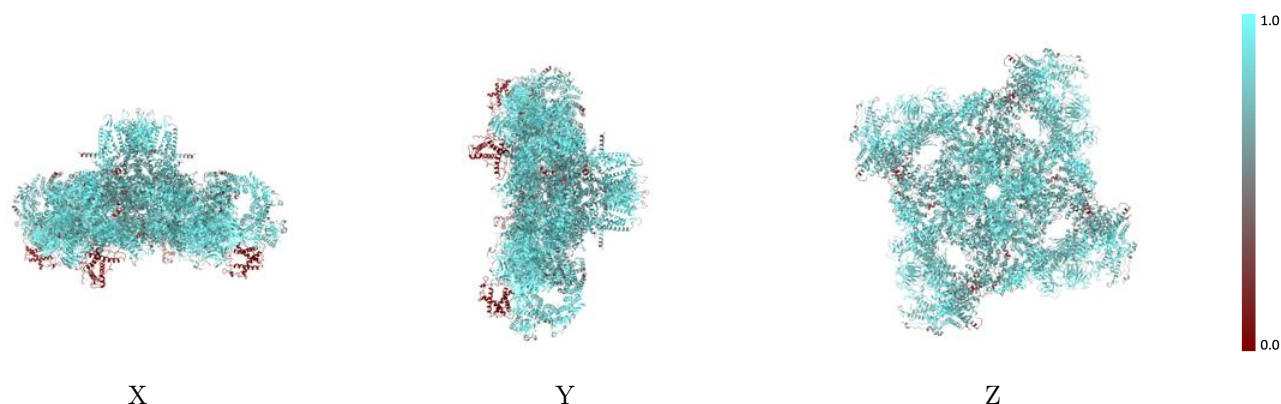
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



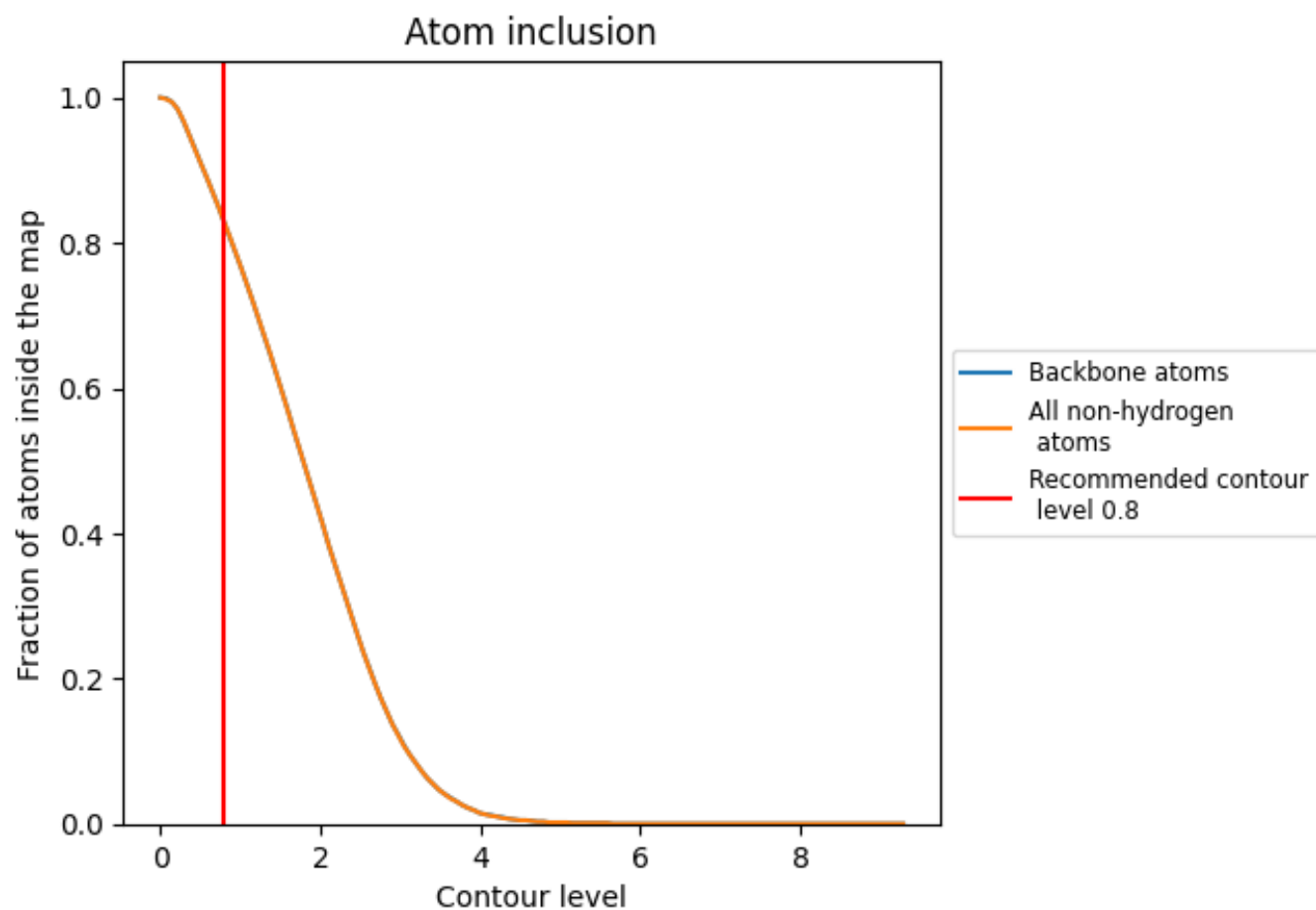
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.6170
A	0.8380	0.6200
B	0.8380	0.6190
C	0.8380	0.6190
D	0.8380	0.6190
E	0.9120	0.6580
F	0.9020	0.6550
G	0.9030	0.6560
H	0.9070	0.6560
I	0.5510	0.5010
J	0.5450	0.5020
K	0.5660	0.5100
L	0.5500	0.5020

1.0

0.0

<0.0