



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 01:54 AM JST

PDB ID : 7VNP  
EMDB ID : EMD-32044  
Title : Structure of human KCNQ4-ML213 complex with PIP2  
Authors : Xu, F.; Zheng, Y.  
Deposited on : 2021-10-11  
Resolution : 2.79 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](mailto: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>.

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

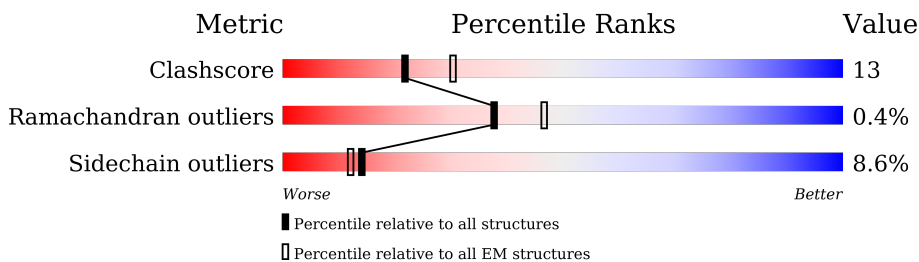
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 2.79 Å.

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



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

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	
1	C	1049	
1	E	1049	
1	G	1049	
2	B	149	
2	D	149	
2	F	149	
2	H	149	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 15196 atoms, of which 540 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 Potassium voltage-gated channel subfamily KQT member 4, Maltodextrin-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	332	2701	1773	474	442	12	0	0
1	C	332	2701	1773	474	442	12	0	0
1	E	332	2701	1773	474	442	12	0	0
1	G	332	2701	1773	474	442	12	0	0

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P56696
A	-6	ASP	-	expression tag	UNP P56696
A	-5	TYR	-	expression tag	UNP P56696
A	-4	LYS	-	expression tag	UNP P56696
A	-3	ASP	-	expression tag	UNP P56696
A	-2	ASP	-	expression tag	UNP P56696
A	-1	ASP	-	expression tag	UNP P56696
A	0	ASP	-	expression tag	UNP P56696
A	1	LYS	-	expression tag	UNP P56696
A	651	LEU	-	linker	UNP P56696
A	652	GLU	-	linker	UNP P56696
A	653	VAL	-	linker	UNP P56696
A	654	LEU	-	linker	UNP P56696
A	655	PHE	-	linker	UNP P56696
A	656	GLN	-	linker	UNP P56696
A	657	GLY	-	linker	UNP P56696
A	658	PRO	-	linker	UNP P56696
A	659	MET	-	linker	UNP P56696
A	1027	ASN	-	expression tag	UNP A0A140NCD0
A	1028	ALA	-	expression tag	UNP A0A140NCD0
A	1029	ALA	-	expression tag	UNP A0A140NCD0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1030	ALA	-	expression tag	UNP A0A140NCD0
A	1031	GLU	-	expression tag	UNP A0A140NCD0
A	1032	HIS	-	expression tag	UNP A0A140NCD0
A	1033	HIS	-	expression tag	UNP A0A140NCD0
A	1034	HIS	-	expression tag	UNP A0A140NCD0
A	1035	HIS	-	expression tag	UNP A0A140NCD0
A	1036	HIS	-	expression tag	UNP A0A140NCD0
A	1037	HIS	-	expression tag	UNP A0A140NCD0
A	1038	HIS	-	expression tag	UNP A0A140NCD0
A	1039	HIS	-	expression tag	UNP A0A140NCD0
A	1040	HIS	-	expression tag	UNP A0A140NCD0
A	1041	HIS	-	expression tag	UNP A0A140NCD0
C	-7	MET	-	initiating methionine	UNP P56696
C	-6	ASP	-	expression tag	UNP P56696
C	-5	TYR	-	expression tag	UNP P56696
C	-4	LYS	-	expression tag	UNP P56696
C	-3	ASP	-	expression tag	UNP P56696
C	-2	ASP	-	expression tag	UNP P56696
C	-1	ASP	-	expression tag	UNP P56696
C	0	ASP	-	expression tag	UNP P56696
C	1	LYS	-	expression tag	UNP P56696
C	651	LEU	-	linker	UNP P56696
C	652	GLU	-	linker	UNP P56696
C	653	VAL	-	linker	UNP P56696
C	654	LEU	-	linker	UNP P56696
C	655	PHE	-	linker	UNP P56696
C	656	GLN	-	linker	UNP P56696
C	657	GLY	-	linker	UNP P56696
C	658	PRO	-	linker	UNP P56696
C	659	MET	-	linker	UNP P56696
C	1027	ASN	-	expression tag	UNP A0A140NCD0
C	1028	ALA	-	expression tag	UNP A0A140NCD0
C	1029	ALA	-	expression tag	UNP A0A140NCD0
C	1030	ALA	-	expression tag	UNP A0A140NCD0
C	1031	GLU	-	expression tag	UNP A0A140NCD0
C	1032	HIS	-	expression tag	UNP A0A140NCD0
C	1033	HIS	-	expression tag	UNP A0A140NCD0
C	1034	HIS	-	expression tag	UNP A0A140NCD0
C	1035	HIS	-	expression tag	UNP A0A140NCD0
C	1036	HIS	-	expression tag	UNP A0A140NCD0
C	1037	HIS	-	expression tag	UNP A0A140NCD0
C	1038	HIS	-	expression tag	UNP A0A140NCD0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1039	HIS	-	expression tag	UNP A0A140NCD0
C	1040	HIS	-	expression tag	UNP A0A140NCD0
C	1041	HIS	-	expression tag	UNP A0A140NCD0
E	-7	MET	-	initiating methionine	UNP P56696
E	-6	ASP	-	expression tag	UNP P56696
E	-5	TYR	-	expression tag	UNP P56696
E	-4	LYS	-	expression tag	UNP P56696
E	-3	ASP	-	expression tag	UNP P56696
E	-2	ASP	-	expression tag	UNP P56696
E	-1	ASP	-	expression tag	UNP P56696
E	0	ASP	-	expression tag	UNP P56696
E	1	LYS	-	expression tag	UNP P56696
E	651	LEU	-	linker	UNP P56696
E	652	GLU	-	linker	UNP P56696
E	653	VAL	-	linker	UNP P56696
E	654	LEU	-	linker	UNP P56696
E	655	PHE	-	linker	UNP P56696
E	656	GLN	-	linker	UNP P56696
E	657	GLY	-	linker	UNP P56696
E	658	PRO	-	linker	UNP P56696
E	659	MET	-	linker	UNP P56696
E	1027	ASN	-	expression tag	UNP A0A140NCD0
E	1028	ALA	-	expression tag	UNP A0A140NCD0
E	1029	ALA	-	expression tag	UNP A0A140NCD0
E	1030	ALA	-	expression tag	UNP A0A140NCD0
E	1031	GLU	-	expression tag	UNP A0A140NCD0
E	1032	HIS	-	expression tag	UNP A0A140NCD0
E	1033	HIS	-	expression tag	UNP A0A140NCD0
E	1034	HIS	-	expression tag	UNP A0A140NCD0
E	1035	HIS	-	expression tag	UNP A0A140NCD0
E	1036	HIS	-	expression tag	UNP A0A140NCD0
E	1037	HIS	-	expression tag	UNP A0A140NCD0
E	1038	HIS	-	expression tag	UNP A0A140NCD0
E	1039	HIS	-	expression tag	UNP A0A140NCD0
E	1040	HIS	-	expression tag	UNP A0A140NCD0
E	1041	HIS	-	expression tag	UNP A0A140NCD0
G	-7	MET	-	initiating methionine	UNP P56696
G	-6	ASP	-	expression tag	UNP P56696
G	-5	TYR	-	expression tag	UNP P56696
G	-4	LYS	-	expression tag	UNP P56696
G	-3	ASP	-	expression tag	UNP P56696
G	-2	ASP	-	expression tag	UNP P56696

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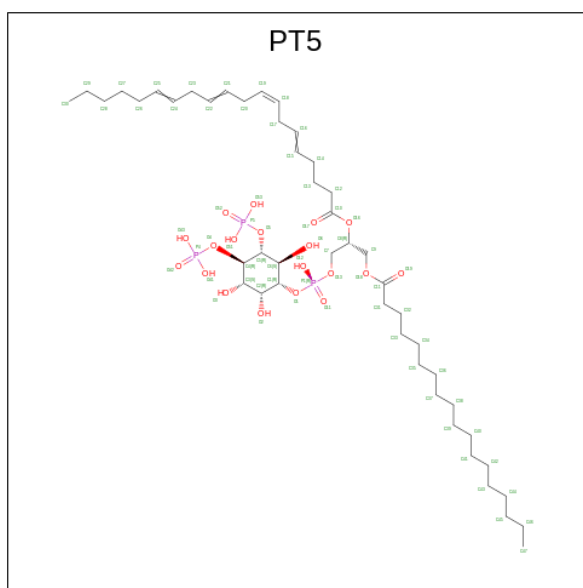
Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	ASP	-	expression tag	UNP P56696
G	0	ASP	-	expression tag	UNP P56696
G	1	LYS	-	expression tag	UNP P56696
G	651	LEU	-	linker	UNP P56696
G	652	GLU	-	linker	UNP P56696
G	653	VAL	-	linker	UNP P56696
G	654	LEU	-	linker	UNP P56696
G	655	PHE	-	linker	UNP P56696
G	656	GLN	-	linker	UNP P56696
G	657	GLY	-	linker	UNP P56696
G	658	PRO	-	linker	UNP P56696
G	659	MET	-	linker	UNP P56696
G	1027	ASN	-	expression tag	UNP A0A140NCD0
G	1028	ALA	-	expression tag	UNP A0A140NCD0
G	1029	ALA	-	expression tag	UNP A0A140NCD0
G	1030	ALA	-	expression tag	UNP A0A140NCD0
G	1031	GLU	-	expression tag	UNP A0A140NCD0
G	1032	HIS	-	expression tag	UNP A0A140NCD0
G	1033	HIS	-	expression tag	UNP A0A140NCD0
G	1034	HIS	-	expression tag	UNP A0A140NCD0
G	1035	HIS	-	expression tag	UNP A0A140NCD0
G	1036	HIS	-	expression tag	UNP A0A140NCD0
G	1037	HIS	-	expression tag	UNP A0A140NCD0
G	1038	HIS	-	expression tag	UNP A0A140NCD0
G	1039	HIS	-	expression tag	UNP A0A140NCD0
G	1040	HIS	-	expression tag	UNP A0A140NCD0
G	1041	HIS	-	expression tag	UNP A0A140NCD0

- Molecule 2 is a protein called Calmodulin-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	144	Total	C	N	O	S	0	0
			828	520	154	152	2		
2	D	144	Total	C	N	O	S	0	0
			828	520	154	152	2		
2	F	144	Total	C	N	O	S	0	0
			828	520	154	152	2		
2	H	144	Total	C	N	O	S	0	0
			828	520	154	152	2		

- Molecule 3 is [(2R)-1-octadecanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (8Z)-icosa-5,8,11,14-tetraenoate (three-letter code: PT5) (formula: C<sub>47</sub>H<sub>85</sub>O<sub>19</sub>P<sub>3</sub>) (labeled as "Ligand of Interest")

by depositor).

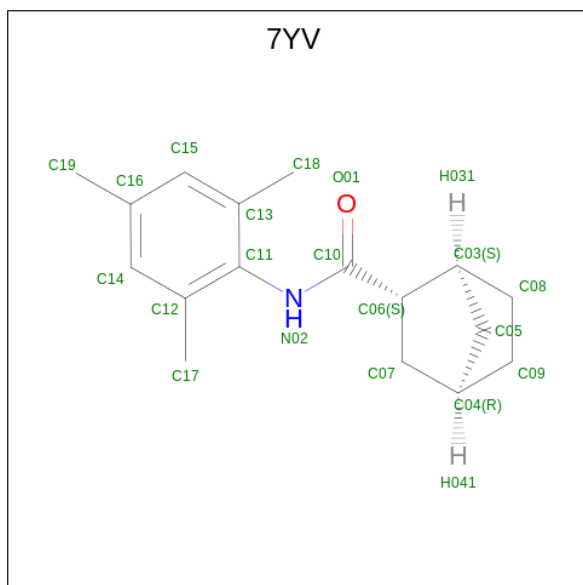


Mol	Chain	Residues	Atoms				AltConf	
			Total	C	H	O		P
3	A	1	227	71	112	38	6	0
3	A	1	227	71	112	38	6	0
3	C	1	227	71	112	38	6	0
3	C	1	227	71	112	38	6	0
3	E	1	227	71	112	38	6	0
3	E	1	227	71	112	38	6	0
3	G	1	227	71	112	38	6	0
3	G	1	227	71	112	38	6	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
4	A	4	Total	K	0
			4	4	

- Molecule 5 is (1S,2S,4R)-N-(2,4,6-trimethylphenyl)bicyclo[2.2.1]heptane-2-carboxamid (three-letter code: 7YV) (formula: C<sub>17</sub>H<sub>23</sub>NO).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
5	A	1	Total	C	H	N	O	0
			84	34	46	2	2	
5	A	1	Total	C	H	N	O	0
			84	34	46	2	2	
5	C	1	Total	C	H	N	O	0
			42	17	23	1	1	
5	E	1	Total	C	H	N	O	0
			42	17	23	1	1	



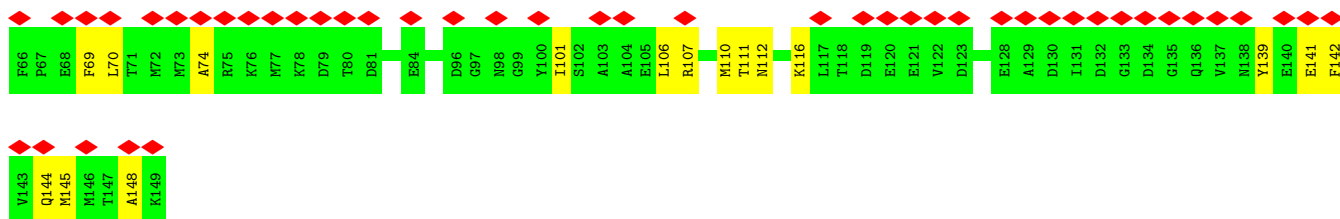




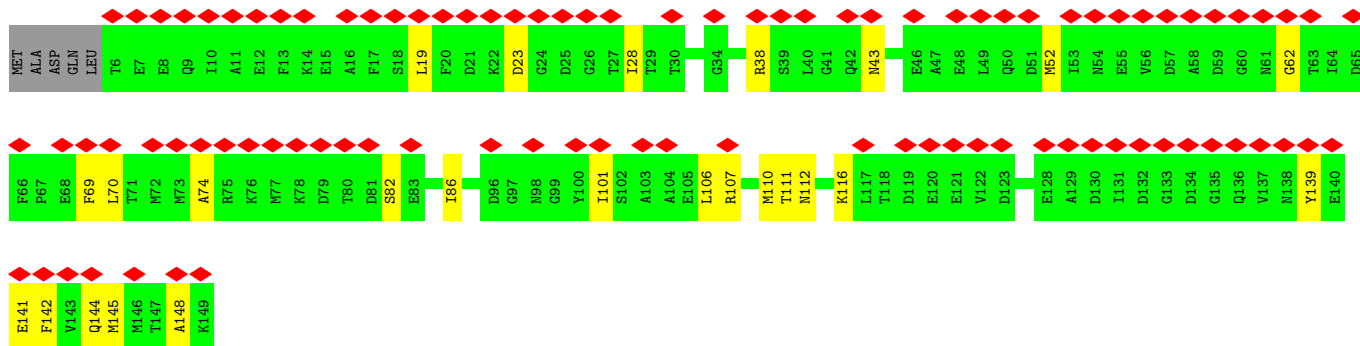
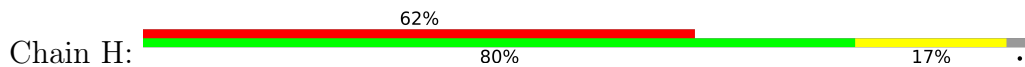








• Molecule 2: Calmodulin-3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	16.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.241	Depositor
Minimum map value	-0.794	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	246.0, 246.0, 246.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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: PT5, 7YV, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.53	0/2769	0.56	0/3743
1	C	0.53	0/2769	0.56	0/3743
1	E	0.53	0/2769	0.57	0/3743
1	G	0.53	0/2769	0.57	0/3743
2	B	0.30	0/838	0.46	0/1152
2	D	0.30	0/838	0.46	0/1152
2	F	0.30	0/838	0.47	0/1152
2	H	0.30	0/838	0.46	0/1152
All	All	0.49	0/14428	0.54	0/19580

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	A	2701	0	2771	68	0
1	C	2701	0	2771	67	0
1	E	2701	0	2771	66	0
1	G	2701	0	2771	65	0
2	B	828	0	549	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	828	0	549	15	0
2	F	828	0	549	15	0
2	H	828	0	549	16	0
3	A	115	112	108	17	0
3	C	115	112	108	18	0
3	E	115	112	108	18	0
3	G	115	112	108	18	0
4	A	4	0	0	0	0
5	A	38	46	0	12	0
5	C	19	23	0	5	0
5	E	19	23	0	6	0
All	All	14656	540	13712	367	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 13.

All (367) 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)
5:E:1103:7YV:C08	1:G:306:LEU:HD23	1.89	1.02
5:C:1103:7YV:C08	1:E:306:LEU:HD23	2.02	0.90
5:A:1107:7YV:C08	1:C:306:LEU:HD23	2.02	0.89
5:E:1103:7YV:C08	1:G:306:LEU:CD2	2.53	0.87
1:A:306:LEU:HD23	5:A:1108:7YV:C08	2.05	0.86
5:A:1107:7YV:C08	1:C:306:LEU:CD2	2.62	0.78
5:C:1103:7YV:C08	1:E:306:LEU:CD2	2.64	0.75
3:A:1101:PT5:O6	3:A:1101:PT5:O41	2.05	0.75
3:E:1101:PT5:O6	3:E:1101:PT5:O41	2.05	0.74
3:C:1101:PT5:O6	3:C:1101:PT5:O41	2.05	0.73
3:A:1101:PT5:O5	3:A:1101:PT5:O2	2.07	0.72
3:G:1101:PT5:O6	3:G:1101:PT5:O41	2.05	0.72
1:A:306:LEU:CD2	5:A:1108:7YV:C08	2.69	0.71
3:G:1101:PT5:O5	3:G:1101:PT5:O2	2.07	0.70
1:E:283:THR:HG22	1:E:308:ILE:HD12	1.75	0.69
1:G:283:THR:HG22	1:G:308:ILE:HD12	1.75	0.69
1:C:307:GLY:O	1:C:310:PHE:N	2.27	0.68
3:E:1101:PT5:O5	3:E:1101:PT5:O2	2.07	0.68
1:A:572:MET:HG3	1:C:573:LEU:HB3	1.74	0.68
1:A:283:THR:HG22	1:A:308:ILE:HD12	1.75	0.68
1:C:283:THR:HG22	1:C:308:ILE:HD12	1.75	0.68
1:E:307:GLY:O	1:E:310:PHE:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1102:PT5:O12	3:G:1102:PT5:O2	2.12	0.67
1:G:307:GLY:O	1:G:310:PHE:N	2.27	0.67
3:C:1101:PT5:O5	3:C:1101:PT5:O2	2.07	0.67
3:A:1102:PT5:O12	3:A:1102:PT5:O2	2.12	0.67
3:C:1102:PT5:O12	3:C:1102:PT5:O2	2.12	0.66
1:A:572:MET:HG3	1:C:573:LEU:CB	2.24	0.66
3:E:1102:PT5:O12	3:E:1102:PT5:O2	2.12	0.66
2:D:28:ILE:HA	2:D:62:GLY:HA3	1.78	0.65
1:A:84:GLN:OE1	1:A:153:SER:HA	1.97	0.65
1:A:307:GLY:O	1:A:310:PHE:N	2.27	0.65
1:C:123:GLU:OE2	1:C:124:HIS:ND1	2.26	0.65
1:C:84:GLN:OE1	1:C:153:SER:HA	1.97	0.65
1:E:84:GLN:OE1	1:E:153:SER:HA	1.97	0.65
2:B:28:ILE:HA	2:B:62:GLY:HA3	1.78	0.65
2:F:28:ILE:HA	2:F:62:GLY:HA3	1.78	0.64
2:H:28:ILE:HA	2:H:62:GLY:HA3	1.78	0.64
2:D:101:ILE:HD12	2:D:106:LEU:HD21	1.79	0.64
1:G:84:GLN:OE1	1:G:153:SER:HA	1.97	0.64
1:G:123:GLU:OE2	1:G:124:HIS:ND1	2.26	0.64
2:F:101:ILE:HD12	2:F:106:LEU:HD21	1.79	0.64
2:B:101:ILE:HD12	2:B:106:LEU:HD21	1.79	0.63
3:C:1101:PT5:O52	3:C:1101:PT5:H4	1.99	0.63
3:A:1101:PT5:O52	3:A:1101:PT5:H4	1.99	0.63
2:H:101:ILE:HD12	2:H:106:LEU:HD21	1.79	0.62
5:A:1107:7YV:C15	3:G:1102:PT5:H80	2.30	0.62
1:C:572:MET:HG3	1:E:573:LEU:HB3	1.81	0.62
3:G:1101:PT5:H4	3:G:1101:PT5:O52	1.99	0.62
3:E:1101:PT5:O52	3:E:1101:PT5:H4	1.99	0.62
1:E:95:ARG:H	1:E:98:ALA:HB3	1.65	0.61
1:A:123:GLU:OE2	1:A:124:HIS:ND1	2.26	0.61
1:E:123:GLU:OE2	1:E:124:HIS:ND1	2.26	0.61
1:E:146:GLU:OE2	1:E:150:ARG:NH2	2.34	0.61
1:G:95:ARG:H	1:G:98:ALA:HB3	1.65	0.61
1:G:146:GLU:OE2	1:G:150:ARG:NH2	2.34	0.61
1:A:95:ARG:H	1:A:98:ALA:HB3	1.65	0.60
3:E:1101:PT5:P4	3:E:1101:PT5:HO6	2.24	0.60
3:G:1101:PT5:O17	3:G:1101:PT5:H15	2.01	0.60
1:A:146:GLU:OE2	1:A:150:ARG:NH2	2.34	0.60
1:C:146:GLU:OE2	1:C:150:ARG:NH2	2.34	0.60
3:A:1102:PT5:H2	3:A:1102:PT5:O13	2.01	0.60
1:C:95:ARG:H	1:C:98:ALA:HB3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1102:PT5:H2	3:C:1102:PT5:O13	2.01	0.60
3:E:1101:PT5:H35	1:G:251:PHE:CD2	2.37	0.60
3:G:1102:PT5:H2	3:G:1102:PT5:O13	2.01	0.60
3:C:1101:PT5:H15	3:C:1101:PT5:O17	2.01	0.60
3:A:1101:PT5:H15	3:A:1101:PT5:O17	2.01	0.60
5:A:1107:7YV:C15	3:G:1102:PT5:C45	2.79	0.60
3:A:1102:PT5:HO2	3:A:1102:PT5:P1	2.25	0.60
1:C:266:ASP:HB3	1:C:289:LYS:HG2	1.84	0.60
1:E:266:ASP:HB3	1:E:289:LYS:HG2	1.84	0.59
2:B:139:TYR:HA	2:B:142:PHE:HD2	1.68	0.59
2:H:19:LEU:HA	2:H:23:ASP:H	1.67	0.59
1:A:266:ASP:HB3	1:A:289:LYS:HG2	1.84	0.59
3:E:1101:PT5:O17	3:E:1101:PT5:H15	2.01	0.59
3:E:1102:PT5:H2	3:E:1102:PT5:O13	2.01	0.59
3:G:1102:PT5:HO2	3:G:1102:PT5:P1	2.25	0.59
1:A:176:VAL:O	1:A:180:ILE:HD12	2.02	0.59
3:G:1101:PT5:P4	3:G:1101:PT5:HO6	2.26	0.59
2:D:19:LEU:HA	2:D:23:ASP:H	1.67	0.59
2:F:19:LEU:HA	2:F:23:ASP:H	1.67	0.59
2:H:139:TYR:HA	2:H:142:PHE:HD2	1.68	0.59
2:F:139:TYR:HA	2:F:142:PHE:HD2	1.68	0.59
2:B:19:LEU:HA	2:B:23:ASP:H	1.67	0.58
2:D:139:TYR:HA	2:D:142:PHE:HD2	1.68	0.58
1:G:176:VAL:O	1:G:180:ILE:HD12	2.02	0.58
1:C:176:VAL:O	1:C:180:ILE:HD12	2.02	0.58
1:G:266:ASP:HB3	1:G:289:LYS:HG2	1.84	0.58
3:C:1101:PT5:P4	3:C:1101:PT5:HO6	2.25	0.58
1:E:223:THR:HG22	1:G:240:THR:HA	1.84	0.58
3:A:1101:PT5:HO6	3:A:1101:PT5:P4	2.26	0.58
1:E:176:VAL:O	1:E:180:ILE:HD12	2.02	0.58
1:C:539:ILE:HG13	1:C:540:LEU:N	2.20	0.57
1:A:240:THR:HA	1:G:223:THR:HG22	1.87	0.57
1:A:573:LEU:HB3	1:G:572:MET:HG3	1.86	0.57
1:A:539:ILE:HG13	1:A:540:LEU:N	2.20	0.56
1:E:539:ILE:HG13	1:E:540:LEU:N	2.20	0.56
3:A:1102:PT5:H80	5:C:1103:7YV:C15	2.36	0.56
1:G:539:ILE:HG13	1:G:540:LEU:N	2.20	0.56
3:C:1102:PT5:H80	5:E:1103:7YV:C15	2.36	0.56
1:A:288:ASP:OD1	1:A:288:ASP:N	2.39	0.56
1:G:288:ASP:N	1:G:288:ASP:OD1	2.39	0.56
1:E:183:VAL:HA	1:E:186:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:VAL:HA	1:G:186:VAL:HG22	1.88	0.55
3:C:1101:PT5:HO2	3:C:1101:PT5:C5	2.16	0.55
5:A:1108:7YV:C15	3:E:1102:PT5:H80	2.37	0.55
1:E:272:ASP:HB3	1:E:289:LYS:HE3	1.89	0.55
2:H:107:ARG:O	2:H:111:THR:OG1	2.22	0.55
1:A:539:ILE:HG13	1:A:540:LEU:H	1.72	0.55
1:G:272:ASP:HB3	1:G:289:LYS:HE3	1.89	0.55
1:C:539:ILE:HG13	1:C:540:LEU:H	1.72	0.55
5:A:1107:7YV:C19	3:G:1102:PT5:C46	2.85	0.54
1:E:539:ILE:HG13	1:E:540:LEU:H	1.72	0.54
2:F:70:LEU:O	2:F:74:ALA:HB3	2.08	0.54
1:A:573:LEU:CB	1:G:572:MET:HG3	2.38	0.54
1:C:272:ASP:HB3	1:C:289:LYS:HE3	1.89	0.54
2:H:70:LEU:O	2:H:74:ALA:HB3	2.08	0.54
3:C:1102:PT5:HO2	3:C:1102:PT5:P1	2.30	0.54
1:A:183:VAL:HA	1:A:186:VAL:HG22	1.88	0.54
1:G:539:ILE:HG13	1:G:540:LEU:H	1.72	0.54
2:D:107:ARG:O	2:D:111:THR:OG1	2.22	0.54
1:C:183:VAL:HA	1:C:186:VAL:HG22	1.88	0.54
3:C:1102:PT5:C45	5:E:1103:7YV:C15	2.85	0.54
1:A:272:ASP:HB3	1:A:289:LYS:HE3	1.89	0.54
1:E:177:ILE:CD1	1:E:216:ARG:HG3	2.38	0.54
1:C:177:ILE:CD1	1:C:216:ARG:HG3	2.38	0.53
1:A:223:THR:HG22	1:C:240:THR:HA	1.90	0.53
1:C:223:THR:HG22	1:E:240:THR:HA	1.89	0.53
1:E:572:MET:HG3	1:G:573:LEU:HB3	1.89	0.53
1:G:260:GLU:OE2	1:G:291:PRO:HB3	2.08	0.53
1:E:260:GLU:OE2	1:E:291:PRO:HB3	2.08	0.53
1:A:260:GLU:OE2	1:A:291:PRO:HB3	2.08	0.53
1:G:177:ILE:CD1	1:G:216:ARG:HG3	2.38	0.53
1:G:209:LEU:O	1:G:212:LEU:HB3	2.09	0.53
3:A:1102:PT5:C45	5:C:1103:7YV:C15	2.86	0.53
2:B:70:LEU:O	2:B:74:ALA:HB3	2.08	0.53
1:C:260:GLU:OE2	1:C:291:PRO:HB3	2.08	0.53
1:E:209:LEU:O	1:E:212:LEU:HB3	2.09	0.53
2:D:70:LEU:O	2:D:74:ALA:HB3	2.08	0.52
1:G:74:SER:N	1:G:78:LYS:HZ3	2.08	0.52
1:A:209:LEU:O	1:A:212:LEU:HB3	2.09	0.52
2:F:107:ARG:O	2:F:111:THR:OG1	2.21	0.52
1:A:177:ILE:CD1	1:A:216:ARG:HG3	2.38	0.52
1:E:288:ASP:OD1	1:E:288:ASP:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:ILE:HG12	2:D:139:TYR:HE1	1.75	0.52
1:C:288:ASP:OD1	1:C:288:ASP:N	2.39	0.52
3:C:1101:PT5:H5	3:C:1101:PT5:O42	2.10	0.52
3:E:1102:PT5:HO2	3:E:1102:PT5:P1	2.32	0.52
3:A:1101:PT5:O53	3:A:1101:PT5:O3	2.27	0.52
1:C:209:LEU:O	1:C:212:LEU:HB3	2.09	0.52
1:C:572:MET:HG3	1:E:573:LEU:CB	2.40	0.52
2:F:101:ILE:HG12	2:F:139:TYR:HE1	1.75	0.51
1:E:74:SER:N	1:E:78:LYS:HZ3	2.08	0.51
3:E:1101:PT5:H5	3:E:1101:PT5:O42	2.10	0.51
3:C:1101:PT5:O53	3:C:1101:PT5:O3	2.27	0.51
1:A:74:SER:N	1:A:78:LYS:HZ3	2.08	0.51
3:G:1101:PT5:H5	3:G:1101:PT5:O42	2.10	0.51
1:C:74:SER:N	1:C:78:LYS:HZ3	2.08	0.51
3:E:1101:PT5:HO2	3:E:1101:PT5:C5	2.17	0.51
5:A:1108:7YV:C15	3:E:1102:PT5:C45	2.89	0.51
3:E:1101:PT5:O53	3:E:1101:PT5:O3	2.27	0.51
3:A:1101:PT5:H5	3:A:1101:PT5:O42	2.10	0.50
2:B:107:ARG:O	2:B:111:THR:OG1	2.21	0.50
2:H:141:GLU:O	2:H:145:MET:N	2.39	0.50
1:A:247:LEU:HD11	1:G:215:VAL:HG12	1.93	0.50
2:F:38:ARG:HA	2:F:43:ASN:H	1.77	0.50
2:B:38:ARG:HA	2:B:43:ASN:H	1.77	0.50
2:B:101:ILE:HG12	2:B:139:TYR:HE1	1.75	0.50
2:D:38:ARG:HA	2:D:43:ASN:H	1.77	0.50
1:G:341:PRO:HB2	1:G:549:PHE:HD1	1.77	0.50
1:C:341:PRO:HB2	1:C:549:PHE:HD1	1.77	0.50
2:H:101:ILE:HG12	2:H:139:TYR:HE1	1.75	0.50
1:E:215:VAL:HG12	1:G:247:LEU:HD11	1.94	0.50
1:A:341:PRO:HB2	1:A:549:PHE:HD1	1.77	0.49
1:E:177:ILE:HD12	1:E:216:ARG:HG3	1.94	0.49
1:E:341:PRO:HB2	1:E:549:PHE:HD1	1.77	0.49
1:E:150:ARG:NH1	1:E:178:ASP:OD2	2.46	0.49
1:A:150:ARG:NH1	1:A:178:ASP:OD2	2.46	0.49
1:C:266:ASP:OD2	1:C:289:LYS:HA	2.13	0.49
1:G:546:LYS:O	1:G:550:LYS:HG2	2.12	0.49
3:G:1101:PT5:O53	3:G:1101:PT5:O3	2.28	0.49
2:H:38:ARG:HA	2:H:43:ASN:H	1.77	0.49
1:C:546:LYS:O	1:C:550:LYS:HG2	2.12	0.48
1:G:177:ILE:HD12	1:G:216:ARG:HG3	1.94	0.48
1:C:150:ARG:NH1	1:C:178:ASP:OD2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:ARG:NH1	1:G:178:ASP:OD2	2.46	0.48
1:A:266:ASP:OD2	1:A:289:LYS:HA	2.13	0.48
1:C:177:ILE:HD12	1:C:216:ARG:HG3	1.94	0.48
3:G:1101:PT5:HO2	3:G:1101:PT5:C5	2.17	0.48
3:C:1102:PT5:C46	5:E:1103:7YV:C19	2.91	0.48
3:E:1101:PT5:H35	1:G:251:PHE:CE2	2.48	0.48
1:A:546:LYS:O	1:A:550:LYS:HG2	2.13	0.48
1:E:546:LYS:O	1:E:550:LYS:HG2	2.13	0.48
1:A:177:ILE:HD12	1:A:216:ARG:HG3	1.94	0.48
1:A:572:MET:HG3	1:C:573:LEU:HB2	1.95	0.48
1:E:572:MET:HG3	1:G:573:LEU:CB	2.44	0.48
1:G:87:VAL:HA	1:G:90:VAL:HG12	1.96	0.48
2:F:110:MET:O	2:F:116:LYS:HA	2.14	0.47
2:H:110:MET:O	2:H:116:LYS:HA	2.14	0.47
3:A:1101:PT5:H35	1:C:251:PHE:CD2	2.50	0.47
1:E:266:ASP:OD2	1:E:289:LYS:HA	2.13	0.47
2:D:110:MET:O	2:D:116:LYS:HA	2.14	0.47
1:G:266:ASP:OD2	1:G:289:LYS:HA	2.13	0.47
1:A:126:GLU:HG2	1:A:127:LEU:N	2.30	0.47
2:B:110:MET:O	2:B:116:LYS:HA	2.14	0.47
1:E:87:VAL:HA	1:E:90:VAL:HG12	1.96	0.47
1:G:126:GLU:HG2	1:G:127:LEU:N	2.30	0.47
1:C:126:GLU:HG2	1:C:127:LEU:N	2.30	0.47
1:E:184:ALA:O	1:E:188:VAL:HG23	2.15	0.47
1:A:87:VAL:HA	1:A:90:VAL:HG12	1.96	0.47
1:A:276:TRP:HD1	1:A:289:LYS:O	1.98	0.47
1:G:103:VAL:O	1:G:107:LEU:HD23	2.15	0.47
1:G:275:TRP:HD1	1:G:289:LYS:HD2	1.80	0.47
1:C:103:VAL:O	1:C:107:LEU:HD23	2.15	0.47
1:E:103:VAL:O	1:E:107:LEU:HD23	2.15	0.47
1:G:184:ALA:O	1:G:188:VAL:HG23	2.15	0.47
1:C:184:ALA:O	1:C:188:VAL:HG23	2.15	0.46
1:E:126:GLU:HG2	1:E:127:LEU:N	2.30	0.46
3:A:1102:PT5:C46	5:C:1103:7YV:C19	2.93	0.46
1:A:184:ALA:O	1:A:188:VAL:HG23	2.15	0.46
5:A:1107:7YV:C19	3:G:1102:PT5:H81	2.46	0.46
2:B:141:GLU:O	2:B:145:MET:N	2.39	0.46
1:C:87:VAL:HA	1:C:90:VAL:HG12	1.96	0.46
1:C:171:ARG:HD2	1:C:171:ARG:HA	1.67	0.46
2:D:141:GLU:O	2:D:145:MET:N	2.39	0.46
1:E:275:TRP:HD1	1:E:289:LYS:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:ILE:HD12	1:G:346:ILE:HA	1.74	0.46
1:C:275:TRP:HD1	1:C:289:LYS:HD2	1.80	0.46
1:G:171:ARG:HA	1:G:171:ARG:HD2	1.67	0.46
1:A:275:TRP:HD1	1:A:289:LYS:HD2	1.80	0.45
1:G:562:ILE:H	1:G:562:ILE:HG12	1.31	0.45
1:A:103:VAL:O	1:A:107:LEU:HD23	2.15	0.45
1:C:152:TRP:C	1:C:154:ALA:H	2.20	0.45
1:A:180:ILE:HA	1:A:183:VAL:HG22	1.99	0.45
1:A:152:TRP:C	1:A:154:ALA:H	2.20	0.45
1:A:283:THR:CG2	1:A:308:ILE:HD12	2.45	0.45
1:C:335:PHE:HZ	1:C:560:ASP:HB2	1.81	0.45
1:G:276:TRP:HD1	1:G:289:LYS:O	1.98	0.45
1:A:335:PHE:HZ	1:A:560:ASP:HB2	1.81	0.45
1:E:276:TRP:HD1	1:E:289:LYS:O	1.98	0.45
1:C:276:TRP:HD1	1:C:289:LYS:O	1.98	0.45
1:G:260:GLU:OE2	1:G:296:GLY:HA3	2.17	0.45
1:G:335:PHE:HZ	1:G:560:ASP:HB2	1.81	0.45
1:G:541:LYS:HD3	1:G:541:LYS:HA	1.76	0.45
1:A:171:ARG:HA	1:A:171:ARG:HD2	1.66	0.45
1:C:180:ILE:HA	1:C:183:VAL:HG22	1.99	0.45
1:E:152:TRP:C	1:E:154:ALA:H	2.20	0.45
1:A:183:VAL:O	1:A:186:VAL:HG22	2.17	0.45
1:E:183:VAL:O	1:E:186:VAL:HG22	2.17	0.45
1:E:335:PHE:HZ	1:E:560:ASP:HB2	1.81	0.45
2:F:116:LYS:HD2	2:F:116:LYS:N	2.32	0.45
1:G:140:ILE:HA	1:G:140:ILE:HD13	1.68	0.45
1:A:260:GLU:OE2	1:A:296:GLY:HA3	2.17	0.44
2:D:116:LYS:N	2:D:116:LYS:HD2	2.32	0.44
1:E:180:ILE:HA	1:E:183:VAL:HG22	1.99	0.44
1:G:183:VAL:O	1:G:186:VAL:HG22	2.17	0.44
1:C:183:VAL:O	1:C:186:VAL:HG22	2.17	0.44
1:A:82:ARG:HD2	1:A:83:LEU:HD22	1.99	0.44
1:A:558:VAL:HB	1:A:559:LYS:H	1.67	0.44
1:C:260:GLU:OE2	1:C:296:GLY:HA3	2.17	0.44
1:C:283:THR:CG2	1:C:308:ILE:HD12	2.45	0.44
1:E:260:GLU:OE2	1:E:296:GLY:HA3	2.17	0.44
1:G:152:TRP:C	1:G:154:ALA:H	2.20	0.44
1:C:82:ARG:HD2	1:C:83:LEU:HD22	1.99	0.44
1:C:541:LYS:HD3	1:C:541:LYS:HA	1.76	0.44
1:E:168:ARG:HE	1:E:171:ARG:HB2	1.82	0.44
1:E:562:ILE:H	1:E:562:ILE:HG12	1.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ARG:HE	1:A:171:ARG:HB2	1.82	0.44
2:B:116:LYS:N	2:B:116:LYS:HD2	2.32	0.44
1:E:82:ARG:HD2	1:E:83:LEU:HD22	1.99	0.44
1:E:140:ILE:HD13	1:E:140:ILE:HA	1.68	0.44
2:B:112:ASN:C	2:B:116:LYS:HE3	2.38	0.44
1:E:279:ILE:HD13	1:E:279:ILE:HA	1.79	0.44
2:H:116:LYS:HD2	2:H:116:LYS:N	2.32	0.44
2:D:112:ASN:C	2:D:116:LYS:HE3	2.39	0.43
1:E:541:LYS:HD3	1:E:541:LYS:HA	1.76	0.43
1:C:569:HIS:NE2	1:E:569:HIS:CD2	2.86	0.43
2:H:112:ASN:C	2:H:116:LYS:HE3	2.39	0.43
1:A:251:PHE:CD2	3:G:1101:PT5:H35	2.53	0.43
1:G:82:ARG:HD2	1:G:83:LEU:HD22	1.99	0.43
1:A:583:VAL:HG22	1:C:583:VAL:HG11	2.00	0.43
1:E:535:ARG:HH22	2:F:69:PHE:HA	1.84	0.43
1:G:180:ILE:HA	1:G:183:VAL:HG22	1.99	0.43
3:A:1101:PT5:HO2	3:A:1101:PT5:C5	2.17	0.43
1:C:554:ARG:N	1:C:555:PRO:HD3	2.34	0.43
1:E:283:THR:CG2	1:E:308:ILE:HD12	2.46	0.43
2:F:112:ASN:C	2:F:116:LYS:HE3	2.38	0.43
2:F:144:GLN:O	2:F:148:ALA:N	2.52	0.43
1:C:535:ARG:HH22	2:D:69:PHE:HA	1.84	0.43
3:E:1102:PT5:H2	3:E:1102:PT5:C7	2.49	0.43
1:G:115:LEU:HD12	1:G:115:LEU:HA	1.85	0.43
1:G:554:ARG:N	1:G:555:PRO:HD3	2.34	0.43
3:G:1102:PT5:H2	3:G:1102:PT5:C7	2.49	0.43
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.87	0.43
1:A:535:ARG:HH22	2:B:69:PHE:HA	1.83	0.43
3:C:1102:PT5:H2	3:C:1102:PT5:C7	2.49	0.43
1:E:554:ARG:N	1:E:555:PRO:HD3	2.34	0.43
1:G:168:ARG:HE	1:G:171:ARG:HB2	1.82	0.43
1:C:168:ARG:HE	1:C:171:ARG:HB2	1.82	0.43
1:E:238:LEU:HD23	1:E:238:LEU:HA	1.81	0.43
2:H:144:GLN:O	2:H:148:ALA:N	2.52	0.43
1:C:140:ILE:HA	1:C:140:ILE:HD13	1.68	0.43
1:E:166:ARG:HA	1:E:166:ARG:HD3	1.75	0.43
2:F:141:GLU:O	2:F:145:MET:N	2.39	0.43
3:A:1102:PT5:H2	3:A:1102:PT5:C7	2.49	0.42
1:G:221:GLY:O	1:G:225:LYS:HD2	2.19	0.42
1:E:558:VAL:HB	1:E:559:LYS:H	1.67	0.42
1:A:221:GLY:O	1:A:225:LYS:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ARG:N	1:A:555:PRO:HD3	2.34	0.42
2:D:144:GLN:O	2:D:148:ALA:N	2.52	0.42
1:A:541:LYS:HD3	1:A:541:LYS:HA	1.76	0.42
1:G:535:ARG:HH22	2:H:69:PHE:HA	1.83	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.80	0.42
1:C:215:VAL:HG12	1:E:247:LEU:HD11	2.01	0.42
1:C:548:LYS:O	1:C:552:THR:HG23	2.20	0.42
1:C:221:GLY:O	1:C:225:LYS:HD2	2.19	0.42
1:A:548:LYS:O	1:A:552:THR:HG23	2.20	0.41
5:A:1107:7YV:C15	3:G:1102:PT5:H79	2.48	0.41
1:E:221:GLY:O	1:E:225:LYS:HD2	2.20	0.41
3:A:1101:PT5:H35	1:C:251:PHE:CE2	2.56	0.41
1:C:238:LEU:HD23	1:C:238:LEU:HA	1.80	0.41
1:C:338:ARG:HD3	1:C:553:LEU:HA	2.02	0.41
1:G:212:LEU:HA	1:G:215:VAL:HG22	2.03	0.41
1:C:212:LEU:HA	1:C:215:VAL:HG22	2.03	0.41
1:E:548:LYS:O	1:E:552:THR:HG23	2.20	0.41
3:C:1102:PT5:H81	5:E:1103:7YV:C19	2.50	0.41
1:E:352:LEU:HD21	1:E:537:ILE:HG22	2.03	0.41
1:G:548:LYS:O	1:G:552:THR:HG23	2.20	0.41
1:A:208:PHE:HD1	1:A:208:PHE:O	2.04	0.41
1:A:215:VAL:HG12	1:C:247:LEU:HD11	2.01	0.41
1:A:352:LEU:HD21	1:A:537:ILE:HG22	2.03	0.41
1:C:208:PHE:HD1	1:C:208:PHE:O	2.04	0.41
3:C:1101:PT5:H35	1:E:251:PHE:CD2	2.55	0.41
1:E:212:LEU:HA	1:E:215:VAL:HG22	2.03	0.41
1:E:281:LEU:HD22	1:E:307:GLY:HA3	2.03	0.41
1:E:338:ARG:HD3	1:E:553:LEU:HA	2.02	0.41
1:A:140:ILE:HA	1:A:140:ILE:HD13	1.68	0.41
1:E:346:ILE:HD12	1:E:346:ILE:HA	1.74	0.41
1:G:283:THR:CG2	1:G:308:ILE:HD12	2.45	0.41
1:C:281:LEU:HD22	1:C:307:GLY:HA3	2.03	0.41
1:A:576:ILE:HD13	1:A:576:ILE:HA	1.87	0.40
2:B:82:SER:O	2:B:86:ILE:HG12	2.21	0.40
1:E:572:MET:HA	1:E:575:ARG:HD2	2.02	0.40
1:G:108:LEU:HD12	1:G:108:LEU:HA	1.94	0.40
1:C:558:VAL:HB	1:C:559:LYS:H	1.67	0.40
1:G:338:ARG:HD3	1:G:553:LEU:HA	2.02	0.40
1:G:543:LEU:HD11	2:H:52:MET:HA	2.03	0.40
2:H:82:SER:O	2:H:86:ILE:HG12	2.21	0.40
1:A:340:MET:HB2	1:A:341:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LEU:HA	1:C:313:LEU:HD12	1.89	0.40
1:E:543:LEU:HD11	2:F:52:MET:HA	2.04	0.40
3:E:1101:PT5:H35	1:G:251:PHE:HD2	1.84	0.40
1:A:75:ALA:O	1:A:79:ARG:HG3	2.22	0.40
1:A:212:LEU:HA	1:A:215:VAL:HG22	2.03	0.40
1:A:258:LEU:HD23	1:A:258:LEU:HA	1.87	0.40
1:A:338:ARG:HD3	1:A:553:LEU:HA	2.02	0.40
1:C:352:LEU:HD21	1:C:537:ILE:HG22	2.03	0.40
1:C:565:TYR:HD1	1:C:565:TYR:HA	1.81	0.40
2:D:82:SER:O	2:D:86:ILE:HG12	2.21	0.40
1:G:281:LEU:HD22	1:G:307:GLY:HA3	2.03	0.40
1:G:340:MET:HB2	1:G:341:PRO:HD3	2.04	0.40
1:A:161:ARG:HD2	1:A:166:ARG:HH21	1.87	0.40
5:A:1108:7YV:C19	3:E:1102:PT5:C46	2.99	0.40
2:B:89:ALA:O	2:B:92:VAL:HG22	2.22	0.40
2:B:144:GLN:O	2:B:148:ALA:N	2.52	0.40
3:C:1101:PT5:O6	3:C:1101:PT5:P4	2.79	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/1049 (31%)	304 (93%)	20 (6%)	2 (1%)	25	56
1	C	326/1049 (31%)	304 (93%)	20 (6%)	2 (1%)	25	56
1	E	326/1049 (31%)	304 (93%)	20 (6%)	2 (1%)	25	56
1	G	326/1049 (31%)	304 (93%)	20 (6%)	2 (1%)	25	56
2	B	142/149 (95%)	134 (94%)	8 (6%)	0	100	100
2	D	142/149 (95%)	134 (94%)	8 (6%)	0	100	100
2	F	142/149 (95%)	134 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	142/149 (95%)	134 (94%)	8 (6%)	0	100	100
All	All	1872/4792 (39%)	1752 (94%)	112 (6%)	8 (0%)	38	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	VAL
1	C	558	VAL
1	E	558	VAL
1	G	558	VAL
1	A	222	GLY
1	C	222	GLY
1	E	222	GLY
1	G	222	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/860 (33%)	255 (90%)	27 (10%)	8	24
1	C	282/860 (33%)	255 (90%)	27 (10%)	8	24
1	E	282/860 (33%)	255 (90%)	27 (10%)	8	24
1	G	282/860 (33%)	255 (90%)	27 (10%)	8	24
2	B	31/127 (24%)	31 (100%)	0	100	100
2	D	31/127 (24%)	31 (100%)	0	100	100
2	F	31/127 (24%)	31 (100%)	0	100	100
2	H	31/127 (24%)	31 (100%)	0	100	100
All	All	1252/3948 (32%)	1144 (91%)	108 (9%)	14	30

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	95	ARG
1	A	140	ILE
1	A	156	CYS
1	A	167	PHE
1	A	168	ARG
1	A	208	PHE
1	A	216	ARG
1	A	217	MET
1	A	219	ARG
1	A	220	ARG
1	A	345	LEU
1	A	346	ILE
1	A	352	LEU
1	A	558	VAL
1	A	559	LYS
1	A	562	ILE
1	A	563	GLU
1	A	565	TYR
1	A	570	LEU
1	A	572	MET
1	A	575	ARG
1	A	577	LYS
1	A	578	SER
1	A	579	LEU
1	A	580	GLN
1	A	582	ARG
1	C	82	ARG
1	C	95	ARG
1	C	140	ILE
1	C	156	CYS
1	C	167	PHE
1	C	168	ARG
1	C	208	PHE
1	C	216	ARG
1	C	217	MET
1	C	219	ARG
1	C	220	ARG
1	C	345	LEU
1	C	346	ILE
1	C	352	LEU
1	C	558	VAL
1	C	559	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	562	ILE
1	C	563	GLU
1	C	565	TYR
1	C	570	LEU
1	C	572	MET
1	C	575	ARG
1	C	577	LYS
1	C	578	SER
1	C	579	LEU
1	C	580	GLN
1	C	582	ARG
1	E	82	ARG
1	E	95	ARG
1	E	140	ILE
1	E	156	CYS
1	E	167	PHE
1	E	168	ARG
1	E	208	PHE
1	E	216	ARG
1	E	217	MET
1	E	219	ARG
1	E	220	ARG
1	E	345	LEU
1	E	346	ILE
1	E	352	LEU
1	E	558	VAL
1	E	559	LYS
1	E	562	ILE
1	E	563	GLU
1	E	565	TYR
1	E	570	LEU
1	E	572	MET
1	E	575	ARG
1	E	577	LYS
1	E	578	SER
1	E	579	LEU
1	E	580	GLN
1	E	582	ARG
1	G	82	ARG
1	G	95	ARG
1	G	140	ILE
1	G	156	CYS

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Mol	Chain	Res	Type
1	G	167	PHE
1	G	168	ARG
1	G	208	PHE
1	G	216	ARG
1	G	217	MET
1	G	219	ARG
1	G	220	ARG
1	G	345	LEU
1	G	346	ILE
1	G	352	LEU
1	G	558	VAL
1	G	559	LYS
1	G	562	ILE
1	G	563	GLU
1	G	565	TYR
1	G	570	LEU
1	G	572	MET
1	G	575	ARG
1	G	577	LYS
1	G	578	SER
1	G	579	LEU
1	G	580	GLN
1	G	582	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PT5	G	1102	-	64,64,69	0.42	0	78,82,87	0.39	0
3	PT5	E	1101	-	51,51,69	0.44	0	64,69,87	0.41	0
3	PT5	G	1101	-	51,51,69	0.45	0	64,69,87	0.42	0
5	7YV	A	1108	-	21,21,21	3.46	13 (61%)	28,31,31	2.67	12 (42%)
5	7YV	C	1103	-	21,21,21	3.46	13 (61%)	28,31,31	2.67	12 (42%)
3	PT5	C	1102	-	64,64,69	0.41	0	78,82,87	0.39	0
3	PT5	A	1101	-	51,51,69	0.45	0	64,69,87	0.42	0
5	7YV	A	1107	-	21,21,21	3.46	13 (61%)	28,31,31	2.67	12 (42%)
3	PT5	C	1101	-	51,51,69	0.44	0	64,69,87	0.42	0
5	7YV	E	1103	-	21,21,21	3.45	13 (61%)	28,31,31	2.67	12 (42%)
3	PT5	E	1102	-	64,64,69	0.42	0	78,82,87	0.39	0
3	PT5	A	1102	-	64,64,69	0.42	0	78,82,87	0.39	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
3	PT5	G	1102	-	-	25/61/85/90	0/1/1/1
3	PT5	E	1101	-	-	25/48/72/90	0/1/1/1
3	PT5	G	1101	-	-	25/48/72/90	0/1/1/1
5	7YV	A	1108	-	-	2/8/25/25	0/4/3/3
5	7YV	C	1103	-	-	2/8/25/25	0/4/3/3
3	PT5	C	1102	-	-	25/61/85/90	0/1/1/1
3	PT5	A	1101	-	-	25/48/72/90	0/1/1/1
5	7YV	A	1107	-	-	2/8/25/25	0/4/3/3
3	PT5	C	1101	-	-	25/48/72/90	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	7YV	E	1103	-	-	2/8/25/25	0/4/3/3
3	PT5	E	1102	-	-	25/61/85/90	0/1/1/1
3	PT5	A	1102	-	-	25/61/85/90	0/1/1/1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1107	7YV	C05-C03	-8.65	1.30	1.53
5	E	1103	7YV	C05-C03	-8.65	1.30	1.53
5	A	1108	7YV	C05-C03	-8.64	1.30	1.53
5	C	1103	7YV	C05-C03	-8.62	1.31	1.53
5	C	1103	7YV	C05-C04	-4.93	1.30	1.52
5	A	1108	7YV	C05-C04	-4.93	1.30	1.52
5	E	1103	7YV	C05-C04	-4.93	1.30	1.52
5	A	1107	7YV	C05-C04	-4.93	1.30	1.52
5	A	1107	7YV	C11-C13	-4.76	1.32	1.40
5	A	1108	7YV	C11-C13	-4.75	1.32	1.40
5	C	1103	7YV	C11-C13	-4.75	1.32	1.40
5	E	1103	7YV	C11-C13	-4.73	1.32	1.40
5	E	1103	7YV	C09-C08	4.65	1.66	1.54
5	A	1108	7YV	C11-C12	-4.65	1.33	1.40
5	A	1107	7YV	C09-C08	4.64	1.66	1.54
5	C	1103	7YV	C09-C08	4.63	1.66	1.54
5	A	1108	7YV	C09-C08	4.63	1.66	1.54
5	A	1107	7YV	C11-C12	-4.62	1.33	1.40
5	C	1103	7YV	C11-C12	-4.61	1.33	1.40
5	E	1103	7YV	C11-C12	-4.60	1.33	1.40
5	C	1103	7YV	C06-C10	-4.45	1.44	1.51
5	A	1108	7YV	C06-C10	-4.43	1.44	1.51
5	A	1107	7YV	C06-C10	-4.39	1.44	1.51
5	E	1103	7YV	C06-C10	-4.36	1.44	1.51
5	E	1103	7YV	C06-C03	-4.16	1.44	1.54
5	C	1103	7YV	C06-C03	-4.15	1.44	1.54
5	A	1107	7YV	C06-C03	-4.13	1.44	1.54
5	A	1108	7YV	C06-C03	-4.12	1.44	1.54
5	A	1107	7YV	C14-C16	-2.98	1.34	1.39
5	A	1108	7YV	C14-C16	-2.96	1.34	1.39
5	C	1103	7YV	C14-C16	-2.96	1.34	1.39
5	E	1103	7YV	C14-C16	-2.95	1.34	1.39
5	C	1103	7YV	O01-C10	-2.94	1.17	1.23
5	E	1103	7YV	O01-C10	-2.94	1.17	1.23
5	A	1108	7YV	O01-C10	-2.93	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1107	7YV	O01-C10	-2.92	1.17	1.23
5	A	1108	7YV	C15-C13	-2.90	1.35	1.39
5	E	1103	7YV	C15-C13	-2.89	1.35	1.39
5	A	1107	7YV	C15-C13	-2.86	1.35	1.39
5	C	1103	7YV	C15-C13	-2.86	1.35	1.39
5	C	1103	7YV	C14-C12	-2.85	1.35	1.39
5	A	1108	7YV	C14-C12	-2.85	1.35	1.39
5	E	1103	7YV	C14-C12	-2.85	1.35	1.39
5	A	1107	7YV	C14-C12	-2.84	1.35	1.39
5	C	1103	7YV	C10-N02	2.47	1.41	1.35
5	A	1108	7YV	C10-N02	2.46	1.41	1.35
5	A	1107	7YV	C10-N02	2.43	1.41	1.35
5	E	1103	7YV	C10-N02	2.39	1.41	1.35
5	A	1107	7YV	C11-N02	-2.10	1.39	1.43
5	E	1103	7YV	C11-N02	-2.09	1.39	1.43
5	A	1108	7YV	C11-N02	-2.09	1.39	1.43
5	C	1103	7YV	C11-N02	-2.06	1.39	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1103	7YV	C09-C08-C03	-6.31	92.63	103.49
5	A	1108	7YV	C09-C08-C03	-6.29	92.66	103.49
5	A	1107	7YV	C09-C08-C03	-6.29	92.68	103.49
5	C	1103	7YV	C09-C08-C03	-6.27	92.70	103.49
5	A	1107	7YV	C13-C15-C16	-5.10	116.94	122.17
5	A	1108	7YV	C13-C15-C16	-5.09	116.94	122.17
5	C	1103	7YV	C13-C15-C16	-5.08	116.96	122.17
5	E	1103	7YV	C13-C15-C16	-5.08	116.96	122.17
5	E	1103	7YV	C18-C13-C11	-4.32	115.87	121.44
5	A	1107	7YV	C18-C13-C11	-4.32	115.87	121.44
5	A	1108	7YV	C18-C13-C11	-4.31	115.89	121.44
5	C	1103	7YV	O01-C10-C06	4.30	126.91	121.73
5	C	1103	7YV	C18-C13-C11	-4.28	115.93	121.44
5	A	1107	7YV	O01-C10-C06	4.27	126.87	121.73
5	A	1108	7YV	O01-C10-C06	4.26	126.86	121.73
5	E	1103	7YV	O01-C10-C06	4.25	126.85	121.73
5	A	1107	7YV	C06-C07-C04	-4.15	94.55	103.47
5	E	1103	7YV	C06-C07-C04	-4.15	94.56	103.47
5	A	1108	7YV	C06-C07-C04	-4.14	94.58	103.47
5	C	1103	7YV	C06-C07-C04	-4.14	94.58	103.47
5	A	1107	7YV	C14-C16-C15	4.03	122.90	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1103	7YV	C14-C16-C15	4.03	122.89	118.09
5	E	1103	7YV	C14-C16-C15	3.99	122.84	118.09
5	A	1108	7YV	C14-C16-C15	3.98	122.84	118.09
5	C	1103	7YV	C06-C10-N02	-3.51	110.17	114.50
5	E	1103	7YV	C06-C10-N02	-3.51	110.18	114.50
5	A	1108	7YV	C06-C10-N02	-3.49	110.20	114.50
5	A	1107	7YV	C06-C10-N02	-3.49	110.20	114.50
5	A	1107	7YV	C12-C14-C16	-3.20	118.88	122.17
5	C	1103	7YV	C12-C14-C16	-3.16	118.92	122.17
5	A	1108	7YV	C12-C14-C16	-3.15	118.93	122.17
5	E	1103	7YV	C12-C14-C16	-3.13	118.95	122.17
5	A	1107	7YV	C18-C13-C15	2.73	124.54	119.49
5	E	1103	7YV	C18-C13-C15	2.73	124.54	119.49
5	C	1103	7YV	C18-C13-C15	2.73	124.54	119.49
5	A	1108	7YV	C18-C13-C15	2.71	124.51	119.49
5	C	1103	7YV	C19-C16-C14	-2.71	116.92	120.94
5	E	1103	7YV	C19-C16-C14	-2.69	116.95	120.94
5	A	1107	7YV	C19-C16-C14	-2.69	116.96	120.94
5	A	1108	7YV	C19-C16-C14	-2.68	116.97	120.94
5	E	1103	7YV	C17-C12-C11	-2.24	118.55	121.44
5	A	1108	7YV	C17-C12-C11	-2.24	118.56	121.44
5	A	1107	7YV	C17-C12-C11	-2.23	118.57	121.44
5	C	1103	7YV	C17-C12-C11	-2.22	118.58	121.44
5	E	1103	7YV	C17-C12-C14	2.13	123.43	119.49
5	C	1103	7YV	C17-C12-C14	2.12	123.41	119.49
5	A	1108	7YV	C17-C12-C14	2.11	123.39	119.49
5	A	1107	7YV	C17-C12-C14	2.09	123.34	119.49

There are no chirality outliers.

All (208) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	PT5	C7-O13-P1-O12
3	A	1101	PT5	C7-O13-P1-O11
3	A	1101	PT5	C7-O13-P1-O1
3	A	1101	PT5	C6-C1-O1-P1
3	A	1101	PT5	C2-C1-O1-P1
3	A	1101	PT5	C3-C4-O4-P4
3	A	1101	PT5	C5-C4-O4-P4
3	A	1101	PT5	C6-C5-O5-P5
3	A	1101	PT5	C4-C5-O5-P5
3	A	1102	PT5	C2-C1-O1-P1

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Mol	Chain	Res	Type	Atoms
3	A	1102	PT5	C19-C20-C21-C22
3	C	1101	PT5	C7-O13-P1-O12
3	C	1101	PT5	C7-O13-P1-O11
3	C	1101	PT5	C7-O13-P1-O1
3	C	1101	PT5	C6-C1-O1-P1
3	C	1101	PT5	C2-C1-O1-P1
3	C	1101	PT5	C3-C4-O4-P4
3	C	1101	PT5	C5-C4-O4-P4
3	C	1101	PT5	C6-C5-O5-P5
3	C	1101	PT5	C4-C5-O5-P5
3	C	1102	PT5	C2-C1-O1-P1
3	C	1102	PT5	C19-C20-C21-C22
3	E	1101	PT5	C7-O13-P1-O12
3	E	1101	PT5	C7-O13-P1-O11
3	E	1101	PT5	C7-O13-P1-O1
3	E	1101	PT5	C6-C1-O1-P1
3	E	1101	PT5	C2-C1-O1-P1
3	E	1101	PT5	C3-C4-O4-P4
3	E	1101	PT5	C5-C4-O4-P4
3	E	1101	PT5	C6-C5-O5-P5
3	E	1101	PT5	C4-C5-O5-P5
3	E	1102	PT5	C2-C1-O1-P1
3	E	1102	PT5	C19-C20-C21-C22
3	G	1101	PT5	C7-O13-P1-O12
3	G	1101	PT5	C7-O13-P1-O11
3	G	1101	PT5	C7-O13-P1-O1
3	G	1101	PT5	C6-C1-O1-P1
3	G	1101	PT5	C2-C1-O1-P1
3	G	1101	PT5	C3-C4-O4-P4
3	G	1101	PT5	C5-C4-O4-P4
3	G	1101	PT5	C6-C5-O5-P5
3	G	1101	PT5	C4-C5-O5-P5
3	G	1102	PT5	C2-C1-O1-P1
3	G	1102	PT5	C19-C20-C21-C22
3	A	1102	PT5	C20-C21-C22-C23
3	C	1102	PT5	C20-C21-C22-C23
3	E	1102	PT5	C20-C21-C22-C23
3	G	1102	PT5	C20-C21-C22-C23
3	A	1101	PT5	C14-C15-C16-C17
3	C	1101	PT5	C14-C15-C16-C17
3	E	1101	PT5	C14-C15-C16-C17
3	G	1101	PT5	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
3	A	1102	PT5	C7-O13-P1-O1
3	C	1102	PT5	C7-O13-P1-O1
3	E	1102	PT5	C7-O13-P1-O1
3	G	1102	PT5	C7-O13-P1-O1
3	A	1102	PT5	C42-C43-C44-C45
3	E	1102	PT5	C42-C43-C44-C45
3	G	1102	PT5	C42-C43-C44-C45
3	C	1102	PT5	C42-C43-C44-C45
3	E	1101	PT5	C31-C11-O18-C9
3	A	1101	PT5	C31-C11-O18-C9
3	C	1101	PT5	C31-C11-O18-C9
3	G	1101	PT5	C31-C11-O18-C9
3	A	1102	PT5	C14-C15-C16-C17
3	C	1102	PT5	C14-C15-C16-C17
3	E	1102	PT5	C14-C15-C16-C17
3	G	1102	PT5	C14-C15-C16-C17
3	A	1101	PT5	O19-C11-O18-C9
3	C	1101	PT5	O19-C11-O18-C9
3	E	1101	PT5	O19-C11-O18-C9
3	G	1101	PT5	O19-C11-O18-C9
3	A	1102	PT5	C44-C45-C46-C47
3	C	1102	PT5	C44-C45-C46-C47
3	E	1102	PT5	C44-C45-C46-C47
3	G	1102	PT5	C44-C45-C46-C47
3	E	1102	PT5	O13-C7-C8-C9
3	A	1101	PT5	C10-C12-C13-C14
3	C	1101	PT5	C10-C12-C13-C14
3	E	1101	PT5	C10-C12-C13-C14
3	G	1101	PT5	C10-C12-C13-C14
3	A	1101	PT5	C32-C33-C34-C35
3	C	1101	PT5	C32-C33-C34-C35
3	E	1101	PT5	C32-C33-C34-C35
3	G	1101	PT5	C32-C33-C34-C35
3	A	1102	PT5	C41-C42-C43-C44
3	C	1102	PT5	C41-C42-C43-C44
3	E	1102	PT5	C41-C42-C43-C44
3	G	1102	PT5	C41-C42-C43-C44
3	A	1102	PT5	O13-C7-C8-C9
3	C	1102	PT5	O13-C7-C8-C9
3	G	1102	PT5	O13-C7-C8-C9
3	A	1102	PT5	C34-C35-C36-C37
3	E	1102	PT5	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
3	C	1102	PT5	C34-C35-C36-C37
3	G	1102	PT5	C34-C35-C36-C37
3	A	1102	PT5	C7-C8-C9-O18
3	C	1102	PT5	C7-C8-C9-O18
3	E	1102	PT5	C7-C8-C9-O18
3	G	1102	PT5	C7-C8-C9-O18
3	A	1101	PT5	C19-C20-C21-C22
3	A	1102	PT5	C15-C16-C17-C18
3	A	1102	PT5	C16-C17-C18-C19
3	C	1101	PT5	C19-C20-C21-C22
3	C	1102	PT5	C15-C16-C17-C18
3	C	1102	PT5	C16-C17-C18-C19
3	E	1101	PT5	C19-C20-C21-C22
3	E	1102	PT5	C15-C16-C17-C18
3	E	1102	PT5	C16-C17-C18-C19
3	G	1101	PT5	C19-C20-C21-C22
3	G	1102	PT5	C15-C16-C17-C18
3	G	1102	PT5	C16-C17-C18-C19
3	A	1102	PT5	O13-C7-C8-O16
3	C	1102	PT5	O13-C7-C8-O16
3	E	1102	PT5	O13-C7-C8-O16
3	G	1102	PT5	O13-C7-C8-O16
3	A	1102	PT5	C43-C44-C45-C46
3	C	1102	PT5	C43-C44-C45-C46
3	G	1102	PT5	C43-C44-C45-C46
3	E	1102	PT5	C43-C44-C45-C46
3	A	1101	PT5	C21-C22-C23-C24
3	C	1101	PT5	C21-C22-C23-C24
3	E	1101	PT5	C21-C22-C23-C24
3	G	1101	PT5	C21-C22-C23-C24
3	A	1101	PT5	C12-C10-O16-C8
3	C	1101	PT5	C12-C10-O16-C8
3	E	1101	PT5	C12-C10-O16-C8
3	G	1101	PT5	C12-C10-O16-C8
3	A	1101	PT5	O17-C10-O16-C8
3	C	1101	PT5	O17-C10-O16-C8
3	E	1101	PT5	O17-C10-O16-C8
3	G	1101	PT5	O17-C10-O16-C8
3	A	1102	PT5	C7-O13-P1-O11
3	C	1102	PT5	C7-O13-P1-O11
3	E	1102	PT5	C7-O13-P1-O11
3	G	1102	PT5	C7-O13-P1-O11

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Mol	Chain	Res	Type	Atoms
3	A	1101	PT5	C17-C18-C19-C20
3	C	1101	PT5	C17-C18-C19-C20
3	E	1101	PT5	C17-C18-C19-C20
3	G	1101	PT5	C17-C18-C19-C20
3	A	1102	PT5	O16-C8-C9-O18
3	C	1102	PT5	O16-C8-C9-O18
3	E	1102	PT5	O16-C8-C9-O18
3	G	1102	PT5	O16-C8-C9-O18
3	C	1102	PT5	C10-C12-C13-C14
3	C	1102	PT5	C32-C33-C34-C35
3	G	1102	PT5	C32-C33-C34-C35
3	A	1102	PT5	C10-C12-C13-C14
3	E	1102	PT5	C10-C12-C13-C14
5	A	1107	7YV	C07-C06-C10-O01
5	A	1108	7YV	C07-C06-C10-O01
5	C	1103	7YV	C07-C06-C10-O01
5	E	1103	7YV	C07-C06-C10-O01
3	A	1102	PT5	C32-C33-C34-C35
3	E	1102	PT5	C32-C33-C34-C35
3	G	1102	PT5	C10-C12-C13-C14
3	A	1101	PT5	C9-C8-O16-C10
3	C	1101	PT5	C9-C8-O16-C10
3	E	1101	PT5	C9-C8-O16-C10
3	G	1101	PT5	C9-C8-O16-C10
3	A	1101	PT5	C15-C16-C17-C18
3	A	1102	PT5	C21-C22-C23-C24
3	C	1101	PT5	C15-C16-C17-C18
3	C	1102	PT5	C21-C22-C23-C24
3	E	1101	PT5	C15-C16-C17-C18
3	E	1102	PT5	C21-C22-C23-C24
3	G	1101	PT5	C15-C16-C17-C18
3	G	1102	PT5	C21-C22-C23-C24
3	C	1101	PT5	C31-C32-C33-C34
3	A	1101	PT5	C31-C32-C33-C34
3	E	1101	PT5	C31-C32-C33-C34
3	G	1101	PT5	C31-C32-C33-C34
3	A	1101	PT5	C13-C14-C15-C16
3	C	1101	PT5	C13-C14-C15-C16
3	E	1101	PT5	C13-C14-C15-C16
3	G	1101	PT5	C13-C14-C15-C16
3	A	1101	PT5	C12-C13-C14-C15
3	C	1101	PT5	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
3	E	1101	PT5	C12-C13-C14-C15
3	G	1101	PT5	C12-C13-C14-C15
3	A	1102	PT5	O17-C10-O16-C8
3	C	1102	PT5	O17-C10-O16-C8
3	E	1102	PT5	O17-C10-O16-C8
3	G	1102	PT5	O17-C10-O16-C8
3	A	1102	PT5	C3-C4-O4-P4
3	C	1102	PT5	C3-C4-O4-P4
3	E	1102	PT5	C3-C4-O4-P4
3	G	1102	PT5	C3-C4-O4-P4
5	A	1107	7YV	C07-C06-C10-N02
5	A	1108	7YV	C07-C06-C10-N02
5	C	1103	7YV	C07-C06-C10-N02
5	E	1103	7YV	C07-C06-C10-N02
3	A	1101	PT5	C7-C8-O16-C10
3	C	1101	PT5	C7-C8-O16-C10
3	E	1101	PT5	C7-C8-O16-C10
3	G	1101	PT5	C7-C8-O16-C10
3	A	1102	PT5	O18-C11-C31-C32
3	G	1102	PT5	O18-C11-C31-C32
3	E	1102	PT5	C12-C10-O16-C8
3	C	1102	PT5	O18-C11-C31-C32
3	E	1102	PT5	O18-C11-C31-C32
3	A	1102	PT5	O19-C11-C31-C32
3	C	1102	PT5	O19-C11-C31-C32
3	E	1102	PT5	O19-C11-C31-C32
3	G	1102	PT5	O19-C11-C31-C32
3	A	1102	PT5	C12-C10-O16-C8
3	C	1102	PT5	C12-C10-O16-C8
3	G	1102	PT5	C12-C10-O16-C8

There are no ring outliers.

12 monomers are involved in 79 short contacts:

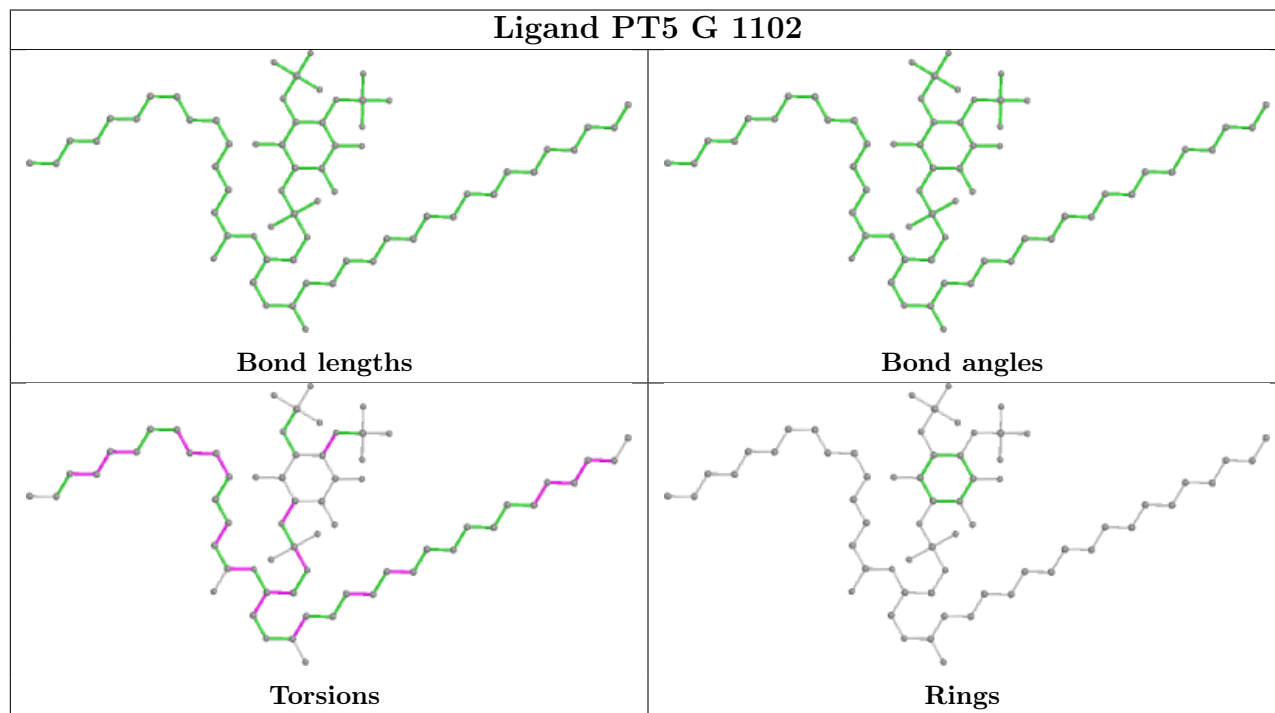
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1102	PT5	9	0
3	E	1101	PT5	11	0
3	G	1101	PT5	9	0
5	A	1108	7YV	5	0
5	C	1103	7YV	5	0
3	C	1102	PT5	8	0
3	A	1101	PT5	10	0

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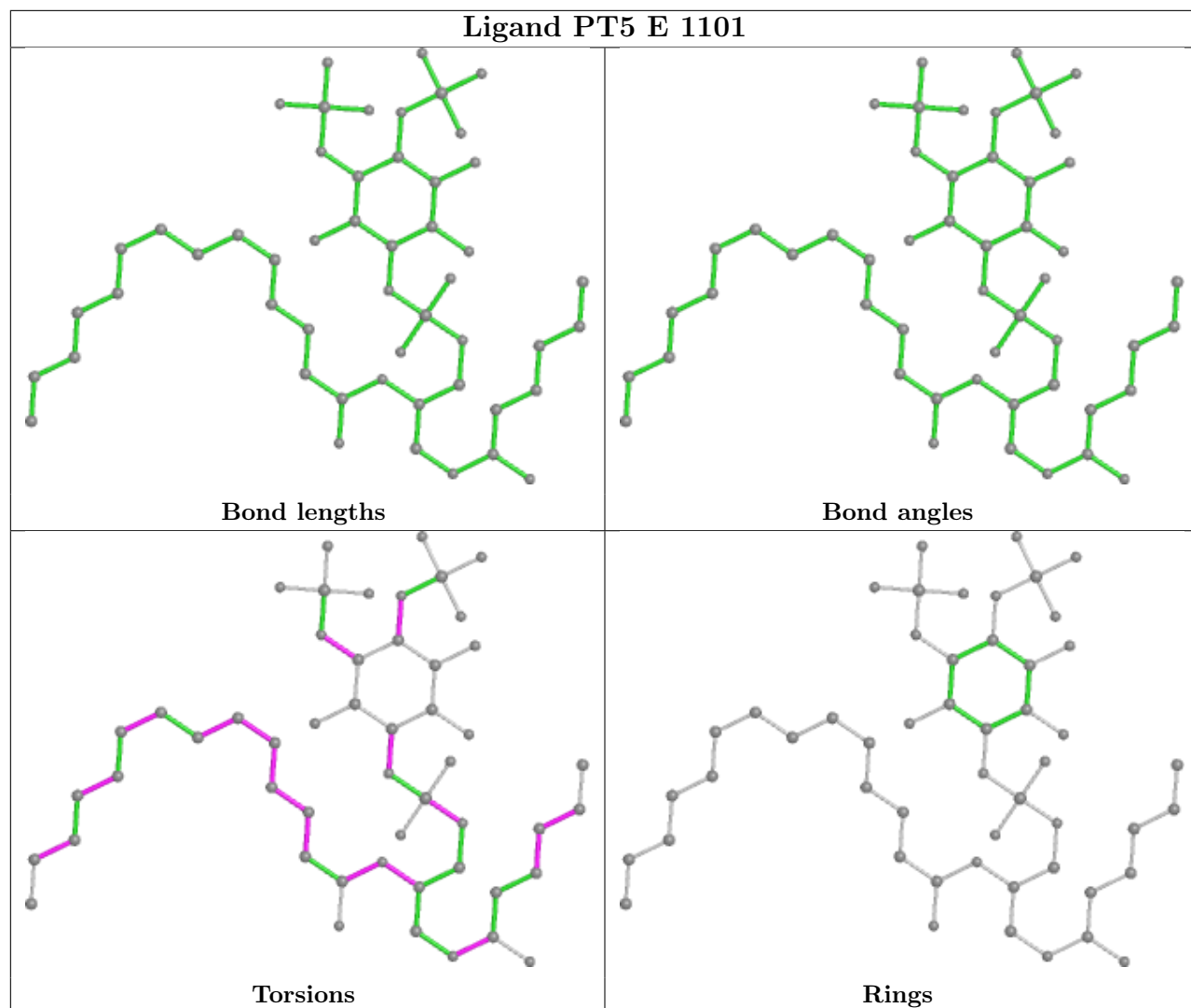
*Continued from previous page...*

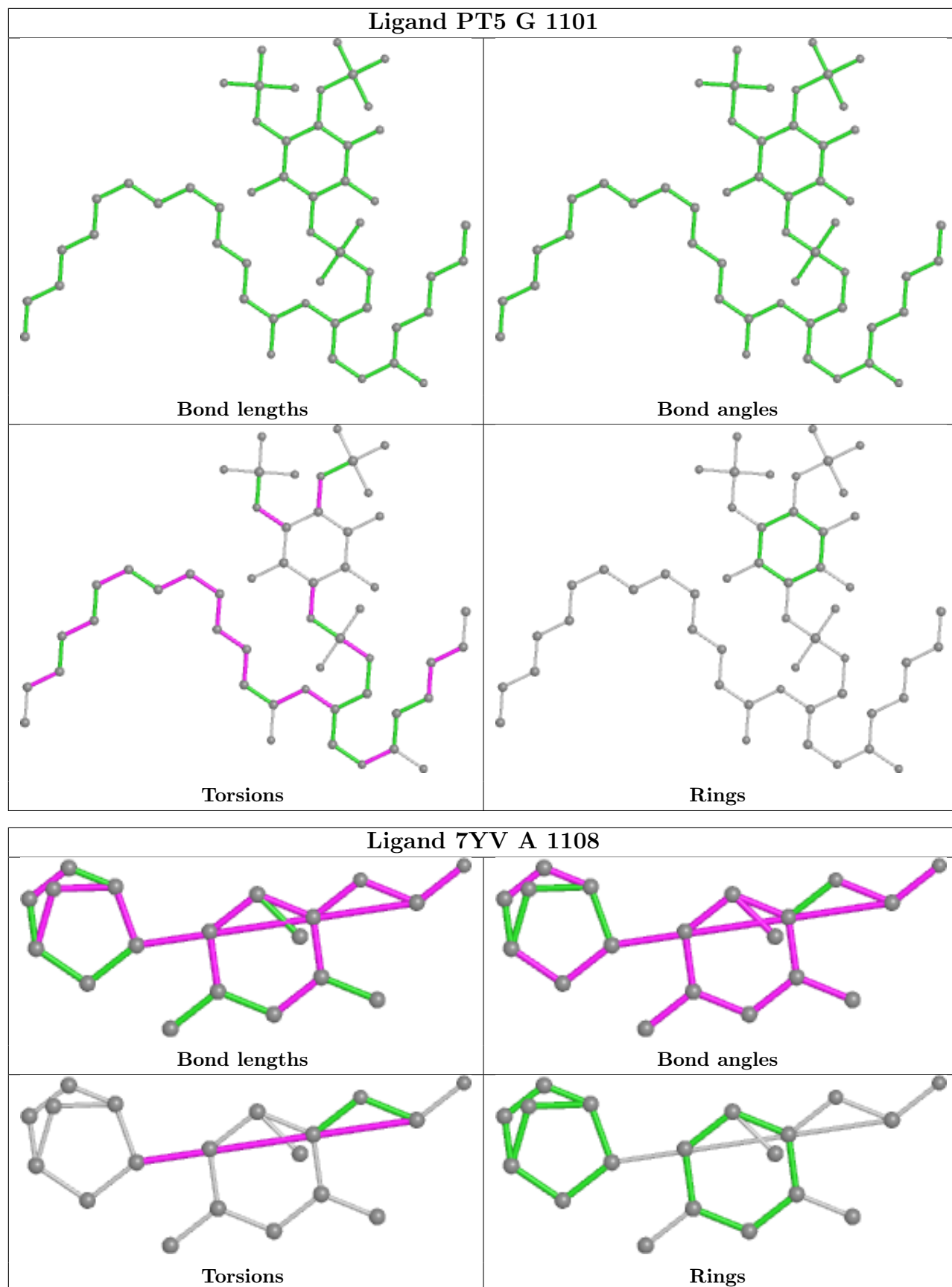
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1107	7YV	7	0
3	C	1101	PT5	10	0
5	E	1103	7YV	6	0
3	E	1102	PT5	7	0
3	A	1102	PT5	7	0

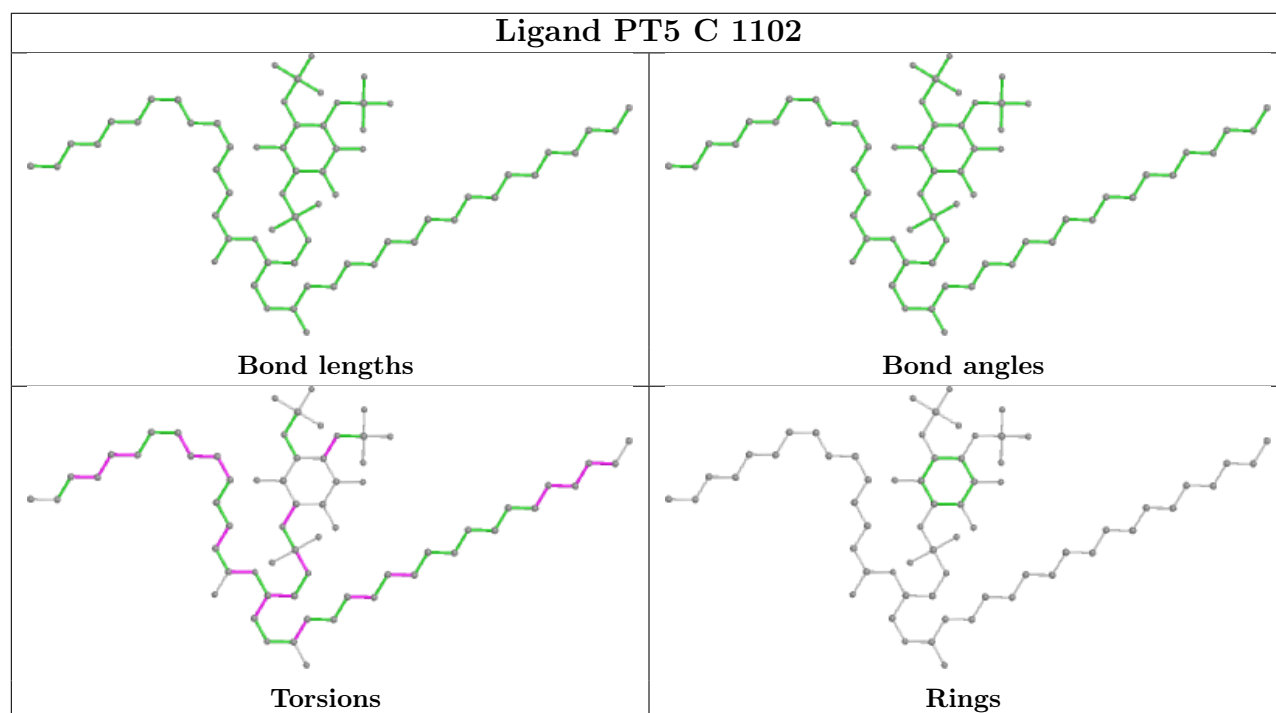
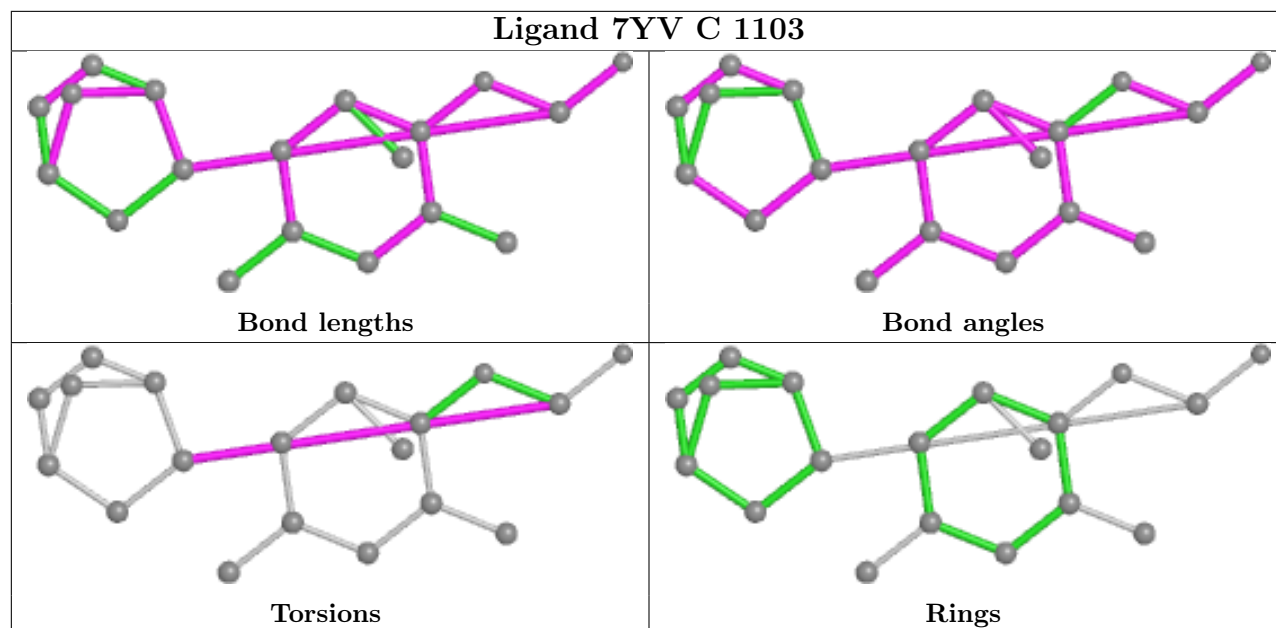
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

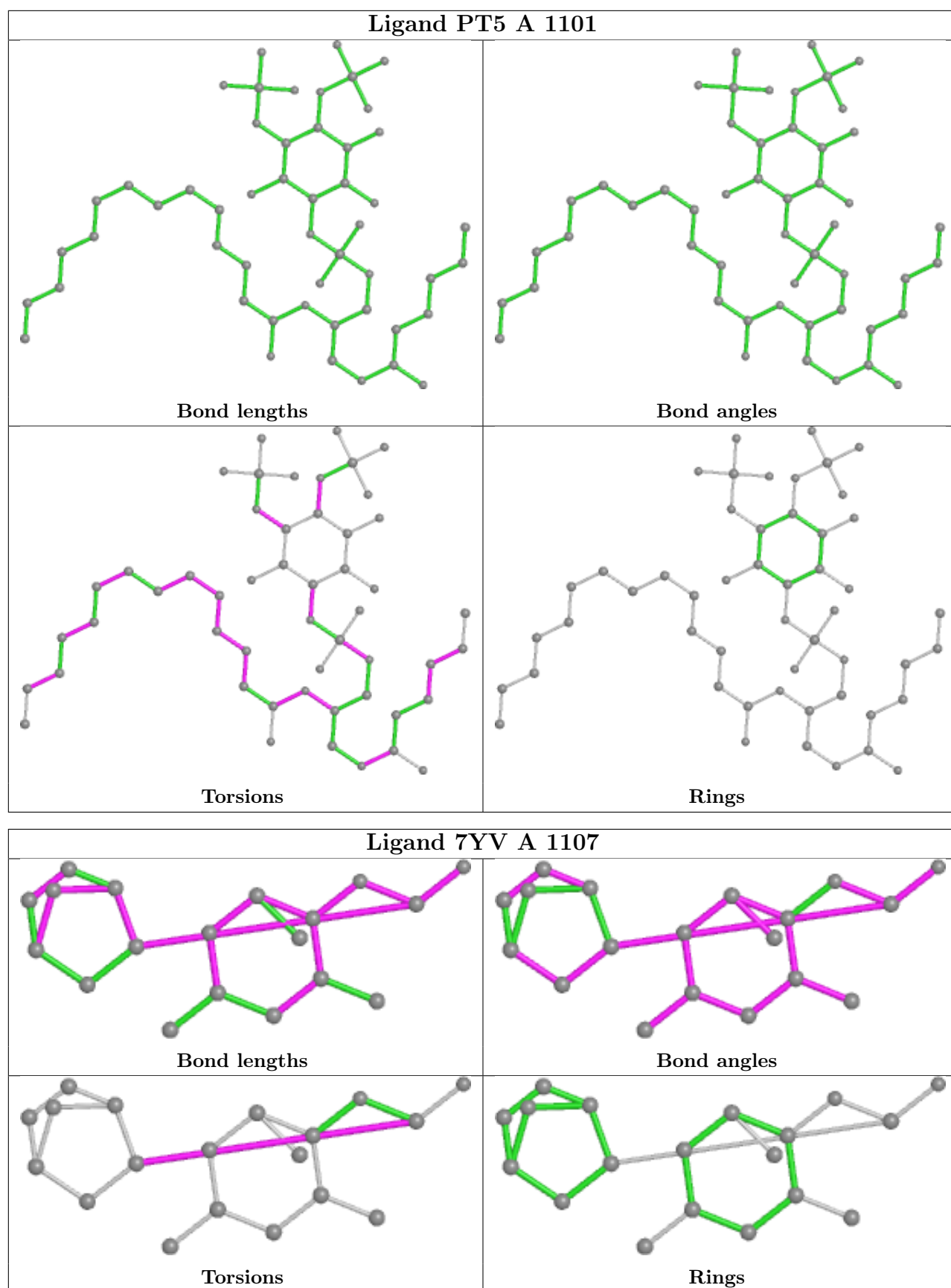


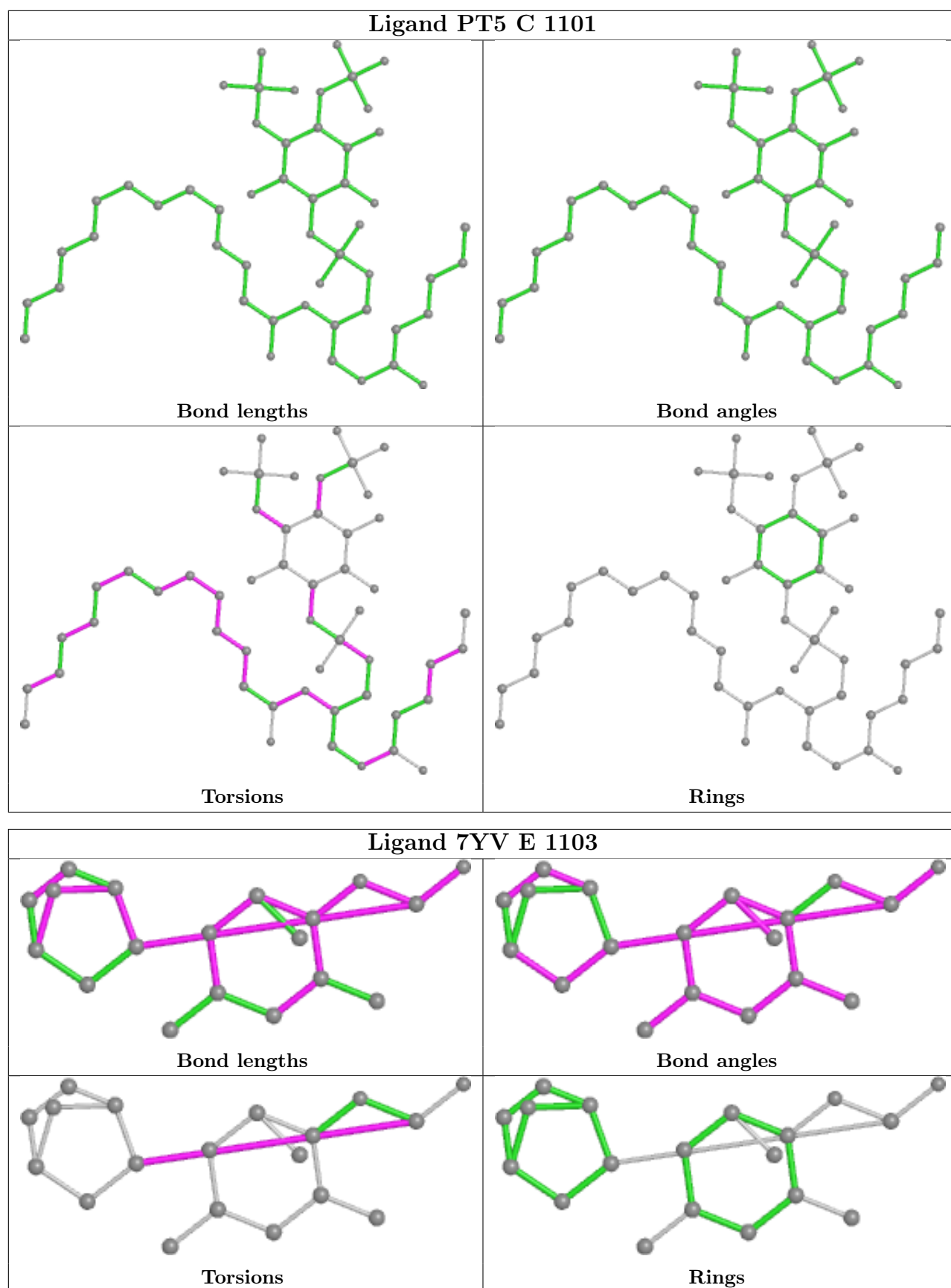


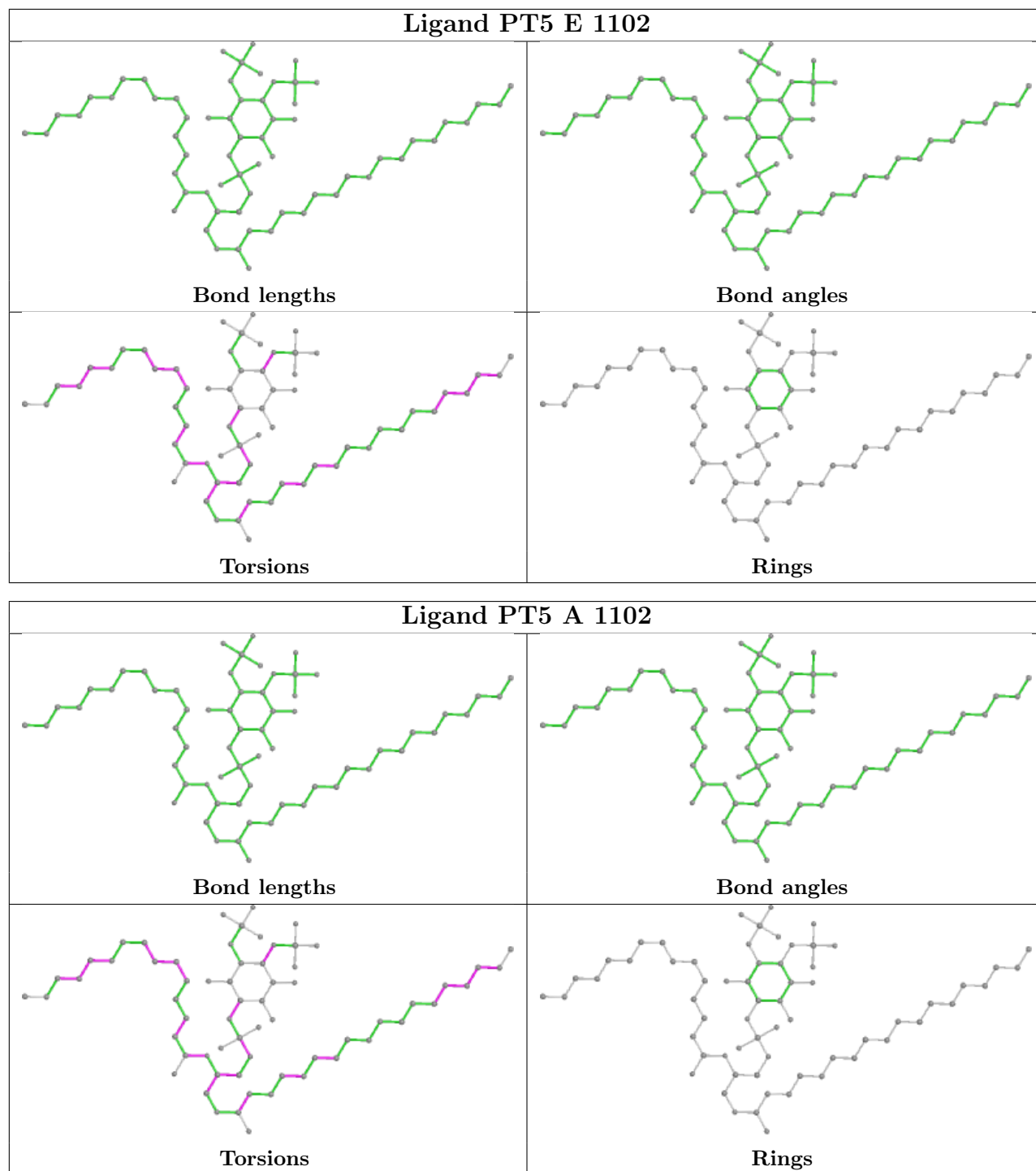












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

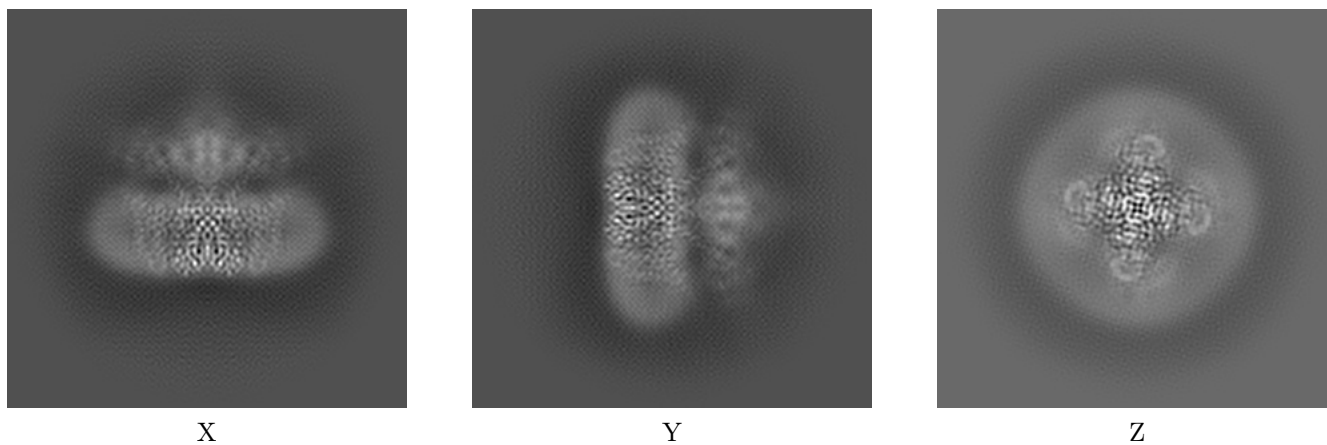
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32044. 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](#)

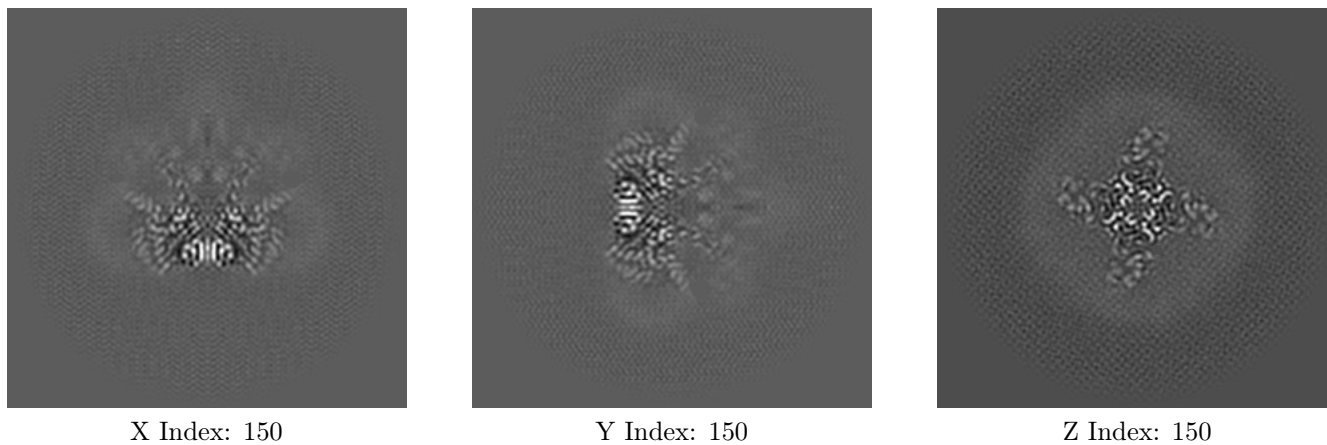
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

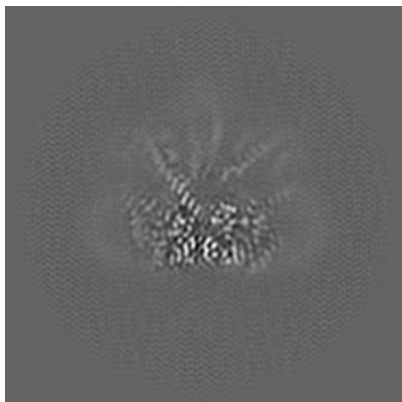
#### 6.2.1 Primary map



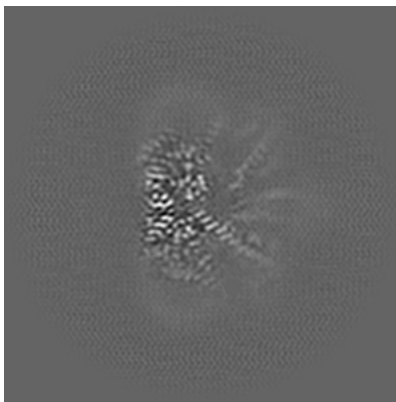
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

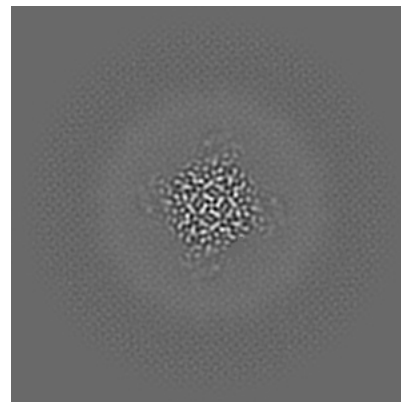
### 6.3.1 Primary map



X Index: 146



Y Index: 154

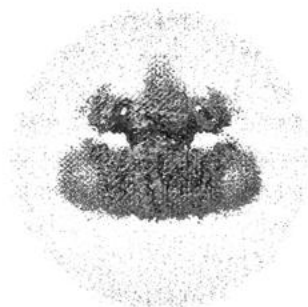


Z Index: 113

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

## 6.4 Orthogonal surface views [i](#)

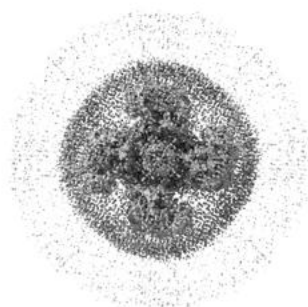
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.077. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



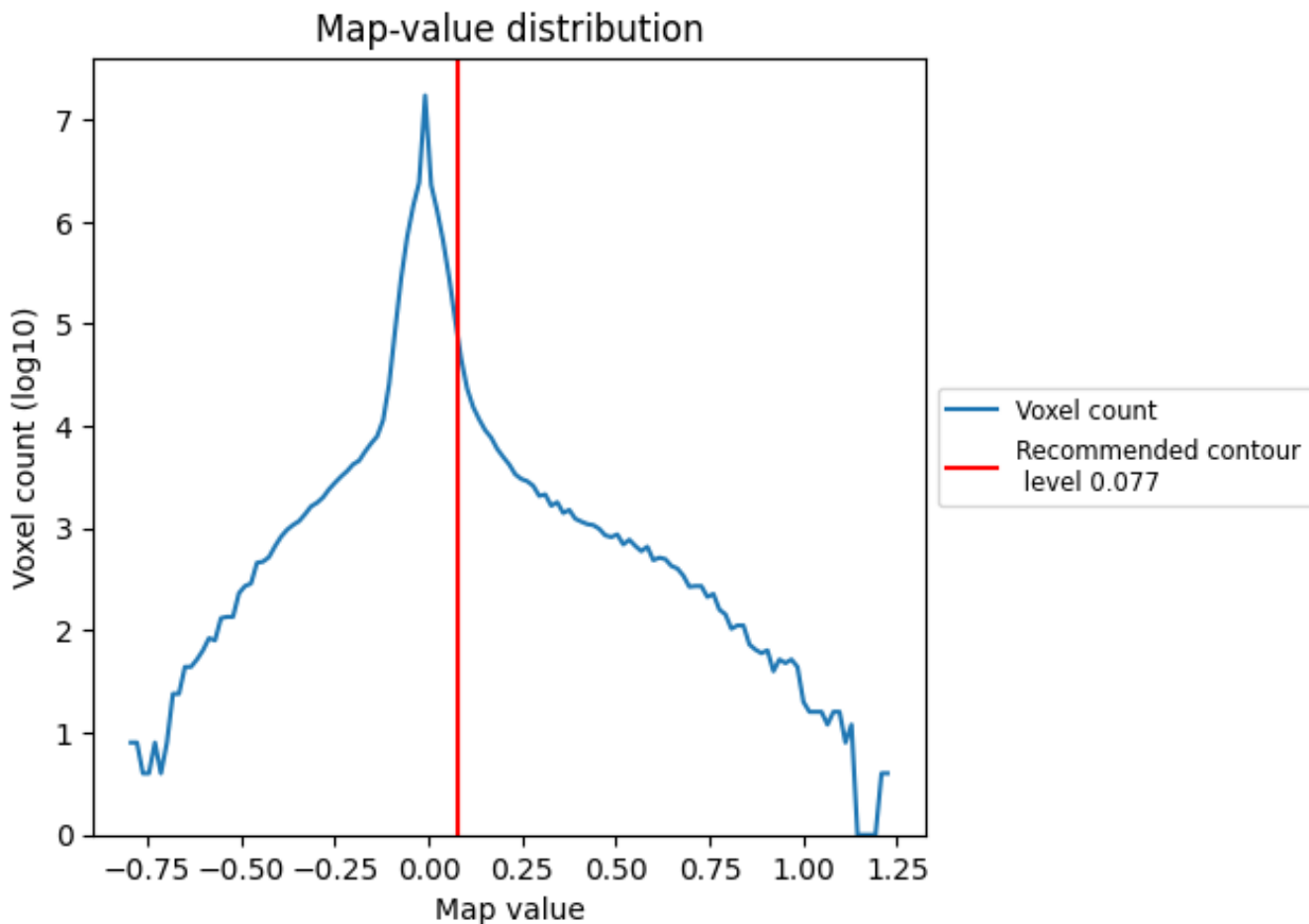
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

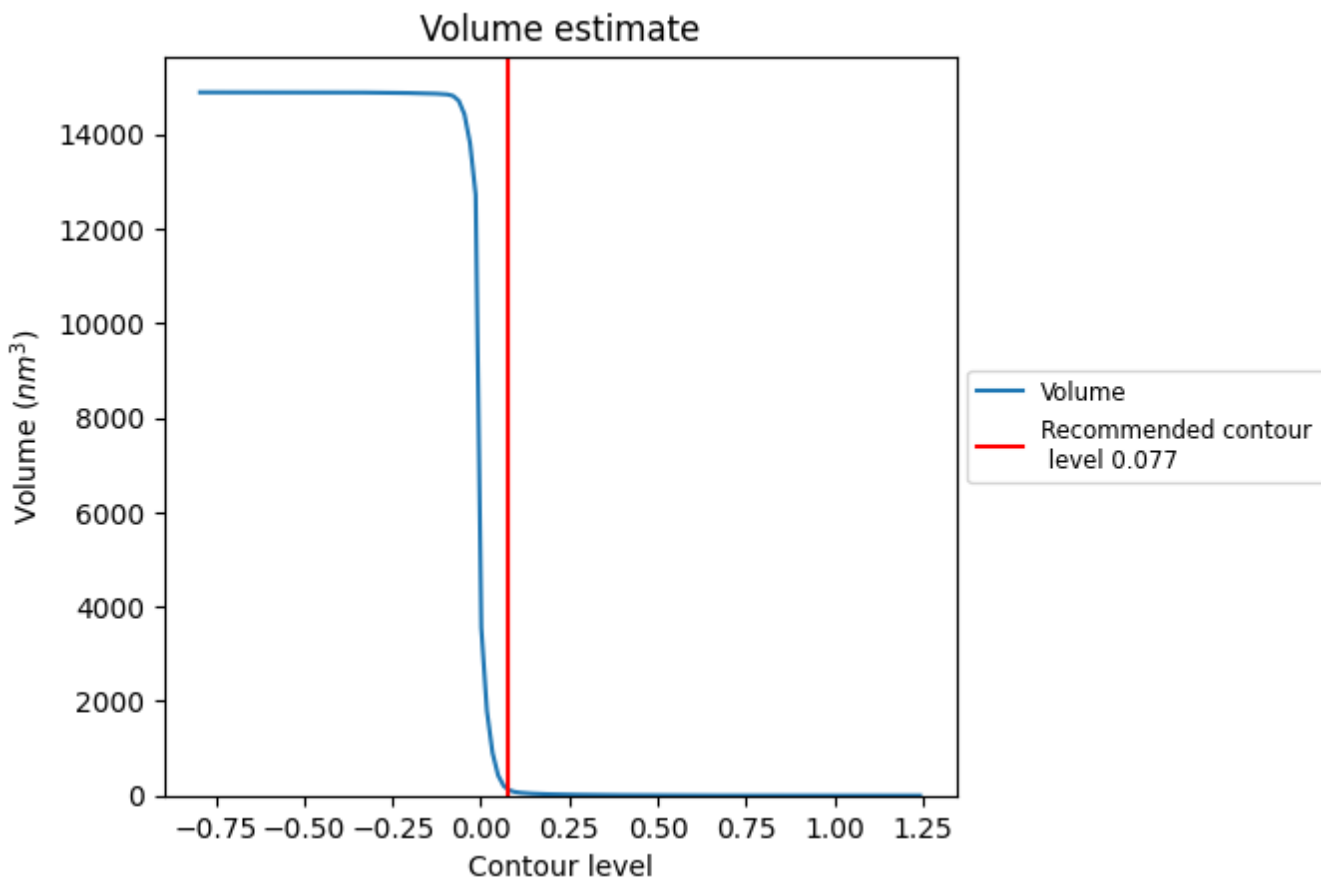
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

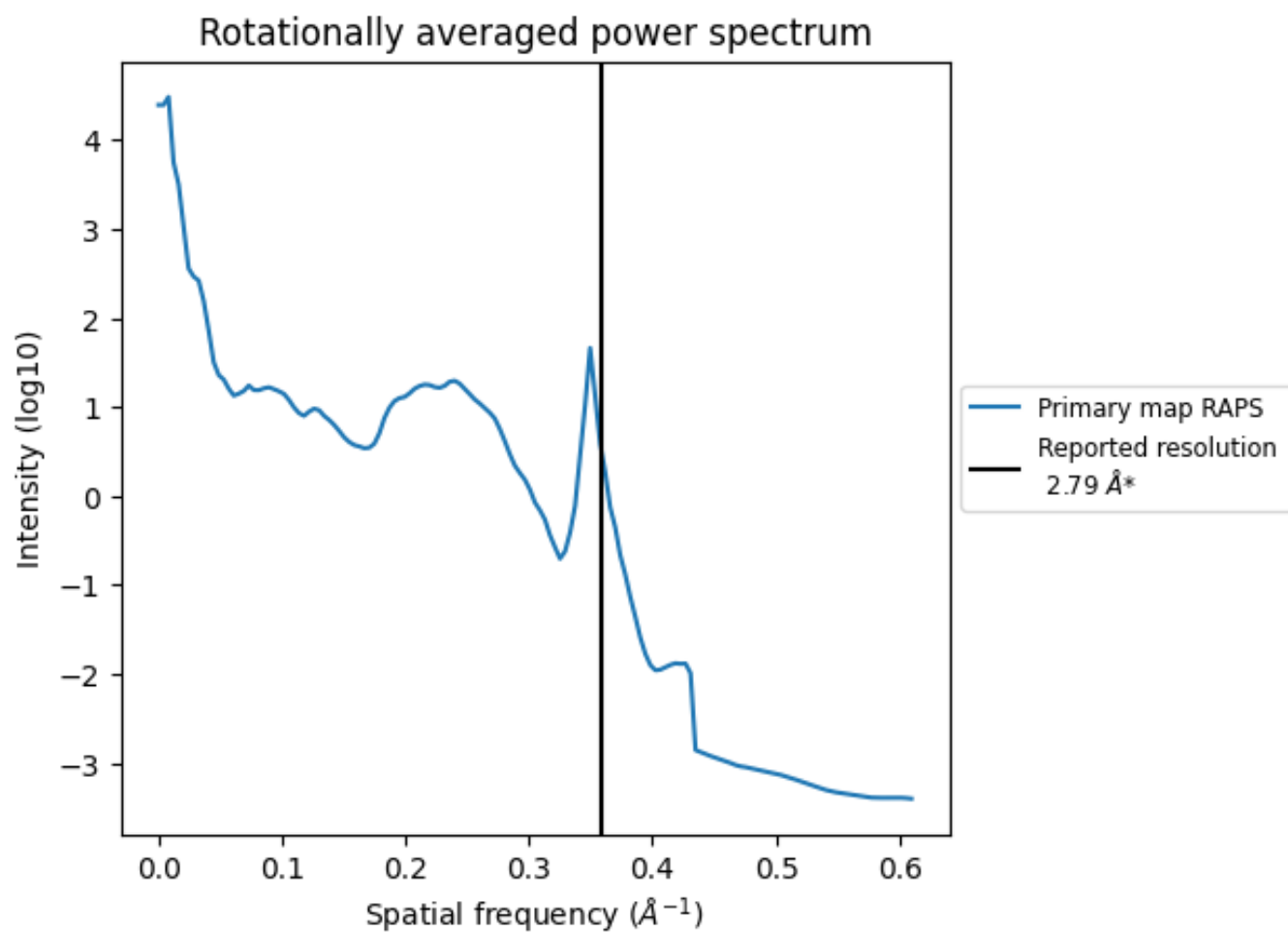
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 133  $\text{nm}^3$ ; this corresponds to an approximate mass of 120 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.358 \text{\AA}^{-1}$

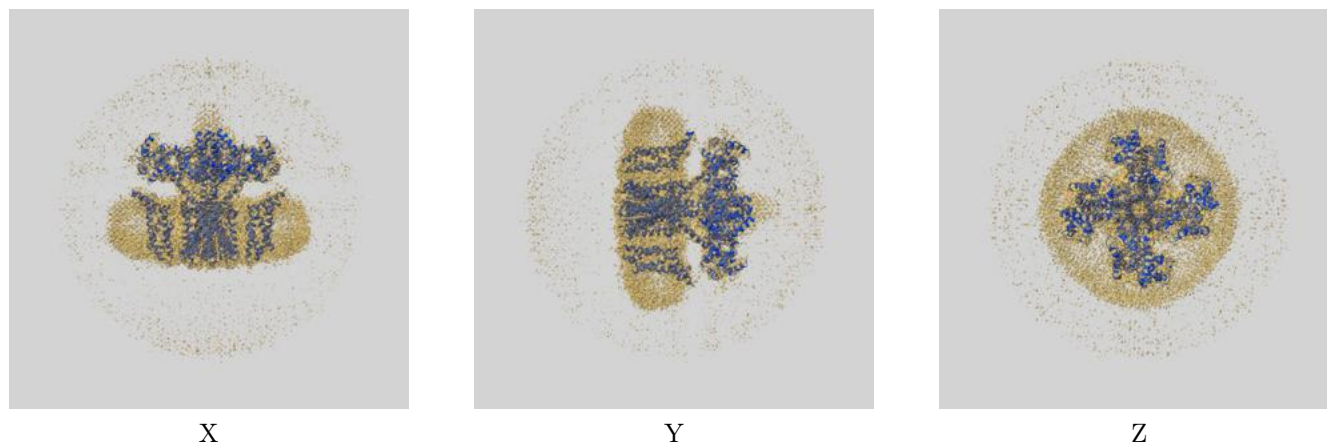
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

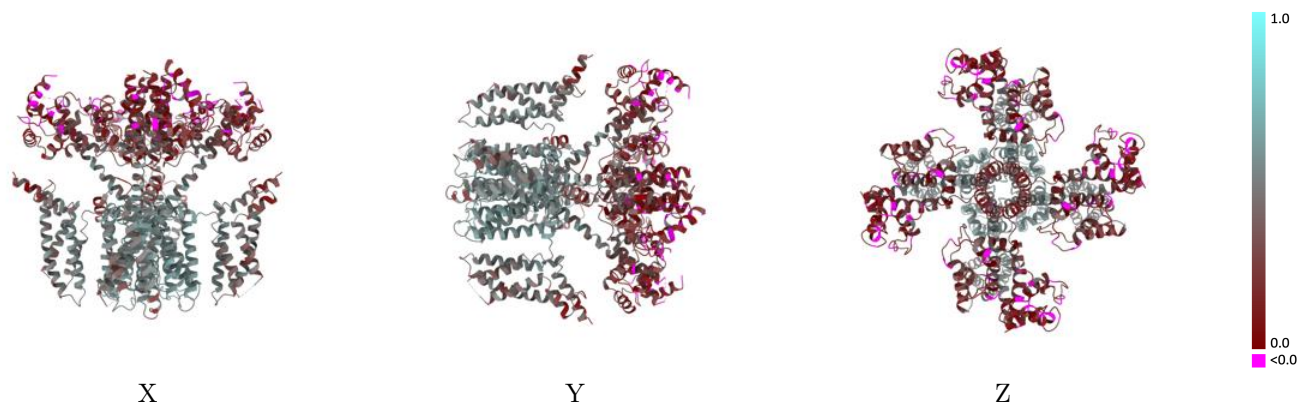
This section contains information regarding the fit between EMDB map EMD-32044 and PDB model 7VNP. Per-residue inclusion information can be found in section 3 on page 9.

### 9.1 Map-model overlay [i](#)



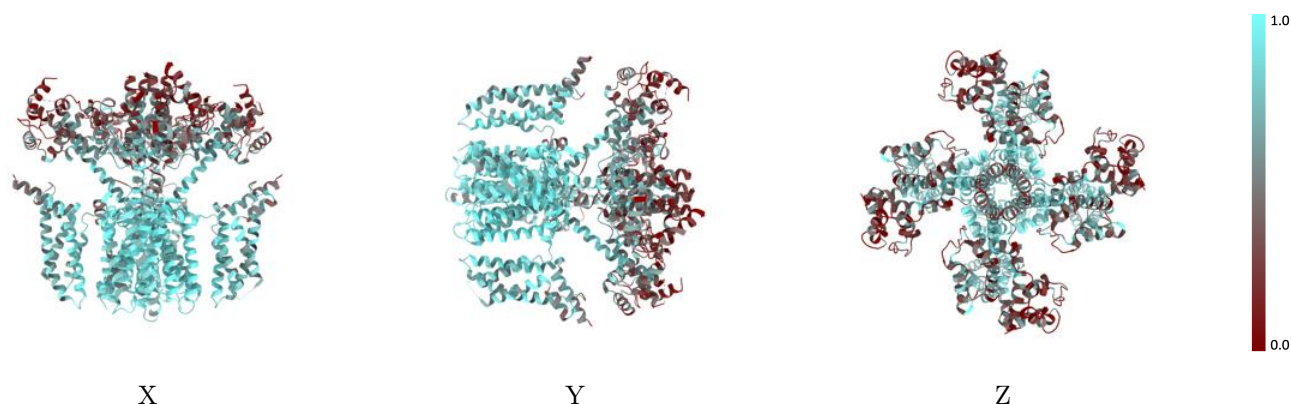
The images above show the 3D surface view of the map at the recommended contour level 0.077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



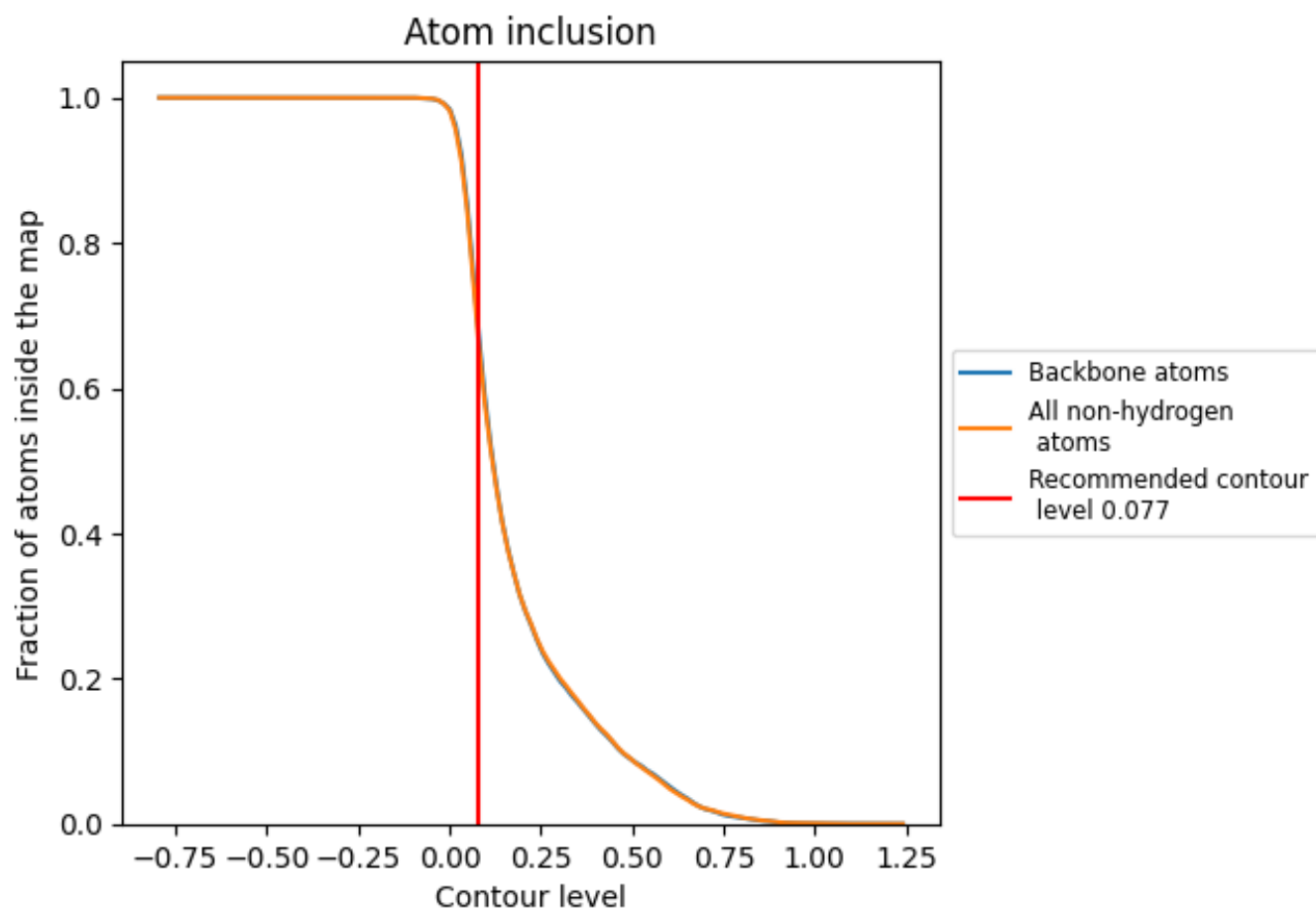
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.077).

## 9.4 Atom inclusion [i](#)





















At the recommended contour level, 69% of all backbone atoms, 68% 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 (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6782	 0.3760
A	 0.7647	 0.4320
B	 0.3637	 0.1860
C	 0.7631	 0.4310
D	 0.3686	 0.1870
E	 0.7649	 0.4320
F	 0.3686	 0.1890
G	 0.7632	 0.4310
H	 0.3686	 0.1860

