



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 02:48 AM UTC

PDB ID : 9PWO / pdb_00009pwo
EMDB ID : EMD-71924
Title : Pig Ryanodine Receptor 1 R615C Mutant: Atorvastatin Bound Open Conformation
Authors : Molinarolo, S.M.; Van Petegem, F.
Deposited on : 2025-08-04
Resolution : 3.36 Å(reported)
Based on initial model : 9OL4

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

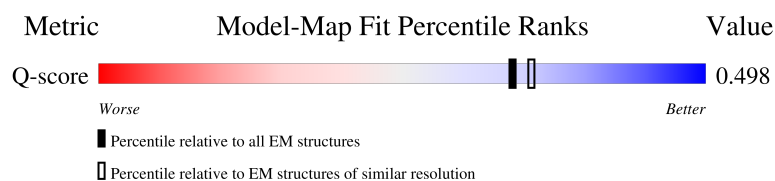
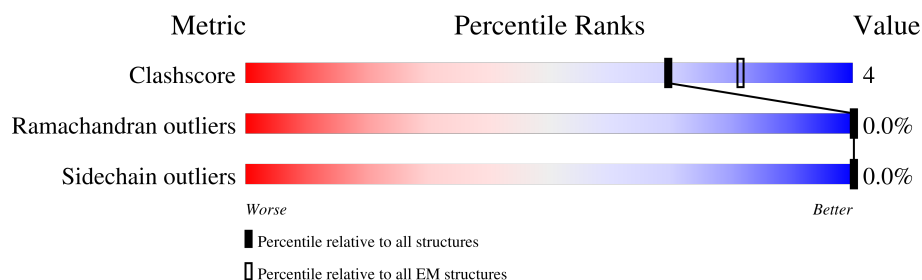
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.36 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	14332 (2.86 - 3.86)

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

Mol	Chain	Length	Quality of chain
1	A	5035	10% 75% 6% 19%
1	G	5035	10% 75% 6% 19%
1	M	5035	9% 75% 6% 19%
1	S	5035	9% 75% 6% 19%

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Mol	Chain	Length	Quality of chain
2	B	111	 80%16%.
2	H	111	 80%16%.
2	N	111	 81%15%.
2	T	111	 80%16%.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 130604 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4103	Total	C	N	O	S	0	0
			31697	20282	5470	5734	211		
1	G	4103	Total	C	N	O	S	0	0
			31697	20282	5470	5734	211		
1	M	4103	Total	C	N	O	S	0	0
			31697	20282	5470	5734	211		
1	S	4103	Total	C	N	O	S	0	0
			31697	20282	5470	5734	211		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	CYS	ARG	variant	UNP P16960
G	615	CYS	ARG	variant	UNP P16960
M	615	CYS	ARG	variant	UNP P16960
S	615	CYS	ARG	variant	UNP P16960

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			815	514	143	154	4		
2	H	107	Total	C	N	O	S	0	0
			815	514	143	154	4		
2	N	107	Total	C	N	O	S	0	0
			815	514	143	154	4		
2	T	107	Total	C	N	O	S	0	0
			815	514	143	154	4		

There are 12 discrepancies between the modelled and reference sequences:

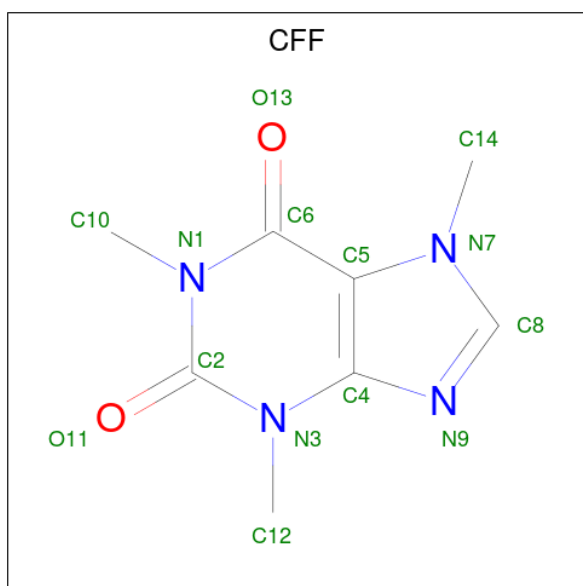
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASN	-	expression tag	UNP P68106
B	0	ALA	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106
H	-1	ASN	-	expression tag	UNP P68106
H	0	ALA	-	expression tag	UNP P68106
N	-2	SER	-	expression tag	UNP P68106
N	-1	ASN	-	expression tag	UNP P68106
N	0	ALA	-	expression tag	UNP P68106
T	-2	SER	-	expression tag	UNP P68106
T	-1	ASN	-	expression tag	UNP P68106
T	0	ALA	-	expression tag	UNP P68106

- Molecule 3 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

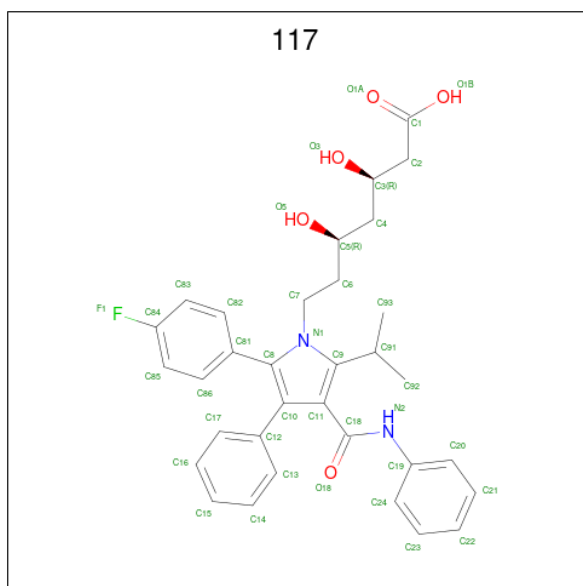


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	4	2	
3	G	1	Total	C	N	O	0
			14	8	4	2	
3	M	1	Total	C	N	O	0
			14	8	4	2	
3	S	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	
4	M	1	Total	Ca	0
			1	1	
4	S	1	Total	Ca	0
			1	1	

- Molecule 5 is 7-[2-(4-FLUORO-PHENYL)-5-ISOPROPYL-3-PHENYL-4-PHENYLCARBAMOYL-PYRROL-1-YL]-3,5-DIHYDROXY-HEPTANOIC ACID (CCD ID: 117) (formula: $C_{33}H_{35}FN_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	A	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	A	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	G	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	G	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	G	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	M	1	Total	C	F	N	O	0
			41	33	1	2	5	

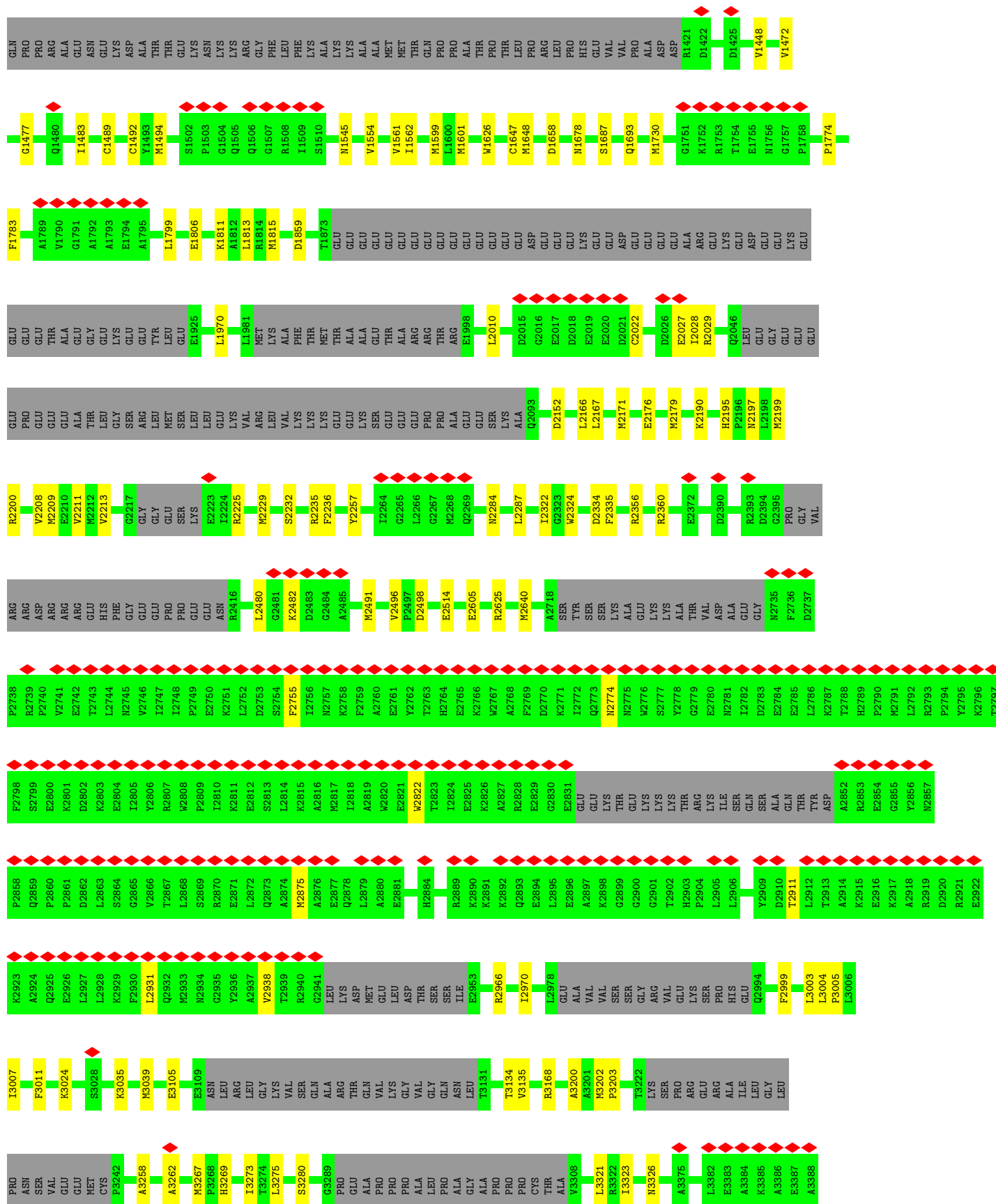
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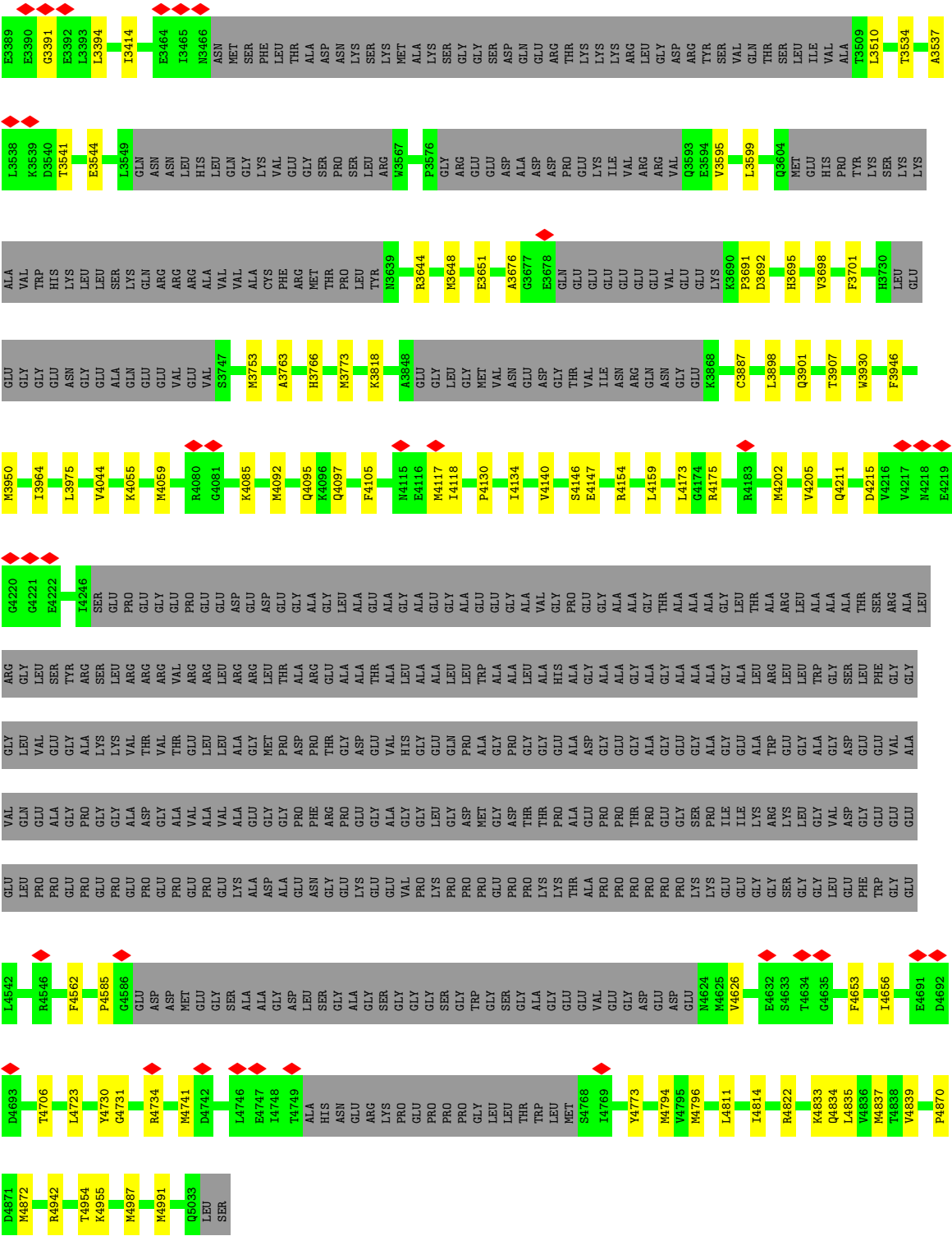
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Mol	Chain	Residues	Atoms					AltConf
5	M	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	M	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	S	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	S	1	Total	C	F	N	O	0
			41	33	1	2	5	
5	S	1	Total	C	F	N	O	0
			41	33	1	2	5	

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

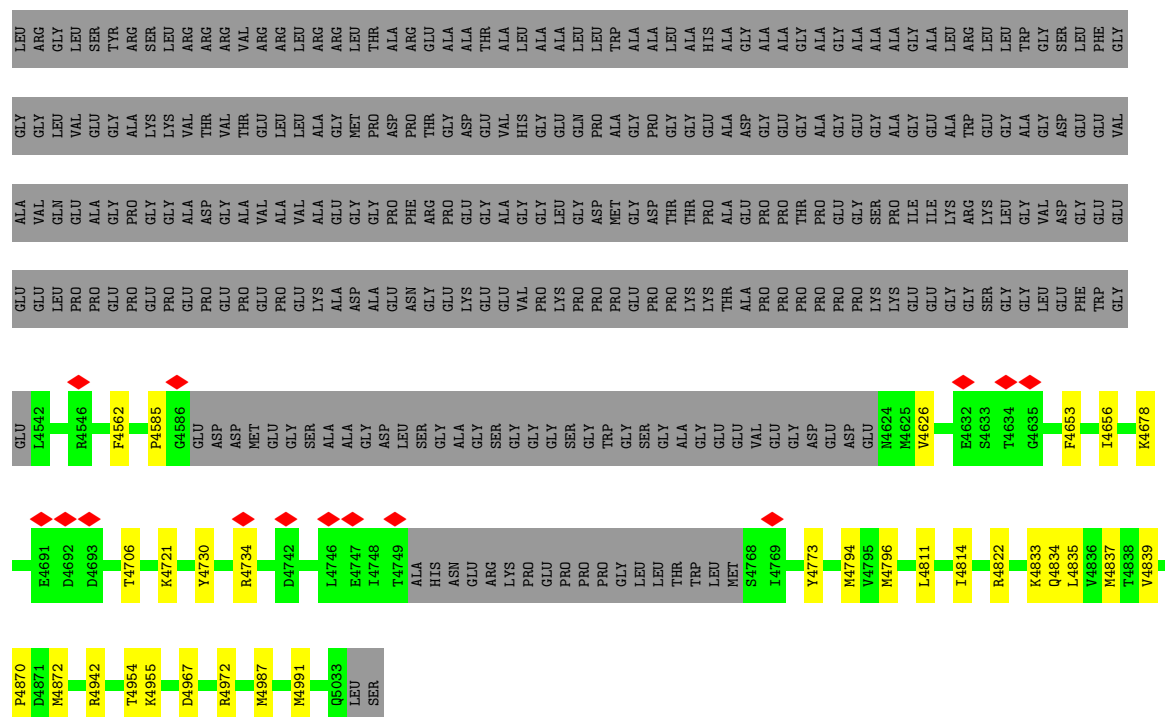
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Zn	0
			1	1	
6	G	1	Total	Zn	0
			1	1	
6	M	1	Total	Zn	0
			1	1	
6	S	1	Total	Zn	0
			1	1	



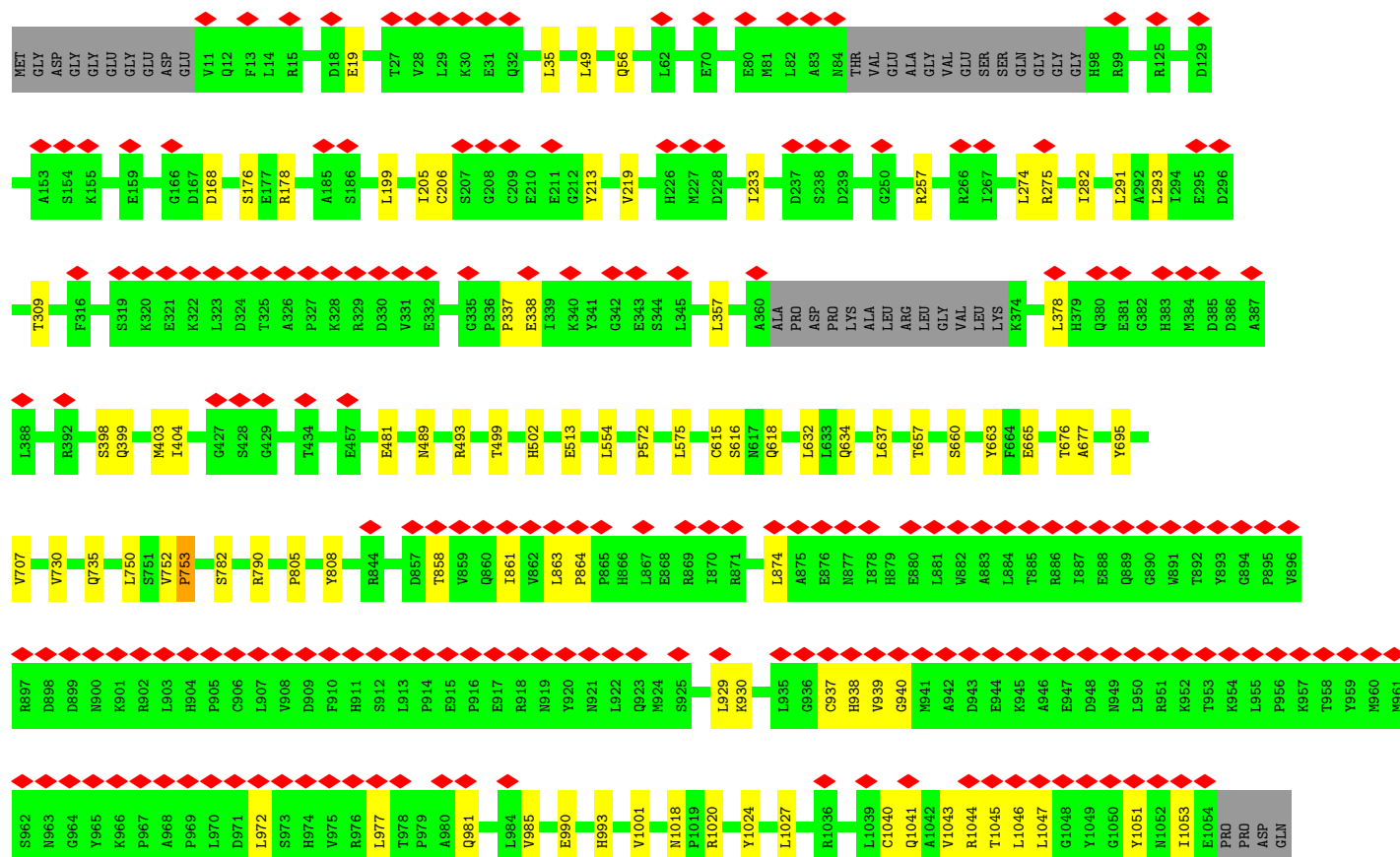
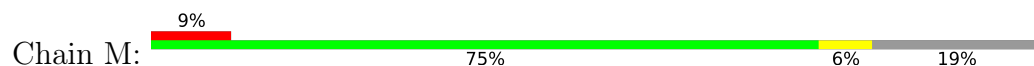








• Molecule 1: Ryanodine receptor 1



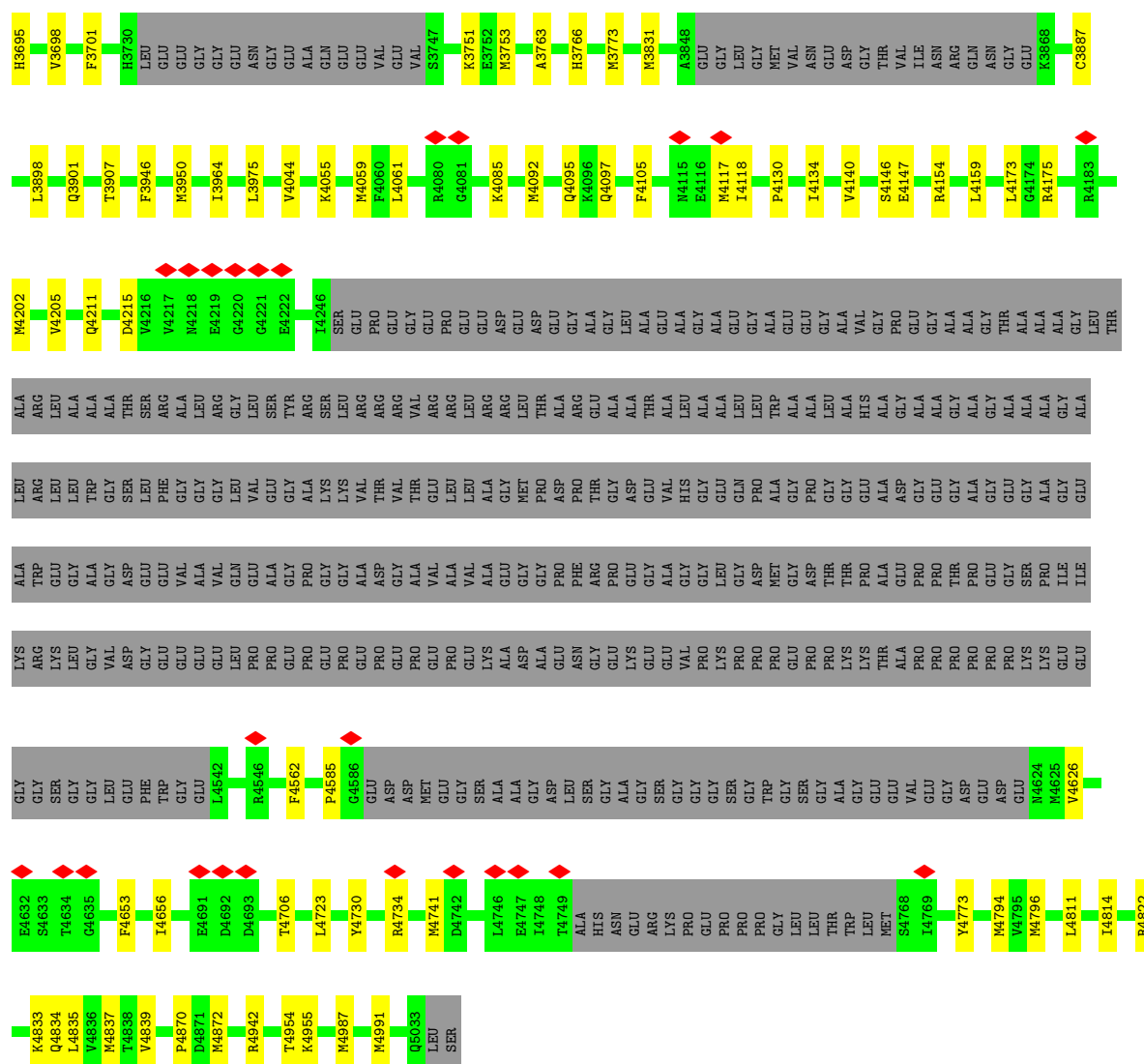




Chain S: 9% 75% 6% 19%







• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain B: 80% 16% .



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 80% 16% .

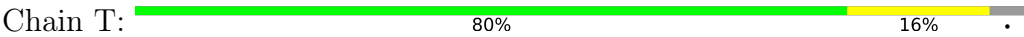


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain N: 81% 15% .



● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	96731	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	491.52, 491.52, 491.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, 117, CFF

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	0.27	0/32418	0.45	1/44019 (0.0%)
1	G	0.27	0/32418	0.45	1/44019 (0.0%)
1	M	0.27	0/32418	0.45	1/44019 (0.0%)
1	S	0.27	0/32418	0.45	1/44019 (0.0%)
2	B	0.15	0/831	0.39	0/1117
2	H	0.15	0/831	0.39	0/1117
2	N	0.15	0/831	0.39	0/1117
2	T	0.15	0/831	0.39	0/1117
All	All	0.27	0/132996	0.45	4/180544 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	2774	ASN	N-CA-C	-5.16	106.83	113.02
1	A	2774	ASN	N-CA-C	-5.14	106.86	113.02
1	G	2774	ASN	N-CA-C	-5.14	106.86	113.02
1	M	2774	ASN	N-CA-C	-5.14	106.86	113.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	31697	0	30659	213	0
1	G	31697	0	30659	217	0
1	M	31697	0	30659	215	0
1	S	31697	0	30659	219	0
2	B	815	0	816	12	0
2	H	815	0	816	12	0
2	N	815	0	816	11	0
2	T	815	0	816	12	0
3	A	14	0	10	0	0
3	G	14	0	10	0	0
3	M	14	0	10	0	0
3	S	14	0	10	0	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
4	M	1	0	0	0	0
4	S	1	0	0	0	0
5	A	123	0	102	10	0
5	G	123	0	102	11	0
5	M	123	0	102	10	0
5	S	123	0	102	10	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
All	All	130604	0	126348	929	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 (929) 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)
1:A:977:LEU:HD21	1:A:1043:VAL:HG12	1.43	1.01
1:G:977:LEU:HD21	1:G:1043:VAL:HG12	1.43	0.99
1:S:977:LEU:HD21	1:S:1043:VAL:HG12	1.43	0.98
1:M:977:LEU:HD21	1:M:1043:VAL:HG12	1.43	0.97
1:A:981:GLN:HG2	1:A:1053:ILE:HD11	1.47	0.96
1:M:981:GLN:HG2	1:M:1053:ILE:HD11	1.47	0.94
1:G:981:GLN:HG2	1:G:1053:ILE:HD11	1.47	0.93
1:S:981:GLN:HG2	1:S:1053:ILE:HD11	1.47	0.93
5:A:5104:117:H83	5:A:5105:117:H931	1.55	0.89
5:G:5104:117:H83	5:G:5105:117:H931	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:5104:117:H83	5:S:5105:117:H931	1.55	0.87
5:M:5104:117:H83	5:M:5105:117:H931	1.55	0.87
1:A:981:GLN:HG2	1:A:1053:ILE:CD1	2.07	0.84
1:S:981:GLN:HG2	1:S:1053:ILE:CD1	2.07	0.84
1:M:937:CYS:SG	1:M:1053:ILE:HB	2.18	0.84
1:G:937:CYS:SG	1:G:1053:ILE:HB	2.18	0.84
1:S:937:CYS:SG	1:S:1053:ILE:HB	2.18	0.84
1:A:937:CYS:SG	1:A:1053:ILE:HB	2.18	0.84
1:G:981:GLN:HG2	1:G:1053:ILE:CD1	2.07	0.84
1:M:981:GLN:HG2	1:M:1053:ILE:CD1	2.07	0.83
1:A:858:THR:O	1:A:861:ILE:HG22	1.84	0.79
1:G:858:THR:O	1:G:861:ILE:HG22	1.84	0.78
1:M:4562:PHE:CE2	5:M:5104:117:H13	2.18	0.78
1:A:4562:PHE:CE2	5:A:5104:117:H13	2.18	0.77
1:S:858:THR:O	1:S:861:ILE:HG22	1.84	0.77
1:G:4562:PHE:CE2	5:G:5104:117:H13	2.18	0.77
1:M:858:THR:O	1:M:861:ILE:HG22	1.84	0.77
1:S:977:LEU:HD21	1:S:1043:VAL:CG1	2.16	0.76
1:S:4562:PHE:CE2	5:S:5104:117:H13	2.18	0.76
1:A:977:LEU:HD21	1:A:1043:VAL:CG1	2.16	0.76
1:M:977:LEU:HD21	1:M:1043:VAL:CG1	2.16	0.76
1:S:985:VAL:HG22	1:S:1043:VAL:HG21	1.68	0.75
1:M:2755:PHE:CZ	1:M:2931:LEU:HG	2.22	0.75
1:M:2755:PHE:HZ	1:M:2931:LEU:HG	1.51	0.75
1:S:2755:PHE:CZ	1:S:2931:LEU:HG	2.22	0.75
1:G:977:LEU:HD21	1:G:1043:VAL:CG1	2.16	0.75
1:G:981:GLN:HG2	1:G:1053:ILE:CG1	2.17	0.75
1:A:981:GLN:HG2	1:A:1053:ILE:CG1	2.17	0.74
1:M:985:VAL:HG22	1:M:1043:VAL:HG21	1.68	0.74
1:A:2755:PHE:HZ	1:A:2931:LEU:HG	1.51	0.74
1:A:985:VAL:HG22	1:A:1043:VAL:HG21	1.68	0.74
1:G:2755:PHE:CZ	1:G:2931:LEU:HG	2.22	0.74
1:A:2755:PHE:CZ	1:A:2931:LEU:HG	2.22	0.74
1:S:2755:PHE:HZ	1:S:2931:LEU:HG	1.51	0.74
1:A:4585:PRO:HD3	1:A:4626:VAL:HG11	1.70	0.74
1:G:2755:PHE:HZ	1:G:2931:LEU:HG	1.51	0.73
1:M:981:GLN:HG2	1:M:1053:ILE:CG1	2.17	0.73
1:S:981:GLN:HG2	1:S:1053:ILE:CG1	2.17	0.73
1:G:972:LEU:HD11	1:G:1045:THR:HA	1.70	0.73
1:G:985:VAL:HG22	1:G:1043:VAL:HG21	1.68	0.73
1:M:972:LEU:HD11	1:M:1045:THR:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4585:PRO:HD3	1:G:4626:VAL:HG11	1.70	0.72
1:A:972:LEU:HD11	1:A:1045:THR:HA	1.70	0.72
1:S:4585:PRO:HD3	1:S:4626:VAL:HG11	1.70	0.72
1:M:4585:PRO:HD3	1:M:4626:VAL:HG11	1.70	0.72
1:G:2755:PHE:CZ	1:G:2931:LEU:CD2	2.73	0.71
1:M:2755:PHE:CZ	1:M:2931:LEU:CD2	2.73	0.71
2:T:5:ILE:HG12	2:T:75:LEU:HD22	1.71	0.71
2:H:5:ILE:HG12	2:H:75:LEU:HD22	1.71	0.71
1:S:2755:PHE:CZ	1:S:2931:LEU:CD2	2.73	0.71
1:A:2755:PHE:CZ	1:A:2931:LEU:CD2	2.73	0.71
1:S:972:LEU:HD11	1:S:1045:THR:HA	1.70	0.71
2:N:5:ILE:HG12	2:N:75:LEU:HD22	1.71	0.70
1:G:977:LEU:CD2	1:G:1043:VAL:HG12	2.21	0.70
2:B:5:ILE:HG12	2:B:75:LEU:HD22	1.71	0.70
1:M:977:LEU:CD2	1:M:1043:VAL:HG12	2.21	0.69
1:M:676:THR:HG22	1:M:677:ALA:H	1.58	0.69
5:M:5104:117:H83	5:M:5105:117:C93	2.23	0.69
1:S:676:THR:HG22	1:S:677:ALA:H	1.58	0.69
1:S:2875:MET:HE1	1:S:2938:VAL:HG12	1.75	0.69
1:G:676:THR:HG22	1:G:677:ALA:H	1.58	0.68
5:G:5104:117:H83	5:G:5105:117:C93	2.23	0.68
5:A:5104:117:H83	5:A:5105:117:C93	2.23	0.68
1:M:2875:MET:HE1	1:M:2938:VAL:HG12	1.75	0.68
1:A:676:THR:HG22	1:A:677:ALA:H	1.58	0.68
1:A:972:LEU:CD1	1:A:1045:THR:HA	2.24	0.68
1:G:2875:MET:HE1	1:G:2938:VAL:HG12	1.75	0.68
1:A:977:LEU:HD23	1:A:1047:LEU:HD12	1.76	0.68
1:G:977:LEU:HD23	1:G:1047:LEU:HD12	1.76	0.68
1:M:2625:ARG:HD3	1:M:2911:THR:HB	1.77	0.68
1:S:404:ILE:HG21	1:S:481:GLU:HG2	1.76	0.68
1:A:977:LEU:CD2	1:A:1043:VAL:HG12	2.21	0.67
1:S:972:LEU:CD1	1:S:1045:THR:HA	2.24	0.67
1:S:977:LEU:CD2	1:S:1043:VAL:HG12	2.21	0.67
5:S:5104:117:H83	5:S:5105:117:C93	2.23	0.67
1:A:2875:MET:HE1	1:A:2938:VAL:HG12	1.75	0.67
1:G:2625:ARG:HD3	1:G:2911:THR:HB	1.77	0.67
1:M:404:ILE:HG21	1:M:481:GLU:HG2	1.76	0.67
1:G:972:LEU:CD1	1:G:1045:THR:HA	2.24	0.67
1:M:977:LEU:HD23	1:M:1047:LEU:HD12	1.76	0.67
1:M:3267:MET:O	1:M:3267:MET:HG3	1.95	0.67
1:S:2625:ARG:HD3	1:S:2911:THR:HB	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:5103:117:H85	5:M:5104:117:H17	1.77	0.67
1:S:977:LEU:HD23	1:S:1047:LEU:HD12	1.76	0.67
1:A:2625:ARG:CD	1:A:2911:THR:HB	2.25	0.67
1:G:2022:CYS:SG	1:G:2029:ARG:NH2	2.68	0.67
1:A:2022:CYS:SG	1:A:2029:ARG:NH2	2.68	0.67
2:T:5:ILE:HG12	2:T:75:LEU:CD2	2.25	0.67
5:G:5103:117:H85	5:G:5104:117:H17	1.77	0.66
1:M:972:LEU:CD1	1:M:1045:THR:HA	2.24	0.66
1:A:2625:ARG:HD3	1:A:2911:THR:HB	1.77	0.66
1:G:404:ILE:HG21	1:G:481:GLU:HG2	1.76	0.66
1:M:2022:CYS:SG	1:M:2029:ARG:NH2	2.68	0.66
1:G:2625:ARG:CD	1:G:2911:THR:HB	2.25	0.66
1:G:3267:MET:O	1:G:3267:MET:HG3	1.95	0.66
1:S:2022:CYS:SG	1:S:2029:ARG:NH2	2.68	0.66
1:A:404:ILE:HG21	1:A:481:GLU:HG2	1.76	0.66
5:A:5103:117:H85	5:A:5104:117:H17	1.77	0.66
1:S:2625:ARG:CD	1:S:2911:THR:HB	2.25	0.66
2:B:5:ILE:HG12	2:B:75:LEU:CD2	2.25	0.66
2:N:5:ILE:HG12	2:N:75:LEU:CD2	2.25	0.66
1:S:2356:ARG:HB3	1:S:2360:ARG:HH12	1.61	0.66
1:M:2625:ARG:CD	1:M:2911:THR:HB	2.25	0.66
1:A:2356:ARG:HB3	1:A:2360:ARG:HH12	1.61	0.65
1:G:2356:ARG:HB3	1:G:2360:ARG:HH12	1.61	0.65
2:H:5:ILE:HG12	2:H:75:LEU:CD2	2.25	0.65
1:M:2356:ARG:HB3	1:M:2360:ARG:HH12	1.61	0.65
5:S:5103:117:H85	5:S:5104:117:H17	1.77	0.65
1:A:3267:MET:O	1:A:3267:MET:HG3	1.95	0.65
1:S:3267:MET:O	1:S:3267:MET:HG3	1.95	0.65
1:A:990:GLU:HG3	1:A:1024:TYR:HB3	1.79	0.65
1:A:2755:PHE:CZ	1:A:2931:LEU:HD23	2.32	0.65
1:M:2755:PHE:CZ	1:M:2931:LEU:HD23	2.32	0.64
1:A:4147:GLU:OE2	1:A:4175:ARG:NH2	2.31	0.64
1:G:990:GLU:HG3	1:G:1024:TYR:HB3	1.79	0.64
1:S:990:GLU:HG3	1:S:1024:TYR:HB3	1.79	0.64
1:M:990:GLU:HG3	1:M:1024:TYR:HB3	1.79	0.64
1:S:1243:PRO:HA	1:S:1601:MET:O	1.98	0.64
1:S:4147:GLU:OE2	1:S:4175:ARG:NH2	2.31	0.64
1:M:1243:PRO:HA	1:M:1601:MET:O	1.98	0.64
1:A:938:HIS:O	1:A:1053:ILE:HA	1.98	0.64
1:A:4656:ILE:HD12	1:A:4794:MET:HE2	1.80	0.63
1:G:4147:GLU:OE2	1:G:4175:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4656:ILE:HD12	1:G:4794:MET:HE2	1.80	0.63
1:M:938:HIS:O	1:M:1053:ILE:HA	1.98	0.63
1:A:1243:PRO:HA	1:A:1601:MET:O	1.98	0.63
1:S:938:HIS:O	1:S:1053:ILE:HA	1.98	0.63
1:S:939:VAL:HG22	1:S:1053:ILE:HG22	1.80	0.63
1:S:3676:ALA:HB2	1:S:3692:ASP:HB3	1.80	0.63
1:S:4656:ILE:HD12	1:S:4794:MET:HE2	1.80	0.63
1:G:939:VAL:HG22	1:G:1053:ILE:HG22	1.80	0.63
1:G:1243:PRO:HA	1:G:1601:MET:O	1.98	0.63
1:G:730:VAL:O	1:G:735:GLN:NE2	2.32	0.63
1:G:2755:PHE:CZ	1:G:2931:LEU:HD23	2.32	0.62
1:G:3676:ALA:HB2	1:G:3692:ASP:HB3	1.80	0.62
1:A:1561:VAL:HG22	1:A:1562:ILE:HG23	1.80	0.62
1:S:977:LEU:HD23	1:S:1047:LEU:CD1	2.29	0.62
1:M:4656:ILE:HD12	1:M:4794:MET:HE2	1.80	0.62
1:M:977:LEU:HD23	1:M:1047:LEU:CD1	2.29	0.62
1:A:977:LEU:HD23	1:A:1047:LEU:CD1	2.29	0.62
1:G:977:LEU:HD23	1:G:1047:LEU:CD1	2.29	0.62
1:M:2284:ASN:HB3	1:M:2287:LEU:HB2	1.82	0.62
1:M:730:VAL:O	1:M:735:GLN:NE2	2.32	0.62
1:A:730:VAL:O	1:A:735:GLN:NE2	2.32	0.62
1:A:939:VAL:HG22	1:A:1053:ILE:HG22	1.80	0.62
1:G:938:HIS:O	1:G:1053:ILE:HA	1.98	0.62
1:G:2284:ASN:HB3	1:G:2287:LEU:HB2	1.82	0.62
1:S:2755:PHE:CZ	1:S:2931:LEU:HD23	2.32	0.62
1:G:176:SER:OG	1:G:178:ARG:NH1	2.33	0.62
1:M:176:SER:OG	1:M:178:ARG:NH1	2.33	0.62
1:S:176:SER:OG	1:S:178:ARG:NH1	2.33	0.62
1:S:1561:VAL:HG22	1:S:1562:ILE:HG23	1.80	0.62
1:S:2284:ASN:HB3	1:S:2287:LEU:HB2	1.82	0.62
1:A:176:SER:OG	1:A:178:ARG:NH1	2.33	0.62
1:M:1561:VAL:HG22	1:M:1562:ILE:HG23	1.80	0.62
1:G:660:SER:HA	1:G:750:LEU:HD12	1.82	0.61
1:S:730:VAL:O	1:S:735:GLN:NE2	2.32	0.61
1:A:3595:VAL:O	1:A:3599:LEU:HD12	2.00	0.61
1:G:1561:VAL:HG22	1:G:1562:ILE:HG23	1.80	0.61
1:G:3595:VAL:O	1:G:3599:LEU:HD12	2.00	0.61
1:M:3676:ALA:HB2	1:M:3692:ASP:HB3	1.80	0.61
1:S:977:LEU:CD2	1:S:1043:VAL:CG1	2.79	0.61
1:A:977:LEU:CD2	1:A:1043:VAL:CG1	2.79	0.61
1:A:2755:PHE:CE1	1:A:2931:LEU:HD23	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3676:ALA:HB2	1:A:3692:ASP:HB3	1.80	0.61
1:S:2755:PHE:CE1	1:S:2931:LEU:HD23	2.36	0.61
1:M:660:SER:HA	1:M:750:LEU:HD12	1.82	0.61
1:M:863:LEU:HD11	1:M:929:LEU:HB3	1.83	0.61
1:M:939:VAL:HG22	1:M:1053:ILE:HG22	1.80	0.61
1:M:4147:GLU:OE2	1:M:4175:ARG:NH2	2.31	0.61
1:M:2755:PHE:CE1	1:M:2931:LEU:HD23	2.36	0.61
1:M:3595:VAL:O	1:M:3599:LEU:HD12	2.00	0.61
1:A:2284:ASN:HB3	1:A:2287:LEU:HB2	1.82	0.61
1:S:657:THR:HG22	1:S:1001:VAL:HG21	1.83	0.61
1:G:863:LEU:HD11	1:G:929:LEU:HB3	1.83	0.60
1:M:657:THR:HG22	1:M:1001:VAL:HG21	1.83	0.60
1:S:3595:VAL:O	1:S:3599:LEU:HD12	2.00	0.60
1:A:657:THR:HG22	1:A:1001:VAL:HG21	1.83	0.60
1:S:660:SER:HA	1:S:750:LEU:HD12	1.82	0.60
1:G:977:LEU:CD2	1:G:1043:VAL:CG1	2.79	0.60
1:A:660:SER:HA	1:A:750:LEU:HD12	1.82	0.60
1:G:2755:PHE:CE1	1:G:2931:LEU:HD23	2.36	0.60
1:M:2496:VAL:HG12	1:M:2498:ASP:H	1.67	0.60
1:G:657:THR:HG22	1:G:1001:VAL:HG21	1.83	0.60
1:G:3763:ALA:HA	1:G:3766:HIS:CD2	2.37	0.60
1:G:707:VAL:HG23	1:G:782:SER:HB3	1.84	0.59
1:M:3763:ALA:HA	1:M:3766:HIS:CD2	2.37	0.59
1:S:3763:ALA:HA	1:S:3766:HIS:CD2	2.37	0.59
1:M:707:VAL:HG23	1:M:782:SER:HB3	1.84	0.59
1:M:977:LEU:CD2	1:M:1043:VAL:CG1	2.79	0.59
5:M:5103:117:C85	5:M:5104:117:H17	2.32	0.59
1:A:3024:LYS:HE2	1:A:3024:LYS:HA	1.84	0.59
1:S:2176:GLU:HA	1:S:2229:MET:HE1	1.85	0.59
1:G:2496:VAL:HG12	1:G:2498:ASP:H	1.67	0.59
5:G:5103:117:C85	5:G:5104:117:H17	2.32	0.59
1:S:2496:VAL:HG12	1:S:2498:ASP:H	1.67	0.59
1:G:3644:ARG:O	1:G:3648:MET:HE3	2.03	0.59
1:A:707:VAL:HG23	1:A:782:SER:HB3	1.84	0.59
1:S:3024:LYS:HA	1:S:3024:LYS:HE2	1.84	0.59
1:A:3763:ALA:HA	1:A:3766:HIS:CD2	2.37	0.59
5:A:5103:117:C85	5:A:5104:117:H17	2.32	0.59
1:M:1040:CYS:O	1:M:1044:ARG:HG3	2.03	0.59
1:S:707:VAL:HG23	1:S:782:SER:HB3	1.84	0.59
1:A:2176:GLU:HA	1:A:2229:MET:HE1	1.85	0.59
1:G:4117:MET:HA	1:G:4117:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:ILE:HD11	2:H:63:GLY:HA2	1.85	0.59
1:S:863:LEU:HD11	1:S:929:LEU:HB3	1.83	0.59
1:S:3644:ARG:O	1:S:3648:MET:HE3	2.03	0.59
5:S:5103:117:C85	5:S:5104:117:H17	2.32	0.59
1:A:863:LEU:HD11	1:A:929:LEU:HB3	1.83	0.58
1:M:3024:LYS:HE2	1:M:3024:LYS:HA	1.84	0.58
1:A:3644:ARG:O	1:A:3648:MET:HE3	2.03	0.58
1:A:4117:MET:HE2	1:A:4117:MET:HA	1.85	0.58
1:A:2496:VAL:HG12	1:A:2498:ASP:H	1.67	0.58
1:G:3024:LYS:HA	1:G:3024:LYS:HE2	1.84	0.58
1:S:513:GLU:OE2	1:S:513:GLU:N	2.35	0.58
1:S:1040:CYS:O	1:S:1044:ARG:HG3	2.03	0.58
2:B:5:ILE:HD11	2:B:63:GLY:HA2	1.85	0.58
1:M:2225:ARG:HD2	1:M:2225:ARG:N	2.19	0.58
1:G:2176:GLU:HA	1:G:2229:MET:HE1	1.85	0.58
1:M:2176:GLU:HA	1:M:2229:MET:HE1	1.85	0.57
1:G:2225:ARG:HD2	1:G:2225:ARG:N	2.19	0.57
1:M:3644:ARG:O	1:M:3648:MET:HE3	2.03	0.57
1:S:2225:ARG:HD2	1:S:2225:ARG:N	2.19	0.57
2:T:5:ILE:HD11	2:T:63:GLY:HA2	1.85	0.57
1:A:1040:CYS:O	1:A:1044:ARG:HG3	2.03	0.57
1:A:2225:ARG:N	1:A:2225:ARG:HD2	2.19	0.57
1:M:4117:MET:HE2	1:M:4117:MET:HA	1.85	0.57
2:N:5:ILE:HD11	2:N:63:GLY:HA2	1.85	0.57
1:G:1040:CYS:O	1:G:1044:ARG:HG3	2.03	0.57
1:M:981:GLN:HG2	1:M:1053:ILE:HG13	1.86	0.57
1:S:4117:MET:HA	1:S:4117:MET:HE2	1.85	0.57
1:S:981:GLN:HG2	1:S:1053:ILE:HG13	1.86	0.57
1:M:2755:PHE:CZ	1:M:2931:LEU:CG	2.88	0.57
1:M:2334:ASP:OD1	1:M:2335:PHE:N	2.39	0.56
1:G:2755:PHE:CZ	1:G:2931:LEU:CG	2.88	0.56
1:A:513:GLU:OE2	1:A:513:GLU:N	2.35	0.56
1:G:2334:ASP:OD1	1:G:2335:PHE:N	2.39	0.56
1:S:2755:PHE:CZ	1:S:2931:LEU:CG	2.88	0.56
1:A:2755:PHE:CZ	1:A:2931:LEU:CG	2.88	0.56
1:A:4954:THR:HG23	1:A:4955:LYS:HG3	1.88	0.56
1:A:981:GLN:HG2	1:A:1053:ILE:HG13	1.86	0.55
1:M:4954:THR:HG23	1:M:4955:LYS:HG3	1.88	0.55
1:S:2334:ASP:OD1	1:S:2335:PHE:N	2.39	0.55
1:A:2334:ASP:OD1	1:A:2335:PHE:N	2.39	0.55
1:A:3258:ALA:HA	1:A:3323:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:106:ASN:OD1	2:T:107:LEU:N	2.39	0.55
1:G:3258:ALA:HA	1:G:3323:ILE:HD11	1.89	0.55
2:H:106:ASN:OD1	2:H:107:LEU:N	2.39	0.55
1:M:3258:ALA:HA	1:M:3323:ILE:HD11	1.89	0.55
1:S:4954:THR:HG23	1:S:4955:LYS:HG3	1.88	0.55
1:G:4954:THR:HG23	1:G:4955:LYS:HG3	1.88	0.55
1:M:513:GLU:N	1:M:513:GLU:OE2	2.35	0.55
1:S:3258:ALA:HA	1:S:3323:ILE:HD11	1.89	0.55
2:B:106:ASN:OD1	2:B:107:LEU:N	2.39	0.54
1:G:513:GLU:OE2	1:G:513:GLU:N	2.35	0.54
1:M:4987:MET:HE3	1:M:4991:MET:SD	2.48	0.54
1:A:35:LEU:HD12	1:A:49:LEU:HD13	1.90	0.54
1:A:805:PRO:HB2	1:A:808:TYR:CD1	2.42	0.54
1:A:4140:VAL:HG22	1:A:4173:LEU:HD21	1.89	0.54
1:M:35:LEU:HD12	1:M:49:LEU:HD13	1.90	0.54
1:M:4140:VAL:HG22	1:M:4173:LEU:HD21	1.89	0.54
1:S:805:PRO:HB2	1:S:808:TYR:CD1	2.42	0.54
1:G:4140:VAL:HG22	1:G:4173:LEU:HD21	1.89	0.54
1:G:4987:MET:HE3	1:G:4991:MET:SD	2.48	0.54
1:S:2197:ASN:OD1	1:S:2200:ARG:NH2	2.41	0.54
1:G:35:LEU:HD12	1:G:49:LEU:HD13	1.90	0.54
1:S:1256:GLU:HB3	1:S:1273:THR:HG23	1.89	0.54
1:A:4987:MET:HE3	1:A:4991:MET:SD	2.48	0.54
1:G:805:PRO:HB2	1:G:808:TYR:CD1	2.42	0.54
1:S:4987:MET:HE3	1:S:4991:MET:SD	2.48	0.54
2:N:22:THR:O	2:N:108:GLU:N	2.34	0.54
2:B:4:GLU:OE1	2:B:4:GLU:N	2.41	0.54
1:G:2197:ASN:OD1	1:G:2200:ARG:NH2	2.41	0.54
1:M:2197:ASN:OD1	1:M:2200:ARG:NH2	2.41	0.54
1:A:1256:GLU:HB3	1:A:1273:THR:HG23	1.89	0.53
1:G:981:GLN:HG2	1:G:1053:ILE:HG13	1.86	0.53
2:H:22:THR:O	2:H:108:GLU:N	2.34	0.53
2:N:106:ASN:OD1	2:N:107:LEU:N	2.39	0.53
1:S:35:LEU:HD12	1:S:49:LEU:HD13	1.90	0.53
1:S:4140:VAL:HG22	1:S:4173:LEU:HD21	1.90	0.53
1:G:1256:GLU:HB3	1:G:1273:THR:HG23	1.89	0.53
2:T:4:GLU:N	2:T:4:GLU:OE1	2.41	0.53
1:M:805:PRO:HB2	1:M:808:TYR:CD1	2.42	0.53
1:A:2197:ASN:OD1	1:A:2200:ARG:NH2	2.41	0.53
2:H:4:GLU:N	2:H:4:GLU:OE1	2.41	0.53
1:M:176:SER:O	1:M:178:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2171:MET:HE3	1:A:2229:MET:HE3	1.91	0.53
2:N:4:GLU:OE1	2:N:4:GLU:N	2.41	0.53
1:G:176:SER:O	1:G:178:ARG:NH1	2.42	0.53
1:M:1256:GLU:HB3	1:M:1273:THR:HG23	1.89	0.53
1:S:176:SER:O	1:S:178:ARG:NH1	2.42	0.53
1:G:2171:MET:HE3	1:G:2229:MET:HE3	1.91	0.53
1:M:2822:TRP:CE3	1:M:2875:MET:CE	2.92	0.53
1:S:2171:MET:HE3	1:S:2229:MET:HE3	1.91	0.53
1:M:2171:MET:HE3	1:M:2229:MET:HE3	1.91	0.52
1:M:2480:LEU:HG	1:M:2482:LYS:H	1.74	0.52
1:A:2480:LEU:HG	1:A:2482:LYS:H	1.74	0.52
1:A:4730:TYR:HB3	1:A:4734:ARG:NH2	2.25	0.52
1:G:4730:TYR:HB3	1:G:4734:ARG:NH2	2.25	0.52
1:M:4730:TYR:HB3	1:M:4734:ARG:NH2	2.25	0.52
1:G:2822:TRP:CE3	1:G:2875:MET:CE	2.92	0.52
1:A:1252:HIS:O	1:A:1275:ARG:NH1	2.43	0.52
1:A:1101:ARG:NH1	1:A:1115:LEU:O	2.43	0.52
1:A:2822:TRP:CE3	1:A:2875:MET:CE	2.92	0.52
1:M:1101:ARG:NH1	1:M:1115:LEU:O	2.43	0.52
1:S:2822:TRP:CE3	1:S:2875:MET:CE	2.92	0.52
1:S:4562:PHE:CD2	5:S:5104:117:H13	2.45	0.52
1:A:176:SER:O	1:A:178:ARG:NH1	2.42	0.52
1:G:2480:LEU:HG	1:G:2482:LYS:H	1.74	0.52
1:A:2167:LEU:HD21	1:A:2211:VAL:HG22	1.92	0.52
1:G:676:THR:HG22	1:G:677:ALA:N	2.25	0.52
1:S:1252:HIS:O	1:S:1275:ARG:NH1	2.43	0.52
1:A:2152:ASP:OD2	1:A:2190:LYS:NZ	2.31	0.52
1:S:4730:TYR:HB3	1:S:4734:ARG:NH2	2.25	0.52
1:G:4562:PHE:CD2	5:G:5104:117:H13	2.45	0.51
1:M:676:THR:HG22	1:M:677:ALA:N	2.25	0.51
1:M:4562:PHE:CD2	5:M:5104:117:H13	2.45	0.51
1:S:2480:LEU:HG	1:S:2482:LYS:H	1.74	0.51
1:M:2167:LEU:HD21	1:M:2211:VAL:HG22	1.92	0.51
5:S:5103:117:H85	5:S:5104:117:C17	2.40	0.51
5:M:5103:117:H85	5:M:5104:117:C17	2.40	0.51
5:A:5103:117:H85	5:A:5104:117:C17	2.40	0.51
1:G:1252:HIS:O	1:G:1275:ARG:NH1	2.43	0.51
1:G:2167:LEU:HD21	1:G:2211:VAL:HG22	1.92	0.51
1:M:3698:VAL:HG13	1:M:3773:MET:HE3	1.93	0.51
1:A:4653:PHE:HD1	1:A:4794:MET:HE1	1.76	0.51
1:M:1252:HIS:O	1:M:1275:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:615:CYS:O	1:M:616:SER:C	2.54	0.51
1:A:4562:PHE:CD2	5:A:5104:117:H13	2.45	0.51
1:S:3698:VAL:HG13	1:S:3773:MET:HE3	1.93	0.51
1:A:676:THR:HG22	1:A:677:ALA:N	2.25	0.51
1:S:3691:PRO:HB2	1:S:3695:HIS:HB3	1.93	0.51
1:G:3691:PRO:HB2	1:G:3695:HIS:HB3	1.93	0.51
1:A:3691:PRO:HB2	1:A:3695:HIS:HB3	1.93	0.50
1:G:615:CYS:O	1:G:616:SER:C	2.54	0.50
1:G:1101:ARG:NH1	1:G:1115:LEU:O	2.43	0.50
1:M:3691:PRO:HB2	1:M:3695:HIS:HB3	1.93	0.50
1:S:1101:ARG:NH1	1:S:1115:LEU:O	2.43	0.50
1:M:4653:PHE:HD1	1:M:4794:MET:HE1	1.76	0.50
1:S:615:CYS:O	1:S:616:SER:C	2.54	0.50
1:S:2167:LEU:HD21	1:S:2211:VAL:HG22	1.92	0.50
1:S:4653:PHE:HD1	1:S:4794:MET:HE1	1.76	0.50
1:A:3698:VAL:HG13	1:A:3773:MET:HE3	1.93	0.50
1:A:615:CYS:O	1:A:616:SER:C	2.54	0.50
1:A:2625:ARG:HD2	1:A:2911:THR:HB	1.94	0.50
1:G:3698:VAL:HG13	1:G:3773:MET:HE3	1.93	0.50
1:A:1098:GLY:O	1:A:1127:HIS:HB2	2.12	0.50
5:G:5103:117:H85	5:G:5104:117:C17	2.40	0.49
1:A:3414:ILE:HD12	1:A:3510:LEU:HD23	1.95	0.49
1:G:3414:ILE:HD12	1:G:3510:LEU:HD23	1.95	0.49
1:G:4653:PHE:HD1	1:G:4794:MET:HE1	1.76	0.49
1:G:2625:ARG:HD2	1:G:2911:THR:HB	1.94	0.49
1:S:4130:PRO:O	1:S:4134:ILE:HG22	2.12	0.49
1:A:858:THR:O	1:A:861:ILE:CG2	2.59	0.49
1:A:4130:PRO:O	1:A:4134:ILE:HG22	2.12	0.49
1:G:3901:GLN:H	1:G:3907:THR:HG23	1.78	0.49
1:G:4130:PRO:O	1:G:4134:ILE:HG22	2.12	0.49
1:M:3901:GLN:H	1:M:3907:THR:HG23	1.78	0.49
1:S:752:VAL:O	1:S:753:PRO:C	2.55	0.49
1:S:1098:GLY:O	1:S:1127:HIS:HB2	2.12	0.49
1:S:3901:GLN:H	1:S:3907:THR:HG23	1.78	0.49
1:G:1098:GLY:O	1:G:1127:HIS:HB2	2.12	0.49
1:G:1970:LEU:HD21	1:G:2010:LEU:HD13	1.95	0.49
1:S:3414:ILE:HD12	1:S:3510:LEU:HD23	1.95	0.49
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	1.95	0.49
2:B:22:THR:O	2:B:108:GLU:N	2.34	0.49
1:G:4811:LEU:O	1:G:4814:ILE:HG22	2.13	0.49
1:M:3414:ILE:HD12	1:M:3510:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4811:LEU:O	1:A:4814:ILE:HG22	2.13	0.49
1:M:1098:GLY:O	1:M:1127:HIS:HB2	2.12	0.49
1:M:4585:PRO:CD	1:M:4626:VAL:HG11	2.42	0.49
1:S:3753:MET:HE2	1:S:3753:MET:HA	1.95	0.49
1:M:274:LEU:HD12	1:M:274:LEU:H	1.78	0.49
5:M:5105:117:N2	5:M:5105:117:H922	2.28	0.49
5:S:5105:117:N2	5:S:5105:117:H922	2.28	0.49
1:G:752:VAL:O	1:G:753:PRO:C	2.55	0.48
5:G:5105:117:N2	5:G:5105:117:H922	2.28	0.48
1:M:3753:MET:HA	1:M:3753:MET:HE2	1.95	0.48
1:S:274:LEU:H	1:S:274:LEU:HD12	1.78	0.48
1:G:3753:MET:HE2	1:G:3753:MET:HA	1.95	0.48
1:A:752:VAL:O	1:A:753:PRO:C	2.55	0.48
1:G:4833:LYS:HG2	1:G:4837:MET:HE2	1.96	0.48
1:M:937:CYS:HG	1:M:1053:ILE:HB	1.77	0.48
1:M:1970:LEU:HD21	1:M:2010:LEU:HD13	1.95	0.48
1:M:2625:ARG:HD2	1:M:2911:THR:HB	1.94	0.48
1:G:219:VAL:HG21	1:G:398:SER:HB3	1.95	0.48
1:M:3391:GLY:O	1:M:3394:LEU:HB3	2.14	0.48
1:M:4130:PRO:O	1:M:4134:ILE:HG22	2.12	0.48
1:S:56:GLN:O	1:S:309:THR:OG1	2.27	0.48
2:T:22:THR:O	2:T:108:GLU:N	2.34	0.48
1:A:213:TYR:CD2	1:A:337:PRO:HB2	2.49	0.48
1:A:1970:LEU:HD21	1:A:2010:LEU:HD13	1.95	0.48
1:G:213:TYR:CD2	1:G:337:PRO:HB2	2.49	0.48
1:G:3035:LYS:HG3	1:G:3039:MET:HE2	1.96	0.48
1:M:4811:LEU:O	1:M:4814:ILE:HG22	2.13	0.48
1:S:4585:PRO:CD	1:S:4626:VAL:HG11	2.42	0.48
1:S:4811:LEU:O	1:S:4814:ILE:HG22	2.13	0.48
1:S:4833:LYS:HG2	1:S:4837:MET:HE2	1.96	0.48
1:G:858:THR:O	1:G:861:ILE:CG2	2.59	0.48
1:M:752:VAL:O	1:M:753:PRO:C	2.55	0.48
1:S:213:TYR:CD2	1:S:337:PRO:HB2	2.49	0.48
1:S:1970:LEU:HD21	1:S:2010:LEU:HD13	1.95	0.48
1:A:3035:LYS:HG3	1:A:3039:MET:HE2	1.96	0.48
1:M:4833:LYS:HG2	1:M:4837:MET:HE2	1.96	0.48
1:A:4833:LYS:HG2	1:A:4837:MET:HE2	1.96	0.48
5:A:5105:117:N2	5:A:5105:117:H922	2.28	0.48
1:G:274:LEU:H	1:G:274:LEU:HD12	1.78	0.48
1:G:3391:GLY:O	1:G:3394:LEU:HB3	2.14	0.48
1:S:3004:LEU:HB2	1:S:3005:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:HD23	1:A:357:LEU:H	1.79	0.48
1:M:213:TYR:CD2	1:M:337:PRO:HB2	2.49	0.48
1:M:219:VAL:HG21	1:M:398:SER:HB3	1.95	0.48
1:A:274:LEU:HD12	1:A:274:LEU:H	1.78	0.48
1:A:282:ILE:HB	1:A:291:LEU:HD22	1.96	0.48
1:A:3134:THR:HG23	1:A:3135:VAL:HG23	1.96	0.48
1:A:3391:GLY:O	1:A:3394:LEU:HB3	2.14	0.48
1:A:3901:GLN:H	1:A:3907:THR:HG23	1.78	0.48
1:G:282:ILE:HB	1:G:291:LEU:HD22	1.96	0.47
1:G:3004:LEU:HB2	1:G:3005:PRO:HD3	1.95	0.47
1:M:3004:LEU:HB2	1:M:3005:PRO:HD3	1.95	0.47
1:S:676:THR:HG22	1:S:677:ALA:N	2.25	0.47
1:S:3391:GLY:O	1:S:3394:LEU:HB3	2.14	0.47
1:A:4585:PRO:CD	1:A:4626:VAL:HG11	2.42	0.47
1:G:357:LEU:HD23	1:G:357:LEU:H	1.79	0.47
1:G:4822:ARG:NH1	5:G:5105:117:O1A	2.48	0.47
1:S:4822:ARG:NH1	5:S:5105:117:O1A	2.48	0.47
1:S:618:GLN:OE1	1:S:1678:ASN:ND2	2.47	0.47
1:S:3134:THR:HG23	1:S:3135:VAL:HG23	1.96	0.47
1:A:4822:ARG:NH1	5:A:5105:117:O1A	2.48	0.47
1:S:282:ILE:HB	1:S:291:LEU:HD22	1.96	0.47
1:S:2625:ARG:HD2	1:S:2911:THR:HB	1.94	0.47
1:A:3753:MET:HA	1:A:3753:MET:HE2	1.95	0.47
2:B:50:ARG:NH1	2:B:53:LYS:HG3	2.30	0.47
1:S:219:VAL:HG21	1:S:398:SER:HB3	1.95	0.47
1:A:618:GLN:OE1	1:A:1678:ASN:ND2	2.47	0.47
1:G:1248:VAL:HG22	1:G:1599:MET:HG2	1.96	0.47
1:M:56:GLN:O	1:M:309:THR:OG1	2.27	0.47
1:M:282:ILE:HB	1:M:291:LEU:HD22	1.96	0.47
1:M:1248:VAL:HG22	1:M:1599:MET:HG2	1.96	0.47
1:M:4822:ARG:NH1	5:M:5105:117:O1A	2.48	0.47
2:N:58:LYS:O	2:N:62:GLU:HG2	2.14	0.47
1:A:219:VAL:HG21	1:A:398:SER:HB3	1.95	0.47
1:A:4085:LYS:HG2	1:A:4118:ILE:HD11	1.97	0.47
2:B:58:LYS:O	2:B:62:GLU:HG2	2.14	0.47
2:H:50:ARG:NH1	2:H:53:LYS:HG3	2.30	0.47
2:H:58:LYS:O	2:H:62:GLU:HG2	2.14	0.47
1:M:357:LEU:HD23	1:M:357:LEU:H	1.79	0.47
1:M:3035:LYS:HG3	1:M:3039:MET:HE2	1.96	0.47
2:T:58:LYS:O	2:T:62:GLU:HG2	2.14	0.47
1:G:3134:THR:HG23	1:G:3135:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4202:MET:O	1:S:4205:VAL:HG22	2.15	0.47
2:T:50:ARG:NH1	2:T:53:LYS:HG3	2.30	0.47
1:G:4085:LYS:HG2	1:G:4118:ILE:HD11	1.97	0.47
1:G:4202:MET:O	1:G:4205:VAL:HG22	2.15	0.47
1:A:2491:MET:HE2	1:A:2491:MET:HA	1.96	0.47
1:M:618:GLN:OE1	1:M:1678:ASN:ND2	2.47	0.47
1:M:3134:THR:HG23	1:M:3135:VAL:HG23	1.96	0.47
1:S:357:LEU:H	1:S:357:LEU:HD23	1.79	0.47
1:S:4835:LEU:O	1:S:4839:VAL:HG13	2.15	0.47
1:A:4835:LEU:O	1:A:4839:VAL:HG13	2.15	0.46
1:G:2491:MET:HE2	1:G:2491:MET:HA	1.96	0.46
1:S:3035:LYS:HG3	1:S:3039:MET:HE2	1.96	0.46
1:G:4585:PRO:CD	1:G:4626:VAL:HG11	2.42	0.46
1:M:2491:MET:HE2	1:M:2491:MET:HA	1.96	0.46
1:M:4095:GLN:OE1	1:M:4097:GLN:HB2	2.16	0.46
1:A:1248:VAL:HG22	1:A:1599:MET:HG2	1.96	0.46
1:A:4095:GLN:OE1	1:A:4097:GLN:HB2	2.16	0.46
1:A:4796:MET:HA	1:A:4796:MET:HE2	1.98	0.46
1:G:618:GLN:OE1	1:G:1678:ASN:ND2	2.47	0.46
1:S:275:ARG:HH21	1:S:338:GLU:HG3	1.81	0.46
1:S:858:THR:O	1:S:861:ILE:CG2	2.59	0.46
1:G:637:LEU:HD13	1:G:1693:GLN:HG2	1.98	0.46
1:G:2356:ARG:O	1:G:2360:ARG:NH1	2.48	0.46
1:G:4095:GLN:OE1	1:G:4097:GLN:HB2	2.16	0.46
2:N:50:ARG:NH1	2:N:53:LYS:HG3	2.30	0.46
1:S:2999:PHE:CD1	1:S:3003:LEU:HD12	2.51	0.46
1:S:4095:GLN:OE1	1:S:4097:GLN:HB2	2.16	0.46
1:A:4706:THR:HG21	1:A:4773:TYR:HB2	1.98	0.46
5:A:5103:117:H41	1:S:4833:LYS:NZ	2.31	0.46
1:G:4796:MET:HE2	1:G:4796:MET:HA	1.98	0.46
1:M:4835:LEU:O	1:M:4839:VAL:HG13	2.15	0.46
1:S:981:GLN:O	1:S:985:VAL:HG23	2.16	0.46
1:A:632:LEU:O	1:A:634:GLN:NE2	2.48	0.46
1:A:637:LEU:HD13	1:A:1693:GLN:HG2	1.98	0.46
1:A:2999:PHE:CD1	1:A:3003:LEU:HD12	2.51	0.46
1:G:4211:GLN:NE2	1:G:4215:ASP:OD2	2.49	0.46
1:G:4835:LEU:O	1:G:4839:VAL:HG13	2.15	0.46
1:M:637:LEU:HD13	1:M:1693:GLN:HG2	1.98	0.46
1:G:4833:LYS:NZ	5:M:5103:117:H41	2.31	0.46
1:M:1561:VAL:HG13	1:M:1562:ILE:H	1.81	0.46
1:S:1248:VAL:HG22	1:S:1599:MET:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2491:MET:HE2	1:S:2491:MET:HA	1.96	0.46
1:S:4085:LYS:HG2	1:S:4118:ILE:HD11	1.97	0.46
1:A:981:GLN:O	1:A:985:VAL:HG23	2.16	0.46
1:A:4833:LYS:NZ	5:G:5103:117:H41	2.31	0.46
1:G:275:ARG:HH21	1:G:338:GLU:HG3	1.81	0.46
1:G:4706:THR:HG21	1:G:4773:TYR:HB2	1.98	0.46
1:M:1041:GLN:OE1	1:M:1041:GLN:HA	2.16	0.46
1:M:2999:PHE:CD1	1:M:3003:LEU:HD12	2.51	0.46
1:M:3007:ILE:HG23	1:M:3011:PHE:CD2	2.51	0.46
1:M:4202:MET:O	1:M:4205:VAL:HG22	2.15	0.46
1:S:2356:ARG:O	1:S:2360:ARG:NH1	2.48	0.46
1:A:1799:LEU:HD23	1:A:1799:LEU:HA	1.72	0.46
1:A:4202:MET:O	1:A:4205:VAL:HG22	2.15	0.46
1:G:3007:ILE:HG23	1:G:3011:PHE:CD2	2.51	0.46
1:M:275:ARG:HH21	1:M:338:GLU:HG3	1.81	0.46
1:S:1811:LYS:O	1:S:1815:MET:HG2	2.16	0.46
1:A:2356:ARG:O	1:A:2360:ARG:NH1	2.48	0.46
1:A:2514:GLU:N	1:A:2514:GLU:OE1	2.49	0.46
1:M:4085:LYS:HG2	1:M:4118:ILE:HD11	1.97	0.46
1:S:554:LEU:HD23	1:S:554:LEU:H	1.81	0.46
1:S:3007:ILE:HG23	1:S:3011:PHE:CD2	2.51	0.46
1:A:554:LEU:H	1:A:554:LEU:HD23	1.81	0.45
1:A:3007:ILE:HG23	1:A:3011:PHE:CD2	2.51	0.45
2:B:52:GLY:N	2:B:61:GLU:OE2	2.42	0.45
1:G:1561:VAL:HG13	1:G:1562:ILE:H	1.81	0.45
1:S:1561:VAL:HG13	1:S:1562:ILE:H	1.81	0.45
1:A:275:ARG:HH21	1:A:338:GLU:HG3	1.81	0.45
1:G:554:LEU:HD23	1:G:554:LEU:H	1.81	0.45
1:G:2514:GLU:OE1	1:G:2514:GLU:N	2.49	0.45
1:S:3262:ALA:HA	1:S:3326:ASN:HB3	1.98	0.45
1:S:4706:THR:HG21	1:S:4773:TYR:HB2	1.98	0.45
1:A:1128:ARG:O	1:A:1129:GLY:C	2.60	0.45
1:A:1811:LYS:O	1:A:1815:MET:HG2	2.16	0.45
1:A:3262:ALA:HA	1:A:3326:ASN:HB3	1.99	0.45
1:G:632:LEU:O	1:G:634:GLN:NE2	2.48	0.45
1:G:981:GLN:O	1:G:985:VAL:HG23	2.16	0.45
1:G:3964:ILE:HG21	1:G:3975:LEU:HD12	1.98	0.45
1:M:858:THR:O	1:M:861:ILE:CG2	2.59	0.45
1:M:2027:GLU:HG2	1:M:2028:ILE:HD13	1.99	0.45
1:S:399:GLN:O	1:S:403:MET:HG3	2.17	0.45
1:S:874:LEU:HD22	1:S:1046:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1128:ARG:O	1:S:1129:GLY:C	2.60	0.45
1:S:2755:PHE:CE1	1:S:2931:LEU:HA	2.52	0.45
1:S:4796:MET:HE2	1:S:4796:MET:HA	1.98	0.45
1:A:615:CYS:O	1:A:618:GLN:N	2.50	0.45
1:A:1041:GLN:OE1	1:A:1041:GLN:HA	2.16	0.45
1:A:1561:VAL:HG13	1:A:1562:ILE:H	1.81	0.45
1:A:3964:ILE:HG21	1:A:3975:LEU:HD12	1.98	0.45
1:M:3964:ILE:HG21	1:M:3975:LEU:HD12	1.98	0.45
1:M:4833:LYS:NZ	5:S:5103:117:H41	2.31	0.45
1:A:56:GLN:O	1:A:309:THR:OG1	2.27	0.45
1:A:489:ASN:O	1:A:493:ARG:HG2	2.17	0.45
1:A:874:LEU:HD22	1:A:1046:LEU:HD21	1.98	0.45
1:A:993:HIS:NE2	1:A:1027:LEU:HD11	2.32	0.45
1:A:4653:PHE:CD1	1:A:4794:MET:HE1	2.51	0.45
1:G:615:CYS:O	1:G:618:GLN:N	2.50	0.45
1:G:1811:LYS:O	1:G:1815:MET:HG2	2.16	0.45
1:M:399:GLN:O	1:M:403:MET:HG3	2.17	0.45
1:M:489:ASN:O	1:M:493:ARG:HG2	2.17	0.45
1:A:1299:GLN:NE2	1:A:1545:ASN:OD1	2.50	0.45
1:G:2999:PHE:CD1	1:G:3003:LEU:HD12	2.51	0.45
1:M:2356:ARG:O	1:M:2360:ARG:NH1	2.48	0.45
1:M:2755:PHE:CE1	1:M:2931:LEU:HA	2.52	0.45
1:S:489:ASN:O	1:S:493:ARG:HG2	2.17	0.45
1:S:637:LEU:HD13	1:S:1693:GLN:HG2	1.98	0.45
1:S:1041:GLN:HA	1:S:1041:GLN:OE1	2.16	0.45
1:A:399:GLN:O	1:A:403:MET:HG3	2.17	0.45
1:A:2755:PHE:CE1	1:A:2931:LEU:HA	2.52	0.45
2:H:52:GLY:N	2:H:61:GLU:OE2	2.42	0.45
1:M:993:HIS:NE2	1:M:1027:LEU:HD11	2.32	0.45
1:M:1448:VAL:HG22	1:M:1554:VAL:HG23	1.99	0.45
1:M:2166:LEU:HB2	1:M:2179:MET:HE2	1.99	0.45
1:M:2514:GLU:N	1:M:2514:GLU:OE1	2.49	0.45
1:M:4653:PHE:CD1	1:M:4794:MET:HE1	2.51	0.45
1:G:499:THR:HG23	1:G:502:HIS:H	1.82	0.45
1:G:2166:LEU:HB2	1:G:2179:MET:HE2	1.99	0.45
1:G:4653:PHE:CD1	1:G:4794:MET:HE1	2.51	0.45
1:M:981:GLN:O	1:M:985:VAL:HG23	2.16	0.45
1:M:4706:THR:HG21	1:M:4773:TYR:HB2	1.98	0.45
1:S:632:LEU:O	1:S:634:GLN:NE2	2.48	0.45
1:A:2166:LEU:HB2	1:A:2179:MET:HE2	1.99	0.45
1:A:4211:GLN:NE2	1:A:4215:ASP:OD2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:489:ASN:O	1:G:493:ARG:HG2	2.17	0.45
1:G:1053:ILE:HG13	1:G:1053:ILE:O	2.17	0.45
1:G:2152:ASP:OD2	1:G:2190:LYS:NZ	2.31	0.45
1:M:1811:LYS:O	1:M:1815:MET:HG2	2.16	0.45
1:S:2027:GLU:HG2	1:S:2028:ILE:HD13	1.99	0.45
1:S:2514:GLU:OE1	1:S:2514:GLU:N	2.49	0.45
1:A:1152:MET:HE2	1:A:1161:ILE:HB	1.99	0.45
1:G:874:LEU:HD22	1:G:1046:LEU:HD21	1.98	0.45
1:G:993:HIS:NE2	1:G:1027:LEU:HD11	2.32	0.45
1:G:1041:GLN:HA	1:G:1041:GLN:OE1	2.16	0.45
2:H:24:VAL:HG22	2:H:48:LYS:HG3	1.99	0.45
1:M:1658:ASP:OD2	1:M:1658:ASP:N	2.50	0.45
1:M:4796:MET:HA	1:M:4796:MET:HE2	1.98	0.45
1:S:1799:LEU:HD23	1:S:1799:LEU:HA	1.72	0.45
1:G:2755:PHE:CE1	1:G:2931:LEU:HA	2.52	0.44
1:M:1128:ARG:O	1:M:1129:GLY:C	2.60	0.44
1:S:615:CYS:O	1:S:618:GLN:N	2.50	0.44
1:S:2166:LEU:HB2	1:S:2179:MET:HE2	1.99	0.44
2:B:24:VAL:HG22	2:B:48:LYS:HG3	1.99	0.44
1:G:399:GLN:O	1:G:403:MET:HG3	2.17	0.44
2:N:24:VAL:HG22	2:N:48:LYS:HG3	1.99	0.44
1:G:1448:VAL:HG22	1:G:1554:VAL:HG23	1.99	0.44
1:M:863:LEU:HD21	1:M:929:LEU:HB2	1.99	0.44
1:M:1152:MET:HE2	1:M:1161:ILE:HB	1.99	0.44
1:S:993:HIS:NE2	1:S:1027:LEU:HD11	2.32	0.44
1:S:1477:GLY:HA2	1:S:1483:ILE:HA	1.99	0.44
1:A:1265:ASP:OD1	1:A:1265:ASP:N	2.51	0.44
1:A:3105:GLU:CD	1:A:3168:ARG:HE	2.26	0.44
1:G:275:ARG:NH2	1:G:336:PRO:O	2.27	0.44
1:G:1128:ARG:O	1:G:1129:GLY:C	2.60	0.44
1:G:1299:GLN:NE2	1:G:1545:ASN:OD1	2.50	0.44
1:G:3541:THR:HG23	1:G:3544:GLU:H	1.82	0.44
1:M:874:LEU:HD22	1:M:1046:LEU:HD21	1.98	0.44
1:S:3964:ILE:HG21	1:S:3975:LEU:HD12	1.98	0.44
1:A:499:THR:HG23	1:A:502:HIS:H	1.82	0.44
1:A:1658:ASP:OD2	1:A:1658:ASP:N	2.50	0.44
1:M:1477:GLY:HA2	1:M:1483:ILE:HA	1.99	0.44
1:M:3105:GLU:CD	1:M:3168:ARG:HE	2.26	0.44
1:S:1658:ASP:OD2	1:S:1658:ASP:N	2.50	0.44
1:G:3262:ALA:HA	1:G:3326:ASN:HB3	1.99	0.44
1:S:3105:GLU:CD	1:S:3168:ARG:HE	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4870:PRO:HB2	1:S:4872:MET:HE3	2.00	0.44
1:A:1477:GLY:HA2	1:A:1483:ILE:HA	1.99	0.44
1:M:554:LEU:H	1:M:554:LEU:HD23	1.81	0.44
1:M:972:LEU:HD13	1:M:1044:ARG:C	2.43	0.44
1:M:3262:ALA:HA	1:M:3326:ASN:HB3	1.99	0.44
1:S:1299:GLN:NE2	1:S:1545:ASN:OD1	2.50	0.44
1:A:3541:THR:HG23	1:A:3544:GLU:H	1.82	0.44
1:A:3648:MET:HA	1:A:3651:GLU:HG2	2.00	0.44
1:G:2195:HIS:O	1:G:2199:MET:HG2	2.18	0.44
1:G:4870:PRO:HB2	1:G:4872:MET:HE3	2.00	0.44
1:M:499:THR:HG23	1:M:502:HIS:H	1.82	0.44
1:S:1448:VAL:HG22	1:S:1554:VAL:HG23	1.99	0.44
1:S:3202:MET:HA	1:S:3203:PRO:HD3	1.88	0.44
1:S:4653:PHE:CD1	1:S:4794:MET:HE1	2.51	0.44
1:G:972:LEU:HD13	1:G:1044:ARG:C	2.43	0.44
1:M:3541:THR:HG23	1:M:3544:GLU:H	1.82	0.44
1:S:1053:ILE:HG13	1:S:1053:ILE:O	2.17	0.44
2:T:24:VAL:HG22	2:T:48:LYS:HG3	1.99	0.44
1:A:863:LEU:HA	1:A:863:LEU:HD12	1.72	0.43
1:A:2027:GLU:HG2	1:A:2028:ILE:HD13	1.99	0.43
1:G:2334:ASP:OD1	1:G:2334:ASP:C	2.61	0.43
1:M:2195:HIS:O	1:M:2199:MET:HG2	2.18	0.43
1:S:3648:MET:HA	1:S:3651:GLU:HG2	2.00	0.43
1:A:863:LEU:HD21	1:A:929:LEU:HB2	1.99	0.43
1:A:3946:PHE:O	1:A:3950:MET:HG3	2.19	0.43
1:A:4870:PRO:HB2	1:A:4872:MET:HE3	2.00	0.43
1:G:3105:GLU:CD	1:G:3168:ARG:HE	2.26	0.43
1:S:275:ARG:NH2	1:S:336:PRO:O	2.27	0.43
1:S:499:THR:HG23	1:S:502:HIS:H	1.82	0.43
1:S:3541:THR:HG23	1:S:3544:GLU:H	1.82	0.43
1:A:1053:ILE:HG13	1:A:1053:ILE:O	2.17	0.43
1:G:663:TYR:OH	1:G:665:GLU:OE2	2.33	0.43
1:G:863:LEU:HD21	1:G:929:LEU:HB2	1.99	0.43
1:M:168:ASP:HB3	1:M:199:LEU:HD12	2.00	0.43
1:M:863:LEU:HD12	1:M:864:PRO:HD2	2.00	0.43
1:M:4870:PRO:HB2	1:M:4872:MET:HE3	2.00	0.43
1:G:56:GLN:O	1:G:309:THR:OG1	2.27	0.43
1:G:2966:ARG:O	1:G:2970:ILE:HG12	2.19	0.43
1:M:1053:ILE:HG13	1:M:1053:ILE:O	2.17	0.43
1:M:1299:GLN:NE2	1:M:1545:ASN:OD1	2.50	0.43
1:M:2966:ARG:O	1:M:2970:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:863:LEU:HD21	1:S:929:LEU:HB2	1.99	0.43
1:S:1813:LEU:HD11	1:S:1859:ASP:HB3	2.01	0.43
1:S:2195:HIS:O	1:S:2199:MET:HG2	2.18	0.43
1:A:1448:VAL:HG22	1:A:1554:VAL:HG23	1.99	0.43
1:A:2822:TRP:CZ3	1:A:2875:MET:HE2	2.54	0.43
1:A:3701:PHE:HB2	1:A:3773:MET:HE2	2.00	0.43
1:G:19:GLU:HB2	1:G:206:CYS:HB3	2.00	0.43
1:G:1265:ASP:OD1	1:G:1265:ASP:N	2.51	0.43
1:G:1286:MET:HE3	1:G:1286:MET:HB3	1.94	0.43
1:M:2822:TRP:CZ3	1:M:2875:MET:HE2	2.54	0.43
1:S:168:ASP:HB3	1:S:199:LEU:HD12	2.00	0.43
1:S:972:LEU:HD13	1:S:1044:ARG:C	2.43	0.43
1:S:2822:TRP:CZ3	1:S:2875:MET:HE2	2.54	0.43
1:A:1078:GLU:HG3	1:A:1237:TRP:NE1	2.34	0.43
1:A:3818:LYS:HA	1:A:3818:LYS:HD3	1.75	0.43
1:M:663:TYR:OH	1:M:665:GLU:OE2	2.33	0.43
1:M:1813:LEU:HD11	1:M:1859:ASP:HB3	2.01	0.43
1:M:2334:ASP:OD1	1:M:2334:ASP:C	2.61	0.43
1:M:4055:LYS:HE3	1:M:4055:LYS:HB3	1.89	0.43
1:S:3831:MET:HE3	1:S:3831:MET:HB2	1.83	0.43
1:A:2195:HIS:O	1:A:2199:MET:HG2	2.18	0.43
1:A:2966:ARG:O	1:A:2970:ILE:HG12	2.19	0.43
1:G:1152:MET:HE2	1:G:1161:ILE:HB	1.99	0.43
1:M:615:CYS:O	1:M:618:GLN:N	2.50	0.43
1:M:3701:PHE:HB2	1:M:3773:MET:HE2	2.00	0.43
1:S:1152:MET:HE2	1:S:1161:ILE:HB	1.99	0.43
1:S:2334:ASP:OD1	1:S:2334:ASP:C	2.61	0.43
1:A:168:ASP:HB3	1:A:199:LEU:HD12	2.00	0.43
1:A:863:LEU:HD12	1:A:864:PRO:HD2	2.00	0.43
1:A:972:LEU:HD13	1:A:1044:ARG:C	2.43	0.43
1:G:168:ASP:HB3	1:G:199:LEU:HD12	2.00	0.43
1:M:293:LEU:HD13	1:M:378:LEU:HD12	2.01	0.43
1:M:1078:GLU:HG3	1:M:1237:TRP:NE1	2.34	0.43
1:S:293:LEU:HD13	1:S:378:LEU:HD12	2.01	0.43
1:S:1078:GLU:HG3	1:S:1237:TRP:NE1	2.34	0.43
1:S:1265:ASP:OD1	1:S:1265:ASP:N	2.51	0.43
1:S:4055:LYS:HE3	1:S:4055:LYS:HB3	1.89	0.43
1:A:940:GLY:C	1:A:1051:TYR:CD1	2.97	0.43
1:G:1477:GLY:HA2	1:G:1483:ILE:HA	1.99	0.43
1:G:2822:TRP:CZ3	1:G:2875:MET:HE2	2.54	0.43
1:G:3648:MET:HA	1:G:3651:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4055:LYS:O	1:G:4059:MET:HG3	2.19	0.43
1:A:4055:LYS:O	1:A:4059:MET:HG3	2.19	0.43
1:A:4059:MET:HE1	1:A:4105:PHE:HD2	1.84	0.43
1:G:863:LEU:HD12	1:G:864:PRO:HD2	2.00	0.43
1:G:1078:GLU:HG3	1:G:1237:TRP:NE1	2.34	0.43
1:M:940:GLY:C	1:M:1051:TYR:CD1	2.97	0.43
1:M:1265:ASP:OD1	1:M:1265:ASP:N	2.51	0.43
1:S:19:GLU:HB2	1:S:206:CYS:HB3	2.00	0.43
1:S:2966:ARG:O	1:S:2970:ILE:HG12	2.19	0.43
1:A:19:GLU:HB2	1:A:206:CYS:HB3	2.00	0.42
1:A:293:LEU:HD13	1:A:378:LEU:HD12	2.01	0.42
1:A:1131:ARG:NH1	1:A:1178:ALA:O	2.52	0.42
1:A:1472:VAL:HG12	1:A:1489:CYS:HB2	2.01	0.42
1:A:2334:ASP:OD1	1:A:2334:ASP:C	2.61	0.42
1:A:4092:MET:HA	1:A:4092:MET:HE2	2.01	0.42
1:M:19:GLU:HB2	1:M:206:CYS:HB3	2.00	0.42
1:M:3648:MET:HA	1:M:3651:GLU:HG2	2.00	0.42
1:M:4211:GLN:NE2	1:M:4215:ASP:OD2	2.49	0.42
1:S:3275:LEU:HD23	1:S:3275:LEU:HA	1.85	0.42
1:S:3946:PHE:O	1:S:3950:MET:HG3	2.19	0.42
1:S:4092:MET:HE2	1:S:4092:MET:HA	2.01	0.42
1:A:1730:MET:HE1	1:A:1774:PRO:HG2	2.01	0.42
1:G:293:LEU:HD13	1:G:378:LEU:HD12	2.01	0.42
1:G:1472:VAL:HG12	1:G:1489:CYS:HB2	2.01	0.42
1:G:2027:GLU:HG2	1:G:2028:ILE:HD13	1.99	0.42
1:G:4059:MET:HE1	1:G:4105:PHE:HD2	1.84	0.42
1:M:403:MET:HE2	1:M:403:MET:HB3	1.89	0.42
1:M:4092:MET:HA	1:M:4092:MET:HE2	2.01	0.42
1:S:940:GLY:C	1:S:1051:TYR:CD1	2.97	0.42
1:S:4059:MET:HE1	1:S:4105:PHE:HD2	1.85	0.42
1:A:4734:ARG:HB3	1:A:4734:ARG:NH1	2.35	0.42
1:G:1813:LEU:HD11	1:G:1859:ASP:HB3	2.01	0.42
1:G:3946:PHE:O	1:G:3950:MET:HG3	2.19	0.42
1:M:1131:ARG:NH1	1:M:1178:ALA:O	2.52	0.42
1:A:1492:CYS:SG	1:A:1494:MET:HG3	2.60	0.42
1:A:2209:MET:HE2	1:A:2209:MET:HB2	1.83	0.42
1:A:2822:TRP:CE3	1:A:2875:MET:HE3	2.55	0.42
1:G:940:GLY:C	1:G:1051:TYR:CD1	2.97	0.42
1:G:1131:ARG:NH1	1:G:1178:ALA:O	2.52	0.42
1:M:790:ARG:HA	1:M:1626:TRP:O	2.20	0.42
1:M:4055:LYS:O	1:M:4059:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:790:ARG:HA	1:S:1626:TRP:O	2.20	0.42
1:S:863:LEU:HD12	1:S:864:PRO:HD2	2.00	0.42
1:S:1730:MET:HE1	1:S:1774:PRO:HG2	2.01	0.42
1:S:4055:LYS:O	1:S:4059:MET:HG3	2.19	0.42
1:A:1813:LEU:HD11	1:A:1859:ASP:HB3	2.01	0.42
1:G:4092:MET:HE2	1:G:4092:MET:HA	2.01	0.42
1:G:4734:ARG:NH1	1:G:4734:ARG:HB3	2.35	0.42
1:M:4059:MET:HE1	1:M:4105:PHE:HD2	1.84	0.42
1:S:1131:ARG:NH1	1:S:1178:ALA:O	2.52	0.42
1:S:4734:ARG:NH1	1:S:4734:ARG:HB3	2.35	0.42
1:A:403:MET:HE2	1:A:403:MET:HB3	1.89	0.42
1:A:790:ARG:HA	1:A:1626:TRP:O	2.20	0.42
1:M:1472:VAL:HG12	1:M:1489:CYS:HB2	2.01	0.42
1:M:2232:SER:O	1:M:2235:ARG:HG2	2.20	0.42
1:M:2822:TRP:CE3	1:M:2875:MET:HE2	2.54	0.42
1:M:4734:ARG:HB3	1:M:4734:ARG:NH1	2.35	0.42
1:S:1492:CYS:SG	1:S:1494:MET:HG3	2.60	0.42
1:G:2822:TRP:CE3	1:G:2875:MET:HE3	2.55	0.42
1:M:1687:SER:HB3	1:M:1783:PHE:CZ	2.55	0.42
1:S:2232:SER:O	1:S:2235:ARG:HG2	2.20	0.42
1:S:3701:PHE:HB2	1:S:3773:MET:HE2	2.00	0.42
1:S:4211:GLN:NE2	1:S:4215:ASP:OD2	2.49	0.42
1:G:1980:ILE:HD13	1:G:1980:ILE:HA	1.92	0.42
1:M:863:LEU:HD13	1:M:930:LYS:CG	2.50	0.42
1:M:2822:TRP:CE3	1:M:2875:MET:HE3	2.55	0.42
1:S:2822:TRP:CE3	1:S:2875:MET:HE3	2.55	0.42
1:S:2208:VAL:HG21	1:S:2236:PHE:CE1	2.55	0.42
1:A:4146:SER:HB2	1:A:4159:LEU:HD11	2.02	0.42
1:G:1687:SER:HB3	1:G:1783:PHE:CZ	2.55	0.42
1:G:2822:TRP:CE3	1:G:2875:MET:HE2	2.54	0.42
1:M:1730:MET:HE1	1:M:1774:PRO:HG2	2.01	0.42
1:M:3946:PHE:O	1:M:3950:MET:HG3	2.19	0.42
2:N:52:GLY:N	2:N:61:GLU:OE2	2.42	0.42
1:S:863:LEU:HD13	1:S:930:LYS:CG	2.50	0.42
1:S:1472:VAL:HG12	1:S:1489:CYS:HB2	2.01	0.42
1:S:2822:TRP:CE3	1:S:2875:MET:HE2	2.54	0.42
1:A:2208:VAL:HG21	1:A:2236:PHE:CE1	2.55	0.41
1:G:4146:SER:HB2	1:G:4159:LEU:HD11	2.02	0.41
1:G:4834:GLN:HE22	1:M:4942:ARG:NH1	2.18	0.41
1:S:663:TYR:OH	1:S:665:GLU:OE2	2.33	0.41
1:A:695:TYR:CD2	1:A:1240:LYS:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2209:MET:HE2	1:M:2209:MET:HB2	1.83	0.41
1:M:4146:SER:HB2	1:M:4159:LEU:HD11	2.02	0.41
1:S:448:LEU:HD23	1:S:448:LEU:HA	1.91	0.41
1:A:1687:SER:HB3	1:A:1783:PHE:CZ	2.55	0.41
1:A:4834:GLN:HE22	1:G:4942:ARG:NH1	2.17	0.41
1:A:4942:ARG:NH1	1:S:4834:GLN:HE22	2.18	0.41
1:G:695:TYR:CD2	1:G:1240:LYS:HE3	2.55	0.41
1:G:790:ARG:HA	1:G:1626:TRP:O	2.20	0.41
1:G:1126:GLY:O	1:G:1127:HIS:C	2.64	0.41
1:G:1730:MET:HE1	1:G:1774:PRO:HG2	2.01	0.41
1:G:2209:MET:HE2	1:G:2209:MET:HB2	1.83	0.41
1:S:1286:MET:HE3	1:S:1286:MET:HB3	1.94	0.41
1:S:2322:ILE:HG22	1:S:2324:TRP:H	1.86	0.41
1:M:19:GLU:O	1:M:205:ILE:HG13	2.20	0.41
1:M:3534:THR:O	1:M:3537:ALA:HB3	2.21	0.41
1:S:19:GLU:O	1:S:205:ILE:HG13	2.20	0.41
1:S:4146:SER:HB2	1:S:4159:LEU:HD11	2.02	0.41
1:A:2232:SER:O	1:A:2235:ARG:HG2	2.20	0.41
1:A:2931:LEU:HD13	1:A:2938:VAL:HG21	2.03	0.41
1:A:3275:LEU:HD23	1:A:3275:LEU:HA	1.85	0.41
1:G:1658:ASP:OD2	1:G:1658:ASP:N	2.50	0.41
1:G:2208:VAL:HG21	1:G:2236:PHE:CE1	2.55	0.41
1:G:2931:LEU:HD13	1:G:2938:VAL:HG21	2.03	0.41
1:M:632:LEU:O	1:M:634:GLN:NE2	2.48	0.41
1:M:2208:VAL:HG21	1:M:2236:PHE:CE1	2.55	0.41
1:A:19:GLU:O	1:A:205:ILE:HG13	2.20	0.41
1:A:2822:TRP:CE3	1:A:2875:MET:HE2	2.54	0.41
1:A:3534:THR:O	1:A:3537:ALA:HB3	2.21	0.41
1:G:2232:SER:O	1:G:2235:ARG:HG2	2.20	0.41
1:G:3701:PHE:HB2	1:G:3773:MET:HE2	2.00	0.41
1:M:2931:LEU:HD13	1:M:2938:VAL:HG21	2.03	0.41
1:S:695:TYR:CD2	1:S:1240:LYS:HE3	2.55	0.41
1:S:1424:PRO:O	1:S:1428:LEU:HD23	2.21	0.41
1:S:1687:SER:HB3	1:S:1783:PHE:CZ	2.55	0.41
1:S:2894:GLU:HG3	1:S:2898:LYS:HD2	2.03	0.41
1:G:403:MET:HE2	1:G:403:MET:HB3	1.89	0.41
1:G:1492:CYS:SG	1:G:1494:MET:HG3	2.60	0.41
1:M:695:TYR:CD2	1:M:1240:LYS:HE3	2.55	0.41
1:M:858:THR:C	1:M:861:ILE:HG22	2.46	0.41
1:M:1799:LEU:HD23	1:M:1799:LEU:HA	1.72	0.41
1:M:2160:LEU:HD13	1:M:2204:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2894:GLU:HG3	1:M:2898:LYS:HD2	2.03	0.41
1:M:3887:CYS:SG	1:M:3898:LEU:HD12	2.61	0.41
1:M:4834:GLN:HE22	1:S:4942:ARG:NH1	2.18	0.41
2:T:52:GLY:N	2:T:61:GLU:OE2	2.42	0.41
2:B:12:ASP:OD1	2:B:12:ASP:C	2.64	0.41
1:G:863:LEU:HD13	1:G:930:LYS:CG	2.50	0.41
1:G:1799:LEU:HD23	1:G:1799:LEU:HA	1.72	0.41
1:M:1492:CYS:SG	1:M:1494:MET:HG3	2.60	0.41
1:S:1647:CYS:SG	1:S:1648:MET:N	2.94	0.41
1:S:2160:LEU:HD13	1:S:2204:MET:HE2	2.02	0.41
1:A:1126:GLY:O	1:A:1127:HIS:C	2.64	0.41
1:A:3200:ALA:HB2	1:A:3280:SER:OG	2.21	0.41
2:B:80:ASP:OD1	2:B:80:ASP:C	2.63	0.41
1:G:19:GLU:O	1:G:205:ILE:HG13	2.20	0.41
1:G:572:PRO:O	1:G:575:LEU:HB2	2.21	0.41
1:G:2322:ILE:HG22	1:G:2324:TRP:H	1.86	0.41
1:G:2605:GLU:HG2	1:G:2640:MET:HG3	2.03	0.41
1:M:1647:CYS:SG	1:M:1648:MET:N	2.94	0.41
1:S:863:LEU:HD12	1:S:863:LEU:HA	1.72	0.41
1:S:2528:LEU:HD12	1:S:2528:LEU:HA	1.92	0.41
1:S:2605:GLU:HG2	1:S:2640:MET:HG3	2.03	0.41
1:S:3534:THR:O	1:S:3537:ALA:HB3	2.21	0.41
1:S:3887:CYS:SG	1:S:3898:LEU:HD12	2.61	0.41
1:S:4044:VAL:HG21	1:S:4154:ARG:HD2	2.03	0.41
2:T:80:ASP:OD1	2:T:80:ASP:C	2.63	0.41
1:A:863:LEU:HD13	1:A:930:LYS:CG	2.50	0.41
1:A:2322:ILE:HG22	1:A:2324:TRP:H	1.86	0.41
1:A:4731:GLY:N	1:A:4734:ARG:HH22	2.19	0.41
1:G:3200:ALA:HB2	1:G:3280:SER:OG	2.21	0.41
1:G:3887:CYS:SG	1:G:3898:LEU:HD12	2.61	0.41
1:M:1228:ILE:HD12	1:M:1228:ILE:HA	1.95	0.41
1:M:1806:GLU:CD	1:M:1806:GLU:H	2.29	0.41
1:M:2322:ILE:HG22	1:M:2324:TRP:H	1.86	0.41
1:S:1228:ILE:HD12	1:S:1228:ILE:HA	1.95	0.41
1:S:3269:HIS:CE1	1:S:3273:ILE:HD12	2.56	0.41
1:S:3282:LEU:HD12	1:S:3316:LEU:HD22	2.03	0.41
1:S:4061:LEU:HD23	1:S:4061:LEU:HA	1.94	0.41
1:G:1018:ASN:OD1	1:G:1020:ARG:HG2	2.21	0.40
1:G:2755:PHE:HE1	1:G:2931:LEU:HA	1.86	0.40
1:G:3176:LEU:HD13	1:G:3176:LEU:HA	1.97	0.40
1:G:3269:HIS:CE1	1:G:3273:ILE:HD12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4721:LYS:HB3	1:G:4721:LYS:HE3	1.97	0.40
2:H:12:ASP:OD1	2:H:12:ASP:C	2.64	0.40
1:M:2966:ARG:HA	1:M:2969:ASP:OD2	2.21	0.40
1:M:3818:LYS:HD3	1:M:3818:LYS:HA	1.75	0.40
1:S:3898:LEU:HD23	1:S:3898:LEU:HA	1.94	0.40
1:A:572:PRO:O	1:A:575:LEU:HB2	2.21	0.40
1:A:2605:GLU:HG2	1:A:2640:MET:HG3	2.03	0.40
1:A:3321:LEU:HD23	1:A:3321:LEU:HA	1.97	0.40
1:A:3887:CYS:SG	1:A:3898:LEU:HD12	2.61	0.40
1:G:1424:PRO:O	1:G:1428:LEU:HD23	2.21	0.40
1:G:1561:VAL:HG13	1:G:1562:ILE:N	2.37	0.40
1:G:1647:CYS:SG	1:G:1648:MET:N	2.94	0.40
1:G:4834:GLN:HE22	1:M:4942:ARG:HH12	1.69	0.40
2:H:80:ASP:OD1	2:H:80:ASP:C	2.63	0.40
1:M:572:PRO:O	1:M:575:LEU:HB2	2.21	0.40
1:M:1126:GLY:O	1:M:1127:HIS:C	2.64	0.40
1:M:3200:ALA:HB2	1:M:3280:SER:OG	2.21	0.40
1:M:3282:LEU:HD12	1:M:3316:LEU:HD22	2.03	0.40
1:S:3200:ALA:HB2	1:S:3280:SER:OG	2.21	0.40
2:T:12:ASP:OD1	2:T:12:ASP:C	2.64	0.40
1:A:80:GLU:HG3	1:G:3930:TRP:CZ3	2.56	0.40
1:A:1018:ASN:OD1	1:A:1020:ARG:HG2	2.21	0.40
1:A:1806:GLU:H	1:A:1806:GLU:CD	2.29	0.40
1:A:2213:VAL:HG22	1:A:2257:TYR:CZ	2.57	0.40
1:A:3898:LEU:HD23	1:A:3898:LEU:HA	1.94	0.40
1:G:449:ILE:HD13	1:G:449:ILE:HA	1.98	0.40
1:M:2755:PHE:HE1	1:M:2931:LEU:HA	1.86	0.40
1:S:1126:GLY:O	1:S:1127:HIS:C	2.64	0.40
1:S:1806:GLU:H	1:S:1806:GLU:CD	2.30	0.40
1:S:2931:LEU:HD13	1:S:2938:VAL:HG21	2.02	0.40
1:S:4730:TYR:HB3	1:S:4734:ARG:HH22	1.86	0.40
1:A:1018:ASN:HA	1:A:1019:PRO:HD3	1.94	0.40
1:A:1647:CYS:SG	1:A:1648:MET:N	2.94	0.40
1:A:3269:HIS:CE1	1:A:3273:ILE:HD12	2.56	0.40
1:A:4044:VAL:HG21	1:A:4154:ARG:HD2	2.03	0.40
1:G:4678:LYS:HB2	1:G:4678:LYS:HE3	1.84	0.40
1:G:4967:ASP:H	1:G:4972:ARG:CB	2.35	0.40
1:M:1424:PRO:O	1:M:1428:LEU:HD23	2.21	0.40
1:M:3275:LEU:HD23	1:M:3275:LEU:HA	1.85	0.40
1:M:4931:GLN:O	1:M:4935:ILE:HG12	2.22	0.40
2:N:12:ASP:C	2:N:12:ASP:OD1	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2228:LYS:HE3	1:S:2228:LYS:HB2	1.96	0.40
1:A:3202:MET:HA	1:A:3203:PRO:HD3	1.88	0.40
1:A:3930:TRP:CZ3	1:S:80:GLU:HG3	2.56	0.40
1:A:4723:LEU:HB2	1:A:4741:MET:HE1	2.04	0.40
1:G:25:ASN:OD1	1:G:26:ALA:N	2.55	0.40
1:G:1806:GLU:CD	1:G:1806:GLU:H	2.29	0.40
1:G:2894:GLU:HG3	1:G:2898:LYS:HD2	2.03	0.40
1:G:2966:ARG:HA	1:G:2969:ASP:OD2	2.21	0.40
1:G:3534:THR:O	1:G:3537:ALA:HB3	2.21	0.40
5:G:5105:117:H62	5:G:5105:117:C81	2.52	0.40
1:M:233:ILE:O	1:M:257:ARG:NH1	2.55	0.40
1:M:1018:ASN:OD1	1:M:1020:ARG:HG2	2.21	0.40
1:M:2605:GLU:HG2	1:M:2640:MET:HG3	2.03	0.40
1:M:2959:GLY:HA2	1:M:2962:GLN:HG2	2.04	0.40
1:S:2213:VAL:HG22	1:S:2257:TYR:CZ	2.57	0.40
1:S:3751:LYS:N	1:S:3751:LYS:HD3	2.37	0.40
1:S:4723:LEU:HB2	1:S:4741:MET:HE1	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	A	4049/5035 (80%)	3974 (98%)	73 (2%)	2 (0%)	100	100
1	G	4049/5035 (80%)	3974 (98%)	73 (2%)	2 (0%)	100	100
1	M	4049/5035 (80%)	3974 (98%)	73 (2%)	2 (0%)	100	100
1	S	4049/5035 (80%)	3974 (98%)	73 (2%)	2 (0%)	100	100
2	B	105/111 (95%)	103 (98%)	2 (2%)	0	100	100
2	H	105/111 (95%)	103 (98%)	2 (2%)	0	100	100
2	N	105/111 (95%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	105/111 (95%)	103 (98%)	2 (2%)	0	100	100
All	All	16616/20584 (81%)	16308 (98%)	300 (2%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1129	GLY
1	G	1129	GLY
1	M	1129	GLY
1	S	1129	GLY
1	A	753	PRO
1	G	753	PRO
1	M	753	PRO
1	S	753	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3283/4284 (77%)	3283 (100%)	0	100	100
1	G	3283/4284 (77%)	3283 (100%)	0	100	100
1	M	3283/4284 (77%)	3283 (100%)	0	100	100
1	S	3283/4284 (77%)	3282 (100%)	1 (0%)	100	100
2	B	87/91 (96%)	87 (100%)	0	100	100
2	H	87/91 (96%)	87 (100%)	0	100	100
2	N	87/91 (96%)	87 (100%)	0	100	100
2	T	87/91 (96%)	87 (100%)	0	100	100
All	All	13480/17500 (77%)	13479 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	218	HIS
1	A	273	HIS
1	A	350	HIS
1	A	379	HIS
1	A	543	ASN
1	A	678	GLN
1	A	725	HIS
1	A	765	GLN
1	A	838	HIS
1	A	866	HIS
1	A	911	HIS
1	A	1299	GLN
1	A	1459	GLN
1	A	1719	HIS
1	A	1942	ASN
1	A	1973	ASN
1	A	2096	GLN
1	A	2108	GLN
1	A	2126	HIS
1	A	2343	ASN
1	A	2757	ASN
1	A	2878	GLN
1	A	3031	HIS
1	A	3922	GLN
1	A	3955	GLN
1	A	4115	ASN
1	A	4148	HIS
1	A	4551	ASN
1	A	4830	HIS
1	A	4834	GLN
1	A	4945	GLN
1	G	203	ASN
1	G	218	HIS
1	G	273	HIS
1	G	350	HIS
1	G	379	HIS
1	G	543	ASN

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Mol	Chain	Res	Type
1	G	678	GLN
1	G	725	HIS
1	G	838	HIS
1	G	866	HIS
1	G	911	HIS
1	G	1299	GLN
1	G	1459	GLN
1	G	1719	HIS
1	G	1942	ASN
1	G	1973	ASN
1	G	2096	GLN
1	G	2108	GLN
1	G	2126	HIS
1	G	2343	ASN
1	G	2445	GLN
1	G	2757	ASN
1	G	2878	GLN
1	G	3031	HIS
1	G	3647	ASN
1	G	3922	GLN
1	G	3955	GLN
1	G	4115	ASN
1	G	4148	HIS
1	G	4551	ASN
1	G	4830	HIS
1	G	4834	GLN
1	G	4945	GLN
1	M	203	ASN
1	M	218	HIS
1	M	273	HIS
1	M	350	HIS
1	M	379	HIS
1	M	543	ASN
1	M	678	GLN
1	M	725	HIS
1	M	735	GLN
1	M	838	HIS
1	M	866	HIS
1	M	911	HIS
1	M	1299	GLN
1	M	1459	GLN
1	M	1719	HIS

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Mol	Chain	Res	Type
1	M	1942	ASN
1	M	1973	ASN
1	M	2037	GLN
1	M	2096	GLN
1	M	2108	GLN
1	M	2126	HIS
1	M	2343	ASN
1	M	2757	ASN
1	M	2878	GLN
1	M	3031	HIS
1	M	3647	ASN
1	M	3922	GLN
1	M	4115	ASN
1	M	4148	HIS
1	M	4551	ASN
1	M	4834	GLN
1	M	4945	GLN
1	S	203	ASN
1	S	218	HIS
1	S	273	HIS
1	S	350	HIS
1	S	379	HIS
1	S	543	ASN
1	S	678	GLN
1	S	725	HIS
1	S	765	GLN
1	S	838	HIS
1	S	866	HIS
1	S	911	HIS
1	S	1127	HIS
1	S	1459	GLN
1	S	1719	HIS
1	S	1942	ASN
1	S	1973	ASN
1	S	2037	GLN
1	S	2096	GLN
1	S	2108	GLN
1	S	2126	HIS
1	S	2343	ASN
1	S	2445	GLN
1	S	2757	ASN
1	S	2878	GLN

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Mol	Chain	Res	Type
1	S	3031	HIS
1	S	3922	GLN
1	S	4115	ASN
1	S	4148	HIS
1	S	4551	ASN
1	S	4830	HIS
1	S	4834	GLN
1	S	4945	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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\# Z > 2$
5	117	A	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.30	5 (9%)
5	117	G	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.30	5 (9%)
3	CFF	A	5101	-	15,15,15	0.55	0	23,23,23	0.68	1 (4%)
3	CFF	G	5101	-	15,15,15	0.55	0	23,23,23	0.68	1 (4%)
5	117	S	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	117	M	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)
5	117	S	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
5	117	A	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
5	117	G	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
3	CFF	S	5101	-	15,15,15	0.54	0	23,23,23	0.69	1 (4%)
5	117	M	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.30	5 (9%)
5	117	M	5105	-	44,44,44	0.78	0	55,61,61	0.95	2 (3%)
3	CFF	M	5101	-	15,15,15	0.55	0	23,23,23	0.68	1 (4%)
5	117	S	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.31	5 (9%)
5	117	G	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)
5	117	A	5104	-	44,44,44	0.79	1 (2%)	55,61,61	0.90	2 (3%)

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
5	117	A	5103	-	-	6/33/33/33	0/4/4/4
5	117	G	5103	-	-	6/33/33/33	0/4/4/4
3	CFF	A	5101	-	-	-	0/2/2/2
3	CFF	G	5101	-	-	-	0/2/2/2
5	117	S	5104	-	-	0/33/33/33	0/4/4/4
5	117	M	5104	-	-	0/33/33/33	0/4/4/4
5	117	S	5105	-	-	9/33/33/33	0/4/4/4
5	117	A	5105	-	-	9/33/33/33	0/4/4/4
5	117	G	5105	-	-	9/33/33/33	0/4/4/4
3	CFF	S	5101	-	-	-	0/2/2/2
5	117	M	5103	-	-	6/33/33/33	0/4/4/4
3	CFF	M	5101	-	-	-	0/2/2/2
5	117	M	5105	-	-	9/33/33/33	0/4/4/4
5	117	S	5103	-	-	6/33/33/33	0/4/4/4
5	117	G	5104	-	-	0/33/33/33	0/4/4/4
5	117	A	5104	-	-	0/33/33/33	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5103	117	C12-C10	-2.29	1.45	1.49
5	G	5103	117	C12-C10	-2.29	1.45	1.49
5	M	5103	117	C12-C10	-2.29	1.45	1.49
5	S	5103	117	C12-C10	-2.29	1.45	1.49
5	A	5104	117	C12-C10	-2.16	1.45	1.49
5	G	5104	117	C12-C10	-2.16	1.45	1.49
5	M	5104	117	C12-C10	-2.16	1.45	1.49
5	S	5104	117	C12-C10	-2.16	1.45	1.49

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	5103	117	C19-N2-C18	-6.08	116.66	127.45
5	G	5103	117	C19-N2-C18	-6.08	116.66	127.45
5	M	5103	117	C19-N2-C18	-6.08	116.66	127.45
5	S	5103	117	C19-N2-C18	-6.08	116.66	127.45
5	A	5105	117	C6-C7-N1	3.32	117.97	112.16
5	G	5105	117	C6-C7-N1	3.32	117.97	112.16
5	M	5105	117	C6-C7-N1	3.32	117.97	112.16
5	S	5105	117	C6-C7-N1	3.32	117.97	112.16
5	A	5104	117	C11-C10-C8	3.14	109.37	106.82
5	G	5104	117	C11-C10-C8	3.14	109.37	106.82
5	M	5104	117	C11-C10-C8	3.14	109.37	106.82
5	S	5104	117	C11-C10-C8	3.14	109.37	106.82
5	A	5104	117	C12-C10-C8	-2.79	121.59	127.01
5	G	5104	117	C12-C10-C8	-2.79	121.59	127.01
5	M	5104	117	C12-C10-C8	-2.79	121.59	127.01
5	S	5104	117	C12-C10-C8	-2.79	121.59	127.01
5	A	5103	117	C5-C4-C3	2.70	118.55	114.28
5	G	5103	117	C5-C4-C3	2.70	118.55	114.28
5	M	5103	117	C5-C4-C3	2.70	118.55	114.28
5	S	5103	117	C5-C4-C3	2.70	118.55	114.28
5	S	5105	117	C5-C4-C3	2.48	118.20	114.28
5	A	5105	117	C5-C4-C3	2.47	118.19	114.28
5	G	5105	117	C5-C4-C3	2.47	118.19	114.28
5	M	5105	117	C5-C4-C3	2.47	118.19	114.28
3	S	5101	CFF	C12-N3-C2	2.26	121.26	117.33
5	A	5103	117	C4-C5-C6	-2.24	107.69	112.42
5	G	5103	117	C4-C5-C6	-2.24	107.69	112.42
5	M	5103	117	C4-C5-C6	-2.24	107.69	112.42
5	S	5103	117	C4-C5-C6	-2.24	107.69	112.42
3	A	5101	CFF	C12-N3-C2	2.23	121.21	117.33
3	G	5101	CFF	C12-N3-C2	2.23	121.21	117.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	5101	CFF	C12-N3-C2	2.23	121.21	117.33
5	S	5103	117	O18-C18-C11	-2.08	118.42	121.53
5	A	5103	117	O18-C18-C11	-2.04	118.47	121.53
5	G	5103	117	O18-C18-C11	-2.04	118.47	121.53
5	M	5103	117	O18-C18-C11	-2.04	118.47	121.53
5	A	5103	117	O3-C3-C4	-2.03	104.76	109.25
5	G	5103	117	O3-C3-C4	-2.03	104.76	109.25
5	M	5103	117	O3-C3-C4	-2.03	104.76	109.25
5	S	5103	117	O3-C3-C4	-2.02	104.78	109.25

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5103	117	C9-C11-C18-O18
5	A	5105	117	O5-C5-C6-C7
5	A	5105	117	C9-C11-C18-N2
5	G	5103	117	C9-C11-C18-O18
5	G	5105	117	O5-C5-C6-C7
5	G	5105	117	C9-C11-C18-N2
5	M	5103	117	C9-C11-C18-O18
5	M	5105	117	O5-C5-C6-C7
5	M	5105	117	C9-C11-C18-N2
5	S	5103	117	C9-C11-C18-O18
5	S	5105	117	O5-C5-C6-C7
5	S	5105	117	C9-C11-C18-N2
5	A	5103	117	C20-C19-N2-C18
5	G	5103	117	C20-C19-N2-C18
5	M	5103	117	C20-C19-N2-C18
5	S	5103	117	C20-C19-N2-C18
5	A	5103	117	C24-C19-N2-C18
5	G	5103	117	C24-C19-N2-C18
5	M	5103	117	C24-C19-N2-C18
5	S	5103	117	C24-C19-N2-C18
5	A	5105	117	C4-C5-C6-C7
5	G	5105	117	C4-C5-C6-C7
5	M	5105	117	C4-C5-C6-C7
5	S	5105	117	C4-C5-C6-C7
5	A	5105	117	C6-C7-N1-C9
5	G	5105	117	C6-C7-N1-C9
5	M	5105	117	C6-C7-N1-C9
5	S	5105	117	C6-C7-N1-C9

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Mol	Chain	Res	Type	Atoms
5	A	5103	117	C10-C11-C18-N2
5	A	5103	117	C10-C11-C18-O18
5	A	5105	117	C10-C11-C18-N2
5	A	5105	117	C10-C11-C18-O18
5	G	5103	117	C10-C11-C18-N2
5	G	5103	117	C10-C11-C18-O18
5	G	5105	117	C10-C11-C18-N2
5	G	5105	117	C10-C11-C18-O18
5	M	5103	117	C10-C11-C18-N2
5	M	5103	117	C10-C11-C18-O18
5	M	5105	117	C10-C11-C18-N2
5	M	5105	117	C10-C11-C18-O18
5	S	5103	117	C10-C11-C18-N2
5	S	5103	117	C10-C11-C18-O18
5	S	5105	117	C10-C11-C18-N2
5	S	5105	117	C10-C11-C18-O18
5	A	5105	117	C9-C11-C18-O18
5	G	5105	117	C9-C11-C18-O18
5	M	5105	117	C9-C11-C18-O18
5	S	5105	117	C9-C11-C18-O18
5	A	5103	117	C9-C11-C18-N2
5	G	5103	117	C9-C11-C18-N2
5	M	5103	117	C9-C11-C18-N2
5	S	5103	117	C9-C11-C18-N2
5	A	5105	117	C6-C7-N1-C8
5	G	5105	117	C6-C7-N1-C8
5	M	5105	117	C6-C7-N1-C8
5	S	5105	117	C6-C7-N1-C8
5	A	5105	117	O1A-C1-C2-C3
5	G	5105	117	O1A-C1-C2-C3
5	M	5105	117	O1A-C1-C2-C3
5	S	5105	117	O1A-C1-C2-C3

There are no ring outliers.

12 monomers are involved in 41 short contacts:

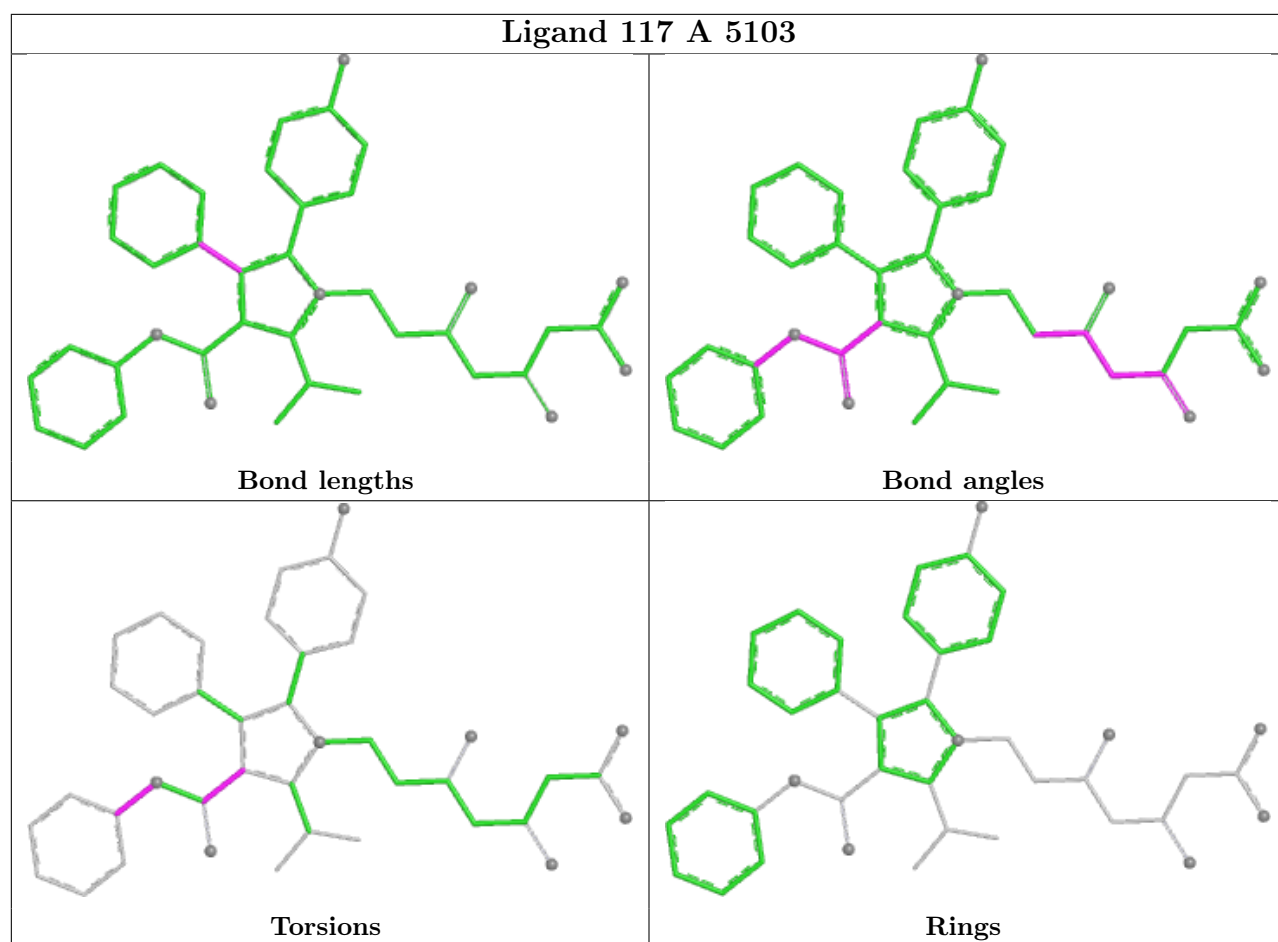
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5103	117	4	0
5	G	5103	117	4	0
5	S	5104	117	7	0
5	M	5104	117	7	0
5	S	5105	117	4	0

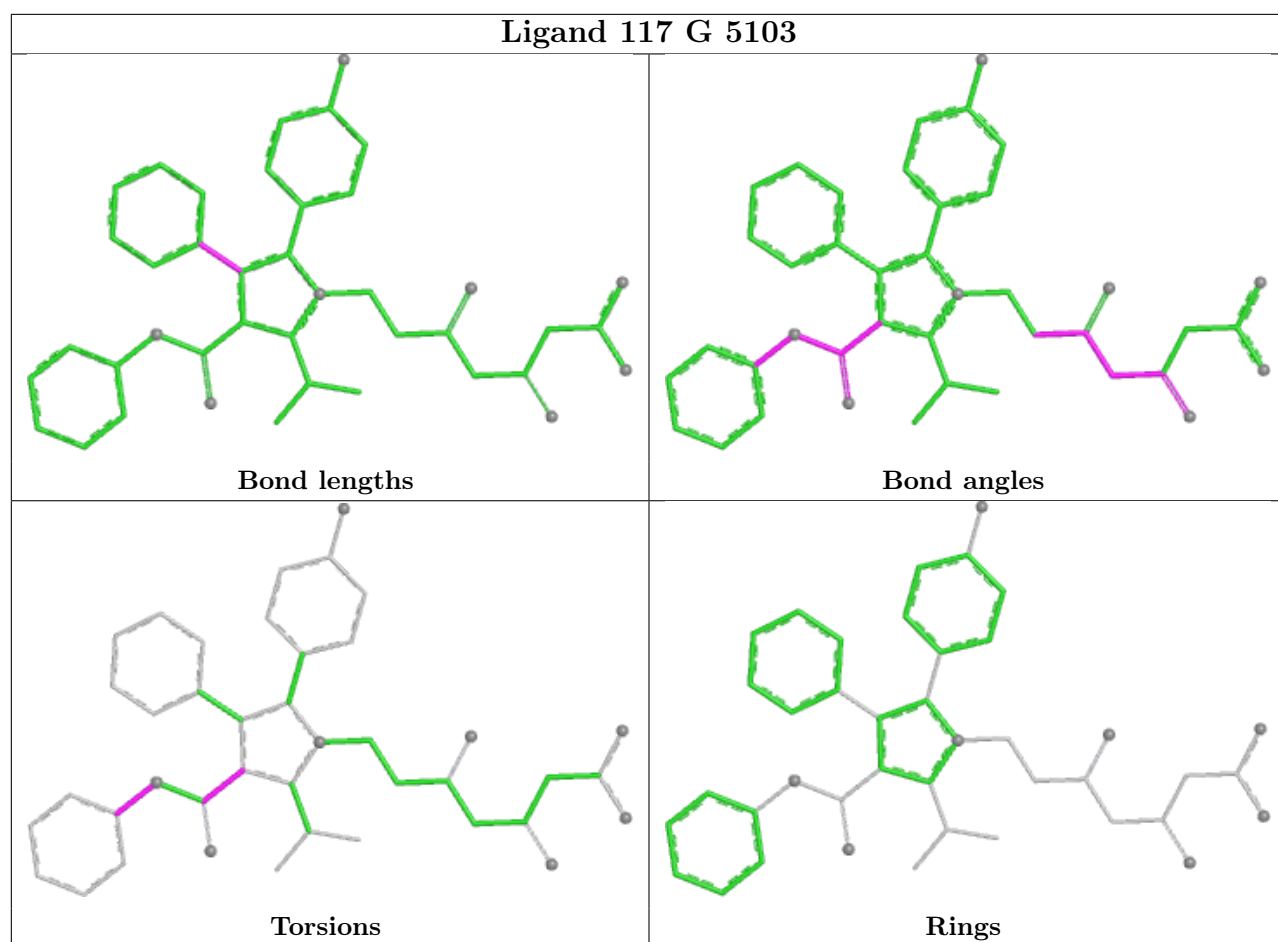
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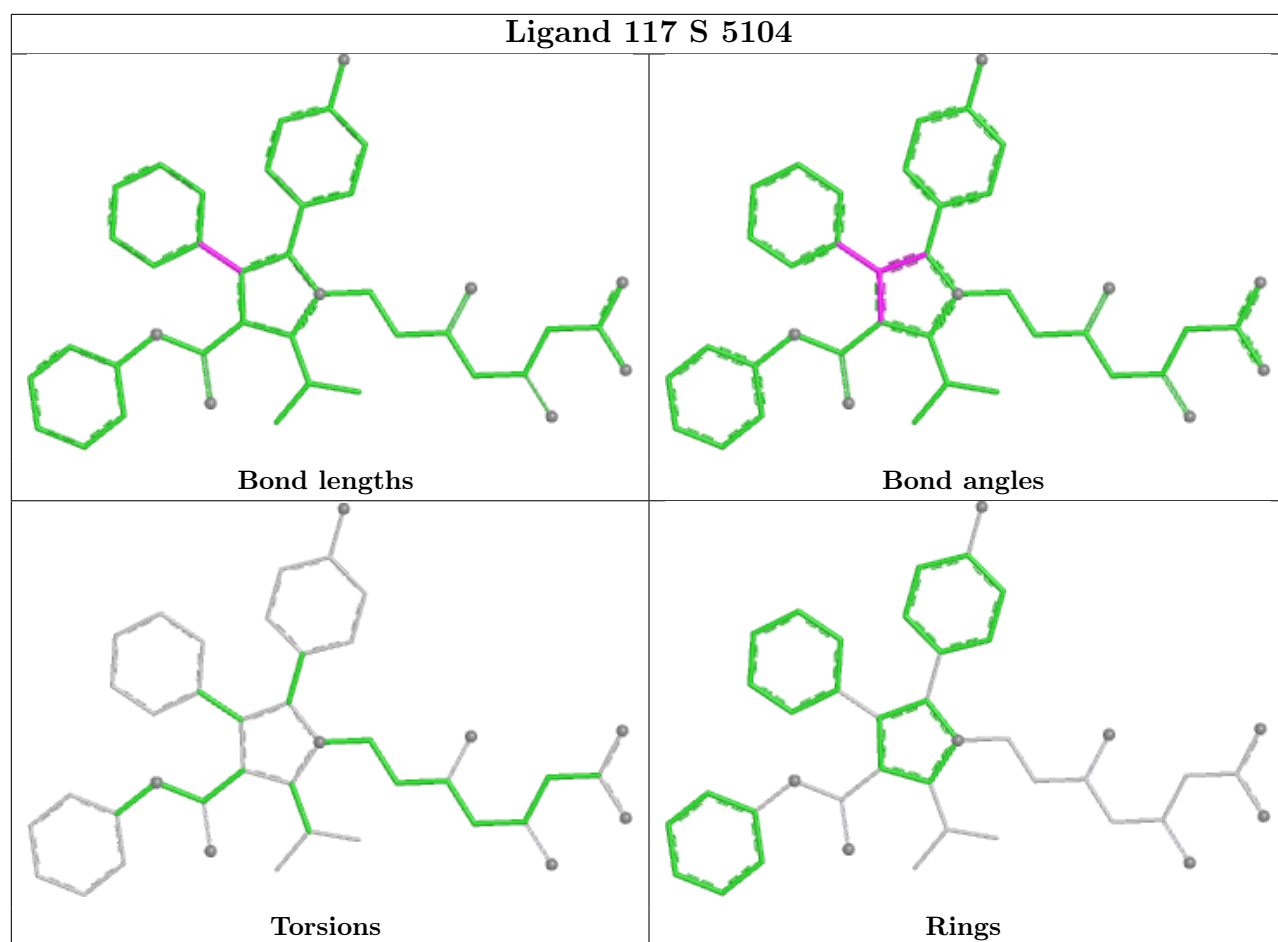
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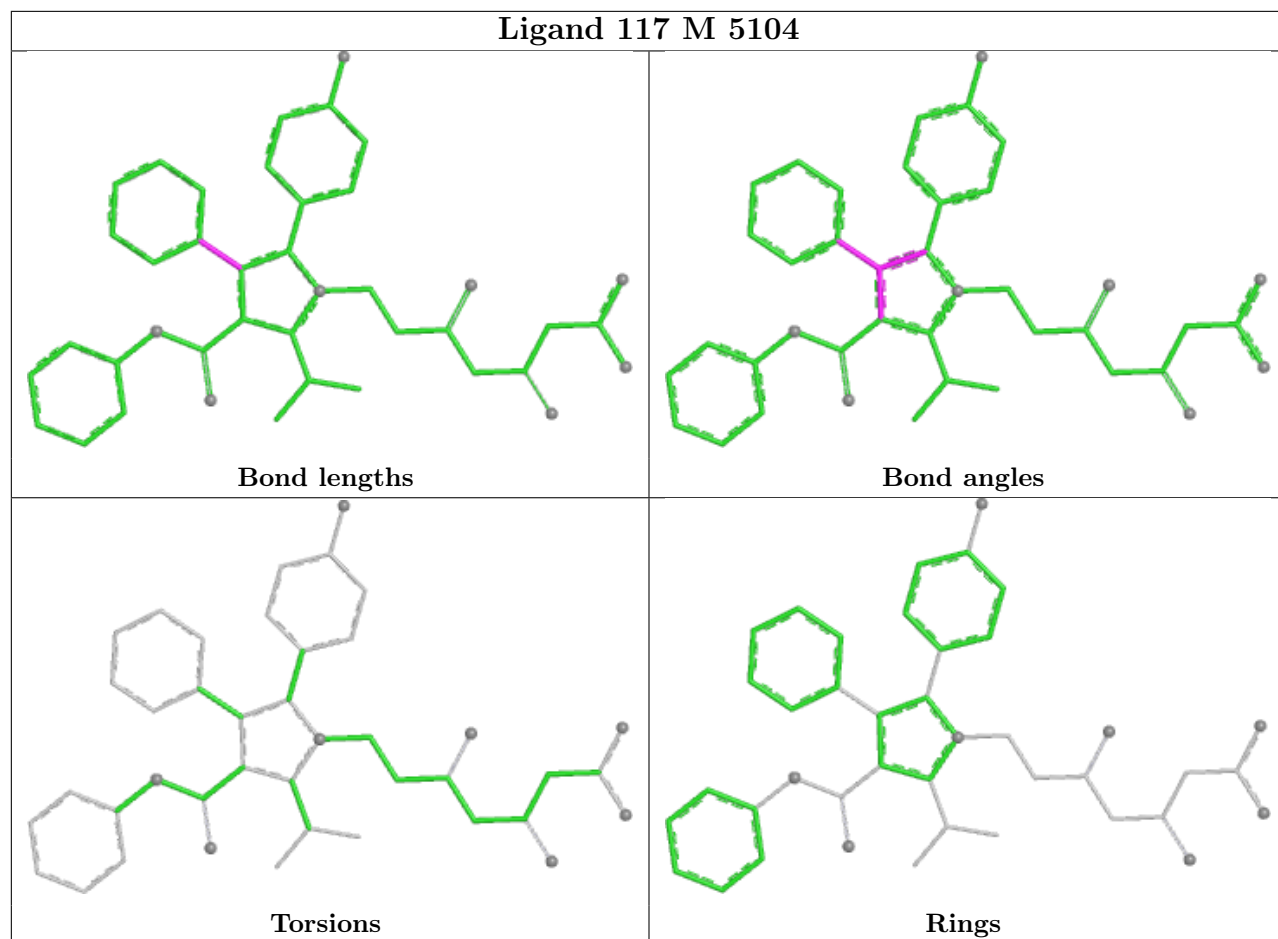
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5105	117	4	0
5	G	5105	117	5	0
5	M	5103	117	4	0
5	M	5105	117	4	0
5	S	5103	117	4	0
5	G	5104	117	7	0
5	A	5104	117	7	0

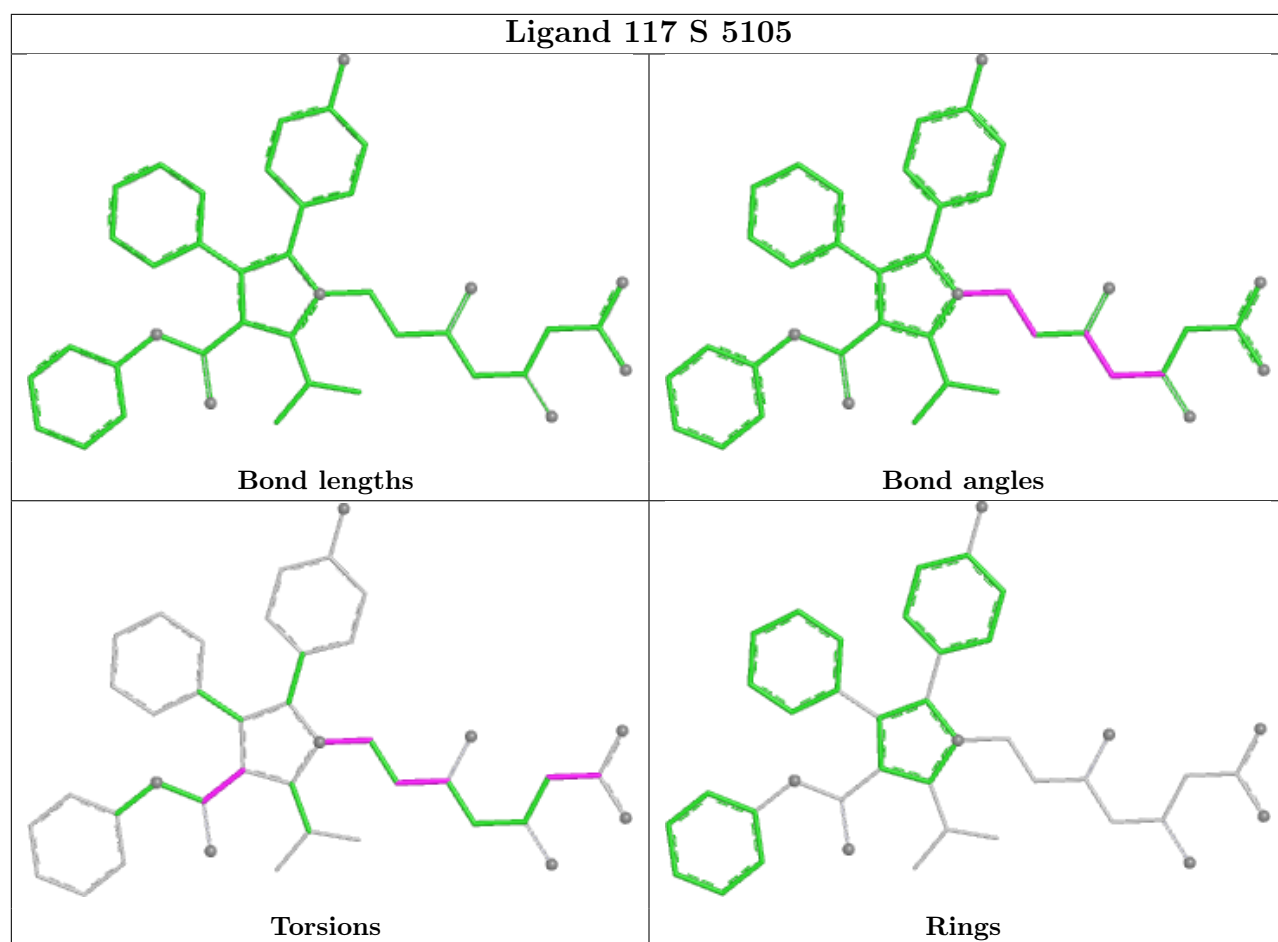
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

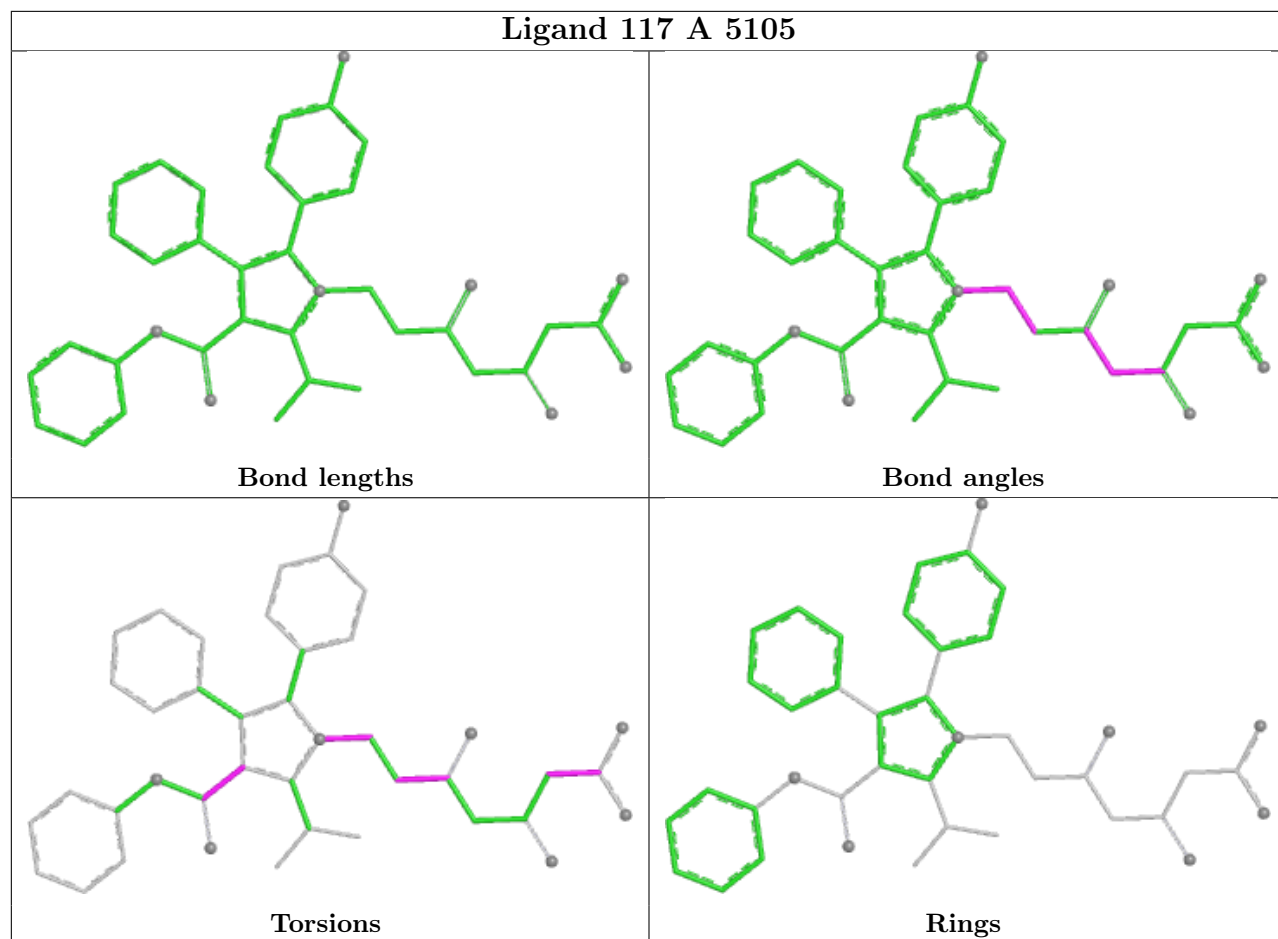


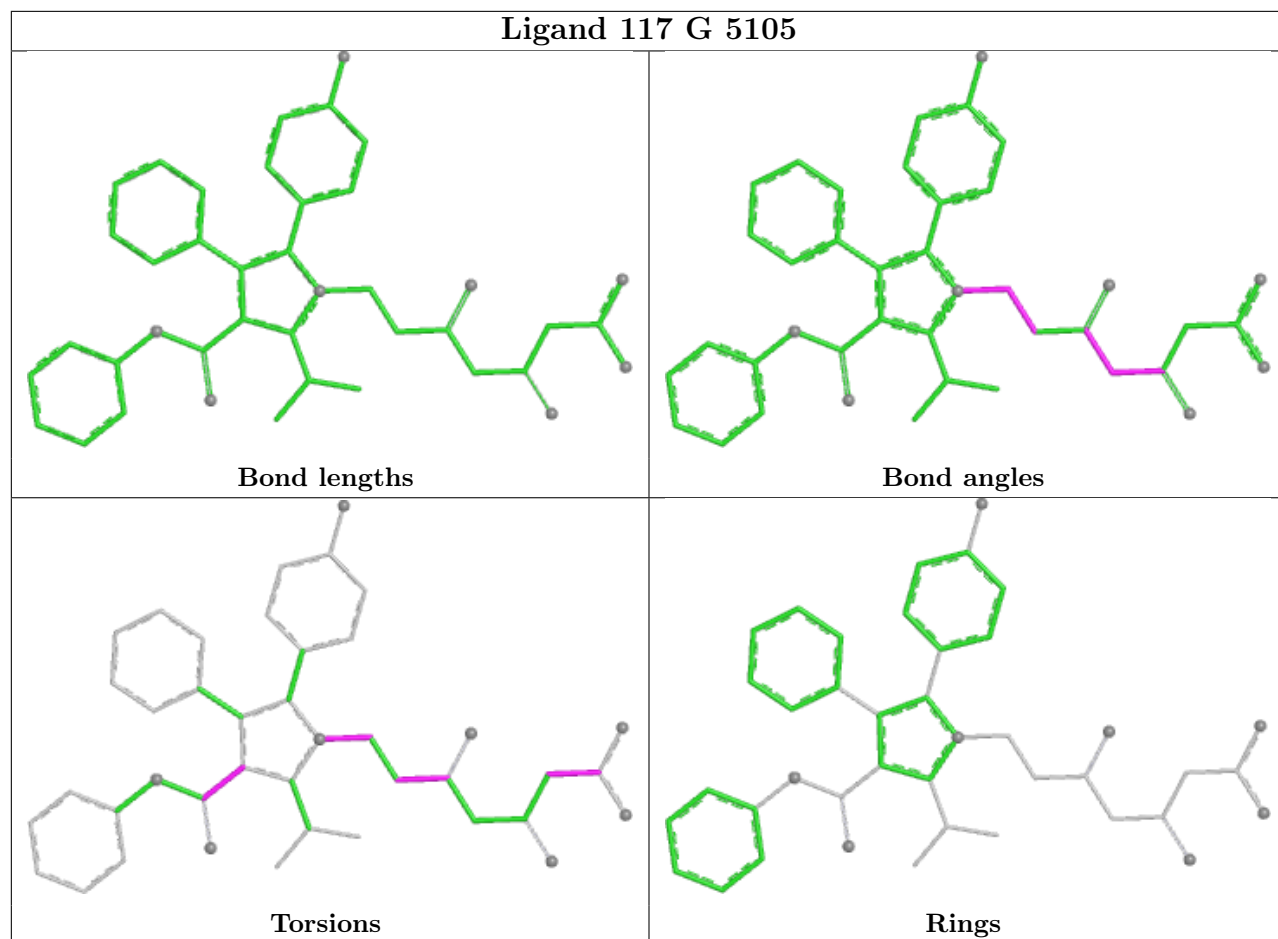


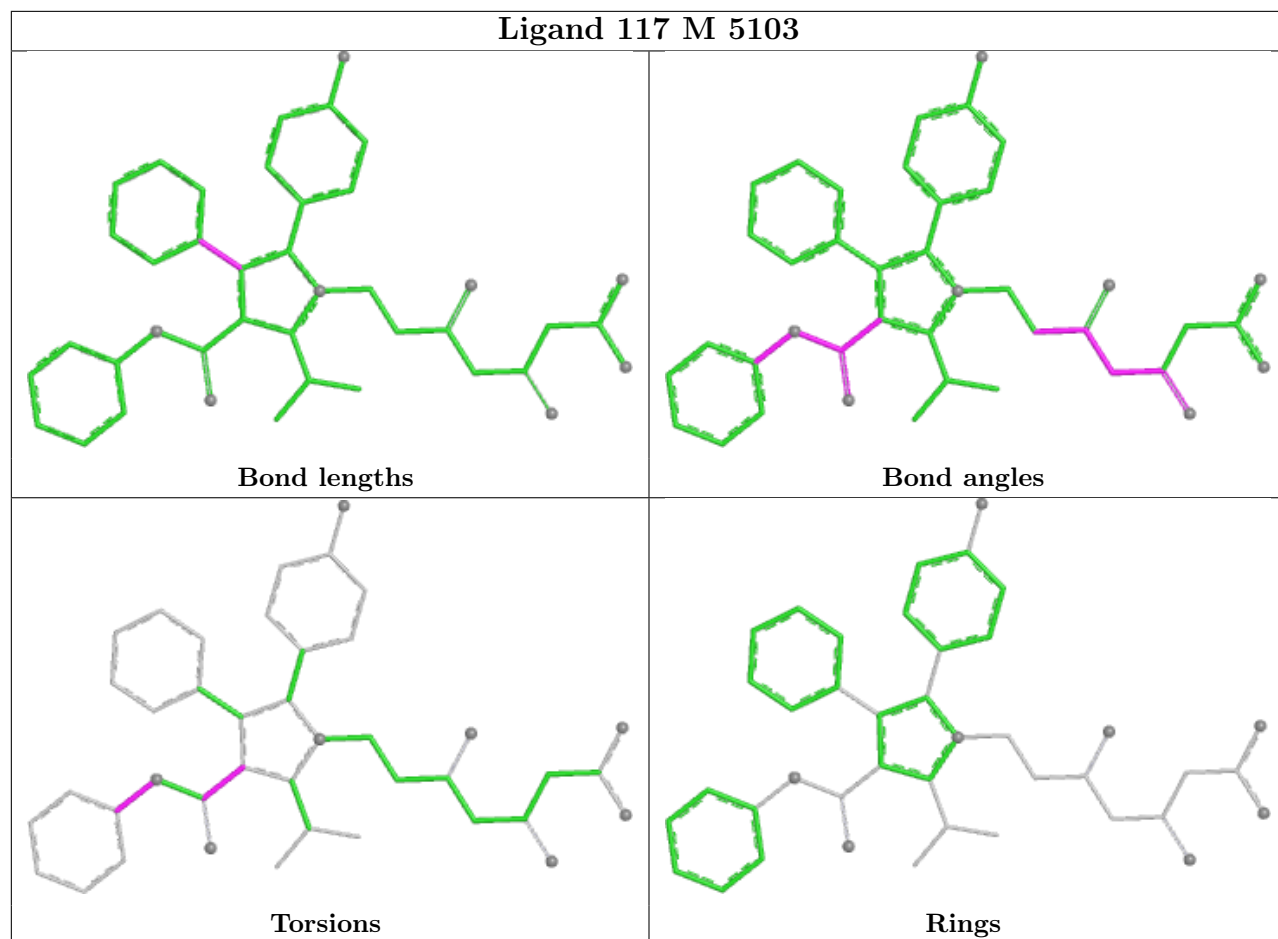


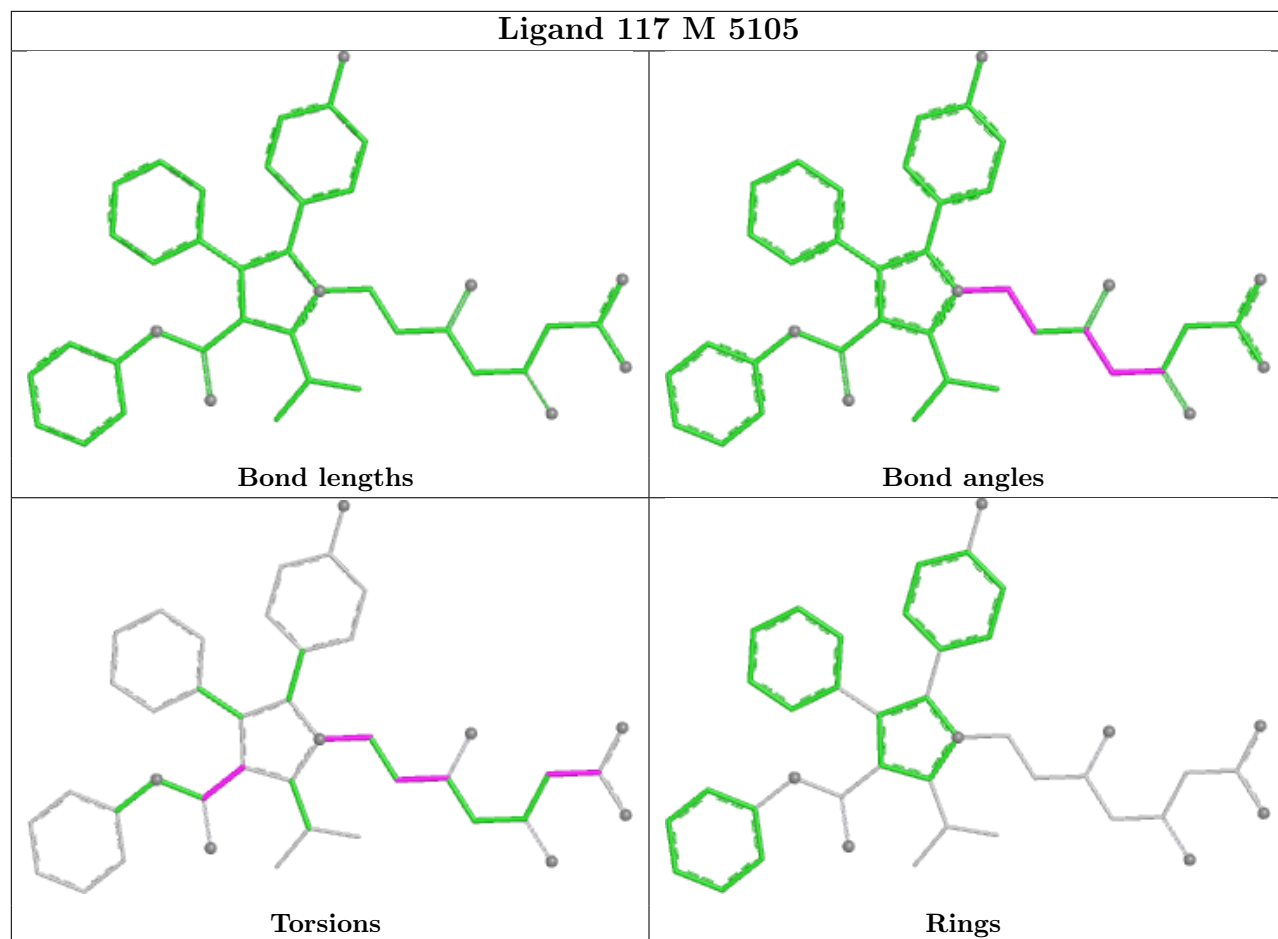


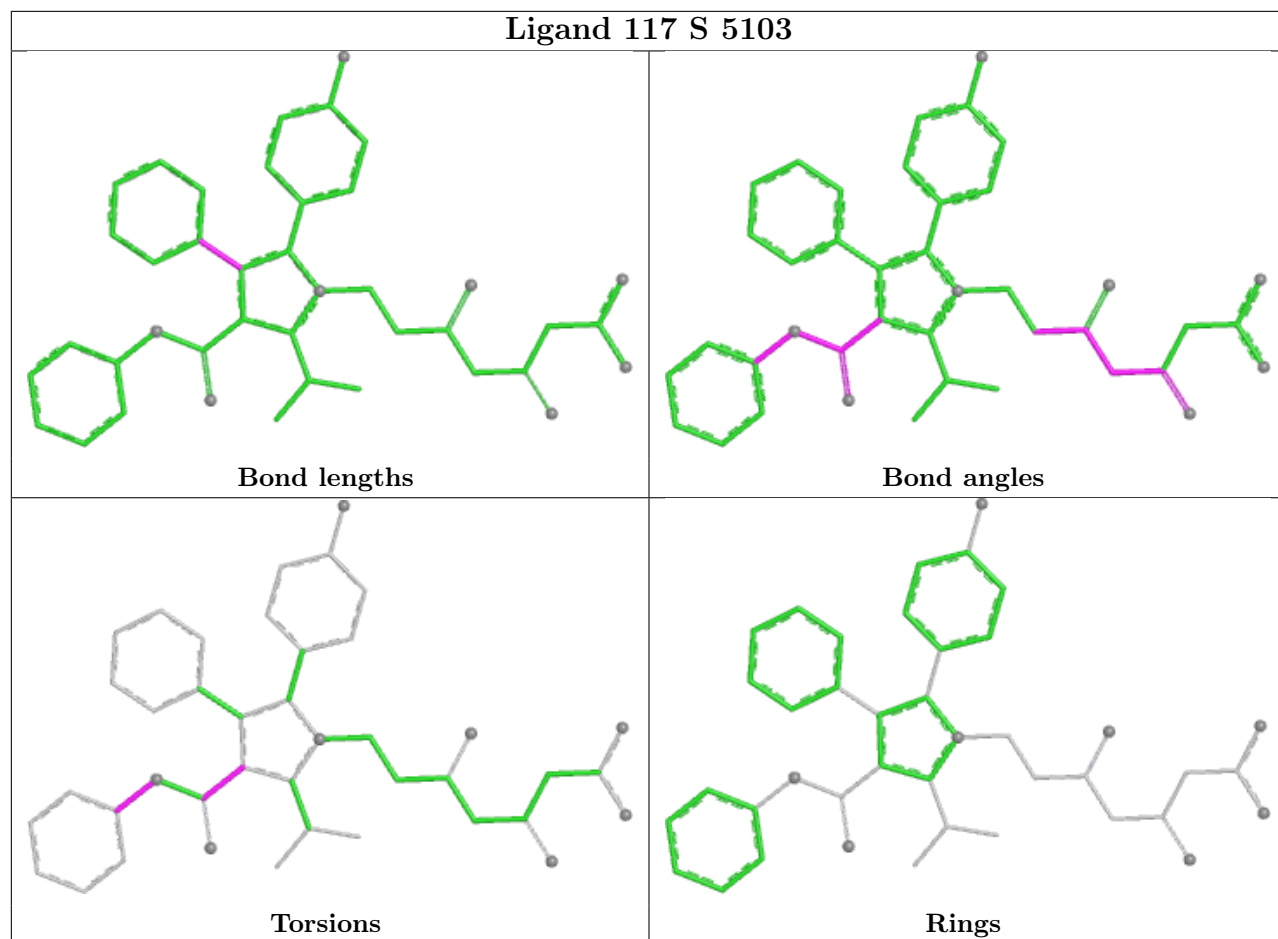


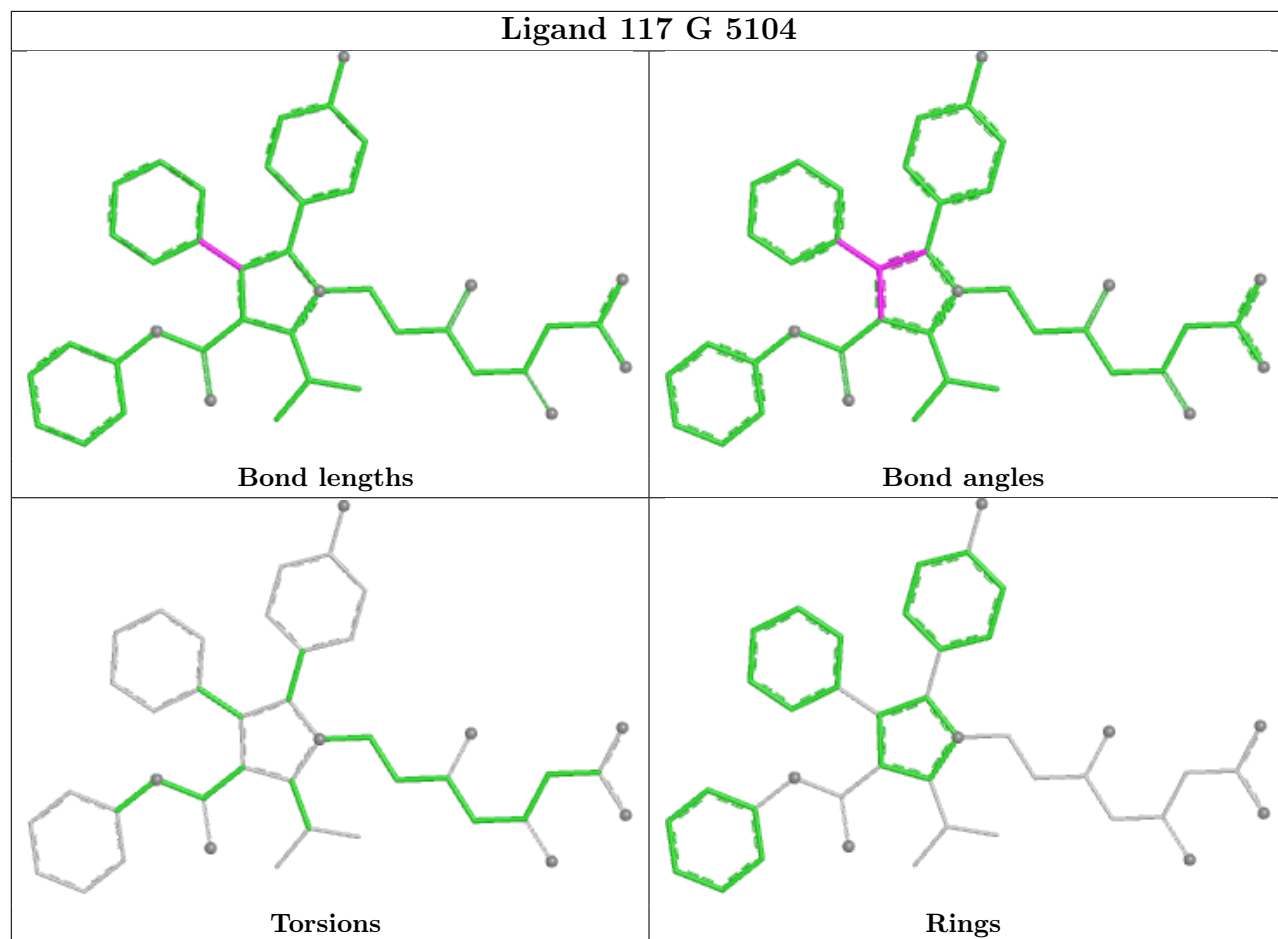


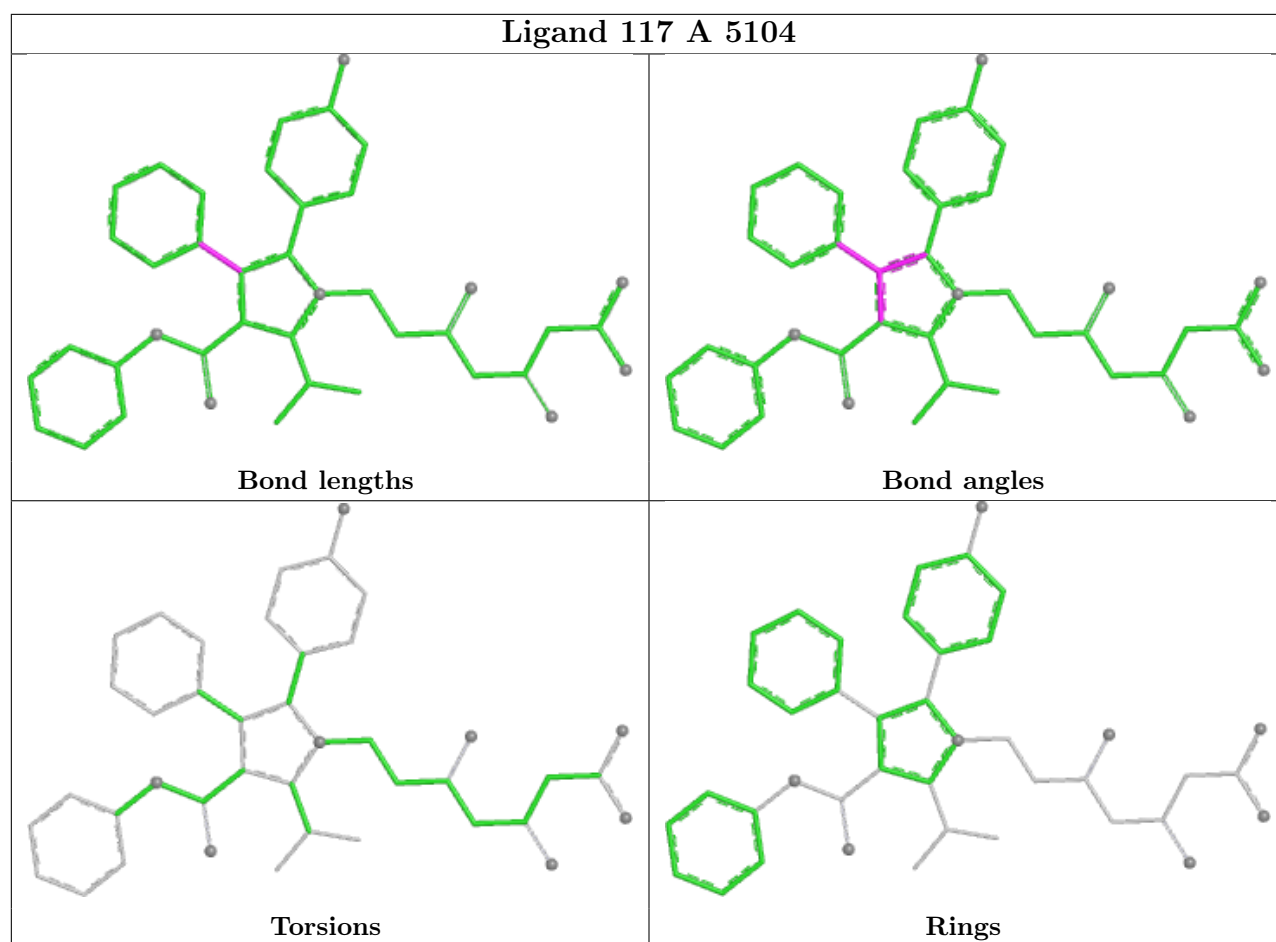












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

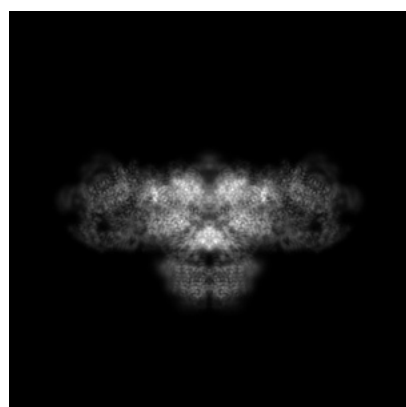
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71924. These allow visual inspection of the internal detail of the map and identification of artifacts.

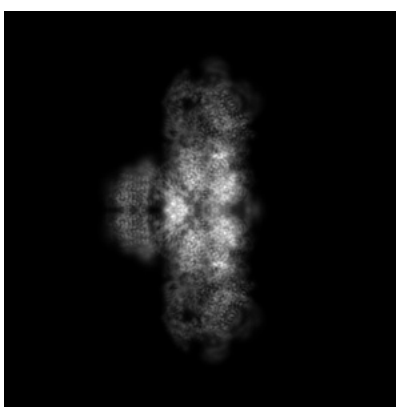
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

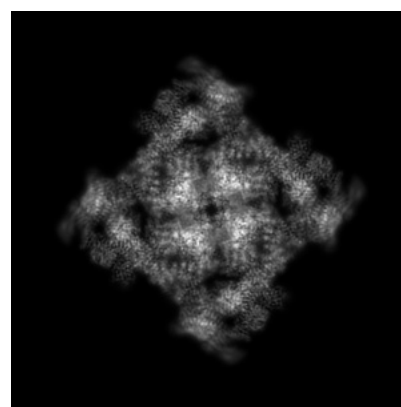
6.1.1 Primary map



X



Y

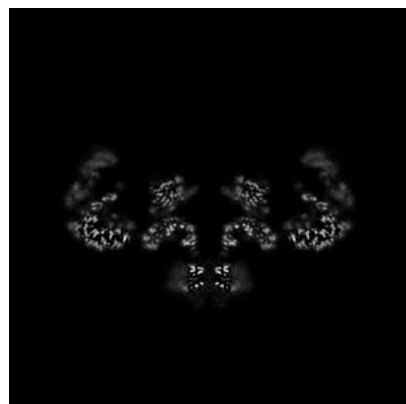


Z

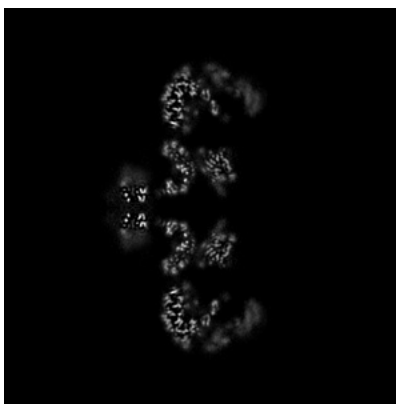
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

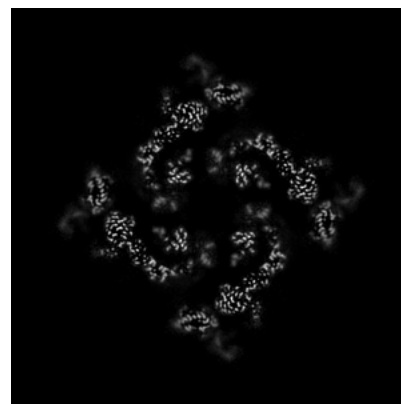
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

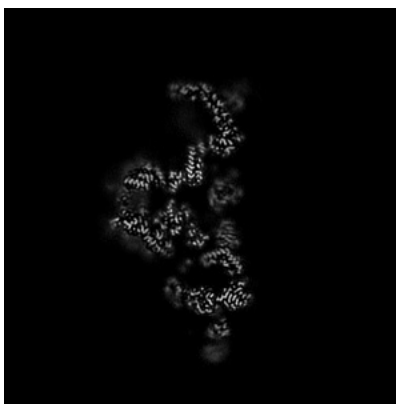
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

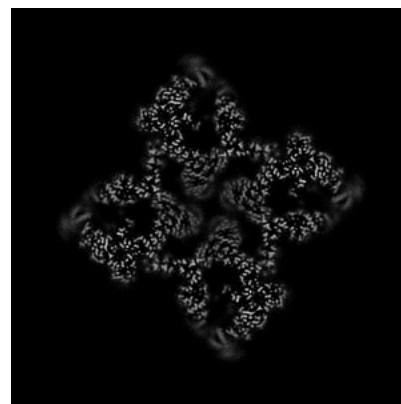
6.3.1 Primary map



X Index: 227



Y Index: 227

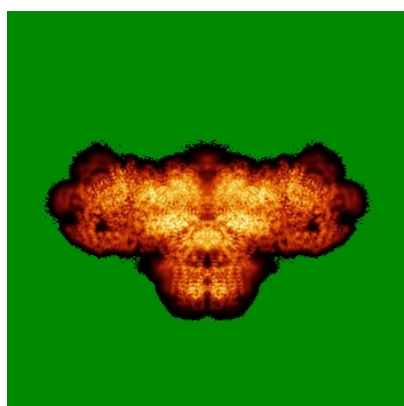


Z Index: 279

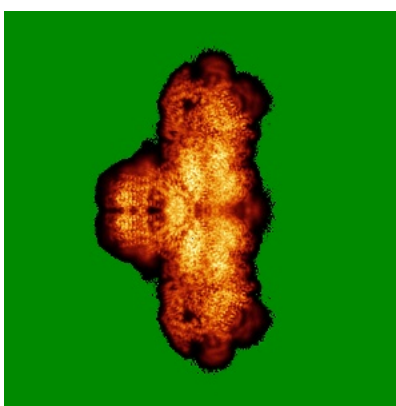
The images above show the largest variance slices of the map in three orthogonal directions.

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

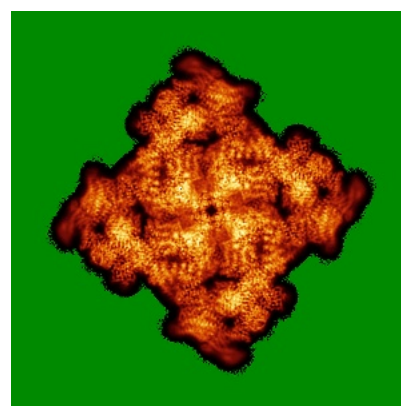
6.4.1 Primary map



X



Y

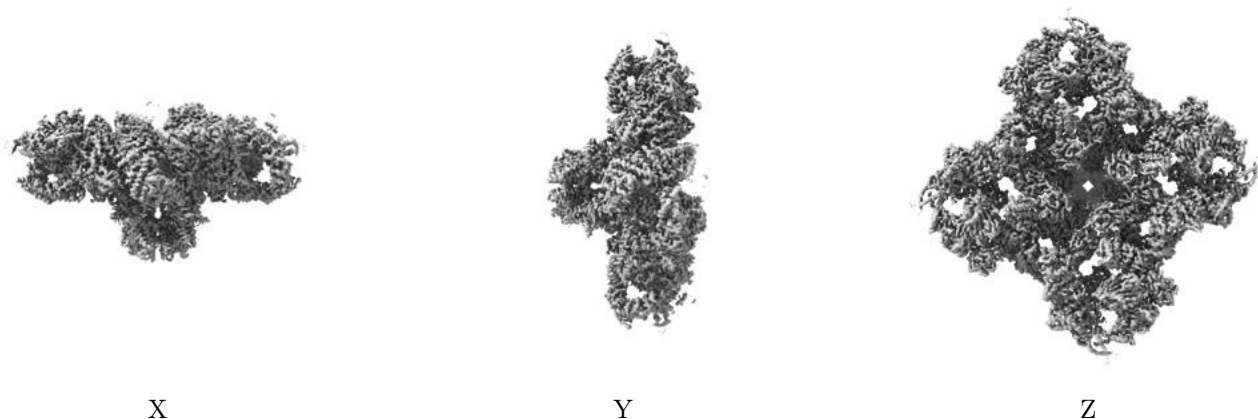


Z

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

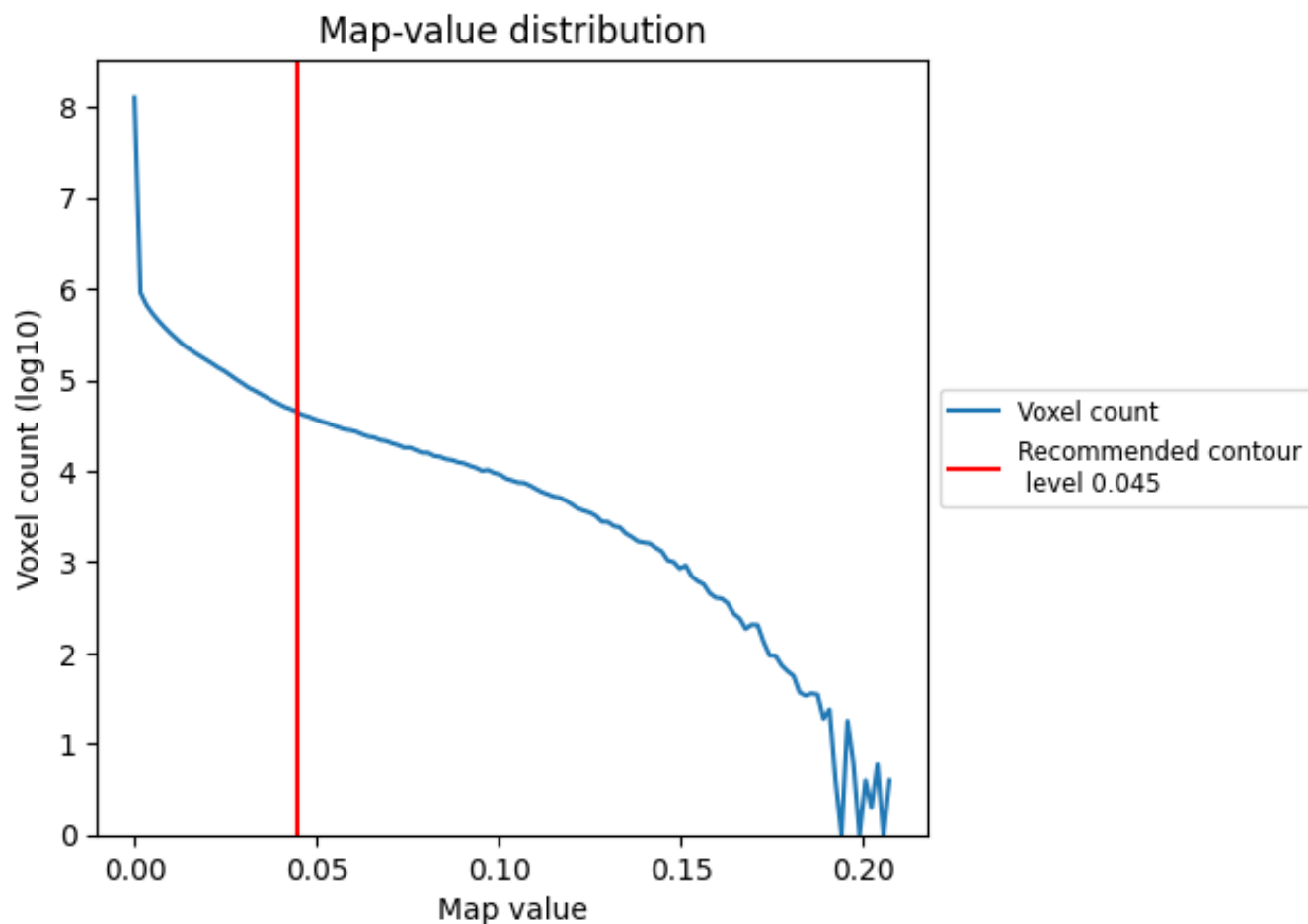
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

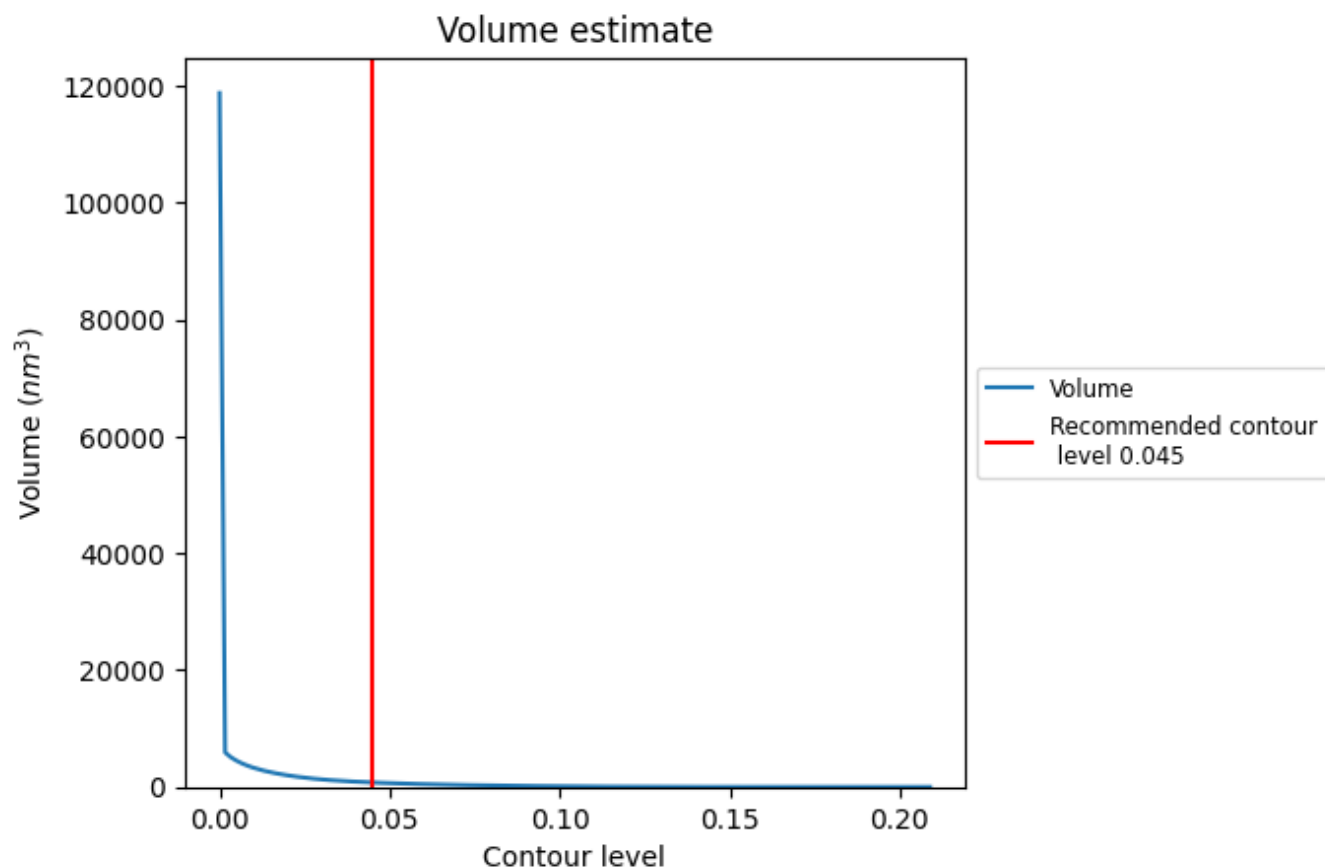
This section contains the results of statistical analysis of the map.

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.

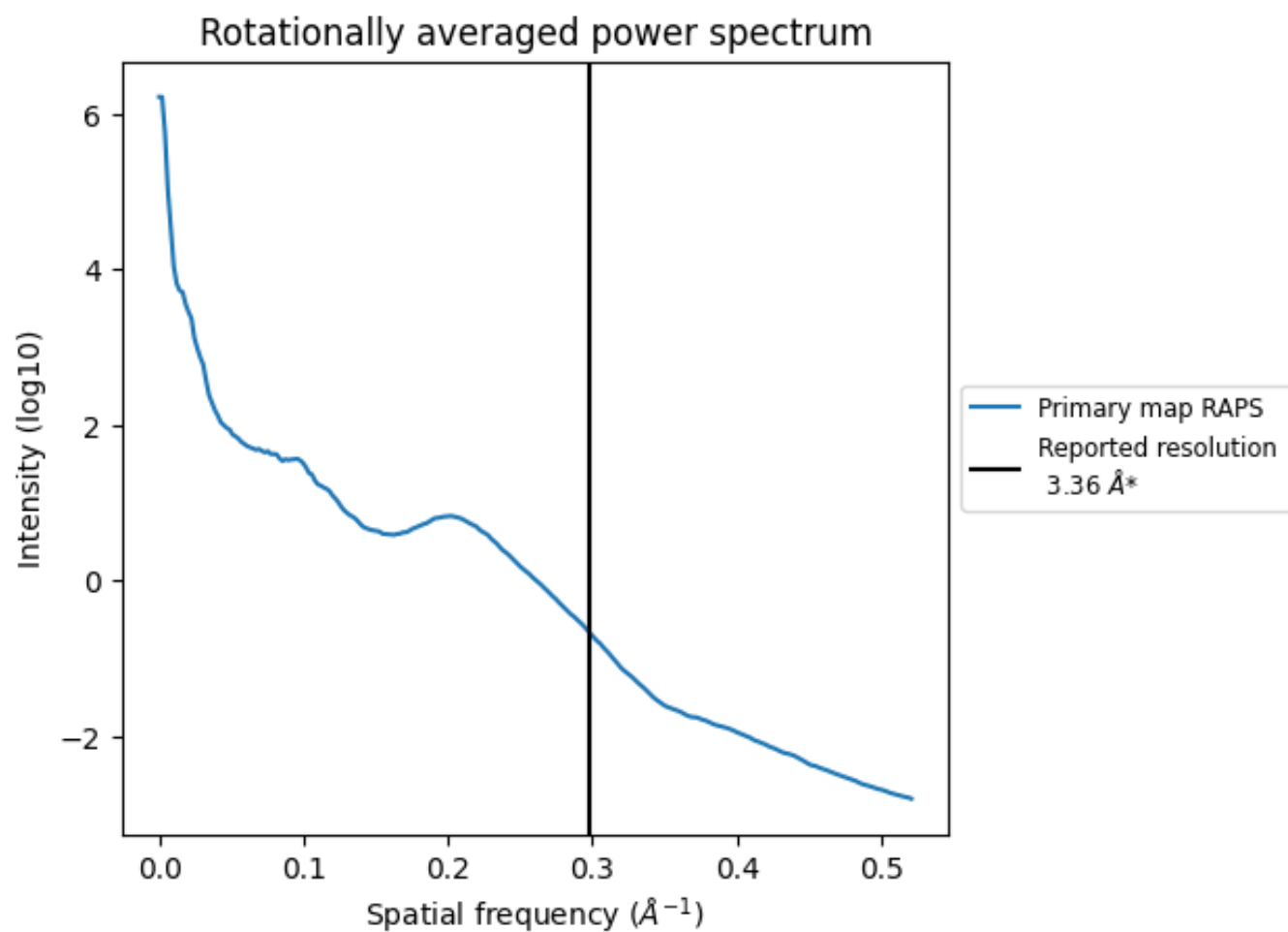
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 765 nm^3 ; this corresponds to an approximate mass of 691 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 0.298 Å⁻¹

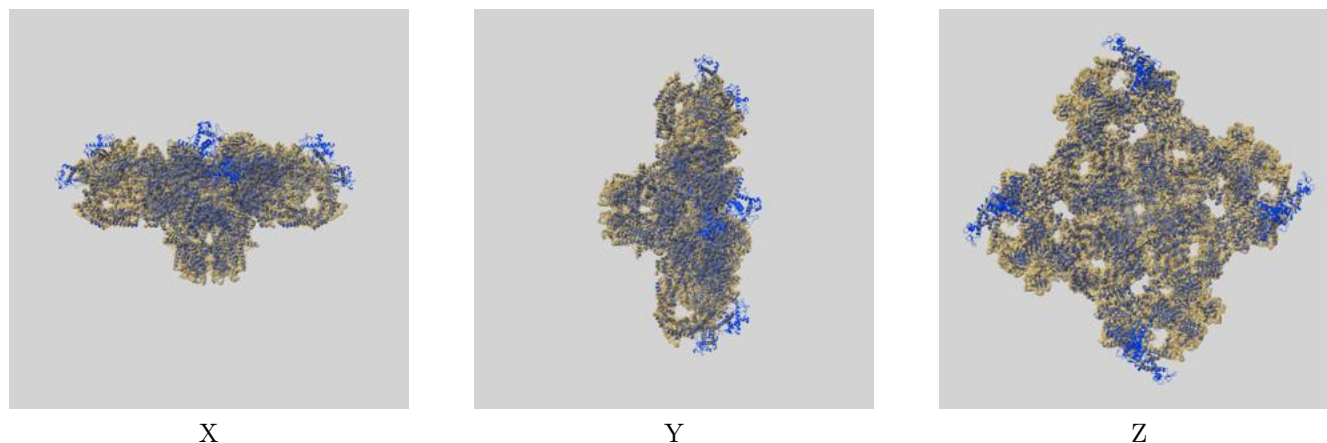
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

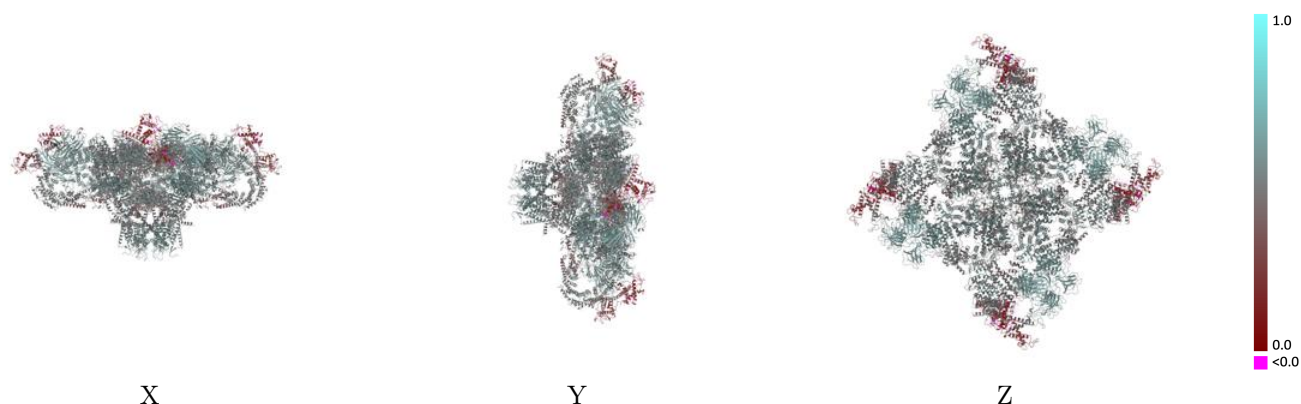
This section contains information regarding the fit between EMDB map EMD-71924 and PDB model 9PWO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



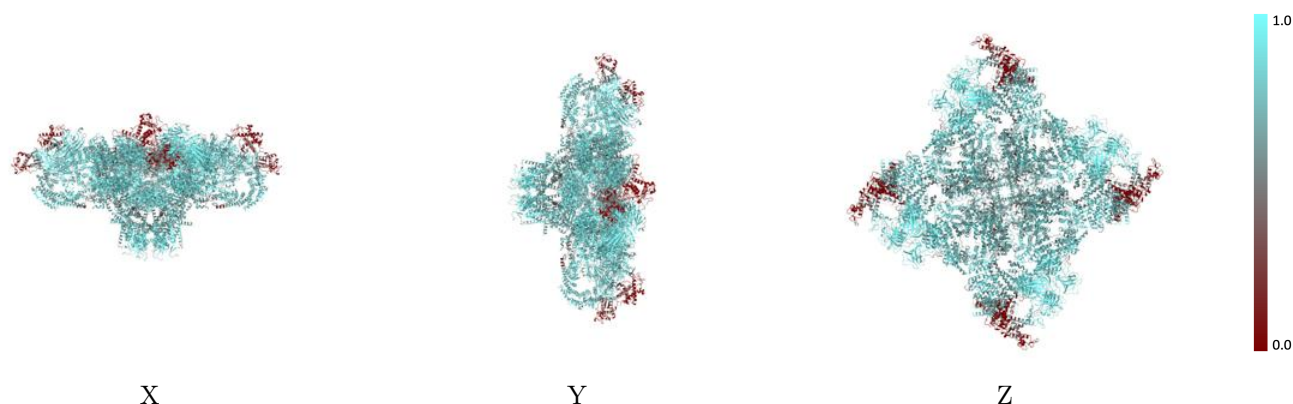
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



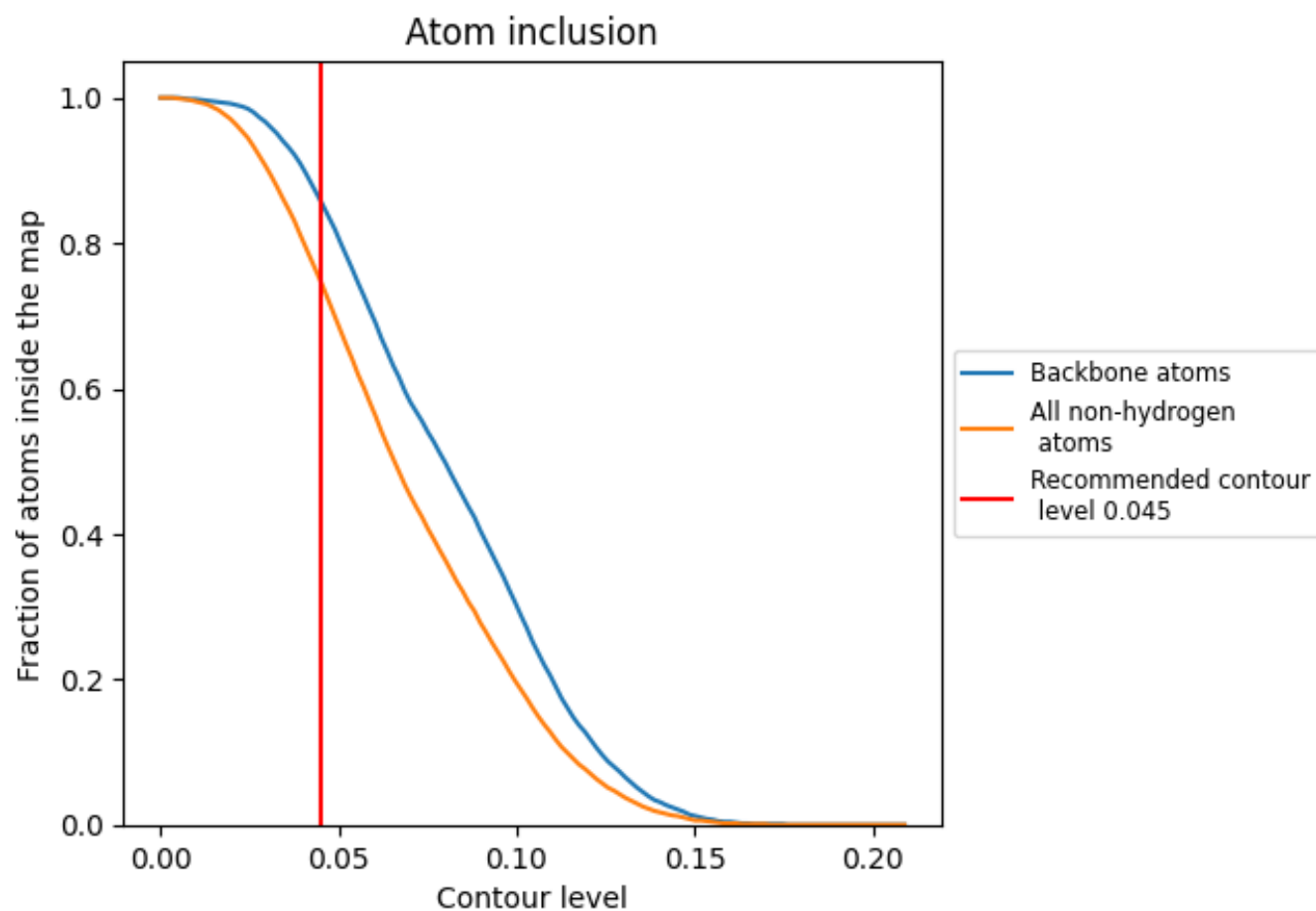
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7470	0.4980
A	0.7440	0.4970
B	0.8630	0.5700
G	0.7430	0.4970
H	0.8630	0.5720
M	0.7440	0.4960
N	0.8630	0.5750
S	0.7440	0.4960
T	0.8630	0.5720

