



Full wwPDB EM Validation Report ⓘ

Nov 8, 2022 – 12:18 AM EST

PDB ID : 6E10
EMDB ID : EMD-8951
Title : PTEX Core Complex in the Engaged (Extended) State
Authors : Ho, C.; Lai, M.; Zhou, Z.H.
Deposited on : 2018-07-08
Resolution : 4.16 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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) : 2.31.2

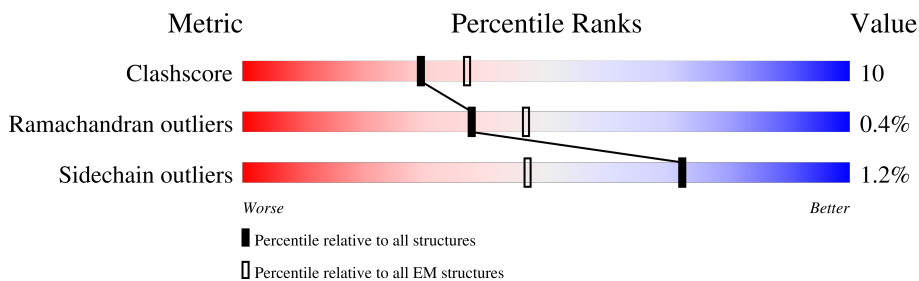
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.16 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 ≥ 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	1	932	
1	2	932	
1	3	932	
1	4	932	
1	5	932	
1	6	932	
2	A	287	
2	B	287	

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Mol	Chain	Length	Quality of chain
2	C	287	
2	D	287	
2	E	287	
2	F	287	
2	G	287	
3	a	207	
3	b	207	
3	c	207	
3	d	207	
3	e	207	
3	f	207	
3	g	207	
3	h	207	
4	0	15	
5	i	58	
5	j	58	
5	k	58	
5	l	58	
5	m	58	
5	n	58	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 57352 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 Heat shock protein 101.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	719	Total	C	N	O	S	0	0
			5763	3693	966	1089	15		
1	2	718	Total	C	N	O	S	0	0
			5759	3691	965	1088	15		
1	3	718	Total	C	N	O	S	0	0
			5759	3691	965	1088	15		
1	4	718	Total	C	N	O	S	0	0
			5759	3691	965	1088	15		
1	5	711	Total	C	N	O	S	0	0
			5701	3654	956	1076	15		
1	6	718	Total	C	N	O	S	0	0
			5759	3691	965	1088	15		

- Molecule 2 is a protein called Exported protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
2	A	189	Total	C	N	O	S	0	0
			1557	1011	269	272	5		
2	G	195	Total	C	N	O	S	0	0
			1604	1039	277	282	6		
2	F	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
2	E	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
2	D	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		
2	C	209	Total	C	N	O	S	0	0
			1715	1107	293	309	6		

- Molecule 3 is a protein called Translocon component PTEX150.

Mol	Chain	Residues	Atoms				AltConf	Trace	
3	a	156	Total	C	N	O	S	0	0
			1287	809	203	274	1		
3	g	156	Total	C	N	O	S	0	0
			1287	809	203	274	1		
3	f	156	Total	C	N	O	S	0	0
			1287	809	203	274	1		
3	e	156	Total	C	N	O	S	0	0
			1287	809	203	274	1		
3	d	156	Total	C	N	O	S	0	0
			1287	809	203	274	1		
3	c	156	Total	C	N	O	S	0	0
			1287	809	203	274	1		
3	b	156	Total	C	N	O	S	0	0
			1287	809	203	274	1		
3	h	50	Total	C	N	O		0	0
			250	150	50	50			

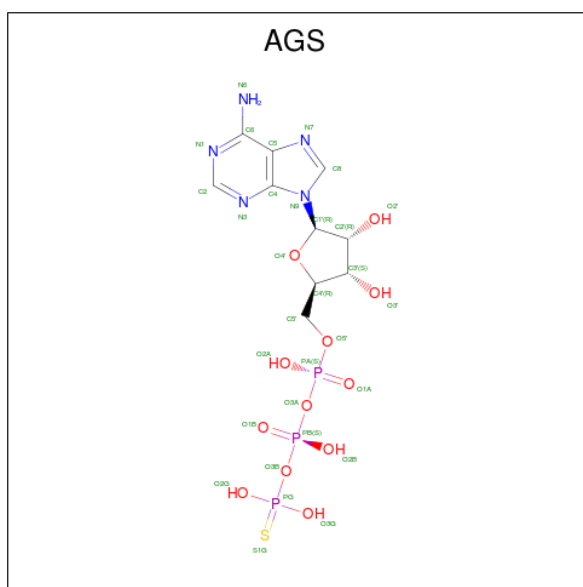
- Molecule 4 is a protein called Endogenous cargo polypeptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	0	15	Total	C	N	O	0	0
			75	45	15	15		

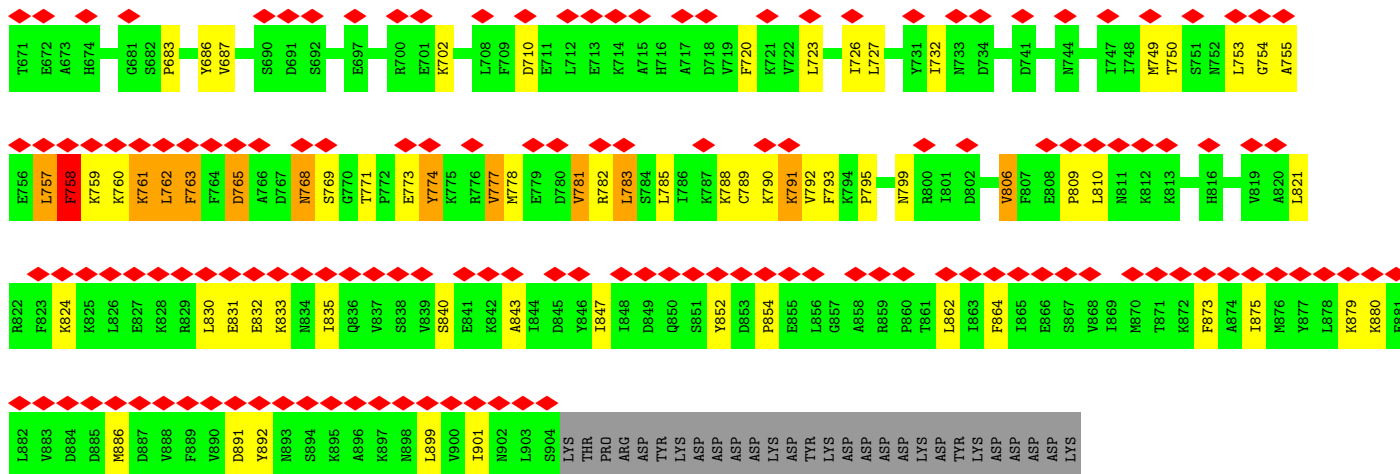
- Molecule 5 is a protein called Unknown (Claw).

Mol	Chain	Residues	Atoms				AltConf	Trace
5	i	46	Total	C	N	O	0	0
			230	138	46	46		
5	j	53	Total	C	N	O	0	0
			265	159	53	53		
5	k	58	Total	C	N	O	0	0
			290	174	58	58		
5	l	57	Total	C	N	O	0	0
			285	171	57	57		
5	m	33	Total	C	N	O	0	0
			165	99	33	33		
5	n	35	Total	C	N	O	0	0
			175	105	35	35		

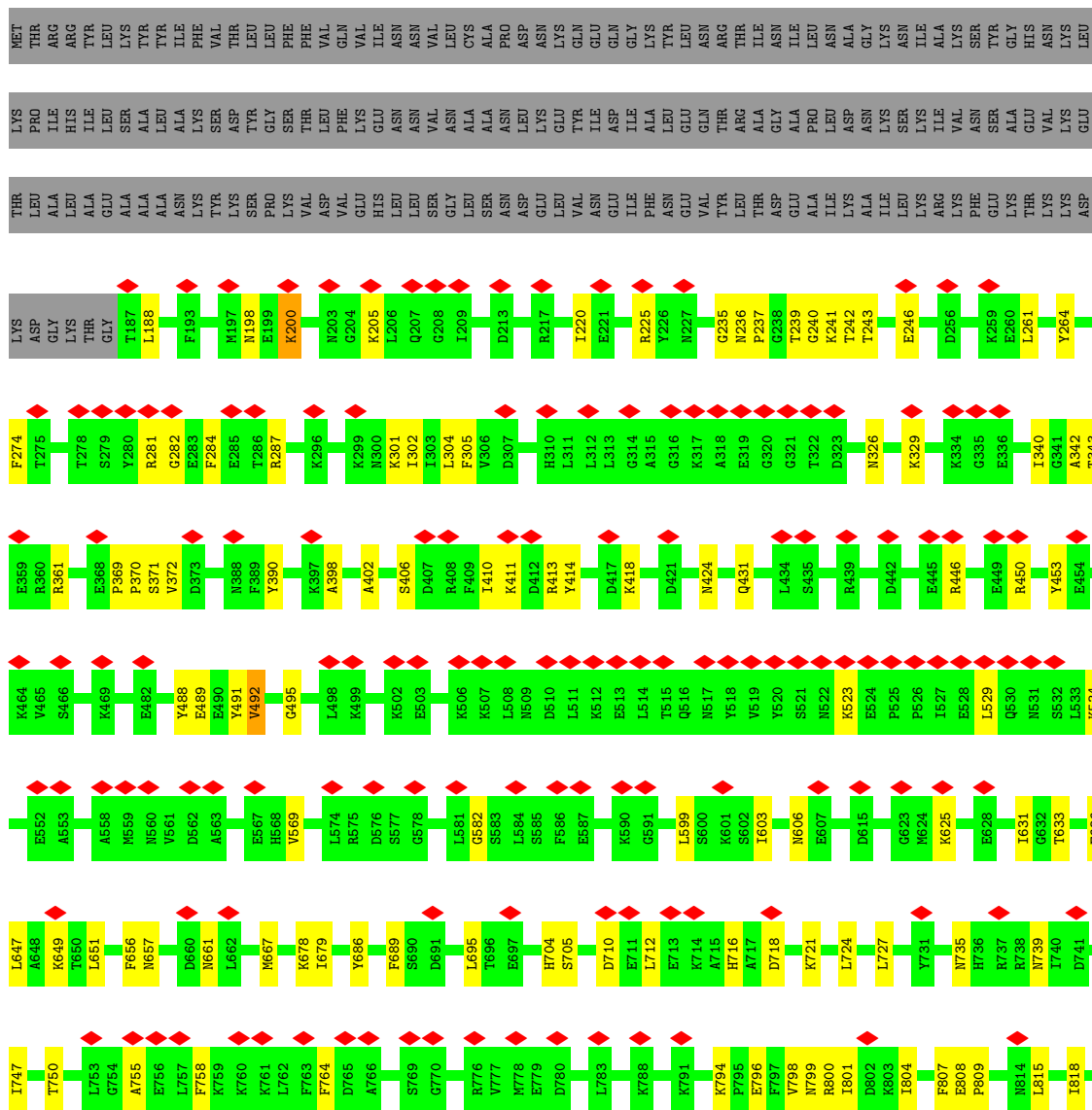
- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).

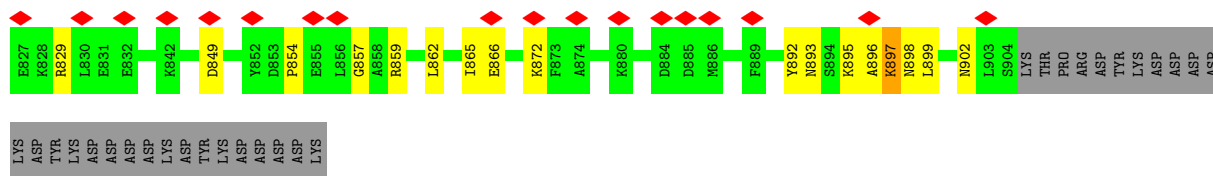


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
6	1	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	1	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	2	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	2	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	3	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	3	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	4	1	Total	C	N	O	P	S	0
			93	30	15	36	9	3	
6	4	1	Total	C	N	O	P	S	0
			93	30	15	36	9	3	
6	4	1	Total	C	N	O	P	S	0
			93	30	15	36	9	3	
6	5	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	6	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
6	6	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

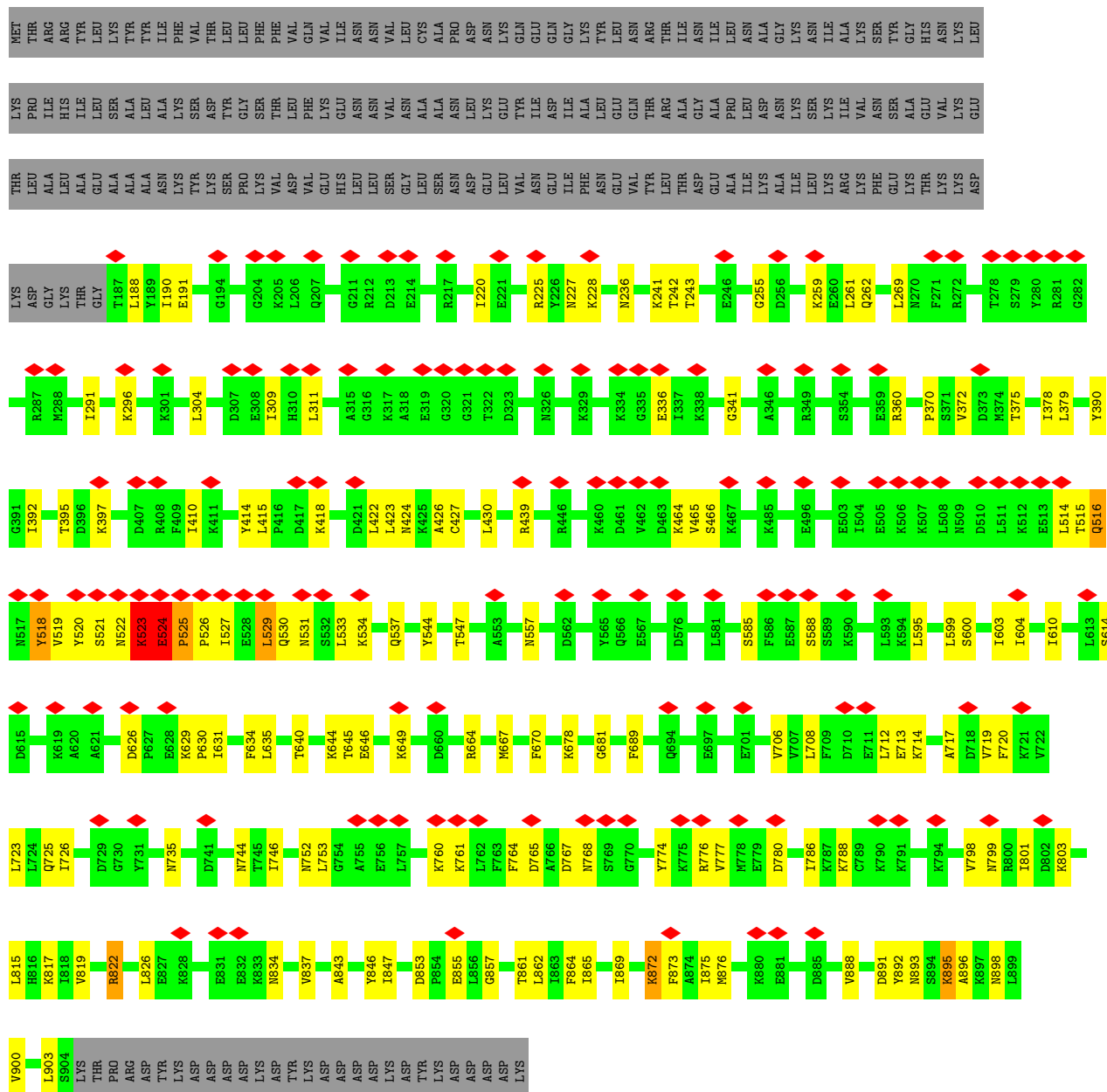


• Molecule 1: Heat shock protein 101



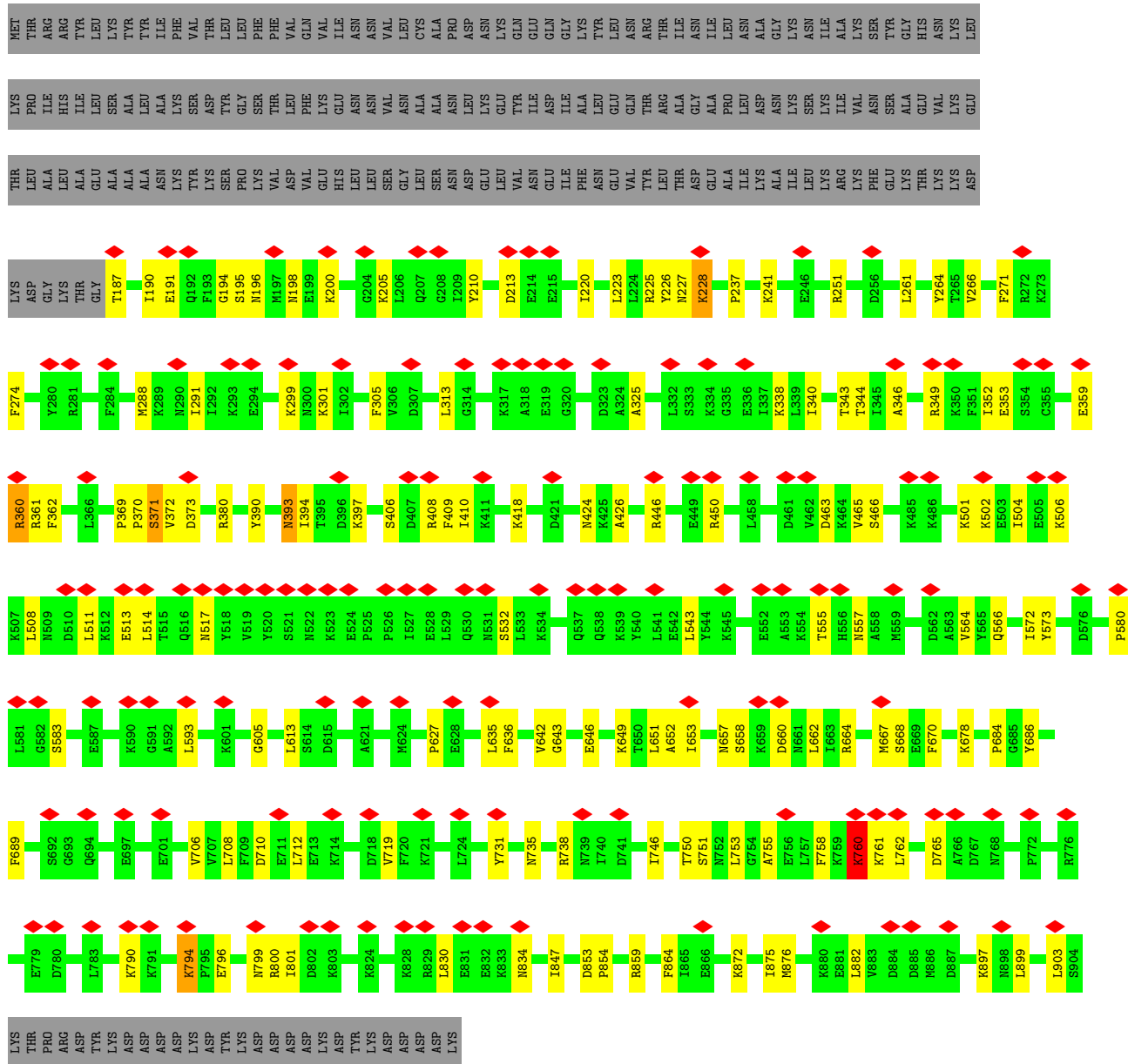


• Molecule 1: Heat shock protein 101

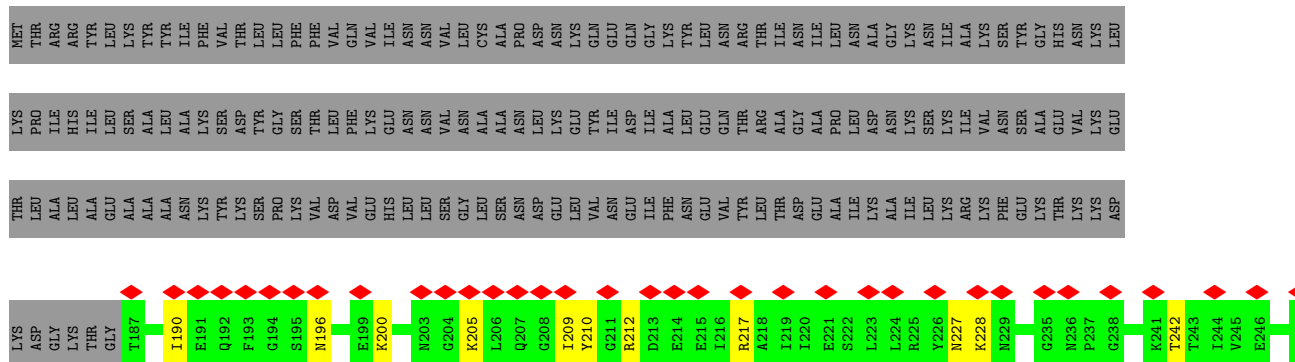


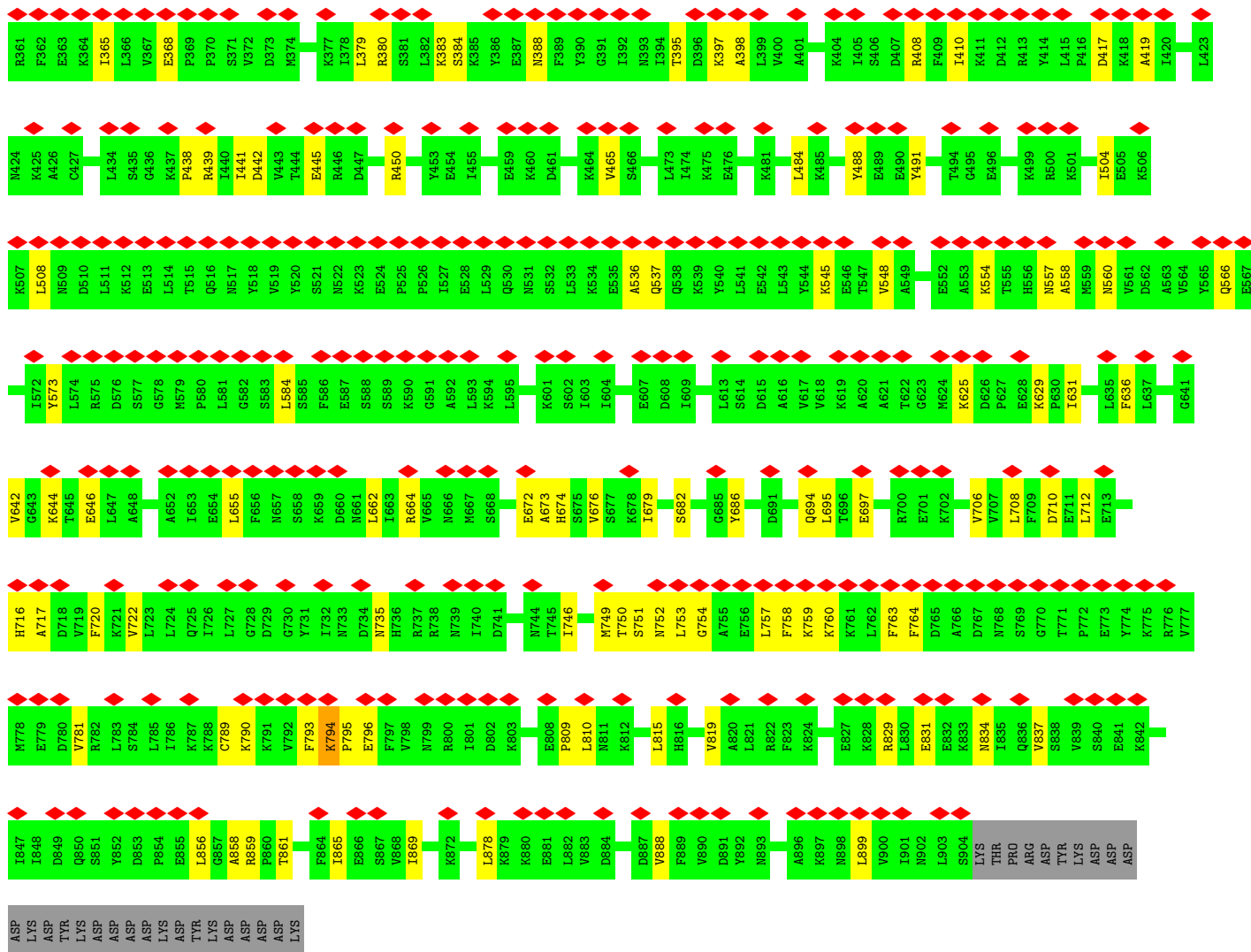
• Molecule 1: Heat shock protein 101



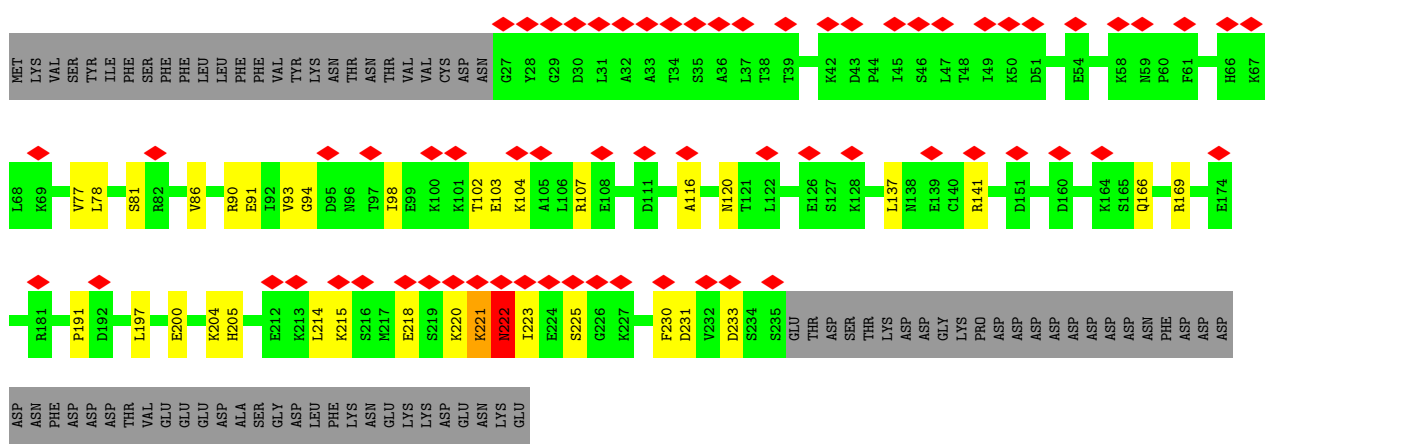


• Molecule 1: Heat shock protein 101





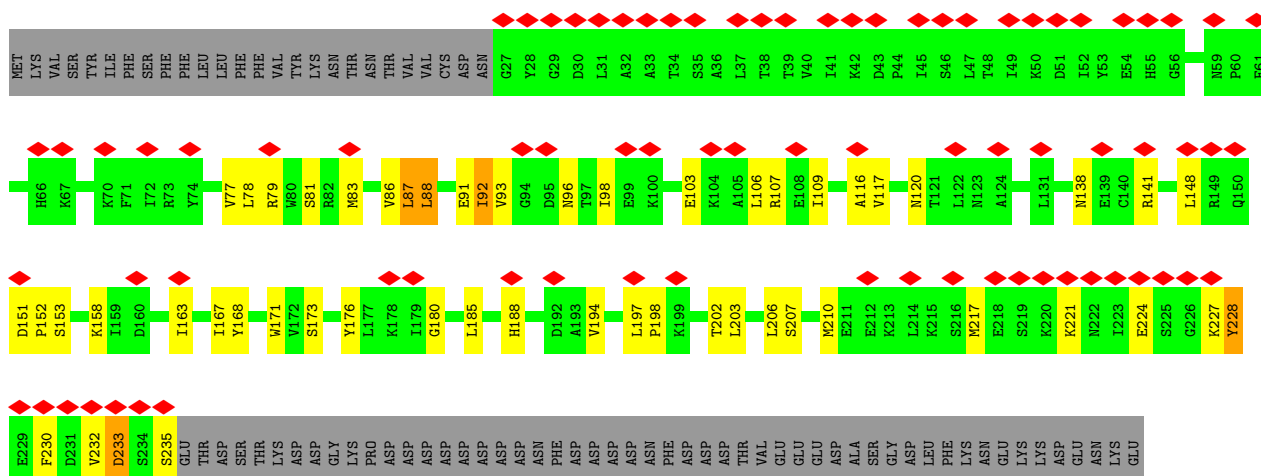
● Molecule 2: Exported protein 2



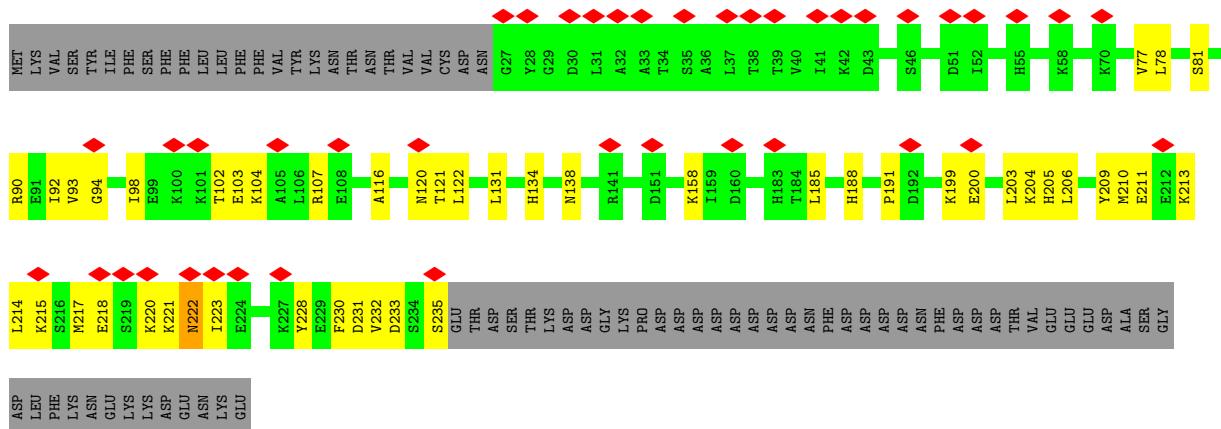
● Molecule 2: Exported protein 2

ASN
LYS
GLU

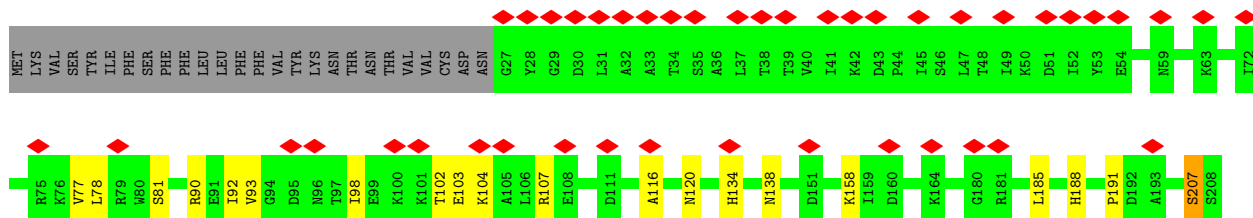
• Molecule 2: Exported protein 2

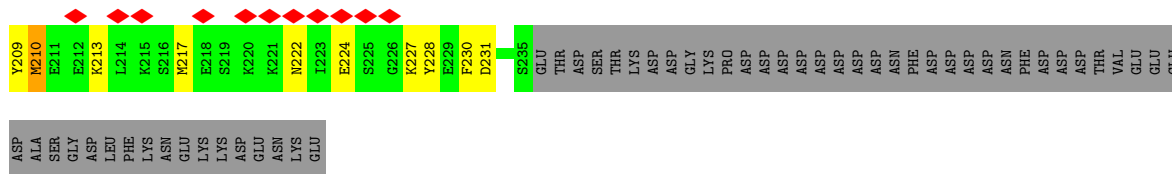


• Molecule 2: Exported protein 2

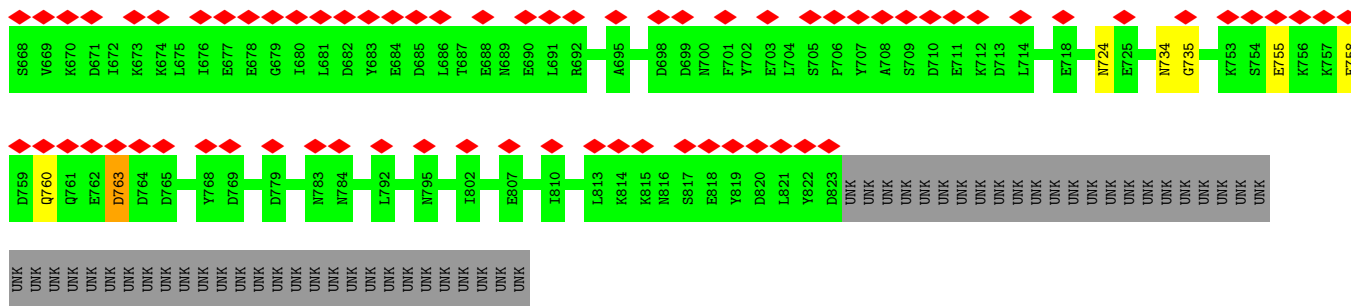


• Molecule 2: Exported protein 2

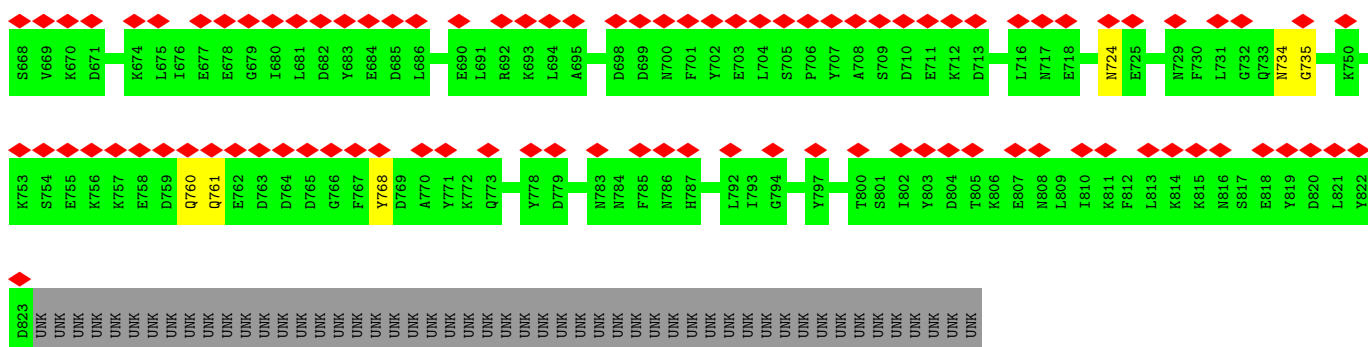
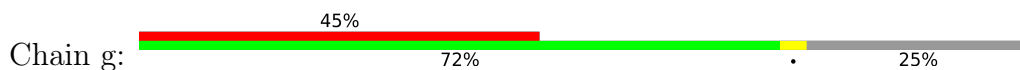




• Molecule 3: Translocon component PTEX150



• Molecule 3: Translocon component PTEX150

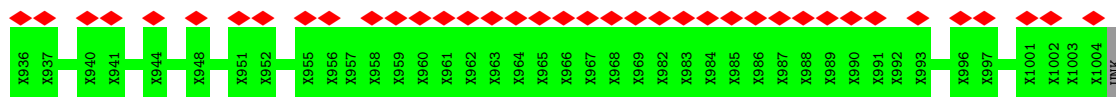


• Molecule 3: Translocon component PTEX150

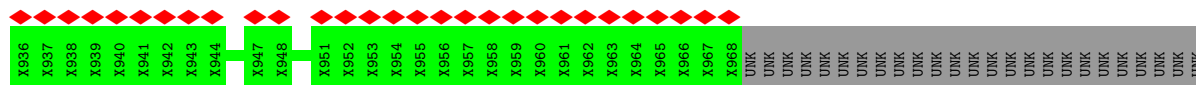


• Molecule 3: Translocon component PTEX150

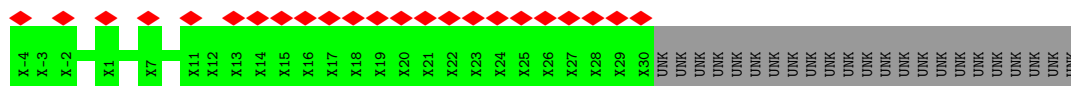
- Molecule 5: Unknown (Claw)



- Molecule 5: Unknown (Claw)



- Molecule 5: Unknown (Claw)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72866	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0424	Depositor
Map size (\AA)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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: AGS

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	1	0.33	1/5854 (0.0%)	0.61	1/7863 (0.0%)
1	2	0.31	0/5850	0.57	1/7858 (0.0%)
1	3	0.33	0/5850	0.60	3/7858 (0.0%)
1	4	0.33	0/5850	0.58	0/7858
1	5	0.33	0/5788	0.55	0/7771
1	6	0.32	0/5850	0.56	0/7858
2	A	0.43	0/1593	0.58	0/2157
2	B	0.47	0/1753	0.64	0/2369
2	C	0.45	0/1753	0.60	0/2369
2	D	0.45	0/1753	0.63	0/2369
2	E	0.46	1/1753 (0.1%)	0.64	0/2369
2	F	0.47	0/1753	0.67	0/2369
2	G	0.42	0/1640	0.57	0/2217
3	a	0.35	0/1311	0.66	0/1764
3	b	0.36	0/1311	0.69	2/1764 (0.1%)
3	c	0.34	0/1311	0.62	0/1764
3	d	0.33	0/1311	0.63	0/1764
3	e	0.34	0/1311	0.64	0/1764
3	f	0.34	0/1311	0.60	0/1764
3	g	0.36	0/1311	0.64	0/1764
All	All	0.36	2/56217 (0.0%)	0.60	7/75633 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	3
1	2	0	3
1	3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	4	0	5
1	5	0	1
2	A	0	1
2	B	0	3
2	C	0	1
2	D	0	1
2	E	0	2
2	G	0	1
3	a	0	2
3	b	0	2
3	c	0	1
3	d	0	2
3	e	0	1
3	f	0	2
3	g	0	2
All	All	0	34

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	809	PRO	N-CD	-6.32	1.39	1.47
2	E	198	PRO	N-CD	5.80	1.55	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	768	TYR	N-CA-CB	8.42	125.75	110.60
3	b	767	PHE	N-CA-C	6.96	129.81	111.00
1	3	873	PHE	N-CA-CB	6.03	121.45	110.60
1	2	240	GLY	N-CA-C	5.26	126.24	113.10
1	3	872	LYS	CB-CA-C	-5.22	99.95	110.40
1	1	500	ARG	N-CA-CB	5.09	119.77	110.60
1	3	777	VAL	N-CA-CB	5.03	122.56	111.50

There are no chirality outliers.

All (34) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	228	LYS	Peptide
1	1	832	GLU	Peptide
1	1	833	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	2	371	SER	Peptide
1	2	414	TYR	Peptide
1	2	794	LYS	Peptide
1	3	414	TYR	Peptide
1	4	228	LYS	Peptide
1	4	371	SER	Peptide
1	4	753	LEU	Peptide
1	4	760	LYS	Peptide
1	4	794	LYS	Peptide
1	5	752	ASN	Peptide
2	A	102	THR	Peptide
2	B	102	THR	Peptide
2	B	221	LYS	Peptide
2	B	222	ASN	Peptide
2	C	102	THR	Peptide
2	D	102	THR	Peptide
2	E	217	MET	Peptide
2	E	221	LYS	Peptide
2	G	102	THR	Peptide
3	a	734	ASN	Peptide
3	a	763	ASP	Peptide
3	b	734	ASN	Peptide
3	b	758	GLU	Peptide
3	c	734	ASN	Peptide
3	d	734	ASN	Peptide
3	d	756	LYS	Peptide
3	e	734	ASN	Peptide
3	f	734	ASN	Peptide
3	f	755	GLU	Mainchain
3	g	734	ASN	Peptide
3	g	760	GLN	Peptide

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	1	5763	0	5968	140	0
1	2	5759	0	5963	119	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	5759	0	5963	129	0
1	4	5759	0	5962	111	0
1	5	5701	0	5911	96	0
1	6	5759	0	5963	88	0
2	A	1557	0	1621	15	0
2	B	1715	0	1767	38	0
2	C	1715	0	1767	25	0
2	D	1715	0	1767	53	0
2	E	1715	0	1767	54	0
2	F	1715	0	1767	41	0
2	G	1604	0	1672	11	0
3	a	1287	0	1211	0	0
3	b	1287	0	1210	0	0
3	c	1287	0	1211	0	0
3	d	1287	0	1210	0	0
3	e	1287	0	1212	0	0
3	f	1287	0	1209	0	0
3	g	1287	0	1213	0	0
3	h	250	0	52	0	0
4	0	75	0	17	10	0
5	i	230	0	50	0	0
5	j	265	0	57	0	0
5	k	290	0	63	0	0
5	l	285	0	64	0	0
5	m	165	0	35	0	0
5	n	175	0	37	0	0
6	1	62	0	24	8	0
6	2	62	0	24	14	0
6	3	62	0	24	11	0
6	4	93	0	36	11	0
6	5	31	0	12	6	0
6	6	62	0	24	7	0
All	All	57352	0	56853	804	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (804) 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)
1:2:489:GLU:O	1:2:492:VAL:HG23	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:224:GLU:HB2	2:E:227:LYS:HB2	1.48	0.95
2:E:168:TYR:HA	2:E:171:TRP:NE1	1.83	0.94
1:1:782:ARG:HH12	2:B:222:ASN:HB3	1.32	0.92
1:1:762:LEU:HD11	1:1:854:PRO:HB3	1.51	0.91
1:3:516:GLN:HA	1:3:516:GLN:NE2	1.87	0.89
1:1:788:LYS:O	1:1:791:LYS:HB3	1.74	0.88
1:1:499:LYS:HE2	1:1:502:LYS:HD2	1.56	0.87
2:E:168:TYR:HA	2:E:171:TRP:CD1	2.11	0.86
2:E:92:ILE:HG21	2:D:122:LEU:HD12	1.55	0.86
1:1:791:LYS:O	1:1:791:LYS:HD3	1.74	0.85
1:3:524:GLU:H	1:3:525:PRO:HD3	1.39	0.85
1:2:237:PRO:O	6:2:1001:AGS:O2G	1.96	0.83
1:2:899:LEU:HB2	2:B:231:ASP:O	1.78	0.82
2:B:90:ARG:NH2	2:B:191:PRO:O	2.13	0.81
1:1:778:MET:O	1:1:781:VAL:HG23	1.79	0.81
1:2:902:ASN:N	2:B:233:ASP:O	2.12	0.81
1:2:488:TYR:O	1:2:492:VAL:HG22	1.80	0.80
1:5:872:LYS:HE2	2:E:230:PHE:HB2	1.63	0.80
1:1:760:LYS:HD2	1:1:760:LYS:O	1.83	0.79
1:3:530:GLN:O	1:3:534:LYS:HG2	1.81	0.79
1:4:853:ASP:OD2	2:D:220:LYS:HB2	1.83	0.79
1:3:524:GLU:H	1:3:525:PRO:CD	1.96	0.79
1:2:898:ASN:O	2:B:230:PHE:HA	1.81	0.78
2:E:138:ASN:OD1	2:E:163:ILE:HD13	1.82	0.77
1:1:499:LYS:CE	1:1:502:LYS:HD2	2.15	0.76
1:1:753:LEU:HD23	1:1:753:LEU:O	1.85	0.76
1:1:762:LEU:CD1	1:1:854:PRO:HB3	2.16	0.76
2:F:209:TYR:CE2	2:F:213:LYS:HD2	2.22	0.75
1:3:891:ASP:O	1:3:900:VAL:HG12	1.87	0.75
1:2:796:GLU:HB2	1:3:640:THR:HG21	1.69	0.75
1:2:796:GLU:CB	1:3:640:THR:HG21	2.18	0.74
1:1:791:LYS:HD3	1:1:791:LYS:C	2.08	0.74
1:5:613:LEU:HD21	1:5:651:LEU:HD11	1.70	0.73
1:3:872:LYS:HD3	1:3:875:ILE:HD11	1.71	0.72
2:E:88:LEU:HD12	2:E:88:LEU:O	1.89	0.72
1:3:527:ILE:N	1:3:527:ILE:HD13	2.03	0.72
1:1:757:LEU:O	1:1:760:LYS:HB3	1.90	0.72
2:E:167:ILE:HD11	2:E:206:LEU:CD2	2.20	0.72
1:2:241:LYS:HE3	1:2:343:THR:O	1.90	0.71
2:F:71:PHE:HE1	2:F:185:LEU:CD2	2.03	0.71
1:2:899:LEU:HA	2:B:230:PHE:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:872:LYS:HG2	2:E:230:PHE:CD2	2.25	0.71
1:3:524:GLU:N	1:3:525:PRO:CD	2.54	0.70
2:B:91:GLU:OE2	2:B:197:LEU:HD12	1.91	0.70
1:2:236:ASN:HB2	1:2:239:THR:HG22	1.74	0.70
1:1:726:ILE:HA	1:1:732:ILE:HD11	1.74	0.70
1:1:243:THR:HG21	6:1:1001:AGS:H2'	1.74	0.70
1:2:893:ASN:HD22	1:2:897:LYS:HD2	1.57	0.70
1:1:637:LEU:N	1:1:637:LEU:HD23	2.07	0.69
1:3:723:LEU:HG	1:3:726:ILE:CG2	2.22	0.69
1:4:735:ASN:O	1:5:694:GLN:NE2	2.25	0.69
1:2:721:LYS:HG2	1:3:714:LYS:HD3	1.74	0.69
1:5:264:TYR:HA	1:5:301:LYS:HB3	1.74	0.69
1:2:236:ASN:HB2	1:2:239:THR:CG2	2.23	0.69
1:1:788:LYS:O	1:1:791:LYS:CB	2.41	0.69
1:3:872:LYS:HA	1:3:875:ILE:HG13	1.75	0.69
1:4:872:LYS:HG2	2:D:230:PHE:CD2	2.28	0.69
2:E:93:VAL:HG21	2:E:98:ILE:HG13	1.73	0.69
1:4:903:LEU:CD2	2:D:235:SER:OG	2.41	0.68
1:5:872:LYS:HE2	2:E:230:PHE:HD2	1.59	0.68
1:3:516:GLN:HA	1:3:516:GLN:HE21	1.59	0.68
1:3:725:GLN:HE21	1:4:668:SER:HB2	1.58	0.68
1:1:862:LEU:HD12	6:1:1002:AGS:O3'	1.93	0.68
1:3:524:GLU:OE1	1:3:524:GLU:HA	1.93	0.68
1:3:634:PHE:CD1	1:3:803:LYS:HB2	2.29	0.68
1:4:872:LYS:HG2	2:D:230:PHE:HD2	1.60	0.67
1:3:723:LEU:HG	1:3:726:ILE:HG22	1.76	0.67
1:1:754:GLY:O	1:1:760:LYS:HB2	1.93	0.67
1:2:686:TYR:CD1	4:0:11:UNK:O	2.48	0.67
2:A:78:LEU:HA	2:A:81:SER:HB3	1.77	0.67
2:E:185:LEU:HB2	2:E:188:HIS:HD2	1.58	0.66
1:1:723:LEU:HD23	1:1:726:ILE:HD12	1.77	0.66
2:C:78:LEU:HA	2:C:81:SER:HB3	1.76	0.66
2:D:78:LEU:HA	2:D:81:SER:HB3	1.76	0.66
2:G:78:LEU:HA	2:G:81:SER:HB3	1.77	0.66
1:1:758:PHE:HB3	1:1:781:VAL:HB	1.78	0.65
1:4:853:ASP:OD1	2:D:220:LYS:HB3	1.96	0.65
1:1:862:LEU:HD23	1:1:862:LEU:O	1.95	0.65
1:2:225:ARG:HD2	1:3:424:ASN:HB3	1.79	0.64
1:4:580:PRO:HG2	1:4:583:SER:HB3	1.79	0.64
2:B:78:LEU:HA	2:B:81:SER:HB3	1.79	0.64
1:5:872:LYS:HE2	2:E:230:PHE:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:PHE:HE1	2:F:185:LEU:HD22	1.62	0.64
1:2:241:LYS:CE	1:2:343:THR:O	2.46	0.64
1:2:329:LYS:HA	1:2:361:ARG:HH12	1.61	0.64
1:5:200:LYS:HD2	1:5:205:LYS:HD2	1.80	0.64
1:5:383:LYS:NZ	1:5:394:ILE:O	2.30	0.64
1:2:411:LYS:HE2	1:2:739:ASN:HD22	1.62	0.64
1:4:511:LEU:HD13	1:4:532:SER:HB2	1.79	0.64
1:3:822:ARG:NH2	6:3:1002:AGS:O3'	2.31	0.64
1:5:872:LYS:HG2	2:E:230:PHE:HD2	1.61	0.64
1:1:332:LEU:HB2	1:1:361:ARG:HD3	1.80	0.64
1:3:888:VAL:HG22	1:3:903:LEU:CD2	2.28	0.64
1:6:625:LYS:HG2	1:6:631:ILE:HG22	1.79	0.64
1:4:664:ARG:HG3	1:4:708:LEU:HD22	1.80	0.63
2:E:152:PRO:HG2	2:D:121:THR:HG22	1.80	0.63
1:2:897:LYS:HG2	1:2:898:ASN:N	2.13	0.63
1:2:243:THR:HG21	6:2:1001:AGS:C5	2.28	0.63
1:2:235:GLY:N	1:2:241:LYS:HZ1	1.96	0.63
1:5:508:LEU:HD11	1:5:539:LYS:HD2	1.81	0.63
2:F:161:GLN:O	2:F:165:SER:OG	2.15	0.63
1:1:753:LEU:HD22	1:1:785:LEU:HD21	1.78	0.63
1:1:778:MET:O	1:1:781:VAL:CG2	2.47	0.62
1:1:635:LEU:HG	1:1:637:LEU:HD21	1.80	0.62
1:3:523:LYS:HD2	1:3:526:PRO:HB3	1.81	0.62
1:4:854:PRO:HD2	2:D:217:MET:CE	2.30	0.62
1:6:445:GLU:OE2	1:6:488:TYR:OH	2.18	0.62
1:3:603:ILE:HD11	1:3:646:GLU:HG3	1.82	0.62
1:4:800:ARG:NH1	6:5:1001:AGS:S1G	2.72	0.62
1:1:777:VAL:O	1:1:781:VAL:HG22	1.98	0.62
1:3:515:THR:HG22	1:3:515:THR:O	2.00	0.62
2:F:79:ARG:HD2	2:F:180:GLY:O	2.00	0.62
2:C:210:MET:CE	2:C:210:MET:HA	2.30	0.62
2:D:232:VAL:HG23	2:D:232:VAL:O	2.00	0.61
1:4:899:LEU:HD11	2:D:233:ASP:OD2	2.01	0.61
1:6:679:ILE:HG23	1:6:695:LEU:HD22	1.81	0.61
1:4:642:VAL:O	6:4:1002:AGS:O1A	2.19	0.61
1:4:864:PHE:HD1	2:D:223:ILE:HG21	1.64	0.61
2:F:90:ARG:NH2	2:F:191:PRO:O	2.33	0.61
1:4:670:PHE:HB3	1:4:719:VAL:HG21	1.83	0.61
2:B:223:ILE:HG12	2:B:225:SER:H	1.65	0.61
1:3:786:ILE:HG21	2:D:221:LYS:HG3	1.83	0.61
2:E:152:PRO:HG2	2:D:121:THR:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:237:PRO:O	6:4:1001:AGS:O2G	2.19	0.61
2:E:152:PRO:HB2	2:D:131:LEU:HB3	1.81	0.61
1:6:271:PHE:HA	1:6:274:PHE:HD2	1.66	0.60
1:2:523:LYS:HG2	1:2:529:LEU:HD22	1.83	0.60
1:3:664:ARG:HA	1:3:708:LEU:HB2	1.83	0.60
1:4:636:PHE:HB2	1:4:750:THR:HG22	1.84	0.60
1:6:504:ILE:HG23	1:6:536:ALA:HB1	1.83	0.60
1:1:755:ALA:O	1:1:760:LYS:HG2	2.02	0.60
1:1:790:LYS:HG2	1:1:795:PRO:HB3	1.83	0.60
1:1:791:LYS:HD2	1:1:792:VAL:HG23	1.82	0.60
1:1:272:ARG:HG2	1:1:273:LYS:HD2	1.84	0.60
1:5:309:ILE:HD11	1:5:341:GLY:HA3	1.82	0.60
1:2:724:LEU:O	1:2:800:ARG:NH1	2.35	0.60
1:2:898:ASN:O	2:B:230:PHE:CA	2.48	0.60
1:1:225:ARG:HH21	1:2:424:ASN:HB3	1.66	0.60
1:1:233:LEU:CD2	1:1:241:LYS:HB2	2.32	0.60
2:G:90:ARG:NH2	2:G:191:PRO:O	2.35	0.60
1:1:252:ILE:HD13	1:1:257:VAL:HG11	1.84	0.60
1:3:667:MET:HG2	1:3:712:LEU:HD23	1.84	0.60
1:5:713:GLU:HG3	1:5:714:LYS:HD2	1.84	0.60
1:1:774:TYR:CE1	1:1:778:MET:SD	2.95	0.59
1:4:264:TYR:HA	1:4:301:LYS:HB3	1.84	0.59
1:6:439:ARG:NH2	1:6:557:ASN:OD1	2.34	0.59
1:6:686:TYR:HA	4:0:3:UNK:O	2.02	0.59
1:1:765:ASP:HB3	2:A:213:LYS:NZ	2.17	0.59
1:1:773:GLU:OE1	1:1:773:GLU:HA	2.01	0.59
1:1:437:LYS:HD3	1:1:441:ILE:HD12	1.83	0.59
1:2:895:LYS:O	1:2:896:ALA:HB3	2.03	0.59
1:5:639:PRO:O	1:5:644:LYS:NZ	2.33	0.59
1:3:872:LYS:HG3	2:C:230:PHE:CD2	2.36	0.59
2:D:94:GLY:O	2:D:204:LYS:NZ	2.31	0.59
1:3:723:LEU:O	1:3:726:ILE:HG22	2.03	0.59
1:5:712:LEU:HD11	1:5:749:MET:HB3	1.85	0.59
2:A:90:ARG:NH2	2:A:191:PRO:O	2.36	0.59
2:F:137:LEU:HD11	2:F:171:TRP:CZ3	2.38	0.59
1:1:233:LEU:HD23	1:1:241:LYS:HB2	1.85	0.58
1:1:642:VAL:HG12	1:1:810:LEU:HG	1.84	0.58
2:C:90:ARG:NH2	2:C:191:PRO:O	2.35	0.58
1:3:670:PHE:HB3	1:3:719:VAL:HG21	1.85	0.58
1:6:438:PRO:HG2	1:6:441:ILE:HD12	1.85	0.58
2:D:214:LEU:O	2:D:218:GLU:N	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:606:ASN:HD21	1:2:808:GLU:H	1.50	0.58
1:2:899:LEU:CB	2:B:231:ASP:O	2.49	0.58
1:6:676:VAL:CG2	1:6:722:VAL:HG21	2.34	0.58
1:2:872:LYS:HG3	2:B:230:PHE:HE1	1.67	0.58
1:3:640:THR:HG22	6:3:1002:AGS:S1G	2.44	0.58
1:4:760:LYS:O	1:4:762:LEU:N	2.36	0.58
1:6:673:ALA:HB2	1:6:716:HIS:CE1	2.38	0.58
1:1:277:GLY:HA3	1:1:287:ARG:HE	1.67	0.58
2:D:90:ARG:NH2	2:D:191:PRO:O	2.36	0.58
1:5:686:TYR:HA	4:0:5:UNK:O	2.04	0.57
2:F:78:LEU:HA	2:F:81:SER:HB3	1.86	0.57
1:1:862:LEU:HD23	1:1:862:LEU:C	2.25	0.57
1:6:408:ARG:NH2	1:6:625:LYS:O	2.34	0.57
1:3:706:VAL:HG12	1:3:746:ILE:HB	1.86	0.57
1:1:309:ILE:HD11	1:1:362:PHE:CZ	2.40	0.57
1:2:667:MET:HG2	1:2:712:LEU:HD23	1.86	0.57
2:E:78:LEU:HA	2:E:81:SER:HB3	1.86	0.57
2:F:86:VAL:CG1	2:F:194:VAL:HG21	2.35	0.57
1:1:835:ILE:HA	1:1:886:MET:HB2	1.86	0.57
1:2:243:THR:HG21	6:2:1001:AGS:C6	2.35	0.57
1:3:649:LYS:HE2	1:3:664:ARG:HH22	1.69	0.57
1:5:604:ILE:H	6:5:1001:AGS:H2	1.69	0.57
1:1:727:LEU:HD11	1:1:749:MET:HE1	1.87	0.56
1:2:796:GLU:CG	1:3:640:THR:HG21	2.35	0.56
1:4:706:VAL:HG12	1:4:746:ILE:HB	1.86	0.56
1:4:712:LEU:HB3	1:4:751:SER:HB3	1.87	0.56
1:3:518:TYR:HD2	1:3:518:TYR:O	1.88	0.56
1:1:381:SER:HA	1:2:453:TYR:HE2	1.71	0.56
1:3:603:ILE:CD1	1:3:646:GLU:HG3	2.34	0.56
2:D:220:LYS:HG3	2:D:221:LYS:HG2	1.85	0.56
1:2:264:TYR:HA	1:2:301:LYS:HB3	1.88	0.56
1:3:717:ALA:HA	1:3:720:PHE:HD2	1.71	0.56
1:4:446:ARG:HB3	1:4:450:ARG:HH12	1.69	0.56
1:3:634:PHE:CE1	1:3:803:LYS:HB2	2.39	0.56
1:5:217:ARG:HH21	1:6:442:ASP:HB3	1.69	0.56
1:5:796:GLU:OE2	1:6:752:ASN:ND2	2.39	0.56
2:F:86:VAL:HG11	2:F:194:VAL:HG21	1.87	0.56
2:F:214:LEU:O	2:F:218:GLU:N	2.38	0.56
1:3:600:SER:HA	1:3:603:ILE:O	2.05	0.56
1:4:605:GLY:HA2	6:4:1002:AGS:HN62	1.69	0.56
1:1:212:ARG:NE	1:1:244:ILE:HD11	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:394:ILE:HA	1:5:564:VAL:HG12	1.87	0.56
1:6:384:SER:O	1:6:388:ASN:ND2	2.39	0.56
1:6:644:LYS:NZ	6:6:1002:AGS:O3G	2.32	0.56
1:2:271:PHE:HA	1:2:274:PHE:HD2	1.71	0.56
1:5:606:ASN:HD21	1:5:808:GLU:H	1.54	0.56
1:1:441:ILE:HG23	1:1:488:TYR:HE1	1.70	0.56
1:4:664:ARG:NH2	1:4:710:ASP:OD2	2.39	0.56
1:5:582:GLY:O	1:5:657:ASN:ND2	2.39	0.56
1:1:382:LEU:HG	1:1:385:LYS:HD2	1.86	0.55
1:4:899:LEU:HD11	2:D:233:ASP:CG	2.25	0.55
1:3:822:ARG:HG2	1:3:862:LEU:HD22	1.89	0.55
1:1:505:GLU:HA	1:1:509:ASN:HD22	1.71	0.55
1:2:849:ASP:O	2:B:220:LYS:HE3	2.05	0.55
1:2:892:TYR:CD1	1:2:897:LYS:O	2.59	0.55
1:4:864:PHE:CD1	2:D:223:ILE:HG21	2.42	0.55
1:2:646:GLU:OE1	6:2:1002:AGS:O2'	2.22	0.55
1:4:686:TYR:HA	4:0:7:UNK:O	2.06	0.55
1:4:876:MET:HG2	1:4:882:LEU:HG	1.87	0.55
2:E:167:ILE:HD11	2:E:206:LEU:HD22	1.88	0.55
1:1:710:ASP:O	1:1:750:THR:OG1	2.20	0.55
1:2:305:PHE:HD1	1:2:340:ILE:HB	1.70	0.55
1:2:489:GLU:HA	1:2:492:VAL:CG2	2.37	0.55
1:4:198:ASN:HD21	1:4:266:VAL:H	1.54	0.55
2:B:94:GLY:O	2:B:204:LYS:NZ	2.30	0.55
1:1:499:LYS:CD	1:1:502:LYS:HD2	2.37	0.55
2:F:87:LEU:HD21	2:F:176:TYR:HE1	1.72	0.55
1:3:846:TYR:OH	2:C:228:TYR:CE1	2.59	0.55
1:6:219:ILE:HG12	1:6:365:ILE:HD13	1.89	0.55
1:6:646:GLU:HG3	6:6:1002:AGS:H2'	1.88	0.55
2:F:137:LEU:HB3	2:F:163:ILE:HD11	1.88	0.55
1:1:236:ASN:HB2	1:1:239:THR:HG23	1.89	0.54
1:4:200:LYS:HB3	1:4:205:LYS:HB2	1.89	0.54
1:2:686:TYR:HD1	4:0:11:UNK:O	1.90	0.54
1:4:658:SER:OG	1:4:660:ASP:OD1	2.25	0.54
1:5:683:PRO:HG3	1:6:674:HIS:CD2	2.42	0.54
2:G:104:LYS:HG2	2:G:107:ARG:HH21	1.71	0.54
1:3:309:ILE:HD11	1:3:341:GLY:HA3	1.90	0.54
1:5:360:ARG:NH2	1:6:417:ASP:OD2	2.40	0.54
2:F:87:LEU:HD21	2:F:176:TYR:CE1	2.43	0.54
1:4:799:ASN:HB3	1:5:859:ARG:HG3	1.89	0.54
1:1:499:LYS:HE2	1:1:502:LYS:CD	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:852:TYR:HE2	1:1:854:PRO:HG3	1.71	0.54
1:3:855:GLU:H	2:C:217:MET:HE1	1.72	0.54
2:F:86:VAL:HG11	2:F:194:VAL:CG2	2.38	0.54
2:C:224:GLU:HB2	2:C:227:LYS:HB2	1.90	0.54
1:1:448:ILE:HG23	1:1:449:GLU:HG2	1.90	0.54
1:1:821:LEU:HD23	1:1:824:LYS:HD2	1.89	0.54
1:1:840:SER:H	1:1:843:ALA:HB3	1.73	0.54
6:4:1003:AGS:O2B	1:5:242:THR:OG1	2.25	0.54
1:1:499:LYS:HD2	1:1:502:LYS:HB3	1.88	0.53
1:3:464:LYS:HG3	1:3:466:SER:H	1.73	0.53
1:3:872:LYS:CD	1:3:875:ILE:HD11	2.37	0.53
1:2:269:LEU:HD21	1:2:304:LEU:HD22	1.90	0.53
1:3:585:SER:O	1:3:588:SER:OG	2.25	0.53
2:D:104:LYS:HG2	2:D:107:ARG:HH21	1.74	0.53
2:A:104:LYS:HG2	2:A:107:ARG:HH21	1.73	0.53
2:E:141:ARG:HD3	2:E:163:ILE:HD12	1.91	0.53
1:3:799:ASN:HB2	1:4:859:ARG:HB2	1.90	0.53
1:1:830:LEU:HB3	1:1:835:ILE:HD12	1.89	0.53
1:6:706:VAL:HG12	1:6:746:ILE:HB	1.91	0.53
1:4:227:ASN:HB3	1:4:228:LYS:HG3	1.91	0.53
2:E:87:LEU:HD11	2:E:197:LEU:HD21	1.91	0.53
1:6:686:TYR:HD1	4:0:3:UNK:O	1.92	0.53
1:6:753:LEU:HD11	1:6:793:PHE:HE2	1.74	0.53
2:F:103:GLU:O	2:F:107:ARG:N	2.40	0.53
1:4:504:ILE:HG23	1:4:508:LEU:HD12	1.91	0.53
1:5:209:ILE:O	1:6:450:ARG:NH2	2.42	0.53
1:1:642:VAL:O	6:1:1002:AGS:O1A	2.27	0.53
1:3:296:LYS:NZ	1:3:336:GLU:OE2	2.42	0.53
1:3:681:GLY:HA3	1:3:735:ASN:HD21	1.74	0.53
2:C:207:SER:O	2:C:210:MET:HB2	2.08	0.53
1:2:235:GLY:CA	1:2:241:LYS:HZ1	2.21	0.52
1:2:633:THR:HA	1:2:747:ILE:HG23	1.91	0.52
1:4:410:ILE:HG21	1:4:418:LYS:HE2	1.90	0.52
2:F:86:VAL:HB	2:F:194:VAL:HG21	1.91	0.52
1:2:643:GLY:N	6:2:1002:AGS:N7	2.56	0.52
1:2:705:SER:O	1:2:745:THR:OG1	2.27	0.52
2:E:116:ALA:O	2:E:120:ASN:ND2	2.43	0.52
1:1:720:PHE:HA	1:1:723:LEU:HD12	1.92	0.52
1:2:721:LYS:HD3	1:3:714:LYS:HB3	1.91	0.52
1:2:862:LEU:HD23	1:2:865:ILE:HD12	1.90	0.52
1:6:508:LEU:HD21	1:6:537:GLN:HE21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:873:PHE:HA	1:1:880:LYS:HD3	1.92	0.52
1:2:348:TYR:HA	1:2:352:ILE:HD12	1.91	0.52
1:6:212:ARG:NH2	1:6:368:GLU:OE1	2.42	0.52
2:C:210:MET:HA	2:C:210:MET:HE3	1.90	0.52
1:2:489:GLU:C	1:2:492:VAL:HG23	2.27	0.52
1:4:731:TYR:O	1:5:666:ASN:ND2	2.42	0.52
2:F:116:ALA:O	2:F:120:ASN:ND2	2.43	0.52
1:5:769:SER:HB3	1:5:771:THR:HG23	1.92	0.52
1:6:200:LYS:HB3	1:6:205:LYS:HB2	1.92	0.52
1:4:225:ARG:HE	1:5:424:ASN:HB3	1.74	0.52
1:6:584:LEU:HD23	1:6:655:LEU:HD23	1.92	0.52
1:1:522:ASN:HB3	1:1:525:PRO:HD3	1.91	0.51
2:E:103:GLU:O	2:E:107:ARG:N	2.40	0.51
2:D:200:GLU:HA	2:D:205:HIS:CD2	2.46	0.51
1:1:768:ASN:H	1:1:768:ASN:ND2	2.08	0.51
1:3:225:ARG:HH12	1:3:228:LYS:HB2	1.74	0.51
1:3:255:GLY:HA2	1:3:262:GLN:HE22	1.74	0.51
1:6:554:LYS:HD2	1:6:557:ASN:HD22	1.74	0.51
1:3:640:THR:HB	6:3:1002:AGS:S1G	2.51	0.51
1:6:837:VAL:HA	1:6:888:VAL:HB	1.92	0.51
2:C:104:LYS:HG2	2:C:107:ARG:HH21	1.74	0.51
1:1:875:ILE:HG21	1:1:879:LYS:HB2	1.91	0.51
1:4:465:VAL:HA	1:4:834:ASN:HD22	1.74	0.51
1:6:395:THR:HG22	1:6:397:LYS:H	1.76	0.51
2:F:82:ARG:HG3	2:F:186:TYR:HB2	1.92	0.51
2:E:153:SER:O	2:E:158:LYS:HE3	2.11	0.51
1:1:379:LEU:HD11	1:1:419:ALA:HB1	1.92	0.51
1:1:683:PRO:HB3	1:2:678:LYS:HE3	1.92	0.51
1:2:796:GLU:HG3	6:3:1002:AGS:S1G	2.50	0.51
1:3:518:TYR:CD2	1:3:522:ASN:HB3	2.45	0.51
1:4:190:ILE:O	1:4:194:GLY:N	2.43	0.51
1:4:353:GLU:OE2	1:5:700:ARG:NH2	2.43	0.51
1:5:379:LEU:HD11	1:5:419:ALA:HB1	1.91	0.51
1:5:607:GLU:HA	1:5:610:ILE:HD12	1.92	0.51
1:1:613:LEU:HD21	1:1:651:LEU:HD11	1.93	0.51
1:6:636:PHE:HB2	1:6:750:THR:HG22	1.92	0.51
2:E:168:TYR:HA	2:E:171:TRP:HE1	1.70	0.51
2:E:173:SER:HB2	2:E:176:TYR:HD2	1.76	0.51
1:2:646:GLU:HG2	1:2:649:LYS:HD2	1.92	0.51
1:4:362:PHE:O	1:5:413:ARG:NH2	2.42	0.51
1:3:526:PRO:HD2	1:3:529:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:533:LEU:O	1:3:537:GLN:NE2	2.42	0.51
2:B:104:LYS:HG2	2:B:107:ARG:HH21	1.74	0.51
1:1:497:ARG:HH12	1:1:550:TYR:HB2	1.76	0.51
1:5:667:MET:HB3	1:5:711:GLU:H	1.76	0.51
1:6:760:LYS:HA	1:6:764:PHE:HE1	1.76	0.51
1:4:426:ALA:HA	1:4:572:ILE:HG13	1.92	0.50
1:5:599:LEU:O	1:5:603:ILE:N	2.44	0.50
1:1:783:LEU:HD21	2:B:221:LYS:HB3	1.92	0.50
1:4:667:MET:HG2	1:4:712:LEU:HA	1.93	0.50
1:6:686:TYR:CD1	4:0:3:UNK:O	2.64	0.50
1:6:858:ALA:O	1:6:861:THR:OG1	2.29	0.50
2:F:169:ARG:O	2:F:172:VAL:N	2.43	0.50
1:1:757:LEU:O	1:1:761:LYS:N	2.44	0.50
1:3:760:LYS:HA	1:3:764:PHE:HD2	1.76	0.50
1:1:319:GLU:HG2	1:1:320:GLY:N	2.26	0.50
1:3:220:ILE:HG23	1:3:261:LEU:HD12	1.91	0.50
1:3:595:LEU:HD23	1:3:614:SER:HA	1.92	0.50
1:4:511:LEU:HA	1:4:514:LEU:HD23	1.93	0.50
1:3:888:VAL:HG22	1:3:903:LEU:HD21	1.92	0.50
1:4:305:PHE:HD1	1:4:340:ILE:HB	1.77	0.50
1:6:694:GLN:HA	1:6:697:GLU:HB3	1.92	0.50
2:B:103:GLU:O	2:B:107:ARG:N	2.42	0.50
1:1:687:VAL:HB	4:0:14:UNK:CB	2.42	0.50
1:2:804:ILE:HB	2:C:222:ASN:HD21	1.77	0.50
1:4:613:LEU:HD21	1:4:651:LEU:HD11	1.94	0.50
1:6:676:VAL:HG23	1:6:722:VAL:HG21	1.93	0.50
2:G:93:VAL:HG21	2:G:98:ILE:HG22	1.94	0.50
2:E:185:LEU:HB2	2:E:188:HIS:CD2	2.44	0.50
1:2:491:TYR:O	1:2:495:GLY:N	2.38	0.50
1:2:796:GLU:HG3	1:3:640:THR:HG21	1.93	0.50
1:4:646:GLU:HA	1:4:649:LYS:HB2	1.94	0.50
1:4:897:LYS:HD3	2:D:231:ASP:OD2	2.12	0.50
1:6:243:THR:HG21	6:6:1001:AGS:H2'	1.94	0.50
1:2:899:LEU:HB3	2:B:231:ASP:HB2	1.94	0.49
1:4:187:THR:N	1:4:191:GLU:OE1	2.45	0.49
1:6:789:CYS:HA	1:6:793:PHE:HD2	1.76	0.49
2:F:86:VAL:CB	2:F:194:VAL:HG21	2.42	0.49
1:2:390:TYR:HD1	1:2:431:GLN:HE21	1.60	0.49
1:3:822:ARG:HG2	1:3:862:LEU:CD2	2.42	0.49
1:4:897:LYS:HD3	2:D:231:ASP:CG	2.33	0.49
1:6:379:LEU:HD21	1:6:419:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:PHE:CE1	2:F:185:LEU:HD22	2.46	0.49
1:4:361:ARG:NH1	6:4:1003:AGS:S1G	2.77	0.49
1:4:646:GLU:HG2	1:4:649:LYS:HD3	1.94	0.49
2:F:93:VAL:HG21	2:F:98:ILE:HG22	1.94	0.49
2:C:209:TYR:CE2	2:C:213:LYS:HE2	2.47	0.49
1:3:645:THR:HG23	6:3:1002:AGS:O1B	2.12	0.49
1:4:790:LYS:HE2	1:5:856:LEU:HD21	1.93	0.49
1:5:508:LEU:HD13	1:5:536:ALA:HA	1.94	0.49
2:D:93:VAL:HG21	2:D:98:ILE:HG22	1.94	0.49
1:1:852:TYR:C	1:1:852:TYR:CD2	2.86	0.49
1:2:859:ARG:NH2	6:2:1002:AGS:O3A	2.46	0.49
1:3:523:LYS:HG2	1:3:525:PRO:HD2	1.94	0.49
2:C:93:VAL:HG21	2:C:98:ILE:HG22	1.94	0.49
1:3:843:ALA:HA	1:3:892:TYR:HB2	1.95	0.49
2:A:93:VAL:HG21	2:A:98:ILE:HG22	1.95	0.49
2:F:162:ILE:HG21	2:F:171:TRP:CH2	2.48	0.49
2:E:86:VAL:HG11	2:E:194:VAL:HG21	1.94	0.49
2:D:206:LEU:O	2:D:210:MET:HG2	2.13	0.49
1:2:326:ASN:HA	1:2:329:LYS:HG2	1.95	0.49
1:4:226:TYR:N	1:5:390:TYR:OH	2.46	0.49
1:5:604:ILE:H	6:5:1001:AGS:C2	2.25	0.49
1:5:404:LYS:HZ1	1:6:831:GLU:HB2	1.78	0.49
2:D:77:VAL:O	2:D:81:SER:N	2.45	0.49
1:2:220:ILE:HG23	1:2:261:LEU:HD22	1.94	0.49
1:2:603:ILE:HD13	1:2:647:LEU:HG	1.94	0.49
1:2:633:THR:HB	1:2:727:LEU:HD22	1.95	0.49
1:3:815:LEU:HD11	1:3:861:THR:HG21	1.93	0.49
1:5:734:ASP:OD2	1:5:738:ARG:NH1	2.45	0.49
1:5:799:ASN:HB2	1:6:859:ARG:HB2	1.95	0.49
2:G:103:GLU:O	2:G:107:ARG:N	2.42	0.49
1:5:872:LYS:CE	2:E:230:PHE:HD2	2.25	0.49
1:6:682:SER:O	1:6:735:ASN:ND2	2.46	0.49
1:1:603:ILE:HD13	6:1:1002:AGS:C2	2.43	0.48
1:4:241:LYS:NZ	1:4:343:THR:O	2.46	0.48
1:1:783:LEU:HD11	2:B:221:LYS:HB2	1.95	0.48
1:2:679:ILE:HG23	1:2:695:LEU:HD12	1.95	0.48
1:3:395:THR:HG22	1:3:397:LYS:H	1.77	0.48
1:6:554:LYS:HG3	1:6:558:ALA:H	1.77	0.48
2:B:93:VAL:HG21	2:B:98:ILE:HG22	1.95	0.48
1:1:201:VAL:HG22	1:1:206:LEU:HD23	1.95	0.48
1:1:765:ASP:HB3	2:A:213:LYS:HZ3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:892:TYR:HE1	1:1:899:LEU:H	1.60	0.48
2:F:161:GLN:HA	2:F:164:LYS:HB2	1.96	0.48
1:2:716:HIS:CD2	1:2:718:ASP:H	2.31	0.48
1:4:271:PHE:HA	1:4:274:PHE:HB3	1.94	0.48
1:5:639:PRO:HB3	1:5:758:PHE:HZ	1.78	0.48
2:E:167:ILE:HD11	2:E:206:LEU:HD23	1.94	0.48
1:1:785:LEU:HD12	1:1:806:VAL:HG13	1.95	0.48
1:1:799:ASN:HB3	1:2:859:ARG:HD2	1.94	0.48
1:4:220:ILE:HG23	1:4:261:LEU:HD12	1.95	0.48
1:4:872:LYS:HA	1:4:875:ILE:HG22	1.94	0.48
2:E:148:LEU:HD13	2:E:151:ASP:OD1	2.14	0.48
1:1:774:TYR:CD1	1:1:774:TYR:C	2.87	0.48
2:F:167:ILE:HD11	2:F:206:LEU:HD22	1.95	0.48
1:1:209:ILE:O	1:2:450:ARG:NH2	2.47	0.48
1:1:774:TYR:HE1	1:1:778:MET:SD	2.34	0.48
1:5:484:LEU:HA	1:5:487:TYR:HB2	1.95	0.48
1:6:223:LEU:O	1:6:229:ASN:ND2	2.46	0.48
2:B:77:VAL:O	2:B:81:SER:N	2.44	0.48
1:1:220:ILE:HG23	1:1:261:LEU:HD12	1.95	0.48
1:1:686:TYR:O	4:0:12:UNK:CB	2.62	0.48
1:3:243:THR:HG21	6:3:1001:AGS:H2'	1.95	0.48
1:3:761:LYS:HD3	1:3:765:ASP:OD2	2.13	0.48
1:4:670:PHE:HE1	1:4:678:LYS:HD2	1.79	0.48
1:5:737:ARG:NH2	1:6:664:ARG:O	2.47	0.48
1:1:758:PHE:HD2	1:1:785:LEU:HG	1.78	0.48
1:1:831:GLU:HA	1:1:835:ILE:H	1.79	0.48
1:6:285:GLU:O	1:6:289:LYS:N	2.44	0.48
1:6:899:LEU:HB3	2:F:233:ASP:OD2	2.12	0.48
1:1:762:LEU:O	1:1:763:PHE:C	2.52	0.47
1:5:555:THR:HG21	1:5:588:SER:H	1.79	0.47
1:5:895:LYS:O	1:5:896:ALA:HB3	2.14	0.47
2:F:152:PRO:HG2	2:E:117:VAL:HG13	1.96	0.47
1:3:723:LEU:HG	1:3:726:ILE:HG21	1.96	0.47
1:5:292:ILE:HG22	1:5:296:LYS:HE3	1.96	0.47
1:5:406:SER:HB2	1:5:418:LYS:HB3	1.96	0.47
2:E:228:TYR:CD2	2:E:228:TYR:N	2.75	0.47
1:2:326:ASN:HD22	1:2:329:LYS:HG3	1.78	0.47
1:2:582:GLY:O	1:2:657:ASN:ND2	2.46	0.47
1:6:712:LEU:HB2	1:6:751:SER:HB3	1.96	0.47
1:3:410:ILE:O	1:3:418:LYS:NZ	2.41	0.47
1:5:379:LEU:HD22	1:5:423:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:819:VAL:HG13	1:5:865:ILE:HD11	1.96	0.47
2:D:116:ALA:O	2:D:120:ASN:ND2	2.48	0.47
2:C:77:VAL:O	2:C:81:SER:N	2.46	0.47
1:1:498:LEU:HD23	1:1:501:LYS:HD2	1.97	0.47
1:4:903:LEU:HD23	2:D:235:SER:OG	2.13	0.47
1:1:265:THR:O	1:1:303:ILE:N	2.47	0.47
1:2:897:LYS:HD3	2:B:231:ASP:OD2	2.15	0.47
1:4:406:SER:HB2	1:4:418:LYS:HG3	1.96	0.47
1:1:492:VAL:O	1:1:496:GLU:N	2.46	0.47
1:3:379:LEU:HD22	1:3:423:LEU:HD12	1.96	0.47
2:C:103:GLU:O	2:C:107:ARG:N	2.44	0.47
1:4:371:SER:O	1:4:373:ASP:N	2.47	0.47
1:6:554:LYS:HD2	1:6:557:ASN:HB2	1.96	0.47
1:2:460:LYS:HG2	1:2:461:ASP:H	1.80	0.47
1:5:295:LEU:HD21	1:5:304:LEU:HD13	1.97	0.47
1:5:528:GLU:HA	1:5:531:ASN:HB2	1.97	0.47
2:B:222:ASN:OD1	2:B:223:ILE:HG22	2.15	0.47
1:6:625:LYS:HE3	1:6:629:LYS:HG3	1.97	0.46
2:A:116:ALA:O	2:A:120:ASN:ND2	2.48	0.46
2:E:88:LEU:HD12	2:E:88:LEU:C	2.35	0.46
1:1:635:LEU:HG	1:1:637:LEU:CD2	2.45	0.46
1:2:281:ARG:HE	1:2:282:GLY:H	1.64	0.46
6:3:1002:AGS:O3B	6:3:1002:AGS:O1A	2.34	0.46
1:4:501:LYS:HD3	1:4:543:LEU:HD22	1.97	0.46
1:6:679:ILE:HG12	1:6:695:LEU:HD13	1.96	0.46
2:F:148:LEU:HD13	2:F:151:ASP:OD1	2.15	0.46
1:1:499:LYS:HG3	1:1:499:LYS:O	2.15	0.46
1:2:242:THR:HG22	1:2:246:GLU:HG3	1.97	0.46
1:4:393:ASN:HD22	1:4:394:ILE:H	1.62	0.46
2:F:71:PHE:HE1	2:F:185:LEU:HD21	1.78	0.46
1:1:364:LYS:HG3	1:2:413:ARG:HH22	1.80	0.46
1:3:370:PRO:HD2	1:3:415:LEU:HB2	1.97	0.46
2:F:79:ARG:CD	2:F:180:GLY:O	2.63	0.46
1:1:640:THR:HA	6:1:1002:AGS:O3G	2.16	0.46
1:4:361:ARG:NH2	6:4:1003:AGS:O1B	2.48	0.46
1:4:686:TYR:OH	1:6:672:GLU:OE1	2.26	0.46
6:5:1001:AGS:O3B	6:5:1001:AGS:O1A	2.34	0.46
2:F:106:LEU:HD23	2:F:109:ILE:HD12	1.98	0.46
1:2:643:GLY:CA	6:2:1002:AGS:N7	2.79	0.46
6:2:1002:AGS:O1A	6:2:1002:AGS:O3B	2.34	0.46
1:3:526:PRO:HD2	1:3:529:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:819:VAL:HG13	1:3:865:ILE:HD11	1.97	0.46
1:4:288:MET:HA	1:4:291:ILE:HD12	1.98	0.46
1:2:656:PHE:HB3	1:2:661:ASN:HD22	1.81	0.46
1:3:900:VAL:HA	2:C:231:ASP:HB3	1.98	0.46
1:5:872:LYS:CG	2:E:230:PHE:HD2	2.27	0.46
1:6:717:ALA:HA	1:6:720:PHE:HD2	1.80	0.46
6:1:1002:AGS:O1A	6:1:1002:AGS:O3B	2.34	0.46
2:E:93:VAL:HG21	2:E:98:ILE:CG1	2.46	0.46
1:1:791:LYS:CD	1:1:792:VAL:HG23	2.46	0.45
1:2:798:VAL:HA	1:2:801:ILE:HD12	1.97	0.45
2:D:203:LEU:O	2:D:204:LYS:C	2.54	0.45
1:1:757:LEU:C	1:1:760:LYS:HB3	2.37	0.45
1:2:895:LYS:O	1:2:896:ALA:CB	2.64	0.45
1:3:776:ARG:O	1:3:780:ASP:HB2	2.16	0.45
2:G:77:VAL:O	2:G:81:SER:N	2.46	0.45
1:4:897:LYS:CD	2:D:231:ASP:OD2	2.64	0.45
1:6:484:LEU:HD22	1:6:488:TYR:HE2	1.81	0.45
1:2:398:ALA:O	1:2:402:ALA:N	2.49	0.45
1:3:767:ASP:O	1:3:774:TYR:OH	2.20	0.45
1:4:794:LYS:O	1:4:796:GLU:N	2.49	0.45
1:6:223:LEU:HD21	1:6:340:ILE:HD11	1.97	0.45
2:E:106:LEU:HD23	2:E:109:ILE:HD12	1.98	0.45
1:1:891:ASP:HB3	1:1:901:ILE:HD12	1.98	0.45
1:4:390:TYR:OH	1:4:424:ASN:OD1	2.31	0.45
1:5:767:ASP:HB2	1:5:811:ASN:HB3	1.99	0.45
2:B:222:ASN:CG	2:B:223:ILE:H	2.19	0.45
2:A:185:LEU:HB2	2:A:188:HIS:HD2	1.82	0.45
2:F:186:TYR:HA	2:F:189:ILE:HD12	1.98	0.45
1:1:361:ARG:NH2	6:2:1001:AGS:O1B	2.50	0.45
1:2:599:LEU:HD21	1:2:651:LEU:HD23	1.99	0.45
1:3:242:THR:OG1	6:3:1001:AGS:O2B	2.29	0.45
1:4:684:PRO:HB2	1:5:682:SER:HB3	1.99	0.45
6:4:1002:AGS:O1A	6:4:1002:AGS:O3B	2.34	0.45
2:D:211:GLU:HB3	2:D:215:LYS:HE2	1.97	0.45
1:2:872:LYS:CG	2:B:230:PHE:HE1	2.28	0.45
1:3:518:TYR:CG	1:3:522:ASN:HB3	2.52	0.45
1:5:190:ILE:HG12	1:5:291:ILE:HG12	1.98	0.45
1:5:261:LEU:HA	1:5:264:TYR:HE2	1.81	0.45
1:6:899:LEU:HD22	2:F:233:ASP:OD1	2.17	0.45
2:A:92:ILE:O	2:A:158:LYS:NZ	2.43	0.45
1:1:420:ILE:HD13	6:1:1001:AGS:H1'	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:369:PRO:HA	1:2:370:PRO:HD3	1.75	0.45
1:2:402:ALA:HA	1:2:569:VAL:HG11	1.99	0.45
1:4:853:ASP:OD2	2:D:220:LYS:CB	2.59	0.45
1:6:465:VAL:HG22	1:6:834:ASN:HB2	1.99	0.45
1:6:757:LEU:HB3	1:6:781:VAL:HG13	1.98	0.45
6:6:1002:AGS:O3B	6:6:1002:AGS:O1A	2.34	0.45
1:1:309:ILE:HG13	1:1:312:LEU:HD12	1.98	0.45
1:2:796:GLU:OE1	1:3:752:ASN:ND2	2.49	0.45
1:3:723:LEU:O	1:3:726:ILE:N	2.47	0.45
1:4:555:THR:OG1	1:4:557:ASN:OD1	2.33	0.45
1:4:652:ALA:HB2	1:4:662:LEU:HB2	1.99	0.45
1:1:774:TYR:CD1	1:1:774:TYR:O	2.70	0.45
1:4:380:ARG:NH1	1:5:458:LEU:HD21	2.32	0.45
1:5:603:ILE:HG12	1:5:647:LEU:HD23	1.99	0.45
1:5:635:LEU:HB2	1:5:801:ILE:HG21	1.99	0.45
1:5:742:PHE:O	1:5:745:THR:OG1	2.28	0.45
2:D:103:GLU:O	2:D:107:ARG:N	2.44	0.45
1:1:765:ASP:HA	2:A:213:LYS:HD3	1.98	0.44
1:2:899:LEU:CA	2:B:231:ASP:O	2.65	0.44
1:3:236:ASN:O	1:3:241:LYS:NZ	2.49	0.44
1:3:853:ASP:O	1:3:857:GLY:N	2.49	0.44
2:B:116:ALA:O	2:B:120:ASN:ND2	2.50	0.44
2:E:79:ARG:CD	2:E:180:GLY:O	2.66	0.44
2:D:185:LEU:HB2	2:D:188:HIS:HD2	1.82	0.44
1:1:286:THR:O	1:1:290:ASN:ND2	2.47	0.44
1:2:534:LYS:O	1:2:538:GLN:N	2.47	0.44
1:2:710:ASP:O	1:2:750:THR:OG1	2.32	0.44
1:4:653:ILE:O	1:4:657:ASN:ND2	2.50	0.44
1:4:854:PRO:HD2	2:D:217:MET:HE1	2.00	0.44
1:5:683:PRO:HG3	1:6:674:HIS:HD2	1.80	0.44
2:D:92:ILE:O	2:D:158:LYS:NZ	2.43	0.44
2:C:185:LEU:HB2	2:C:188:HIS:HD2	1.82	0.44
1:1:686:TYR:HD1	4:0:13:UNK:O	2.00	0.44
1:1:758:PHE:HB3	1:1:781:VAL:CB	2.44	0.44
1:2:897:LYS:HE3	1:2:897:LYS:HB3	1.77	0.44
1:3:713:GLU:HB2	1:3:752:ASN:H	1.82	0.44
1:3:847:ILE:HG23	1:3:864:PHE:HD2	1.83	0.44
1:4:635:LEU:HB2	1:4:801:ILE:HD13	1.98	0.44
1:5:810:LEU:HD11	6:5:1001:AGS:N7	2.32	0.44
1:6:545:LYS:HA	1:6:548:VAL:HB	2.00	0.44
2:F:71:PHE:CE1	2:F:185:LEU:CD2	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:1003:AGS:N1	1:5:210:TYR:HB3	2.32	0.44
1:5:227:ASN:OD1	1:5:228:LYS:N	2.50	0.44
1:1:508:LEU:HD13	1:1:540:TYR:HB2	2.00	0.44
1:2:625:LYS:HE2	1:2:631:ILE:HD11	2.00	0.44
1:3:422:LEU:O	1:3:426:ALA:N	2.46	0.44
1:1:636:PHE:HB2	1:1:750:THR:HA	1.99	0.44
1:2:758:PHE:HZ	1:2:809:PRO:HD3	1.82	0.44
1:3:544:TYR:O	1:3:547:THR:OG1	2.31	0.44
1:3:634:PHE:HD1	1:3:803:LYS:HB2	1.80	0.44
1:3:803:LYS:HD2	2:D:222:ASN:OD1	2.17	0.44
1:4:360:ARG:HH22	1:5:417:ASP:CG	2.21	0.44
1:4:394:ILE:HA	1:4:564:VAL:HG22	2.00	0.44
1:6:710:ASP:O	1:6:750:THR:OG1	2.30	0.44
1:1:583:SER:HB3	1:1:657:ASN:HB2	2.00	0.44
1:2:406:SER:HB2	1:2:418:LYS:HB3	1.99	0.44
1:4:408:ARG:HD2	1:4:627:PRO:HB3	1.99	0.44
1:5:663:ILE:HD12	1:5:707:VAL:HG22	1.99	0.44
1:5:776:ARG:NH2	2:F:222:ASN:HD21	2.16	0.44
1:5:847:ILE:HG23	1:5:864:PHE:HD2	1.82	0.44
2:A:103:GLU:O	2:A:107:ARG:N	2.43	0.44
2:G:185:LEU:HB2	2:G:188:HIS:HD2	1.82	0.44
1:4:864:PHE:HE1	2:D:228:TYR:HD2	1.66	0.44
1:5:799:ASN:HB3	1:6:856:LEU:HB3	1.99	0.44
1:2:636:PHE:HB3	1:2:807:PHE:HE2	1.83	0.44
1:3:518:TYR:O	1:3:518:TYR:CD2	2.70	0.44
1:4:755:ALA:H	1:4:758:PHE:HB2	1.82	0.44
1:4:830:LEU:O	1:4:834:ASN:N	2.51	0.44
1:4:853:ASP:CG	2:D:220:LYS:HB2	2.38	0.44
2:A:77:VAL:O	2:A:81:SER:N	2.46	0.44
1:2:872:LYS:HG3	2:B:230:PHE:CE1	2.51	0.43
1:3:847:ILE:HG12	1:3:869:ILE:HD11	2.00	0.43
1:3:855:GLU:HG3	2:C:217:MET:HE1	1.99	0.43
1:5:727:LEU:HD21	1:5:749:MET:HE2	1.99	0.43
1:6:200:LYS:HA	1:6:203:ASN:HB2	1.99	0.43
2:E:206:LEU:O	2:E:210:MET:HG2	2.18	0.43
1:1:379:LEU:HD22	1:1:423:LEU:HD12	2.00	0.43
1:2:641:GLY:HA3	1:2:857:GLY:HA3	2.00	0.43
1:2:643:GLY:HA3	6:2:1002:AGS:N7	2.33	0.43
1:2:689:PHE:HE1	1:2:735:ASN:HB3	1.83	0.43
1:2:764:PHE:HB3	1:2:854:PRO:HG2	2.00	0.43
1:5:269:LEU:HD12	1:5:306:VAL:HG22	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:589:SER:HA	1:6:878:LEU:HD22	2.00	0.43
1:5:728:GLY:HA3	1:5:800:ARG:HH11	1.82	0.43
1:6:790:LYS:HG2	1:6:795:PRO:HB3	2.00	0.43
1:2:410:ILE:O	1:2:418:LYS:NZ	2.50	0.43
1:2:804:ILE:HB	2:C:222:ASN:ND2	2.33	0.43
1:3:689:PHE:CE1	1:3:735:ASN:HB3	2.53	0.43
1:5:513:GLU:HA	1:5:516:GLN:HB3	2.01	0.43
1:5:667:MET:HA	1:5:670:PHE:HD2	1.83	0.43
1:6:488:TYR:HA	1:6:491:TYR:CE1	2.53	0.43
1:1:758:PHE:HB3	1:1:781:VAL:CG1	2.49	0.43
1:1:778:MET:HA	1:1:781:VAL:CG2	2.47	0.43
2:G:92:ILE:O	2:G:158:LYS:NZ	2.42	0.43
1:1:540:TYR:O	1:1:544:TYR:N	2.49	0.43
1:1:660:ASP:O	1:1:702:LYS:NZ	2.40	0.43
1:2:796:GLU:HG3	1:3:640:THR:CG2	2.49	0.43
1:2:898:ASN:O	2:B:230:PHE:CB	2.66	0.43
1:3:822:ARG:HA	1:3:822:ARG:HD3	1.53	0.43
1:6:248:LEU:HB2	1:6:266:VAL:HG21	2.01	0.43
2:E:77:VAL:O	2:E:81:SER:N	2.50	0.43
1:1:438:PRO:HG2	1:1:441:ILE:HG13	2.00	0.43
1:2:284:PHE:HA	1:2:287:ARG:HB2	2.01	0.43
1:4:854:PRO:HD2	2:D:217:MET:HE3	2.01	0.43
1:4:903:LEU:HD21	2:D:235:SER:OG	2.18	0.43
2:F:148:LEU:HB3	2:F:151:ASP:OD1	2.18	0.43
2:C:116:ALA:O	2:C:120:ASN:ND2	2.51	0.43
1:2:859:ARG:HH21	6:2:1002:AGS:PA	2.42	0.43
1:3:640:THR:CG2	6:3:1002:AGS:S1G	3.06	0.43
1:3:893:ASN:HD22	1:3:896:ALA:HB3	1.84	0.43
1:4:223:LEU:O	1:4:338:LYS:NZ	2.44	0.43
1:6:380:ARG:O	1:6:383:LYS:NZ	2.38	0.43
2:E:87:LEU:HD23	2:E:87:LEU:HA	1.70	0.43
1:4:397:LYS:HB2	1:4:566:GLN:HE21	1.83	0.43
1:4:627:PRO:HD3	1:5:829:ARG:HH11	1.83	0.43
2:E:83:MET:SD	2:E:176:TYR:O	2.77	0.43
1:3:670:PHE:HE1	1:3:678:LYS:HB2	1.83	0.43
1:6:676:VAL:HG21	1:6:722:VAL:HG21	2.01	0.43
2:D:199:LYS:O	2:D:205:HIS:CB	2.67	0.43
1:1:759:LYS:NZ	1:1:778:MET:HG3	2.34	0.43
1:2:899:LEU:HA	2:B:231:ASP:O	2.19	0.43
1:4:200:LYS:HG2	1:4:205:LYS:HD2	2.00	0.43
1:5:484:LEU:HB3	1:5:488:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:729:ASP:HB3	1:5:731:TYR:CE1	2.54	0.43
2:B:166:GLN:O	2:B:169:ARG:NH1	2.52	0.43
1:2:326:ASN:HB3	1:3:311:LEU:HD21	2.01	0.42
1:3:604:ILE:HG21	1:3:817:LYS:HE3	2.01	0.42
1:3:862:LEU:HD23	1:3:865:ILE:HD12	2.01	0.42
2:E:148:LEU:HB3	2:E:151:ASP:OD1	2.19	0.42
1:2:897:LYS:CG	1:2:898:ASN:N	2.81	0.42
1:4:502:LYS:HE2	1:4:506:LYS:HE3	2.00	0.42
1:6:673:ALA:O	1:6:676:VAL:HG12	2.19	0.42
1:6:819:VAL:HG13	1:6:865:ILE:HD11	2.01	0.42
2:F:77:VAL:O	2:F:81:SER:N	2.49	0.42
1:1:757:LEU:CD1	1:1:788:LYS:HE3	2.48	0.42
1:3:631:ILE:HD12	1:3:744:ASN:HA	2.00	0.42
1:3:635:LEU:HB2	1:3:801:ILE:HD13	2.02	0.42
1:4:344:THR:HG22	1:4:346:ALA:H	1.84	0.42
1:6:810:LEU:HD11	6:6:1002:AGS:N7	2.33	0.42
1:3:626:ASP:HB3	1:3:629:LYS:HB3	2.01	0.42
1:3:765:ASP:HB3	2:C:213:LYS:NZ	2.34	0.42
2:E:79:ARG:HD2	2:E:180:GLY:O	2.19	0.42
1:1:360:ARG:NH2	6:2:1001:AGS:H5'2	2.35	0.42
1:1:791:LYS:C	1:1:791:LYS:CD	2.86	0.42
1:2:704:HIS:CD2	1:2:744:ASN:HB3	2.55	0.42
1:3:465:VAL:HG23	1:3:834:ASN:HB2	2.01	0.42
1:3:855:GLU:CD	2:C:217:MET:HE2	2.38	0.42
1:4:213:ASP:OD1	1:4:251:ARG:NH1	2.53	0.42
1:4:593:LEU:HD13	1:5:879:LYS:HE3	2.01	0.42
1:5:473:LEU:O	1:5:477:PHE:N	2.51	0.42
1:5:872:LYS:CD	2:E:230:PHE:HD2	2.32	0.42
1:1:217:ARG:HH22	1:2:446:ARG:HG3	1.84	0.42
1:1:499:LYS:HD2	1:1:502:LYS:HD2	2.00	0.42
1:3:855:GLU:HG3	2:C:217:MET:CE	2.50	0.42
2:E:86:VAL:CG1	2:E:194:VAL:HG21	2.50	0.42
2:E:203:LEU:O	2:E:207:SER:HB3	2.20	0.42
1:1:765:ASP:HB3	2:A:213:LYS:HZ2	1.84	0.42
1:3:640:THR:CB	6:3:1002:AGS:S1G	3.08	0.42
1:6:206:LEU:HD22	1:6:246:GLU:HB3	2.01	0.42
1:1:508:LEU:HD23	1:1:508:LEU:HA	1.89	0.42
1:1:637:LEU:HD12	1:1:785:LEU:HD13	2.01	0.42
1:1:789:CYS:O	1:1:793:PHE:N	2.52	0.42
1:2:544:TYR:O	1:2:547:THR:OG1	2.31	0.42
1:2:892:TYR:CE1	1:2:897:LYS:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:269:LEU:HD11	1:3:304:LEU:HD11	2.02	0.42
1:4:847:ILE:HG23	1:4:864:PHE:HD2	1.85	0.42
1:6:398:ALA:HA	1:6:566:GLN:HG2	2.02	0.42
1:1:498:LEU:O	1:1:501:LYS:HB2	2.20	0.42
1:3:188:LEU:HB2	1:3:191:GLU:HG3	2.00	0.42
1:3:439:ARG:HE	1:3:557:ASN:ND2	2.17	0.42
1:4:352:ILE:HG22	1:4:359:GLU:HB3	2.01	0.42
1:6:642:VAL:O	6:6:1002:AGS:O1A	2.37	0.42
1:6:794:LYS:O	1:6:796:GLU:N	2.52	0.42
2:B:86:VAL:HG11	2:B:191:PRO:HA	2.02	0.42
1:1:212:ARG:HD3	1:1:244:ILE:CG1	2.49	0.42
1:4:513:GLU:O	1:4:517:ASN:N	2.52	0.42
2:A:166:GLN:O	2:A:169:ARG:NH1	2.51	0.42
2:G:116:ALA:O	2:G:120:ASN:ND2	2.52	0.42
2:E:168:TYR:CA	2:E:171:TRP:CD1	2.93	0.42
1:2:188:LEU:HD13	1:2:302:ILE:HD12	2.01	0.41
1:3:599:LEU:CD1	1:3:610:ILE:HG23	2.50	0.41
1:6:759:LYS:HB2	1:6:763:PHE:HB2	2.01	0.41
2:D:94:GLY:O	2:D:204:LYS:CE	2.68	0.41
2:D:209:TYR:CZ	2:D:213:LYS:HE3	2.55	0.41
1:1:438:PRO:HG2	1:1:441:ILE:CG1	2.50	0.41
1:4:689:PHE:CE1	1:4:735:ASN:HB3	2.55	0.41
2:E:93:VAL:HG13	2:E:96:ASN:HB2	2.02	0.41
2:D:134:HIS:O	2:D:138:ASN:ND2	2.53	0.41
1:1:642:VAL:HG23	1:1:644:LYS:HG3	2.01	0.41
1:3:243:THR:CG2	6:3:1001:AGS:H2'	2.49	0.41
1:3:392:ILE:HD13	1:3:430:LEU:HB2	2.02	0.41
1:4:195:SER:OG	1:4:196:ASN:N	2.50	0.41
1:4:313:LEU:HA	1:4:325:ALA:HB2	2.02	0.41
1:5:859:ARG:NH2	6:5:1001:AGS:O3B	2.53	0.41
2:E:152:PRO:HB3	2:D:131:LEU:O	2.21	0.41
1:1:789:CYS:HG	1:1:793:PHE:HD2	1.62	0.41
1:6:662:LEU:HD11	1:6:708:LEU:HG	2.03	0.41
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.93	0.41
2:E:171:TRP:H	2:E:171:TRP:HD1	1.64	0.41
2:C:134:HIS:O	2:C:138:ASN:ND2	2.52	0.41
1:1:209:ILE:HG23	6:1:1001:AGS:N1	2.35	0.41
1:1:409:PHE:HZ	1:1:625:LYS:HE2	1.85	0.41
1:1:554:LYS:HG2	1:1:558:ALA:HA	2.02	0.41
1:3:822:ARG:O	1:3:826:LEU:N	2.52	0.41
2:B:215:LYS:HA	2:B:218:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:514:LEU:C	1:3:516:GLN:H	2.22	0.41
1:5:696:THR:HB	1:5:740:ILE:HD13	2.03	0.41
1:5:860:PRO:HA	1:5:863:ILE:HB	2.03	0.41
1:5:887:ASP:N	1:5:903:LEU:O	2.47	0.41
2:E:86:VAL:HG11	2:E:194:VAL:CG2	2.51	0.41
2:D:203:LEU:HD23	2:D:206:LEU:HD23	2.02	0.41
1:2:200:LYS:HB3	1:2:205:LYS:HB3	2.03	0.41
1:4:409:PHE:HB3	1:4:573:TYR:OH	2.21	0.41
1:6:194:GLY:O	1:6:270:ASN:ND2	2.51	0.41
1:6:758:PHE:HE1	1:6:809:PRO:HB3	1.86	0.41
1:4:765:ASP:OD1	2:D:217:MET:SD	2.78	0.41
6:4:1003:AGS:N6	1:5:212:ARG:HD2	2.35	0.41
1:5:274:PHE:O	1:5:287:ARG:NH1	2.54	0.41
1:5:903:LEU:HA	2:E:235:SER:O	2.20	0.41
1:1:233:LEU:HD23	1:1:241:LYS:CB	2.51	0.41
1:1:236:ASN:HB3	1:1:237:PRO:CD	2.51	0.41
1:2:241:LYS:N	6:2:1001:AGS:O2A	2.54	0.41
1:3:521:SER:C	1:3:523:LYS:H	2.24	0.41
1:3:826:LEU:HD23	1:3:837:VAL:HG11	2.03	0.41
1:4:643:GLY:HA2	6:4:1002:AGS:H5'1	2.02	0.41
1:4:899:LEU:HD23	2:D:231:ASP:HB2	1.08	0.41
1:6:241:LYS:N	6:6:1001:AGS:O2A	2.54	0.41
1:6:264:TYR:HA	1:6:301:LYS:HD3	2.02	0.41
1:6:491:TYR:HB2	1:6:560:ASN:OD1	2.21	0.41
2:G:134:HIS:O	2:G:138:ASN:ND2	2.54	0.41
2:C:92:ILE:O	2:C:158:LYS:NZ	2.43	0.41
1:1:439:ARG:HH21	1:1:557:ASN:HD22	1.68	0.41
1:1:760:LYS:HD2	1:1:760:LYS:C	2.32	0.41
1:3:259:LYS:HA	1:3:262:GLN:HB2	2.02	0.41
1:3:629:LYS:HD2	1:3:630:PRO:HD2	2.01	0.41
1:3:644:LYS:NZ	1:3:752:ASN:OD1	2.39	0.41
1:3:872:LYS:O	1:3:876:MET:HB2	2.21	0.41
1:6:712:LEU:HD11	1:6:749:MET:HB3	2.03	0.41
1:2:815:LEU:HA	1:2:818:ILE:HD12	2.03	0.40
1:2:829:ARG:NH2	1:2:866:GLU:OE1	2.52	0.40
1:3:375:THR:HA	1:3:378:ILE:HD12	2.03	0.40
1:4:210:TYR:HB3	6:4:1001:AGS:N1	2.36	0.40
1:6:328:LEU:O	1:6:332:LEU:N	2.53	0.40
1:5:748:ILE:HG22	1:5:750:THR:HG23	2.03	0.40
1:6:410:ILE:HB	1:6:573:TYR:OH	2.22	0.40
1:6:869:ILE:HG22	2:F:230:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:GLU:HA	2:B:205:HIS:CD2	2.56	0.40
2:B:222:ASN:CG	2:B:223:ILE:N	2.75	0.40
2:F:87:LEU:HD13	2:F:171:TRP:HA	2.02	0.40
2:F:137:LEU:HD11	2:F:171:TRP:HZ3	1.84	0.40
1:3:190:ILE:HG12	1:3:291:ILE:HG12	2.03	0.40
1:4:196:ASN:HD22	1:4:200:LYS:HE3	1.85	0.40
1:4:463:ASP:OD1	1:4:466:SER:OG	2.37	0.40
1:1:261:LEU:HD23	1:1:261:LEU:HA	1.87	0.40
1:1:847:ILE:HG12	1:1:864:PHE:HE2	1.87	0.40
1:2:643:GLY:HA3	6:2:1002:AGS:C5	2.51	0.40
1:2:899:LEU:CA	2:B:230:PHE:HB2	2.47	0.40
1:3:390:TYR:CG	1:3:427:CYS:HB3	2.56	0.40
1:3:753:LEU:HD22	1:3:788:LYS:HG3	2.03	0.40
1:4:369:PRO:HA	1:4:370:PRO:HD3	1.90	0.40
1:5:261:LEU:HA	1:5:264:TYR:CE2	2.57	0.40
1:5:670:PHE:HE1	1:5:678:LYS:HB2	1.87	0.40
1:6:815:LEU:HD23	1:6:815:LEU:HA	1.88	0.40
2:B:137:LEU:O	2:B:141:ARG:N	2.55	0.40
2:G:166:GLN:O	2:G:169:ARG:NH1	2.54	0.40
2:E:152:PRO:CG	2:D:121:THR:CG2	2.98	0.40
1:2:241:LYS:HB3	1:2:342:ALA:HB1	2.03	0.40
1:3:798:VAL:O	2:D:221:LYS:NZ	2.52	0.40
1:5:309:ILE:HG23	1:5:312:LEU:HD12	2.04	0.40
2:A:77:VAL:HG21	2:A:118:TYR:CG	2.57	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	1	717/932 (77%)	661 (92%)	53 (7%)	3 (0%)	34 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	716/932 (77%)	666 (93%)	48 (7%)	2 (0%)	41	76
1	3	716/932 (77%)	668 (93%)	43 (6%)	5 (1%)	22	62
1	4	716/932 (77%)	684 (96%)	29 (4%)	3 (0%)	34	71
1	5	707/932 (76%)	679 (96%)	28 (4%)	0	100	100
1	6	716/932 (77%)	669 (93%)	45 (6%)	2 (0%)	41	76
2	A	187/287 (65%)	182 (97%)	5 (3%)	0	100	100
2	B	207/287 (72%)	199 (96%)	7 (3%)	1 (0%)	29	68
2	C	207/287 (72%)	201 (97%)	6 (3%)	0	100	100
2	D	207/287 (72%)	201 (97%)	5 (2%)	1 (0%)	29	68
2	E	207/287 (72%)	196 (95%)	9 (4%)	2 (1%)	15	53
2	F	207/287 (72%)	198 (96%)	9 (4%)	0	100	100
2	G	193/287 (67%)	189 (98%)	4 (2%)	0	100	100
3	a	154/207 (74%)	138 (90%)	15 (10%)	1 (1%)	25	64
3	b	154/207 (74%)	135 (88%)	18 (12%)	1 (1%)	25	64
3	c	154/207 (74%)	138 (90%)	14 (9%)	2 (1%)	12	48
3	d	154/207 (74%)	138 (90%)	14 (9%)	2 (1%)	12	48
3	e	154/207 (74%)	138 (90%)	15 (10%)	1 (1%)	25	64
3	f	154/207 (74%)	140 (91%)	13 (8%)	1 (1%)	25	64
3	g	154/207 (74%)	138 (90%)	13 (8%)	3 (2%)	8	41
All	All	6781/9050 (75%)	6358 (94%)	393 (6%)	30 (0%)	38	71

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	4	761	LYS
3	a	735	GLY
3	g	735	GLY
3	g	761	GLN
3	f	735	GLY
3	e	735	GLY
3	d	735	GLY
3	c	735	GLY
3	c	758	GLU
3	b	735	GLY
1	2	372	VAL

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Mol	Chain	Res	Type
1	3	525	PRO
1	4	372	VAL
2	B	222	ASN
2	E	233	ASP
1	1	758	PHE
1	3	372	VAL
1	4	760	LYS
2	E	232	VAL
1	2	755	ALA
1	3	523	LYS
1	3	895	LYS
3	g	768	TYR
3	d	757	LYS
2	D	222	ASN
1	1	229	ASN
1	1	757	LEU
1	6	754	GLY
1	3	524	GLU
1	6	794	LYS

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	1	642/830 (77%)	622 (97%)	20 (3%)	40	62
1	2	642/830 (77%)	637 (99%)	5 (1%)	81	89
1	3	642/830 (77%)	628 (98%)	14 (2%)	52	70
1	4	642/830 (77%)	637 (99%)	5 (1%)	81	89
1	5	635/830 (76%)	633 (100%)	2 (0%)	92	95
1	6	642/830 (77%)	640 (100%)	2 (0%)	92	95
2	A	174/268 (65%)	173 (99%)	1 (1%)	86	92
2	B	193/268 (72%)	193 (100%)	0	100	100
2	C	193/268 (72%)	191 (99%)	2 (1%)	76	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	193/268 (72%)	193 (100%)	0	100	100
2	E	193/268 (72%)	186 (96%)	7 (4%)	35	60
2	F	193/268 (72%)	192 (100%)	1 (0%)	88	93
2	G	180/268 (67%)	180 (100%)	0	100	100
3	a	144/144 (100%)	139 (96%)	5 (4%)	36	60
3	b	144/144 (100%)	143 (99%)	1 (1%)	84	90
3	c	144/144 (100%)	142 (99%)	2 (1%)	67	80
3	d	144/144 (100%)	142 (99%)	2 (1%)	67	80
3	e	144/144 (100%)	143 (99%)	1 (1%)	84	90
3	f	144/144 (100%)	143 (99%)	1 (1%)	84	90
3	g	144/144 (100%)	143 (99%)	1 (1%)	84	90
All	All	6172/7864 (78%)	6100 (99%)	72 (1%)	72	83

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	224	LEU
1	1	243	THR
1	1	273	LYS
1	1	437	LYS
1	1	441	ILE
1	1	467	LYS
1	1	758	PHE
1	1	761	LYS
1	1	762	LEU
1	1	763	PHE
1	1	765	ASP
1	1	768	ASN
1	1	769	SER
1	1	771	THR
1	1	774	TYR
1	1	777	VAL
1	1	781	VAL
1	1	783	LEU
1	1	791	LYS
1	1	806	VAL
1	2	198	ASN
1	2	200	LYS

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Mol	Chain	Res	Type
1	2	492	VAL
1	2	799	ASN
1	2	897	LYS
1	3	227	ASN
1	3	360	ARG
1	3	516	GLN
1	3	518	TYR
1	3	519	VAL
1	3	520	TYR
1	3	523	LYS
1	3	524	GLU
1	3	529	LEU
1	3	531	ASN
1	3	768	ASN
1	3	822	ARG
1	3	895	LYS
1	3	898	ASN
1	4	299	LYS
1	4	349	ARG
1	4	360	ARG
1	4	393	ASN
1	4	738	ARG
1	5	196	ASN
1	5	897	LYS
1	6	228	LYS
1	6	829	ARG
3	a	724	ASN
3	a	755	GLU
3	a	758	GLU
3	a	760	GLN
3	a	763	ASP
2	A	164	LYS
3	g	724	ASN
3	f	724	ASN
2	F	206	LEU
3	e	724	ASN
2	E	87	LEU
2	E	88	LEU
2	E	91	GLU
2	E	92	ILE
2	E	202	THR
2	E	228	TYR

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Mol	Chain	Res	Type
2	E	233	ASP
3	d	724	ASN
3	d	755	GLU
3	c	705	SER
3	c	724	ASN
2	C	207	SER
2	C	210	MET
3	b	724	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	509	ASN
1	1	557	ASN
1	1	560	ASN
1	1	768	ASN
1	1	834	ASN
1	2	198	ASN
1	2	431	GLN
1	2	560	ASN
1	2	606	ASN
1	2	661	ASN
1	2	704	HIS
1	2	716	HIS
1	2	799	ASN
1	2	893	ASN
1	3	227	ASN
1	3	262	GLN
1	3	516	GLN
1	3	560	ASN
1	3	661	ASN
1	3	694	GLN
1	3	725	GLN
1	4	196	ASN
1	4	393	ASN
1	4	560	ASN
1	4	566	GLN
1	4	657	ASN
1	4	704	HIS
1	4	834	ASN
1	5	196	ASN
1	5	270	ASN

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Mol	Chain	Res	Type
1	5	560	ASN
1	5	606	ASN
1	5	674	HIS
1	5	768	ASN
1	6	198	ASN
1	6	290	ASN
1	6	388	ASN
1	6	537	GLN
1	6	836	GLN
2	B	134	HIS
2	B	188	HIS
2	B	205	HIS
3	a	717	ASN
3	a	724	ASN
2	A	134	HIS
2	A	188	HIS
3	g	717	ASN
3	g	724	ASN
2	G	134	HIS
2	G	188	HIS
3	f	717	ASN
3	f	724	ASN
3	f	787	HIS
2	F	134	HIS
2	F	222	ASN
3	e	717	ASN
3	e	724	ASN
3	e	783	ASN
3	e	787	HIS
2	E	134	HIS
2	E	188	HIS
2	E	222	ASN
3	d	717	ASN
3	d	724	ASN
2	D	134	HIS
2	D	188	HIS
2	D	205	HIS
3	c	717	ASN
3	c	724	ASN
2	C	134	HIS
2	C	188	HIS
2	C	222	ASN

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Mol	Chain	Res	Type
3	b	717	ASN
3	b	724	ASN

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	AGS	1	1001	-	26,33,33	1.88	3 (11%)	26,52,52	1.57	4 (15%)
6	AGS	4	1003	-	26,33,33	0.79	0	26,52,52	1.31	2 (7%)
6	AGS	3	1001	-	26,33,33	0.77	0	26,52,52	1.31	2 (7%)
6	AGS	4	1002	-	26,33,33	0.89	0	26,52,52	1.61	2 (7%)
6	AGS	4	1001	-	26,33,33	0.77	0	26,52,52	1.31	2 (7%)
6	AGS	6	1002	-	26,33,33	0.88	0	26,52,52	1.62	2 (7%)
6	AGS	2	1002	-	26,33,33	0.89	0	26,52,52	1.62	2 (7%)
6	AGS	1	1002	-	26,33,33	0.88	0	26,52,52	1.61	2 (7%)
6	AGS	2	1001	-	26,33,33	1.88	4 (15%)	26,52,52	1.58	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	AGS	5	1001	-	26,33,33	0.88	0	26,52,52	1.62	2 (7%)
6	AGS	6	1001	-	26,33,33	0.78	1 (3%)	26,52,52	1.31	2 (7%)
6	AGS	3	1002	-	26,33,33	0.88	0	26,52,52	1.62	2 (7%)

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
6	AGS	1	1001	-	-	6/17/38/38	0/3/3/3
6	AGS	4	1003	-	-	6/17/38/38	0/3/3/3
6	AGS	3	1001	-	-	6/17/38/38	0/3/3/3
6	AGS	4	1002	-	-	5/17/38/38	0/3/3/3
6	AGS	4	1001	-	-	6/17/38/38	0/3/3/3
6	AGS	6	1002	-	-	5/17/38/38	0/3/3/3
6	AGS	2	1002	-	-	5/17/38/38	0/3/3/3
6	AGS	1	1002	-	-	5/17/38/38	0/3/3/3
6	AGS	2	1001	-	-	7/17/38/38	0/3/3/3
6	AGS	5	1001	-	-	5/17/38/38	0/3/3/3
6	AGS	6	1001	-	-	6/17/38/38	0/3/3/3
6	AGS	3	1002	-	-	5/17/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	1001	AGS	PG-S1G	7.94	2.07	1.90
6	2	1001	AGS	PG-S1G	7.93	2.07	1.90
6	2	1001	AGS	C5-C4	2.50	1.47	1.40
6	1	1001	AGS	C5-C4	2.50	1.47	1.40
6	2	1001	AGS	PG-O2G	2.02	1.61	1.54
6	1	1001	AGS	PG-O2G	2.02	1.61	1.54
6	2	1001	AGS	PG-O3G	-2.01	1.48	1.54
6	6	1001	AGS	PG-S1G	2.00	1.95	1.90

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	1002	AGS	PA-O3A-PB	-7.13	108.36	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	5	1001	AGS	PA-O3A-PB	-7.12	108.39	132.83
6	1	1002	AGS	PA-O3A-PB	-7.12	108.40	132.83
6	6	1002	AGS	PA-O3A-PB	-7.11	108.42	132.83
6	4	1002	AGS	PA-O3A-PB	-7.11	108.43	132.83
6	3	1002	AGS	PA-O3A-PB	-7.11	108.44	132.83
6	4	1003	AGS	PA-O3A-PB	-5.24	114.86	132.83
6	4	1001	AGS	PA-O3A-PB	-5.23	114.89	132.83
6	6	1001	AGS	PA-O3A-PB	-5.22	114.92	132.83
6	3	1001	AGS	PA-O3A-PB	-5.21	114.94	132.83
6	2	1001	AGS	PA-O3A-PB	-3.61	120.45	132.83
6	1	1001	AGS	PA-O3A-PB	-3.60	120.46	132.83
6	2	1001	AGS	C3'-C2'-C1'	3.39	106.08	100.98
6	1	1001	AGS	C3'-C2'-C1'	3.37	106.05	100.98
6	1	1001	AGS	N3-C2-N1	-3.18	123.70	128.68
6	2	1001	AGS	N3-C2-N1	-3.18	123.72	128.68
6	2	1001	AGS	C4-C5-N7	-2.70	106.58	109.40
6	1	1001	AGS	C4-C5-N7	-2.66	106.63	109.40
6	3	1002	AGS	C5-C6-N6	2.28	123.82	120.35
6	4	1003	AGS	C5-C6-N6	2.25	123.77	120.35
6	4	1001	AGS	C5-C6-N6	2.23	123.75	120.35
6	3	1001	AGS	C5-C6-N6	2.22	123.72	120.35
6	5	1001	AGS	C5-C6-N6	2.20	123.70	120.35
6	6	1002	AGS	C5-C6-N6	2.20	123.69	120.35
6	6	1001	AGS	C5-C6-N6	2.19	123.67	120.35
6	1	1002	AGS	C5-C6-N6	2.16	123.63	120.35
6	4	1002	AGS	C5-C6-N6	2.15	123.62	120.35
6	2	1002	AGS	C5-C6-N6	2.15	123.61	120.35

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	1	1001	AGS	PB-O3B-PG-O2G
6	1	1001	AGS	PB-O3B-PG-O3G
6	1	1001	AGS	C5'-O5'-PA-O1A
6	1	1001	AGS	C5'-O5'-PA-O2A
6	1	1002	AGS	PB-O3B-PG-O2G
6	1	1002	AGS	PB-O3B-PG-O3G
6	1	1002	AGS	C5'-O5'-PA-O3A
6	2	1001	AGS	C5'-O5'-PA-O1A
6	2	1001	AGS	O4'-C4'-C5'-O5'
6	2	1002	AGS	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
6	2	1002	AGS	PB-O3B-PG-O3G
6	2	1002	AGS	C5'-O5'-PA-O3A
6	3	1001	AGS	C5'-O5'-PA-O1A
6	3	1001	AGS	C5'-O5'-PA-O2A
6	3	1002	AGS	PB-O3B-PG-O2G
6	3	1002	AGS	PB-O3B-PG-O3G
6	3	1002	AGS	C5'-O5'-PA-O3A
6	4	1001	AGS	C5'-O5'-PA-O1A
6	4	1001	AGS	C5'-O5'-PA-O2A
6	4	1002	AGS	PB-O3B-PG-O2G
6	4	1002	AGS	PB-O3B-PG-O3G
6	4	1002	AGS	C5'-O5'-PA-O3A
6	4	1003	AGS	C5'-O5'-PA-O1A
6	4	1003	AGS	C5'-O5'-PA-O2A
6	5	1001	AGS	PB-O3B-PG-O2G
6	5	1001	AGS	PB-O3B-PG-O3G
6	5	1001	AGS	C5'-O5'-PA-O3A
6	6	1001	AGS	C5'-O5'-PA-O1A
6	6	1001	AGS	C5'-O5'-PA-O2A
6	6	1002	AGS	PB-O3B-PG-O2G
6	6	1002	AGS	PB-O3B-PG-O3G
6	6	1002	AGS	C5'-O5'-PA-O3A
6	1	1001	AGS	C5'-O5'-PA-O3A
6	1	1002	AGS	C5'-O5'-PA-O2A
6	2	1001	AGS	C5'-O5'-PA-O2A
6	2	1002	AGS	C5'-O5'-PA-O2A
6	3	1002	AGS	C5'-O5'-PA-O2A
6	4	1002	AGS	C5'-O5'-PA-O2A
6	5	1001	AGS	C5'-O5'-PA-O2A
6	6	1002	AGS	C5'-O5'-PA-O2A
6	2	1001	AGS	C3'-C4'-C5'-O5'
6	3	1001	AGS	PB-O3A-PA-O1A
6	3	1001	AGS	PB-O3A-PA-O2A
6	4	1001	AGS	PB-O3A-PA-O1A
6	4	1001	AGS	PB-O3A-PA-O2A
6	4	1003	AGS	PB-O3A-PA-O1A
6	4	1003	AGS	PB-O3A-PA-O2A
6	6	1001	AGS	PB-O3A-PA-O1A
6	6	1001	AGS	PB-O3A-PA-O2A
6	1	1002	AGS	O4'-C4'-C5'-O5'
6	3	1002	AGS	O4'-C4'-C5'-O5'
6	4	1002	AGS	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
6	5	1001	AGS	O4'-C4'-C5'-O5'
6	6	1002	AGS	O4'-C4'-C5'-O5'
6	2	1001	AGS	PB-O3A-PA-O1A
6	2	1002	AGS	O4'-C4'-C5'-O5'
6	3	1001	AGS	O4'-C4'-C5'-O5'
6	4	1003	AGS	O4'-C4'-C5'-O5'
6	6	1001	AGS	O4'-C4'-C5'-O5'
6	2	1001	AGS	C5'-O5'-PA-O3A
6	3	1001	AGS	C5'-O5'-PA-O3A
6	4	1001	AGS	C5'-O5'-PA-O3A
6	4	1003	AGS	C5'-O5'-PA-O3A
6	6	1001	AGS	C5'-O5'-PA-O3A
6	1	1001	AGS	O4'-C4'-C5'-O5'
6	4	1001	AGS	O4'-C4'-C5'-O5'
6	2	1001	AGS	PB-O3A-PA-O2A

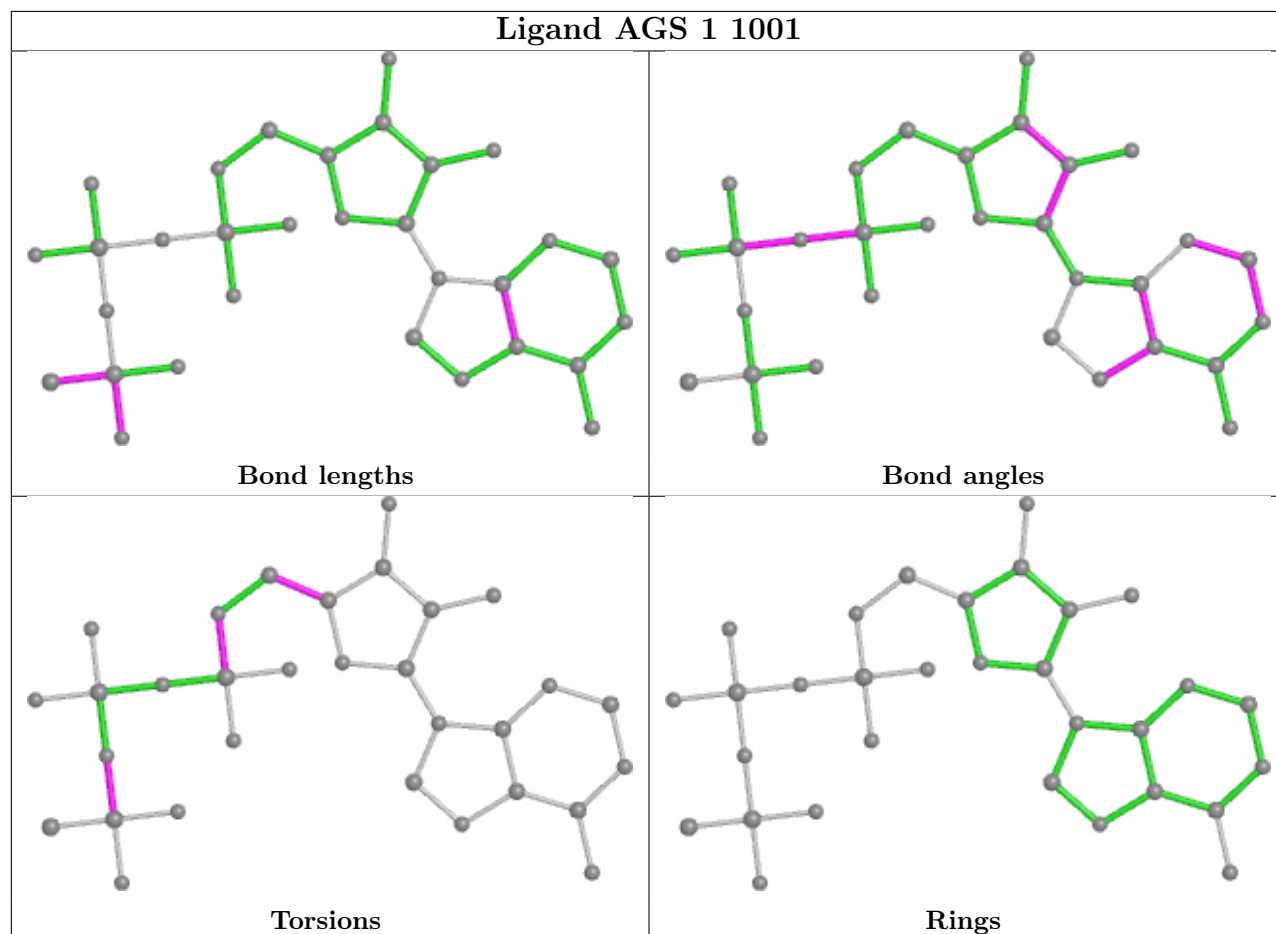
There are no ring outliers.

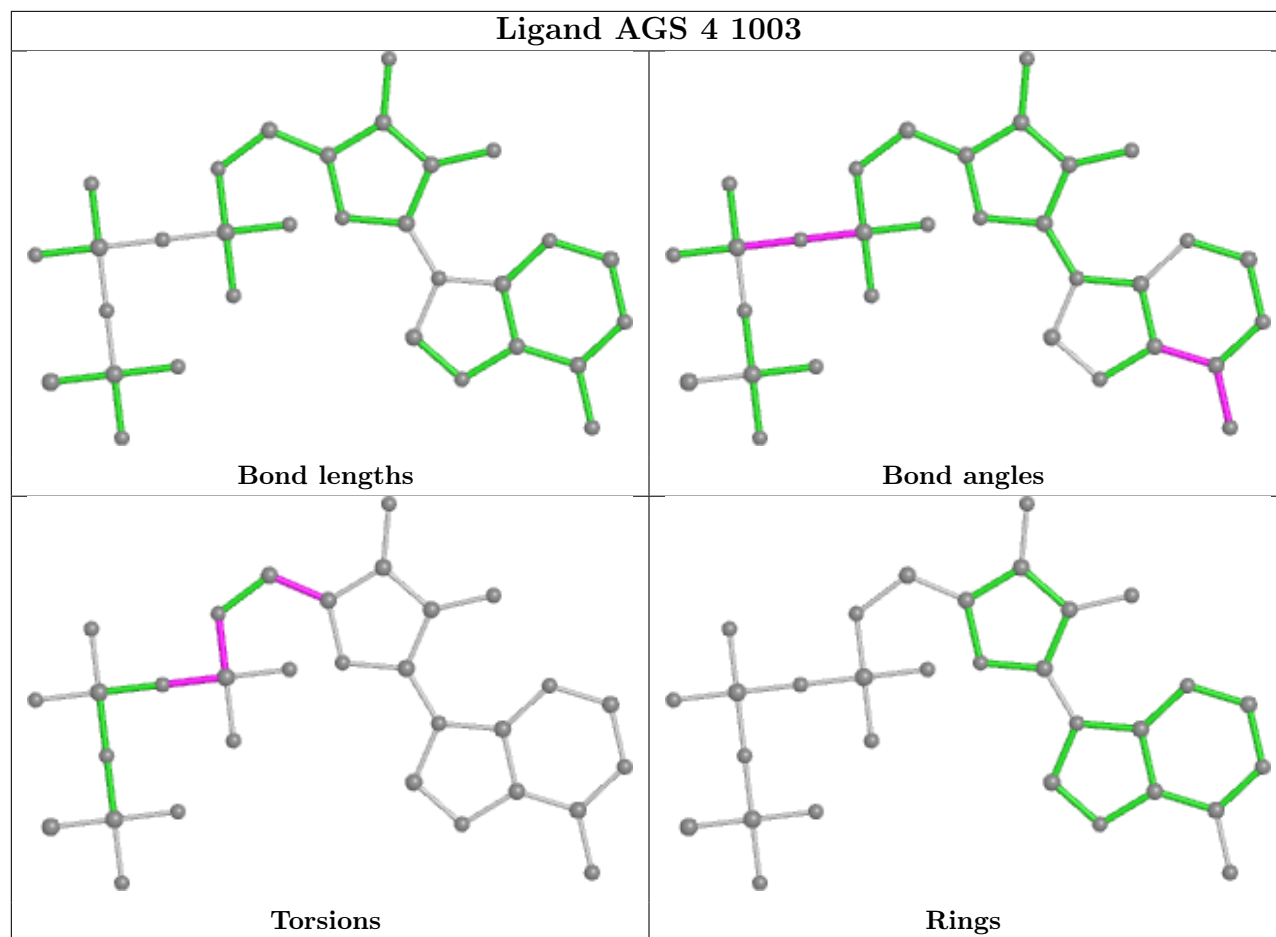
12 monomers are involved in 57 short contacts:

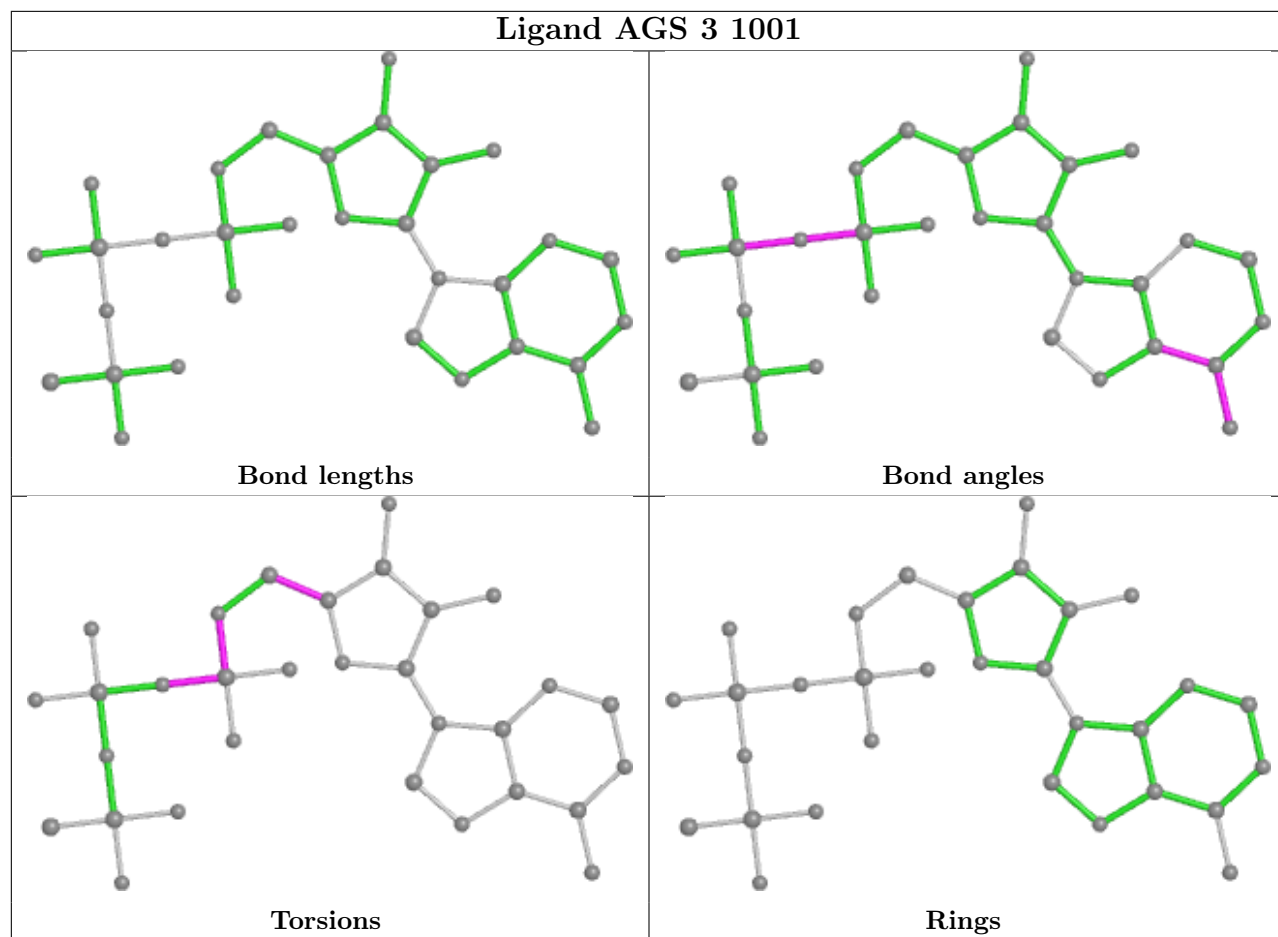
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	1001	AGS	3	0
6	4	1003	AGS	5	0
6	3	1001	AGS	3	0
6	4	1002	AGS	4	0
6	4	1001	AGS	2	0
6	6	1002	AGS	5	0
6	2	1002	AGS	8	0
6	1	1002	AGS	5	0
6	2	1001	AGS	6	0
6	5	1001	AGS	6	0
6	6	1001	AGS	2	0
6	3	1002	AGS	8	0

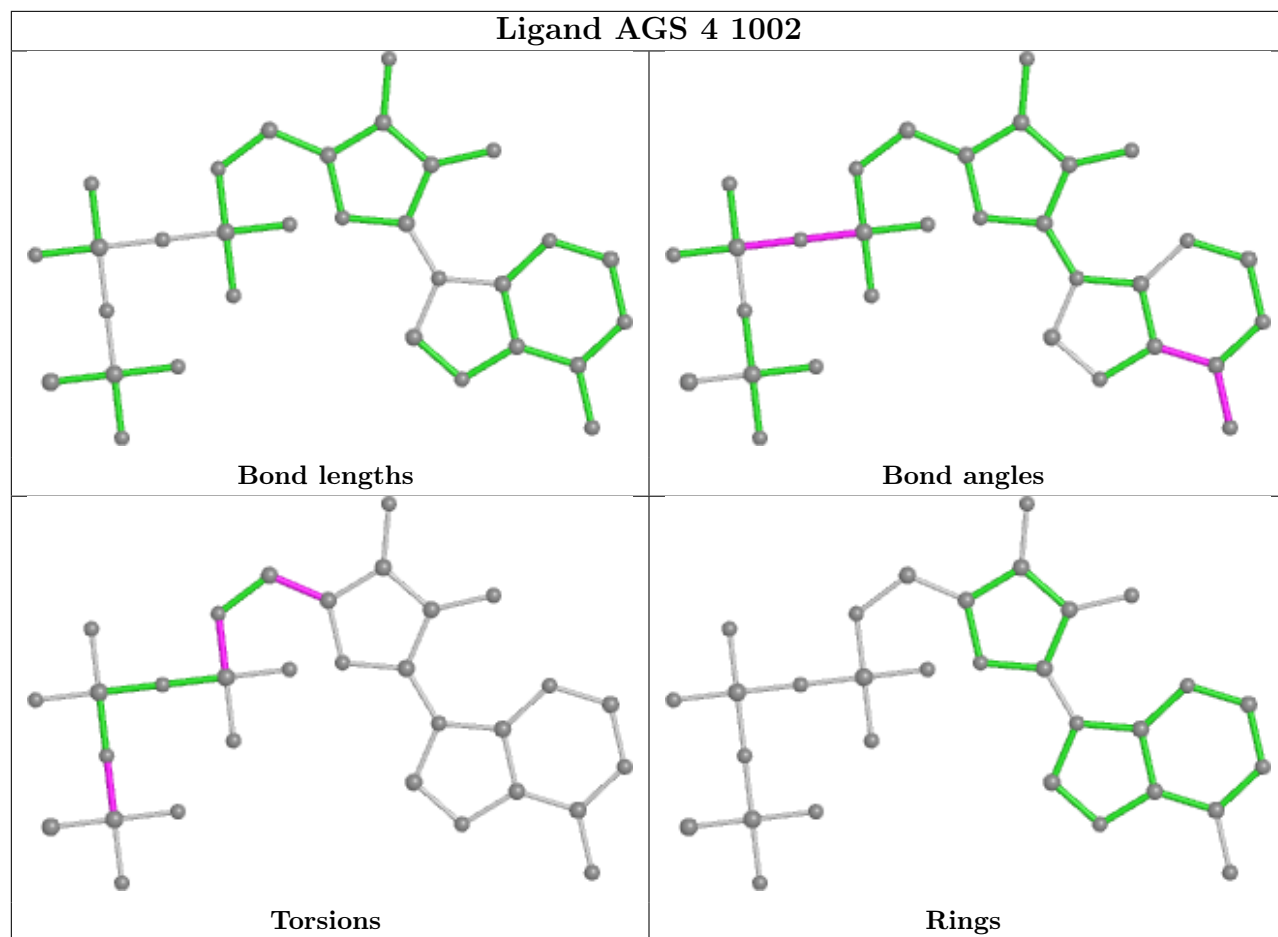
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

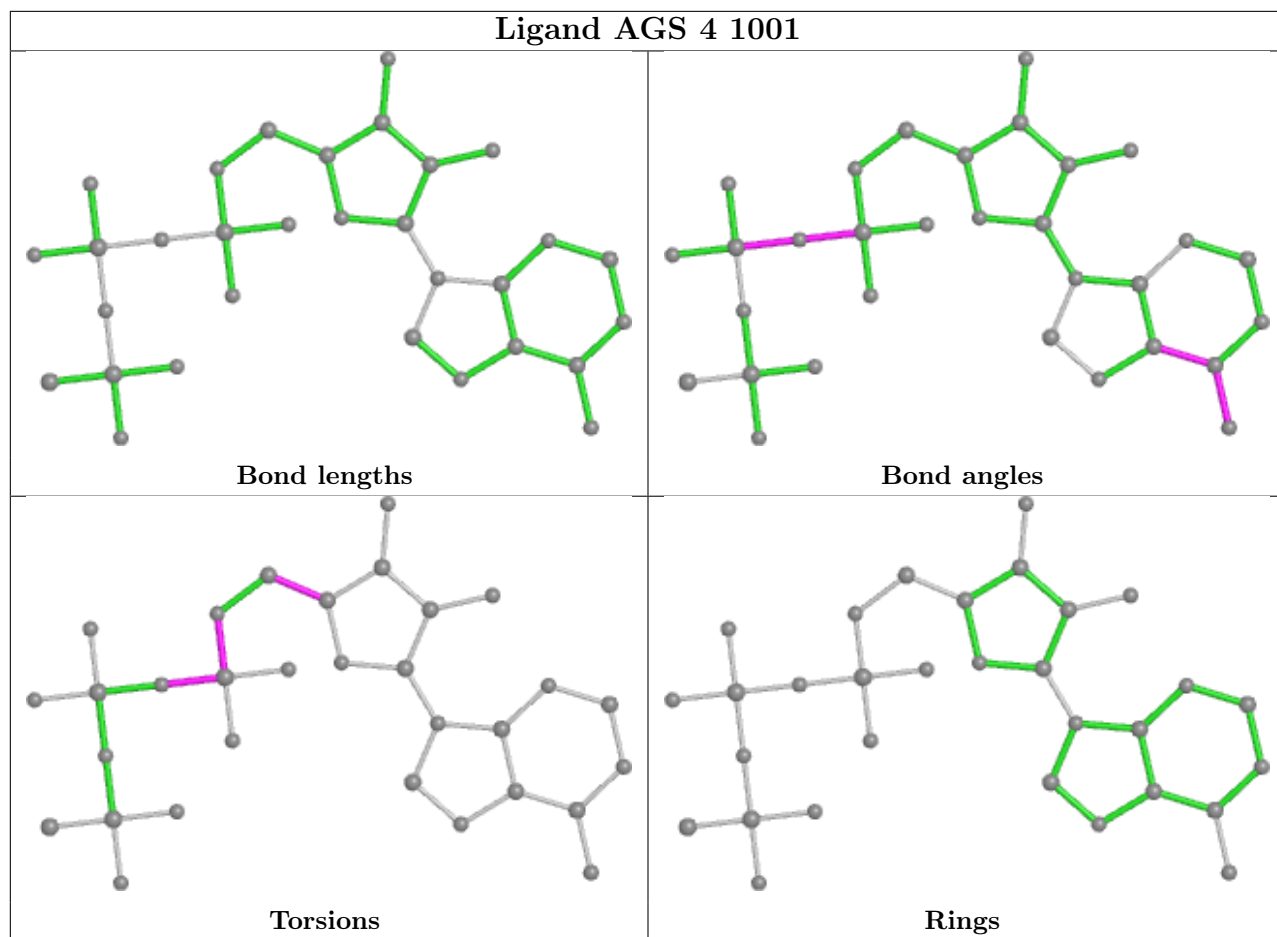
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

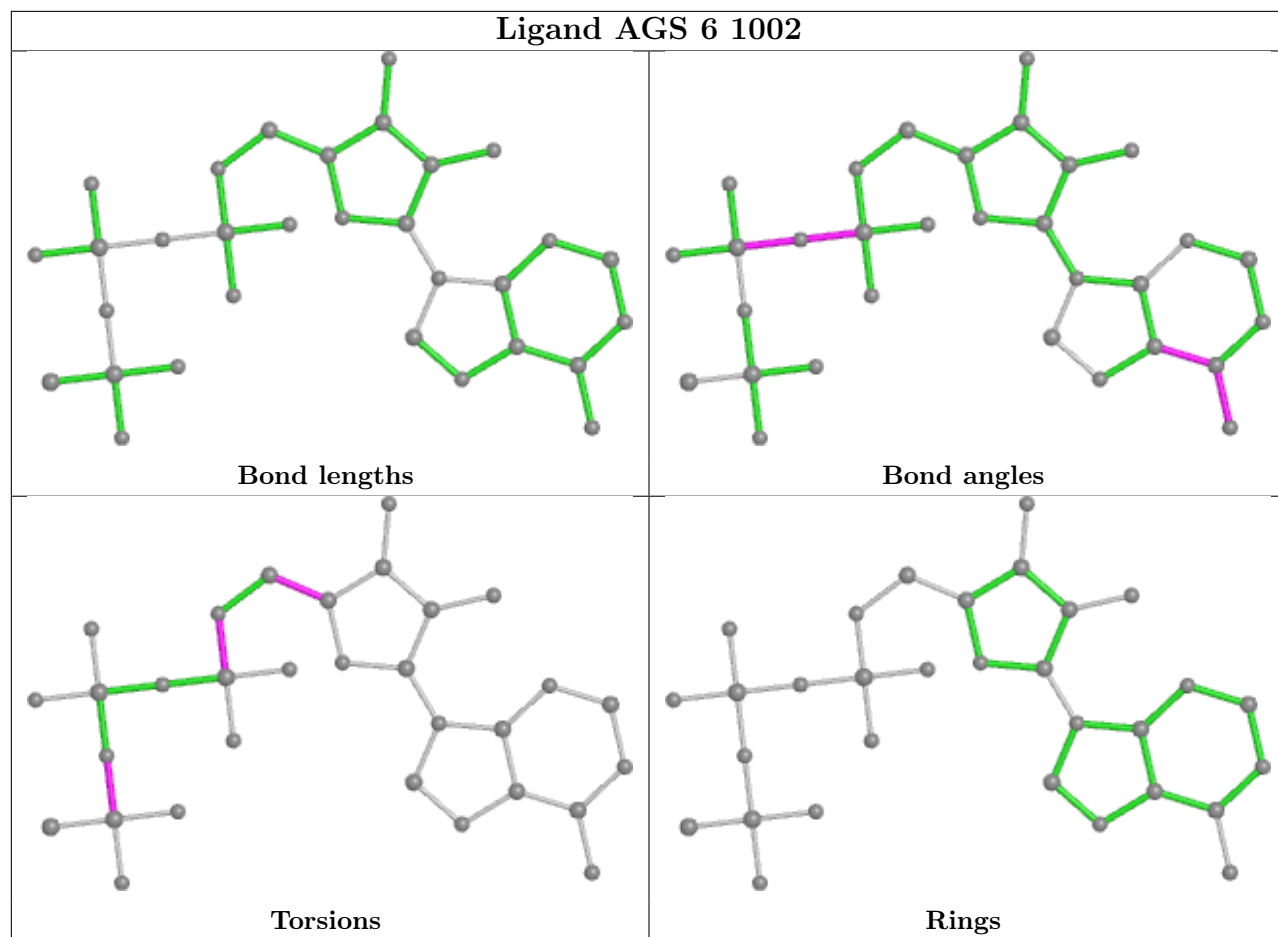


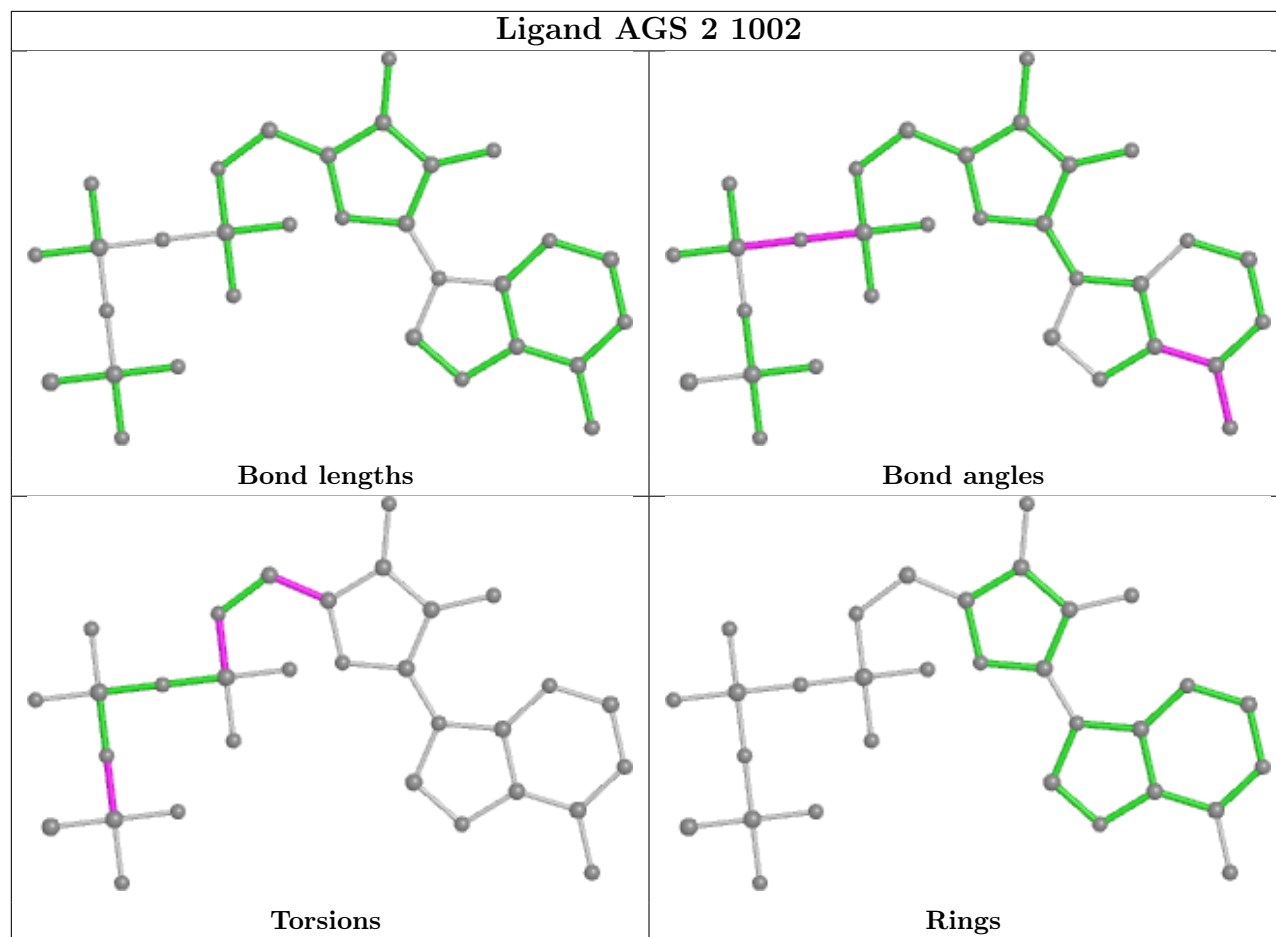


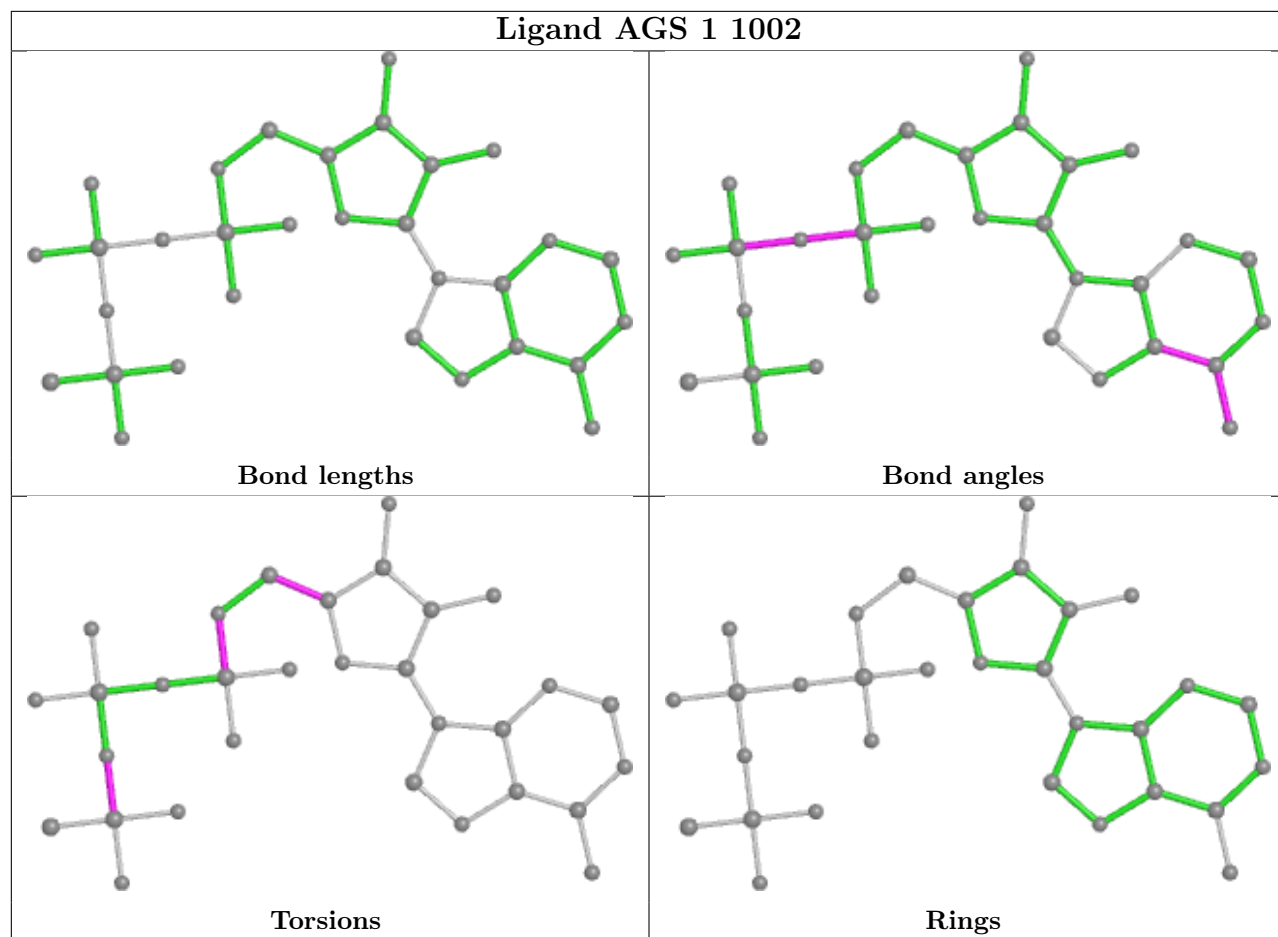


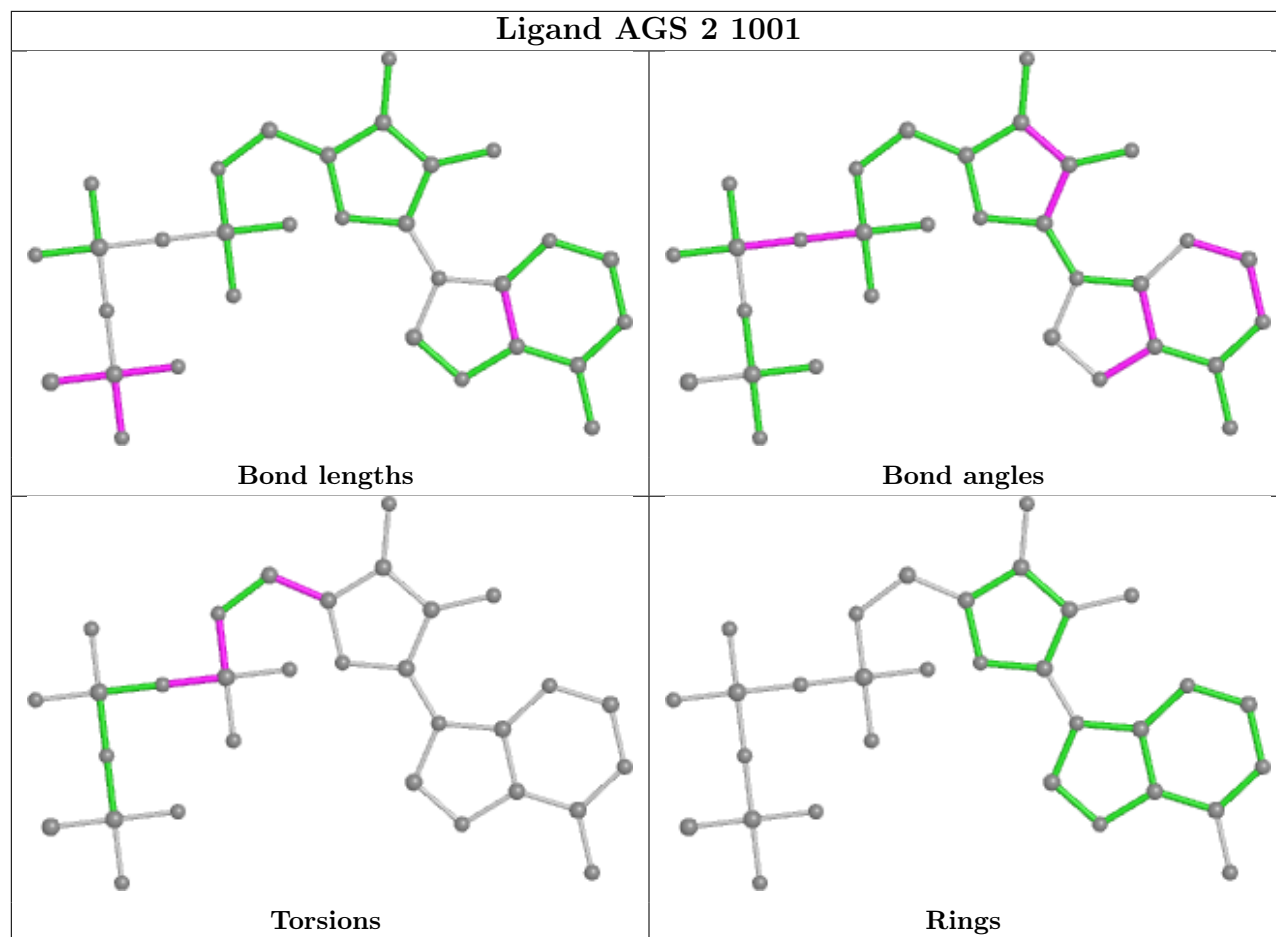


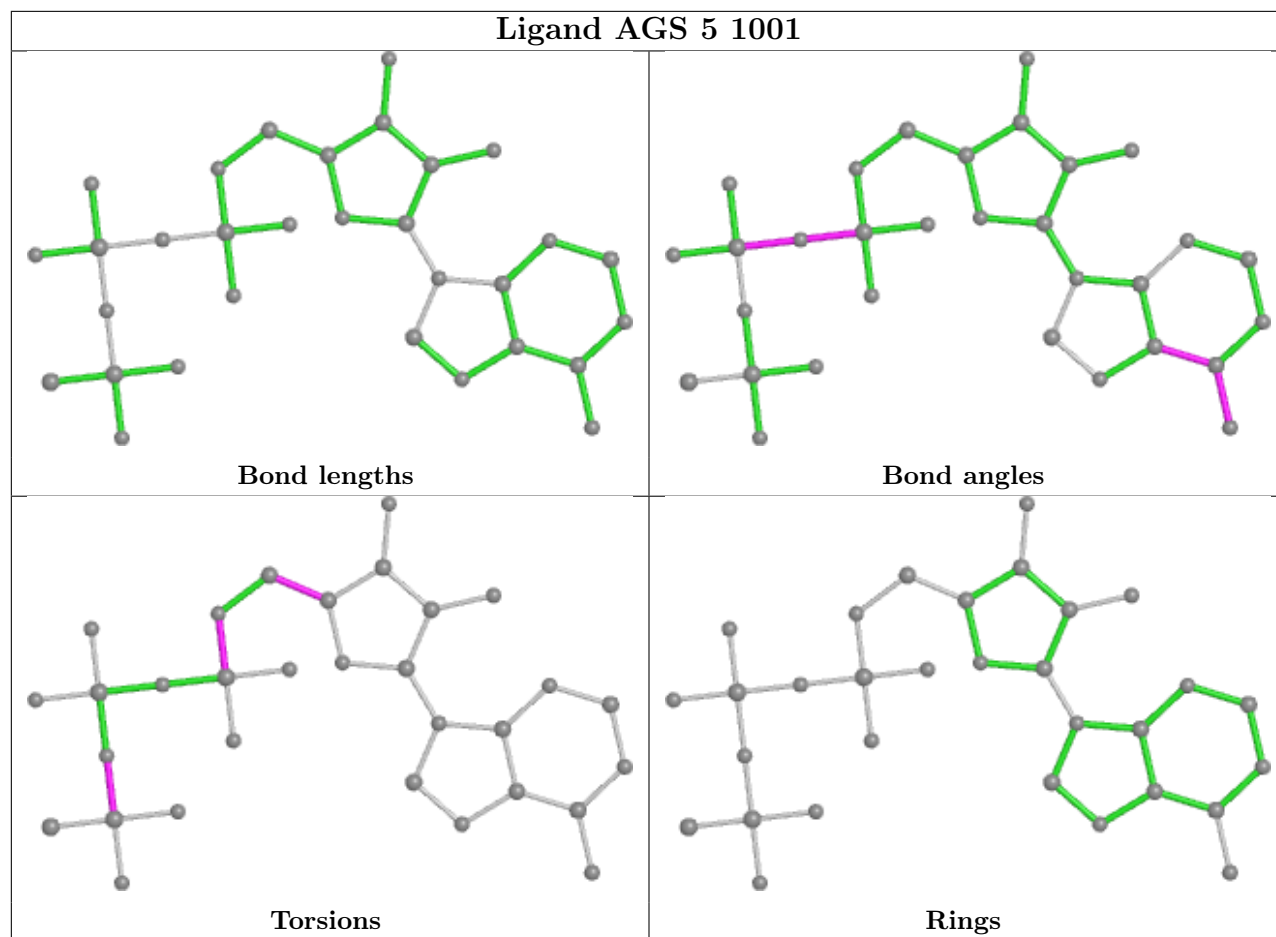


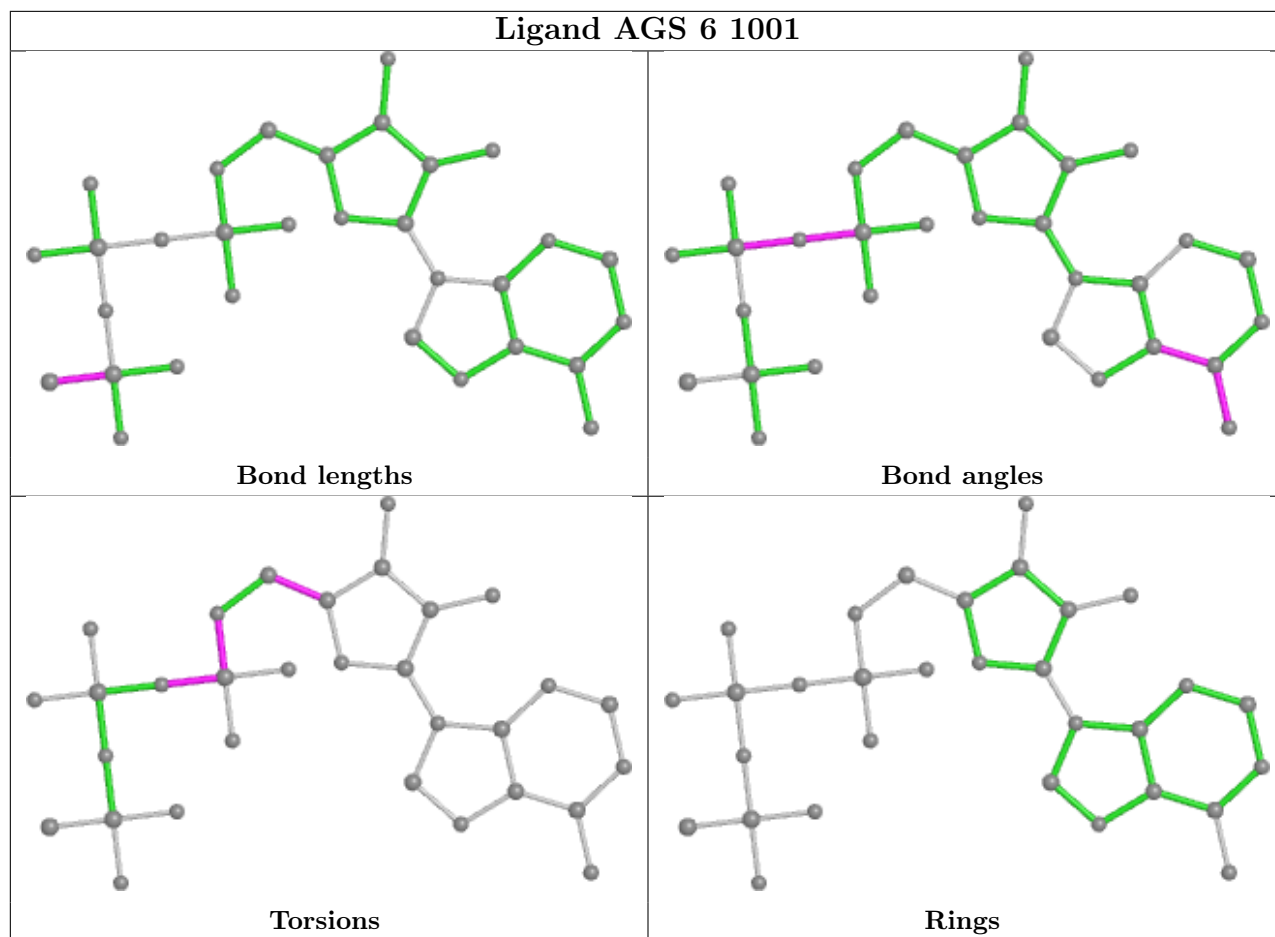


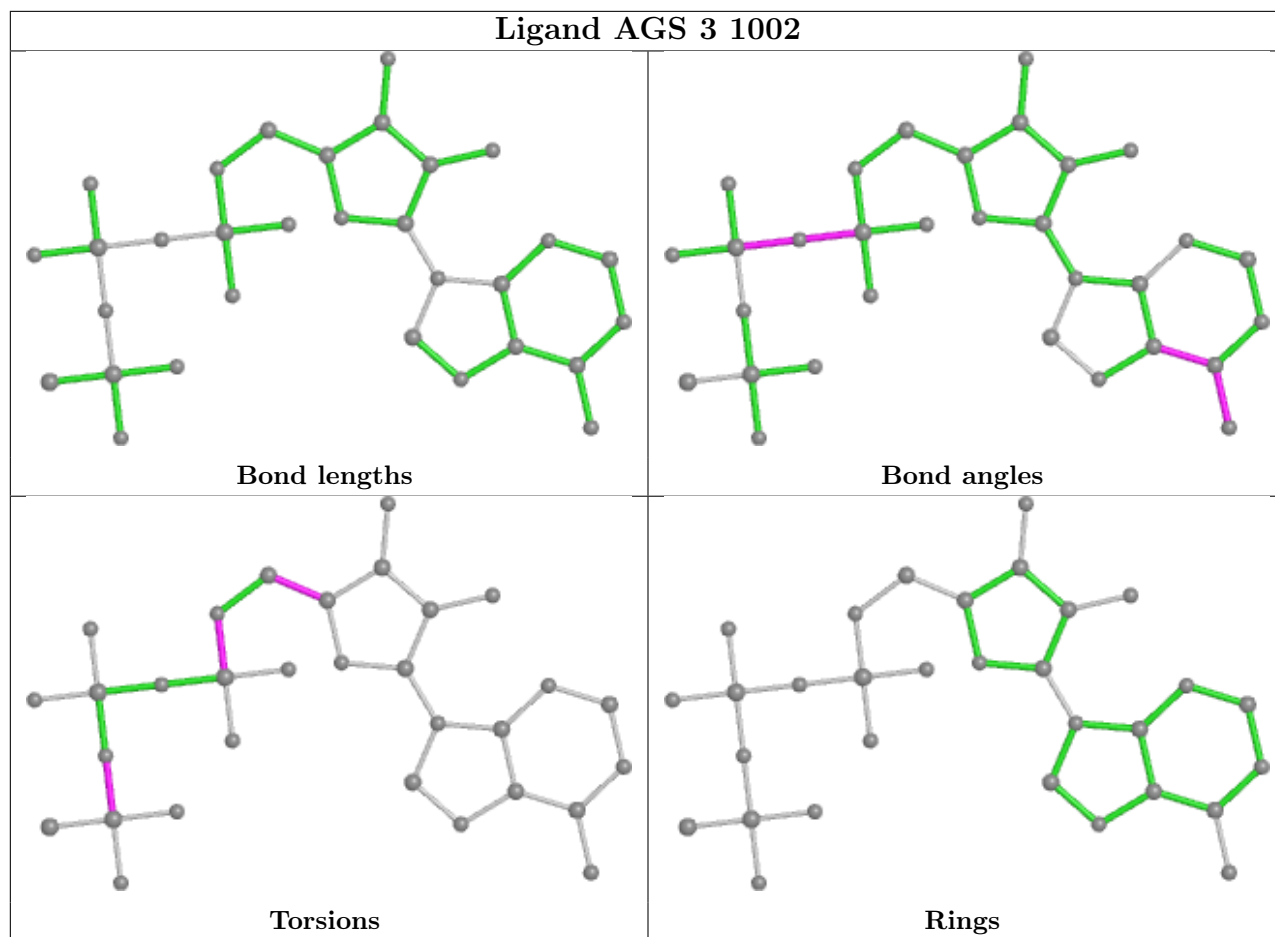












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	h	1
5	i	1
5	j	1
5	l	1
5	k	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	h	966:UNK	C	986:UNK	N	51.66

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	964:UNK	C	988:UNK	N	42.81
1	j	973:UNK	C	988:UNK	N	34.37
1	l	969:UNK	C	982:UNK	N	21.02
1	k	974:UNK	C	980:UNK	N	17.70

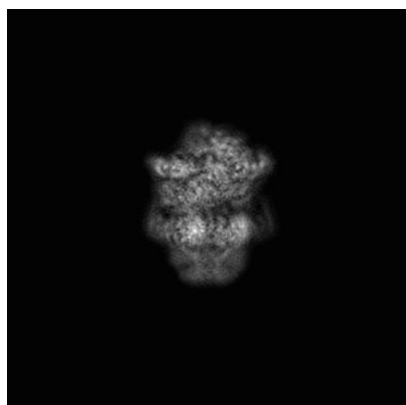
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8951. These allow visual inspection of the internal detail of the map and identification of artifacts.

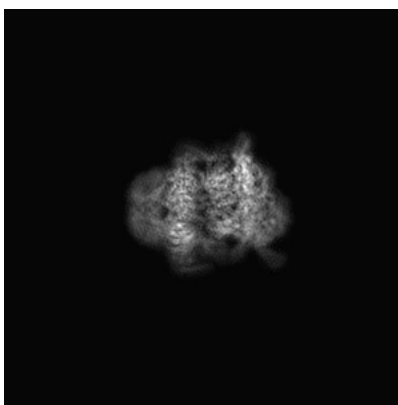
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

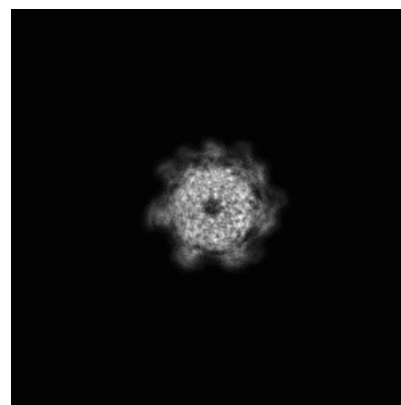
6.1.1 Primary map



X



Y

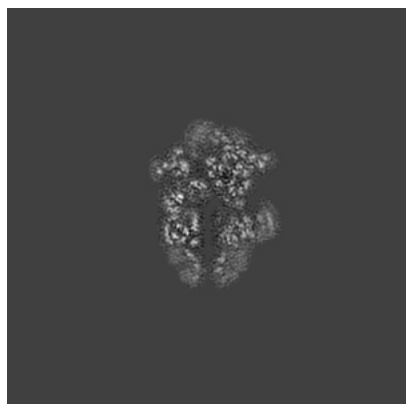


Z

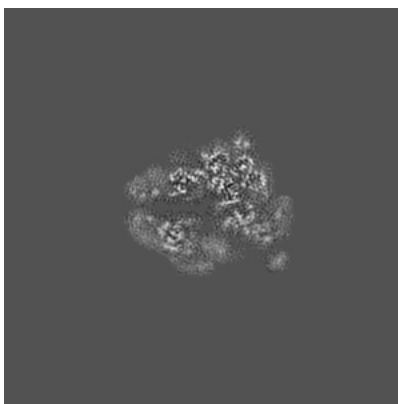
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

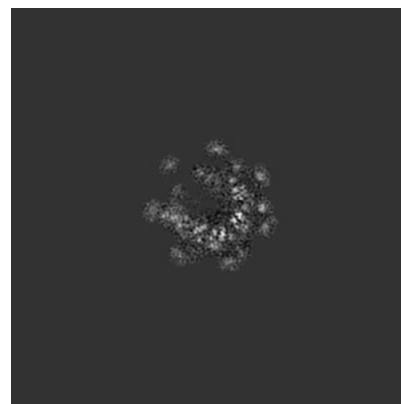
6.2.1 Primary map



X Index: 240



Y Index: 240

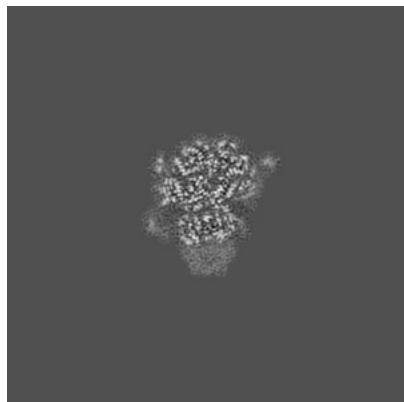


Z Index: 240

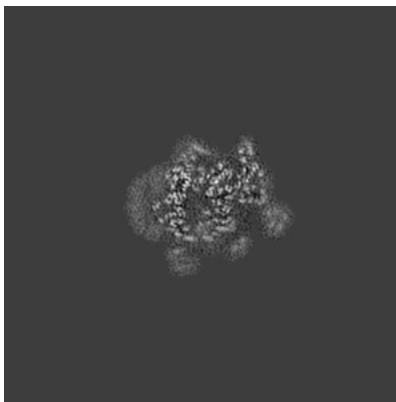
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 276



Y Index: 219



Z Index: 289

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

6.4 Orthogonal surface views [i](#)

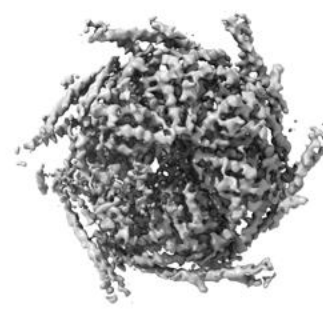
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0424. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

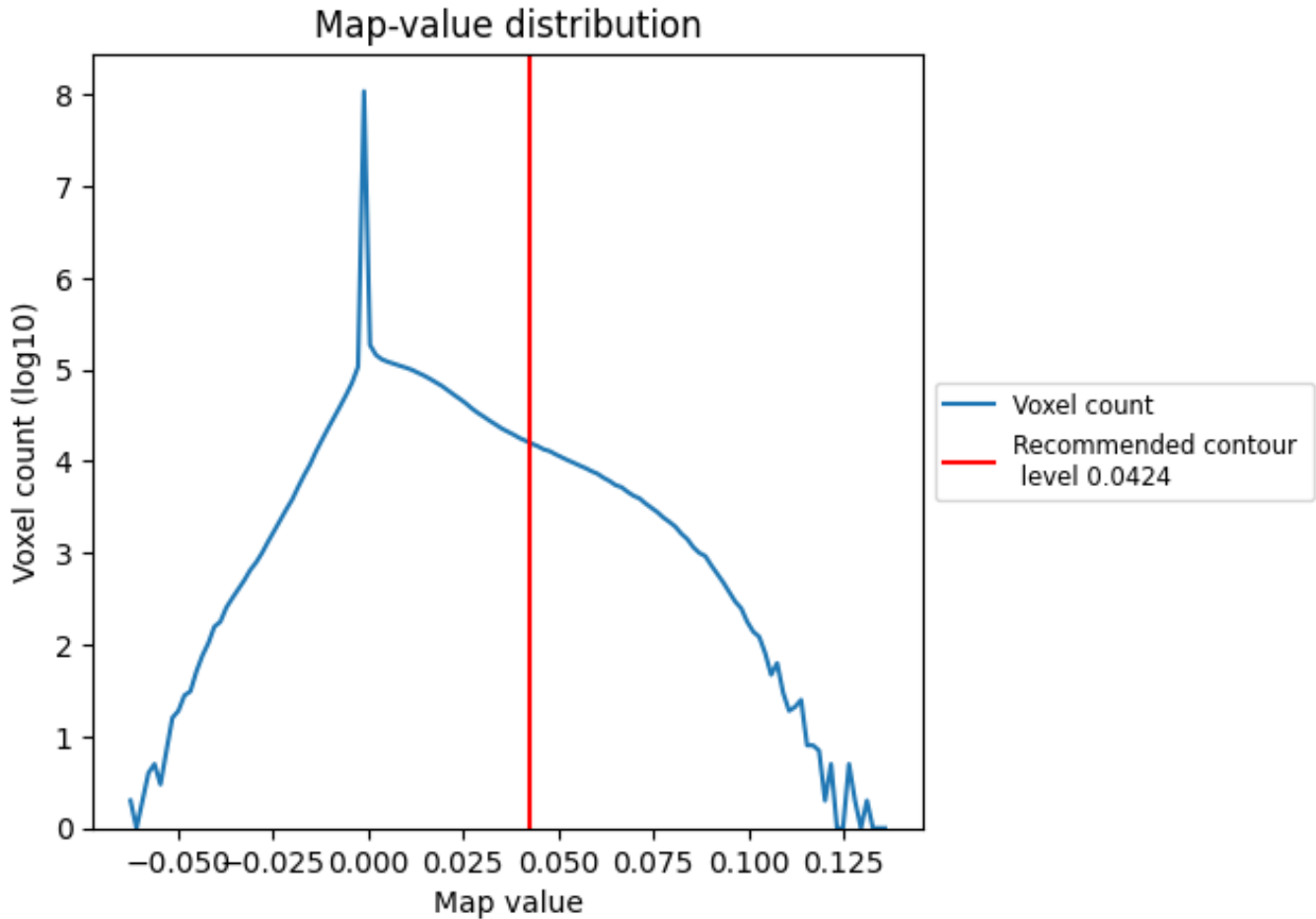
6.5 Mask visualisation

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

7 Map analysis [i](#)

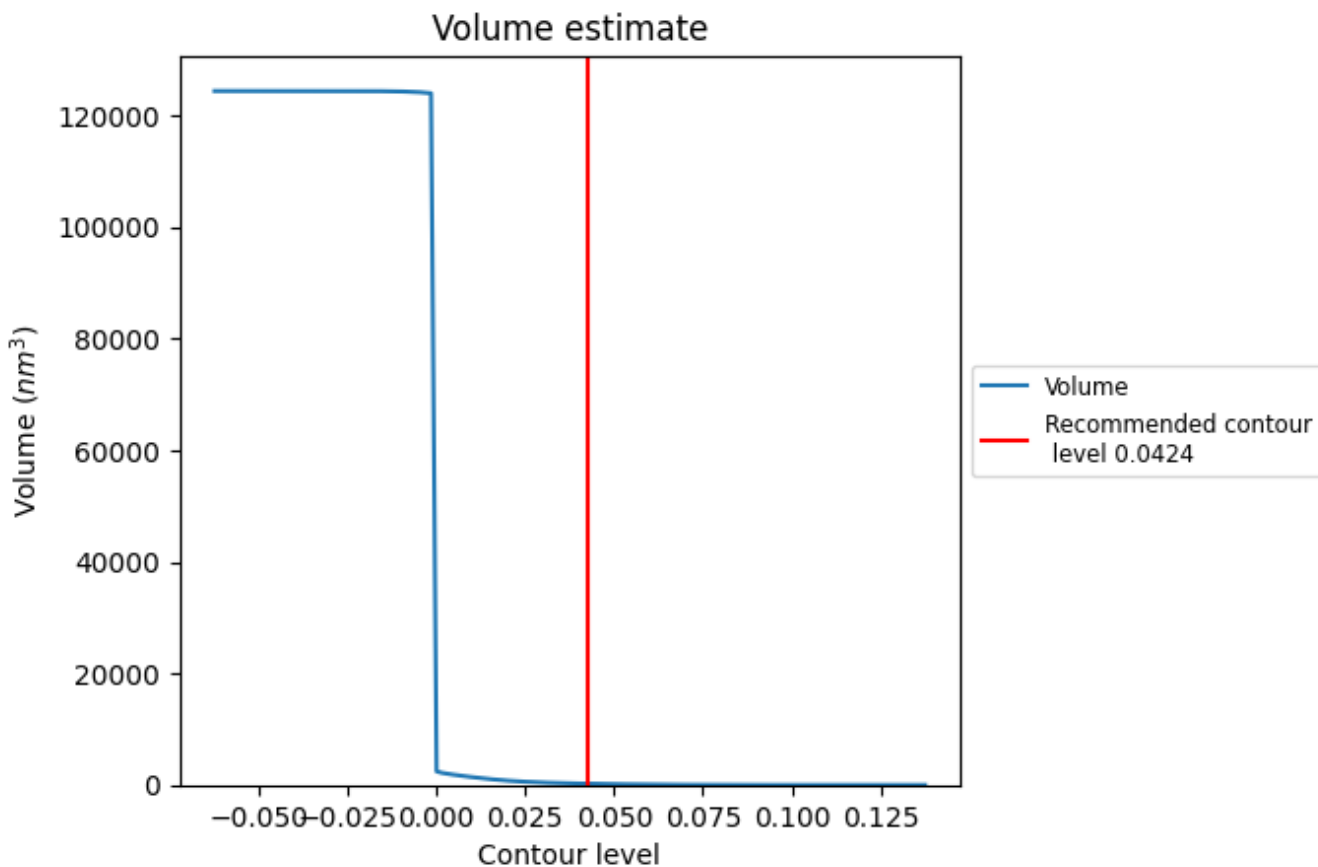
This section contains the results of statistical analysis of the map.

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.

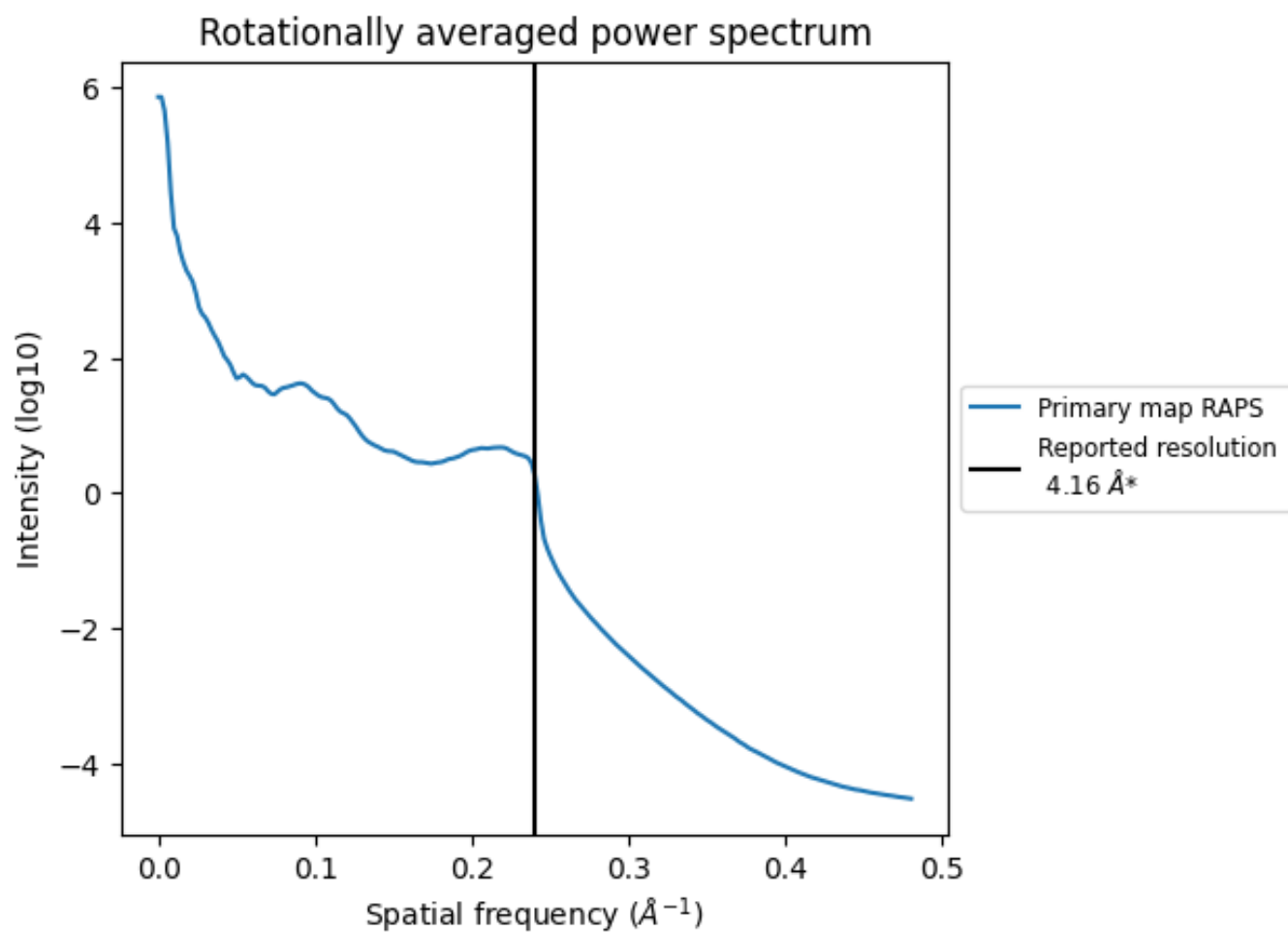
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 226 nm^3 ; this corresponds to an approximate mass of 204 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 0.240\AA^{-1}

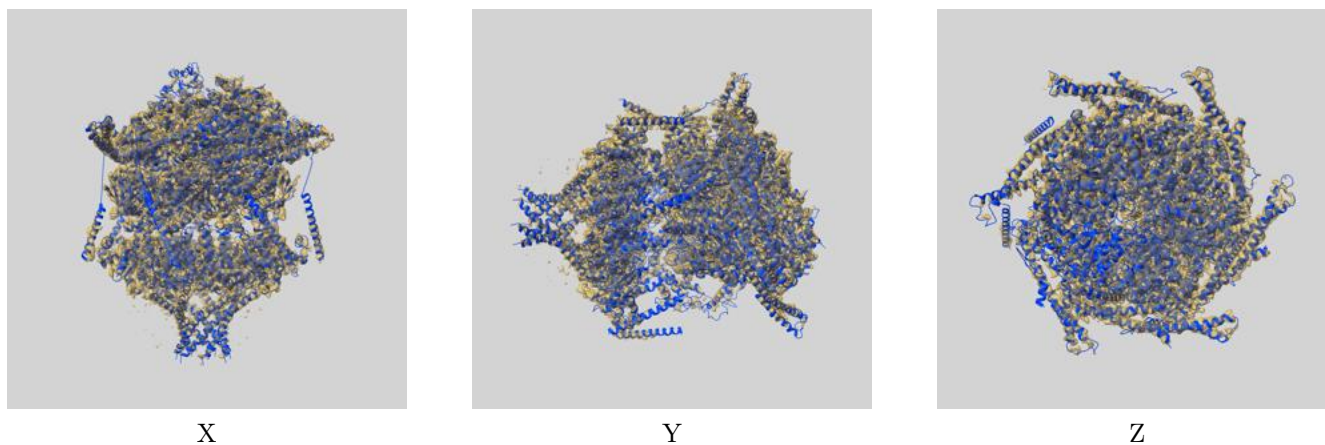
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

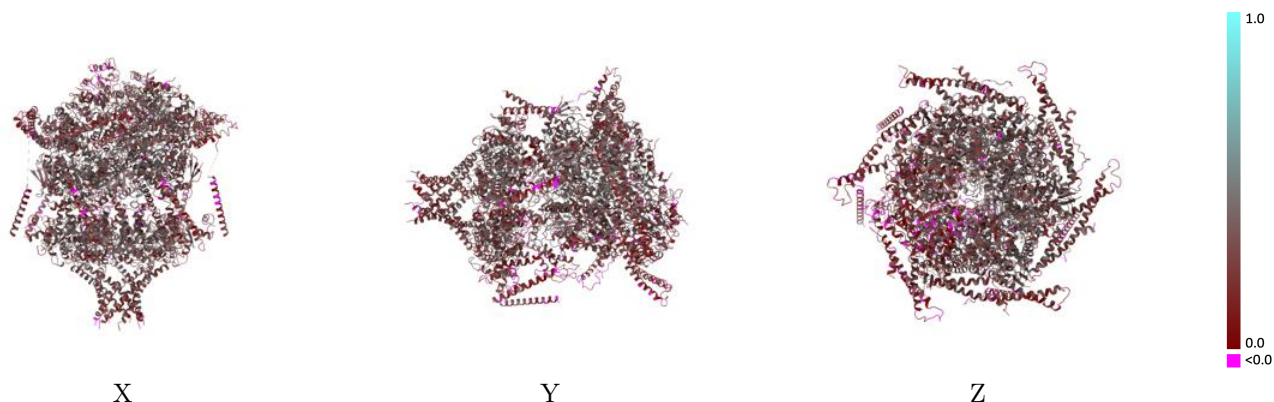
This section contains information regarding the fit between EMDB map EMD-8951 and PDB model 6E10. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



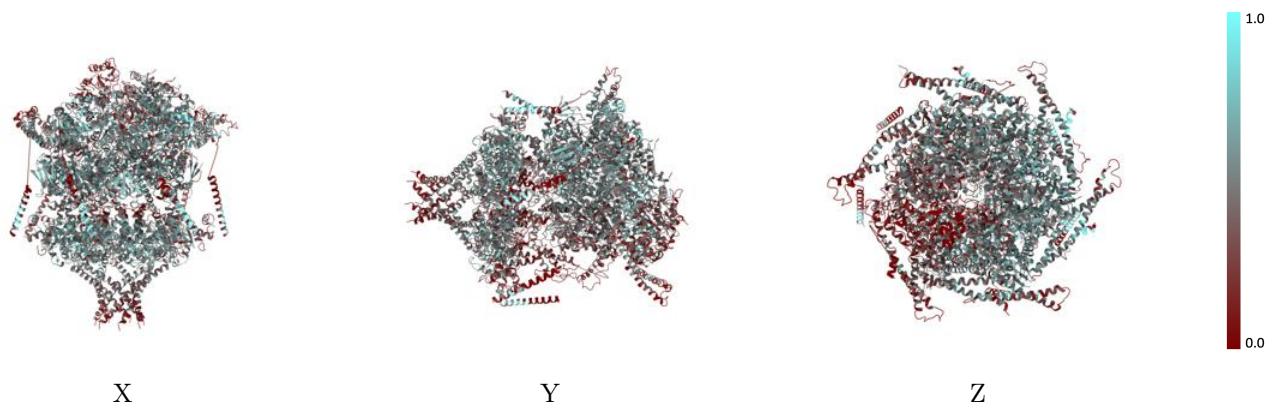
The images above show the 3D surface view of the map at the recommended contour level 0.0424 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



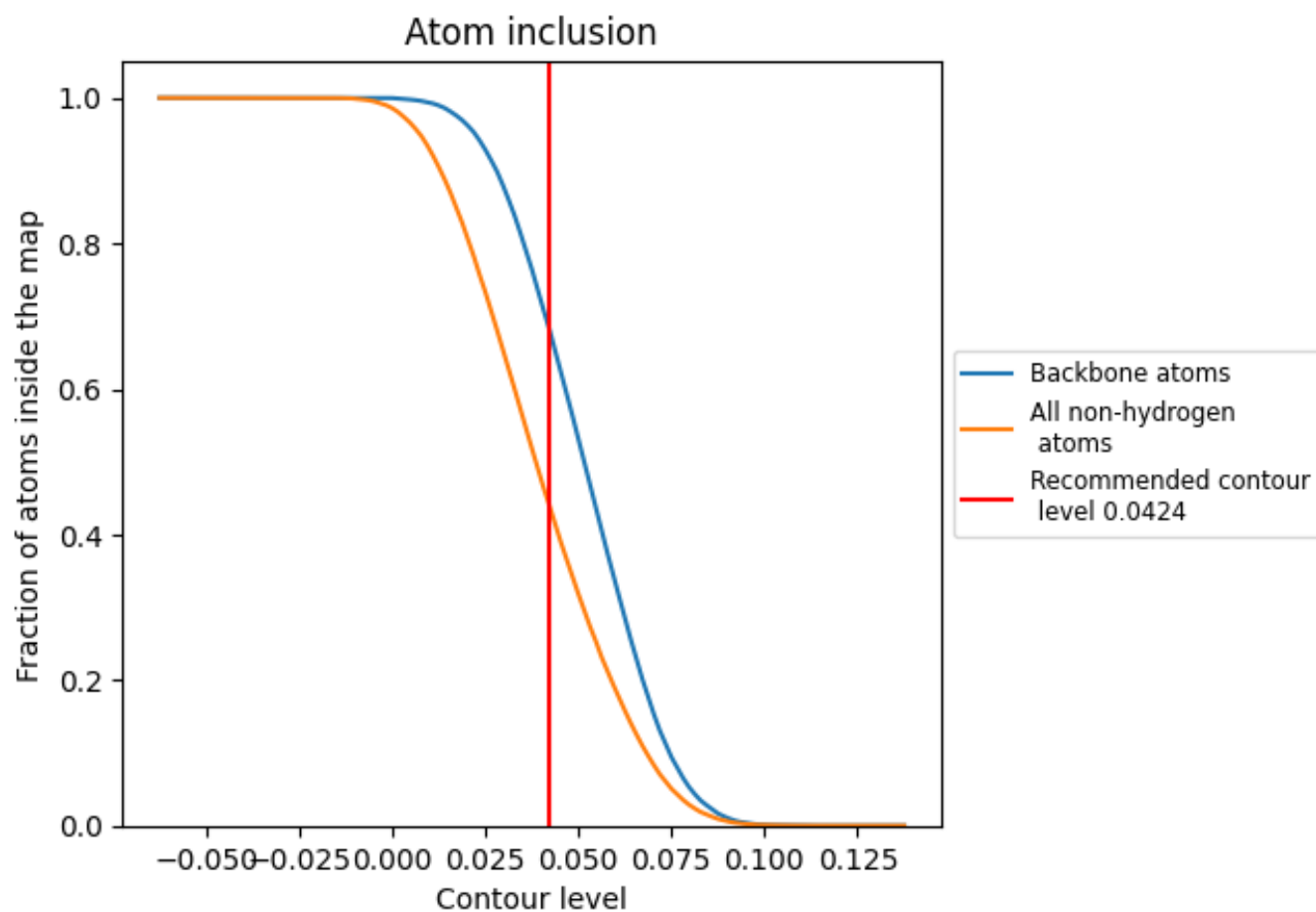
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0424).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 44% 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 (0.0424) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4379	 0.2970
0	 0.6400	 0.4790
1	 0.3345	 0.2440
2	 0.5152	 0.3260
3	 0.5433	 0.3460
4	 0.5341	 0.3480
5	 0.4607	 0.3110
6	 0.2949	 0.2330
A	 0.4744	 0.3050
B	 0.4902	 0.3220
C	 0.5300	 0.3440
D	 0.5271	 0.3420
E	 0.4610	 0.3110
F	 0.4230	 0.2910
G	 0.4316	 0.2770
a	 0.3860	 0.3020
b	 0.4426	 0.3110
c	 0.4410	 0.3110
d	 0.4096	 0.2860
e	 0.3263	 0.2530
f	 0.2752	 0.2370
g	 0.3223	 0.2380
h	 0.1560	 0.1310
i	 0.3435	 0.2240
j	 0.4566	 0.2240
k	 0.4207	 0.2230
l	 0.3228	 0.2130
m	 0.1333	 0.1490
n	 0.3086	 0.1810

