



Full wwPDB EM Validation Report ⓘ

Apr 18, 2026 – 12:20 PM EDT

PDB ID : 9YRC / pdb_00009yrc
EMDB ID : EMD-73365
Title : p97Ufd1-Npl4 complex processing poly-ubiquitinated substrate in the presence of ATP
Authors : Li, H.; Rapoport, T.
Deposited on : 2025-10-16
Resolution : 2.97 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:

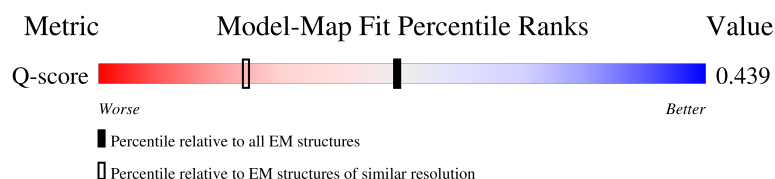
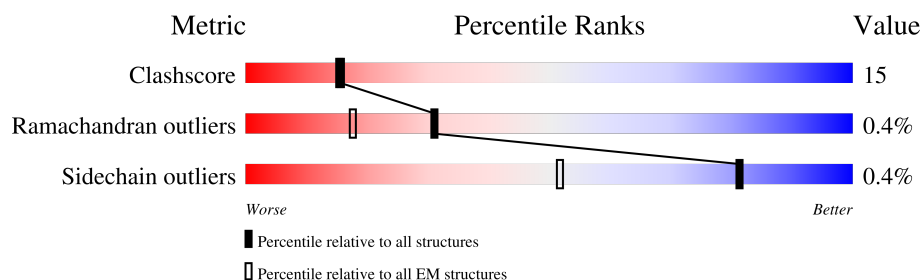
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.97 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	13205 (2.47 - 3.47)

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	806	
1	B	806	
1	C	806	
1	D	806	

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Mol	Chain	Length	Quality of chain
1	E	806	<div><div><div></div><div></div><div></div><div></div></div><div>26%40%28%31%</div></div>
1	F	806	<div><div><div></div><div></div><div></div><div></div></div><div>8%16%17%67%</div></div>
2	G	608	<div><div><div></div><div></div><div></div><div></div></div><div>6%53%21%25%</div></div>
3	H	307	<div><div><div></div><div></div><div></div><div></div></div><div>6%94%</div></div>
4	I	76	<div><div><div></div><div></div><div></div><div></div></div><div>47%16%36%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 28118 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	554	Total	C	N	O	S	0	0
			4295	2703	763	807	22		
1	B	564	Total	C	N	O	S	0	0
			4369	2750	776	821	22		
1	C	551	Total	C	N	O	S	0	0
			4264	2685	754	803	22		
1	D	563	Total	C	N	O	S	0	0
			4367	2751	776	818	22		
1	E	553	Total	C	N	O	S	0	0
			4296	2705	766	804	21		
1	F	262	Total	C	N	O	S	0	0
			2020	1268	359	383	10		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	GLN	GLU	conflict	UNP P55072
B	578	GLN	GLU	conflict	UNP P55072
C	578	GLN	GLU	conflict	UNP P55072
D	578	GLN	GLU	conflict	UNP P55072
E	578	GLN	GLU	conflict	UNP P55072
F	578	GLN	GLU	conflict	UNP P55072

- Molecule 2 is a protein called Nuclear protein localization protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	453	Total	C	N	O	S	0	0
			3632	2303	617	695	17		

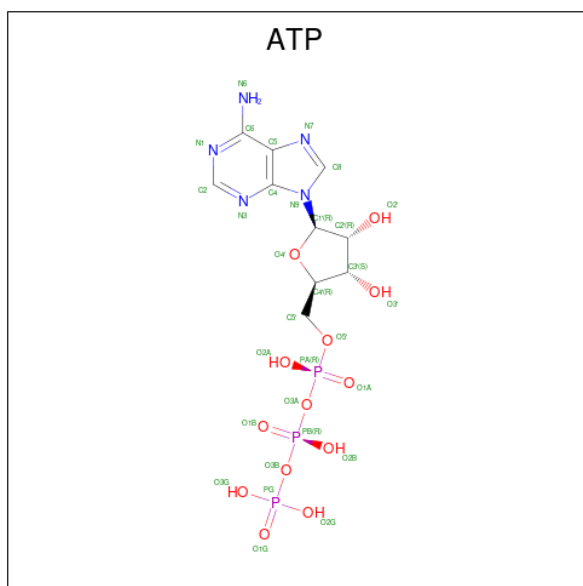
- Molecule 3 is a protein called Ubiquitin recognition factor in ER-associated degradation protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	H	19	Total	C	N	O	0	0
			162	107	30	25		

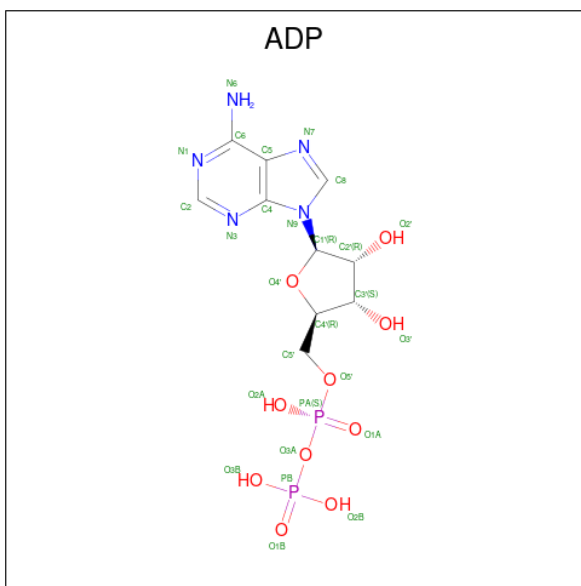
- Molecule 4 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	49	Total	C	N	O	S	0	0
			384	242	64	77	1		

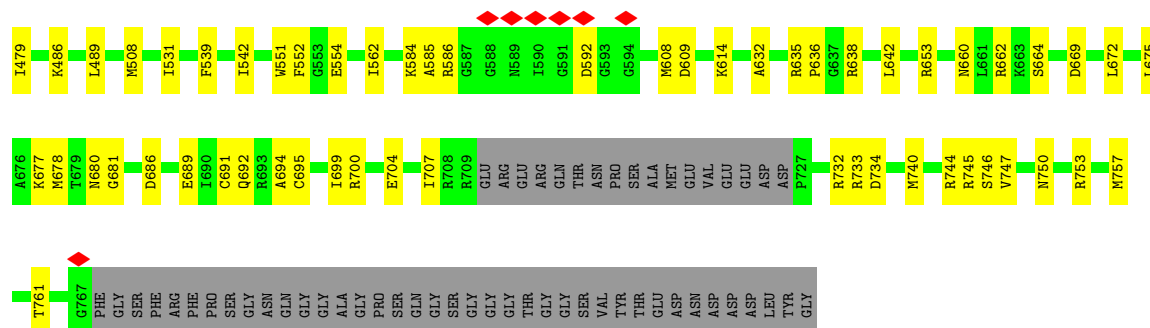
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



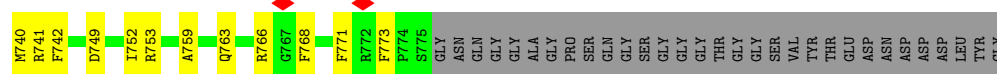
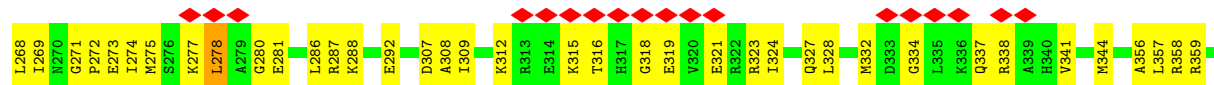
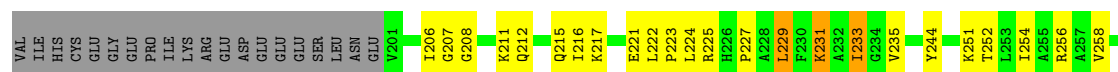
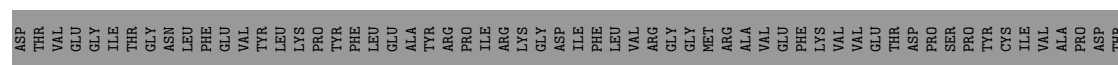
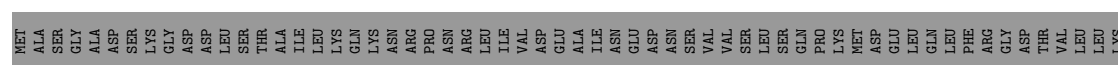
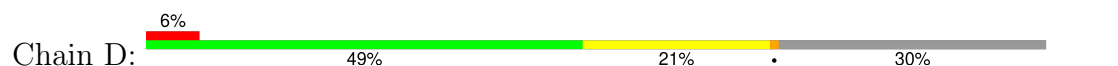
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
6	D	1	Total 27	C 10	N 5	O 10	P 2	0
6	E	1	Total 27	C 10	N 5	O 10	P 2	0
6	E	1	Total 27	C 10	N 5	O 10	P 2	0

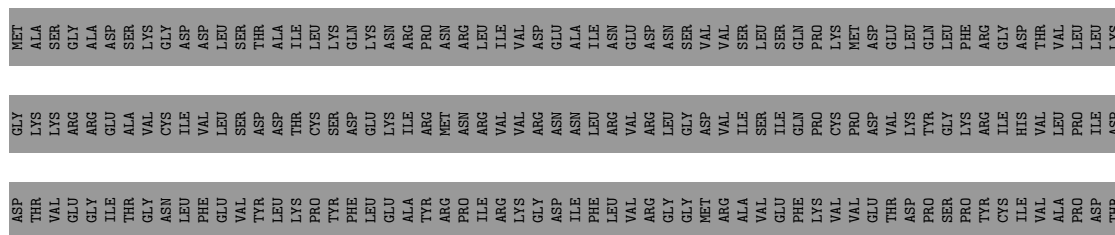


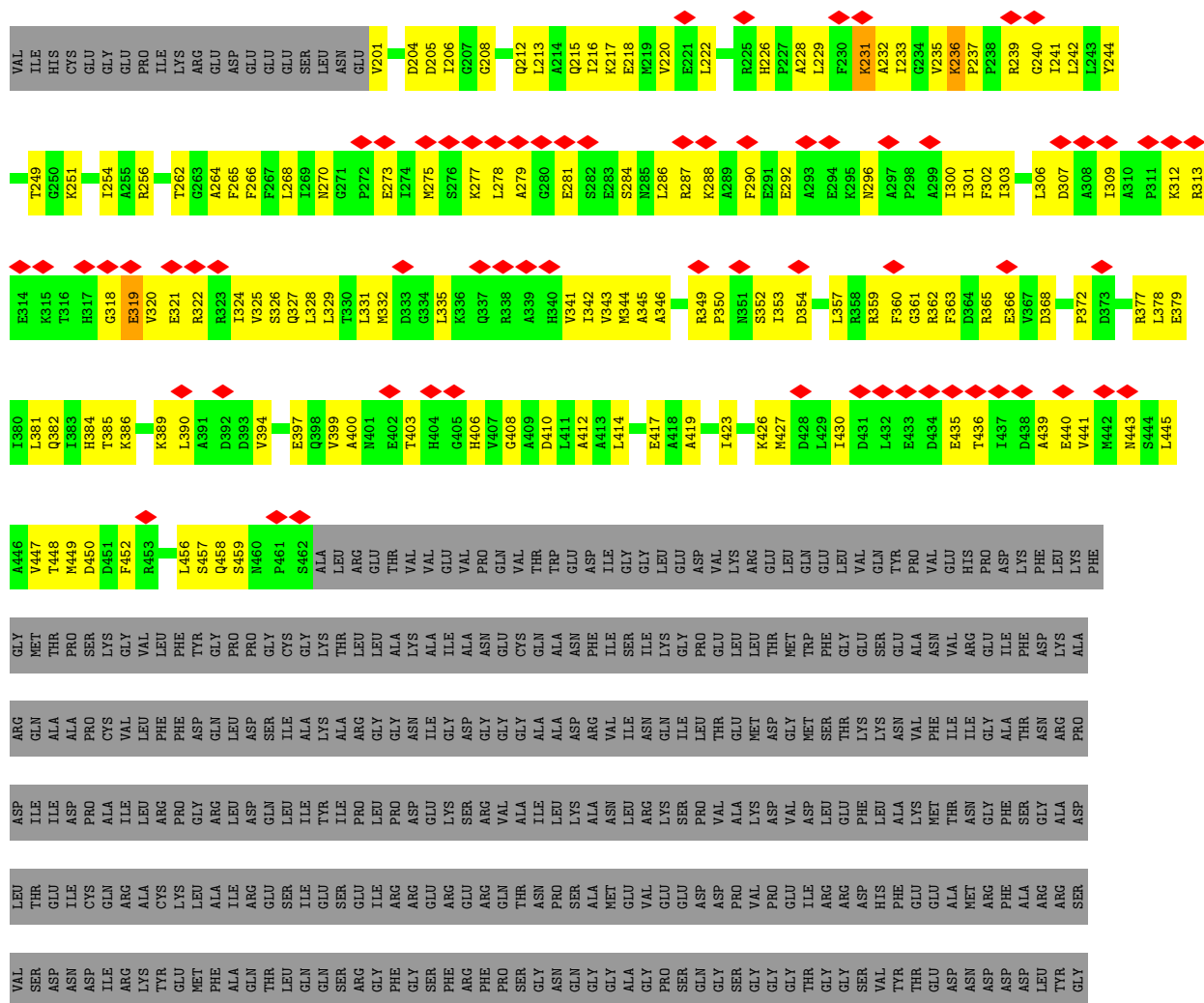
• Molecule 1: Transitional endoplasmic reticulum ATPase

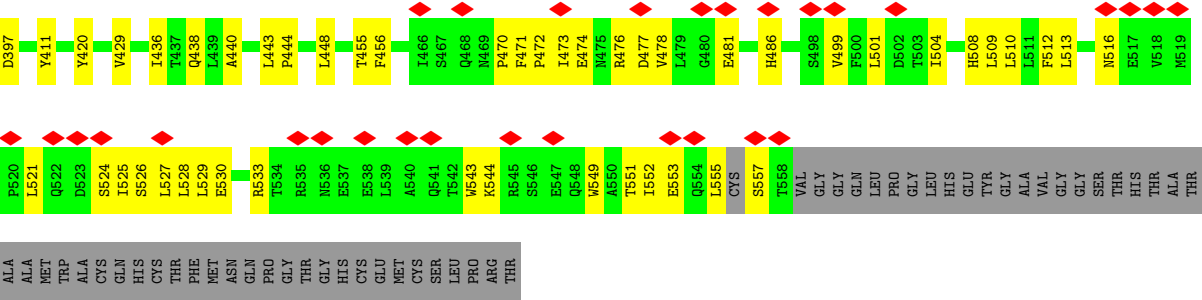


• Molecule 1: Transitional endoplasmic reticulum ATPase



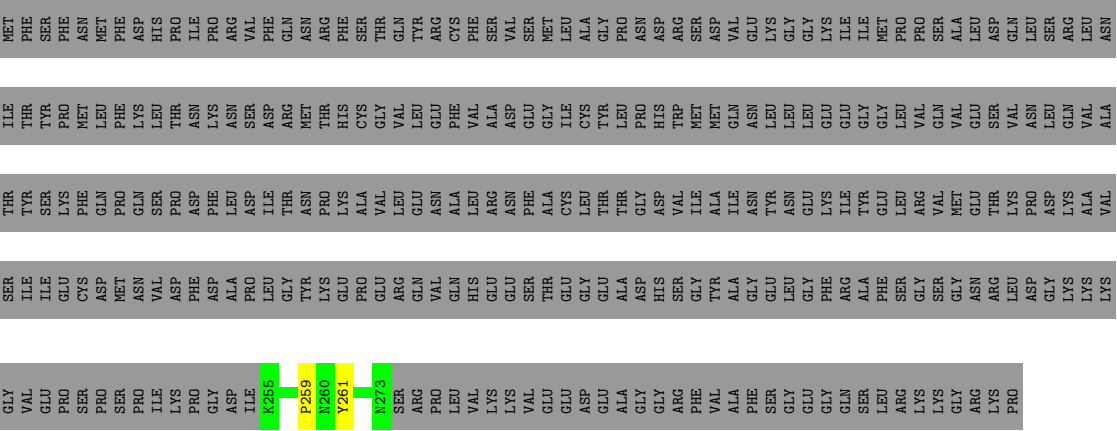






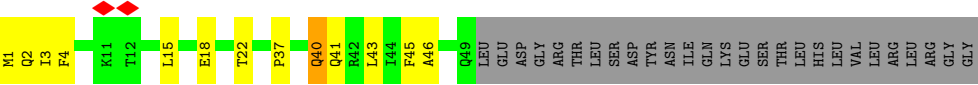
● Molecule 3: Ubiquitin recognition factor in ER-associated degradation protein 1

Chain H: 6% . 94%



● Molecule 4: Ubiquitin

Chain I: 47% 16% 36%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65959	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)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.646	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	330.80002, 330.80002, 330.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/4365	0.51	0/5890
1	B	0.27	0/4442	0.50	3/5993 (0.1%)
1	C	0.30	0/4334	0.48	1/5849 (0.0%)
1	D	0.26	0/4441	0.56	7/5991 (0.1%)
1	E	0.19	0/4369	0.51	0/5891
1	F	0.28	0/2051	0.62	0/2770
2	G	0.24	0/3721	0.46	0/5050
3	H	0.23	0/165	0.61	0/218
4	I	0.27	0/387	0.45	0/519
All	All	0.25	0/28275	0.51	11/38171 (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	A	0	3
2	G	0	1
All	All	0	4

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	695	CYS	CA-CB-SG	13.04	144.40	114.40
1	B	695	CYS	CA-CB-SG	10.08	137.59	114.40
1	C	337	GLN	N-CA-C	7.82	119.53	108.74
1	B	695	CYS	CB-CA-C	7.54	121.03	109.34
1	B	695	CYS	N-CA-CB	-7.30	99.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	691	CYS	N-CA-CB	7.06	120.61	110.16
1	D	695	CYS	N-CA-CB	-6.56	99.40	110.49
1	D	690	ILE	CA-C-N	-6.29	111.35	120.29
1	D	690	ILE	C-N-CA	-6.29	111.35	120.29
1	D	278	LEU	N-CA-C	-6.22	106.92	114.75
1	D	432	LEU	CB-CA-C	-5.69	110.00	116.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	LYS	Peptide
1	A	343	VAL	Peptide
1	A	348	ASN	Peptide
2	G	156	GLU	Peptide

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	4295	0	4332	161	0
1	B	4369	0	4392	95	0
1	C	4264	0	4302	101	0
1	D	4367	0	4398	145	0
1	E	4296	0	4323	187	0
1	F	2020	0	2050	98	0
2	G	3632	0	3521	98	0
3	H	162	0	173	2	0
4	I	384	0	404	17	0
5	A	62	0	24	4	0
5	B	62	0	24	1	0
5	C	62	0	24	4	0
5	D	31	0	12	1	0
5	F	31	0	12	2	0
6	D	27	0	12	1	0
6	E	54	0	24	8	0
All	All	28118	0	28027	817	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 15.

All (817) 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:B:201:VAL:HG21	1:B:256:ARG:HB3	1.45	0.96
1:D:691:CYS:O	1:D:695:CYS:HB3	1.77	0.83
1:A:241:ILE:HD13	1:A:343:VAL:HG22	1.59	0.83
1:C:744:ARG:HH12	1:D:642:LEU:HD13	1.45	0.82
2:G:471:PHE:HD1	2:G:472:PRO:HD2	1.45	0.81
1:A:338:ARG:HD2	1:A:340:HIS:HD2	1.45	0.81
2:G:138:CYS:N	2:G:141:CYS:SG	2.53	0.81
1:B:256:ARG:NH2	1:C:335:LEU:O	2.15	0.80
1:F:385:THR:HB	1:F:390:LEU:HD21	1.63	0.79
1:F:237:PRO:HB2	1:F:342:ILE:HD11	1.63	0.79
1:D:550:MET:HB3	1:E:553:GLY:H	1.48	0.78
1:B:691:CYS:O	1:B:695:CYS:HB3	1.84	0.77
1:A:239:ARG:NH1	1:A:361:GLY:O	2.17	0.77
1:F:275:MET:HE3	1:F:309:ILE:HG22	1.66	0.77
1:F:239:ARG:NH1	1:F:332:MET:O	2.18	0.77
1:A:394:VAL:HA	1:A:449:MET:HE2	1.67	0.76
1:F:240:GLY:HA3	1:F:363:PHE:HA	1.67	0.76
1:D:287:ARG:NH1	2:G:174:GLY:H	1.84	0.75
2:G:227:MET:HE2	2:G:269:GLU:HG2	1.67	0.75
1:E:375:THR:O	1:E:378:LEU:HB3	1.87	0.75
1:D:371:ILE:HD12	1:D:372:PRO:HD2	1.67	0.75
1:B:432:LEU:O	1:C:225:ARG:NH1	2.22	0.73
1:D:448:THR:OG1	1:D:450:ASP:OD1	2.06	0.73
1:F:430:ILE:HD11	1:F:441:VAL:HG11	1.70	0.73
1:A:256:ARG:HD2	1:A:257:ALA:H	1.52	0.73
1:E:499:HIS:ND1	1:E:501:ASP:OD1	2.22	0.73
1:A:349:ARG:H	1:A:349:ARG:HD3	1.50	0.73
1:E:210:ARG:HA	1:E:213:LEU:HG	1.71	0.73
1:F:212:GLN:HA	1:F:215:GLN:HG2	1.69	0.72
1:C:336:LYS:HE2	2:G:207:LYS:HD2	1.71	0.72
1:E:302:PHE:CE2	1:E:304:ASP:HB3	2.25	0.72
1:E:549:THR:HG22	1:E:551:TRP:H	1.54	0.72
4:I:37:PRO:HG2	4:I:40:GLN:HG3	1.71	0.71
1:D:604:ILE:HG22	1:D:608:MET:HE2	1.73	0.71
1:C:608:MET:O	1:C:614:LYS:NZ	2.24	0.71
1:D:208:GLY:N	1:D:379:GLU:OE2	2.17	0.70
1:B:312:LYS:HG2	1:B:355:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:GLY:H	1:C:337:GLN:HE21	1.37	0.70
1:F:435:GLU:HG3	1:F:436:THR:HG23	1.72	0.70
1:F:448:THR:OG1	1:F:450:ASP:OD1	2.09	0.70
1:B:312:LYS:H	1:B:315:LYS:HZ3	1.37	0.69
1:E:772:ARG:NH1	1:E:773:PHE:O	2.25	0.69
1:C:312:LYS:NZ	1:C:351:ASN:O	2.24	0.69
1:D:338:ARG:HB2	1:D:341:VAL:HB	1.73	0.69
1:B:433:GLU:O	1:C:225:ARG:NH2	2.24	0.69
1:F:377:ARG:NH1	1:F:403:THR:O	2.22	0.69
2:G:471:PHE:CD1	2:G:472:PRO:HD2	2.28	0.69
2:G:189:LYS:NZ	2:G:397:ASP:OD1	2.24	0.68
1:F:302:PHE:HD1	1:F:344:MET:HG3	1.59	0.67
1:F:378:LEU:O	1:F:382:GLN:NE2	2.28	0.67
1:F:266:PHE:HE2	1:F:268:LEU:HD12	1.60	0.67
5:B:901:ATP:O1G	1:C:362:ARG:NH2	2.26	0.67
5:C:901:ATP:O2G	1:D:359:ARG:NH1	2.27	0.67
2:G:321:ARG:HG3	2:G:322:LYS:H	1.58	0.67
2:G:501:LEU:HA	2:G:504:ILE:HG22	1.77	0.67
5:A:902:ATP:O3G	1:B:638:ARG:NH2	2.28	0.66
1:B:542:ILE:HG22	1:B:544:GLY:H	1.60	0.66
1:C:388:MET:HE3	1:C:419:ALA:HB2	1.76	0.66
1:F:206:ILE:HG12	1:F:254:ILE:HG22	1.77	0.66
1:D:421:GLN:OE1	1:D:424:ARG:NH2	2.28	0.66
1:E:269:ILE:HD11	1:E:303:ILE:HG23	1.77	0.66
1:C:334:GLY:H	1:C:337:GLN:NE2	1.93	0.66
1:E:449:MET:O	1:E:453:ARG:NH1	2.29	0.66
1:C:584:LYS:HG2	1:C:585:ALA:H	1.61	0.66
1:C:744:ARG:NH1	1:D:642:LEU:HD13	2.10	0.66
1:D:424:ARG:HA	1:D:427:MET:HG3	1.77	0.66
2:G:105:VAL:HG12	2:G:106:VAL:HG23	1.78	0.66
1:E:381:LEU:HD13	1:E:396:LEU:HD21	1.76	0.66
1:A:657:LEU:HB3	1:A:672:LEU:HD12	1.78	0.66
1:A:256:ARG:HD2	1:A:257:ALA:N	2.11	0.66
1:A:426:LYS:NZ	1:A:444:SER:O	2.29	0.65
1:D:256:ARG:NH2	1:D:268:LEU:HD21	2.09	0.65
1:A:290:PHE:HE1	1:A:342:ILE:HD11	1.61	0.65
1:D:207:GLY:O	6:D:902:ADP:N6	2.28	0.65
1:B:437:ILE:HD11	1:C:226:HIS:HD2	1.62	0.65
1:D:693:ARG:NH2	1:E:641:GLN:OE1	2.30	0.65
2:G:530:GLU:HA	2:G:533:ARG:HG2	1.77	0.65
1:B:302:PHE:HD1	1:B:344:MET:HG3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:THR:OG1	6:E:902:ADP:O1A	2.13	0.65
2:G:544:LYS:HD2	2:G:549:TRP:CD1	2.32	0.65
1:F:266:PHE:HD1	1:F:300:ILE:HG23	1.60	0.65
2:G:186:ILE:O	2:G:396:ARG:NH2	2.30	0.65
1:B:439:ALA:O	1:B:443:ASN:ND2	2.30	0.65
1:A:335:LEU:HD23	1:A:338:ARG:HD3	1.78	0.64
1:A:268:LEU:HA	1:A:303:ILE:HD11	1.78	0.64
1:C:359:ARG:HD2	1:C:360:PHE:H	1.60	0.64
1:A:243:LEU:HA	1:A:345:ALA:HB3	1.78	0.64
1:A:362:ARG:O	1:A:364:ASP:N	2.29	0.64
1:D:763:GLN:OE1	1:D:766:ARG:NH1	2.26	0.64
1:A:542:ILE:HG21	1:A:562:ILE:HD11	1.79	0.64
1:C:219:MET:HE1	1:C:365:ARG:HD2	1.79	0.64
1:A:221:GLU:HB2	1:A:300:ILE:HD12	1.80	0.64
1:F:220:VAL:HG12	1:F:342:ILE:HG21	1.80	0.64
1:B:277:LYS:NZ	4:I:18:GLU:OE2	2.26	0.63
1:C:691:CYS:O	1:C:694:ALA:N	2.31	0.63
1:E:754:LYS:HA	1:E:757:MET:HG3	1.80	0.63
2:G:525:ILE:HG13	2:G:528:LEU:HD23	1.80	0.63
1:E:207:GLY:O	6:E:902:ADP:N6	2.23	0.63
1:D:273:GLU:OE2	2:G:140:HIS:NE2	2.30	0.63
2:G:553:GLU:O	2:G:557:SER:N	2.32	0.63
1:A:203:TYR:OH	1:A:255:ALA:O	2.12	0.63
1:A:598:ASP:OD1	1:A:599:ARG:N	2.31	0.63
1:B:597:ALA:O	1:B:601:ILE:HD12	1.99	0.63
1:C:330:THR:O	1:C:337:GLN:NE2	2.31	0.63
1:E:283:GLU:OE2	1:E:323:ARG:NH1	2.31	0.63
1:A:238:PRO:C	1:A:239:ARG:HD2	2.24	0.63
1:F:208:GLY:N	1:F:379:GLU:OE1	2.32	0.63
1:A:223:PRO:HA	1:A:227:PRO:HB3	1.81	0.63
1:E:377:ARG:HB3	1:E:411:LEU:HB2	1.81	0.63
1:B:625:ARG:NH1	1:C:586:ARG:O	2.32	0.63
1:F:417:GLU:OE2	1:F:458:GLN:NE2	2.29	0.62
1:D:337:GLN:OE1	1:D:338:ARG:NH1	2.32	0.62
1:D:689:GLU:HA	1:D:692:GLN:HB3	1.80	0.62
1:C:359:ARG:HD2	1:C:360:PHE:N	2.15	0.61
2:G:243:LYS:NZ	2:G:481:GLU:OE2	2.33	0.61
2:G:512:PHE:O	2:G:516:ASN:ND2	2.33	0.61
1:D:738:GLU:HA	1:D:741:ARG:HD3	1.82	0.61
1:B:356:ALA:O	1:B:362:ARG:NH1	2.33	0.61
1:F:306:LEU:HD11	1:F:345:ALA:HB1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:ARG:HH11	2:G:174:GLY:H	1.46	0.61
1:F:322:ARG:HA	1:F:325:VAL:HG12	1.82	0.61
1:D:221:GLU:O	1:D:225:ARG:HB3	2.00	0.61
1:E:300:ILE:HG22	1:E:342:ILE:HB	1.82	0.61
1:F:318:GLY:O	1:F:321:GLU:N	2.19	0.61
1:F:457:SER:OG	1:F:458:GLN:OE1	2.18	0.61
1:E:679:THR:HB	1:E:682:PHE:HB2	1.82	0.61
2:G:456:PHE:HD2	4:I:43:LEU:HD12	1.66	0.60
1:D:691:CYS:O	1:D:692:GLN:C	2.44	0.60
1:F:249:THR:O	5:F:901:ATP:N6	2.33	0.60
1:E:320:VAL:HG22	1:E:323:ARG:HH21	1.65	0.60
1:E:477:GLU:HG2	1:E:662:ARG:HH11	1.66	0.60
1:A:244:TYR:HB2	1:A:368:ASP:HA	1.82	0.60
1:C:700:ARG:NH2	1:D:491:GLU:OE1	2.34	0.60
1:D:288:LYS:NZ	2:G:148:ASP:OD2	2.35	0.60
1:A:349:ARG:HD3	1:A:349:ARG:N	2.13	0.60
1:E:377:ARG:NH2	1:E:414:LEU:O	2.34	0.60
1:E:525:THR:OG1	6:E:901:ADP:O1A	2.19	0.60
1:C:333:ASP:HB3	1:C:362:ARG:HD2	1.83	0.60
1:F:372:PRO:HG3	1:F:408:GLY:H	1.66	0.59
1:A:221:GLU:HG3	1:A:224:LEU:HB3	1.83	0.59
1:B:270:ASN:H	2:G:206:THR:HG21	1.66	0.59
1:B:297:ALA:HB1	1:B:298:PRO:HD2	1.85	0.59
1:D:212:GLN:O	1:D:216:ILE:HD12	2.02	0.59
1:E:406:HIS:HA	1:E:461:PRO:HB3	1.83	0.59
1:A:377:ARG:NH1	1:A:400:ALA:O	2.34	0.59
1:D:759:ALA:O	1:D:763:GLN:HG2	2.02	0.59
1:D:426:LYS:HD3	1:D:445:LEU:HD23	1.85	0.59
1:D:692:GLN:NE2	1:E:509:THR:O	2.35	0.59
1:D:741:ARG:NH1	1:E:769:GLY:O	2.35	0.59
2:G:324:THR:HG23	2:G:378:ASN:HB3	1.84	0.59
1:B:256:ARG:NH1	1:C:335:LEU:HG	2.18	0.59
1:B:419:ALA:HB1	1:C:233:ILE:HG21	1.83	0.59
1:C:489:LEU:HD13	1:C:531:ILE:HD11	1.85	0.59
1:A:402:GLU:N	1:A:402:GLU:OE1	2.36	0.58
1:B:637:GLY:N	1:B:640:ASP:OD1	2.30	0.58
1:D:648:PRO:O	1:D:653:ARG:NH1	2.36	0.58
1:C:466:GLU:OE1	1:C:466:GLU:N	2.29	0.58
1:D:334:GLY:H	1:D:337:GLN:HB3	1.67	0.58
1:E:697:LEU:HD23	1:E:700:ARG:HE	1.68	0.58
1:A:220:VAL:HG22	1:A:221:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:MET:O	1:C:338:ARG:NH1	2.36	0.58
2:G:551:THR:O	2:G:555:LEU:HD23	2.03	0.58
1:A:253:LEU:HD22	5:A:901:ATP:H2'	1.85	0.58
1:D:736:PHE:O	1:D:740:MET:HG3	2.04	0.58
1:F:394:VAL:HA	1:F:449:MET:SD	2.43	0.58
1:E:381:LEU:O	1:E:385:THR:OG1	2.21	0.58
1:B:319:GLU:OE1	1:B:322:ARG:NH2	2.37	0.57
1:E:445:LEU:HD21	1:F:233:ILE:HD12	1.85	0.57
1:B:390:LEU:HG	1:B:394:VAL:HG11	1.85	0.57
1:D:450:ASP:OD1	1:D:451:ASP:N	2.37	0.57
1:E:317:HIS:O	1:F:322:ARG:NH2	2.37	0.57
1:D:423:ILE:HD11	1:E:233:ILE:HG21	1.86	0.57
1:E:650:GLU:OE2	1:E:653:ARG:NH2	2.38	0.57
1:A:224:LEU:HD22	1:A:298:PRO:HB2	1.87	0.57
1:D:550:MET:HE1	4:I:2:GLN:NE2	2.19	0.57
1:A:406:HIS:NE2	1:A:459:SER:OG	2.35	0.57
1:E:524:LYS:NZ	6:E:901:ADP:O2B	2.35	0.57
1:A:278:LEU:HD23	1:B:323:ARG:NH1	2.19	0.57
2:G:510:LEU:HD23	2:G:529:LEU:HD23	1.86	0.57
1:B:594:GLY:O	1:B:599:ARG:NH1	2.37	0.56
1:D:321:GLU:HA	1:D:324:ILE:HG22	1.86	0.56
1:A:222:LEU:HD12	1:A:226:HIS:H	1.70	0.56
1:A:294:GLU:C	1:A:340:HIS:HE1	2.12	0.56
1:C:462:SER:O	1:C:465:ARG:HB2	2.05	0.56
1:E:474:VAL:HG13	1:E:478:ASP:HB2	1.88	0.56
1:A:301:ILE:HD12	1:A:342:ILE:HG12	1.86	0.56
1:A:310:ALA:HA	1:A:325:VAL:HG12	1.87	0.56
1:B:312:LYS:HB3	1:B:314:GLU:OE1	2.05	0.56
1:D:394:VAL:HA	1:D:449:MET:SD	2.45	0.56
1:E:509:THR:HG22	1:E:615:LYS:HE2	1.88	0.56
1:F:320:VAL:O	1:F:324:ILE:HG12	2.05	0.56
1:F:381:LEU:HD12	1:F:400:ALA:HB2	1.87	0.56
1:D:318:GLY:O	1:D:321:GLU:HG3	2.05	0.56
1:A:293:ALA:O	1:A:295:LYS:N	2.38	0.56
1:C:239:ARG:HB2	1:C:338:ARG:HH21	1.71	0.56
1:E:256:ARG:NH1	1:E:260:ASN:OD1	2.38	0.56
1:E:311:PRO:HD2	1:E:321:GLU:HB2	1.87	0.56
1:F:228:ALA:HA	1:F:231:LYS:HD2	1.87	0.56
1:E:272:PRO:HA	1:F:326:SER:HB2	1.87	0.56
1:F:354:ASP:HB3	1:F:357:LEU:HD23	1.87	0.56
1:C:745:ARG:NH1	1:C:747:VAL:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:399:VAL:HG21	1:F:452:PHE:HD2	1.69	0.56
1:C:675:LEU:HD22	1:C:740:MET:HE1	1.87	0.56
1:E:240:GLY:HA3	1:E:363:PHE:HA	1.87	0.56
1:E:313:ARG:O	1:E:322:ARG:NH2	2.39	0.56
1:F:284:SER:HA	1:F:287:ARG:HE	1.69	0.56
1:E:253:LEU:HD22	6:E:902:ADP:H2'	1.87	0.56
1:F:423:ILE:O	1:F:427:MET:HG2	2.06	0.56
1:A:357:LEU:HB3	1:A:363:PHE:HD2	1.70	0.55
1:E:265:PHE:HE2	1:E:267:PHE:HB2	1.71	0.55
1:E:292:GLU:HA	1:E:295:LYS:HG2	1.89	0.55
1:A:306:LEU:HA	1:A:309:ILE:HG22	1.88	0.55
1:B:691:CYS:SG	1:C:508:MET:HG3	2.46	0.55
1:B:734:ASP:OD1	1:B:735:HIS:N	2.38	0.55
1:E:748:SER:OG	1:E:750:ASN:OD1	2.24	0.55
1:A:350:PRO:HA	1:A:358:ARG:HH12	1.71	0.55
1:E:586:ARG:NH1	1:E:630:ASP:OD2	2.39	0.55
1:B:253:LEU:O	1:B:256:ARG:HB2	2.05	0.55
1:E:561:GLU:HG3	1:E:565:LYS:HE3	1.87	0.55
1:D:695:CYS:O	1:D:699:ILE:HG12	2.06	0.55
1:F:378:LEU:HD11	1:F:397:GLU:HA	1.87	0.55
1:F:278:LEU:HD23	1:F:279:ALA:N	2.22	0.55
1:A:561:GLU:HG2	1:A:565:LYS:HE2	1.89	0.55
1:B:294:GLU:HG2	1:B:338:ARG:HB2	1.88	0.55
1:B:312:LYS:HG2	1:B:354:ASP:HA	1.88	0.55
2:G:183:LEU:HD11	2:G:357:LEU:HB3	1.89	0.55
1:F:439:ALA:O	1:F:443:ASN:ND2	2.40	0.55
1:A:295:LYS:HD2	1:A:340:HIS:NE2	2.22	0.55
1:C:438:ASP:HB3	1:C:441:VAL:HG22	1.89	0.55
1:E:421:GLN:HG2	1:E:424:ARG:HD3	1.88	0.55
1:A:205:ASP:OD1	1:A:386:LYS:NZ	2.35	0.55
1:B:218:GLU:HA	1:B:222:LEU:HD13	1.89	0.55
1:E:608:MET:HE2	1:E:638:ARG:HB3	1.88	0.55
1:F:384:HIS:CE1	1:F:412:ALA:HB2	2.42	0.55
1:A:398:GLN:NE2	1:A:402:GLU:OE2	2.40	0.54
1:A:543:LYS:N	1:A:546:GLU:OE1	2.40	0.54
1:A:700:ARG:NH2	1:B:491:GLU:OE1	2.39	0.54
1:C:691:CYS:O	1:C:692:GLN:C	2.50	0.54
1:D:438:ASP:HB2	1:D:441:VAL:HG22	1.88	0.54
1:E:512:LYS:HD3	1:E:618:PHE:HD1	1.71	0.54
1:E:523:GLY:O	1:E:527:LEU:N	2.32	0.54
1:A:266:PHE:CE2	1:A:302:PHE:HD2	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:ASP:OD1	1:C:746:SER:OG	2.24	0.54
2:G:314:ASP:OD2	2:G:329:ARG:NE	2.40	0.54
1:E:583:ALA:HA	1:E:601:ILE:HD12	1.90	0.54
1:A:233:ILE:HD12	1:F:419:ALA:HB1	1.89	0.54
1:B:608:MET:HE1	1:B:639:LEU:HG	1.89	0.54
1:D:288:LYS:O	1:D:292:GLU:HG2	2.08	0.54
1:D:357:LEU:O	1:D:363:PHE:HB2	2.08	0.54
1:B:751:ASP:HA	1:B:754:LYS:HE2	1.90	0.54
2:G:254:GLY:HA3	2:G:269:GLU:O	2.08	0.54
1:A:235:VAL:HA	1:A:336:LYS:NZ	2.23	0.54
2:G:205:CYS:N	2:G:208:CYS:SG	2.77	0.54
1:C:356:ALA:O	1:C:362:ARG:NH1	2.40	0.53
1:E:457:SER:OG	1:E:458:GLN:OE1	2.22	0.53
1:F:419:ALA:O	1:F:423:ILE:HG12	2.08	0.53
1:A:243:LEU:HD11	1:A:363:PHE:HB3	1.89	0.53
1:C:333:ASP:OD2	1:C:359:ARG:NH2	2.41	0.53
1:E:265:PHE:HZ	1:E:293:ALA:HA	1.73	0.53
1:F:456:LEU:HA	1:F:459:SER:HB3	1.90	0.53
1:D:233:ILE:HG23	1:D:235:VAL:HG12	1.90	0.53
1:D:673:GLU:O	1:D:677:LYS:HG2	2.08	0.53
1:C:695:CYS:SG	1:D:508:MET:HG3	2.49	0.53
1:D:691:CYS:C	1:D:695:CYS:HB3	2.33	0.53
1:D:206:ILE:HD12	1:D:254:ILE:HD13	1.90	0.53
1:F:426:LYS:O	1:F:430:ILE:HG12	2.09	0.53
1:D:278:LEU:HD22	1:D:281:GLU:HB2	1.90	0.53
1:F:288:LYS:O	1:F:292:GLU:HG2	2.08	0.53
1:A:384:HIS:CE1	5:A:901:ATP:H1'	2.44	0.53
1:B:702:SER:O	1:B:705:SER:OG	2.19	0.53
1:D:258:VAL:HG11	1:D:344:MET:HE1	1.91	0.53
1:E:540:ILE:HB	1:E:574:LEU:HD23	1.91	0.53
1:A:359:ARG:HG2	1:A:360:PHE:H	1.74	0.53
1:A:384:HIS:CE1	1:A:412:ALA:HB2	2.43	0.53
1:F:440:GLU:HA	1:F:443:ASN:HD21	1.73	0.53
2:G:337:SER:N	2:G:340:GLU:OE1	2.35	0.53
1:A:241:ILE:HB	1:A:343:VAL:HG13	1.91	0.52
1:A:257:ALA:O	1:A:259:ALA:N	2.33	0.52
1:E:524:LYS:HG2	1:E:645:ILE:HG13	1.90	0.52
1:E:709:ARG:NH2	1:E:710:GLU:OE2	2.42	0.52
1:A:222:LEU:HA	1:A:225:ARG:HB3	1.90	0.52
1:C:699:ILE:HD12	1:D:502:LYS:HB3	1.91	0.52
1:E:431:ASP:HB2	1:E:434:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ILE:HD11	1:C:226:HIS:CD2	2.44	0.52
1:D:515:LEU:HB3	1:D:642:LEU:HG	1.91	0.52
1:E:471:VAL:HG13	1:E:536:GLN:HA	1.91	0.52
2:G:228:PHE:HB2	2:G:456:PHE:CE1	2.45	0.52
1:D:286:LEU:HD21	1:D:328:LEU:HD13	1.91	0.52
2:G:440:ALA:HB1	2:G:443:LEU:HD13	1.90	0.52
1:C:225:ARG:O	1:C:225:ARG:HD3	2.10	0.52
1:C:426:LYS:HD3	1:C:441:VAL:HB	1.91	0.52
5:C:902:ATP:H5'1	1:D:635:ARG:HH12	1.73	0.52
1:E:445:LEU:HD21	1:F:233:ILE:CD1	2.40	0.52
1:A:349:ARG:HB3	1:A:353:ILE:HG12	1.91	0.52
1:B:691:CYS:O	1:B:692:GLN:C	2.52	0.52
1:E:314:GLU:HG3	1:E:315:LYS:H	1.73	0.52
1:A:222:LEU:HD13	1:A:225:ARG:NH2	2.25	0.52
1:A:312:LYS:N	1:A:352:SER:O	2.43	0.52
1:B:291:GLU:OE2	1:B:295:LYS:NZ	2.26	0.52
1:B:489:LEU:HD13	1:B:531:ILE:HD11	1.90	0.52
2:G:313:THR:HG22	2:G:372:ALA:HB3	1.92	0.52
1:A:678:MET:HG3	1:B:771:PHE:HE1	1.75	0.52
1:E:374:ALA:O	1:E:377:ARG:HG2	2.10	0.52
1:A:265:PHE:HD2	1:A:299:ALA:HB2	1.74	0.52
1:E:273:GLU:HG3	1:E:277:LYS:NZ	2.25	0.52
1:E:317:HIS:CE1	1:F:313:ARG:HB3	2.45	0.52
1:E:423:ILE:HG13	1:F:229:LEU:HD22	1.92	0.52
2:G:329:ARG:NH2	2:G:340:GLU:OE2	2.40	0.52
1:A:306:LEU:C	1:A:308:ALA:H	2.17	0.52
1:D:277:LYS:O	1:D:278:LEU:HD12	2.09	0.52
1:B:377:ARG:HG2	1:B:411:LEU:HD11	1.92	0.51
1:E:336:LYS:HD2	1:E:336:LYS:O	2.10	0.51
4:I:41:GLN:HG3	4:I:43:LEU:HG	1.92	0.51
1:D:692:GLN:O	1:D:696:LYS:HB2	2.10	0.51
1:E:625:ARG:HG3	1:E:754:LYS:NZ	2.25	0.51
1:A:222:LEU:HD13	1:A:225:ARG:HH21	1.76	0.51
1:A:278:LEU:O	1:A:280:GLY:N	2.44	0.51
1:B:268:LEU:CD2	1:C:335:LEU:HD22	2.41	0.51
2:G:310:TRP:NE1	2:G:369:THR:OG1	2.42	0.51
1:A:318:GLY:N	1:A:321:GLU:OE2	2.44	0.51
1:E:336:LYS:O	1:E:337:GLN:HG3	2.11	0.51
1:B:256:ARG:HH12	1:C:335:LEU:HG	1.76	0.51
1:F:239:ARG:NH1	1:F:335:LEU:O	2.44	0.51
2:G:321:ARG:HG3	2:G:322:LYS:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG23	1:A:213:LEU:HD11	1.93	0.51
1:B:334:GLY:O	1:B:337:GLN:NE2	2.42	0.51
1:A:303:ILE:HA	1:A:344:MET:SD	2.51	0.51
1:D:244:TYR:HE1	1:D:366:GLU:HB3	1.76	0.51
1:D:691:CYS:O	1:D:694:ALA:N	2.44	0.51
1:E:397:GLU:N	1:E:397:GLU:OE1	2.44	0.51
1:E:669:ASP:OD1	1:E:670:VAL:N	2.43	0.51
1:A:203:TYR:OH	1:A:258:VAL:HG12	2.10	0.51
1:A:268:LEU:HD12	1:A:303:ILE:CD1	2.40	0.51
1:B:691:CYS:O	1:B:695:CYS:CB	2.56	0.51
1:E:379:GLU:HA	1:E:382:GLN:NE2	2.26	0.51
1:E:607:GLU:O	1:E:611:MET:N	2.44	0.51
1:E:762:LEU:HG	1:E:766:ARG:HE	1.75	0.50
1:C:323:ARG:HH22	4:I:15:LEU:HD21	1.75	0.50
1:C:470:GLU:OE1	1:D:613:THR:OG1	2.19	0.50
1:E:274:ILE:HG23	1:E:282:SER:HB2	1.93	0.50
2:G:391:CYS:HB2	2:G:448:LEU:HD22	1.93	0.50
1:E:515:LEU:HD12	1:E:639:LEU:HD13	1.93	0.50
1:F:301:ILE:HB	1:F:343:VAL:HG12	1.92	0.50
1:D:462:SER:HA	1:D:465:ARG:HG2	1.93	0.50
1:E:564:ASP:O	1:E:567:ARG:HB2	2.11	0.50
2:G:231:HIS:HE1	2:G:235:ASP:OD2	1.94	0.50
1:A:565:LYS:HA	1:A:568:GLN:HB2	1.94	0.50
1:B:662:ARG:HG3	1:B:663:LYS:HD3	1.93	0.50
1:D:608:MET:HE1	1:D:633:ILE:HG23	1.94	0.50
1:A:734:ASP:OD1	1:A:735:HIS:N	2.45	0.50
1:B:364:ASP:OD1	1:B:365:ARG:HG2	2.12	0.50
1:E:293:ALA:HB2	1:E:301:ILE:HD11	1.93	0.50
1:E:489:LEU:HB3	1:E:531:ILE:HD13	1.93	0.50
1:E:751:ASP:O	1:E:754:LYS:HG3	2.12	0.50
2:G:160:LYS:HG2	2:G:217:ARG:HH22	1.76	0.50
1:B:388:MET:HA	1:C:233:ILE:O	2.12	0.50
1:D:256:ARG:HH22	1:D:268:LEU:HD21	1.77	0.50
1:E:220:VAL:HG23	1:E:342:ILE:HG21	1.93	0.50
1:F:406:HIS:NE2	1:F:459:SER:HB2	2.27	0.50
2:G:526:SER:O	2:G:529:LEU:HB2	2.12	0.50
1:A:275:MET:HG3	1:A:308:ALA:O	2.13	0.49
1:A:349:ARG:CB	1:A:353:ILE:HG12	2.42	0.49
1:C:478:ASP:OD1	1:C:662:ARG:NH2	2.44	0.49
1:C:678:MET:HE2	1:C:678:MET:HA	1.94	0.49
1:D:653:ARG:HD2	1:D:679:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:512:LYS:HG3	1:E:615:LYS:HD2	1.93	0.49
1:A:230:PHE:HB3	1:A:236:LYS:HG3	1.94	0.49
1:A:214:ALA:O	1:A:217:LYS:N	2.46	0.49
1:A:522:CYS:HB3	1:A:645:ILE:HG22	1.93	0.49
2:G:521:LEU:HD11	2:G:552:ILE:HD11	1.93	0.49
1:E:417:GLU:OE2	1:E:459:SER:OG	2.27	0.49
1:A:335:LEU:H	1:A:338:ARG:HE	1.58	0.49
1:A:384:HIS:HE1	5:A:901:ATP:H1'	1.77	0.49
1:C:377:ARG:HB2	1:C:411:LEU:HD11	1.95	0.49
1:D:426:LYS:NZ	1:D:444:SER:OG	2.40	0.49
1:E:450:ASP:N	1:E:450:ASP:OD1	2.44	0.49
1:E:519:PRO:HG2	1:E:522:CYS:SG	2.53	0.49
1:F:410:ASP:O	1:F:414:LEU:HD23	2.11	0.49
1:B:744:ARG:NH2	1:C:642:LEU:HD13	2.26	0.49
1:C:660:ASN:O	1:D:508:MET:HE1	2.13	0.49
5:C:902:ATP:O3G	1:D:638:ARG:NH1	2.43	0.49
2:G:248:HIS:H	2:G:313:THR:HG1	1.55	0.49
1:A:586:ARG:HG2	1:A:630:ASP:OD1	2.13	0.49
1:B:268:LEU:HB3	2:G:205:CYS:HA	1.95	0.49
1:C:377:ARG:HD2	1:C:400:ALA:O	2.13	0.49
1:F:222:LEU:HA	1:F:226:HIS:HD2	1.77	0.49
1:F:359:ARG:HD2	1:F:360:PHE:N	2.27	0.49
1:A:704:GLU:HA	1:A:707:ILE:HG22	1.94	0.49
1:D:277:LYS:HD3	1:E:319:GLU:HB3	1.94	0.49
1:D:749:ASP:N	1:D:749:ASP:OD1	2.42	0.49
2:G:456:PHE:CD2	4:I:43:LEU:HD12	2.48	0.49
1:E:669:ASP:O	1:E:733:ARG:NH1	2.46	0.49
1:D:662:ARG:HG3	1:D:663:LYS:HE3	1.95	0.48
1:A:250:GLY:O	1:A:254:ILE:N	2.42	0.48
1:A:601:ILE:HA	1:A:604:ILE:HG22	1.94	0.48
1:E:360:PHE:HA	1:E:364:ASP:OD1	2.13	0.48
1:E:640:ASP:OD1	1:E:640:ASP:N	2.47	0.48
2:G:376:PRO:HD2	2:G:381:HIS:CE1	2.48	0.48
1:A:256:ARG:HH12	1:A:259:ALA:HB2	1.77	0.48
1:A:338:ARG:HD2	1:A:340:HIS:CD2	2.37	0.48
1:A:359:ARG:HE	1:A:362:ARG:NH2	2.12	0.48
1:D:216:ILE:HD11	1:D:367:VAL:HG11	1.96	0.48
1:D:701:GLU:OE1	1:D:735:HIS:NE2	2.42	0.48
1:E:265:PHE:CZ	1:E:293:ALA:HA	2.48	0.48
1:E:449:MET:HB2	1:E:453:ARG:HH12	1.78	0.48
2:G:132:HIS:NE2	2:G:138:CYS:SG	2.80	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLN:HE21	1:A:454:TRP:NE1	2.12	0.48
1:A:567:ARG:HG2	1:A:615:LYS:HG2	1.94	0.48
1:D:319:GLU:O	1:D:323:ARG:HG3	2.14	0.48
1:A:256:ARG:HH12	1:A:259:ALA:CB	2.26	0.48
1:D:637:GLY:N	1:D:640:ASP:OD1	2.31	0.48
2:G:231:HIS:CE1	4:I:45:PHE:CE2	3.02	0.48
2:G:509:LEU:O	2:G:513:LEU:HG	2.14	0.48
1:C:704:GLU:HA	1:C:707:ILE:HG22	1.95	0.48
1:D:625:ARG:HH12	1:E:586:ARG:NE	2.12	0.48
1:E:597:ALA:O	1:E:600:VAL:HG12	2.13	0.48
1:E:702:SER:O	1:E:706:GLU:HG2	2.14	0.48
1:F:222:LEU:HD21	1:F:229:LEU:HD13	1.96	0.48
1:B:635:ARG:HE	1:B:638:ARG:NH2	2.12	0.48
1:D:269:ILE:HD12	1:D:274:ILE:HD12	1.96	0.48
1:E:310:ALA:HB1	1:E:325:VAL:HG22	1.96	0.48
1:F:242:LEU:HB3	1:F:366:GLU:HG2	1.96	0.48
1:E:475:THR:HG23	1:E:477:GLU:H	1.79	0.48
1:A:314:GLU:HA	1:A:322:ARG:HH11	1.79	0.47
1:A:497:VAL:HG23	1:A:498:GLU:HG2	1.96	0.47
1:A:586:ARG:HH12	1:A:598:ASP:HB3	1.77	0.47
1:D:271:GLY:O	1:D:275:MET:HG2	2.14	0.47
1:E:763:GLN:O	1:E:767:GLY:N	2.47	0.47
2:G:228:PHE:HB2	2:G:456:PHE:CD1	2.49	0.47
1:A:255:ALA:HB2	1:A:344:MET:HE1	1.95	0.47
1:A:417:GLU:OE2	1:A:424:ARG:NH2	2.47	0.47
1:C:338:ARG:HD2	1:C:341:VAL:HG23	1.94	0.47
1:C:691:CYS:SG	1:D:508:MET:HG3	2.54	0.47
1:F:270:ASN:HB2	1:F:273:GLU:OE1	2.14	0.47
2:G:253:TYR:OH	2:G:297:ASP:OD1	2.25	0.47
1:A:672:LEU:HD13	1:A:675:LEU:HD12	1.94	0.47
1:A:737:GLU:OE2	1:B:772:ARG:NH2	2.47	0.47
1:D:356:ALA:O	1:D:362:ARG:HD2	2.14	0.47
2:G:132:HIS:NE2	2:G:141:CYS:SG	2.88	0.47
1:C:423:ILE:HD11	1:D:233:ILE:HG21	1.96	0.47
1:E:403:THR:HG22	1:E:406:HIS:HD2	1.78	0.47
1:A:489:LEU:HD22	1:A:531:ILE:HD11	1.97	0.47
1:D:670:VAL:HG21	1:D:736:PHE:HE2	1.79	0.47
1:C:653:ARG:NH1	1:C:680:ASN:O	2.47	0.47
1:F:262:THR:HG23	1:F:264:ALA:H	1.80	0.47
1:F:307:ASP:OD1	1:F:307:ASP:N	2.47	0.47
2:G:455:THR:HB	4:I:40:GLN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HD12	1:A:345:ALA:HB2	1.97	0.47
1:A:543:LYS:HG2	1:B:606:THR:HB	1.97	0.47
1:E:377:ARG:O	1:E:381:LEU:N	2.42	0.47
1:F:201:VAL:HA	1:F:205:ASP:OD2	2.15	0.47
1:A:323:ARG:HG2	1:F:275:MET:O	2.15	0.47
1:B:756:GLU:O	1:B:759:ALA:N	2.47	0.47
1:C:695:CYS:O	1:C:699:ILE:HG12	2.15	0.47
1:E:417:GLU:HA	1:E:420:LEU:HD23	1.96	0.47
2:G:261:ASP:OD2	4:I:37:PRO:HB3	2.15	0.47
1:B:440:GLU:HG2	1:B:441:VAL:N	2.30	0.47
1:B:398:GLN:O	1:B:401:ASN:N	2.48	0.46
1:E:578:GLN:O	1:E:581:SER:OG	2.22	0.46
1:A:381:LEU:HB3	1:A:396:LEU:HD12	1.97	0.46
1:E:419:ALA:HB1	1:E:447:VAL:HG11	1.97	0.46
1:B:327:GLN:HE21	1:B:331:LEU:HG	1.80	0.46
1:B:362:ARG:O	1:B:364:ASP:N	2.48	0.46
1:C:669:ASP:HB2	1:C:733:ARG:NH2	2.30	0.46
1:D:244:TYR:CE1	1:D:366:GLU:HB3	2.51	0.46
1:D:667:ALA:HB3	1:D:670:VAL:HG23	1.97	0.46
1:E:474:VAL:HG21	1:E:526:LEU:HD22	1.97	0.46
1:E:689:GLU:HB3	1:E:693:ARG:HE	1.80	0.46
2:G:146:PRO:HG3	2:G:151:TYR:CZ	2.51	0.46
2:G:477:ASP:OD1	2:G:478:VAL:N	2.48	0.46
1:A:240:GLY:CA	1:A:363:PHE:HD1	2.28	0.46
1:A:313:ARG:NH1	1:A:354:ASP:HB2	2.31	0.46
1:A:662:ARG:CZ	1:A:663:LYS:HZ2	2.28	0.46
1:D:268:LEU:HA	1:D:268:LEU:HD23	1.66	0.46
1:E:226:HIS:O	1:E:226:HIS:ND1	2.49	0.46
1:F:287:ARG:O	1:F:290:PHE:N	2.48	0.46
1:A:212:GLN:O	1:A:216:ILE:HG12	2.16	0.46
1:B:228:ALA:HA	1:B:231:LYS:HD2	1.96	0.46
1:F:241:ILE:HD12	1:F:365:ARG:O	2.16	0.46
1:A:307:ASP:OD2	1:A:346:ALA:HB3	2.15	0.46
1:A:315:LYS:HG3	1:A:316:THR:N	2.30	0.46
5:C:902:ATP:O3G	1:D:635:ARG:NH2	2.49	0.46
1:D:421:GLN:HE21	1:D:425:LYS:HE2	1.81	0.46
1:F:318:GLY:O	1:F:320:VAL:N	2.48	0.46
1:F:349:ARG:HH21	1:F:350:PRO:HG2	1.80	0.46
1:F:361:GLY:C	1:F:362:ARG:HD2	2.40	0.46
1:A:241:ILE:HD12	1:A:241:ILE:H	1.80	0.46
1:B:633:ILE:HG22	1:B:639:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:LYS:HB2	1:D:315:LYS:HB2	1.97	0.46
1:F:382:GLN:O	1:F:386:LYS:HG2	2.15	0.46
1:F:423:ILE:HD13	1:F:445:LEU:HD11	1.98	0.46
1:A:427:MET:HE1	1:A:432:LEU:HB3	1.98	0.46
1:A:493:VAL:HG21	1:A:535:CYS:SG	2.56	0.46
1:E:563:PHE:CD1	1:E:611:MET:HG3	2.50	0.46
1:F:381:LEU:O	1:F:385:THR:OG1	2.20	0.46
2:G:210:PRO:HD2	2:G:420:TYR:CE2	2.51	0.46
2:G:544:LYS:HD2	2:G:549:TRP:HD1	1.79	0.46
1:A:277:LYS:O	1:A:281:GLU:HB3	2.15	0.46
1:E:422:ALA:HB2	1:E:447:VAL:HG12	1.98	0.46
2:G:194:CYS:SG	2:G:197:HIS:HD2	2.38	0.46
2:G:200:TRP:CG	2:G:201:PRO:HA	2.50	0.46
1:A:377:ARG:HG2	1:A:411:LEU:HD11	1.98	0.46
1:B:654:VAL:HG12	1:B:658:LYS:HD2	1.98	0.46
1:E:231:LYS:HA	1:E:231:LYS:HD3	1.71	0.46
1:E:516:PHE:HD1	1:E:643:ILE:HB	1.81	0.46
2:G:165:HIS:HB3	2:G:264:LEU:HD23	1.98	0.46
1:A:432:LEU:HD21	1:B:226:HIS:CE1	2.52	0.45
1:C:271:GLY:O	1:C:309:ILE:HD11	2.15	0.45
1:D:277:LYS:O	1:D:277:LYS:HG3	2.16	0.45
1:E:422:ALA:HB1	1:E:445:LEU:HD11	1.98	0.45
1:E:608:MET:O	1:E:612:SER:N	2.44	0.45
1:F:349:ARG:NH2	1:F:350:PRO:HG2	2.31	0.45
2:G:106:VAL:O	2:G:106:VAL:HG12	2.16	0.45
1:A:615:LYS:HG3	1:A:617:VAL:HG23	1.98	0.45
1:B:297:ALA:HB1	1:B:298:PRO:CD	2.46	0.45
1:B:609:ASP:OD2	1:B:635:ARG:NH2	2.40	0.45
1:C:313:ARG:HG2	1:C:322:ARG:HG2	1.98	0.45
1:C:334:GLY:N	1:C:337:GLN:NE2	2.63	0.45
1:D:222:LEU:HB3	1:D:223:PRO:HD3	1.99	0.45
1:D:316:THR:HG23	1:D:321:GLU:CD	2.42	0.45
1:D:545:PRO:HG3	1:D:581:SER:HB2	1.98	0.45
1:E:300:ILE:HA	1:E:342:ILE:O	2.16	0.45
2:G:236:ARG:HH12	2:G:470:PRO:CB	2.29	0.45
1:F:303:ILE:O	1:F:303:ILE:HG13	2.17	0.45
1:A:421:GLN:HE21	1:A:454:TRP:CD1	2.34	0.45
1:B:426:LYS:HG3	1:B:445:LEU:CD2	2.47	0.45
1:C:592:ASP:HA	1:D:594:GLY:HA3	1.98	0.45
1:D:217:LYS:O	1:D:221:GLU:HG2	2.17	0.45
1:D:277:LYS:HZ2	1:E:319:GLU:C	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:GLU:HA	1:E:295:LYS:HE3	1.98	0.45
1:E:548:LEU:HD23	1:E:549:THR:N	2.30	0.45
1:F:389:LYS:HG3	1:F:445:LEU:O	2.16	0.45
2:G:227:MET:HA	2:G:455:THR:O	2.17	0.45
1:B:749:ASP:O	1:B:753:ARG:HG3	2.17	0.45
1:C:336:LYS:C	1:C:337:GLN:HG2	2.41	0.45
1:D:211:LYS:O	1:D:215:GLN:HG3	2.16	0.45
1:A:539:PHE:CE1	1:B:611:MET:HE1	2.51	0.45
1:A:682:PHE:HE2	1:A:743:ALA:HB1	1.81	0.45
1:E:226:HIS:HE1	1:E:229:LEU:HD22	1.81	0.45
1:E:597:ALA:O	1:E:601:ILE:HG12	2.16	0.45
1:F:328:LEU:O	1:F:332:MET:HG2	2.17	0.45
1:F:384:HIS:CE1	5:F:901:ATP:H1'	2.51	0.45
1:A:697:LEU:HD13	1:A:738:GLU:HB3	1.99	0.45
1:E:425:LYS:C	1:E:426:LYS:HD3	2.42	0.45
1:A:487:ARG:O	1:A:491:GLU:HG3	2.16	0.45
1:B:709:ARG:O	1:B:712:GLU:HG3	2.17	0.45
1:E:273:GLU:O	1:E:277:LYS:NZ	2.42	0.45
1:E:750:ASN:HA	1:E:753:ARG:HD3	1.99	0.45
1:F:213:LEU:O	1:F:217:LYS:HD3	2.17	0.45
1:F:329:LEU:HD21	1:F:357:LEU:HD22	1.99	0.45
1:A:388:MET:HE1	1:A:415:CYS:HB3	1.99	0.45
1:A:424:ARG:HH22	1:A:454:TRP:HE1	1.65	0.45
1:A:426:LYS:NZ	1:A:445:LEU:HA	2.32	0.45
1:D:332:MET:HE1	1:D:363:PHE:CE2	2.52	0.45
1:E:636:PRO:HA	1:E:640:ASP:HB3	1.99	0.45
2:G:321:ARG:O	2:G:322:LYS:HE2	2.17	0.45
1:A:312:LYS:HD2	1:A:314:GLU:HG3	1.99	0.45
1:A:349:ARG:HB3	1:A:352:SER:OG	2.17	0.45
1:E:690:ILE:HG12	1:E:740:MET:HA	1.99	0.45
1:F:204:ASP:OD1	1:F:204:ASP:N	2.49	0.45
2:G:329:ARG:HH22	2:G:340:GLU:CD	2.25	0.45
2:G:473:ILE:HB	2:G:476:ARG:HG3	1.98	0.44
1:D:277:LYS:HD3	1:E:319:GLU:CB	2.47	0.44
1:D:549:THR:O	1:D:555:SER:OG	2.35	0.44
2:G:183:LEU:HD23	2:G:183:LEU:H	1.83	0.44
1:A:242:LEU:C	1:A:243:LEU:HD12	2.42	0.44
1:B:515:LEU:HD22	1:B:634:LEU:HD21	1.99	0.44
1:F:349:ARG:HG3	1:F:352:SER:HB3	1.99	0.44
1:A:457:SER:OG	1:A:458:GLN:NE2	2.34	0.44
1:E:247:PRO:HA	1:E:348:ASN:HD22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:625:ARG:HG3	1:E:754:LYS:HZ3	1.81	0.44
1:E:644:TYR:CZ	1:E:646:PRO:HB3	2.52	0.44
2:G:229:GLU:HG3	2:G:270:VAL:O	2.18	0.44
1:A:315:LYS:HG3	1:A:316:THR:H	1.83	0.44
1:C:231:LYS:HA	1:C:231:LYS:HD2	1.60	0.44
1:C:431:ASP:O	1:C:432:LEU:HB2	2.17	0.44
1:C:757:MET:O	1:C:761:THR:HG23	2.18	0.44
1:A:242:LEU:HD11	1:A:344:MET:HG3	1.99	0.44
1:B:312:LYS:H	1:B:315:LYS:NZ	2.12	0.44
1:B:752:ILE:O	1:B:756:GLU:HG2	2.18	0.44
1:C:222:LEU:HB3	1:C:223:PRO:HD3	1.99	0.44
1:C:297:ALA:O	1:C:298:PRO:C	2.61	0.44
1:C:677:LYS:HB2	1:C:677:LYS:HE2	1.65	0.44
1:E:385:THR:O	1:E:388:MET:HG2	2.17	0.44
2:G:474:GLU:OE1	2:G:508:HIS:ND1	2.46	0.44
1:E:237:PRO:HD2	1:E:337:GLN:HE22	1.83	0.44
1:E:290:PHE:CD2	1:E:331:LEU:HD13	2.53	0.44
2:G:281:THR:OG1	2:G:284:SER:OG	2.25	0.44
1:A:517:TYR:HE1	1:A:642:LEU:HB3	1.83	0.44
1:B:704:GLU:HA	1:B:707:ILE:HG22	2.00	0.44
1:C:455:ALA:O	1:C:459:SER:N	2.51	0.44
1:D:385:THR:HG22	1:D:388:MET:SD	2.58	0.44
2:G:114:LEU:HD22	2:G:264:LEU:HA	2.00	0.44
1:A:393:ASP:OD1	1:A:393:ASP:N	2.47	0.43
1:B:326:SER:O	1:B:330:THR:HG23	2.18	0.43
1:B:417:GLU:OE1	1:C:365:ARG:NH2	2.51	0.43
1:D:649:ASP:O	1:D:653:ARG:N	2.46	0.43
1:E:555:SER:O	1:E:559:VAL:HG23	2.18	0.43
1:E:648:PRO:O	1:E:653:ARG:NH1	2.50	0.43
2:G:499:VAL:HB	2:G:501:LEU:HD23	2.00	0.43
1:D:252:THR:O	1:D:256:ARG:HG2	2.18	0.43
1:D:287:ARG:HG3	1:D:327:GLN:NE2	2.32	0.43
1:D:489:LEU:HD11	1:D:516:PHE:CZ	2.53	0.43
1:A:279:ALA:O	1:A:282:SER:N	2.50	0.43
1:C:239:ARG:NH2	1:C:338:ARG:O	2.51	0.43
1:E:210:ARG:HA	1:E:213:LEU:CG	2.46	0.43
1:E:321:GLU:O	1:E:325:VAL:HG23	2.18	0.43
1:E:398:GLN:HG2	1:E:399:VAL:N	2.32	0.43
1:F:236:LYS:HE2	1:F:237:PRO:HD2	2.00	0.43
1:B:438:ASP:HB2	1:B:441:VAL:HG22	1.99	0.43
1:B:635:ARG:HH21	1:B:638:ARG:CZ	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:681:GLY:HA3	1:C:745:ARG:HD2	1.99	0.43
1:E:515:LEU:HG	1:E:621:GLY:O	2.18	0.43
1:E:582:ILE:O	1:E:601:ILE:HD11	2.18	0.43
1:F:244:TYR:CE1	1:F:368:ASP:HB2	2.53	0.43
1:F:251:LYS:HD3	1:F:346:ALA:HB1	2.01	0.43
1:F:328:LEU:HA	1:F:331:LEU:HD12	2.01	0.43
2:G:132:HIS:CD2	2:G:138:CYS:HB3	2.53	0.43
1:C:539:PHE:CE1	1:D:611:MET:HE1	2.52	0.43
1:D:224:LEU:O	1:D:227:PRO:HD3	2.18	0.43
1:D:271:GLY:HA2	1:D:309:ILE:HG13	1.99	0.43
1:D:428:ASP:OD1	1:D:429:LEU:N	2.50	0.43
1:E:567:ARG:NH2	1:E:614:LYS:HG2	2.33	0.43
1:E:653:ARG:NH2	1:E:680:ASN:HA	2.34	0.43
1:A:220:VAL:C	1:A:222:LEU:H	2.26	0.43
1:A:250:GLY:O	1:A:254:ILE:HG12	2.17	0.43
1:D:440:GLU:HG2	1:D:441:VAL:N	2.34	0.43
1:D:708:ARG:NH1	1:D:709:ARG:HE	2.17	0.43
2:G:411:TYR:CD1	3:H:259:PRO:HG3	2.53	0.43
1:C:664:SER:HB3	1:D:508:MET:HE2	2.01	0.43
1:E:514:VAL:HG13	1:E:618:PHE:HZ	1.83	0.43
1:A:220:VAL:HG22	1:A:221:GLU:N	2.33	0.43
1:D:737:GLU:OE2	1:E:773:PHE:HB3	2.19	0.43
1:E:382:GLN:HB2	1:E:386:LYS:HE3	2.00	0.43
1:E:477:GLU:HG2	1:E:662:ARG:NH1	2.32	0.43
2:G:197:HIS:ND1	2:G:203:GLY:O	2.52	0.43
2:G:234:ALA:HB1	2:G:382:PHE:CZ	2.54	0.43
2:G:555:LEU:O	2:G:557:SER:N	2.52	0.43
1:D:647:LEU:HD12	1:D:752:ILE:HD12	2.00	0.43
1:E:247:PRO:HA	1:E:348:ASN:ND2	2.33	0.43
1:E:399:VAL:HG11	1:E:452:PHE:CD1	2.53	0.43
1:E:526:LEU:HD11	6:E:901:ADP:H2'	2.00	0.43
2:G:513:LEU:HB3	2:G:521:LEU:HD12	2.01	0.43
2:G:524:SER:O	2:G:543:TRP:NE1	2.49	0.43
1:C:750:ASN:O	1:C:753:ARG:HG2	2.18	0.42
1:D:278:LEU:C	1:D:280:GLY:H	2.26	0.42
1:D:489:LEU:HD11	1:D:516:PHE:HZ	1.84	0.42
1:E:261:GLU:O	1:E:261:GLU:HG2	2.19	0.42
1:E:438:ASP:HB2	1:E:440:GLU:OE1	2.18	0.42
1:F:277:LYS:HB3	1:F:281:GLU:HG2	2.00	0.42
1:C:609:ASP:OD2	1:C:635:ARG:NH2	2.46	0.42
1:D:271:GLY:O	1:D:274:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:465:ARG:HH12	1:D:358:ARG:CZ	2.33	0.42
1:C:732:ARG:HG3	1:C:734:ASP:OD1	2.19	0.42
1:D:427:MET:HA	1:D:430:ILE:HG12	2.02	0.42
1:D:629:ILE:HG21	1:D:634:LEU:HD21	2.01	0.42
1:E:321:GLU:HG2	1:E:322:ARG:N	2.35	0.42
1:E:395:ASP:H	1:E:449:MET:HE3	1.84	0.42
2:G:155:LEU:HD12	2:G:157:PRO:HD2	2.01	0.42
2:G:295:VAL:O	2:G:299:ILE:HG12	2.19	0.42
1:A:439:ALA:O	1:A:442:MET:HB2	2.19	0.42
1:C:219:MET:CE	1:C:365:ARG:HD2	2.46	0.42
1:C:672:LEU:HD23	1:C:675:LEU:HD12	2.01	0.42
1:D:272:PRO:HB3	1:E:313:ARG:HH12	1.84	0.42
1:D:307:ASP:OD1	1:D:308:ALA:N	2.52	0.42
1:D:550:MET:O	4:I:1:MET:N	2.45	0.42
1:F:319:GLU:O	1:F:322:ARG:HG2	2.19	0.42
1:A:265:PHE:O	1:A:300:ILE:HG22	2.19	0.42
1:A:338:ARG:HB2	1:A:340:HIS:CD2	2.54	0.42
1:E:408:GLY:HA2	1:E:411:LEU:HD22	2.02	0.42
1:F:302:PHE:HA	1:F:344:MET:O	2.19	0.42
1:C:427:MET:HE3	1:C:432:LEU:HD21	2.01	0.42
1:C:439:ALA:HA	1:C:442:MET:HB3	2.01	0.42
1:D:523:GLY:N	5:D:901:ATP:O2B	2.52	0.42
1:E:250:GLY:O	1:E:253:LEU:HG	2.20	0.42
1:E:377:ARG:HH11	1:E:403:THR:HG21	1.85	0.42
1:E:449:MET:HA	1:E:452:PHE:HD2	1.84	0.42
1:E:495:TYR:HA	1:E:502:LYS:HE3	2.01	0.42
1:B:268:LEU:HD22	1:C:335:LEU:HD22	2.00	0.42
1:B:691:CYS:C	1:B:695:CYS:HB3	2.42	0.42
1:D:332:MET:HE1	1:D:363:PHE:CZ	2.55	0.42
1:D:479:ILE:HB	1:D:486:LYS:HE2	2.01	0.42
1:B:426:LYS:HG3	1:B:445:LEU:HD21	2.01	0.42
1:C:689:GLU:HB2	1:D:636:PRO:HB3	2.02	0.42
1:F:447:VAL:HG22	1:F:452:PHE:HE1	1.85	0.42
1:A:440:GLU:OE2	1:A:444:SER:OG	2.37	0.42
1:B:349:ARG:HG3	1:B:352:SER:OG	2.19	0.42
1:D:515:LEU:HB2	1:D:639:LEU:HD13	2.02	0.42
1:E:388:MET:HG3	1:E:390:LEU:HG	2.02	0.42
1:E:699:ILE:O	1:E:703:ILE:HG13	2.19	0.42
1:F:325:VAL:O	1:F:329:LEU:HG	2.20	0.42
1:A:653:ARG:NH1	1:A:680:ASN:O	2.53	0.42
1:B:203:TYR:CD1	1:B:257:ALA:HB1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:MET:HE2	1:D:319:GLU:CD	2.45	0.42
1:D:629:ILE:HB	1:D:634:LEU:HD11	2.02	0.42
1:E:757:MET:O	1:E:761:THR:HG23	2.20	0.42
1:F:215:GLN:HA	1:F:218:GLU:OE2	2.19	0.42
1:A:354:ASP:OD1	1:A:354:ASP:N	2.52	0.41
1:B:695:CYS:O	1:B:699:ILE:HG12	2.19	0.41
1:E:249:THR:HG22	1:E:251:LYS:HZ2	1.85	0.41
1:A:357:LEU:O	1:A:363:PHE:N	2.52	0.41
1:B:515:LEU:HB3	1:B:642:LEU:HD22	2.01	0.41
1:C:632:ALA:O	1:C:638:ARG:NH1	2.51	0.41
1:C:675:LEU:HD21	1:D:773:PHE:CZ	2.55	0.41
1:E:606:THR:O	1:E:610:GLY:N	2.52	0.41
2:G:242:ARG:NH2	4:I:46:ALA:O	2.47	0.41
2:G:443:LEU:HD12	2:G:444:PRO:HD2	2.02	0.41
1:A:388:MET:HG3	1:B:233:ILE:HG22	2.02	0.41
1:C:388:MET:HA	1:D:233:ILE:O	2.20	0.41
1:C:428:ASP:OD1	1:C:429:LEU:N	2.54	0.41
1:E:216:ILE:O	1:E:220:VAL:HG12	2.20	0.41
1:E:608:MET:HE3	1:E:619:ILE:HD12	2.02	0.41
2:G:165:HIS:O	2:G:169:ARG:HG2	2.19	0.41
2:G:282:GLN:OE1	2:G:283:ASN:ND2	2.54	0.41
2:G:436:ILE:HD11	2:G:438:GLN:HE21	1.85	0.41
1:A:206:ILE:HG13	1:A:206:ILE:O	2.20	0.41
1:A:238:PRO:HB2	1:A:341:VAL:HA	2.02	0.41
1:B:292:GLU:HG3	2:G:420:TYR:HE1	1.85	0.41
1:D:739:ALA:O	1:D:742:PHE:N	2.45	0.41
1:E:649:ASP:OD1	1:E:649:ASP:N	2.51	0.41
4:I:41:GLN:NE2	4:I:43:LEU:HD11	2.36	0.41
1:A:332:MET:HE1	1:A:363:PHE:CE2	2.55	0.41
1:A:390:LEU:HB3	1:A:394:VAL:HG11	2.02	0.41
1:A:545:PRO:HG3	1:A:581:SER:HB3	2.02	0.41
1:C:349:ARG:HG3	1:C:349:ARG:O	2.20	0.41
1:E:246:PRO:HG2	1:E:249:THR:HB	2.03	0.41
1:E:252:THR:OG1	6:E:902:ADP:O1B	2.36	0.41
1:E:394:VAL:HG23	1:E:448:THR:HA	2.03	0.41
2:G:213:ILE:HG22	2:G:213:ILE:O	2.20	0.41
2:G:252:LEU:HD22	2:G:270:VAL:HG11	2.03	0.41
3:H:259:PRO:HB2	3:H:261:TYR:CE2	2.56	0.41
1:B:652:SER:O	1:B:656:ILE:HG13	2.20	0.41
1:D:521:GLY:HA3	1:E:635:ARG:HD2	2.02	0.41
1:E:385:THR:HA	1:E:388:MET:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:PRO:HB2	1:E:512:LYS:HE3	2.02	0.41
1:F:240:GLY:HA2	1:F:363:PHE:CD1	2.55	0.41
1:F:335:LEU:HD21	1:F:341:VAL:HB	2.03	0.41
1:A:221:GLU:O	1:A:225:ARG:N	2.53	0.41
1:A:517:TYR:CZ	1:A:644:TYR:HB2	2.56	0.41
1:B:200:GLU:OE1	1:B:200:GLU:N	2.54	0.41
1:E:528:ALA:O	1:E:531:ILE:HG22	2.20	0.41
1:F:201:VAL:O	1:F:256:ARG:NH1	2.54	0.41
1:F:216:ILE:O	1:F:220:VAL:HG22	2.20	0.41
2:G:429:VAL:HG23	4:I:22:THR:HG21	2.01	0.41
2:G:527:LEU:HD21	2:G:543:TRP:HD1	1.86	0.41
1:A:287:ARG:HB2	1:A:291:GLU:OE1	2.21	0.41
1:A:682:PHE:CE2	1:A:743:ALA:HB1	2.56	0.41
1:D:749:ASP:O	1:D:753:ARG:HG3	2.20	0.41
1:E:258:VAL:O	1:E:262:THR:HG22	2.20	0.41
1:E:540:ILE:O	1:E:575:PHE:N	2.49	0.41
1:E:639:LEU:HD23	1:E:639:LEU:HA	1.89	0.41
1:F:244:TYR:CE2	1:F:350:PRO:HG3	2.55	0.41
1:A:212:GLN:HG2	1:A:369:ILE:HD13	2.02	0.41
1:A:243:LEU:O	1:A:244:TYR:HD1	2.03	0.41
1:A:516:PHE:HD1	1:A:643:ILE:HB	1.86	0.41
1:B:273:GLU:OE2	2:G:206:THR:HG23	2.21	0.41
1:B:702:SER:O	1:B:706:GLU:OE1	2.39	0.41
1:C:433:GLU:HA	1:D:225:ARG:NH2	2.35	0.41
1:D:221:GLU:O	1:D:225:ARG:CB	2.67	0.41
1:D:551:TRP:CZ3	4:I:4:PHE:HZ	2.38	0.41
1:E:231:LYS:HZ3	1:E:231:LYS:HG2	1.76	0.41
1:E:602:ASN:O	1:E:606:THR:HG23	2.21	0.41
1:E:612:SER:O	1:E:615:LYS:HD3	2.21	0.41
1:E:656:ILE:HG12	6:E:901:ADP:C6	2.56	0.41
1:F:265:PHE:HB2	1:F:296:ASN:HD22	1.85	0.41
2:G:200:TRP:CD2	2:G:201:PRO:HA	2.55	0.41
2:G:231:HIS:CE1	4:I:45:PHE:HE2	2.39	0.41
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.56	0.41
1:B:686:ASP:OD1	1:C:636:PRO:HG2	2.21	0.41
1:C:297:ALA:HB1	1:C:298:PRO:HD2	2.03	0.41
1:D:229:LEU:HD13	1:D:229:LEU:HA	1.81	0.41
1:D:338:ARG:H	1:D:338:ARG:HD3	1.86	0.41
1:D:496:PRO:HB3	1:D:510:PRO:HG3	2.02	0.41
1:D:699:ILE:O	1:D:703:ILE:HG12	2.21	0.41
1:E:484:ASP:OD1	1:E:485:VAL:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:327:GLN:HE22	1:F:331:LEU:HD11	1.86	0.41
1:F:353:ILE:HD12	1:F:353:ILE:H	1.86	0.41
1:A:228:ALA:HA	1:A:231:LYS:HD2	2.03	0.40
1:A:242:LEU:O	1:A:243:LEU:HD12	2.21	0.40
1:A:407:VAL:HG12	1:A:408:GLY:N	2.35	0.40
1:B:693:ARG:C	1:B:695:CYS:H	2.29	0.40
1:C:551:TRP:HB2	1:C:554:GLU:HG2	2.02	0.40
1:D:233:ILE:CG2	1:D:235:VAL:HG12	2.51	0.40
1:E:510:PRO:HG2	1:E:615:LYS:HE3	2.03	0.40
2:G:147:PHE:HA	2:G:170:LYS:HG3	2.02	0.40
2:G:218:GLN:HG2	2:G:220:TYR:H	1.85	0.40
1:B:544:GLY:HA3	1:B:545:PRO:HD3	1.89	0.40
1:C:479:ILE:HB	1:C:486:LYS:HE2	2.03	0.40
1:D:231:LYS:HD2	1:D:231:LYS:HA	1.52	0.40
1:E:236:LYS:HB3	1:E:337:GLN:HE21	1.86	0.40
1:A:266:PHE:CE2	1:A:302:PHE:CD2	3.08	0.40
1:A:334:GLY:HA3	1:A:338:ARG:NE	2.36	0.40
1:B:251:LYS:HB2	1:B:251:LYS:HE2	1.91	0.40
1:C:542:ILE:HD11	1:C:562:ILE:HG12	2.03	0.40
1:C:678:MET:HG2	1:D:771:PHE:CD2	2.57	0.40
1:E:244:TYR:OH	1:E:368:ASP:HB2	2.20	0.40
1:E:335:LEU:H	1:E:335:LEU:HD23	1.86	0.40
1:E:516:PHE:HE1	1:E:643:ILE:HD12	1.86	0.40
1:A:608:MET:HE3	1:A:638:ARG:HD2	2.04	0.40
1:C:552:PHE:HA	4:I:3:ILE:HG21	2.03	0.40
1:D:727:PRO:HB2	1:D:728:VAL:H	1.74	0.40
1:E:244:TYR:HB2	1:E:350:PRO:HB3	2.04	0.40
1:E:309:ILE:HB	1:E:324:ILE:HG21	2.03	0.40
1:E:539:PHE:CE1	1:E:575:PHE:HB2	2.57	0.40
1:E:659:ALA:O	1:E:662:ARG:NE	2.51	0.40
1:F:312:LYS:HE3	1:F:352:SER:HA	2.03	0.40
2:G:146:PRO:O	2:G:147:PHE:HB2	2.21	0.40
1:A:294:GLU:OE1	1:A:301:ILE:HD11	2.22	0.40
1:A:403:THR:HG22	1:A:406:HIS:HB2	2.02	0.40
1:A:681:GLY:HA3	1:A:745:ARG:HE	1.85	0.40
1:B:321:GLU:O	1:B:325:VAL:HG23	2.21	0.40
1:D:514:VAL:HG13	1:D:643:ILE:HD13	2.04	0.40
1:E:277:LYS:HG2	1:E:281:GLU:OE1	2.21	0.40
1:E:583:ALA:HA	1:E:601:ILE:CD1	2.52	0.40
1:E:610:GLY:O	1:E:611:MET:HE2	2.21	0.40
1:F:286:LEU:HD12	1:F:286:LEU:HA	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:280:GLY:HA2	2:G:285:LEU:HA	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	550/806 (68%)	496 (90%)	48 (9%)	6 (1%)	11	40
1	B	560/806 (70%)	530 (95%)	29 (5%)	1 (0%)	43	73
1	C	547/806 (68%)	513 (94%)	34 (6%)	0	100	100
1	D	559/806 (69%)	525 (94%)	32 (6%)	2 (0%)	30	62
1	E	547/806 (68%)	500 (91%)	44 (8%)	3 (0%)	24	58
1	F	260/806 (32%)	229 (88%)	29 (11%)	2 (1%)	16	47
2	G	449/608 (74%)	427 (95%)	21 (5%)	1 (0%)	43	73
3	H	17/307 (6%)	15 (88%)	2 (12%)	0	100	100
4	I	47/76 (62%)	43 (92%)	4 (8%)	0	100	100
All	All	3536/5827 (61%)	3278 (93%)	243 (7%)	15 (0%)	31	62

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	ILE
1	A	279	ALA
1	B	297	ALA
2	G	147	PHE
1	E	548	LEU
1	E	549	THR
1	A	258	VAL

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Mol	Chain	Res	Type
1	F	232	ALA
1	F	319	GLU
1	A	303	ILE
1	A	435	GLU
1	D	251	LYS
1	D	768	PHE
1	E	472	PRO
1	A	237	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	453/678 (67%)	452 (100%)	1 (0%)	87	92
1	B	460/678 (68%)	458 (100%)	2 (0%)	84	90
1	C	451/678 (66%)	450 (100%)	1 (0%)	87	92
1	D	461/678 (68%)	458 (99%)	3 (1%)	76	87
1	E	453/678 (67%)	452 (100%)	1 (0%)	87	92
1	F	214/678 (32%)	211 (99%)	3 (1%)	59	80
2	G	405/531 (76%)	404 (100%)	1 (0%)	87	92
3	H	17/267 (6%)	17 (100%)	0	100	100
4	I	45/69 (65%)	44 (98%)	1 (2%)	45	73
All	All	2959/4935 (60%)	2946 (100%)	13 (0%)	81	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	LEU
1	B	231	LYS
1	B	233	ILE
1	C	231	LYS
1	D	229	LEU
1	D	231	LYS

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Mol	Chain	Res	Type
1	D	233	ILE
1	E	231	LYS
1	F	231	LYS
1	F	235	VAL
1	F	236	LYS
2	G	486	HIS
4	I	40	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	HIS
1	A	499	HIS
1	B	443	ASN
1	B	680	ASN
1	C	226	HIS
1	C	603	GLN
1	C	624	ASN
1	D	401	ASN
1	D	443	ASN
1	D	692	GLN
1	E	317	HIS
1	E	327	GLN
1	E	337	GLN
1	E	348	ASN
1	E	603	GLN
1	F	348	ASN
1	F	351	ASN
1	F	443	ASN
2	G	231	HIS
2	G	246	ASN
2	G	283	ASN
2	G	381	HIS
4	I	31	GLN
4	I	41	GLN

5.3.3 RNA ⓘ

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](#)

11 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$
5	ATP	B	901	-	32,33,33	0.66	1 (3%)	48,52,52	0.33	0
5	ATP	A	902	-	32,33,33	0.47	0	48,52,52	0.29	0
5	ATP	B	902	-	32,33,33	0.75	2 (6%)	48,52,52	0.32	0
6	ADP	E	901	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
6	ADP	D	902	-	28,29,29	1.36	3 (10%)	43,45,45	1.86	9 (20%)
5	ATP	A	901	-	32,33,33	0.61	1 (3%)	48,52,52	0.31	0
5	ATP	C	901	-	32,33,33	0.68	2 (6%)	48,52,52	0.33	0
5	ATP	C	902	-	32,33,33	0.68	2 (6%)	48,52,52	0.32	0
5	ATP	F	901	-	32,33,33	0.48	0	48,52,52	0.32	0
5	ATP	D	901	-	32,33,33	0.56	0	48,52,52	0.31	0
6	ADP	E	902	-	28,29,29	1.42	4 (14%)	43,45,45	1.87	8 (18%)

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	ATP	B	901	-	-	2/22/38/38	0/3/3/3
5	ATP	A	902	-	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	902	-	-	8/22/38/38	0/3/3/3
6	ADP	E	901	-	-	3/16/32/32	0/3/3/3
6	ADP	D	902	-	-	5/16/32/32	0/3/3/3
5	ATP	A	901	-	-	4/22/38/38	0/3/3/3
5	ATP	C	901	-	-	4/22/38/38	0/3/3/3
5	ATP	C	902	-	-	8/22/38/38	0/3/3/3
5	ATP	F	901	-	-	7/22/38/38	0/3/3/3
5	ATP	D	901	-	-	5/22/38/38	0/3/3/3
6	ADP	E	902	-	-	3/16/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	902	ADP	C5-C4	4.75	1.47	1.39
6	E	901	ADP	C5-C4	4.74	1.47	1.39
6	D	902	ADP	C5-C4	4.43	1.47	1.39
5	B	902	ATP	PB-O3B	-2.99	1.56	1.59
5	B	901	ATP	PB-O3B	-2.75	1.56	1.59
6	E	901	ADP	C5-C6	2.69	1.48	1.41
6	D	902	ADP	C5-N7	-2.68	1.34	1.39
6	E	902	ADP	C5-N7	-2.57	1.34	1.39
5	C	902	ATP	PB-O3B	-2.48	1.56	1.59
6	E	902	ADP	C5-C6	2.42	1.47	1.41
5	C	901	ATP	PB-O3B	-2.42	1.56	1.59
6	E	901	ADP	C5-N7	-2.37	1.34	1.39
6	D	902	ADP	C5-C6	2.35	1.47	1.41
5	C	901	ATP	PA-O3A	-2.27	1.57	1.59
6	E	901	ADP	C8-N7	2.23	1.36	1.31
5	A	901	ATP	PA-O3A	-2.18	1.57	1.59
6	E	902	ADP	C8-N7	2.17	1.35	1.31
5	B	902	ATP	PA-O3A	-2.17	1.57	1.59
5	C	902	ATP	PA-O3A	-2.12	1.57	1.59

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	901	ADP	C5-C4-N3	-6.11	118.31	126.72
6	D	902	ADP	C5-C4-N3	-6.08	118.34	126.72
6	E	902	ADP	C5-C4-N3	-6.08	118.35	126.72
6	D	902	ADP	N3-C4-N9	5.10	135.84	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	902	ADP	N3-C4-N9	5.10	135.84	127.17
6	E	901	ADP	N3-C4-N9	5.00	135.67	127.17
6	E	901	ADP	C2-N3-C4	3.79	121.08	111.83
6	E	902	ADP	C2-N3-C4	3.63	120.70	111.83
6	D	902	ADP	C2-N3-C4	3.51	120.41	111.83
6	E	901	ADP	C4-C5-N7	-3.29	106.81	110.58
6	E	901	ADP	N3-C2-N1	-3.17	123.78	128.58
6	E	902	ADP	N3-C2-N1	-3.09	123.91	128.58
6	E	902	ADP	C4-C5-N7	-3.05	107.10	110.58
6	D	902	ADP	C4-C5-N7	-2.91	107.25	110.58
6	D	902	ADP	N3-C2-N1	-2.72	124.46	128.58
6	E	901	ADP	C4-N9-C8	2.62	108.49	105.74
6	E	902	ADP	C4-N9-C8	2.61	108.48	105.74
6	D	902	ADP	C3'-C2'-C1'	2.57	106.33	101.46
6	D	902	ADP	C4-N9-C8	2.55	108.42	105.74
6	E	902	ADP	C3'-C2'-C1'	2.53	106.26	101.46
6	E	901	ADP	C5-N7-C8	2.52	107.41	103.45
6	E	901	ADP	C3'-C2'-C1'	2.46	106.12	101.46
6	E	902	ADP	C5-N7-C8	2.23	106.95	103.45
6	D	902	ADP	C5-N7-C8	2.20	106.90	103.45
6	D	902	ADP	C2'-C3'-C4'	2.14	106.74	102.61

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	902	ATP	PB-O3B-PG-O3G
5	A	902	ATP	C5'-O5'-PA-O1A
5	A	902	ATP	C5'-O5'-PA-O3A
5	B	902	ATP	PB-O3B-PG-O3G
5	B	902	ATP	C5'-O5'-PA-O1A
5	B	902	ATP	C5'-O5'-PA-O2A
5	B	902	ATP	C5'-O5'-PA-O3A
5	B	902	ATP	O4'-C4'-C5'-O5'
5	C	901	ATP	C5'-O5'-PA-O1A
5	C	901	ATP	C5'-O5'-PA-O3A
5	C	902	ATP	PB-O3B-PG-O3G
5	C	902	ATP	C5'-O5'-PA-O1A
5	C	902	ATP	C5'-O5'-PA-O2A
5	C	902	ATP	C5'-O5'-PA-O3A
5	C	902	ATP	O4'-C4'-C5'-O5'
5	D	901	ATP	PB-O3B-PG-O3G

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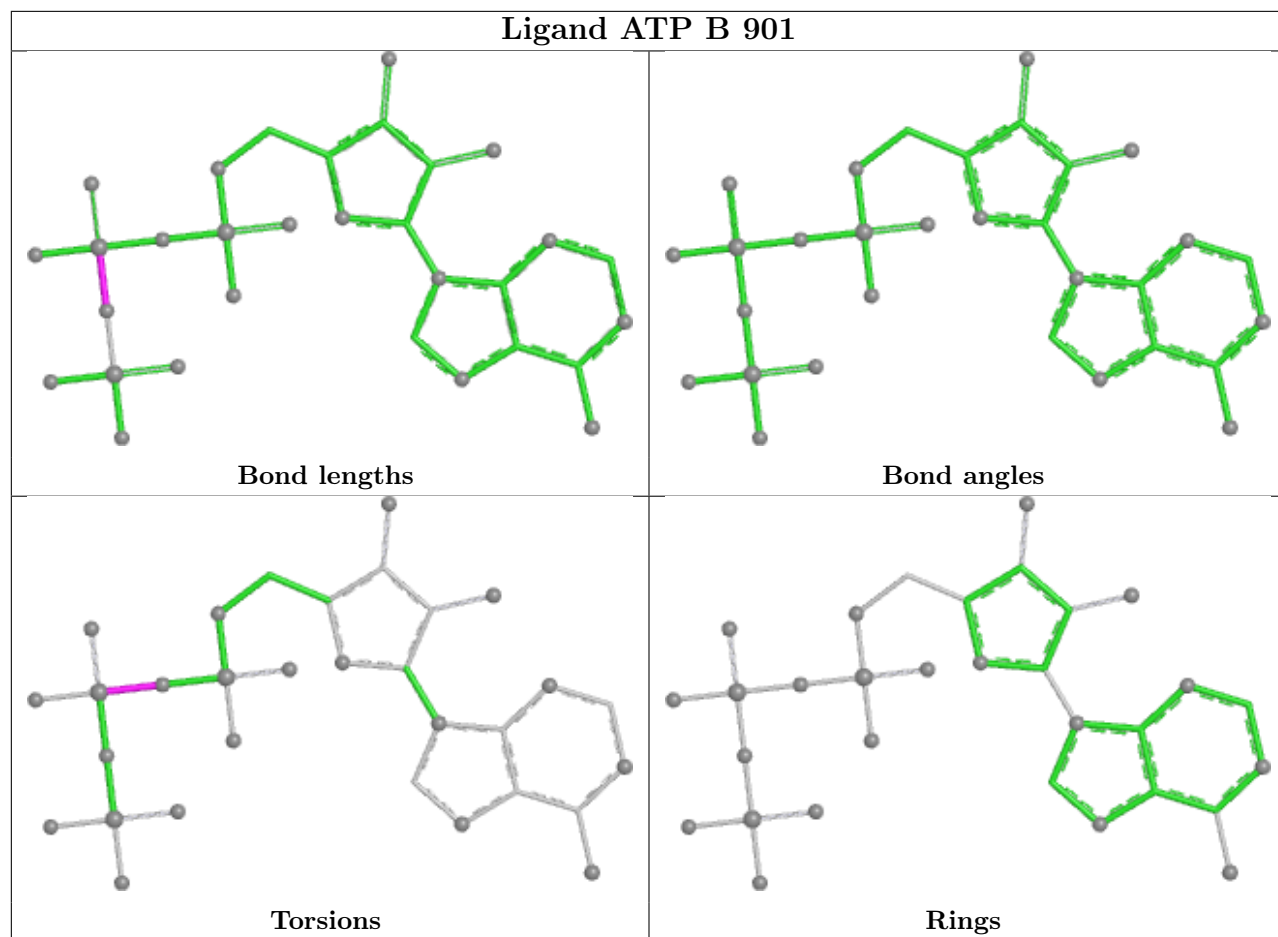
Mol	Chain	Res	Type	Atoms
5	D	901	ATP	O4'-C4'-C5'-O5'
6	E	901	ADP	C5'-O5'-PA-O1A
6	E	901	ADP	O4'-C4'-C5'-O5'
6	E	901	ADP	C3'-C4'-C5'-O5'
6	E	902	ADP	C5'-O5'-PA-O1A
6	E	902	ADP	C5'-O5'-PA-O2A
6	E	902	ADP	C5'-O5'-PA-O3A
5	B	902	ATP	C3'-C4'-C5'-O5'
5	D	901	ATP	C3'-C4'-C5'-O5'
5	C	902	ATP	C3'-C4'-C5'-O5'
5	A	901	ATP	C3'-C4'-C5'-O5'
5	A	901	ATP	O4'-C4'-C5'-O5'
5	F	901	ATP	O4'-C4'-C5'-O5'
6	D	902	ADP	O4'-C4'-C5'-O5'
6	D	902	ADP	C3'-C4'-C5'-O5'
6	D	902	ADP	PA-O3A-PB-O1B
5	A	901	ATP	PA-O3A-PB-O1B
5	D	901	ATP	PA-O3A-PB-O1B
5	F	901	ATP	PA-O3A-PB-O1B
5	C	901	ATP	C5'-O5'-PA-O2A
5	C	901	ATP	PA-O3A-PB-O2B
5	F	901	ATP	PA-O3A-PB-O2B
5	F	901	ATP	C4'-C5'-O5'-PA
5	B	901	ATP	PA-O3A-PB-O2B
5	B	902	ATP	PG-O3B-PB-O1B
5	C	902	ATP	PG-O3B-PB-O1B
5	F	901	ATP	PB-O3B-PG-O2G
6	D	902	ADP	PA-O3A-PB-O2B
6	D	902	ADP	PA-O3A-PB-O3B
5	A	901	ATP	PA-O3A-PB-O2B
5	A	902	ATP	PA-O3A-PB-O1B
5	A	902	ATP	PA-O3A-PB-O2B
5	B	901	ATP	PA-O3A-PB-O1B
5	C	902	ATP	PG-O3B-PB-O2B
5	F	901	ATP	C3'-C4'-C5'-O5'
5	A	902	ATP	PG-O3B-PB-O2B
5	B	902	ATP	PG-O3B-PB-O2B
5	D	901	ATP	PA-O3A-PB-O2B
5	F	901	ATP	PG-O3B-PB-O2B

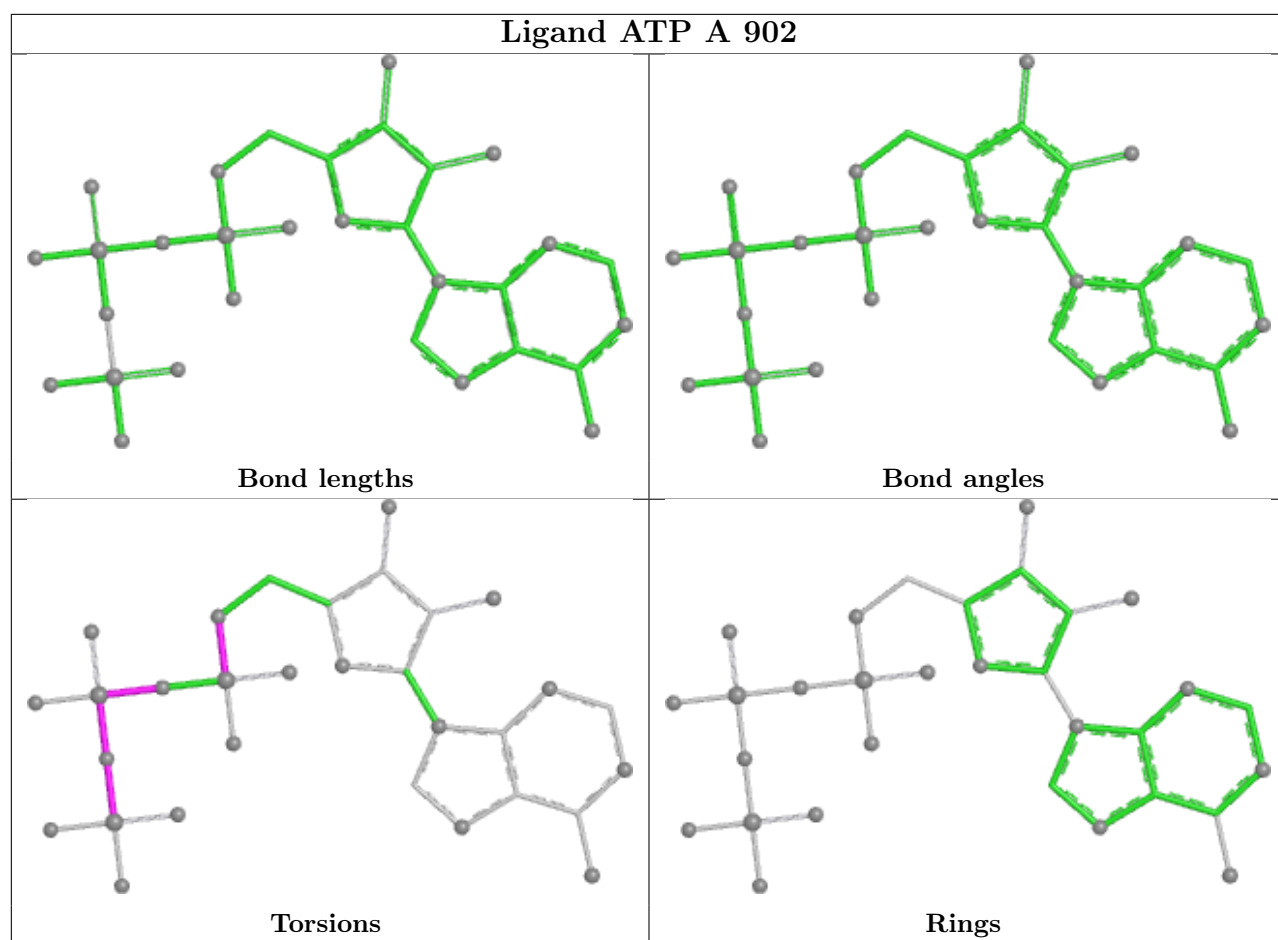
There are no ring outliers.

10 monomers are involved in 21 short contacts:

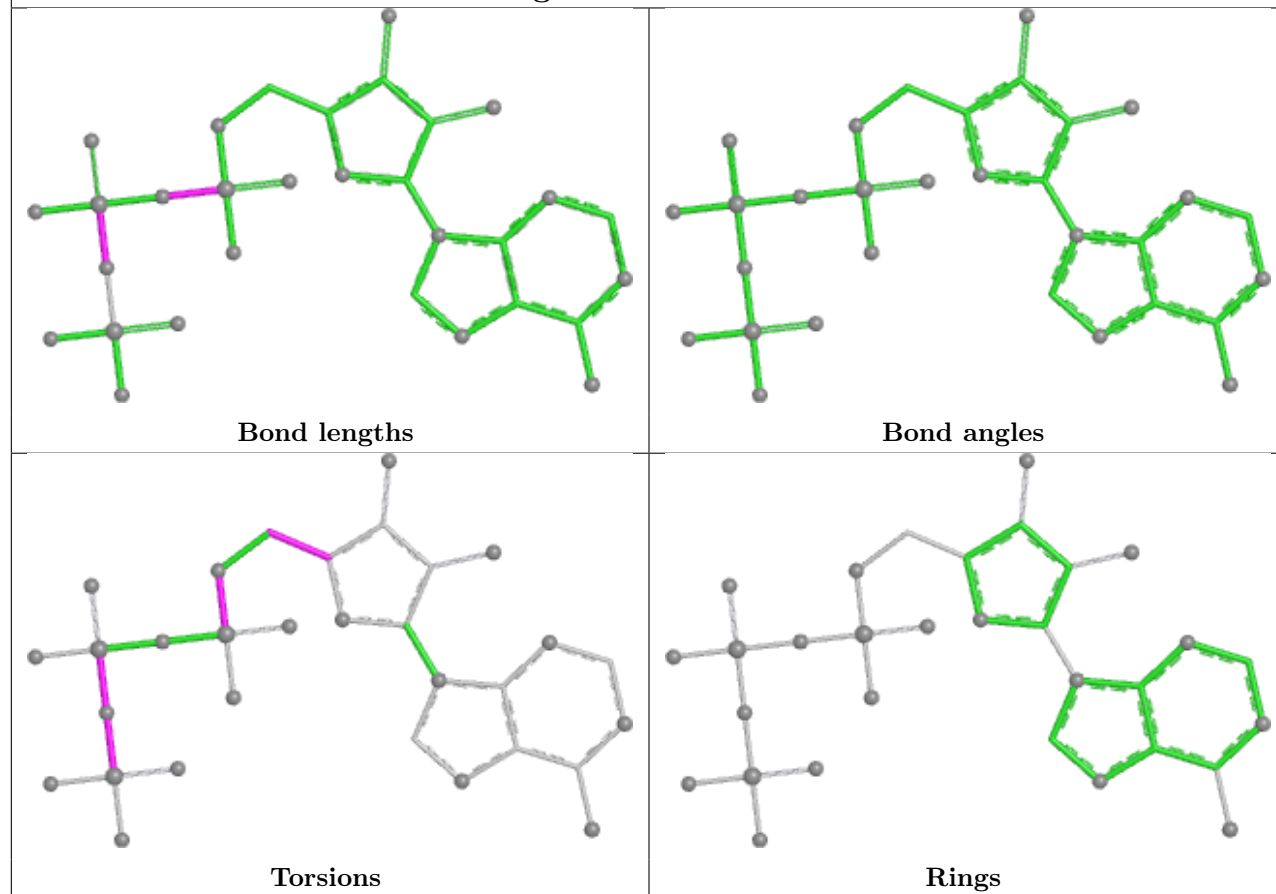
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	901	ATP	1	0
5	A	902	ATP	1	0
6	E	901	ADP	4	0
6	D	902	ADP	1	0
5	A	901	ATP	3	0
5	C	901	ATP	1	0
5	C	902	ATP	3	0
5	F	901	ATP	2	0
5	D	901	ATP	1	0
6	E	902	ADP	4	0

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

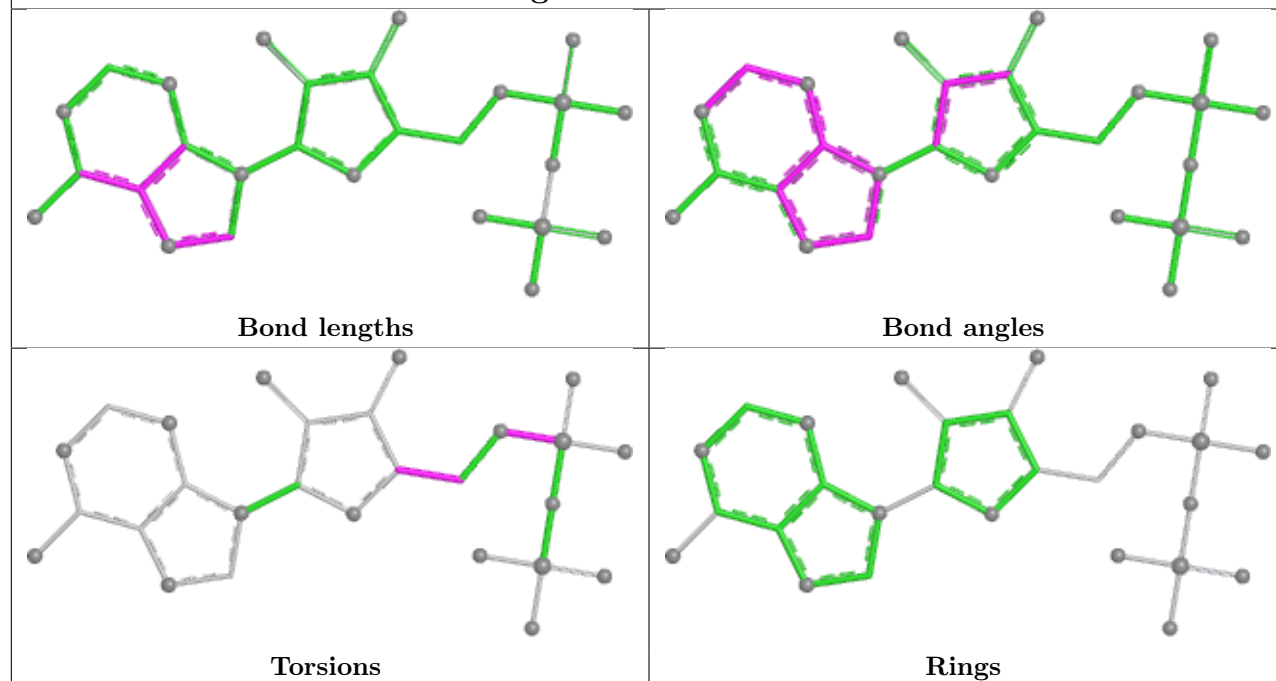


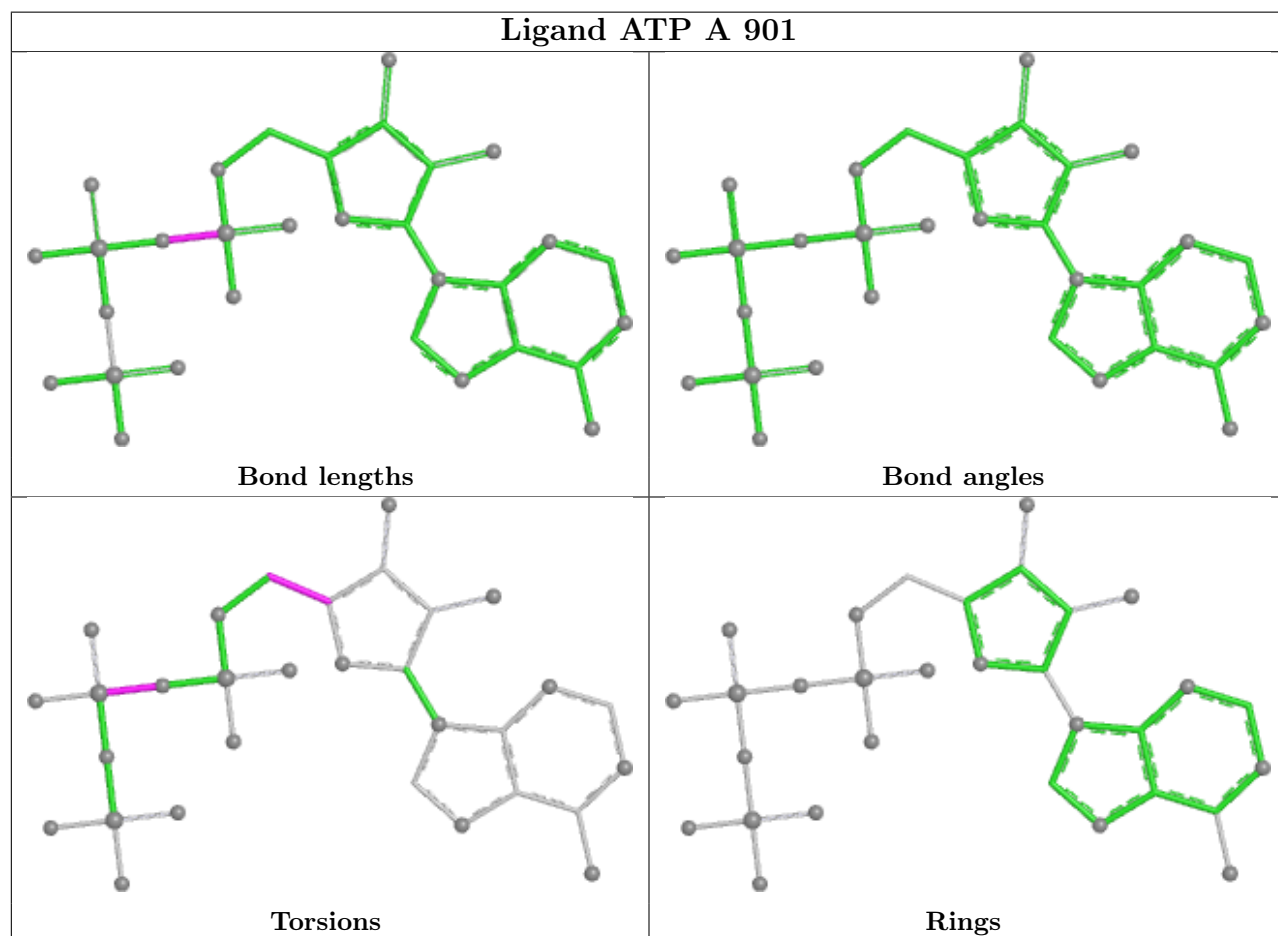
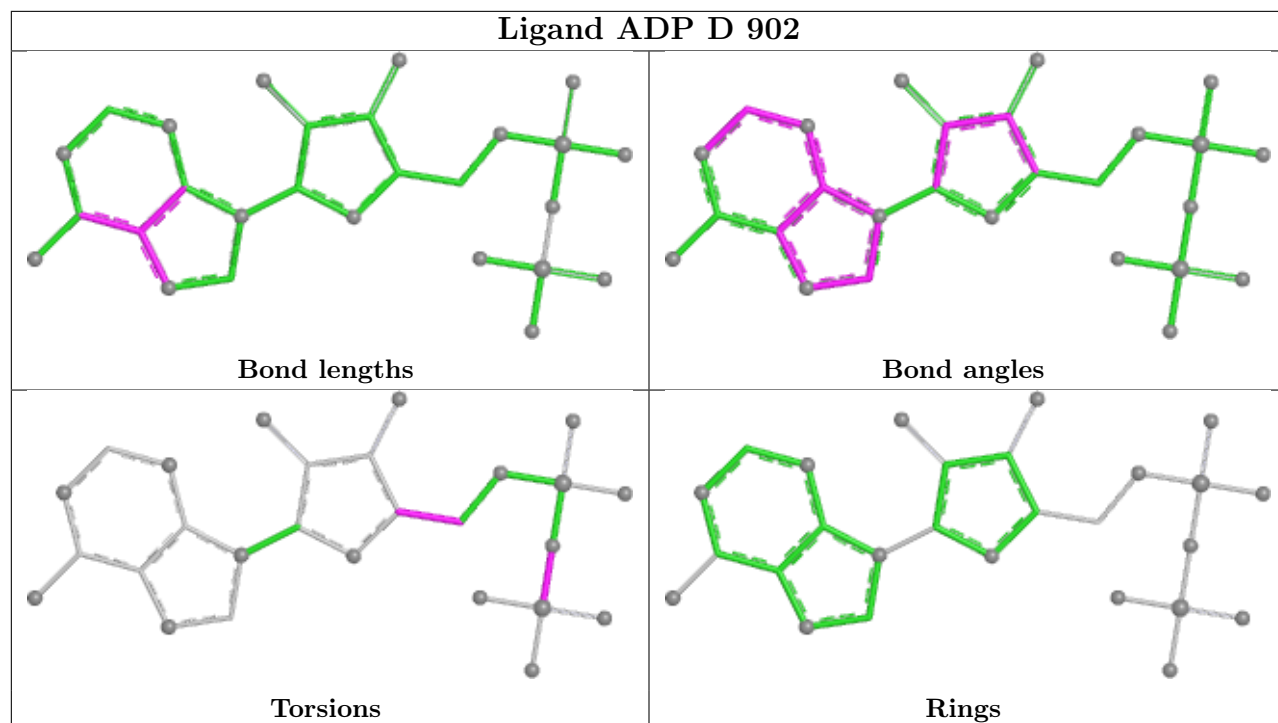


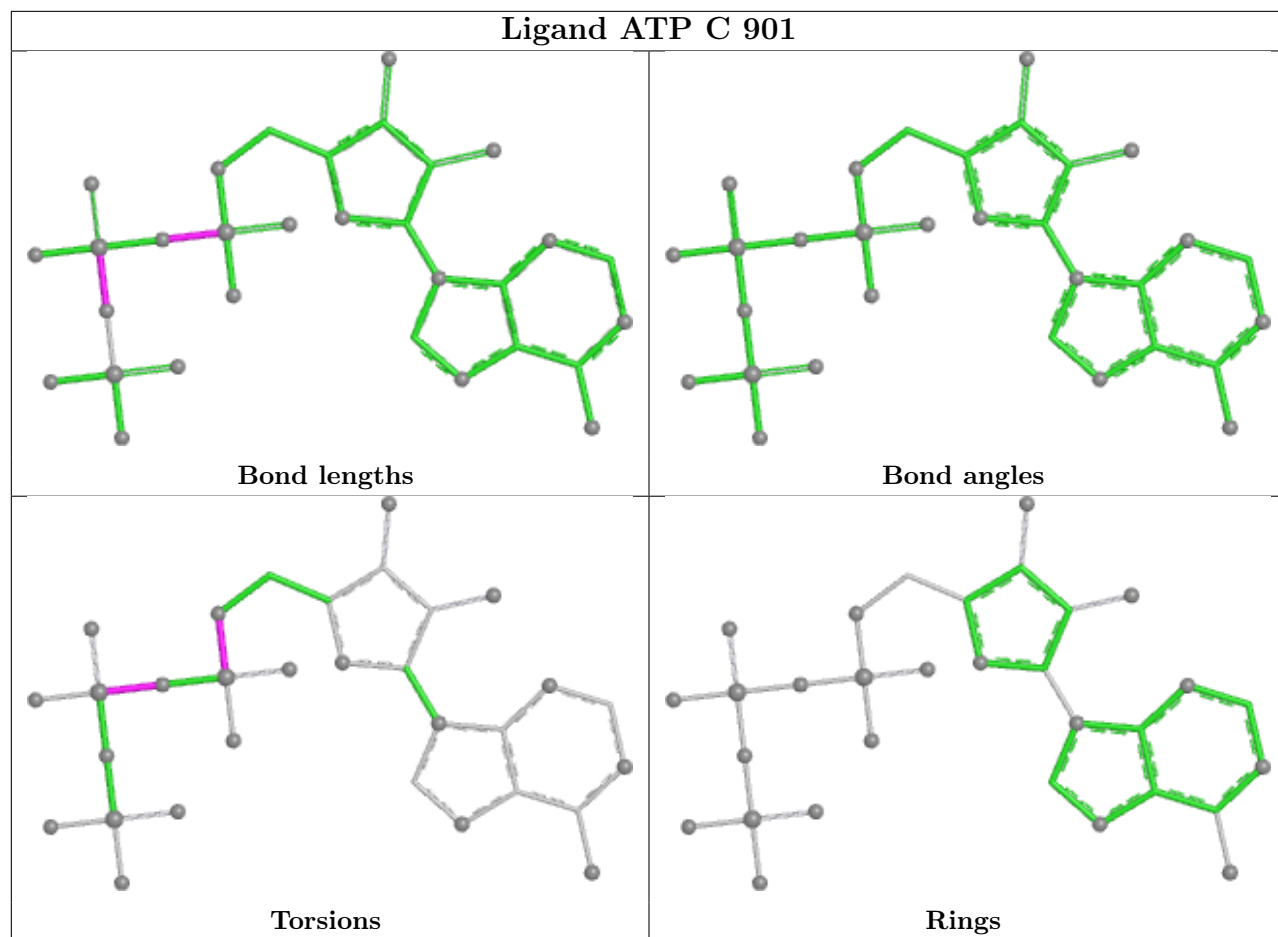
Ligand ATP B 902

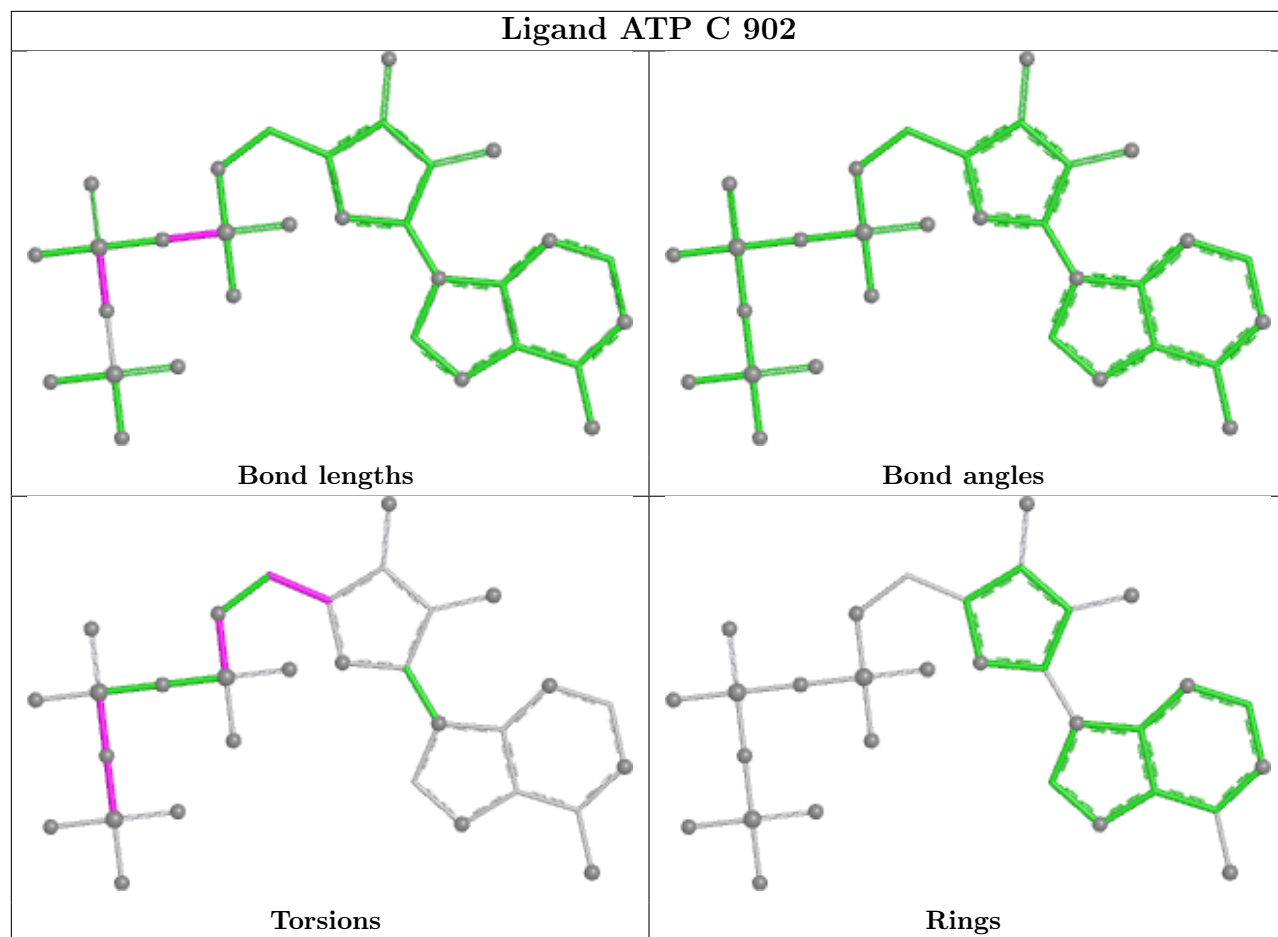


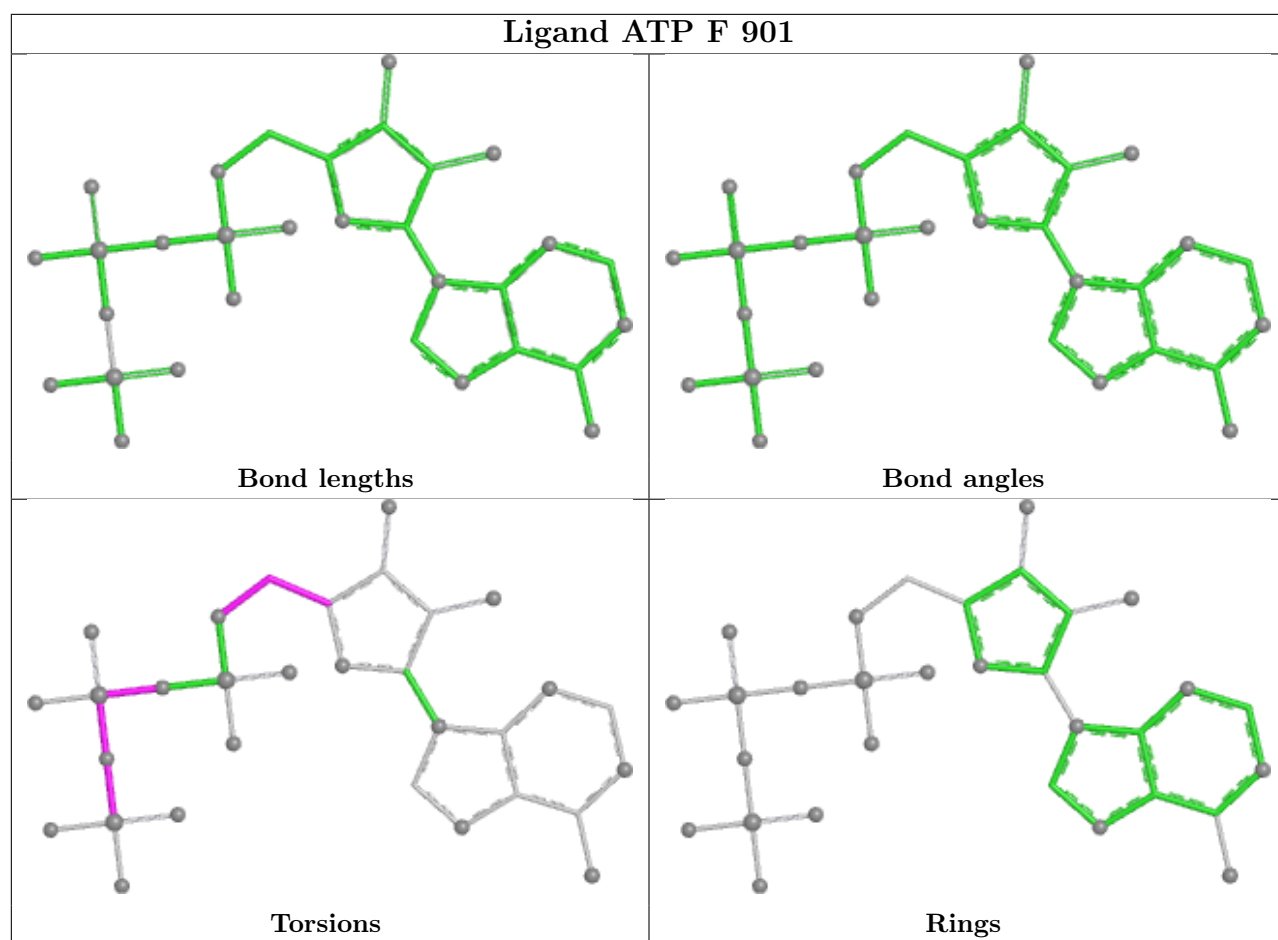
Ligand ADP E 901

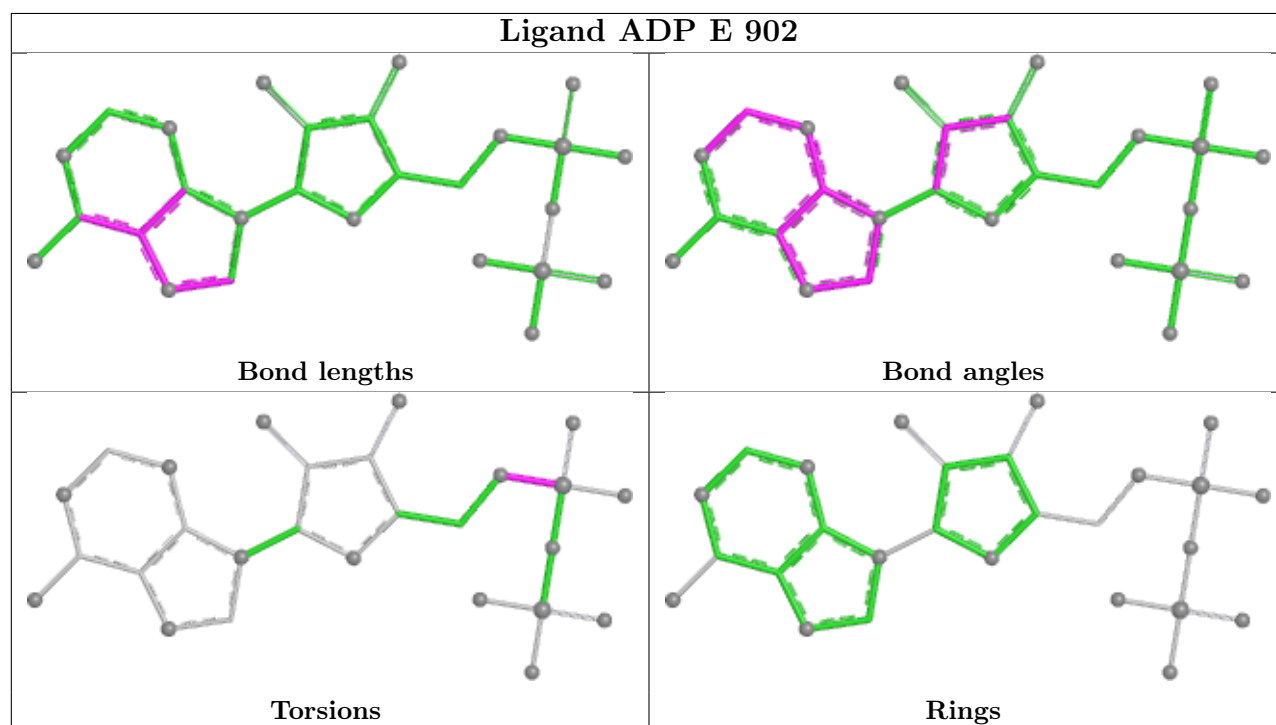
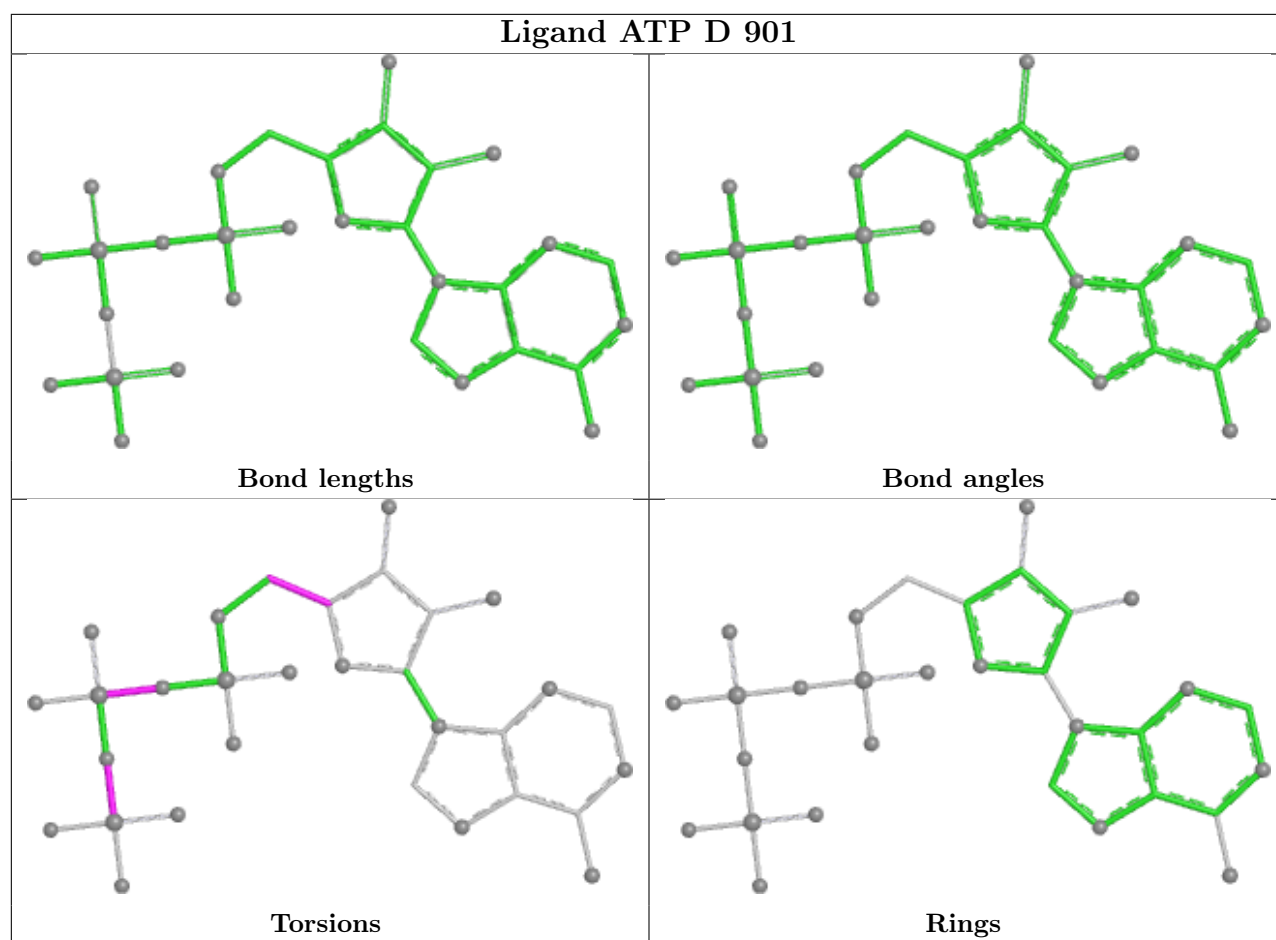












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

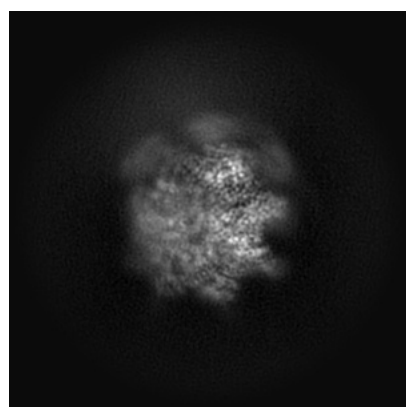
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73365. These allow visual inspection of the internal detail of the map and identification of artifacts.

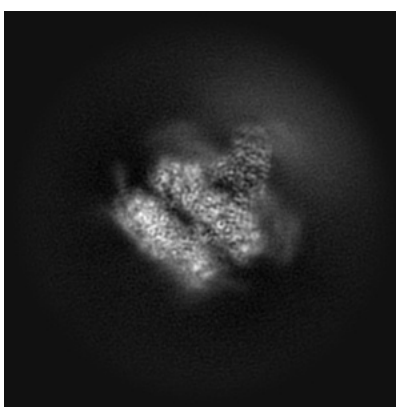
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

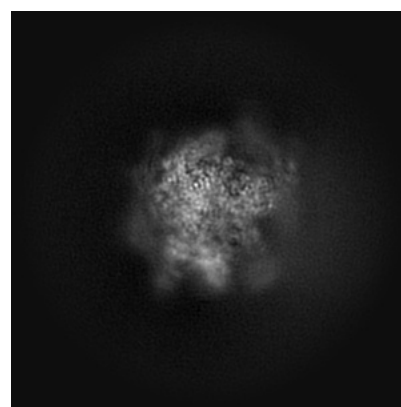
6.1.1 Primary map



X



Y

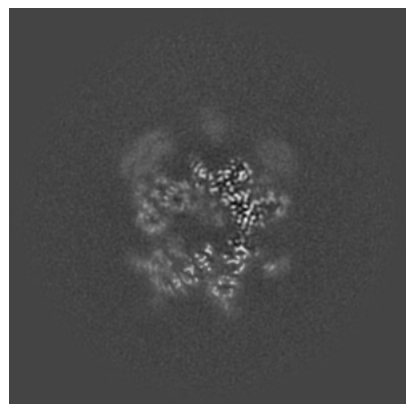


Z

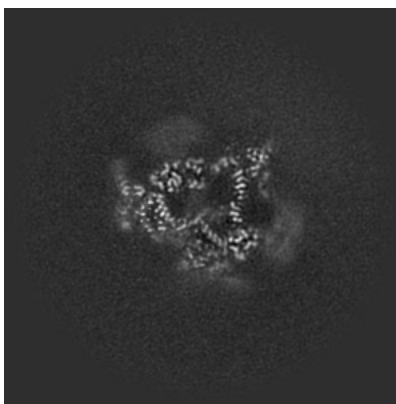
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

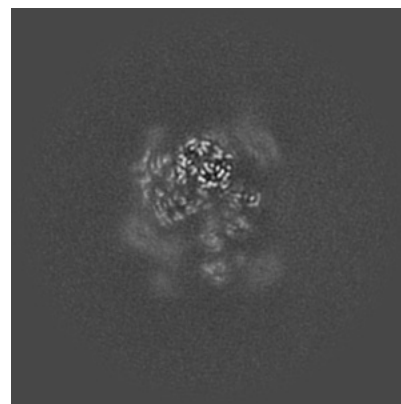
6.2.1 Primary map



X Index: 200



Y Index: 200

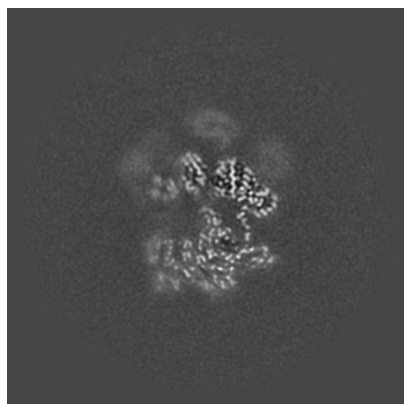


Z Index: 200

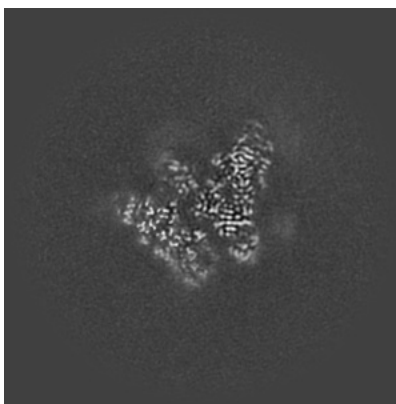
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

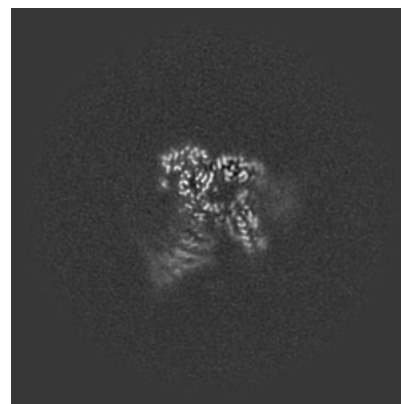
6.3.1 Primary map



X Index: 184



Y Index: 225

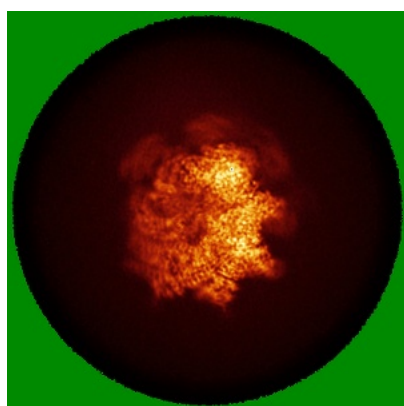


Z Index: 159

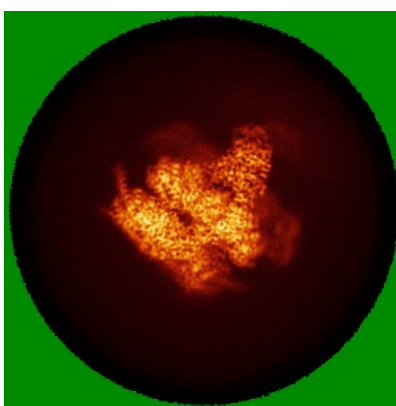
The images above show the largest variance slices of the map in three orthogonal directions.

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

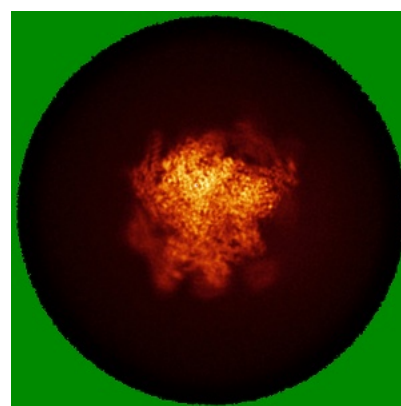
6.4.1 Primary map



X



Y

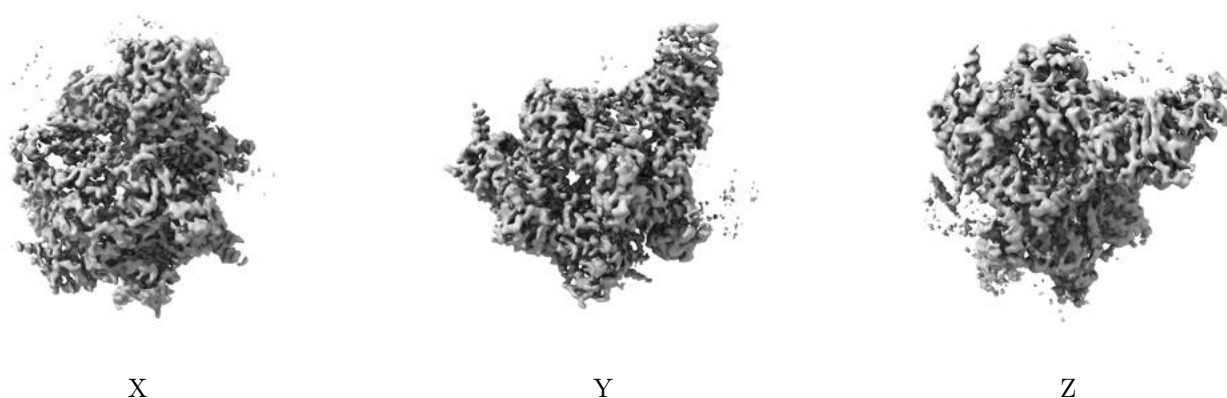


Z

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

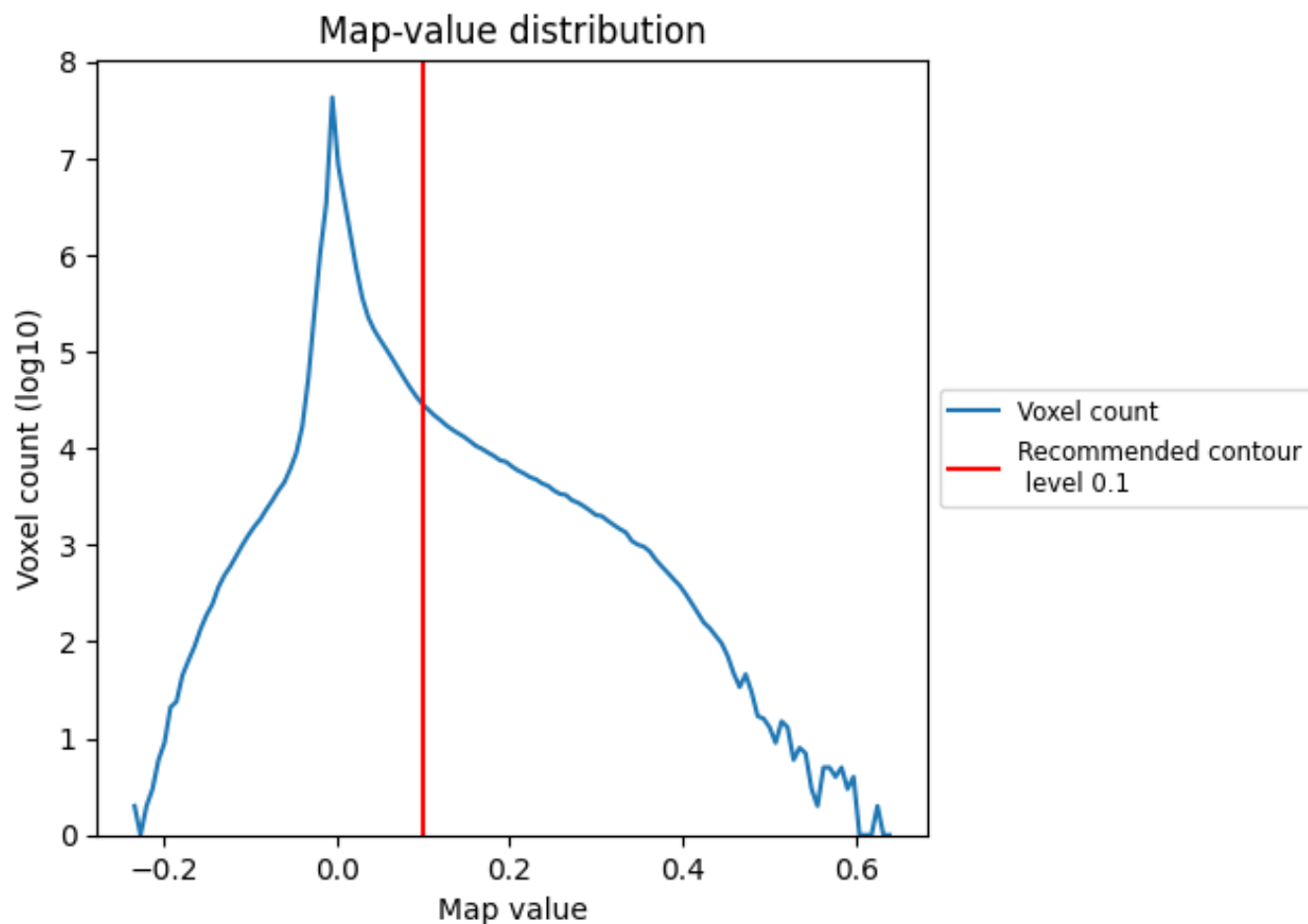
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

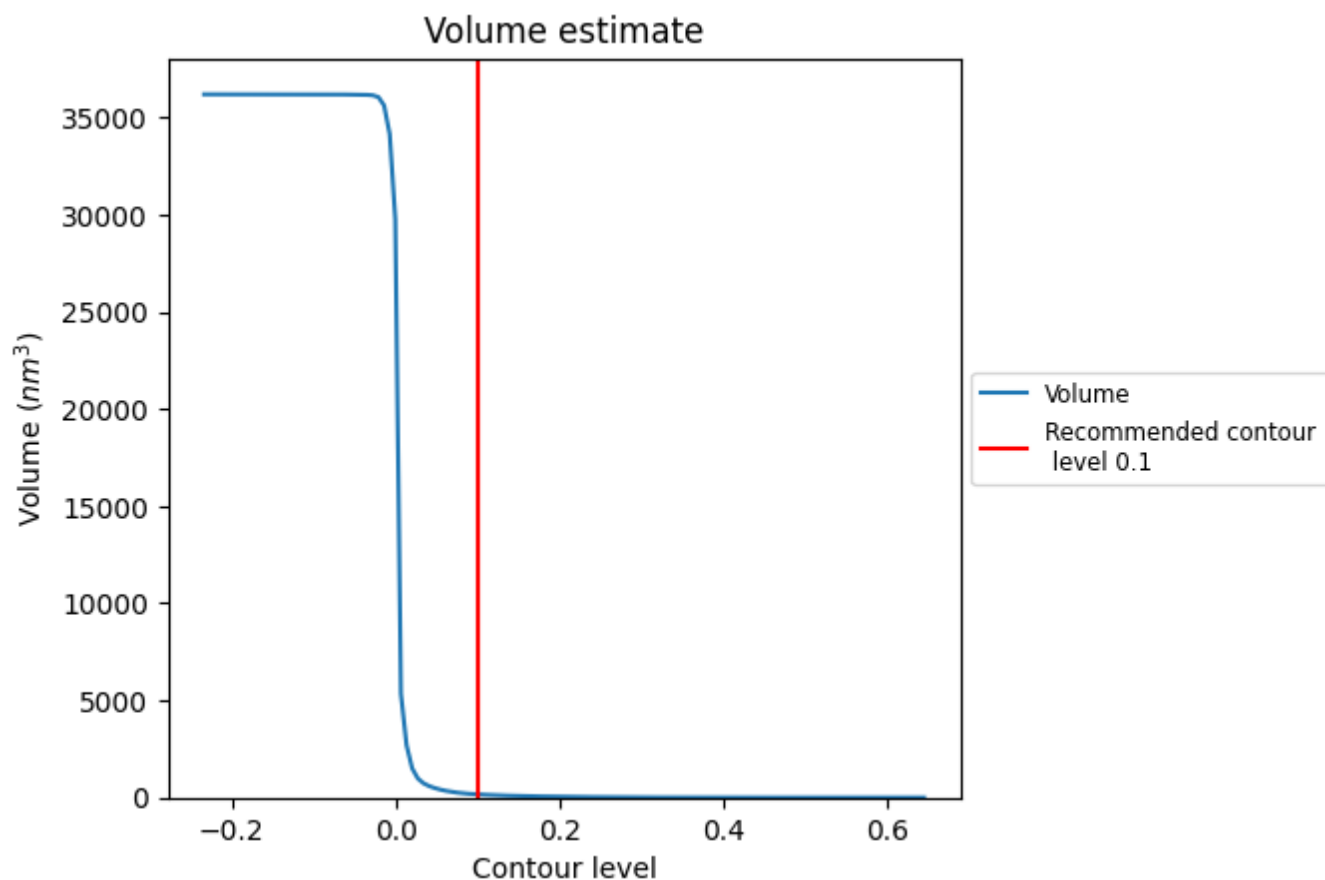
This section contains the results of statistical analysis of the map.

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.

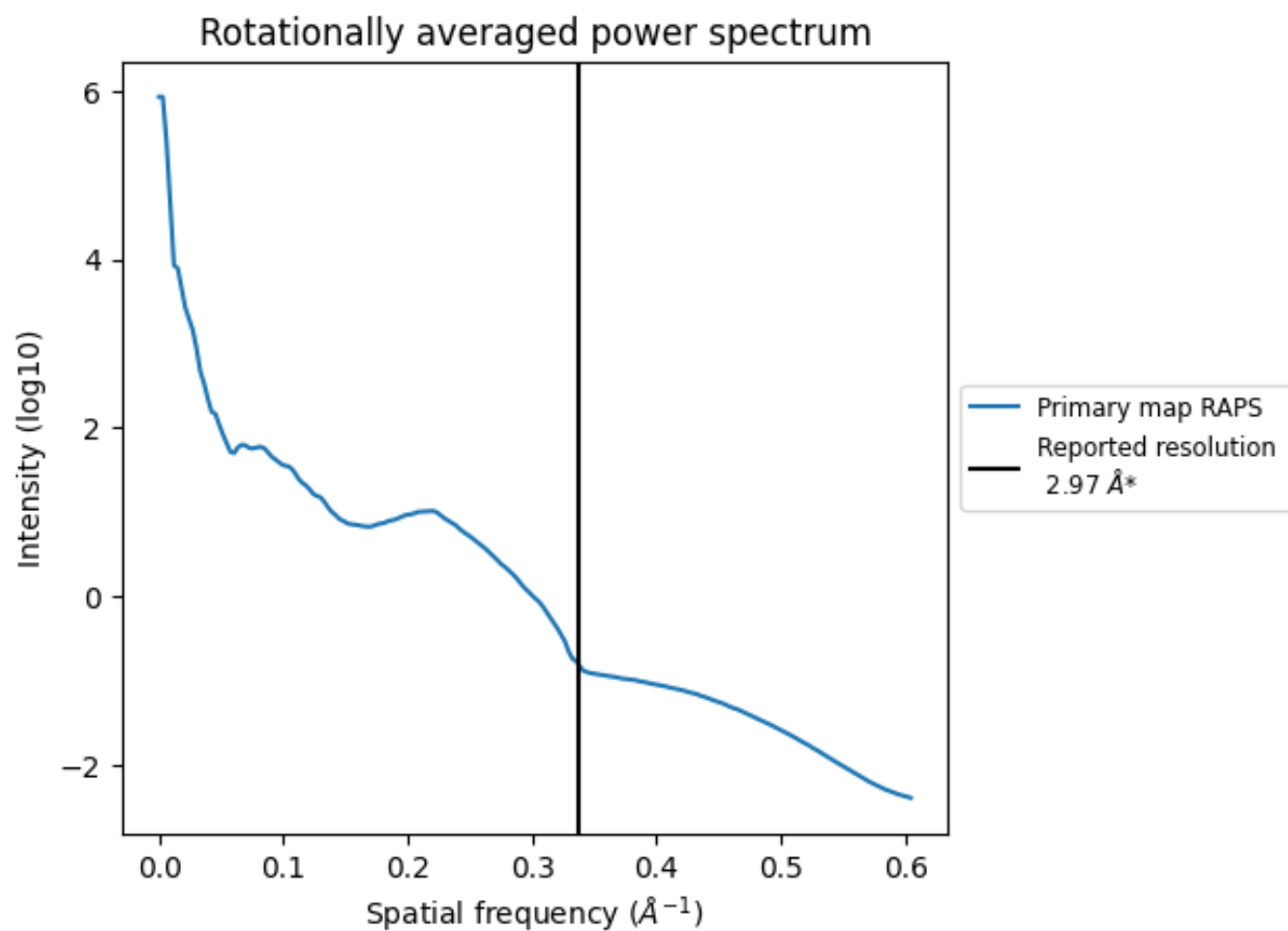
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 165 nm^3 ; this corresponds to an approximate mass of 149 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 0.337 Å⁻¹

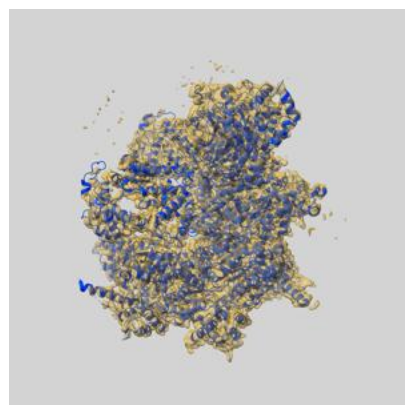
8 Fourier-Shell correlation

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

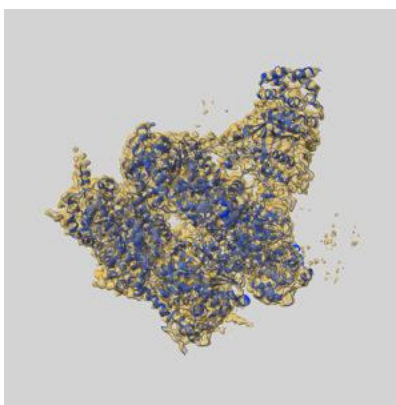
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73365 and PDB model 9YRC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

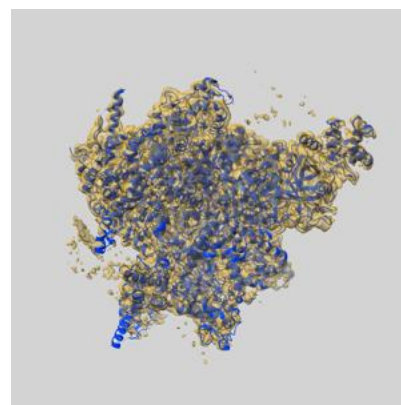
9.1 Map-model overlay [i](#)



X



Y



Z

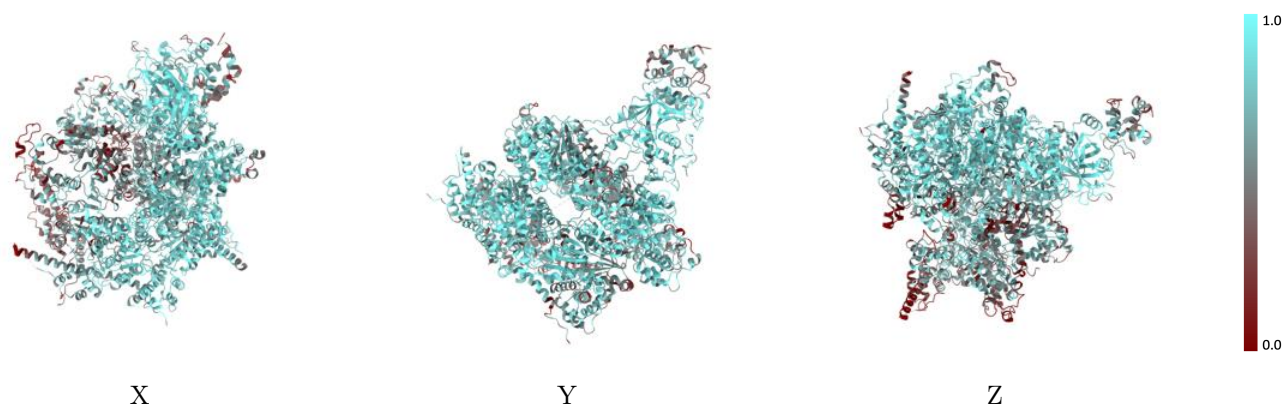
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



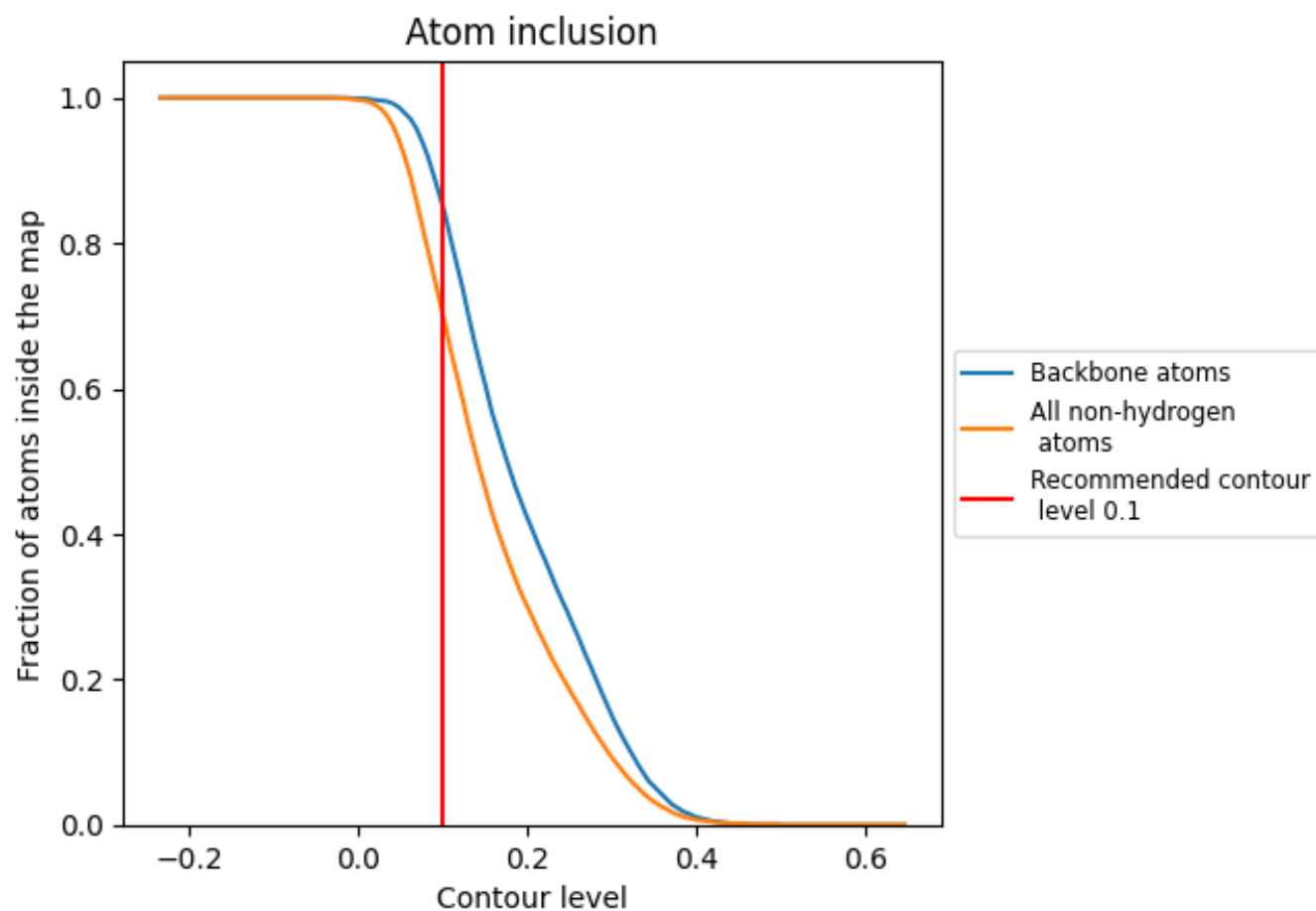
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 70% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7020	<div></div> 0.4390
A	<div></div> 0.6470	<div></div> 0.4230
B	<div></div> 0.8240	<div></div> 0.5110
C	<div></div> 0.8430	<div></div> 0.5130
D	<div></div> 0.7360	<div></div> 0.4460
E	<div></div> 0.4760	<div></div> 0.2850
F	<div></div> 0.5360	<div></div> 0.3300
G	<div></div> 0.7660	<div></div> 0.5090
H	<div></div> 0.7900	<div></div> 0.4980
I	<div></div> 0.7150	<div></div> 0.5040

1.0

0.0

<0.0