



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 04:43 AM UTC

PDB ID : 3J8A / pdb_00003j8a
EMDB ID : EMD-6124
Title : Structure of the F-actin-tropomyosin complex
Authors : von der Ecken, J.; Mueller, M.; Lehman, W.; Manstein, J.M.; Penczek, A.P.;
Raunser, S.
Deposited on : 2014-10-08
Resolution : 3.70 Å(reported)
Based on initial model : 4A7N

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:

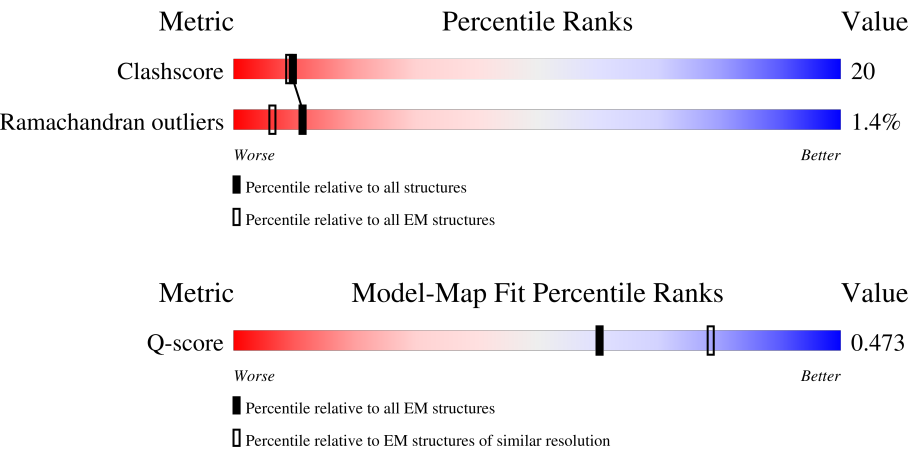
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	F	135	40% 99% .
1	G	135	33% 99% .
2	A	375	6% 57% 39% ..
2	B	375	7% 55% 41% ..
2	C	375	8% 54% 42% ..

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Mol	Chain	Length	Quality of chain
2	D	375	9% 56% 40% ..
2	E	375	5% 54% 42% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15800 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 tropomyosin alpha-1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	F	135	Total	C	N	O	0	0
			675	405	135	135		
1	G	135	Total	C	N	O	0	0
			675	405	135	135		

- Molecule 2 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
2	B	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
2	C	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
2	D	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		
2	E	367	Total	C	N	O	S	0	0
			2862	1813	481	548	20		

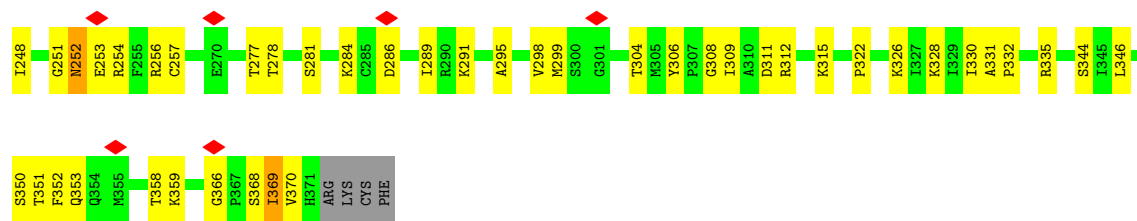
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	

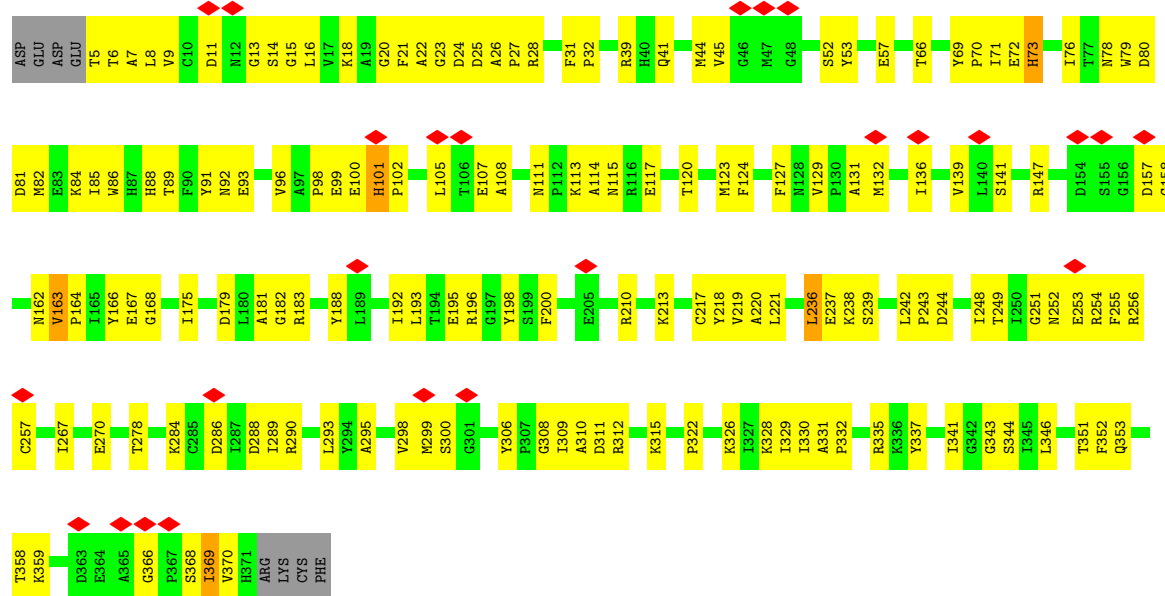
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



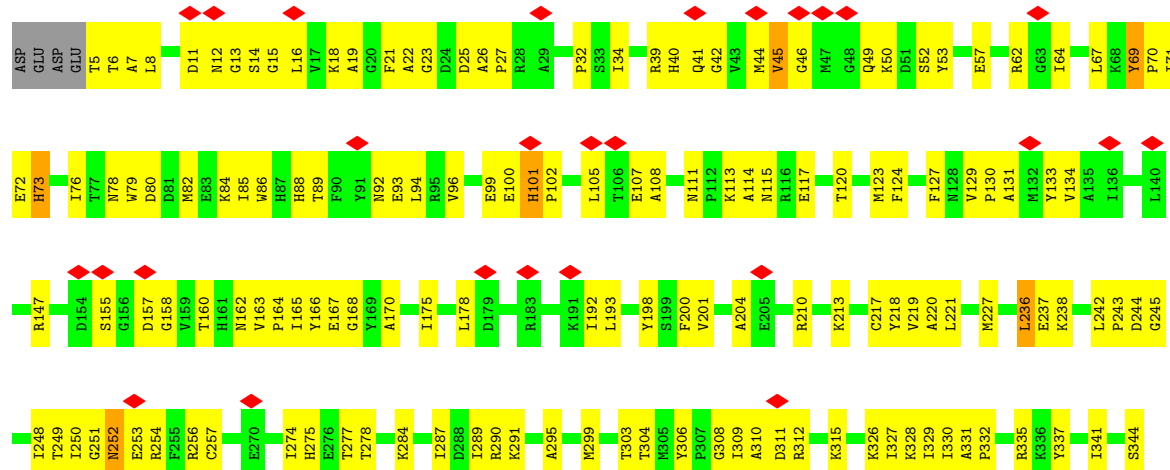
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0

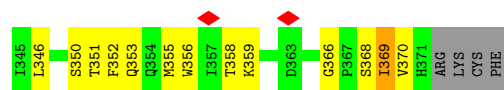


• Molecule 2: Actin, alpha skeletal muscle

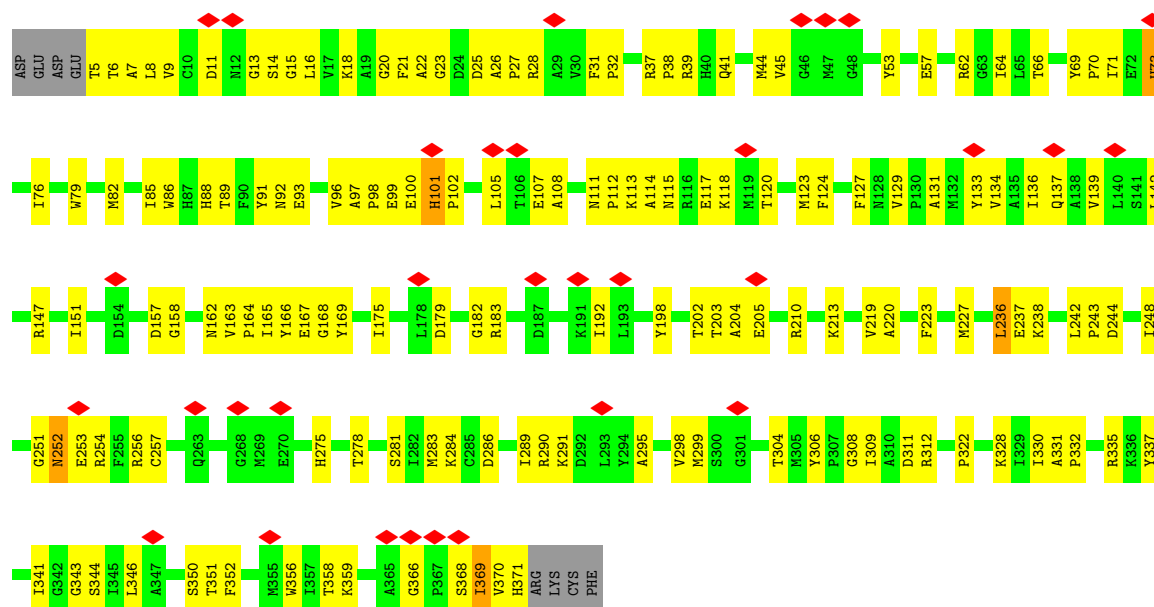


• Molecule 2: Actin, alpha skeletal muscle

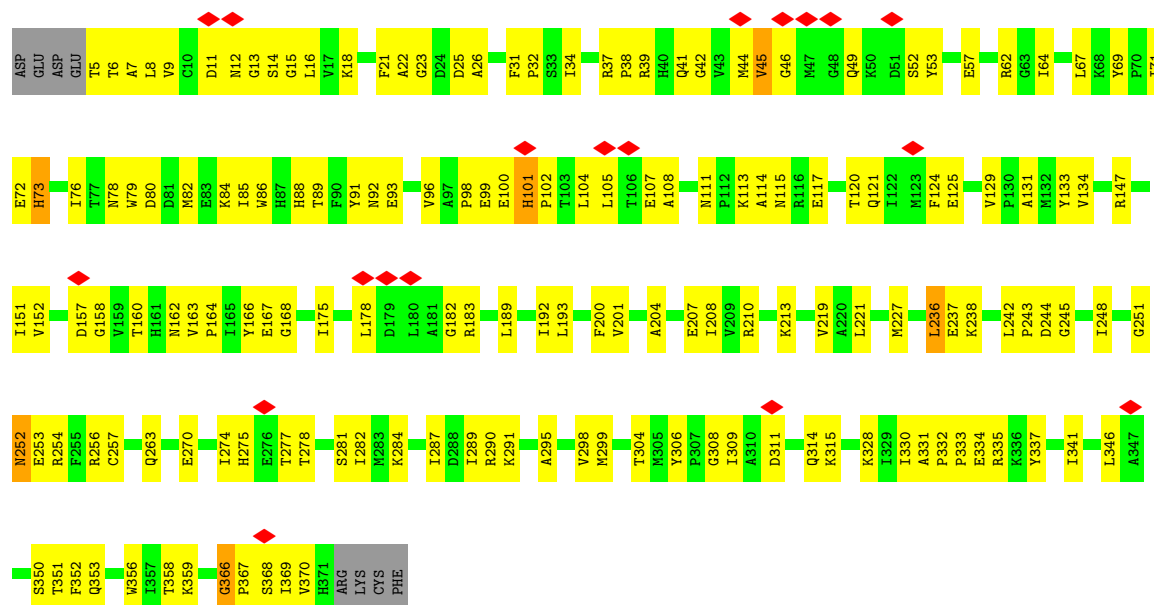




• Molecule 2: Actin, alpha skeletal muscle



• Molecule 2: Actin, alpha skeletal muscle



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=166.4°, rise=27.5 Å, axial sym=C1	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	14.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	16.164	Depositor
Minimum map value	-8.480	Depositor
Average map value	0.038	Depositor
Map value standard deviation	1.493	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	115.36, 103.04, 203.84	wwPDB
Map dimensions	103, 92, 182	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	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, HIC, MG

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	$\# Z > 5$
2	A	0.36	0/2911	0.91	7/3945 (0.2%)
2	B	0.35	0/2911	0.89	7/3945 (0.2%)
2	C	0.36	0/2911	0.91	10/3945 (0.3%)
2	D	0.36	0/2911	0.90	7/3945 (0.2%)
2	E	0.35	0/2911	0.92	8/3945 (0.2%)
All	All	0.35	0/14555	0.91	39/19725 (0.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	263	GLN	CA-C-N	-7.88	109.99	119.84
2	E	263	GLN	C-N-CA	-7.88	109.99	119.84
2	E	201	VAL	N-CA-C	7.54	118.31	110.62
2	A	236	LEU	N-CA-C	-7.41	104.27	112.72
2	C	201	VAL	N-CA-C	7.23	117.99	110.62
2	D	236	LEU	N-CA-C	-7.04	104.70	112.72
2	E	236	LEU	N-CA-C	-6.77	105.00	112.72
2	D	311	ASP	N-CA-C	-6.71	105.09	113.28
2	B	236	LEU	N-CA-C	-6.47	105.35	112.72
2	D	366	GLY	CA-C-N	6.11	126.55	119.47
2	D	366	GLY	C-N-CA	6.11	126.55	119.47
2	C	236	LEU	N-CA-C	-6.03	105.85	112.72
2	E	366	GLY	CA-C-N	5.96	127.30	119.84
2	E	366	GLY	C-N-CA	5.96	127.30	119.84
2	E	101	HIS	CA-C-N	5.92	126.82	120.13
2	E	101	HIS	C-N-CA	5.92	126.82	120.13
2	A	311	ASP	N-CA-C	-5.87	106.12	113.28
2	B	163	VAL	N-CA-C	5.81	114.36	107.73
2	C	311	ASP	N-CA-C	-5.73	106.28	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	HIS	CA-C-N	5.70	126.57	120.13
2	A	101	HIS	C-N-CA	5.70	126.57	120.13
2	B	101	HIS	CA-C-N	5.69	126.56	120.13
2	B	101	HIS	C-N-CA	5.69	126.56	120.13
2	C	69	TYR	CA-C-N	5.57	125.19	119.56
2	C	69	TYR	C-N-CA	5.57	125.19	119.56
2	C	101	HIS	CA-C-N	5.51	126.35	120.13
2	C	101	HIS	C-N-CA	5.51	126.35	120.13
2	D	64	ILE	N-CA-C	-5.46	107.16	112.29
2	B	311	ASP	N-CA-C	-5.38	106.72	113.28
2	C	327	ILE	N-CA-C	5.38	114.54	106.42
2	B	366	GLY	CA-C-N	5.37	126.55	119.84
2	B	366	GLY	C-N-CA	5.37	126.55	119.84
2	D	101	HIS	CA-C-N	5.28	126.10	120.13
2	D	101	HIS	C-N-CA	5.28	126.10	120.13
2	A	366	GLY	CA-C-N	5.27	126.43	119.84
2	A	366	GLY	C-N-CA	5.27	126.43	119.84
2	A	201	VAL	N-CA-C	5.22	115.95	110.62
2	C	366	GLY	CA-C-N	5.17	126.30	119.84
2	C	366	GLY	C-N-CA	5.17	126.30	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	675	0	137	1	0
1	G	675	0	137	1	0
2	A	2862	0	2832	127	0
2	B	2862	0	2832	127	0
2	C	2862	0	2832	124	0
2	D	2862	0	2832	121	0
2	E	2862	0	2832	122	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	2	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
All	All	15800	0	14494	597	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 20.

All (597) 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)
2:B:102:PRO:HB3	2:B:131:ALA:HB3	1.57	0.87
2:A:114:ALA:HB1	2:A:117:GLU:HB2	1.55	0.86
2:E:114:ALA:HB1	2:E:117:GLU:HB2	1.56	0.85
2:B:124:PHE:HE1	2:B:359:LYS:HG3	1.41	0.84
2:E:102:PRO:HB3	2:E:131:ALA:HB3	1.59	0.84
2:D:102:PRO:HB3	2:D:131:ALA:HB3	1.58	0.84
2:A:102:PRO:HB3	2:A:131:ALA:HB3	1.61	0.81
2:B:219:VAL:HB	2:B:308:GLY:HA3	1.60	0.81
2:A:286:ASP:OD2	2:C:39:ARG:NH2	2.15	0.80
2:D:114:ALA:HB1	2:D:117:GLU:HB2	1.63	0.79
2:B:147:ARG:HH22	2:B:330:ILE:HG21	1.48	0.79
2:B:52:SER:OG	2:B:84:LYS:NZ	2.15	0.78
2:A:242:LEU:HG	2:A:243:PRO:HD2	1.66	0.78
2:C:102:PRO:HB3	2:C:131:ALA:HB3	1.66	0.78
2:D:286:ASP:OD2	2:E:39:ARG:NH2	2.17	0.77
2:B:162:ASN:HD21	2:B:278:THR:HA	1.50	0.76
2:C:114:ALA:HB1	2:C:117:GLU:HB2	1.67	0.76
2:E:219:VAL:HB	2:E:308:GLY:HA3	1.68	0.76
2:C:219:VAL:HB	2:C:308:GLY:HA3	1.68	0.75
2:D:219:VAL:HB	2:D:308:GLY:HA3	1.67	0.75
2:E:192:ILE:HD12	2:E:253:GLU:HB2	1.69	0.74
2:E:242:LEU:HG	2:E:243:PRO:HD2	1.69	0.74
2:C:192:ILE:HD12	2:C:253:GLU:HB2	1.69	0.74
2:C:332:PRO:O	2:C:335:ARG:NH1	2.21	0.73
2:B:114:ALA:HB1	2:B:117:GLU:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:124:PHE:HE1	2:E:359:LYS:HG3	1.53	0.73
2:A:219:VAL:HB	2:A:308:GLY:HA3	1.71	0.72
2:B:242:LEU:HG	2:B:243:PRO:HD2	1.71	0.72
2:B:123:MET:HG3	2:B:127:PHE:HD2	1.53	0.72
2:E:332:PRO:O	2:E:335:ARG:NH1	2.23	0.72
2:D:253:GLU:HA	2:D:256:ARG:HB3	1.71	0.71
2:A:96:VAL:HG21	2:A:101:HIS:HE1	1.55	0.71
2:C:147:ARG:HH12	2:C:330:ILE:HB	1.56	0.71
2:A:39:ARG:NH2	2:B:286:ASP:OD2	2.23	0.71
2:A:245:GLY:HA3	2:B:322:PRO:HB2	1.72	0.71
2:A:53:TYR:HB3	2:A:57:GLU:HG3	1.71	0.71
2:B:299:MET:HE1	2:B:309:ILE:HD13	1.72	0.71
2:B:332:PRO:O	2:B:335:ARG:NH1	2.23	0.71
2:C:242:LEU:HG	2:C:243:PRO:HD2	1.73	0.71
2:A:62:ARG:HB3	2:A:204:ALA:HB1	1.73	0.70
2:A:332:PRO:O	2:A:335:ARG:NH1	2.24	0.70
2:A:192:ILE:HD12	2:A:253:GLU:HB2	1.74	0.70
2:D:332:PRO:O	2:D:335:ARG:NH1	2.25	0.70
2:C:6:THR:O	2:C:101:HIS:HB3	1.92	0.70
2:E:52:SER:OG	2:E:84:LYS:NZ	2.22	0.69
2:D:192:ILE:HD12	2:D:253:GLU:HB2	1.73	0.69
2:A:193:LEU:HD23	2:A:200:PHE:HE2	1.56	0.69
2:D:242:LEU:HG	2:D:243:PRO:HD2	1.75	0.69
2:D:322:PRO:HB2	2:E:245:GLY:HA3	1.74	0.69
2:E:147:ARG:HH12	2:E:330:ILE:HB	1.57	0.69
2:E:193:LEU:HD23	2:E:200:PHE:HE2	1.58	0.68
2:B:100:GLU:HB3	2:B:101:HIS:ND1	2.09	0.67
2:C:52:SER:OG	2:C:84:LYS:NZ	2.25	0.67
2:C:105:LEU:HB2	2:C:134:VAL:HG22	1.76	0.67
2:A:322:PRO:HB2	2:C:245:GLY:HA3	1.76	0.67
2:B:295:ALA:HA	2:B:328:LYS:H	1.60	0.67
2:A:147:ARG:HH22	2:A:330:ILE:HG21	1.60	0.67
2:B:270:GLU:OE2	2:D:203:THR:N	2.26	0.66
2:D:304:THR:O	2:D:335:ARG:NH2	2.25	0.66
2:B:5:THR:N	2:B:100:GLU:OE2	2.28	0.66
2:E:105:LEU:HB2	2:E:134:VAL:HG22	1.77	0.66
2:A:147:ARG:HH12	2:A:330:ILE:HB	1.60	0.66
2:B:147:ARG:HH12	2:B:330:ILE:HB	1.61	0.66
2:A:192:ILE:HD11	2:A:257:CYS:HB2	1.78	0.66
2:E:96:VAL:HG21	2:E:101:HIS:HE1	1.59	0.66
2:A:105:LEU:HB2	2:A:134:VAL:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:GLU:HB3	2:D:101:HIS:ND1	2.12	0.65
2:A:16:LEU:H	2:A:32:PRO:HA	1.62	0.65
2:D:73:HIC:HD2	2:D:179:ASP:OD1	1.96	0.65
2:A:21:PHE:O	2:A:23:GLY:N	2.30	0.65
2:B:96:VAL:HG21	2:B:101:HIS:HE1	1.60	0.65
2:A:227:MET:HE1	2:A:252:ASN:HD21	1.61	0.65
2:B:120:THR:O	2:B:124:PHE:HB2	1.97	0.64
2:B:295:ALA:HA	2:B:328:LYS:N	2.12	0.64
2:E:53:TYR:HB3	2:E:57:GLU:HG3	1.80	0.64
2:E:111:ASN:ND2	2:E:115:ASN:OD1	2.31	0.64
2:B:11:ASP:OD1	2:B:18:LYS:HB2	1.98	0.64
2:E:79:TRP:HA	2:E:82:MET:HB3	1.80	0.64
2:D:16:LEU:H	2:D:32:PRO:HA	1.63	0.64
2:B:253:GLU:HA	2:B:256:ARG:HB3	1.80	0.64
2:C:147:ARG:HH22	2:C:330:ILE:HG21	1.63	0.64
2:C:5:THR:N	2:C:100:GLU:OE2	2.31	0.63
2:C:253:GLU:HA	2:C:256:ARG:HB3	1.80	0.63
2:D:120:THR:O	2:D:124:PHE:HB2	1.98	0.63
2:A:64:ILE:HD12	2:B:166:TYR:HB3	1.81	0.63
2:E:16:LEU:H	2:E:32:PRO:HA	1.63	0.63
2:A:242:LEU:HD13	2:A:248:ILE:HD12	1.80	0.63
2:C:250:ILE:HD12	2:C:254:ARG:HB2	1.80	0.63
2:C:113:LYS:HA	2:C:115:ASN:H	1.63	0.63
2:E:72:GLU:HG2	2:E:73:HIC:HD2	1.80	0.63
2:C:120:THR:O	2:C:124:PHE:HB2	1.99	0.63
2:D:76:ILE:HD11	2:D:79:TRP:CD2	2.34	0.63
2:E:162:ASN:ND2	2:E:278:THR:HA	2.14	0.63
2:A:253:GLU:HA	2:A:256:ARG:HB3	1.81	0.63
2:C:12:ASN:HD21	2:C:82:MET:HE1	1.63	0.63
2:E:124:PHE:CE1	2:E:359:LYS:HG3	2.34	0.62
2:E:162:ASN:HD21	2:E:278:THR:HA	1.63	0.62
2:C:11:ASP:OD1	2:C:18:LYS:HB2	1.99	0.62
2:E:100:GLU:HB3	2:E:101:HIS:ND1	2.14	0.62
2:E:147:ARG:HH22	2:E:330:ILE:HG21	1.63	0.62
2:B:16:LEU:H	2:B:32:PRO:HA	1.65	0.62
2:A:11:ASP:OD1	2:A:18:LYS:HB2	1.99	0.62
2:D:21:PHE:O	2:D:23:GLY:N	2.33	0.62
2:A:12:ASN:HD21	2:A:82:MET:HE1	1.63	0.62
2:D:96:VAL:HG21	2:D:101:HIS:HE1	1.65	0.62
2:E:5:THR:N	2:E:100:GLU:OE2	2.32	0.62
2:E:251:GLY:O	2:E:253:GLU:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:79:TRP:HA	2:A:82:MET:HB3	1.82	0.61
2:C:41:GLN:N	2:C:41:GLN:OE1	2.31	0.61
2:D:5:THR:N	2:D:100:GLU:OE2	2.33	0.61
2:A:5:THR:N	2:A:100:GLU:OE2	2.33	0.61
2:C:53:TYR:HB3	2:C:57:GLU:HG3	1.81	0.61
2:E:41:GLN:OE1	2:E:41:GLN:N	2.32	0.61
2:A:299:MET:HE1	2:A:309:ILE:HD13	1.80	0.61
2:A:166:TYR:HB3	2:C:64:ILE:HD12	1.81	0.60
2:B:192:ILE:HD12	2:B:253:GLU:HB2	1.83	0.60
2:D:18:LYS:HB3	2:D:27:PRO:HG3	1.83	0.60
2:E:178:LEU:HD11	2:E:277:THR:HG21	1.82	0.60
2:B:123:MET:HE3	2:B:132:MET:HE1	1.83	0.60
2:B:237:GLU:HB2	2:B:251:GLY:HA3	1.84	0.60
2:B:89:THR:HA	2:B:93:GLU:CD	2.27	0.60
2:E:11:ASP:OD1	2:E:18:LYS:HB2	2.01	0.60
2:C:16:LEU:H	2:C:32:PRO:HA	1.66	0.60
2:A:41:GLN:OE1	2:A:41:GLN:N	2.32	0.59
2:D:358:THR:OG1	2:D:359:LYS:N	2.28	0.59
2:C:251:GLY:O	2:C:253:GLU:N	2.36	0.59
2:C:89:THR:HA	2:C:93:GLU:CD	2.27	0.59
2:E:89:THR:HA	2:E:93:GLU:CD	2.28	0.59
2:A:100:GLU:HB3	2:A:101:HIS:ND1	2.18	0.59
2:A:251:GLY:O	2:A:253:GLU:N	2.35	0.59
2:E:21:PHE:O	2:E:23:GLY:N	2.35	0.59
2:E:221:LEU:O	2:E:315:LYS:NZ	2.22	0.59
2:C:193:LEU:HD23	2:C:200:PHE:HE2	1.68	0.59
2:D:11:ASP:OD1	2:D:18:LYS:HB2	2.02	0.59
2:E:287:ILE:HG13	2:E:290:ARG:HH22	1.66	0.59
2:B:162:ASN:ND2	2:B:278:THR:HA	2.16	0.58
2:D:163:VAL:HA	2:D:175:ILE:HG22	1.85	0.58
2:C:111:ASN:ND2	2:C:115:ASN:OD1	2.36	0.58
2:A:164:PRO:HD2	2:A:175:ILE:HG22	1.86	0.58
2:C:21:PHE:O	2:C:23:GLY:N	2.37	0.57
2:C:242:LEU:HD13	2:C:248:ILE:HD12	1.85	0.57
2:D:53:TYR:HB3	2:D:57:GLU:HG3	1.86	0.57
2:B:124:PHE:CE1	2:B:359:LYS:HG3	2.32	0.57
2:D:41:GLN:OE1	2:D:41:GLN:N	2.32	0.57
2:A:89:THR:HA	2:A:93:GLU:CD	2.29	0.57
2:C:7:ALA:HA	2:C:101:HIS:HB3	1.87	0.57
2:D:242:LEU:HD13	2:D:248:ILE:HD12	1.86	0.57
2:E:120:THR:O	2:E:124:PHE:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ARG:HB3	2:B:66:THR:HG23	1.87	0.57
2:B:131:ALA:HA	2:B:358:THR:HA	1.87	0.57
2:D:275:HIS:C	2:D:275:HIS:CD2	2.82	0.57
2:A:358:THR:OG1	2:A:359:LYS:N	2.37	0.57
2:C:275:HIS:C	2:C:275:HIS:CD2	2.83	0.57
2:E:295:ALA:HA	2:E:328:LYS:H	1.70	0.57
2:B:193:LEU:HD23	2:B:200:PHE:HE2	1.69	0.57
2:C:79:TRP:HA	2:C:82:MET:HB3	1.87	0.57
2:C:124:PHE:HE1	2:C:359:LYS:HG2	1.70	0.56
2:D:89:THR:HA	2:D:93:GLU:CD	2.30	0.56
2:E:295:ALA:HA	2:E:328:LYS:N	2.20	0.56
2:A:72:GLU:HG2	2:A:73:HIC:HD2	1.88	0.56
2:C:304:THR:O	2:C:335:ARG:NH2	2.35	0.56
2:C:72:GLU:HG2	2:C:73:HIC:HD2	1.87	0.56
2:C:287:ILE:HG13	2:C:290:ARG:HH22	1.71	0.56
2:D:82:MET:SD	2:D:86:TRP:NE1	2.78	0.56
2:A:169:TYR:HB2	2:C:64:ILE:HD11	1.87	0.56
2:B:123:MET:HG3	2:B:127:PHE:CD2	2.37	0.56
2:E:76:ILE:HD11	2:E:79:TRP:CD2	2.40	0.56
2:C:107:GLU:HG2	2:C:108:ALA:H	1.71	0.56
2:A:82:MET:SD	2:A:86:TRP:NE1	2.79	0.56
2:B:41:GLN:OE1	2:B:41:GLN:N	2.31	0.55
2:C:164:PRO:HD2	2:C:175:ILE:HG22	1.87	0.55
2:C:82:MET:SD	2:C:86:TRP:NE1	2.80	0.55
2:D:251:GLY:O	2:D:253:GLU:N	2.39	0.55
2:E:253:GLU:HA	2:E:256:ARG:HB3	1.87	0.55
2:B:163:VAL:HA	2:B:175:ILE:HG22	1.88	0.55
2:A:163:VAL:HA	2:A:175:ILE:HG22	1.88	0.55
2:B:196:ARG:NH2	2:B:251:GLY:H	2.04	0.55
2:A:210:ARG:O	2:A:213:LYS:HB3	2.07	0.55
2:E:52:SER:HG	2:E:84:LYS:HZ3	1.49	0.55
2:D:162:ASN:HD21	2:D:278:THR:HA	1.72	0.55
2:E:192:ILE:HD11	2:E:257:CYS:HB2	1.89	0.55
2:B:15:GLY:HA3	2:B:16:LEU:HB2	1.89	0.54
2:B:88:HIS:CD2	2:B:92:ASN:HD21	2.25	0.54
2:D:23:GLY:HA2	2:D:344:SER:HB3	1.88	0.54
2:D:295:ALA:HA	2:D:328:LYS:N	2.22	0.54
2:B:306:TYR:CE1	4:B:402:ADP:H2	2.26	0.54
2:A:295:ALA:HA	2:A:328:LYS:N	2.23	0.54
2:E:237:GLU:HB2	2:E:251:GLY:HA3	1.89	0.54
2:B:21:PHE:O	2:B:23:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:ALA:HA	2:D:328:LYS:H	1.73	0.54
2:B:111:ASN:ND2	2:B:115:ASN:OD1	2.41	0.54
2:E:210:ARG:O	2:E:213:LYS:HB3	2.07	0.54
2:C:358:THR:OG1	2:C:359:LYS:N	2.40	0.54
2:A:76:ILE:HD11	2:A:79:TRP:CD2	2.43	0.54
2:C:210:ARG:O	2:C:213:LYS:HB3	2.08	0.54
2:D:13:GLY:C	2:D:15:GLY:H	2.16	0.54
2:E:358:THR:OG1	2:E:359:LYS:N	2.40	0.54
2:A:88:HIS:CG	2:A:92:ASN:HD21	2.25	0.53
2:C:162:ASN:ND2	2:C:278:THR:HA	2.23	0.53
2:C:76:ILE:HD11	2:C:79:TRP:CD2	2.43	0.53
2:D:88:HIS:CD2	2:D:92:ASN:HD21	2.25	0.53
2:E:113:LYS:HA	2:E:115:ASN:H	1.73	0.53
2:D:113:LYS:HA	2:D:115:ASN:H	1.73	0.53
2:A:295:ALA:HB1	2:A:328:LYS:HG2	1.91	0.53
2:D:147:ARG:HH22	2:D:330:ILE:HG13	1.74	0.53
2:E:44:MET:HG3	2:E:44:MET:O	2.09	0.53
2:C:25:ASP:CG	2:C:26:ALA:H	2.16	0.53
2:C:71:ILE:HA	2:C:76:ILE:HA	1.90	0.53
2:D:25:ASP:CG	2:D:26:ALA:H	2.17	0.53
2:D:39:ARG:HB3	2:D:66:THR:HG23	1.90	0.53
2:A:295:ALA:HA	2:A:328:LYS:H	1.74	0.53
2:B:88:HIS:CG	2:B:92:ASN:HD21	2.25	0.53
2:C:100:GLU:HB3	2:C:101:HIS:ND1	2.23	0.53
2:A:306:TYR:CE1	4:A:402:ADP:H2	2.26	0.53
2:B:53:TYR:HB3	2:B:57:GLU:HG3	1.90	0.53
2:B:358:THR:OG1	2:B:359:LYS:N	2.40	0.53
2:E:368:SER:O	2:E:370:VAL:N	2.40	0.53
2:A:107:GLU:HG2	2:A:108:ALA:H	1.74	0.53
2:D:15:GLY:HA3	2:D:16:LEU:HB2	1.91	0.53
2:D:162:ASN:ND2	2:D:278:THR:HA	2.23	0.53
2:E:25:ASP:CG	2:E:26:ALA:H	2.17	0.53
2:E:163:VAL:HA	2:E:175:ILE:HG22	1.90	0.52
2:A:88:HIS:CD2	2:A:92:ASN:HD21	2.27	0.52
2:E:6:THR:O	2:E:101:HIS:HB3	2.09	0.52
2:B:52:SER:HG	2:B:84:LYS:HZ3	1.50	0.52
2:B:210:ARG:O	2:B:213:LYS:HB3	2.09	0.52
2:C:192:ILE:HD11	2:C:257:CYS:HB2	1.92	0.52
2:D:62:ARG:HB3	2:D:204:ALA:HB1	1.91	0.52
2:A:6:THR:O	2:A:101:HIS:HB3	2.09	0.52
2:B:25:ASP:CG	2:B:26:ALA:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ILE:HA	2:B:76:ILE:HA	1.91	0.52
2:B:13:GLY:C	2:B:15:GLY:H	2.18	0.52
2:D:88:HIS:CG	2:D:92:ASN:HD21	2.27	0.52
2:A:25:ASP:CG	2:A:26:ALA:H	2.18	0.52
2:D:299:MET:HE1	2:D:309:ILE:HD13	1.92	0.52
2:B:82:MET:SD	2:B:86:TRP:NE1	2.82	0.52
2:C:88:HIS:CD2	2:C:92:ASN:HD21	2.27	0.51
2:B:136:ILE:HD11	2:B:139:VAL:HG23	1.93	0.51
2:D:131:ALA:HA	2:D:358:THR:HA	1.92	0.51
2:E:227:MET:HE1	2:E:252:ASN:HD21	1.75	0.51
2:C:162:ASN:HD21	2:C:278:THR:HA	1.75	0.51
2:E:107:GLU:HG2	2:E:108:ALA:H	1.75	0.51
2:A:237:GLU:HB2	2:A:251:GLY:HA3	1.92	0.51
2:B:23:GLY:HA2	2:B:344:SER:HB3	1.93	0.51
2:C:352:PHE:HB2	2:C:355:MET:HE3	1.93	0.51
2:B:18:LYS:HB3	2:B:27:PRO:HG3	1.93	0.51
2:B:331:ALA:HB1	2:B:335:ARG:HD3	1.93	0.51
2:B:251:GLY:O	2:B:253:GLU:N	2.44	0.51
2:E:86:TRP:O	2:E:89:THR:OG1	2.23	0.51
2:E:178:LEU:HD12	2:E:274:ILE:HD13	1.93	0.51
2:E:62:ARG:HB3	2:E:204:ALA:HB1	1.93	0.50
2:A:13:GLY:C	2:A:15:GLY:H	2.20	0.50
2:A:157:ASP:HA	2:A:182:GLY:H	1.75	0.50
2:C:101:HIS:O	2:C:129:VAL:HG13	2.11	0.50
2:A:113:LYS:HA	2:A:115:ASN:H	1.76	0.50
2:B:6:THR:O	2:B:101:HIS:HB3	2.11	0.50
2:D:111:ASN:ND2	2:D:115:ASN:OD1	2.45	0.50
2:E:121:GLN:O	2:E:125:GLU:HG2	2.11	0.50
2:B:238:LYS:HE2	2:B:254:ARG:HH22	1.76	0.50
2:A:7:ALA:HA	2:A:101:HIS:CB	2.42	0.50
2:A:120:THR:O	2:A:124:PHE:HB2	2.11	0.50
2:B:289:ILE:HG23	2:B:293:LEU:HG	1.93	0.50
2:E:12:ASN:HD21	2:E:82:MET:HE1	1.76	0.50
2:C:221:LEU:HD11	2:C:315:LYS:HD3	1.93	0.50
2:D:164:PRO:HD2	2:D:175:ILE:HG22	1.92	0.50
2:D:166:TYR:CE2	2:D:289:ILE:HD11	2.46	0.50
2:D:346:LEU:HG	2:D:352:PHE:CZ	2.46	0.50
2:A:14:SER:HB2	2:A:157:ASP:O	2.12	0.50
2:B:157:ASP:OD1	2:B:183:ARG:HG3	2.12	0.50
2:D:14:SER:HB2	2:D:157:ASP:O	2.12	0.50
2:D:123:MET:HG3	2:D:127:PHE:HD2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:GLU:HG2	2:D:108:ALA:H	1.76	0.49
2:A:15:GLY:HA3	2:A:16:LEU:HB2	1.94	0.49
2:B:105:LEU:HD11	2:B:123:MET:HE1	1.93	0.49
2:E:162:ASN:ND2	2:E:281:SER:OG	2.46	0.49
2:E:337:TYR:O	2:E:341:ILE:HG13	2.11	0.49
2:C:227:MET:HE1	2:C:252:ASN:HD21	1.77	0.49
2:D:166:TYR:HB3	2:E:64:ILE:HD12	1.94	0.49
2:A:8:LEU:HB3	2:A:101:HIS:NE2	2.27	0.49
2:C:96:VAL:HG21	2:C:101:HIS:HE1	1.77	0.49
2:A:101:HIS:O	2:A:129:VAL:HG13	2.11	0.49
2:B:7:ALA:HA	2:B:101:HIS:CB	2.42	0.49
2:D:105:LEU:HB2	2:D:134:VAL:HG22	1.93	0.49
2:E:7:ALA:HA	2:E:101:HIS:CB	2.42	0.49
2:B:120:THR:HG23	2:B:132:MET:HE3	1.94	0.49
2:D:162:ASN:ND2	2:D:281:SER:OG	2.46	0.49
2:A:169:TYR:HA	2:C:42:GLY:HA2	1.94	0.49
2:D:306:TYR:CE1	4:D:402:ADP:H2	2.31	0.49
2:E:14:SER:HB2	2:E:157:ASP:O	2.12	0.49
2:C:346:LEU:HG	2:C:352:PHE:CZ	2.48	0.49
2:D:101:HIS:O	2:D:129:VAL:HG13	2.12	0.49
2:D:210:ARG:O	2:D:213:LYS:HB3	2.13	0.49
2:A:78:ASN:ND2	2:A:80:ASP:HB3	2.28	0.49
2:B:72:GLU:HG2	2:B:73:HIC:HD2	1.95	0.49
2:C:299:MET:HE1	2:C:309:ILE:HD13	1.94	0.49
2:B:76:ILE:HD11	2:B:79:TRP:CD2	2.48	0.48
2:C:23:GLY:HA2	2:C:344:SER:HB3	1.95	0.48
2:C:220:ALA:O	2:C:312:ARG:HD3	2.13	0.48
2:E:88:HIS:CD2	2:E:92:ASN:HD21	2.31	0.48
2:E:8:LEU:HB3	2:E:101:HIS:NE2	2.28	0.48
2:A:221:LEU:O	2:A:315:LYS:NZ	2.28	0.48
2:B:79:TRP:HA	2:B:82:MET:HB3	1.96	0.48
2:C:15:GLY:HA3	2:C:16:LEU:HB2	1.94	0.48
2:C:88:HIS:CG	2:C:92:ASN:HD21	2.32	0.48
2:D:198:TYR:CZ	2:D:248:ILE:HG23	2.48	0.48
2:E:15:GLY:HA3	2:E:16:LEU:HB2	1.93	0.48
2:E:69:TYR:OH	2:E:207:GLU:OE2	2.30	0.48
2:E:82:MET:SD	2:E:86:TRP:NE1	2.86	0.48
2:A:162:ASN:ND2	2:A:278:THR:HA	2.29	0.48
2:B:164:PRO:HD2	2:B:175:ILE:HG22	1.95	0.48
2:C:7:ALA:HA	2:C:101:HIS:CB	2.44	0.48
2:E:157:ASP:HA	2:E:158:GLY:HA2	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:PRO:HD2	2:E:175:ILE:HG22	1.95	0.48
2:D:7:ALA:HA	2:D:101:HIS:CB	2.43	0.48
2:A:123:MET:HG3	2:A:127:PHE:HD2	1.79	0.48
2:B:91:TYR:HE1	2:B:98:PRO:HG3	1.78	0.48
2:B:368:SER:C	2:B:370:VAL:H	2.21	0.48
2:D:332:PRO:O	2:D:335:ARG:HG3	2.14	0.48
2:B:14:SER:HB2	2:B:157:ASP:O	2.13	0.48
2:E:13:GLY:C	2:E:15:GLY:H	2.21	0.48
2:B:31:PHE:HB2	2:B:32:PRO:HD2	1.95	0.48
2:C:18:LYS:HB3	2:C:27:PRO:HG3	1.96	0.47
2:C:123:MET:HG3	2:C:127:PHE:HD2	1.78	0.47
2:D:85:ILE:O	2:D:89:THR:HG23	2.14	0.47
2:E:91:TYR:HE1	2:E:98:PRO:HG3	1.78	0.47
2:C:310:ALA:HB1	2:C:329:ILE:HD13	1.96	0.47
2:A:86:TRP:O	2:A:89:THR:OG1	2.25	0.47
2:D:169:TYR:OH	2:E:49:GLN:HB3	2.15	0.47
2:D:237:GLU:HB2	2:D:251:GLY:HA3	1.96	0.47
2:A:178:LEU:HD11	2:A:277:THR:HG21	1.96	0.47
2:A:195:GLU:HA	2:D:112:PRO:HA	1.96	0.47
2:C:238:LYS:HE2	2:C:254:ARG:HH22	1.79	0.47
2:D:169:TYR:HB2	2:E:64:ILE:HD11	1.96	0.47
2:B:157:ASP:HA	2:B:158:GLY:HA2	1.55	0.47
2:D:157:ASP:OD1	2:D:183:ARG:HG3	2.15	0.47
2:D:169:TYR:HA	2:E:42:GLY:HA2	1.97	0.47
2:D:192:ILE:HD11	2:D:257:CYS:HB2	1.96	0.47
2:E:88:HIS:CG	2:E:92:ASN:HD21	2.33	0.47
2:A:220:ALA:O	2:A:312:ARG:HD3	2.14	0.47
2:A:368:SER:O	2:A:370:VAL:N	2.48	0.47
2:B:337:TYR:O	2:B:341:ILE:HG13	2.15	0.47
2:C:19:ALA:HB1	2:C:94:LEU:HD11	1.97	0.47
2:E:101:HIS:O	2:E:129:VAL:HG13	2.15	0.47
2:A:107:GLU:O	2:A:137:GLN:HB2	2.14	0.47
2:B:167:GLU:HA	2:B:168:GLY:HA2	1.56	0.47
2:B:220:ALA:O	2:B:312:ARG:HD3	2.14	0.47
2:C:287:ILE:HG13	2:C:290:ARG:NH2	2.30	0.47
2:D:79:TRP:CZ2	2:D:118:LYS:HB2	2.49	0.47
2:B:7:ALA:HA	2:B:101:HIS:HB3	1.97	0.47
2:C:13:GLY:C	2:C:15:GLY:H	2.23	0.47
2:C:163:VAL:HA	2:C:175:ILE:HG22	1.98	0.47
2:D:299:MET:HB3	2:D:304:THR:HG21	1.96	0.47
2:B:346:LEU:HG	2:B:352:PHE:CZ	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:291:LYS:HD2	2:E:291:LYS:O	2.15	0.46
2:B:107:GLU:HG2	2:B:108:ALA:H	1.79	0.46
2:D:69:TYR:HA	2:D:70:PRO:HD3	1.79	0.46
2:E:34:ILE:HG21	2:E:67:LEU:HB3	1.97	0.46
2:A:131:ALA:HA	2:A:358:THR:HA	1.98	0.46
2:B:332:PRO:O	2:B:335:ARG:HG3	2.15	0.46
2:C:193:LEU:HD23	2:C:200:PHE:CE2	2.50	0.46
2:E:167:GLU:HA	2:E:168:GLY:HA2	1.57	0.46
2:C:251:GLY:O	2:C:253:GLU:HG2	2.15	0.46
2:A:162:ASN:HD21	2:A:278:THR:HA	1.79	0.46
2:C:133:TYR:HB2	2:C:356:TRP:CD1	2.51	0.46
2:D:167:GLU:HA	2:D:168:GLY:HA2	1.56	0.46
2:A:198:TYR:CZ	2:A:248:ILE:HG23	2.51	0.46
2:B:85:ILE:O	2:B:89:THR:HG23	2.16	0.46
2:C:124:PHE:CE1	2:C:359:LYS:HG2	2.50	0.46
2:C:284:LYS:HD2	2:C:284:LYS:HA	1.77	0.46
2:C:368:SER:C	2:C:370:VAL:H	2.23	0.46
2:D:91:TYR:HE1	2:D:98:PRO:HG3	1.80	0.46
2:B:310:ALA:HB1	2:B:329:ILE:HG21	1.98	0.46
2:C:101:HIS:O	2:C:130:PRO:HD2	2.16	0.46
2:D:368:SER:C	2:D:370:VAL:H	2.24	0.46
2:E:368:SER:C	2:E:370:VAL:H	2.22	0.46
2:D:220:ALA:O	2:D:312:ARG:HD3	2.16	0.46
2:D:284:LYS:HD2	2:D:284:LYS:HA	1.77	0.46
2:E:131:ALA:HA	2:E:358:THR:HA	1.97	0.46
2:E:331:ALA:HB1	2:E:335:ARG:HD3	1.97	0.46
2:A:79:TRP:CZ2	2:A:118:LYS:HB2	2.51	0.46
2:B:44:MET:O	2:B:44:MET:HG2	2.16	0.46
2:B:73:HIC:ND1	2:B:179:ASP:OD1	2.49	0.46
2:B:221:LEU:HD11	2:B:315:LYS:HD3	1.98	0.46
2:E:71:ILE:HA	2:E:76:ILE:HA	1.97	0.46
2:B:99:GLU:OE1	2:B:99:GLU:N	2.49	0.46
2:D:99:GLU:N	2:D:99:GLU:OE1	2.49	0.46
2:D:113:LYS:HD2	2:D:371:HIS:NE2	2.31	0.46
2:E:368:SER:O	2:E:370:VAL:HG23	2.16	0.46
2:B:8:LEU:HB3	2:B:101:HIS:CD2	2.51	0.45
2:A:81:ASP:O	2:A:85:ILE:HG12	2.16	0.45
2:C:69:TYR:HA	2:C:70:PRO:HD3	1.71	0.45
2:D:71:ILE:HA	2:D:76:ILE:HA	1.98	0.45
2:A:245:GLY:HA3	2:B:322:PRO:CB	2.45	0.45
2:B:147:ARG:NH2	2:B:330:ILE:HG21	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:284:LYS:HA	2:A:284:LYS:HD2	1.75	0.45
2:A:332:PRO:O	2:A:335:ARG:HG3	2.15	0.45
2:B:188:TYR:HB2	2:B:267:ILE:HD11	1.99	0.45
2:C:44:MET:O	2:C:44:MET:HG2	2.16	0.45
2:D:157:ASP:HA	2:D:158:GLY:HA2	1.58	0.45
2:C:39:ARG:NE	2:E:270:GLU:OE2	2.50	0.45
2:B:192:ILE:O	2:B:195:GLU:HB2	2.16	0.45
2:C:62:ARG:HB3	2:C:204:ALA:HB1	1.99	0.45
2:C:167:GLU:HA	2:C:168:GLY:HA2	1.55	0.45
2:E:157:ASP:HA	2:E:182:GLY:H	1.81	0.45
2:E:332:PRO:O	2:E:335:ARG:HG3	2.16	0.45
1:F:155:UNK:HA	1:G:155:UNK:HA	1.98	0.45
2:B:132:MET:HE2	2:B:132:MET:HB2	1.86	0.45
2:A:244:ASP:OD2	2:B:290:ARG:NH2	2.29	0.45
2:C:108:ALA:HB3	2:C:111:ASN:HB2	1.99	0.45
2:C:368:SER:O	2:C:369:ILE:HG22	2.17	0.45
2:E:304:THR:O	2:E:335:ARG:NH2	2.42	0.45
2:A:71:ILE:HA	2:A:76:ILE:HA	1.99	0.45
2:A:96:VAL:HG23	2:A:100:GLU:HG3	1.99	0.45
2:B:69:TYR:HA	2:B:70:PRO:HD3	1.77	0.45
2:D:107:GLU:O	2:D:137:GLN:HB2	2.17	0.45
2:A:158:GLY:HA2	2:A:182:GLY:H	1.82	0.45
2:A:193:LEU:HD23	2:A:200:PHE:CE2	2.45	0.45
2:B:351:THR:C	2:B:353:GLN:H	2.24	0.45
2:A:331:ALA:HB1	2:A:335:ARG:HD3	1.98	0.44
2:A:62:ARG:HB2	2:B:288:ASP:OD2	2.17	0.44
2:C:198:TYR:CZ	2:C:248:ILE:HG23	2.51	0.44
2:D:8:LEU:HB3	2:D:101:HIS:NE2	2.31	0.44
2:A:166:TYR:CZ	2:A:289:ILE:HD11	2.52	0.44
2:A:346:LEU:HG	2:A:352:PHE:CZ	2.53	0.44
2:B:298:VAL:HA	2:B:330:ILE:O	2.17	0.44
2:C:85:ILE:O	2:C:89:THR:HG23	2.17	0.44
2:C:368:SER:O	2:C:370:VAL:HG23	2.17	0.44
2:E:275:HIS:CD2	2:E:275:HIS:C	2.93	0.44
2:B:96:VAL:HG23	2:B:100:GLU:HG3	1.99	0.44
2:C:45:VAL:HG12	2:C:46:GLY:N	2.32	0.44
2:C:166:TYR:CE2	2:C:289:ILE:HD11	2.51	0.44
2:C:236:LEU:HD12	2:C:236:LEU:HA	1.65	0.44
2:E:287:ILE:HG13	2:E:290:ARG:NH2	2.31	0.44
2:E:299:MET:HE1	2:E:309:ILE:HD13	2.00	0.44
2:A:85:ILE:O	2:A:89:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:TYR:HE1	2:A:98:PRO:HG3	1.82	0.44
2:C:157:ASP:HA	2:C:158:GLY:HA2	1.57	0.44
2:C:306:TYR:CE1	4:C:402:ADP:H2	2.36	0.44
2:E:45:VAL:HG12	2:E:46:GLY:N	2.33	0.44
2:A:44:MET:O	2:A:44:MET:HG3	2.17	0.44
2:C:155:SER:O	2:C:303:THR:OG1	2.27	0.44
2:D:6:THR:O	2:D:101:HIS:HB3	2.17	0.44
2:D:291:LYS:HD2	2:D:291:LYS:O	2.18	0.44
2:E:351:THR:C	2:E:353:GLN:H	2.25	0.44
2:A:368:SER:C	2:A:370:VAL:H	2.25	0.44
2:E:189:LEU:HB2	2:E:257:CYS:SG	2.58	0.44
2:A:167:GLU:HA	2:A:168:GLY:HA2	1.59	0.44
2:B:78:ASN:ND2	2:B:80:ASP:HB3	2.33	0.44
2:C:351:THR:C	2:C:353:GLN:H	2.26	0.44
2:E:117:GLU:O	2:E:120:THR:N	2.51	0.44
2:A:7:ALA:HA	2:A:101:HIS:HB3	1.99	0.44
2:D:31:PHE:HB2	2:D:32:PRO:HD2	2.00	0.44
2:E:152:VAL:HG22	2:E:298:VAL:HG13	1.98	0.44
2:A:45:VAL:HG12	2:A:46:GLY:N	2.33	0.43
2:C:34:ILE:HG21	2:C:67:LEU:HB3	1.99	0.43
2:D:236:LEU:HA	2:D:236:LEU:HD12	1.70	0.43
2:E:346:LEU:HG	2:E:352:PHE:CZ	2.53	0.43
2:D:238:LYS:HE2	2:D:254:ARG:HH22	1.82	0.43
2:E:85:ILE:O	2:E:89:THR:HG23	2.17	0.43
2:E:208:ILE:HD12	2:E:243:PRO:HG3	2.00	0.43
2:B:331:ALA:HA	2:B:332:PRO:HD3	1.82	0.43
2:A:169:TYR:OH	2:C:49:GLN:HB3	2.19	0.43
2:D:151:ILE:HA	2:D:164:PRO:HA	2.01	0.43
2:D:337:TYR:O	2:D:341:ILE:HG13	2.18	0.43
2:B:181:ALA:HA	2:B:182:GLY:HA2	1.82	0.43
2:A:291:LYS:HD2	2:A:291:LYS:O	2.19	0.43
2:D:322:PRO:CB	2:E:245:GLY:HA3	2.47	0.43
2:E:31:PHE:HB2	2:E:32:PRO:HD2	1.99	0.43
2:E:151:ILE:HG21	2:E:282:ILE:HD11	2.01	0.43
2:E:193:LEU:HD23	2:E:200:PHE:CE2	2.46	0.43
2:A:23:GLY:HA2	2:A:344:SER:HB3	2.01	0.43
2:A:99:GLU:N	2:A:99:GLU:OE1	2.52	0.43
2:D:37:ARG:HA	2:D:38:PRO:HD3	1.87	0.43
2:D:96:VAL:HG23	2:D:100:GLU:HG3	2.01	0.43
2:A:157:ASP:OD1	2:A:183:ARG:HG3	2.19	0.43
2:B:81:ASP:O	2:B:85:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:SER:OG	2:B:300:SER:OG	2.26	0.43
2:B:198:TYR:CZ	2:B:248:ILE:HG23	2.54	0.43
2:D:44:MET:O	2:D:44:MET:HG2	2.17	0.43
2:A:295:ALA:HB2	2:A:326:LYS:O	2.18	0.43
2:B:9:VAL:HG21	2:B:343:GLY:HA3	1.99	0.43
2:B:117:GLU:O	2:B:120:THR:N	2.52	0.43
2:B:368:SER:O	2:B:370:VAL:HG23	2.19	0.43
2:C:237:GLU:OE2	2:C:249:THR:HB	2.19	0.43
2:D:79:TRP:HA	2:D:82:MET:HB3	2.01	0.43
2:D:142:LEU:HD12	2:D:165:ILE:HD12	2.01	0.43
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.72	0.42
2:D:9:VAL:HG21	2:D:343:GLY:HA3	2.00	0.42
2:E:99:GLU:OE1	2:E:99:GLU:N	2.52	0.42
2:A:166:TYR:CE2	2:A:289:ILE:HD11	2.53	0.42
2:A:169:TYR:CZ	2:C:49:GLN:HB3	2.53	0.42
2:D:136:ILE:HD11	2:D:139:VAL:HG23	2.00	0.42
2:D:157:ASP:HA	2:D:182:GLY:H	1.85	0.42
2:A:69:TYR:HA	2:A:70:PRO:HD3	1.75	0.42
2:D:20:GLY:HA2	2:D:28:ARG:HG2	2.00	0.42
2:E:236:LEU:HA	2:E:236:LEU:HD12	1.70	0.42
2:E:306:TYR:CE1	4:E:402:ADP:H2	2.37	0.42
2:A:322:PRO:CB	2:C:245:GLY:HA3	2.48	0.42
2:B:166:TYR:CE2	2:B:289:ILE:HD11	2.55	0.42
2:B:218:TYR:CZ	2:B:255:PHE:HB3	2.55	0.42
2:A:217:CYS:SG	2:A:218:TYR:N	2.92	0.42
2:A:304:THR:O	2:A:335:ARG:NH2	2.45	0.42
2:C:8:LEU:HB3	2:C:101:HIS:CD2	2.55	0.42
2:C:295:ALA:HB2	2:C:326:LYS:O	2.20	0.42
2:D:133:TYR:HB2	2:D:356:TRP:CD1	2.55	0.42
2:A:351:THR:C	2:A:353:GLN:H	2.26	0.42
2:B:20:GLY:HA2	2:B:28:ARG:HG2	2.00	0.42
2:B:239:SER:HB3	2:B:249:THR:HG22	2.00	0.42
2:C:96:VAL:HG23	2:C:100:GLU:HG3	2.01	0.42
2:C:117:GLU:O	2:C:120:THR:N	2.52	0.42
2:D:368:SER:O	2:D:370:VAL:N	2.52	0.42
2:C:14:SER:HB2	2:C:157:ASP:O	2.19	0.42
2:C:238:LYS:HE2	2:C:254:ARG:NH2	2.34	0.42
2:D:350:SER:HA	2:D:351:THR:HA	1.84	0.42
2:E:9:VAL:HG23	2:E:104:LEU:HD22	2.00	0.42
2:E:251:GLY:O	2:E:252:ASN:C	2.62	0.42
2:E:284:LYS:HD2	2:E:284:LYS:HA	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:236:LEU:HD12	2:A:236:LEU:HA	1.65	0.42
2:B:236:LEU:HD12	2:B:236:LEU:HA	1.63	0.42
2:C:165:ILE:HG23	2:C:170:ALA:HB2	2.01	0.42
2:C:178:LEU:HD12	2:C:274:ILE:HD13	2.02	0.42
2:A:350:SER:HA	2:A:351:THR:HA	1.79	0.42
2:B:295:ALA:HB2	2:B:326:LYS:O	2.19	0.42
2:C:99:GLU:N	2:C:99:GLU:OE1	2.52	0.42
2:D:202:THR:HG23	2:D:205:GLU:HB2	2.02	0.42
2:A:108:ALA:HB3	2:A:111:ASN:HB2	2.02	0.42
2:B:101:HIS:O	2:B:129:VAL:HG13	2.19	0.42
2:B:284:LYS:HD2	2:B:284:LYS:HA	1.77	0.42
2:C:193:LEU:HD12	2:C:193:LEU:HA	1.80	0.42
2:D:368:SER:O	2:D:369:ILE:HG22	2.19	0.42
2:E:133:TYR:HB2	2:E:356:TRP:CD1	2.55	0.42
2:C:217:CYS:SG	2:C:218:TYR:N	2.93	0.41
2:E:311:ASP:HA	2:E:314:GLN:HB3	2.02	0.41
2:A:39:ARG:HB3	2:A:66:THR:HG23	2.02	0.41
2:B:192:ILE:HD11	2:B:257:CYS:HB2	2.02	0.41
2:B:217:CYS:SG	2:B:218:TYR:N	2.93	0.41
2:D:147:ARG:HH12	2:D:330:ILE:HB	1.85	0.41
2:D:223:PHE:CZ	2:D:227:MET:HE3	2.55	0.41
2:A:111:ASN:ND2	2:A:115:ASN:OD1	2.53	0.41
2:A:328:LYS:HG2	2:A:328:LYS:H	1.59	0.41
2:B:368:SER:O	2:B:369:ILE:HG22	2.20	0.41
2:D:117:GLU:O	2:D:120:THR:N	2.53	0.41
2:E:166:TYR:CE2	2:E:289:ILE:HD11	2.55	0.41
2:D:331:ALA:HB1	2:D:335:ARG:HD3	2.02	0.41
2:E:242:LEU:HD13	2:E:248:ILE:HD12	2.02	0.41
2:E:333:PRO:O	2:E:334:GLU:HG2	2.20	0.41
2:A:331:ALA:HA	2:A:332:PRO:HD3	1.89	0.41
2:C:291:LYS:HD2	2:C:291:LYS:O	2.20	0.41
2:E:350:SER:HA	2:E:351:THR:HA	1.82	0.41
2:A:162:ASN:ND2	2:A:281:SER:OG	2.53	0.41
2:A:368:SER:O	2:A:370:VAL:HG23	2.20	0.41
2:E:78:ASN:ND2	2:E:80:ASP:HB3	2.35	0.41
2:B:15:GLY:CA	2:B:16:LEU:HB2	2.50	0.41
2:B:157:ASP:HA	2:B:182:GLY:H	1.86	0.41
2:C:78:ASN:ND2	2:C:80:ASP:HB3	2.36	0.41
2:C:237:GLU:HB2	2:C:251:GLY:HA3	2.02	0.41
2:D:96:VAL:HG22	2:D:97:ALA:O	2.20	0.41
2:E:238:LYS:HE2	2:E:254:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:152:VAL:HG22	2:A:298:VAL:HG13	2.03	0.41
2:B:238:LYS:HE2	2:B:254:ARG:NH2	2.36	0.41
2:D:7:ALA:HA	2:D:101:HIS:CG	2.55	0.41
2:D:309:ILE:H	2:D:309:ILE:HG13	1.65	0.41
2:E:105:LEU:O	2:E:134:VAL:HA	2.20	0.41
2:E:160:THR:HG22	2:E:178:LEU:O	2.21	0.41
2:A:171:LEU:HD22	2:C:40:HIS:CE1	2.56	0.41
2:A:193:LEU:HD12	2:A:193:LEU:HA	1.74	0.41
2:A:368:SER:O	2:A:369:ILE:HG22	2.21	0.41
2:B:328:LYS:N	2:B:328:LYS:HD3	2.36	0.41
2:C:160:THR:HG22	2:C:178:LEU:O	2.21	0.41
2:C:178:LEU:HD11	2:C:277:THR:HG21	2.01	0.41
2:C:326:LYS:HE3	2:C:328:LYS:HE3	2.03	0.41
2:C:331:ALA:HA	2:C:332:PRO:HD3	1.85	0.41
2:D:283:MET:HA	2:D:290:ARG:HD3	2.02	0.41
2:D:298:VAL:HA	2:D:330:ILE:O	2.21	0.41
2:D:359:LYS:HA	2:D:359:LYS:HD2	1.84	0.41
2:A:31:PHE:HB2	2:A:32:PRO:HD2	2.02	0.41
2:A:346:LEU:O	2:A:352:PHE:HE1	2.04	0.41
2:D:16:LEU:HB3	2:D:18:LYS:HE3	2.03	0.41
2:E:157:ASP:OD1	2:E:183:ARG:HG3	2.21	0.41
2:E:366:GLY:HA3	2:E:367:PRO:HD3	1.91	0.41
2:A:37:ARG:HA	2:A:38:PRO:HD3	1.84	0.40
2:A:238:LYS:HE2	2:A:254:ARG:HH22	1.86	0.40
2:B:346:LEU:O	2:B:352:PHE:HE1	2.04	0.40
2:C:350:SER:HA	2:C:351:THR:HA	1.81	0.40
2:D:198:TYR:CE2	2:D:248:ILE:HG12	2.55	0.40
2:A:19:ALA:HB1	2:A:94:LEU:HD11	2.03	0.40
2:B:306:TYR:HE1	4:B:402:ADP:H2	1.68	0.40
2:C:337:TYR:O	2:C:341:ILE:HG13	2.21	0.40
2:D:238:LYS:HE2	2:D:254:ARG:NH2	2.35	0.40
2:C:295:ALA:HA	2:C:328:LYS:N	2.35	0.40
2:E:37:ARG:HA	2:E:38:PRO:HD3	1.84	0.40
2:B:23:GLY:HA2	2:B:24:ASP:HA	1.93	0.40
2:B:113:LYS:HA	2:B:115:ASN:H	1.86	0.40
2:C:50:LYS:HB2	2:C:53:TYR:CD1	2.56	0.40
2:D:251:GLY:O	2:D:252:ASN:C	2.64	0.40
2:E:96:VAL:HG23	2:E:100:GLU:HG3	2.03	0.40
2:D:15:GLY:CA	2:D:16:LEU:HB2	2.51	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	
2	A	364/375 (97%)	318 (87%)	41 (11%)	5 (1%)	9	37
2	B	364/375 (97%)	317 (87%)	42 (12%)	5 (1%)	9	37
2	C	364/375 (97%)	318 (87%)	41 (11%)	5 (1%)	9	37
2	D	364/375 (97%)	316 (87%)	43 (12%)	5 (1%)	9	37
2	E	364/375 (97%)	318 (87%)	41 (11%)	5 (1%)	9	37
All	All	1820/1875 (97%)	1587 (87%)	208 (11%)	25 (1%)	11	37

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	22	ALA
2	A	45	VAL
2	A	252	ASN
2	A	369	ILE
2	B	22	ALA
2	B	45	VAL
2	B	369	ILE
2	C	22	ALA
2	C	45	VAL
2	C	252	ASN
2	C	369	ILE
2	D	22	ALA
2	D	45	VAL
2	D	252	ASN
2	D	369	ILE
2	E	22	ALA
2	E	45	VAL
2	E	252	ASN
2	E	369	ILE
2	B	252	ASN
2	A	244	ASP

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Mol	Chain	Res	Type
2	B	244	ASP
2	C	244	ASP
2	D	244	ASP
2	E	244	ASP

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

5 non-standard protein/DNA/RNA residues 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
2	HIC	A	73	2	10,11,12	2.39	1 (10%)	9,14,16	4.07	3 (33%)
2	HIC	D	73	2	10,11,12	2.37	1 (10%)	9,14,16	4.47	3 (33%)
2	HIC	E	73	2	10,11,12	2.38	1 (10%)	9,14,16	4.07	3 (33%)
2	HIC	C	73	2	10,11,12	2.38	1 (10%)	9,14,16	4.16	3 (33%)
2	HIC	B	73	2	10,11,12	2.38	1 (10%)	9,14,16	4.14	3 (33%)

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
2	HIC	A	73	2	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HIC	D	73	2	-	0/5/6/8	0/1/1/1
2	HIC	E	73	2	-	0/5/6/8	0/1/1/1
2	HIC	C	73	2	-	0/5/6/8	0/1/1/1
2	HIC	B	73	2	-	0/5/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	73	HIC	CZ-NE2	-7.36	1.27	1.46
2	B	73	HIC	CZ-NE2	-7.33	1.27	1.46
2	D	73	HIC	CZ-NE2	-7.33	1.27	1.46
2	C	73	HIC	CZ-NE2	-7.33	1.27	1.46
2	E	73	HIC	CZ-NE2	-7.32	1.27	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	73	HIC	NE2-CE1-ND1	-11.67	108.19	112.66
2	C	73	HIC	NE2-CE1-ND1	-10.92	108.48	112.66
2	B	73	HIC	NE2-CE1-ND1	-10.86	108.50	112.66
2	E	73	HIC	NE2-CE1-ND1	-10.77	108.54	112.66
2	A	73	HIC	NE2-CE1-ND1	-10.73	108.56	112.66
2	D	73	HIC	CD2-NE2-CE1	5.92	109.05	106.71
2	B	73	HIC	CD2-NE2-CE1	5.38	108.84	106.71
2	C	73	HIC	CD2-NE2-CE1	5.33	108.82	106.71
2	A	73	HIC	CD2-NE2-CE1	5.14	108.74	106.71
2	E	73	HIC	CD2-NE2-CE1	5.09	108.72	106.71
2	D	73	HIC	CE1-ND1-CG	2.30	109.48	105.80
2	C	73	HIC	CE1-ND1-CG	2.17	109.28	105.80
2	A	73	HIC	CE1-ND1-CG	2.11	109.18	105.80
2	B	73	HIC	CE1-ND1-CG	2.10	109.17	105.80
2	E	73	HIC	CE1-ND1-CG	2.07	109.12	105.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	73	HIC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	73	HIC	1	0
2	E	73	HIC	1	0
2	C	73	HIC	1	0
2	B	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	D	402	3	28,29,29	1.41	4 (14%)	43,45,45	1.84	10 (23%)
4	ADP	E	402	3	28,29,29	1.39	4 (14%)	43,45,45	1.82	10 (23%)
4	ADP	C	402	3	28,29,29	1.41	4 (14%)	43,45,45	1.83	10 (23%)
4	ADP	A	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.82	10 (23%)
4	ADP	B	402	3	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	D	402	3	-	5/16/32/32	0/3/3/3
4	ADP	E	402	3	-	4/16/32/32	0/3/3/3
4	ADP	C	402	3	-	3/16/32/32	0/3/3/3
4	ADP	A	402	3	-	3/16/32/32	0/3/3/3
4	ADP	B	402	3	-	1/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	ADP	C5-C4	4.75	1.47	1.39
4	D	402	ADP	C5-C4	4.73	1.47	1.39
4	A	402	ADP	C5-C4	4.68	1.47	1.39
4	B	402	ADP	C5-C4	4.61	1.47	1.39
4	E	402	ADP	C5-C4	4.54	1.47	1.39
4	B	402	ADP	C5-C6	2.84	1.48	1.41
4	E	402	ADP	C5-C6	2.83	1.48	1.41
4	A	402	ADP	C5-C6	2.81	1.48	1.41
4	C	402	ADP	C5-C6	2.81	1.48	1.41
4	D	402	ADP	C5-C6	2.76	1.48	1.41
4	A	402	ADP	C8-N7	2.44	1.36	1.31
4	E	402	ADP	C8-N7	2.37	1.36	1.31
4	B	402	ADP	C8-N7	2.37	1.36	1.31
4	C	402	ADP	C8-N7	2.35	1.36	1.31
4	D	402	ADP	C8-N7	2.34	1.36	1.31
4	D	402	ADP	C5-N7	-2.25	1.35	1.39
4	B	402	ADP	C5-N7	-2.22	1.35	1.39
4	A	402	ADP	C5-N7	-2.19	1.35	1.39
4	C	402	ADP	C5-N7	-2.18	1.35	1.39
4	E	402	ADP	C5-N7	-2.18	1.35	1.39

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	ADP	C5-C4-N3	-5.73	118.83	126.72
4	C	402	ADP	C5-C4-N3	-5.70	118.86	126.72
4	D	402	ADP	C5-C4-N3	-5.70	118.87	126.72
4	A	402	ADP	C5-C4-N3	-5.69	118.88	126.72
4	E	402	ADP	C5-C4-N3	-5.66	118.92	126.72
4	D	402	ADP	N3-C4-N9	4.49	134.81	127.17
4	A	402	ADP	N3-C4-N9	4.36	134.58	127.17
4	C	402	ADP	N3-C4-N9	4.33	134.53	127.17
4	B	402	ADP	N3-C4-N9	4.32	134.52	127.17
4	E	402	ADP	N3-C4-N9	4.28	134.45	127.17
4	B	402	ADP	C4-C5-N7	-3.88	106.15	110.58
4	C	402	ADP	C4-C5-N7	-3.84	106.19	110.58
4	A	402	ADP	C4-C5-N7	-3.79	106.25	110.58
4	E	402	ADP	C4-C5-N7	-3.75	106.30	110.58
4	E	402	ADP	C2-N3-C4	3.64	120.73	111.83
4	B	402	ADP	C2-N3-C4	3.63	120.70	111.83
4	A	402	ADP	C2-N3-C4	3.58	120.58	111.83
4	C	402	ADP	C2-N3-C4	3.57	120.56	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	ADP	C4-C5-N7	-3.55	106.52	110.58
4	D	402	ADP	C2-N3-C4	3.55	120.50	111.83
4	E	402	ADP	N3-C2-N1	-3.22	123.71	128.58
4	C	402	ADP	N3-C2-N1	-3.07	123.93	128.58
4	B	402	ADP	N3-C2-N1	-3.04	123.98	128.58
4	A	402	ADP	N3-C2-N1	-2.99	124.06	128.58
4	D	402	ADP	N3-C2-N1	-2.99	124.06	128.58
4	B	402	ADP	C5-N7-C8	2.91	108.03	103.45
4	A	402	ADP	C5-N7-C8	2.82	107.89	103.45
4	C	402	ADP	C5-N7-C8	2.81	107.87	103.45
4	E	402	ADP	C5-N7-C8	2.81	107.87	103.45
4	D	402	ADP	C4-N9-C8	2.80	108.68	105.74
4	A	402	ADP	C4-N9-C8	2.74	108.62	105.74
4	B	402	ADP	C4-N9-C8	2.71	108.58	105.74
4	D	402	ADP	C5-N7-C8	2.70	107.69	103.45
4	E	402	ADP	C4-N9-C8	2.57	108.44	105.74
4	C	402	ADP	C4-N9-C8	2.57	108.44	105.74
4	B	402	ADP	C6-C5-N7	2.36	136.63	132.09
4	B	402	ADP	N9-C8-N7	-2.35	110.60	113.94
4	C	402	ADP	C3'-C2'-C1'	2.33	105.88	101.46
4	A	402	ADP	N9-C8-N7	-2.27	110.72	113.94
4	D	402	ADP	C3'-C2'-C1'	2.26	105.74	101.46
4	E	402	ADP	C6-C5-N7	2.26	136.44	132.09
4	C	402	ADP	C6-C5-N7	2.25	136.43	132.09
4	A	402	ADP	C6-C5-N7	2.24	136.41	132.09
4	E	402	ADP	N9-C8-N7	-2.24	110.76	113.94
4	D	402	ADP	N9-C8-N7	-2.21	110.80	113.94
4	B	402	ADP	C3'-C2'-C1'	2.18	105.59	101.46
4	A	402	ADP	C3'-C2'-C1'	2.18	105.58	101.46
4	E	402	ADP	C3'-C2'-C1'	2.17	105.57	101.46
4	C	402	ADP	N9-C8-N7	-2.15	110.89	113.94
4	D	402	ADP	C6-C5-N7	2.10	136.13	132.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	ADP	C5'-O5'-PA-O1A
4	A	402	ADP	C5'-O5'-PA-O2A
4	A	402	ADP	C5'-O5'-PA-O3A
4	B	402	ADP	C5'-O5'-PA-O2A
4	C	402	ADP	C5'-O5'-PA-O1A

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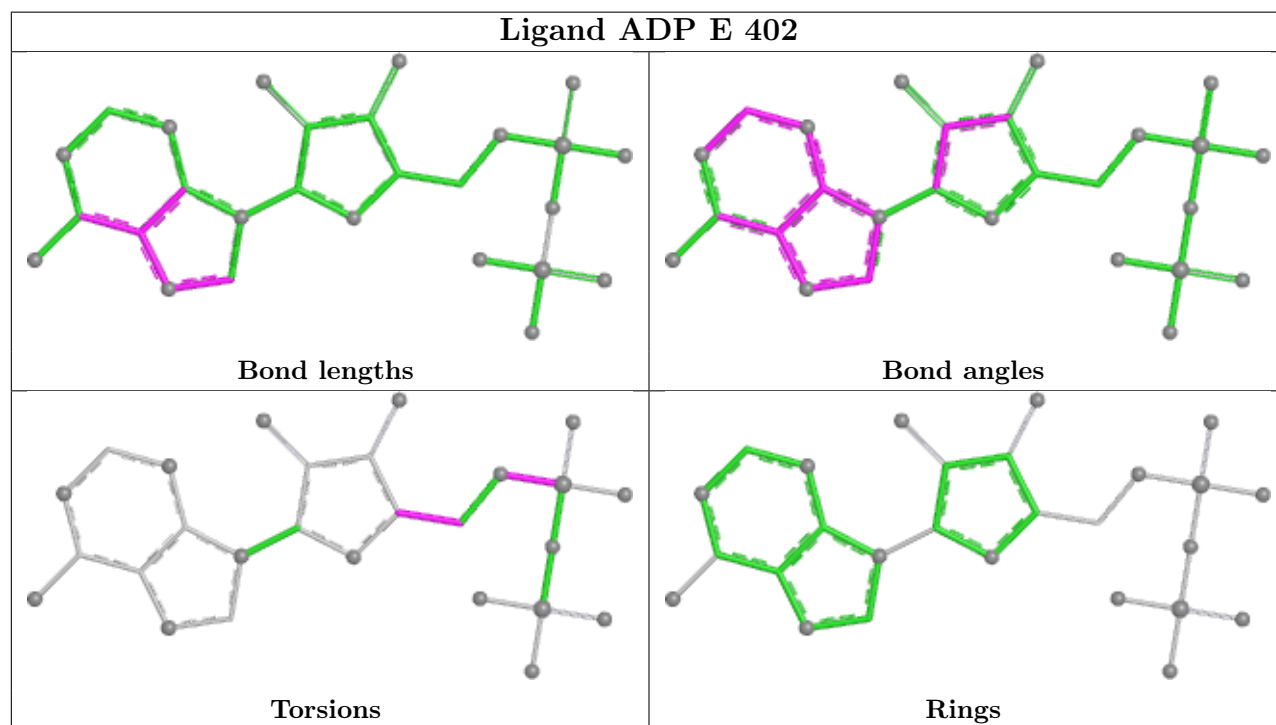
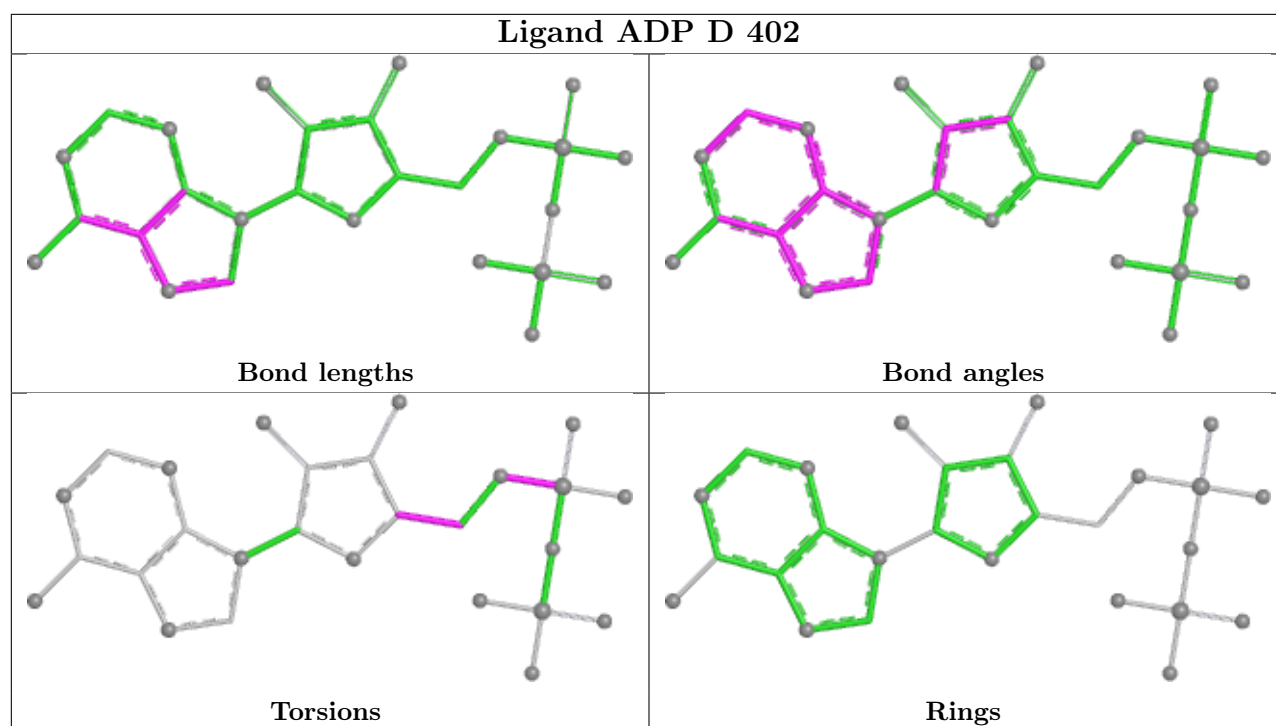
Mol	Chain	Res	Type	Atoms
4	C	402	ADP	C5'-O5'-PA-O2A
4	C	402	ADP	C5'-O5'-PA-O3A
4	D	402	ADP	C5'-O5'-PA-O1A
4	D	402	ADP	C5'-O5'-PA-O3A
4	E	402	ADP	C5'-O5'-PA-O1A
4	E	402	ADP	C5'-O5'-PA-O2A
4	E	402	ADP	C5'-O5'-PA-O3A
4	D	402	ADP	C3'-C4'-C5'-O5'
4	E	402	ADP	C3'-C4'-C5'-O5'
4	D	402	ADP	C5'-O5'-PA-O2A
4	D	402	ADP	O4'-C4'-C5'-O5'

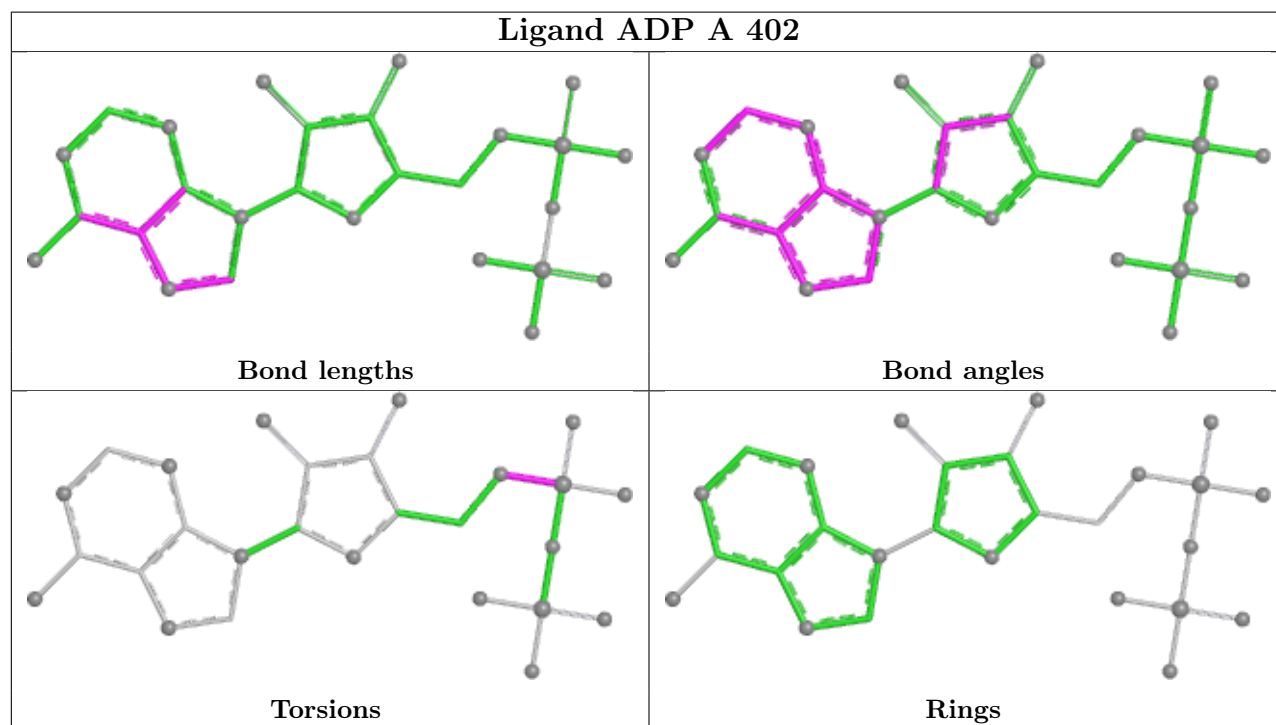
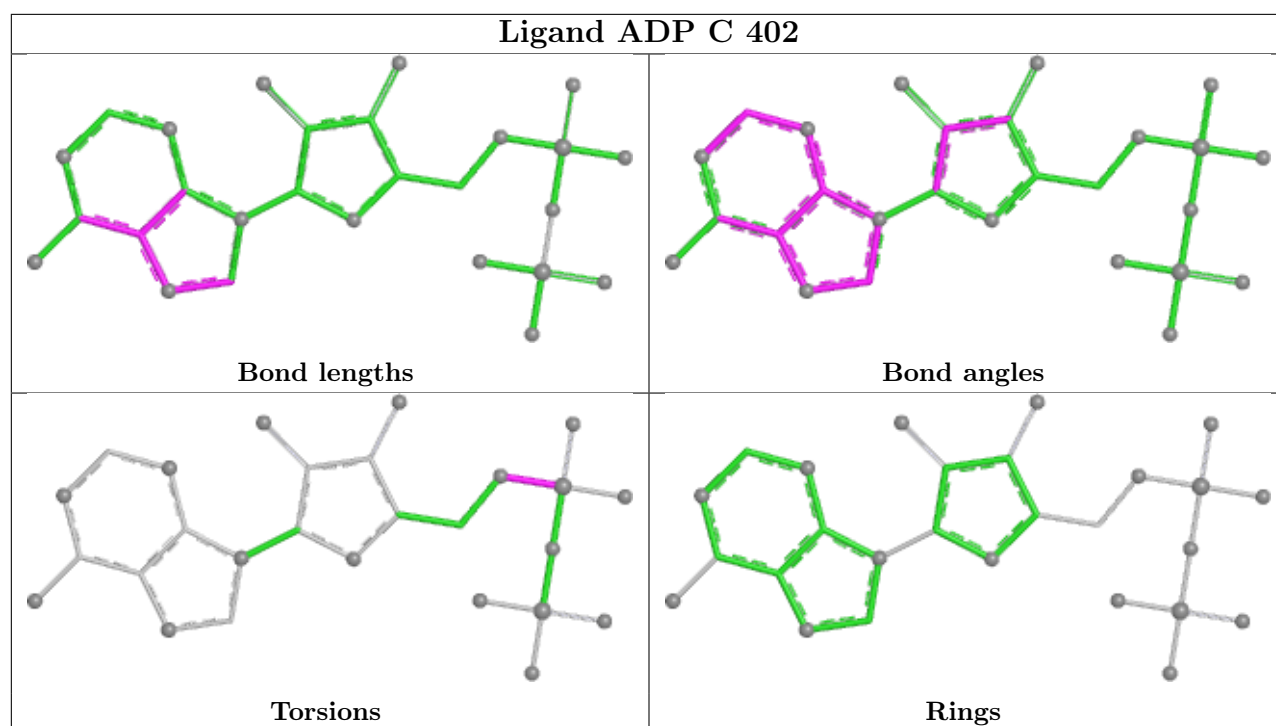
There are no ring outliers.

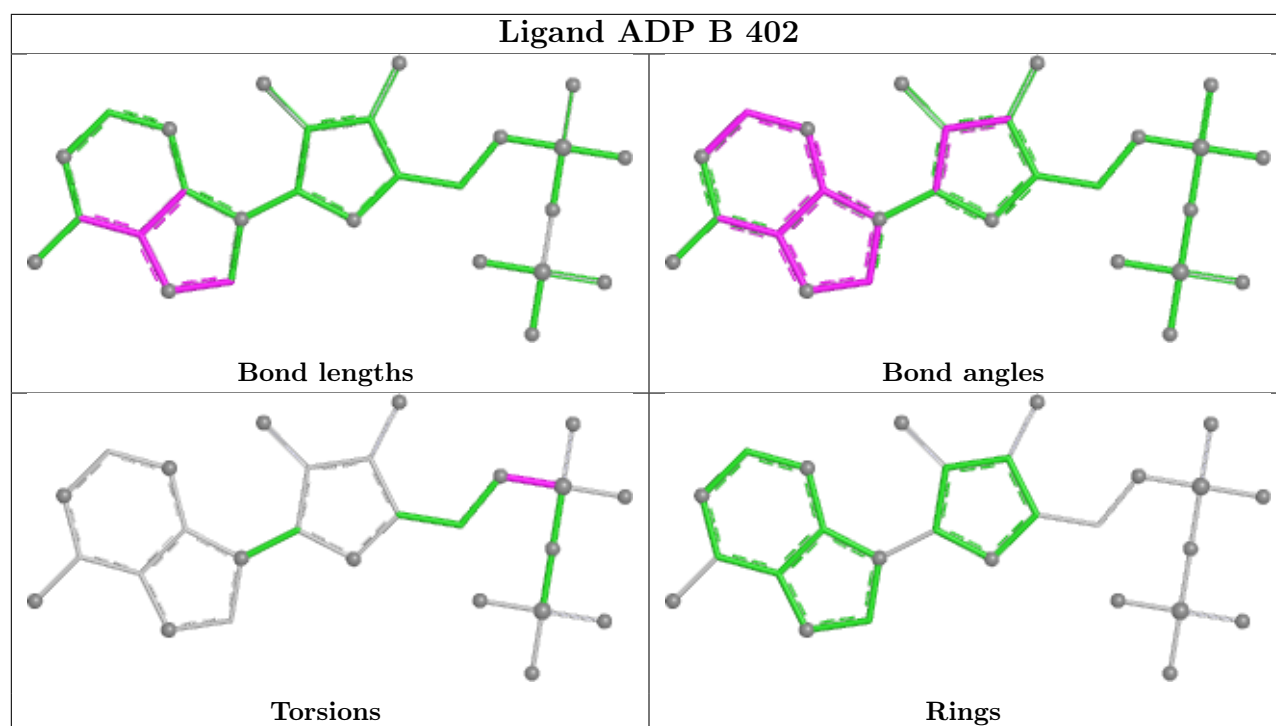
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	402	ADP	1	0
4	E	402	ADP	1	0
4	C	402	ADP	1	0
4	A	402	ADP	1	0
4	B	402	ADP	2	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

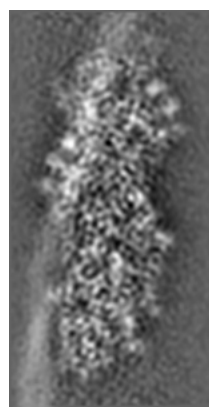
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6124. These allow visual inspection of the internal detail of the map and identification of artifacts.

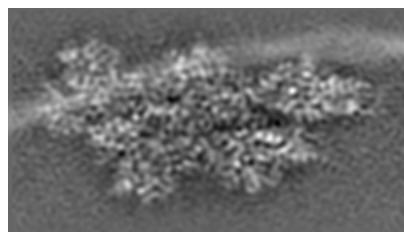
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

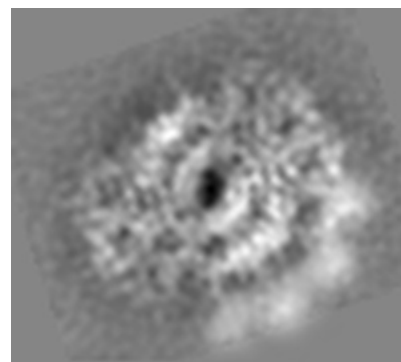
6.1.1 Primary map



X



Y

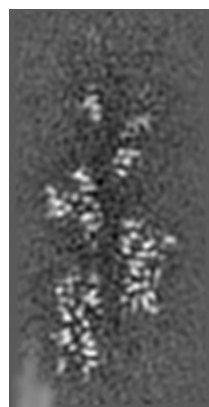


Z

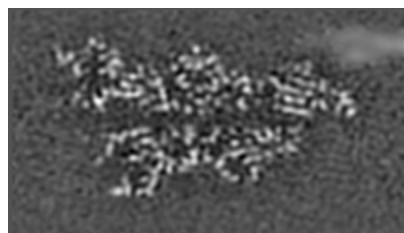
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

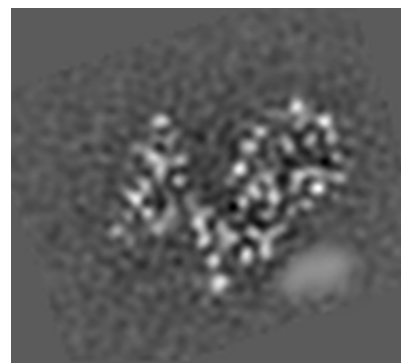
6.2.1 Primary map



X Index: 51



Y Index: 46

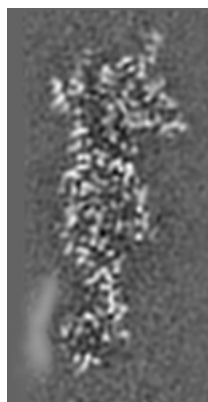


Z Index: 91

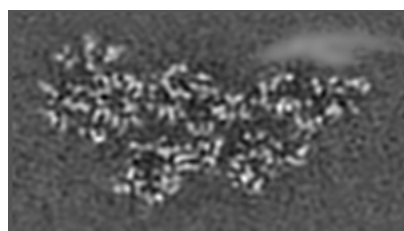
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

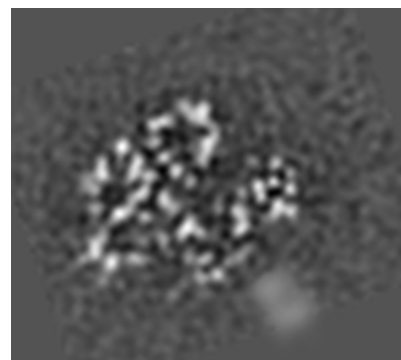
6.3.1 Primary map



X Index: 64



Y Index: 39

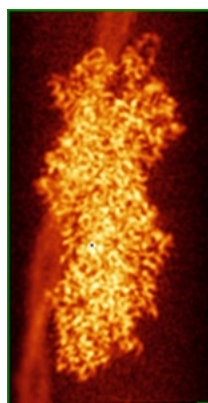


Z Index: 55

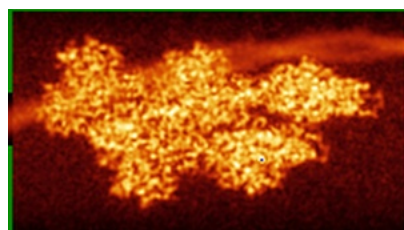
The images above show the largest variance slices of the map in three orthogonal directions.

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

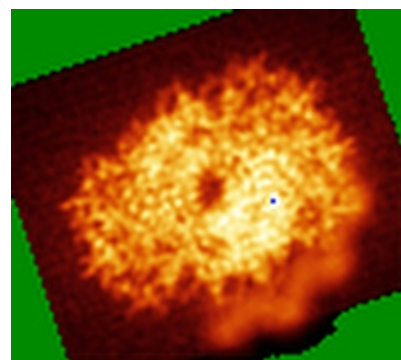
6.4.1 Primary map



X



Y



Z

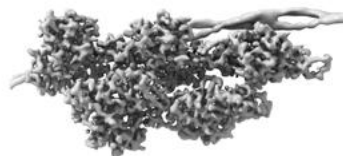
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

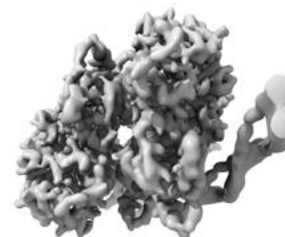
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

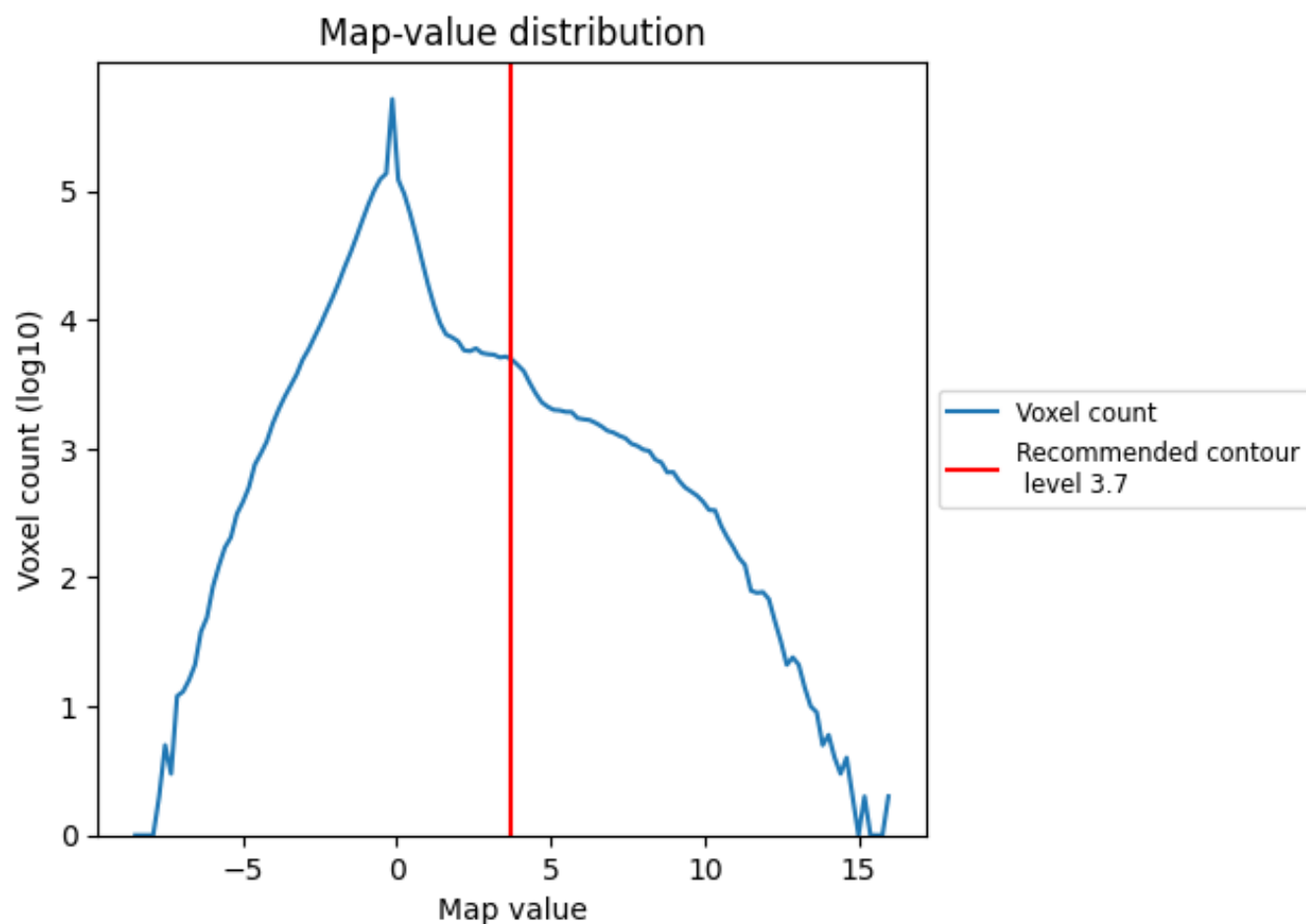
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

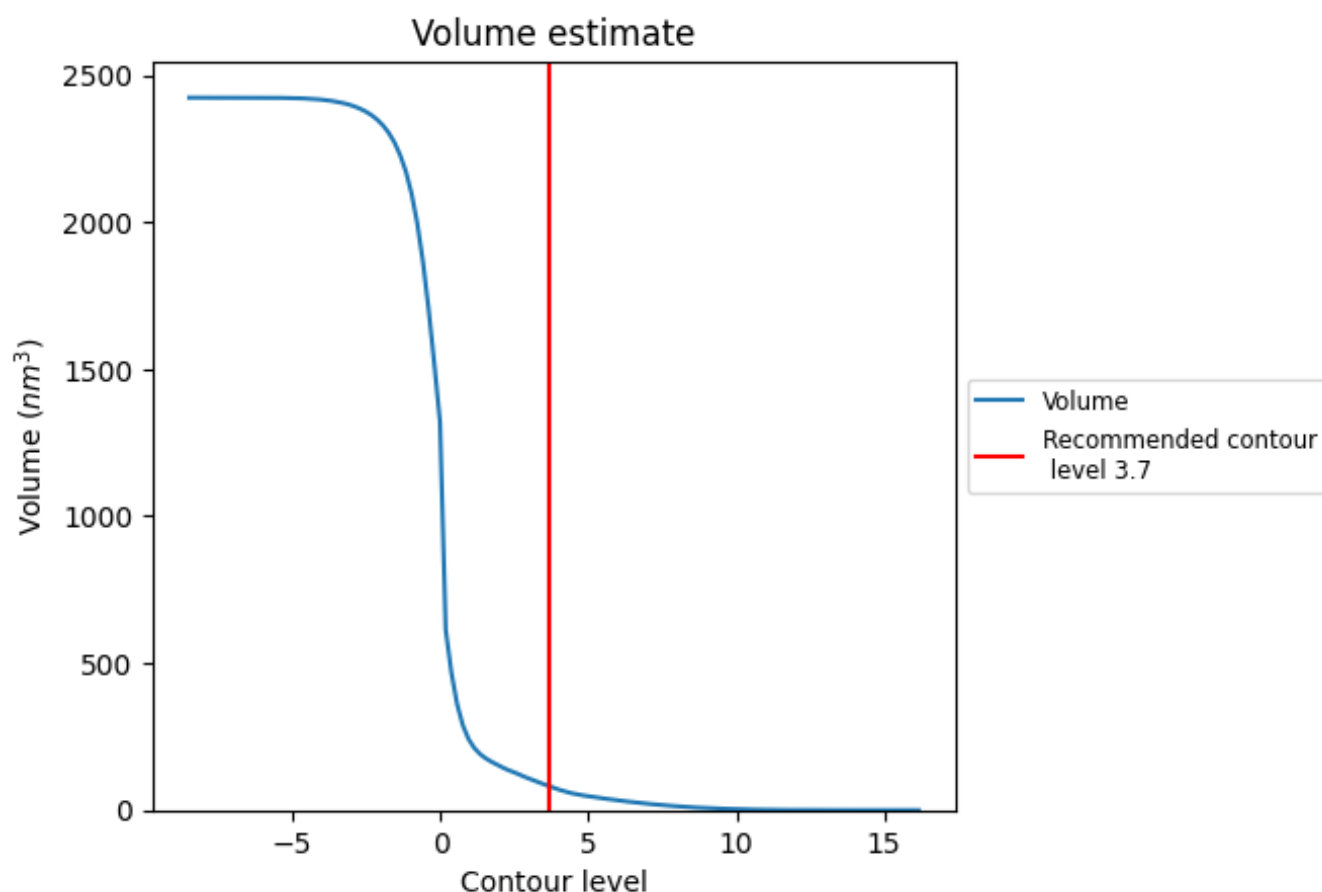
This section contains the results of statistical analysis of the map.

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 81 nm³; this corresponds to an approximate mass of 73 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

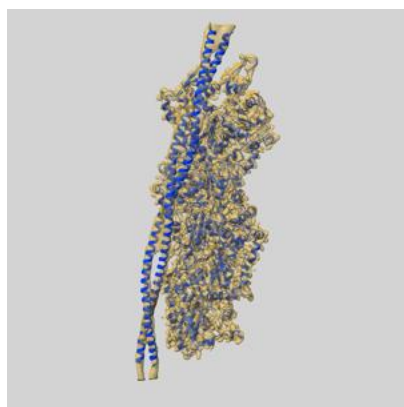
8 Fourier-Shell correlation ⓘ

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

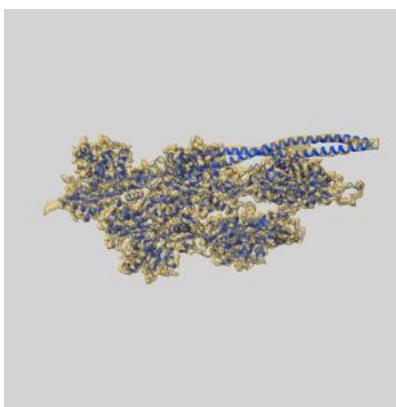
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6124 and PDB model 3J8A. Per-residue inclusion information can be found in section [3](#) on page [6](#).

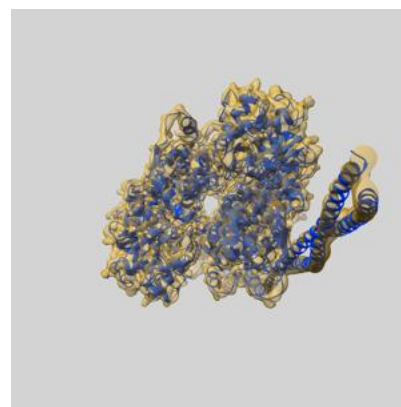
9.1 Map-model overlay [i](#)



X



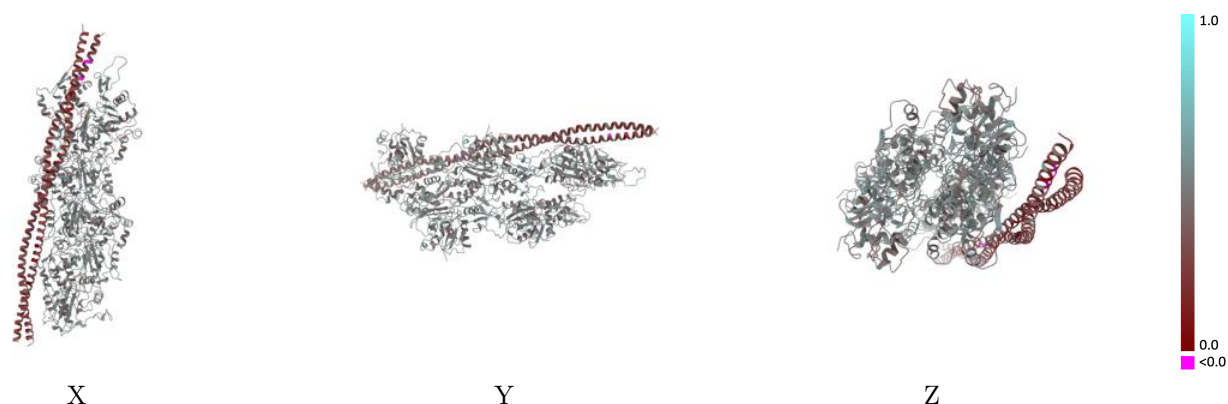
Y



Z

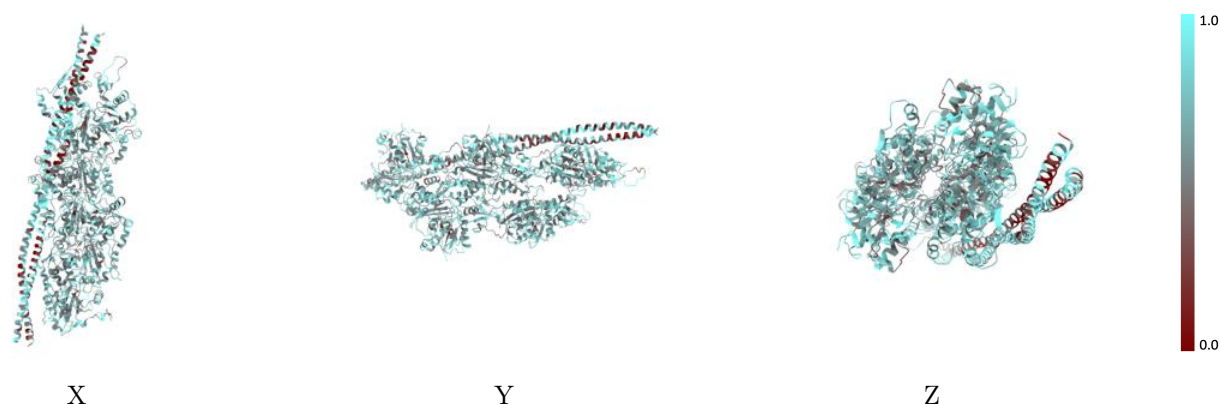
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



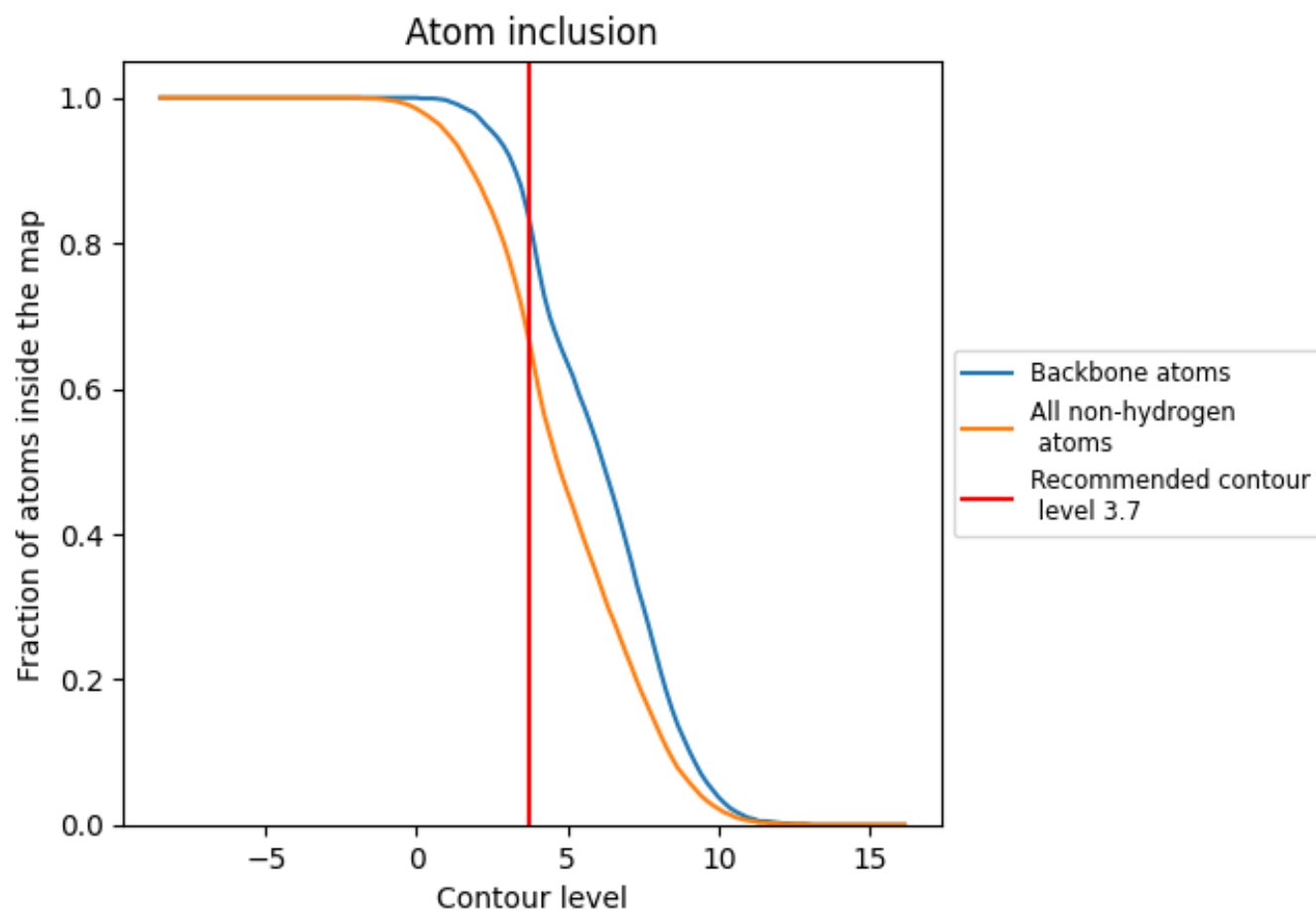
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.7).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 67% 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 (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6710	0.4730
A	0.6700	0.4980
B	0.6830	0.4890
C	0.6820	0.4920
D	0.6730	0.4920
E	0.6820	0.4940
F	0.5990	0.2590
G	0.6020	0.2570

1.0

0.0

<0.0