



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 03:08 AM UTC

PDB ID : 7P1G / pdb_00007p1g
EMDB ID : EMD-13158
Title : Structure of the *P. aeruginosa* ExoY-F-actin complex
Authors : Belyy, A.; Merino, F.; Raunser, S.
Deposited on : 2021-07-01
Resolution : 3.20 Å (reported)
Based on initial models : 7AD9, 5XNW

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

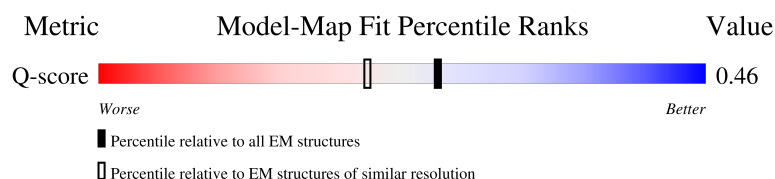
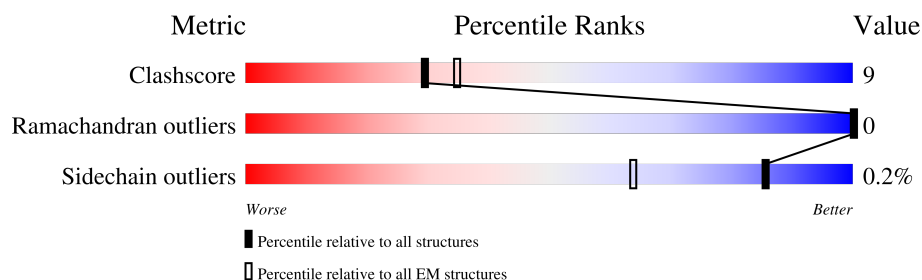
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



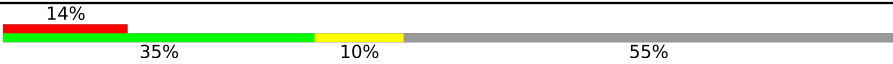
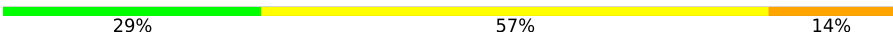
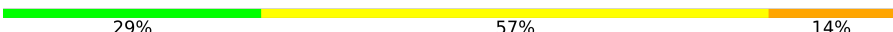
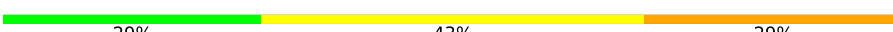
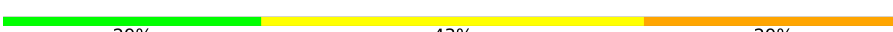
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	K	773	10% 35% 10% 55%
1	L	773	10% 36% 9% 55%
1	M	773	7% 35% 10% 55%
1	N	773	9% 36% 9% 55%

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Mol	Chain	Length	Quality of chain
1	O	773	
2	A	377	
2	B	377	
2	C	377	
2	D	377	
2	E	377	
3	F	7	
3	G	7	
3	H	7	
3	I	7	
3	J	7	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28580 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 Maltose/maltodextrin-binding periplasmic protein,Adenylate cyclase ExoY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	K	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	L	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	N	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		
1	O	347	Total	C	N	O	S	0	0
			2697	1680	500	504	13		

There are 155 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-394	MET	-	initiating methionine	UNP P0AEX9
M	-393	GLY	-	expression tag	UNP P0AEX9
M	-392	SER	-	expression tag	UNP P0AEX9
M	-391	SER	-	expression tag	UNP P0AEX9
M	-390	HIS	-	expression tag	UNP P0AEX9
M	-389	HIS	-	expression tag	UNP P0AEX9
M	-388	HIS	-	expression tag	UNP P0AEX9
M	-387	HIS	-	expression tag	UNP P0AEX9
M	-386	HIS	-	expression tag	UNP P0AEX9
M	-385	HIS	-	expression tag	UNP P0AEX9
M	-384	SER	-	expression tag	UNP P0AEX9
M	-383	SER	-	expression tag	UNP P0AEX9
M	-382	GLY	-	expression tag	UNP P0AEX9
M	-381	LEU	-	expression tag	UNP P0AEX9
M	-380	VAL	-	expression tag	UNP P0AEX9
M	-379	PRO	-	expression tag	UNP P0AEX9
M	-378	ARG	-	expression tag	UNP P0AEX9
M	-377	GLY	-	expression tag	UNP P0AEX9
M	-376	SER	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-375	HIS	-	expression tag	UNP P0AEX9
M	-374	MET	-	expression tag	UNP P0AEX9
M	-62	VAL	ALA	conflict	UNP P0AEX9
M	-7	ASN	-	linker	UNP P0AEX9
M	-6	SER	-	linker	UNP P0AEX9
M	-5	GLY	-	linker	UNP P0AEX9
M	-4	SER	-	linker	UNP P0AEX9
M	-3	SER	-	linker	UNP P0AEX9
M	-2	GLY	-	linker	UNP P0AEX9
M	-1	SER	-	linker	UNP P0AEX9
M	0	SER	-	linker	UNP P0AEX9
M	1	GLY	-	linker	UNP P0AEX9
K	-394	MET	-	initiating methionine	UNP P0AEX9
K	-393	GLY	-	expression tag	UNP P0AEX9
K	-392	SER	-	expression tag	UNP P0AEX9
K	-391	SER	-	expression tag	UNP P0AEX9
K	-390	HIS	-	expression tag	UNP P0AEX9
K	-389	HIS	-	expression tag	UNP P0AEX9
K	-388	HIS	-	expression tag	UNP P0AEX9
K	-387	HIS	-	expression tag	UNP P0AEX9
K	-386	HIS	-	expression tag	UNP P0AEX9
K	-385	HIS	-	expression tag	UNP P0AEX9
K	-384	SER	-	expression tag	UNP P0AEX9
K	-383	SER	-	expression tag	UNP P0AEX9
K	-382	GLY	-	expression tag	UNP P0AEX9
K	-381	LEU	-	expression tag	UNP P0AEX9
K	-380	VAL	-	expression tag	UNP P0AEX9
K	-379	PRO	-	expression tag	UNP P0AEX9
K	-378	ARG	-	expression tag	UNP P0AEX9
K	-377	GLY	-	expression tag	UNP P0AEX9
K	-376	SER	-	expression tag	UNP P0AEX9
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K	-6	SER	-	linker	UNP P0AEX9
K	-5	GLY	-	linker	UNP P0AEX9
K	-4	SER	-	linker	UNP P0AEX9
K	-3	SER	-	linker	UNP P0AEX9
K	-2	GLY	-	linker	UNP P0AEX9
K	-1	SER	-	linker	UNP P0AEX9
K	0	SER	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1	GLY	-	linker	UNP P0AEX9
L	-394	MET	-	initiating methionine	UNP P0AEX9
L	-393	GLY	-	expression tag	UNP P0AEX9
L	-392	SER	-	expression tag	UNP P0AEX9
L	-391	SER	-	expression tag	UNP P0AEX9
L	-390	HIS	-	expression tag	UNP P0AEX9
L	-389	HIS	-	expression tag	UNP P0AEX9
L	-388	HIS	-	expression tag	UNP P0AEX9
L	-387	HIS	-	expression tag	UNP P0AEX9
L	-386	HIS	-	expression tag	UNP P0AEX9
L	-385	HIS	-	expression tag	UNP P0AEX9
L	-384	SER	-	expression tag	UNP P0AEX9
L	-383	SER	-	expression tag	UNP P0AEX9
L	-382	GLY	-	expression tag	UNP P0AEX9
L	-381	LEU	-	expression tag	UNP P0AEX9
L	-380	VAL	-	expression tag	UNP P0AEX9
L	-379	PRO	-	expression tag	UNP P0AEX9
L	-378	ARG	-	expression tag	UNP P0AEX9
L	-377	GLY	-	expression tag	UNP P0AEX9
L	-376	SER	-	expression tag	UNP P0AEX9
L	-375	HIS	-	expression tag	UNP P0AEX9
L	-374	MET	-	expression tag	UNP P0AEX9
L	-62	VAL	ALA	conflict	UNP P0AEX9
L	-7	ASN	-	linker	UNP P0AEX9
L	-6	SER	-	linker	UNP P0AEX9
L	-5	GLY	-	linker	UNP P0AEX9
L	-4	SER	-	linker	UNP P0AEX9
L	-3	SER	-	linker	UNP P0AEX9
L	-2	GLY	-	linker	UNP P0AEX9
L	-1	SER	-	linker	UNP P0AEX9
L	0	SER	-	linker	UNP P0AEX9
L	1	GLY	-	linker	UNP P0AEX9
N	-394	MET	-	initiating methionine	UNP P0AEX9
N	-393	GLY	-	expression tag	UNP P0AEX9
N	-392	SER	-	expression tag	UNP P0AEX9
N	-391	SER	-	expression tag	UNP P0AEX9
N	-390	HIS	-	expression tag	UNP P0AEX9
N	-389	HIS	-	expression tag	UNP P0AEX9
N	-388	HIS	-	expression tag	UNP P0AEX9
N	-387	HIS	-	expression tag	UNP P0AEX9
N	-386	HIS	-	expression tag	UNP P0AEX9
N	-385	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-384	SER	-	expression tag	UNP P0AEX9
N	-383	SER	-	expression tag	UNP P0AEX9
N	-382	GLY	-	expression tag	UNP P0AEX9
N	-381	LEU	-	expression tag	UNP P0AEX9
N	-380	VAL	-	expression tag	UNP P0AEX9
N	-379	PRO	-	expression tag	UNP P0AEX9
N	-378	ARG	-	expression tag	UNP P0AEX9
N	-377	GLY	-	expression tag	UNP P0AEX9
N	-376	SER	-	expression tag	UNP P0AEX9
N	-375	HIS	-	expression tag	UNP P0AEX9
N	-374	MET	-	expression tag	UNP P0AEX9
N	-62	VAL	ALA	conflict	UNP P0AEX9
N	-7	ASN	-	linker	UNP P0AEX9
N	-6	SER	-	linker	UNP P0AEX9
N	-5	GLY	-	linker	UNP P0AEX9
N	-4	SER	-	linker	UNP P0AEX9
N	-3	SER	-	linker	UNP P0AEX9
N	-2	GLY	-	linker	UNP P0AEX9
N	-1	SER	-	linker	UNP P0AEX9
N	0	SER	-	linker	UNP P0AEX9
N	1	GLY	-	linker	UNP P0AEX9
O	-394	MET	-	initiating methionine	UNP P0AEX9
O	-393	GLY	-	expression tag	UNP P0AEX9
O	-392	SER	-	expression tag	UNP P0AEX9
O	-391	SER	-	expression tag	UNP P0AEX9
O	-390	HIS	-	expression tag	UNP P0AEX9
O	-389	HIS	-	expression tag	UNP P0AEX9
O	-388	HIS	-	expression tag	UNP P0AEX9
O	-387	HIS	-	expression tag	UNP P0AEX9
O	-386	HIS	-	expression tag	UNP P0AEX9
O	-385	HIS	-	expression tag	UNP P0AEX9
O	-384	SER	-	expression tag	UNP P0AEX9
O	-383	SER	-	expression tag	UNP P0AEX9
O	-382	GLY	-	expression tag	UNP P0AEX9
O	-381	LEU	-	expression tag	UNP P0AEX9
O	-380	VAL	-	expression tag	UNP P0AEX9
O	-379	PRO	-	expression tag	UNP P0AEX9
O	-378	ARG	-	expression tag	UNP P0AEX9
O	-377	GLY	-	expression tag	UNP P0AEX9
O	-376	SER	-	expression tag	UNP P0AEX9
O	-375	HIS	-	expression tag	UNP P0AEX9
O	-374	MET	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-62	VAL	ALA	conflict	UNP P0AEX9
O	-7	ASN	-	linker	UNP P0AEX9
O	-6	SER	-	linker	UNP P0AEX9
O	-5	GLY	-	linker	UNP P0AEX9
O	-4	SER	-	linker	UNP P0AEX9
O	-3	SER	-	linker	UNP P0AEX9
O	-2	GLY	-	linker	UNP P0AEX9
O	-1	SER	-	linker	UNP P0AEX9
O	0	SER	-	linker	UNP P0AEX9
O	1	GLY	-	linker	UNP P0AEX9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	A	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	B	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	D	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		
2	E	371	Total	C	N	O	S	0	0
			2899	1836	489	553	21		

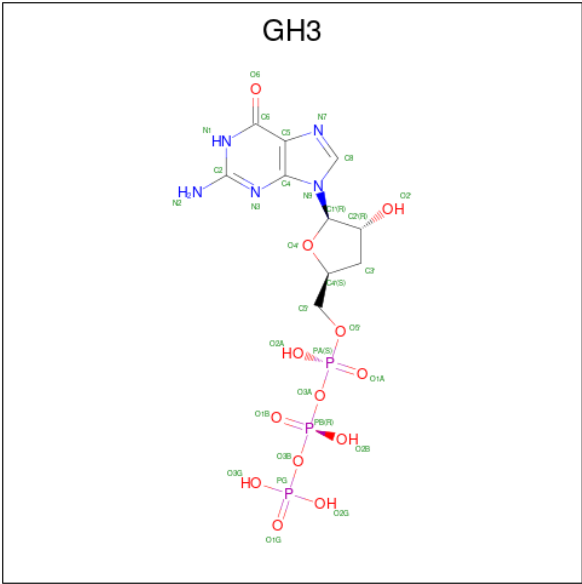
- Molecule 3 is a protein called Phalloidin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	F	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	G	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	I	7	Total	C	N	O	S	0	0
			55	35	8	11	1		
3	J	7	Total	C	N	O	S	0	0
			55	35	8	11	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	M	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	L	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	N	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	O	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	

- Molecule 5 is 3'-DEOXY-GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GH3) (formula: C₁₀H₁₆N₅O₁₃P₃).



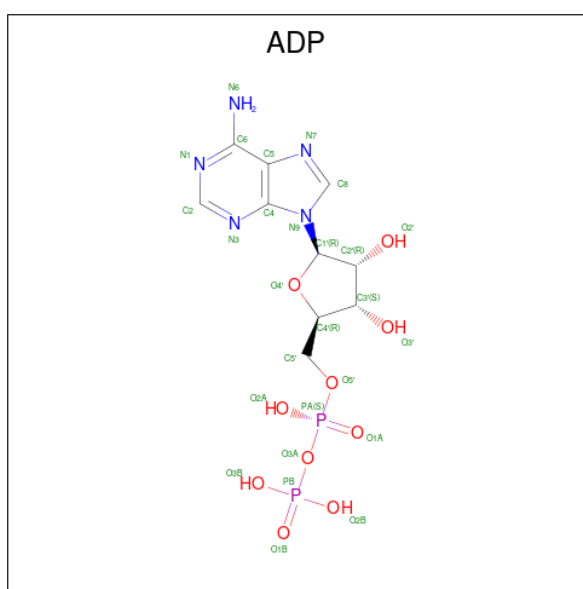
Mol	Chain	Residues	Atoms					AltConf
5	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

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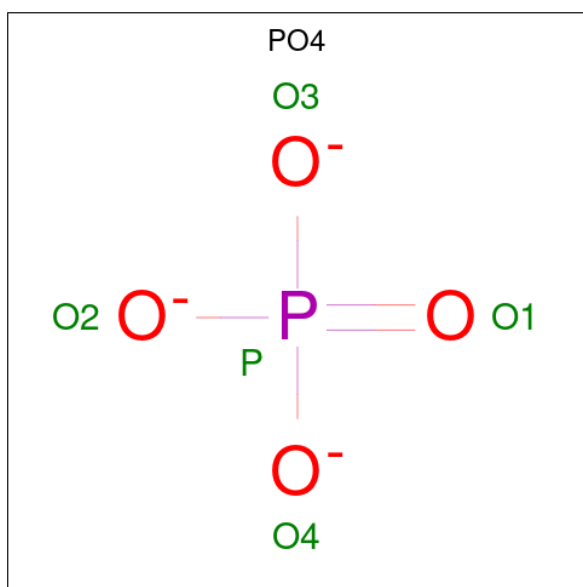
Mol	Chain	Residues	Atoms					AltConf
5	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	N	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
6	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

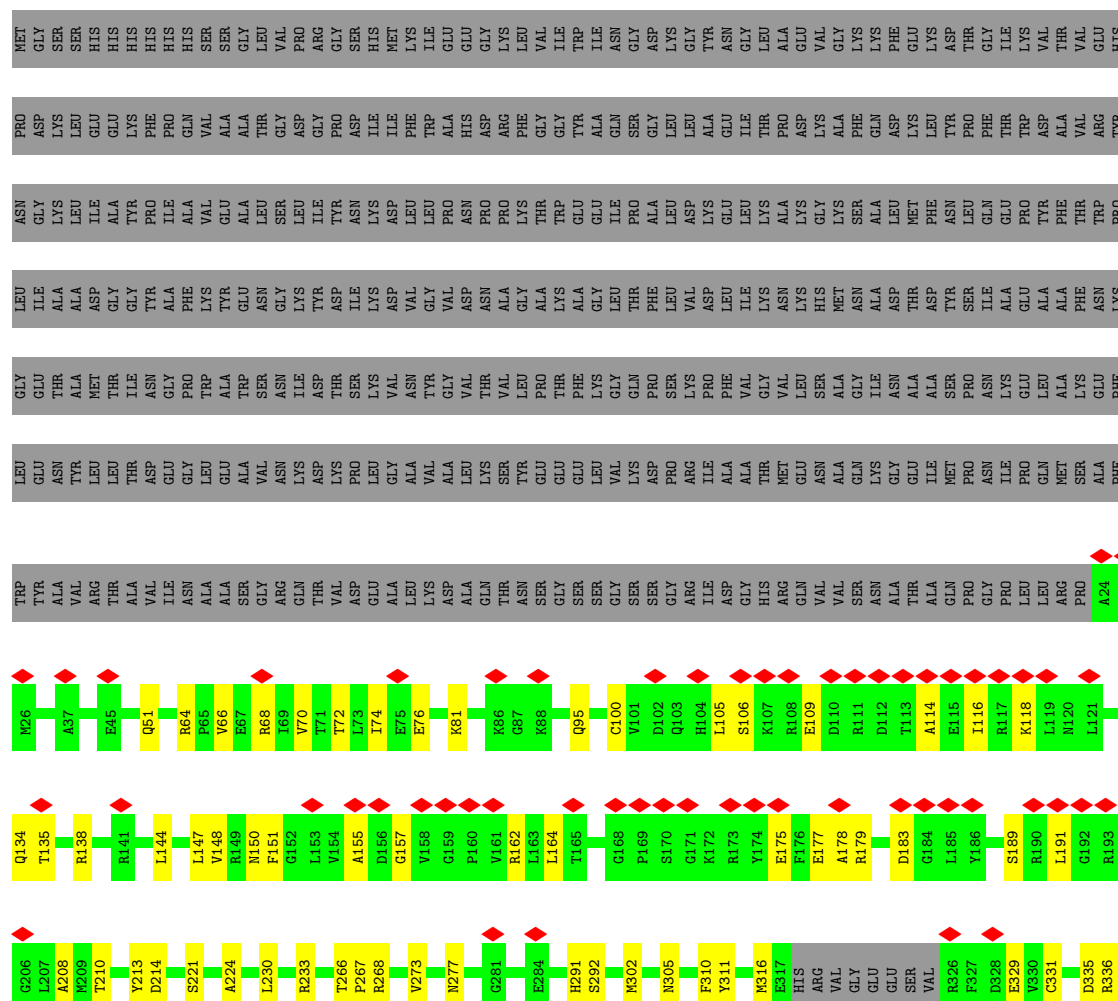
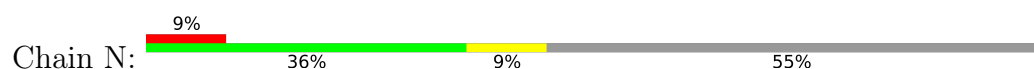
- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	O	P	0
			5	4	1	
7	A	1	Total	O	P	0
			5	4	1	
7	B	1	Total	O	P	0
			5	4	1	
7	D	1	Total	O	P	0
			5	4	1	
7	E	1	Total	O	P	0
			5	4	1	



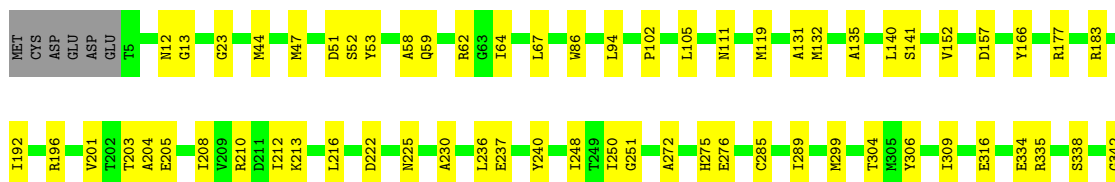
- Molecule 1: Maltose/maltodextrin-binding periplasmic protein, Adenylate cyclase ExoY





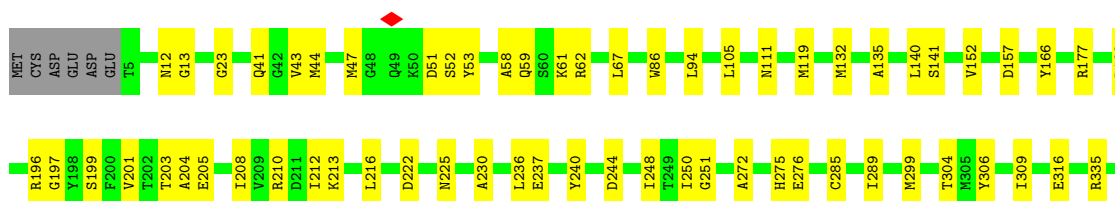
- Molecule 2: Actin, alpha skeletal muscle

Chain A: 81% 17%



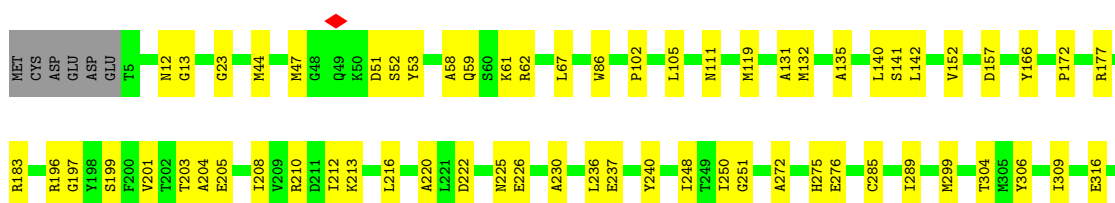
- Molecule 2: Actin, alpha skeletal muscle

Chain B: 81% 17%



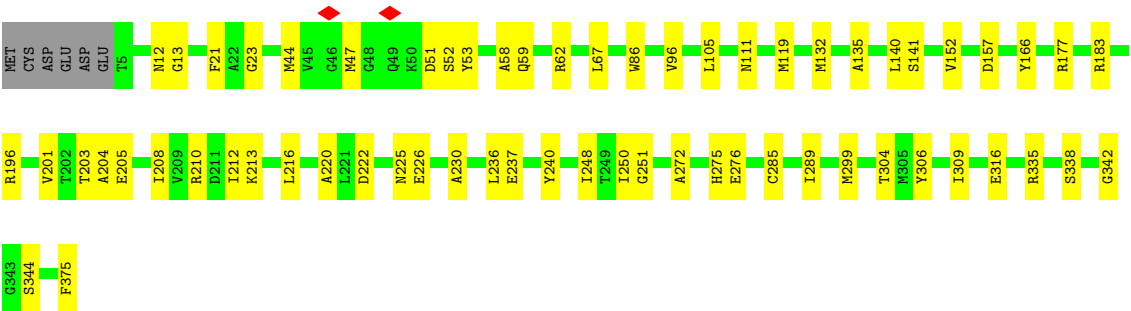
- Molecule 2: Actin, alpha skeletal muscle

Chain D: 80% 18%

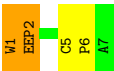


- Molecule 2: Actin, alpha skeletal muscle

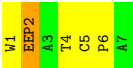
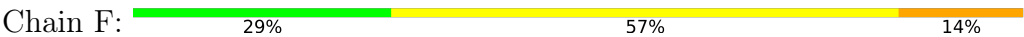
Chain E: 82% 17%



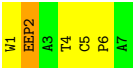
● Molecule 3: Phalloidin



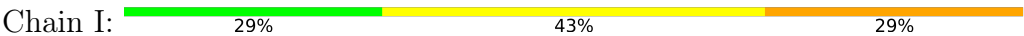
● Molecule 3: Phalloidin



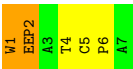
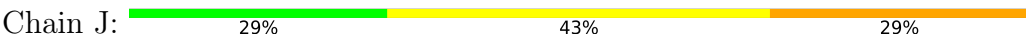
● Molecule 3: Phalloidin



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● Molecule 3: Phalloidin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1535755	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	93	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.263	Depositor
Minimum map value	-0.148	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.023	Depositor
Map size ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EEP, DTH, HYP, PO4, MG, ADP, GH3

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	K	0.56	0/2752	0.66	0/3717
1	L	0.56	0/2752	0.66	0/3717
1	M	0.56	0/2752	0.66	0/3717
1	N	0.56	0/2752	0.66	0/3717
1	O	0.56	0/2752	0.66	0/3717
2	A	0.94	0/2962	0.77	0/4012
2	B	0.94	0/2962	0.77	0/4012
2	C	0.94	0/2962	0.77	0/4012
2	D	0.94	0/2962	0.77	0/4012
2	E	0.94	0/2962	0.77	0/4012
3	F	2.26	0/28	2.58	3/33 (9.1%)
3	G	2.26	0/28	2.56	3/33 (9.1%)
3	H	2.25	0/28	2.57	3/33 (9.1%)
3	I	2.25	0/28	2.57	3/33 (9.1%)
3	J	2.25	0/28	2.56	3/33 (9.1%)
All	All	0.80	0/28710	0.74	15/38810 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	TRP	CB-CA-C	-5.97	98.76	110.10
3	H	1	TRP	CB-CA-C	-5.96	98.78	110.10
3	F	1	TRP	CB-CA-C	-5.96	98.79	110.10
3	J	1	TRP	CB-CA-C	-5.95	98.80	110.10
3	G	1	TRP	CB-CA-C	-5.94	98.81	110.10
3	F	1	TRP	CD2-CE2-CZ2	-5.75	116.65	122.40
3	J	1	TRP	CD2-CE2-CZ2	-5.68	116.72	122.40
3	H	1	TRP	CD2-CE2-CZ2	-5.67	116.72	122.40
3	G	1	TRP	CD2-CE2-CZ2	-5.66	116.74	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1	TRP	CD2-CE2-CZ2	-5.66	116.74	122.40
3	F	1	TRP	N-CA-CB	-5.29	101.51	110.50
3	H	1	TRP	N-CA-CB	-5.28	101.53	110.50
3	I	1	TRP	N-CA-CB	-5.27	101.54	110.50
3	G	1	TRP	N-CA-CB	-5.26	101.56	110.50
3	J	1	TRP	N-CA-CB	-5.25	101.57	110.50

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	K	2697	0	2634	50	0
1	L	2697	0	2634	48	0
1	M	2697	0	2634	51	0
1	N	2697	0	2634	46	0
1	O	2697	0	2634	52	0
2	A	2899	0	2871	48	0
2	B	2899	0	2871	52	0
2	C	2899	0	2871	53	0
2	D	2899	0	2871	54	0
2	E	2899	0	2871	46	0
3	F	55	0	38	2	0
3	G	55	0	38	2	0
3	H	55	0	38	4	0
3	I	55	0	38	5	0
3	J	55	0	38	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	1	0	0	0	0
4	O	1	0	0	0	0
5	K	31	0	12	4	0
5	L	31	0	12	5	0
5	M	31	0	12	5	0
5	N	31	0	12	5	0
5	O	31	0	12	5	0
6	A	27	0	12	4	0
6	B	27	0	12	4	0
6	C	27	0	12	4	0
6	D	27	0	12	4	0
6	E	27	0	12	4	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
7	D	5	0	0	0	0
7	E	5	0	0	0	0
All	All	28580	0	27835	516	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 9.

All (516) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:402:GH3:O4'	5:K:402:GH3:C1'	1.69	1.32
5:L:402:GH3:O4'	5:L:402:GH3:C1'	1.69	1.25
5:N:402:GH3:O4'	5:N:402:GH3:C1'	1.69	1.24
5:O:402:GH3:O4'	5:O:402:GH3:C1'	1.69	1.20
5:M:402:GH3:O4'	5:M:402:GH3:C1'	1.69	1.20
2:B:43:VAL:HG11	2:D:375:PHE:HZ	1.42	0.85
2:D:197:GLY:O	3:J:1:TRP:HE3	1.60	0.83
2:B:59:GLN:OE1	2:B:210:ARG:NH2	2.12	0.83
2:C:59:GLN:OE1	2:C:210:ARG:NH2	2.12	0.83
2:E:59:GLN:OE1	2:E:210:ARG:NH2	2.12	0.83
2:D:59:GLN:OE1	2:D:210:ARG:NH2	2.12	0.82
2:A:59:GLN:OE1	2:A:210:ARG:NH2	2.12	0.82
1:K:292:SER:OG	5:K:402:GH3:N2	2.15	0.80
1:N:292:SER:OG	5:N:402:GH3:N2	2.15	0.80
1:O:292:SER:OG	5:O:402:GH3:N2	2.15	0.80
1:L:292:SER:OG	5:L:402:GH3:N2	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:292:SER:OG	5:M:402:GH3:N2	2.15	0.79
1:M:68:ARG:NH2	1:M:150:ASN:OD1	2.17	0.78
1:O:68:ARG:NH2	1:O:150:ASN:OD1	2.17	0.78
1:K:68:ARG:NH2	1:K:150:ASN:OD1	2.17	0.77
1:N:68:ARG:NH2	1:N:150:ASN:OD1	2.17	0.76
1:L:68:ARG:NH2	1:L:150:ASN:OD1	2.17	0.75
2:E:304:THR:O	2:E:335:ARG:NH1	2.23	0.72
2:A:304:THR:O	2:A:335:ARG:NH1	2.23	0.72
2:D:304:THR:O	2:D:335:ARG:NH1	2.23	0.72
2:B:304:THR:O	2:B:335:ARG:NH1	2.23	0.71
2:C:304:THR:O	2:C:335:ARG:NH1	2.23	0.71
2:B:43:VAL:HG11	2:D:375:PHE:CZ	2.25	0.70
2:C:47:MET:HE3	1:O:378:VAL:HB	1.74	0.69
1:L:346:ILE:HG23	1:L:351:TYR:HB2	1.76	0.68
1:M:378:VAL:HB	2:A:47:MET:HE3	1.74	0.68
1:N:346:ILE:HG23	1:N:351:TYR:HB2	1.76	0.68
1:K:346:ILE:HG23	1:K:351:TYR:HB2	1.76	0.67
1:M:346:ILE:HG23	1:M:351:TYR:HB2	1.76	0.67
3:H:1:TRP:HE3	2:B:197:GLY:O	1.78	0.66
1:O:346:ILE:HG23	1:O:351:TYR:HB2	1.76	0.66
1:L:105:LEU:O	1:L:109:GLU:N	2.28	0.65
1:M:336:ARG:NH2	1:M:359:TRP:O	2.30	0.65
1:K:336:ARG:NH2	1:K:359:TRP:O	2.30	0.65
1:N:105:LEU:O	1:N:109:GLU:N	2.28	0.65
1:O:336:ARG:NH2	1:O:359:TRP:O	2.30	0.65
1:L:336:ARG:NH2	1:L:359:TRP:O	2.30	0.65
2:A:285:CYS:HB3	2:A:289:ILE:HD11	1.80	0.64
2:B:285:CYS:HB3	2:B:289:ILE:HD11	1.80	0.64
2:D:197:GLY:O	3:J:1:TRP:CE3	2.46	0.64
1:N:336:ARG:NH2	1:N:359:TRP:O	2.30	0.64
2:C:285:CYS:HB3	2:C:289:ILE:HD11	1.80	0.64
1:O:105:LEU:O	1:O:109:GLU:N	2.28	0.64
2:D:285:CYS:HB3	2:D:289:ILE:HD11	1.80	0.64
1:M:105:LEU:O	1:M:109:GLU:N	2.28	0.63
1:M:144:LEU:HD21	1:M:164:LEU:HD21	1.81	0.63
3:I:2:EEP:N	3:I:2:EEP:O1	2.31	0.63
1:O:144:LEU:HD21	1:O:164:LEU:HD21	1.81	0.63
2:E:285:CYS:HB3	2:E:289:ILE:HD11	1.80	0.63
1:K:144:LEU:HD21	1:K:164:LEU:HD21	1.81	0.63
3:J:2:EEP:N	3:J:2:EEP:O1	2.30	0.63
2:D:111:ASN:HB3	2:D:177:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:ASN:HB3	2:B:177:ARG:NH1	2.15	0.62
3:G:2:EEP:N	3:G:2:EEP:O1	2.31	0.62
1:K:105:LEU:O	1:K:109:GLU:N	2.28	0.62
2:D:59:GLN:O	2:D:62:ARG:HB2	2.00	0.62
2:E:59:GLN:O	2:E:62:ARG:HB2	2.00	0.62
2:A:157:ASP:OD2	2:A:183:ARG:NH2	2.30	0.62
2:B:157:ASP:OD2	2:B:183:ARG:NH2	2.30	0.62
1:N:144:LEU:HD21	1:N:164:LEU:HD21	1.81	0.62
2:A:111:ASN:HB3	2:A:177:ARG:NH1	2.15	0.62
2:B:59:GLN:O	2:B:62:ARG:HB2	2.00	0.62
2:E:111:ASN:HB3	2:E:177:ARG:NH1	2.15	0.62
2:C:59:GLN:O	2:C:62:ARG:HB2	1.99	0.61
2:C:157:ASP:OD2	2:C:183:ARG:NH2	2.30	0.61
3:H:2:EEP:N	3:H:2:EEP:O1	2.30	0.61
1:L:144:LEU:HD21	1:L:164:LEU:HD21	1.81	0.61
2:A:59:GLN:O	2:A:62:ARG:HB2	1.99	0.61
2:C:111:ASN:HB3	2:C:177:ARG:NH1	2.15	0.61
1:O:138:ARG:NH2	1:O:183:ASP:OD2	2.26	0.61
1:O:302:MET:HG2	1:O:336:ARG:HE	1.67	0.60
1:N:302:MET:HG2	1:N:336:ARG:HE	1.67	0.60
1:L:302:MET:HG2	1:L:336:ARG:HE	1.67	0.60
2:D:111:ASN:HB3	2:D:177:ARG:HH12	1.67	0.60
2:A:213:LYS:NZ	6:A:402:ADP:O2'	2.35	0.60
1:M:302:MET:HG2	1:M:336:ARG:HE	1.67	0.59
2:C:213:LYS:NZ	6:C:402:ADP:O2'	2.35	0.59
2:B:213:LYS:NZ	6:B:402:ADP:O2'	2.35	0.59
1:M:138:ARG:NH2	1:M:183:ASP:OD2	2.26	0.59
2:B:111:ASN:HB3	2:B:177:ARG:HH12	1.67	0.59
1:N:138:ARG:NH2	1:N:183:ASP:OD2	2.26	0.59
2:A:111:ASN:HB3	2:A:177:ARG:HH12	1.67	0.59
3:F:2:EEP:N	3:F:2:EEP:O1	2.30	0.59
1:K:302:MET:HG2	1:K:336:ARG:HE	1.67	0.58
2:C:111:ASN:HB3	2:C:177:ARG:HH12	1.67	0.58
1:L:138:ARG:NH2	1:L:183:ASP:OD2	2.26	0.58
2:E:213:LYS:NZ	6:E:402:ADP:O2'	2.35	0.58
2:E:201:VAL:N	2:E:205:GLU:OE2	2.33	0.57
2:C:201:VAL:N	2:C:205:GLU:OE2	2.34	0.57
2:D:213:LYS:NZ	6:D:402:ADP:O2'	2.35	0.57
2:A:201:VAL:N	2:A:205:GLU:OE2	2.34	0.57
2:E:111:ASN:HB3	2:E:177:ARG:HH12	1.67	0.57
2:A:222:ASP:OD2	2:A:225:ASN:ND2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:GLY:O	3:I:1:TRP:HE3	1.88	0.56
1:K:138:ARG:NH2	1:K:183:ASP:OD2	2.26	0.56
1:O:316:MET:N	1:O:329:GLU:OE1	2.38	0.56
2:E:157:ASP:OD2	2:E:183:ARG:NH2	2.30	0.56
2:B:201:VAL:N	2:B:205:GLU:OE2	2.33	0.56
1:M:316:MET:N	1:M:329:GLU:OE1	2.38	0.56
2:D:157:ASP:OD2	2:D:183:ARG:NH2	2.30	0.56
1:K:316:MET:N	1:K:329:GLU:OE1	2.38	0.56
1:N:316:MET:N	1:N:329:GLU:OE1	2.38	0.56
1:L:316:MET:N	1:L:329:GLU:OE1	2.38	0.55
2:B:222:ASP:OD2	2:B:225:ASN:ND2	2.34	0.55
1:M:135:THR:O	1:M:196:ALA:HB1	2.06	0.55
1:L:329:GLU:N	1:L:329:GLU:OE2	2.40	0.55
1:N:135:THR:O	1:N:196:ALA:HB1	2.06	0.55
1:N:329:GLU:OE2	1:N:329:GLU:N	2.40	0.55
1:O:329:GLU:N	1:O:329:GLU:OE2	2.40	0.55
1:O:177:GLU:OE1	1:O:179:ARG:NE	2.37	0.55
1:M:329:GLU:N	1:M:329:GLU:OE2	2.40	0.55
1:K:329:GLU:OE2	1:K:329:GLU:N	2.40	0.55
1:O:175:GLU:HB2	1:O:191:LEU:HD13	1.89	0.55
1:L:135:THR:O	1:L:196:ALA:HB1	2.06	0.54
2:B:141:SER:HB2	2:B:152:VAL:HG11	1.90	0.54
2:D:222:ASP:OD2	2:D:225:ASN:ND2	2.34	0.54
2:D:201:VAL:N	2:D:205:GLU:OE2	2.33	0.54
1:M:175:GLU:HB2	1:M:191:LEU:HD13	1.89	0.54
2:C:196:ARG:NH1	2:C:250:ILE:O	2.41	0.54
2:A:196:ARG:NH1	2:A:250:ILE:O	2.41	0.54
2:D:141:SER:HB2	2:D:152:VAL:HG11	1.90	0.54
1:O:64:ARG:NH2	1:O:305:ASN:OD1	2.38	0.54
1:K:135:THR:O	1:K:196:ALA:HB1	2.06	0.54
1:N:175:GLU:HB2	1:N:191:LEU:HD13	1.89	0.54
1:L:175:GLU:HB2	1:L:191:LEU:HD13	1.89	0.54
1:O:135:THR:O	1:O:196:ALA:HB1	2.06	0.54
2:B:196:ARG:NH1	2:B:250:ILE:O	2.41	0.54
2:D:196:ARG:NH1	2:D:250:ILE:O	2.41	0.54
2:E:222:ASP:OD2	2:E:225:ASN:ND2	2.34	0.54
1:L:177:GLU:OE1	1:L:179:ARG:NE	2.37	0.54
1:K:175:GLU:HB2	1:K:191:LEU:HD13	1.89	0.53
2:E:47:MET:N	2:E:47:MET:SD	2.80	0.53
2:E:196:ARG:NH1	2:E:250:ILE:O	2.41	0.53
1:O:335:ASP:OD2	1:O:337:LYS:NZ	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:SER:OG	1:N:116:ILE:O	2.24	0.53
2:C:141:SER:HB2	2:C:152:VAL:HG11	1.90	0.53
2:B:304:THR:HA	2:B:309:ILE:HD13	1.91	0.53
1:O:106:SER:OG	1:O:116:ILE:O	2.24	0.53
2:C:222:ASP:OD2	2:C:225:ASN:ND2	2.34	0.53
1:K:106:SER:OG	1:K:116:ILE:O	2.24	0.53
1:K:335:ASP:OD2	1:K:337:LYS:NZ	2.35	0.52
2:A:141:SER:HB2	2:A:152:VAL:HG11	1.90	0.52
2:E:141:SER:HB2	2:E:152:VAL:HG11	1.90	0.52
1:M:64:ARG:NH2	1:M:305:ASN:OD1	2.39	0.52
2:D:304:THR:HA	2:D:309:ILE:HD13	1.91	0.52
2:B:41:GLN:NE2	2:D:172:PRO:HG3	2.25	0.52
1:M:135:THR:HA	1:M:198:GLN:HG2	1.92	0.52
1:L:135:THR:HA	1:L:198:GLN:HG2	1.92	0.52
1:K:135:THR:HA	1:K:198:GLN:HG2	1.92	0.52
1:M:51:GLN:NE2	1:M:329:GLU:HB3	2.25	0.52
2:C:157:ASP:N	6:C:402:ADP:O3B	2.41	0.52
2:A:304:THR:HA	2:A:309:ILE:HD13	1.91	0.52
1:K:64:ARG:NH2	1:K:305:ASN:OD1	2.38	0.52
1:O:51:GLN:NE2	1:O:329:GLU:HB3	2.25	0.52
1:O:135:THR:HA	1:O:198:GLN:HG2	1.92	0.52
1:L:106:SER:OG	1:L:116:ILE:O	2.24	0.52
1:N:51:GLN:NE2	1:N:329:GLU:HB3	2.25	0.51
1:N:135:THR:HA	1:N:198:GLN:HG2	1.92	0.51
2:E:304:THR:HA	2:E:309:ILE:HD13	1.91	0.51
2:C:304:THR:HA	2:C:309:ILE:HD13	1.91	0.51
1:K:177:GLU:OE1	1:K:179:ARG:NE	2.38	0.51
1:M:106:SER:OG	1:M:116:ILE:O	2.24	0.51
2:E:216:LEU:HD22	2:E:250:ILE:HD12	1.93	0.51
1:K:51:GLN:NE2	1:K:329:GLU:HB3	2.25	0.51
1:L:51:GLN:NE2	1:L:329:GLU:HB3	2.25	0.51
1:L:316:MET:HE3	1:L:345:CYS:SG	2.51	0.51
1:O:316:MET:HE3	1:O:345:CYS:SG	2.51	0.51
2:A:216:LEU:HD22	2:A:250:ILE:HD12	1.93	0.51
2:D:157:ASP:N	6:D:402:ADP:O3B	2.41	0.51
2:E:140:LEU:O	2:E:342:GLY:HA3	2.11	0.51
2:C:216:LEU:HD22	2:C:250:ILE:HD12	1.93	0.51
2:B:140:LEU:O	2:B:342:GLY:HA3	2.10	0.50
2:C:140:LEU:O	2:C:342:GLY:HA3	2.11	0.50
2:A:140:LEU:O	2:A:342:GLY:HA3	2.10	0.50
1:N:335:ASP:OD2	1:N:337:LYS:NZ	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ILE:O	2:D:212:ILE:HG13	2.12	0.50
1:M:316:MET:HE3	1:M:345:CYS:SG	2.51	0.50
1:N:177:GLU:OE1	1:N:179:ARG:NE	2.38	0.50
1:N:316:MET:HE3	1:N:345:CYS:SG	2.51	0.50
1:K:316:MET:HE3	1:K:345:CYS:SG	2.51	0.50
2:A:208:ILE:O	2:A:212:ILE:HG13	2.12	0.50
1:L:64:ARG:NH2	1:L:305:ASN:OD1	2.39	0.50
1:L:310:PHE:HB2	1:L:331:CYS:SG	2.52	0.50
1:K:189:SER:OG	1:K:194:SER:HA	2.12	0.50
1:L:335:ASP:OD2	1:L:337:LYS:NZ	2.35	0.50
2:B:230:ALA:HB2	2:B:236:LEU:HD22	1.93	0.50
1:K:310:PHE:HB2	1:K:331:CYS:SG	2.52	0.50
2:A:86:TRP:HH2	2:A:119:MET:HG2	1.77	0.50
2:B:86:TRP:HH2	2:B:119:MET:HG2	1.77	0.50
2:E:208:ILE:O	2:E:212:ILE:HG13	2.12	0.50
1:L:189:SER:OG	1:L:194:SER:HA	2.12	0.50
2:D:140:LEU:O	2:D:342:GLY:HA3	2.11	0.50
2:D:216:LEU:HD22	2:D:250:ILE:HD12	1.93	0.50
2:D:237:GLU:HA	2:D:251:GLY:HA2	1.94	0.50
2:B:208:ILE:O	2:B:212:ILE:HG13	2.12	0.49
1:N:189:SER:OG	1:N:194:SER:HA	2.12	0.49
2:D:230:ALA:HB2	2:D:236:LEU:HD22	1.93	0.49
2:C:230:ALA:HB2	2:C:236:LEU:HD22	1.93	0.49
2:A:230:ALA:HB2	2:A:236:LEU:HD22	1.93	0.49
1:O:189:SER:OG	1:O:194:SER:HA	2.12	0.49
2:B:12:ASN:CG	2:B:86:TRP:HE1	2.21	0.49
2:B:216:LEU:HD22	2:B:250:ILE:HD12	1.93	0.49
2:C:237:GLU:HA	2:C:251:GLY:HA2	1.94	0.49
2:A:237:GLU:HA	2:A:251:GLY:HA2	1.94	0.49
2:E:237:GLU:HA	2:E:251:GLY:HA2	1.95	0.49
1:M:310:PHE:HB2	1:M:331:CYS:SG	2.52	0.49
2:C:208:ILE:O	2:C:212:ILE:HG13	2.12	0.49
1:N:310:PHE:HB2	1:N:331:CYS:SG	2.52	0.49
2:E:230:ALA:HB2	2:E:236:LEU:HD22	1.93	0.49
1:O:114:ALA:O	1:O:118:LYS:HB2	2.13	0.49
1:O:310:PHE:HB2	1:O:331:CYS:SG	2.52	0.49
1:K:157:GLY:HA3	1:K:162:ARG:HH11	1.78	0.49
2:E:86:TRP:HH2	2:E:119:MET:HG2	1.77	0.49
1:M:189:SER:OG	1:M:194:SER:HA	2.12	0.49
1:K:201:ALA:HA	1:K:208:ALA:HA	1.95	0.49
1:L:114:ALA:O	1:L:118:LYS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:114:ALA:O	1:M:118:LYS:HB2	2.13	0.49
1:N:114:ALA:O	1:N:118:LYS:HB2	2.13	0.49
1:O:157:GLY:HA3	1:O:162:ARG:HH11	1.78	0.49
2:D:12:ASN:CG	2:D:86:TRP:HE1	2.21	0.48
2:D:86:TRP:HH2	2:D:119:MET:HG2	1.77	0.48
5:K:402:GH3:H4'	5:K:402:GH3:O2A	2.13	0.48
2:B:157:ASP:N	6:B:402:ADP:O3B	2.41	0.48
2:B:237:GLU:HA	2:B:251:GLY:HA2	1.94	0.48
1:L:157:GLY:HA3	1:L:162:ARG:HH11	1.78	0.48
2:E:157:ASP:N	6:E:402:ADP:O3B	2.41	0.48
1:M:157:GLY:HA3	1:M:162:ARG:HH11	1.78	0.48
5:M:402:GH3:O2A	5:M:402:GH3:H4'	2.13	0.48
1:N:64:ARG:NH2	1:N:305:ASN:OD1	2.38	0.48
1:M:201:ALA:HA	1:M:208:ALA:HA	1.95	0.48
5:K:402:GH3:N3	5:K:402:GH3:H2'	2.29	0.48
2:C:12:ASN:CG	2:C:86:TRP:HE1	2.21	0.48
2:A:299:MET:HE1	2:A:309:ILE:HG23	1.95	0.48
1:N:72:THR:O	1:N:76:GLU:HG2	2.14	0.48
5:O:402:GH3:N3	5:O:402:GH3:H2'	2.28	0.48
5:O:402:GH3:O2A	5:O:402:GH3:H4'	2.13	0.48
2:A:12:ASN:CG	2:A:86:TRP:HE1	2.21	0.48
1:L:201:ALA:HA	1:L:208:ALA:HA	1.95	0.48
2:D:299:MET:HE1	2:D:309:ILE:HG23	1.96	0.48
2:E:12:ASN:CG	2:E:86:TRP:HE1	2.21	0.48
1:K:114:ALA:O	1:K:118:LYS:HB2	2.13	0.48
1:N:157:GLY:HA3	1:N:162:ARG:HH11	1.78	0.48
1:L:233:ARG:HA	1:L:266:THR:HG22	1.96	0.48
1:O:201:ALA:HA	1:O:208:ALA:HA	1.95	0.48
5:L:402:GH3:H2'	5:L:402:GH3:N3	2.29	0.48
1:N:233:ARG:HA	1:N:266:THR:HG22	1.96	0.48
2:C:86:TRP:HH2	2:C:119:MET:HG2	1.77	0.47
2:E:53:TYR:HB2	2:E:58:ALA:HB2	1.96	0.47
2:C:299:MET:HE1	2:C:309:ILE:HG23	1.96	0.47
5:L:402:GH3:O2A	5:L:402:GH3:H4'	2.13	0.47
2:B:299:MET:HE1	2:B:309:ILE:HG23	1.96	0.47
1:N:201:ALA:HA	1:N:208:ALA:HA	1.95	0.47
5:N:402:GH3:H4'	5:N:402:GH3:O2A	2.13	0.47
1:O:72:THR:O	1:O:76:GLU:HG2	2.14	0.47
1:O:233:ARG:HA	1:O:266:THR:HG22	1.96	0.47
2:E:166:TYR:CD1	2:E:289:ILE:HB	2.49	0.47
1:M:72:THR:O	1:M:76:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:166:TYR:CD1	2:C:289:ILE:HB	2.49	0.47
2:A:157:ASP:N	6:A:402:ADP:O3B	2.41	0.47
1:L:72:THR:O	1:L:76:GLU:HG2	2.14	0.47
2:C:53:TYR:HB2	2:C:58:ALA:HB2	1.96	0.47
2:E:299:MET:HE1	2:E:309:ILE:HG23	1.96	0.47
2:E:51:ASP:OD1	2:E:52:SER:N	2.48	0.47
1:M:177:GLU:OE1	1:M:179:ARG:NE	2.37	0.47
2:A:53:TYR:HB2	2:A:58:ALA:HB2	1.96	0.47
2:A:166:TYR:CD1	2:A:289:ILE:HB	2.49	0.47
2:B:306:TYR:CE1	6:B:402:ADP:H2	2.33	0.47
1:M:233:ARG:HA	1:M:266:THR:HG22	1.96	0.47
5:M:402:GH3:H2'	5:M:402:GH3:N3	2.28	0.47
1:K:72:THR:O	1:K:76:GLU:HG2	2.14	0.47
2:D:51:ASP:OD1	2:D:52:SER:N	2.48	0.47
1:K:81:LYS:N	1:K:210:THR:O	2.48	0.47
1:K:233:ARG:HA	1:K:266:THR:HG22	1.96	0.46
2:B:51:ASP:OD1	2:B:52:SER:N	2.48	0.46
1:O:147:LEU:HA	1:O:151:PHE:HD1	1.80	0.46
2:A:51:ASP:OD1	2:A:52:SER:N	2.48	0.46
2:D:53:TYR:HB2	2:D:58:ALA:HB2	1.96	0.46
2:D:199:SER:HB2	3:J:1:TRP:CE2	2.50	0.46
1:K:147:LEU:HA	1:K:151:PHE:HD1	1.80	0.46
5:N:402:GH3:H2'	5:N:402:GH3:N3	2.29	0.46
2:C:306:TYR:CE1	6:C:402:ADP:H2	2.33	0.46
2:A:306:TYR:CE1	6:A:402:ADP:H2	2.33	0.46
2:B:166:TYR:CD1	2:B:289:ILE:HB	2.49	0.46
2:D:166:TYR:CD1	2:D:289:ILE:HB	2.49	0.46
2:D:306:TYR:CE1	6:D:402:ADP:H2	2.33	0.46
2:E:306:TYR:CE1	6:E:402:ADP:H2	2.33	0.46
2:A:275:HIS:CD2	2:A:316:GLU:HB3	2.50	0.46
1:L:51:GLN:HE22	1:L:329:GLU:HB3	1.81	0.46
1:O:81:LYS:N	1:O:210:THR:O	2.48	0.46
1:M:147:LEU:HA	1:M:151:PHE:HD1	1.80	0.46
2:C:51:ASP:OD1	2:C:52:SER:N	2.48	0.46
2:B:53:TYR:HB2	2:B:58:ALA:HB2	1.96	0.46
1:N:147:LEU:HA	1:N:151:PHE:HD1	1.80	0.46
2:D:275:HIS:CD2	2:D:316:GLU:HB3	2.50	0.46
2:E:132:MET:HE2	2:E:132:MET:HB2	1.78	0.46
2:D:203:THR:O	2:D:204:ALA:HB3	2.16	0.45
1:L:157:GLY:HA3	1:L:162:ARG:NH1	2.31	0.45
1:M:81:LYS:N	1:M:210:THR:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:275:HIS:CD2	2:C:316:GLU:HB3	2.50	0.45
2:B:275:HIS:CD2	2:B:316:GLU:HB3	2.50	0.45
1:N:81:LYS:N	1:N:210:THR:O	2.48	0.45
2:E:203:THR:O	2:E:204:ALA:HB3	2.16	0.45
2:E:275:HIS:CD2	2:E:316:GLU:HB3	2.50	0.45
1:M:81:LYS:NZ	5:M:402:GH3:O2A	2.41	0.45
1:N:230:LEU:HA	1:N:267:PRO:HB2	1.98	0.45
2:C:47:MET:N	2:C:47:MET:SD	2.81	0.45
1:L:81:LYS:N	1:L:210:THR:O	2.48	0.45
2:B:203:THR:O	2:B:204:ALA:HB3	2.16	0.45
1:M:51:GLN:HE22	1:M:329:GLU:HB3	1.81	0.45
1:O:51:GLN:HE22	1:O:329:GLU:HB3	1.81	0.45
1:K:157:GLY:HA3	1:K:162:ARG:NH1	2.32	0.45
1:L:147:LEU:HA	1:L:151:PHE:HD1	1.80	0.45
2:C:203:THR:O	2:C:204:ALA:HB3	2.16	0.45
1:M:157:GLY:HA3	1:M:162:ARG:NH1	2.32	0.45
2:C:105:LEU:HD12	2:C:132:MET:HE1	1.99	0.45
1:K:51:GLN:HE22	1:K:329:GLU:HB3	1.81	0.45
1:O:70:VAL:HG12	1:O:74:ILE:HG13	1.99	0.45
2:B:272:ALA:HB1	2:B:276:GLU:HB2	1.99	0.44
2:D:105:LEU:HD12	2:D:132:MET:HE1	1.99	0.44
2:A:105:LEU:HD12	2:A:132:MET:HE1	1.99	0.44
2:A:203:THR:O	2:A:204:ALA:HB3	2.16	0.44
1:N:162:ARG:O	1:N:178:ALA:HB3	2.17	0.44
1:M:230:LEU:HA	1:M:267:PRO:HB2	1.99	0.44
2:C:143:TYR:OH	2:A:44:MET:HA	2.16	0.44
1:L:162:ARG:O	1:L:178:ALA:HB3	2.17	0.44
1:N:51:GLN:HE22	1:N:329:GLU:HB3	1.81	0.44
1:N:70:VAL:HG12	1:N:74:ILE:HG13	1.99	0.44
1:N:157:GLY:HA3	1:N:162:ARG:NH1	2.31	0.44
2:A:94:LEU:HD23	2:A:94:LEU:HA	1.78	0.44
1:L:230:LEU:HA	1:L:267:PRO:HB2	1.99	0.44
2:B:105:LEU:HD12	2:B:132:MET:HE1	1.99	0.44
1:K:162:ARG:O	1:K:178:ALA:HB3	2.17	0.44
2:D:47:MET:SD	2:D:47:MET:N	2.81	0.44
1:O:134:GLN:O	1:O:198:GLN:HA	2.18	0.44
2:E:105:LEU:HD12	2:E:132:MET:HE1	1.99	0.44
1:M:70:VAL:HG12	1:M:74:ILE:HG13	1.99	0.44
1:K:230:LEU:HA	1:K:267:PRO:HB2	1.98	0.44
2:D:216:LEU:CD2	2:D:250:ILE:HD12	2.48	0.44
2:D:272:ALA:HB1	2:D:276:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:272:ALA:HB1	2:A:276:GLU:HB2	1.99	0.44
2:B:47:MET:SD	2:B:47:MET:N	2.81	0.44
1:O:162:ARG:O	1:O:178:ALA:HB3	2.17	0.44
1:L:70:VAL:HG12	1:L:74:ILE:HG13	2.00	0.44
2:B:216:LEU:CD2	2:B:250:ILE:HD12	2.48	0.44
1:O:157:GLY:HA3	1:O:162:ARG:NH1	2.31	0.44
1:K:70:VAL:HG12	1:K:74:ILE:HG13	2.00	0.44
3:I:4:DTH:H	3:I:4:DTH:HG23	1.48	0.44
2:A:62:ARG:HG3	2:A:67:LEU:HD11	2.00	0.43
2:B:61:LYS:HE2	2:B:61:LYS:HB2	1.78	0.43
2:D:135:ALA:HB3	2:D:140:LEU:HD11	2.00	0.43
1:M:221:SER:O	1:M:224:ALA:N	2.50	0.43
2:B:62:ARG:HG3	2:B:67:LEU:HD11	2.00	0.43
2:D:62:ARG:HG3	2:D:67:LEU:HD11	2.00	0.43
2:E:216:LEU:CD2	2:E:250:ILE:HD12	2.48	0.43
1:M:162:ARG:O	1:M:178:ALA:HB3	2.17	0.43
1:M:311:TYR:CD1	1:M:311:TYR:N	2.87	0.43
2:C:23:GLY:N	2:C:344:SER:OG	2.51	0.43
1:L:221:SER:O	1:L:224:ALA:N	2.50	0.43
1:L:311:TYR:CD1	1:L:311:TYR:N	2.87	0.43
2:B:244:ASP:O	2:D:322:PRO:HG3	2.18	0.43
1:K:311:TYR:N	1:K:311:TYR:CD1	2.86	0.43
2:B:135:ALA:HB3	2:B:140:LEU:HD11	2.01	0.43
1:N:346:ILE:CG2	1:N:351:TYR:HB2	2.46	0.43
1:M:134:GLN:O	1:M:198:GLN:HA	2.18	0.43
2:C:216:LEU:CD2	2:C:250:ILE:HD12	2.48	0.43
1:O:214:ASP:OD2	1:O:291:HIS:HE1	2.02	0.43
1:O:230:LEU:HA	1:O:267:PRO:HB2	1.98	0.43
1:N:134:GLN:O	1:N:198:GLN:HA	2.18	0.43
1:N:311:TYR:CD1	1:N:311:TYR:N	2.86	0.43
2:D:142:LEU:HD23	2:D:142:LEU:HA	1.81	0.43
1:O:135:THR:HA	1:O:198:GLN:HA	2.01	0.43
2:E:23:GLY:N	2:E:344:SER:OG	2.51	0.43
2:E:135:ALA:HB3	2:E:140:LEU:HD11	2.00	0.43
1:M:214:ASP:OD2	1:M:291:HIS:HE1	2.02	0.43
1:M:280:LEU:HD23	1:M:280:LEU:HA	1.85	0.43
2:A:64:ILE:HD13	2:A:64:ILE:HA	1.79	0.43
2:C:62:ARG:HG3	2:C:67:LEU:HD11	2.00	0.43
3:H:1:TRP:CE3	2:B:197:GLY:O	2.64	0.43
1:L:135:THR:HA	1:L:198:GLN:HA	2.01	0.43
2:B:248:ILE:HD13	2:B:248:ILE:HG21	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:240:TYR:O	2:E:248:ILE:HG22	2.19	0.43
2:E:272:ALA:HB1	2:E:276:GLU:HB2	2.00	0.43
3:J:4:DTH:H	3:J:4:DTH:HG23	1.48	0.43
2:C:272:ALA:HB1	2:C:276:GLU:HB2	2.00	0.43
2:B:23:GLY:N	2:B:344:SER:OG	2.51	0.43
2:D:240:TYR:O	2:D:248:ILE:HG22	2.19	0.43
1:K:134:GLN:O	1:K:198:GLN:HA	2.18	0.43
1:K:214:ASP:OD2	1:K:291:HIS:HE1	2.02	0.43
2:A:216:LEU:CD2	2:A:250:ILE:HD12	2.48	0.43
1:O:346:ILE:CG2	1:O:351:TYR:HB2	2.46	0.43
1:M:135:THR:HA	1:M:198:GLN:HA	2.01	0.42
2:C:135:ALA:HB3	2:C:140:LEU:HD11	2.01	0.42
2:C:197:GLY:O	3:I:1:TRP:CE3	2.70	0.42
2:B:240:TYR:O	2:B:248:ILE:HG22	2.19	0.42
1:N:132:TYR:CG	1:N:133:THR:N	2.87	0.42
1:N:135:THR:HA	1:N:198:GLN:HA	2.01	0.42
2:A:240:TYR:O	2:A:248:ILE:HG22	2.19	0.42
2:C:240:TYR:O	2:C:248:ILE:HG22	2.19	0.42
1:L:134:GLN:O	1:L:198:GLN:HA	2.18	0.42
1:O:230:LEU:HB3	1:O:268:ARG:HB2	2.01	0.42
2:E:13:GLY:HA3	6:E:402:ADP:O2B	2.19	0.42
2:C:248:ILE:HD13	2:C:248:ILE:HG21	1.73	0.42
1:K:230:LEU:HB3	1:K:268:ARG:HB2	2.01	0.42
1:N:214:ASP:OD2	1:N:291:HIS:HE1	2.01	0.42
1:O:81:LYS:NZ	5:O:402:GH3:O2A	2.41	0.42
1:L:132:TYR:CG	1:L:133:THR:N	2.88	0.42
1:L:214:ASP:OD2	1:L:291:HIS:HE1	2.01	0.42
1:N:148:VAL:HG21	1:N:155:ALA:HB2	2.02	0.42
2:D:61:LYS:HE2	2:D:61:LYS:HB2	1.78	0.42
2:E:62:ARG:HG3	2:E:67:LEU:HD11	2.00	0.42
1:M:335:ASP:OD2	1:M:337:LYS:NZ	2.35	0.42
2:D:44:MET:HB3	2:D:47:MET:HE1	2.02	0.42
2:A:135:ALA:HB3	2:A:140:LEU:HD11	2.00	0.42
2:B:12:ASN:ND2	2:B:86:TRP:HE1	2.18	0.42
1:M:230:LEU:HB3	1:M:268:ARG:HB2	2.01	0.42
1:L:81:LYS:NZ	5:L:402:GH3:O2A	2.41	0.42
2:D:23:GLY:N	2:D:344:SER:OG	2.51	0.42
2:D:199:SER:HB2	3:J:1:TRP:CD2	2.55	0.42
2:E:12:ASN:ND2	2:E:86:TRP:HE1	2.18	0.42
2:A:192:ILE:HD12	2:A:192:ILE:HG23	1.90	0.42
1:L:346:ILE:CG2	1:L:351:TYR:HB2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:81:LYS:NZ	5:N:402:GH3:O2A	2.41	0.42
1:O:132:TYR:CG	1:O:133:THR:N	2.87	0.42
1:O:311:TYR:CD1	1:O:311:TYR:N	2.87	0.42
3:F:4:DTH:H	3:F:4:DTH:HG23	1.48	0.42
2:B:44:MET:HB3	2:B:47:MET:HE1	2.02	0.42
1:O:95:GLN:HG3	1:O:100:CYS:SG	2.60	0.42
1:K:135:THR:HA	1:K:198:GLN:HA	2.01	0.41
2:D:248:ILE:HD13	2:D:248:ILE:HG21	1.73	0.41
1:O:148:VAL:HG21	1:O:155:ALA:HB2	2.02	0.41
2:E:44:MET:HB3	2:E:47:MET:HE1	2.02	0.41
1:M:95:GLN:HG3	1:M:100:CYS:SG	2.60	0.41
1:M:132:TYR:CG	1:M:133:THR:N	2.87	0.41
2:E:248:ILE:HD13	2:E:248:ILE:HG21	1.73	0.41
1:M:148:VAL:HG21	1:M:155:ALA:HB2	2.02	0.41
1:M:346:ILE:CG2	1:M:351:TYR:HB2	2.46	0.41
2:C:12:ASN:ND2	2:C:86:TRP:HE1	2.18	0.41
3:H:1:TRP:CD2	2:B:199:SER:HB2	2.55	0.41
1:K:148:VAL:HG21	1:K:155:ALA:HB2	2.02	0.41
2:D:132:MET:HE2	2:D:132:MET:HB2	1.78	0.41
2:C:13:GLY:HA3	6:C:402:ADP:O2B	2.19	0.41
2:A:13:GLY:HA3	6:A:402:ADP:O2B	2.19	0.41
2:B:132:MET:HB2	2:B:132:MET:HE2	1.78	0.41
1:N:221:SER:O	1:N:224:ALA:N	2.50	0.41
1:N:273:VAL:O	1:N:277:ASN:ND2	2.50	0.41
2:E:220:ALA:HB1	2:E:226:GLU:HG3	2.03	0.41
2:C:335:ARG:HA	2:C:338:SER:OG	2.21	0.41
1:K:132:TYR:CG	1:K:133:THR:N	2.87	0.41
2:B:94:LEU:HA	2:B:94:LEU:HD23	1.78	0.41
1:O:273:VAL:O	1:O:277:ASN:ND2	2.50	0.41
1:M:329:GLU:N	1:M:329:GLU:CD	2.79	0.41
2:C:61:LYS:HB2	2:C:61:LYS:HE2	1.78	0.41
2:C:220:ALA:HB1	2:C:226:GLU:HG3	2.03	0.41
1:K:95:GLN:HG3	1:K:100:CYS:SG	2.60	0.41
1:K:329:GLU:N	1:K:329:GLU:CD	2.79	0.41
2:B:13:GLY:HA3	6:B:402:ADP:O2B	2.19	0.41
2:D:13:GLY:HA3	6:D:402:ADP:O2B	2.20	0.41
2:E:237:GLU:HA	2:E:251:GLY:CA	2.51	0.41
1:K:273:VAL:O	1:K:277:ASN:ND2	2.50	0.41
2:A:44:MET:HB3	2:A:47:MET:HE1	2.02	0.41
1:L:230:LEU:HB3	1:L:268:ARG:HB2	2.01	0.41
2:B:335:ARG:HA	2:B:338:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:66:VAL:HG21	1:N:213:TYR:CD2	2.56	0.41
2:D:12:ASN:ND2	2:D:86:TRP:HE1	2.18	0.41
2:C:43:VAL:HG11	2:E:375:PHE:HZ	1.86	0.41
2:C:44:MET:HB3	2:C:47:MET:HE1	2.02	0.41
2:C:53:TYR:CB	2:C:58:ALA:HB2	2.51	0.41
2:C:64:ILE:HA	2:C:64:ILE:HD13	1.79	0.41
2:C:237:GLU:HA	2:C:251:GLY:CA	2.51	0.41
2:A:47:MET:N	2:A:47:MET:SD	2.80	0.41
1:L:95:GLN:HG3	1:L:100:CYS:SG	2.60	0.41
1:L:329:GLU:N	1:L:329:GLU:CD	2.79	0.41
1:N:230:LEU:HB3	1:N:268:ARG:HB2	2.01	0.41
1:O:329:GLU:N	1:O:329:GLU:CD	2.79	0.41
2:C:132:MET:HE2	2:C:132:MET:HB2	1.78	0.41
3:I:1:TRP:CD1	3:I:1:TRP:H3	2.39	0.41
1:M:41:GLY:N	1:M:66:VAL:O	2.53	0.40
1:K:173:ARG:HH11	1:K:173:ARG:HD3	1.78	0.40
1:K:346:ILE:CG2	1:K:351:TYR:HB2	2.46	0.40
2:D:102:PRO:HA	2:D:131:ALA:O	2.22	0.40
1:O:221:SER:O	1:O:224:ALA:N	2.50	0.40
2:E:335:ARG:HA	2:E:338:SER:OG	2.21	0.40
1:M:66:VAL:HG21	1:M:213:TYR:CD2	2.56	0.40
2:A:23:GLY:N	2:A:344:SER:OG	2.51	0.40
1:L:66:VAL:HG21	1:L:213:TYR:CD2	2.56	0.40
2:B:53:TYR:CB	2:B:58:ALA:HB2	2.51	0.40
1:N:95:GLN:HG3	1:N:100:CYS:SG	2.60	0.40
1:M:99:ILE:HG21	1:M:200:LEU:HD12	2.04	0.40
1:K:63:ILE:HG22	1:K:64:ARG:O	2.22	0.40
1:K:66:VAL:HG21	1:K:213:TYR:CD2	2.56	0.40
1:K:364:ARG:NH2	2:A:334:GLU:OE2	2.54	0.40
2:A:12:ASN:ND2	2:A:86:TRP:HE1	2.18	0.40
2:A:237:GLU:HA	2:A:251:GLY:CA	2.51	0.40
1:L:148:VAL:HG21	1:L:155:ALA:HB2	2.02	0.40
3:G:4:DTH:H	3:G:4:DTH:HG23	1.48	0.40
2:D:335:ARG:HA	2:D:338:SER:OG	2.21	0.40
1:O:66:VAL:HG21	1:O:213:TYR:CD2	2.56	0.40
1:O:138:ARG:HB3	1:O:185:LEU:HD13	2.03	0.40
2:C:153:LEU:O	2:C:153:LEU:HG	2.22	0.40
1:K:99:ILE:HG21	1:K:200:LEU:HD12	2.04	0.40
2:A:102:PRO:HA	2:A:131:ALA:O	2.22	0.40
1:L:82:GLY:HA2	1:L:290:HIS:ND1	2.36	0.40
1:M:273:VAL:O	1:M:277:ASN:ND2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:82:GLY:HA2	1:K:290:HIS:ND1	2.36	0.40
2:A:335:ARG:HA	2:A:338:SER:OG	2.21	0.40
1:L:138:ARG:HB3	1:L:185:LEU:HD13	2.03	0.40
2:D:220:ALA:HB1	2:D:226:GLU:HG3	2.03	0.40
1:O:82:GLY:HA2	1:O:290:HIS:ND1	2.36	0.40
1:O:99:ILE:HG21	1:O:200:LEU:HD12	2.04	0.40
1:O:326:ARG:HG3	1:O:327:PHE:CD1	2.57	0.40
2:E:21:PHE:CE1	2:E:96:VAL:HG11	2.57	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	K	343/773 (44%)	325 (95%)	18 (5%)	0	100	100
1	L	343/773 (44%)	325 (95%)	18 (5%)	0	100	100
1	M	343/773 (44%)	325 (95%)	18 (5%)	0	100	100
1	N	343/773 (44%)	324 (94%)	19 (6%)	0	100	100
1	O	343/773 (44%)	324 (94%)	19 (6%)	0	100	100
2	A	369/377 (98%)	345 (94%)	24 (6%)	0	100	100
2	B	369/377 (98%)	344 (93%)	25 (7%)	0	100	100
2	C	369/377 (98%)	345 (94%)	24 (6%)	0	100	100
2	D	369/377 (98%)	344 (93%)	25 (7%)	0	100	100
2	E	369/377 (98%)	345 (94%)	24 (6%)	0	100	100
3	F	2/7 (29%)	2 (100%)	0	0	100	100
3	G	2/7 (29%)	2 (100%)	0	0	100	100
3	H	2/7 (29%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	2/7 (29%)	2 (100%)	0	0	100	100
3	J	2/7 (29%)	2 (100%)	0	0	100	100
All	All	3570/5785 (62%)	3356 (94%)	214 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	K	280/623 (45%)	280 (100%)	0	100	100
1	L	280/623 (45%)	280 (100%)	0	100	100
1	M	280/623 (45%)	280 (100%)	0	100	100
1	N	280/623 (45%)	280 (100%)	0	100	100
1	O	280/623 (45%)	280 (100%)	0	100	100
2	A	314/320 (98%)	314 (100%)	0	100	100
2	B	314/320 (98%)	314 (100%)	0	100	100
2	C	314/320 (98%)	314 (100%)	0	100	100
2	D	314/320 (98%)	314 (100%)	0	100	100
2	E	314/320 (98%)	314 (100%)	0	100	100
3	F	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	G	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	H	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	I	2/2 (100%)	1 (50%)	1 (50%)	0	0
3	J	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	2980/4725 (63%)	2975 (100%)	5 (0%)	85	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	5	CYS
3	F	5	CYS
3	G	5	CYS
3	I	5	CYS
3	J	5	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	73	HIS
2	C	92	ASN
2	C	121	GLN
2	C	246	GLN
2	A	121	GLN
2	A	246	GLN
2	B	41	GLN
2	B	92	ASN
2	B	246	GLN
2	D	92	ASN
2	D	121	GLN
2	D	246	GLN
2	E	73	HIS
2	E	121	GLN
2	E	246	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

15 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
3	HYP	F	6	3	7,8,9	1.31	0	5,10,12	1.41	1 (20%)
3	EEP	F	2	3	7,9,10	2.67	3 (42%)	3,12,14	1.24	0
3	EEP	I	2	3	7,9,10	2.67	3 (42%)	3,12,14	1.23	0
3	HYP	H	6	3	7,8,9	1.32	0	5,10,12	1.40	1 (20%)
3	HYP	G	6	3	7,8,9	1.32	0	5,10,12	1.40	1 (20%)
3	EEP	G	2	3	7,9,10	2.68	3 (42%)	3,12,14	1.23	0
3	HYP	J	6	3	7,8,9	1.33	0	5,10,12	1.40	1 (20%)
3	EEP	J	2	3	7,9,10	2.68	3 (42%)	3,12,14	1.23	0
3	EEP	H	2	3	7,9,10	2.67	3 (42%)	3,12,14	1.24	0
3	HYP	I	6	3	7,8,9	1.32	0	5,10,12	1.41	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HYP	F	6	3	-	0/0/11/13	0/1/1/1
3	EEP	F	2	3	-	3/9/10/12	-
3	EEP	I	2	3	-	3/9/10/12	-
3	HYP	H	6	3	-	0/0/11/13	0/1/1/1
3	HYP	G	6	3	-	0/0/11/13	0/1/1/1
3	EEP	G	2	3	-	3/9/10/12	-
3	HYP	J	6	3	-	0/0/11/13	0/1/1/1
3	EEP	J	2	3	-	3/9/10/12	-
3	EEP	H	2	3	-	3/9/10/12	-
3	HYP	I	6	3	-	0/0/11/13	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	EEP	CB-CA	-5.20	1.47	1.54
3	G	2	EEP	CB-CA	-5.17	1.47	1.54
3	F	2	EEP	CB-CA	-5.17	1.47	1.54
3	H	2	EEP	CB-CA	-5.16	1.47	1.54
3	I	2	EEP	CB-CA	-5.15	1.47	1.54
3	F	2	EEP	O1-CG	-3.04	1.40	1.44
3	H	2	EEP	O1-CG	-3.02	1.40	1.44
3	G	2	EEP	O1-CG	-3.01	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	2	EEP	O1-CG	-3.00	1.40	1.44
3	I	2	EEP	CD2-CG	-2.99	1.49	1.52
3	I	2	EEP	O1-CG	-2.99	1.40	1.44
3	G	2	EEP	CD2-CG	-2.98	1.49	1.52
3	J	2	EEP	CD2-CG	-2.97	1.49	1.52
3	H	2	EEP	CD2-CG	-2.95	1.49	1.52
3	F	2	EEP	CD2-CG	-2.92	1.49	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	6	HYP	O-C-CA	-2.62	118.02	124.77
3	F	6	HYP	O-C-CA	-2.62	118.04	124.77
3	I	6	HYP	O-C-CA	-2.62	118.04	124.77
3	G	6	HYP	O-C-CA	-2.61	118.06	124.77
3	H	6	HYP	O-C-CA	-2.61	118.06	124.77

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	2	EEP	O2-CD1-CG-CB
3	H	2	EEP	O2-CD1-CG-O1
3	H	2	EEP	O2-CD1-CG-CD2
3	F	2	EEP	O2-CD1-CG-CB
3	F	2	EEP	O2-CD1-CG-O1
3	F	2	EEP	O2-CD1-CG-CD2
3	G	2	EEP	O2-CD1-CG-CB
3	G	2	EEP	O2-CD1-CG-O1
3	G	2	EEP	O2-CD1-CG-CD2
3	I	2	EEP	O2-CD1-CG-CB
3	I	2	EEP	O2-CD1-CG-O1
3	I	2	EEP	O2-CD1-CG-CD2
3	J	2	EEP	O2-CD1-CG-CB
3	J	2	EEP	O2-CD1-CG-O1
3	J	2	EEP	O2-CD1-CG-CD2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	EEP	1	0
3	I	2	EEP	1	0
3	G	2	EEP	1	0
3	J	2	EEP	1	0
3	H	2	EEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 10 are monoatomic - leaving 15 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	$\# Z > 2$
6	ADP	B	402	4	28,29,29	1.56	5 (17%)	43,45,45	1.94	13 (30%)
7	PO4	E	403	4	4,4,4	1.18	0	6,6,6	0.86	0
5	GH3	M	402	-	31,33,33	5.81	20 (64%)	44,52,52	1.85	9 (20%)
5	GH3	K	402	-	31,33,33	5.81	20 (64%)	44,52,52	1.85	9 (20%)
5	GH3	O	402	-	31,33,33	5.81	20 (64%)	44,52,52	1.86	9 (20%)
6	ADP	C	402	4	28,29,29	1.57	5 (17%)	43,45,45	1.95	13 (30%)
6	ADP	D	402	4	28,29,29	1.56	5 (17%)	43,45,45	1.95	13 (30%)
7	PO4	C	403	4	4,4,4	1.18	0	6,6,6	0.85	0
6	ADP	A	402	4	28,29,29	1.57	5 (17%)	43,45,45	1.95	13 (30%)
5	GH3	N	402	-	31,33,33	5.80	20 (64%)	44,52,52	1.85	9 (20%)
6	ADP	E	402	4	28,29,29	1.56	5 (17%)	43,45,45	1.94	13 (30%)
7	PO4	B	403	4	4,4,4	1.18	0	6,6,6	0.86	0
7	PO4	A	403	4	4,4,4	1.19	0	6,6,6	0.86	0
7	PO4	D	403	4	4,4,4	1.18	0	6,6,6	0.85	0
5	GH3	L	402	-	31,33,33	5.81	20 (64%)	44,52,52	1.86	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	B	402	4	-	0/16/32/32	0/3/3/3
5	GH3	M	402	-	-	5/22/34/34	0/3/3/3
5	GH3	K	402	-	-	5/22/34/34	0/3/3/3
5	GH3	O	402	-	-	5/22/34/34	0/3/3/3
6	ADP	C	402	4	-	0/16/32/32	0/3/3/3
6	ADP	D	402	4	-	0/16/32/32	0/3/3/3
6	ADP	A	402	4	-	0/16/32/32	0/3/3/3
5	GH3	N	402	-	-	5/22/34/34	0/3/3/3
6	ADP	E	402	4	-	0/16/32/32	0/3/3/3
5	GH3	L	402	-	-	5/22/34/34	0/3/3/3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	402	GH3	PB-O3B	13.29	1.73	1.59
5	L	402	GH3	PA-O3A	13.28	1.73	1.59
5	K	402	GH3	PA-O3A	13.27	1.73	1.59
5	K	402	GH3	PB-O3B	13.26	1.73	1.59
5	M	402	GH3	PB-O3B	13.25	1.73	1.59
5	M	402	GH3	PA-O3A	13.25	1.73	1.59
5	N	402	GH3	PB-O3B	13.24	1.73	1.59
5	O	402	GH3	PA-O3A	13.24	1.73	1.59
5	L	402	GH3	PB-O3B	13.24	1.73	1.59
5	N	402	GH3	PA-O3A	13.23	1.73	1.59
5	M	402	GH3	PB-O3A	12.34	1.72	1.59
5	O	402	GH3	PB-O3A	12.32	1.72	1.59
5	K	402	GH3	PB-O3A	12.30	1.72	1.59
5	L	402	GH3	PB-O3A	12.30	1.72	1.59
5	N	402	GH3	PB-O3A	12.30	1.72	1.59
5	K	402	GH3	O4'-C1'	11.96	1.69	1.42
5	N	402	GH3	O4'-C1'	11.95	1.69	1.42
5	L	402	GH3	O4'-C1'	11.95	1.69	1.42
5	M	402	GH3	O4'-C1'	11.94	1.69	1.42
5	O	402	GH3	O4'-C1'	11.94	1.69	1.42
5	L	402	GH3	O6-C6	11.30	1.45	1.23
5	M	402	GH3	O6-C6	11.29	1.45	1.23
5	O	402	GH3	O6-C6	11.28	1.45	1.23
5	K	402	GH3	O6-C6	11.28	1.45	1.23
5	N	402	GH3	O6-C6	11.26	1.44	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	402	GH3	C2-N2	8.27	1.53	1.34
5	L	402	GH3	C2-N2	8.27	1.53	1.34
5	M	402	GH3	C2-N2	8.26	1.53	1.34
5	O	402	GH3	C2-N2	8.25	1.53	1.34
5	N	402	GH3	C2-N2	8.25	1.53	1.34
5	L	402	GH3	C3'-C4'	6.56	1.66	1.52
5	N	402	GH3	C3'-C4'	6.55	1.66	1.52
5	K	402	GH3	C3'-C4'	6.54	1.66	1.52
5	M	402	GH3	C3'-C4'	6.53	1.66	1.52
5	O	402	GH3	C3'-C4'	6.53	1.66	1.52
5	K	402	GH3	O2'-C2'	6.36	1.56	1.43
5	N	402	GH3	O2'-C2'	6.36	1.56	1.43
5	M	402	GH3	O2'-C2'	6.36	1.56	1.43
5	L	402	GH3	O2'-C2'	6.35	1.56	1.43
5	O	402	GH3	O2'-C2'	6.34	1.56	1.43
5	N	402	GH3	O4'-C4'	-5.05	1.35	1.44
5	O	402	GH3	O4'-C4'	-5.04	1.35	1.44
5	K	402	GH3	O4'-C4'	-5.03	1.35	1.44
5	M	402	GH3	O4'-C4'	-5.03	1.35	1.44
5	L	402	GH3	O4'-C4'	-4.98	1.35	1.44
5	N	402	GH3	PA-O5'	4.44	1.76	1.59
5	O	402	GH3	PA-O5'	4.44	1.76	1.59
5	M	402	GH3	PA-O5'	4.43	1.76	1.59
5	K	402	GH3	PA-O5'	4.42	1.76	1.59
5	L	402	GH3	PA-O5'	4.41	1.76	1.59
5	O	402	GH3	C5'-C4'	4.16	1.63	1.50
5	M	402	GH3	C5'-C4'	4.15	1.63	1.50
5	L	402	GH3	C5'-C4'	4.15	1.63	1.50
5	N	402	GH3	C5'-C4'	4.14	1.63	1.50
5	K	402	GH3	C5'-C4'	4.13	1.63	1.50
6	A	402	ADP	C5-N7	-3.32	1.33	1.39
6	E	402	ADP	C5-N7	-3.29	1.33	1.39
6	C	402	ADP	C5-N7	-3.28	1.33	1.39
6	D	402	ADP	C5-N7	-3.27	1.33	1.39
6	B	402	ADP	C5-N7	-3.25	1.33	1.39
6	C	402	ADP	C4-N9	-3.25	1.30	1.37
6	A	402	ADP	C4-N9	-3.25	1.30	1.37
6	D	402	ADP	C4-N9	-3.24	1.31	1.37
6	B	402	ADP	C4-N9	-3.23	1.31	1.37
6	E	402	ADP	C4-N9	-3.22	1.31	1.37
5	N	402	GH3	C4-N3	2.87	1.40	1.34
5	O	402	GH3	C4-N3	2.86	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	402	GH3	C4-N3	2.85	1.40	1.34
5	M	402	GH3	C4-N3	2.84	1.40	1.34
5	L	402	GH3	C4-N3	2.84	1.40	1.34
6	A	402	ADP	C5-C4	2.76	1.44	1.39
6	D	402	ADP	C5-C4	2.73	1.43	1.39
6	E	402	ADP	C5-C4	2.72	1.43	1.39
6	C	402	ADP	C5-C4	2.72	1.43	1.39
6	B	402	ADP	C5-C4	2.71	1.43	1.39
6	A	402	ADP	C8-N9	-2.62	1.33	1.37
6	C	402	ADP	C8-N9	-2.61	1.33	1.37
6	B	402	ADP	C8-N9	-2.61	1.33	1.37
6	D	402	ADP	C8-N9	-2.59	1.33	1.37
6	E	402	ADP	C8-N9	-2.58	1.33	1.37
5	M	402	GH3	C2-N3	2.49	1.39	1.33
5	M	402	GH3	C8-N7	2.49	1.39	1.32
5	O	402	GH3	C8-N7	2.49	1.39	1.32
5	N	402	GH3	C2-N3	2.48	1.39	1.33
5	K	402	GH3	C8-N7	2.48	1.39	1.32
5	K	402	GH3	C2-N3	2.48	1.39	1.33
5	L	402	GH3	C8-N7	2.48	1.39	1.32
5	O	402	GH3	C2-N3	2.48	1.39	1.33
5	L	402	GH3	C2-N3	2.48	1.39	1.33
5	N	402	GH3	C8-N7	2.47	1.39	1.32
5	L	402	GH3	PB-O1B	2.44	1.59	1.50
5	K	402	GH3	PB-O1B	2.43	1.59	1.50
5	N	402	GH3	PB-O1B	2.43	1.59	1.50
5	M	402	GH3	PB-O1B	2.43	1.59	1.50
5	O	402	GH3	PB-O1B	2.43	1.59	1.50
5	O	402	GH3	PA-O1A	2.37	1.59	1.50
5	L	402	GH3	PA-O1A	2.37	1.59	1.50
5	K	402	GH3	PA-O1A	2.35	1.59	1.50
5	M	402	GH3	PA-O1A	2.35	1.59	1.50
5	N	402	GH3	PA-O1A	2.34	1.58	1.50
5	L	402	GH3	C5-C4	2.32	1.45	1.38
5	N	402	GH3	C3'-C2'	2.32	1.58	1.52
5	O	402	GH3	C3'-C2'	2.32	1.58	1.52
5	M	402	GH3	C3'-C2'	2.32	1.58	1.52
5	K	402	GH3	C3'-C2'	2.32	1.58	1.52
5	M	402	GH3	C5-C4	2.31	1.45	1.38
5	O	402	GH3	C5-C4	2.30	1.45	1.38
5	N	402	GH3	C5-C4	2.30	1.45	1.38
5	L	402	GH3	C3'-C2'	2.30	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	402	GH3	C5-C4	2.29	1.45	1.38
5	N	402	GH3	PG-O1G	2.25	1.57	1.50
5	K	402	GH3	PG-O1G	2.24	1.57	1.50
5	O	402	GH3	PG-O1G	2.24	1.57	1.50
5	M	402	GH3	PG-O1G	2.24	1.57	1.50
5	L	402	GH3	PG-O1G	2.23	1.57	1.50
5	K	402	GH3	C4-N9	2.20	1.43	1.38
5	M	402	GH3	C4-N9	2.17	1.43	1.38
5	N	402	GH3	C4-N9	2.15	1.43	1.38
5	O	402	GH3	C4-N9	2.14	1.43	1.38
5	L	402	GH3	C4-N9	2.13	1.43	1.38
6	A	402	ADP	C2'-C3'	-2.08	1.47	1.53
6	E	402	ADP	C2'-C3'	-2.06	1.47	1.53
6	C	402	ADP	C2'-C3'	-2.05	1.47	1.53
6	D	402	ADP	C2'-C3'	-2.04	1.47	1.53
6	B	402	ADP	C2'-C3'	-2.02	1.47	1.53

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	GH3	C5-C4-N3	-6.50	118.04	128.39
5	O	402	GH3	C5-C4-N3	-6.49	118.06	128.39
5	N	402	GH3	C5-C4-N3	-6.48	118.08	128.39
5	M	402	GH3	C5-C4-N3	-6.47	118.09	128.39
5	K	402	GH3	C5-C4-N3	-6.45	118.12	128.39
6	A	402	ADP	C5-C4-N3	-5.08	119.72	126.72
6	D	402	ADP	C5-C4-N3	-5.06	119.75	126.72
6	C	402	ADP	C5-C4-N3	-5.06	119.75	126.72
6	B	402	ADP	C5-C4-N3	-5.04	119.78	126.72
6	E	402	ADP	C5-C4-N3	-5.02	119.80	126.72
5	L	402	GH3	N9-C4-N3	4.42	134.80	125.95
5	N	402	GH3	N9-C4-N3	4.42	134.78	125.95
5	O	402	GH3	N9-C4-N3	4.41	134.78	125.95
5	M	402	GH3	N9-C4-N3	4.41	134.77	125.95
5	K	402	GH3	N9-C4-N3	4.40	134.76	125.95
5	L	402	GH3	C2-N3-C4	4.34	119.77	112.30
5	O	402	GH3	C2-N3-C4	4.33	119.76	112.30
6	A	402	ADP	N3-C4-N9	4.32	134.51	127.17
5	M	402	GH3	C2-N3-C4	4.31	119.73	112.30
5	N	402	GH3	C2-N3-C4	4.31	119.72	112.30
6	C	402	ADP	N3-C4-N9	4.29	134.47	127.17
6	D	402	ADP	N3-C4-N9	4.29	134.46	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	402	ADP	N3-C4-N9	4.28	134.44	127.17
5	K	402	GH3	C2-N3-C4	4.27	119.66	112.30
6	E	402	ADP	N3-C4-N9	4.26	134.41	127.17
6	C	402	ADP	C4-N9-C8	3.64	109.56	105.74
6	A	402	ADP	C4-N9-C8	3.63	109.55	105.74
6	D	402	ADP	C4-N9-C8	3.63	109.55	105.74
6	B	402	ADP	C4-N9-C8	3.62	109.53	105.74
6	E	402	ADP	C4-N9-C8	3.60	109.52	105.74
6	A	402	ADP	O4'-C1'-N9	3.40	114.63	108.09
6	D	402	ADP	O4'-C1'-N9	3.39	114.60	108.09
6	C	402	ADP	O4'-C1'-N9	3.39	114.59	108.09
6	E	402	ADP	O4'-C1'-N9	3.38	114.59	108.09
6	B	402	ADP	O4'-C1'-N9	3.38	114.57	108.09
6	A	402	ADP	C2-N3-C4	3.22	119.68	111.83
6	D	402	ADP	C2-N3-C4	3.21	119.67	111.83
6	C	402	ADP	C2-N3-C4	3.20	119.65	111.83
6	B	402	ADP	C2-N3-C4	3.20	119.64	111.83
6	E	402	ADP	C2-N3-C4	3.17	119.57	111.83
5	L	402	GH3	C2-N1-C6	-2.85	119.95	125.11
5	K	402	GH3	C2-N1-C6	-2.84	119.96	125.11
5	M	402	GH3	C2-N1-C6	-2.83	119.98	125.11
5	N	402	GH3	C2-N1-C6	-2.82	119.99	125.11
5	O	402	GH3	C4'-O4'-C1'	-2.82	105.74	109.69
5	L	402	GH3	C4'-O4'-C1'	-2.82	105.74	109.69
5	O	402	GH3	C2-N1-C6	-2.82	120.00	125.11
6	B	402	ADP	N3-C2-N1	-2.82	124.31	128.58
6	D	402	ADP	N3-C2-N1	-2.80	124.34	128.58
5	M	402	GH3	C4'-O4'-C1'	-2.80	105.77	109.69
6	C	402	ADP	N3-C2-N1	-2.80	124.35	128.58
5	N	402	GH3	C4'-O4'-C1'	-2.79	105.78	109.69
6	A	402	ADP	N3-C2-N1	-2.78	124.38	128.58
6	E	402	ADP	N3-C2-N1	-2.77	124.39	128.58
5	K	402	GH3	C4'-O4'-C1'	-2.77	105.81	109.69
6	D	402	ADP	C2'-C1'-N9	-2.70	106.61	113.30
6	B	402	ADP	C2'-C1'-N9	-2.68	106.64	113.30
6	C	402	ADP	C2'-C1'-N9	-2.67	106.67	113.30
6	E	402	ADP	C2'-C1'-N9	-2.66	106.69	113.30
6	A	402	ADP	C2'-C1'-N9	-2.66	106.70	113.30
6	D	402	ADP	C4-C5-N7	-2.65	107.55	110.58
5	L	402	GH3	C4-C5-N7	-2.65	106.48	110.67
6	E	402	ADP	C4-C5-N7	-2.64	107.56	110.58
5	O	402	GH3	C4-C5-N7	-2.64	106.49	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	402	ADP	O3'-C3'-C2'	-2.63	103.39	111.82
5	K	402	GH3	C4-C5-N7	-2.63	106.51	110.67
6	C	402	ADP	O3'-C3'-C2'	-2.63	103.40	111.82
6	C	402	ADP	C4-C5-N7	-2.63	107.58	110.58
5	N	402	GH3	C4-C5-N7	-2.63	106.51	110.67
5	M	402	GH3	C4-C5-N7	-2.62	106.51	110.67
6	A	402	ADP	C4-C5-N7	-2.62	107.58	110.58
6	E	402	ADP	O3'-C3'-C2'	-2.62	103.42	111.82
6	B	402	ADP	C4-C5-N7	-2.62	107.59	110.58
6	A	402	ADP	O3'-C3'-C2'	-2.62	103.43	111.82
6	D	402	ADP	O3'-C3'-C2'	-2.61	103.46	111.82
6	D	402	ADP	N9-C8-N7	-2.59	110.26	113.94
6	E	402	ADP	N9-C8-N7	-2.58	110.27	113.94
6	C	402	ADP	N9-C8-N7	-2.58	110.27	113.94
6	A	402	ADP	N9-C8-N7	-2.58	110.28	113.94
5	K	402	GH3	C8-N7-C5	2.56	108.81	104.26
6	B	402	ADP	N9-C8-N7	-2.55	110.31	113.94
5	L	402	GH3	C8-N7-C5	2.55	108.79	104.26
5	N	402	GH3	C8-N7-C5	2.54	108.79	104.26
5	O	402	GH3	C8-N7-C5	2.54	108.79	104.26
5	M	402	GH3	C8-N7-C5	2.54	108.78	104.26
6	A	402	ADP	O3A-PA-O1A	-2.45	103.33	110.70
6	D	402	ADP	O3A-PA-O1A	-2.45	103.33	110.70
6	E	402	ADP	O3A-PA-O1A	-2.45	103.34	110.70
6	C	402	ADP	O3A-PA-O1A	-2.44	103.35	110.70
6	B	402	ADP	O3A-PA-O1A	-2.43	103.41	110.70
5	N	402	GH3	O6-C6-C5	-2.25	120.60	126.53
5	O	402	GH3	O6-C6-C5	-2.24	120.62	126.53
5	M	402	GH3	O6-C6-C5	-2.24	120.62	126.53
5	K	402	GH3	O6-C6-C5	-2.24	120.62	126.53
5	L	402	GH3	O6-C6-C5	-2.24	120.63	126.53
6	D	402	ADP	O5'-C5'-C4'	-2.18	101.57	108.99
6	C	402	ADP	O5'-C5'-C4'	-2.18	101.58	108.99
6	E	402	ADP	O5'-C5'-C4'	-2.18	101.58	108.99
6	A	402	ADP	O5'-C5'-C4'	-2.17	101.60	108.99
6	B	402	ADP	O5'-C5'-C4'	-2.17	101.60	108.99
6	E	402	ADP	C5-N7-C8	2.17	106.86	103.45
6	D	402	ADP	C5-N7-C8	2.16	106.85	103.45
6	A	402	ADP	C5-N7-C8	2.14	106.81	103.45
6	C	402	ADP	C5-N7-C8	2.13	106.81	103.45
6	B	402	ADP	C5-N7-C8	2.12	106.79	103.45
5	M	402	GH3	C5-C6-N1	2.05	118.46	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	402	GH3	C5-C6-N1	2.04	118.46	113.25
5	O	402	GH3	C5-C6-N1	2.04	118.45	113.25
5	N	402	GH3	C5-C6-N1	2.04	118.44	113.25
5	K	402	GH3	C5-C6-N1	2.04	118.44	113.25

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	402	GH3	C4'-C5'-O5'-PA
5	M	402	GH3	O4'-C4'-C5'-O5'
5	M	402	GH3	C3'-C4'-C5'-O5'
5	K	402	GH3	C4'-C5'-O5'-PA
5	K	402	GH3	O4'-C4'-C5'-O5'
5	K	402	GH3	C3'-C4'-C5'-O5'
5	L	402	GH3	C4'-C5'-O5'-PA
5	L	402	GH3	O4'-C4'-C5'-O5'
5	L	402	GH3	C3'-C4'-C5'-O5'
5	N	402	GH3	C4'-C5'-O5'-PA
5	N	402	GH3	O4'-C4'-C5'-O5'
5	N	402	GH3	C3'-C4'-C5'-O5'
5	O	402	GH3	C4'-C5'-O5'-PA
5	O	402	GH3	O4'-C4'-C5'-O5'
5	O	402	GH3	C3'-C4'-C5'-O5'
5	M	402	GH3	C2'-C1'-N9-C4
5	K	402	GH3	C2'-C1'-N9-C4
5	L	402	GH3	C2'-C1'-N9-C4
5	N	402	GH3	C2'-C1'-N9-C4
5	O	402	GH3	C2'-C1'-N9-C4
5	M	402	GH3	PG-O3B-PB-O2B
5	K	402	GH3	PG-O3B-PB-O2B
5	L	402	GH3	PG-O3B-PB-O2B
5	N	402	GH3	PG-O3B-PB-O2B
5	O	402	GH3	PG-O3B-PB-O2B

There are no ring outliers.

10 monomers are involved in 44 short contacts:

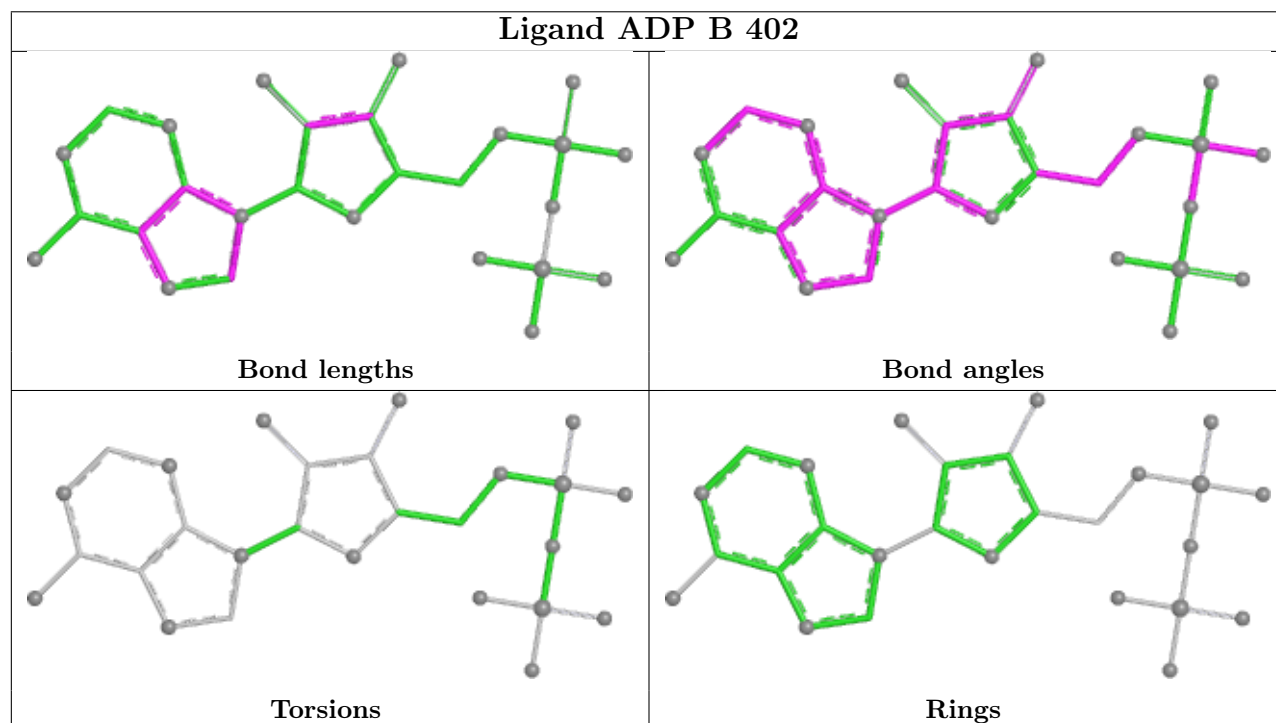
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	402	ADP	4	0
5	M	402	GH3	5	0

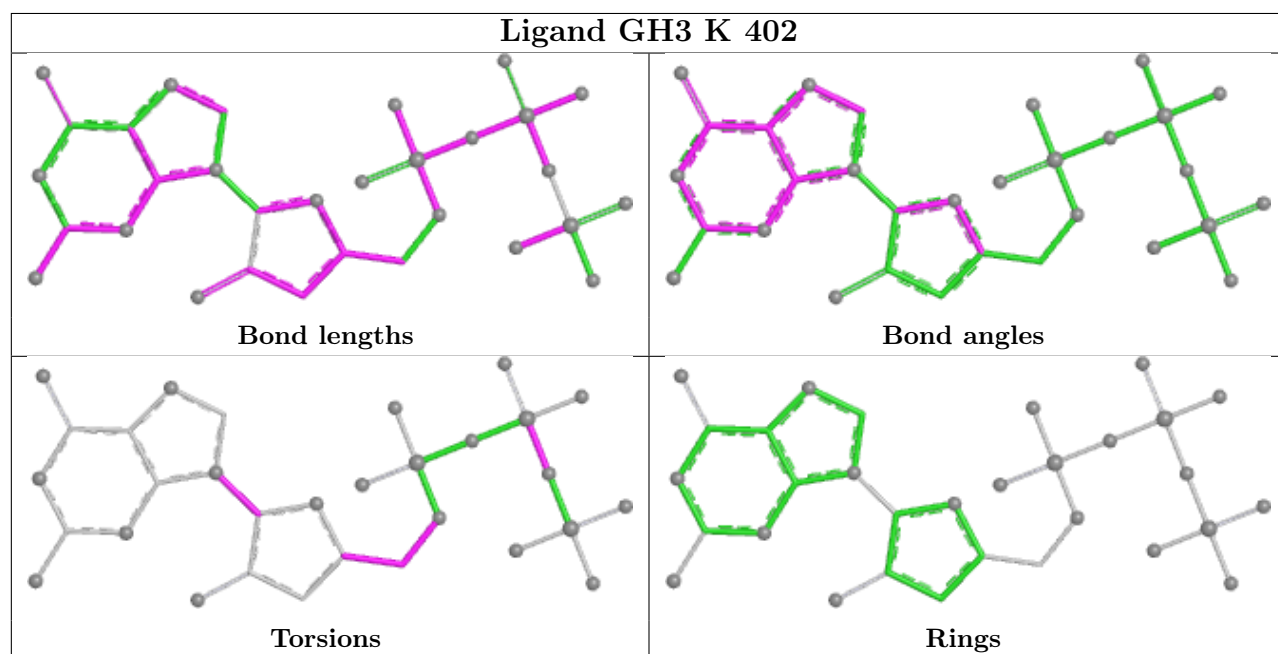
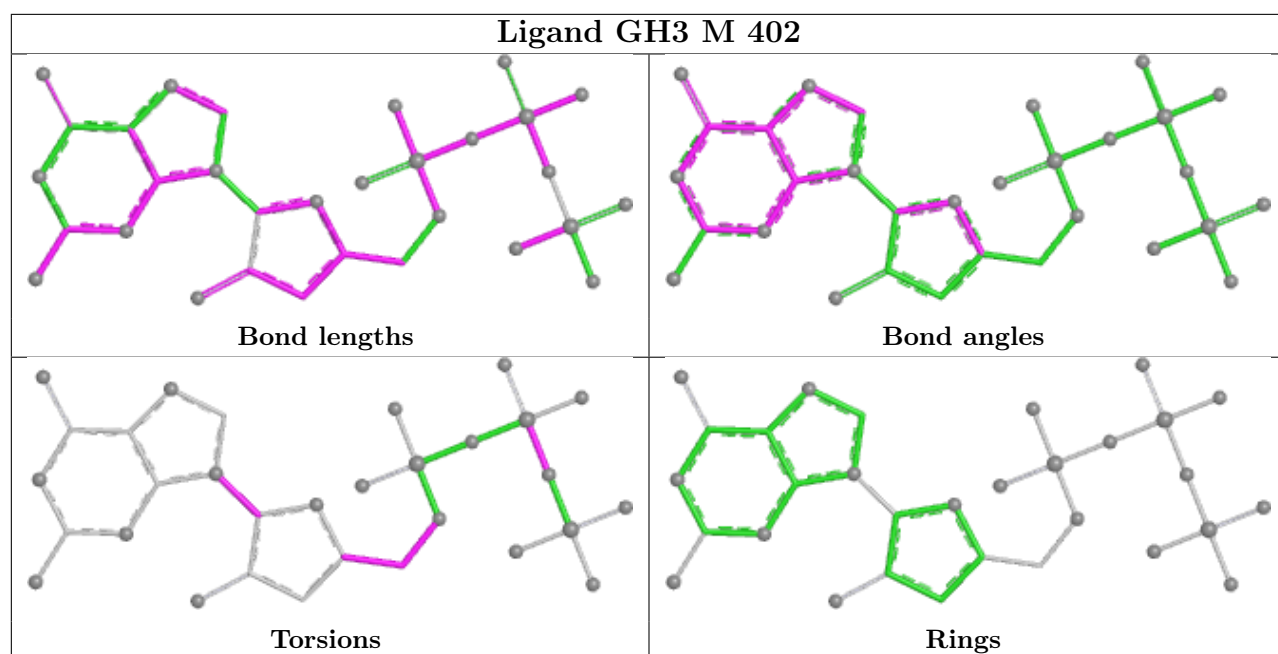
Continued on next page...

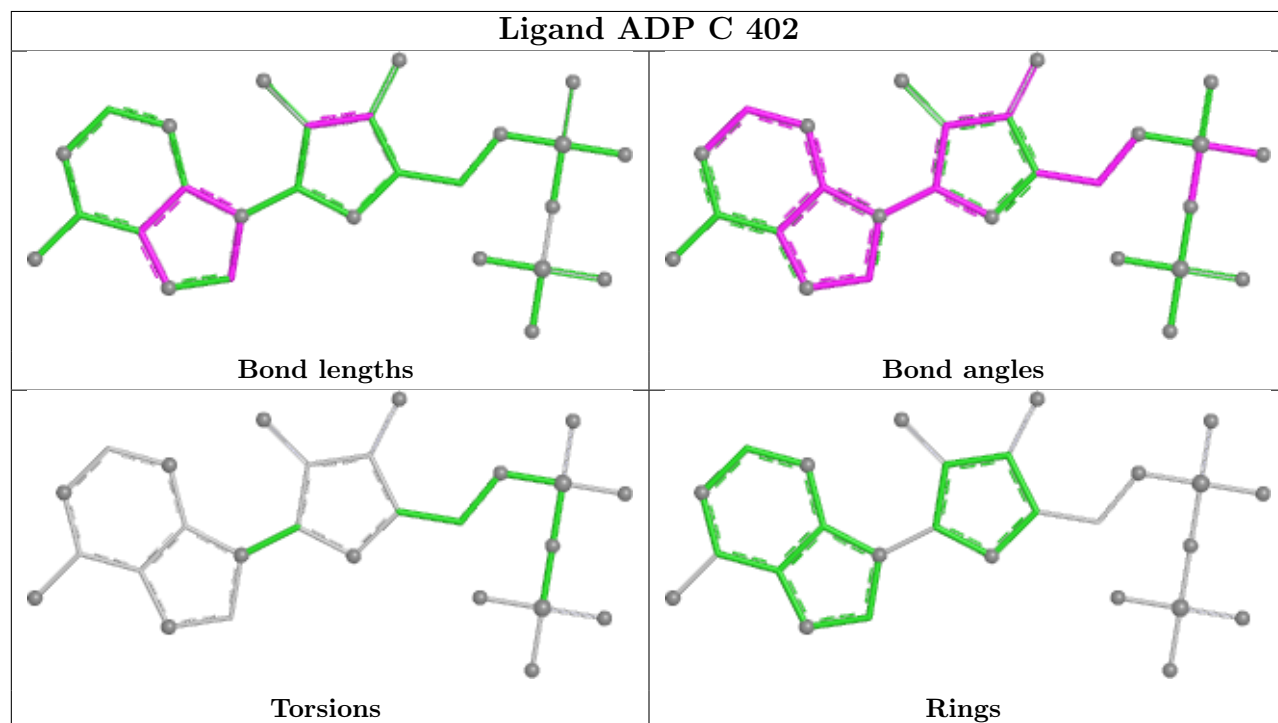
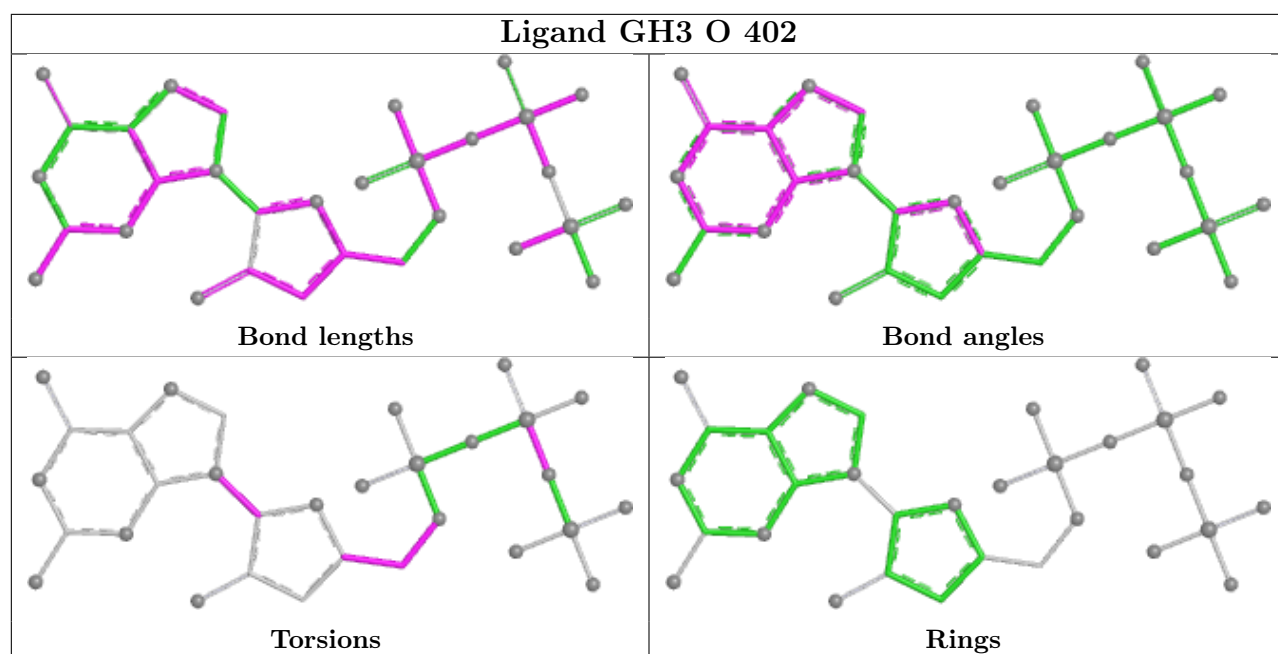
Continued from previous page...

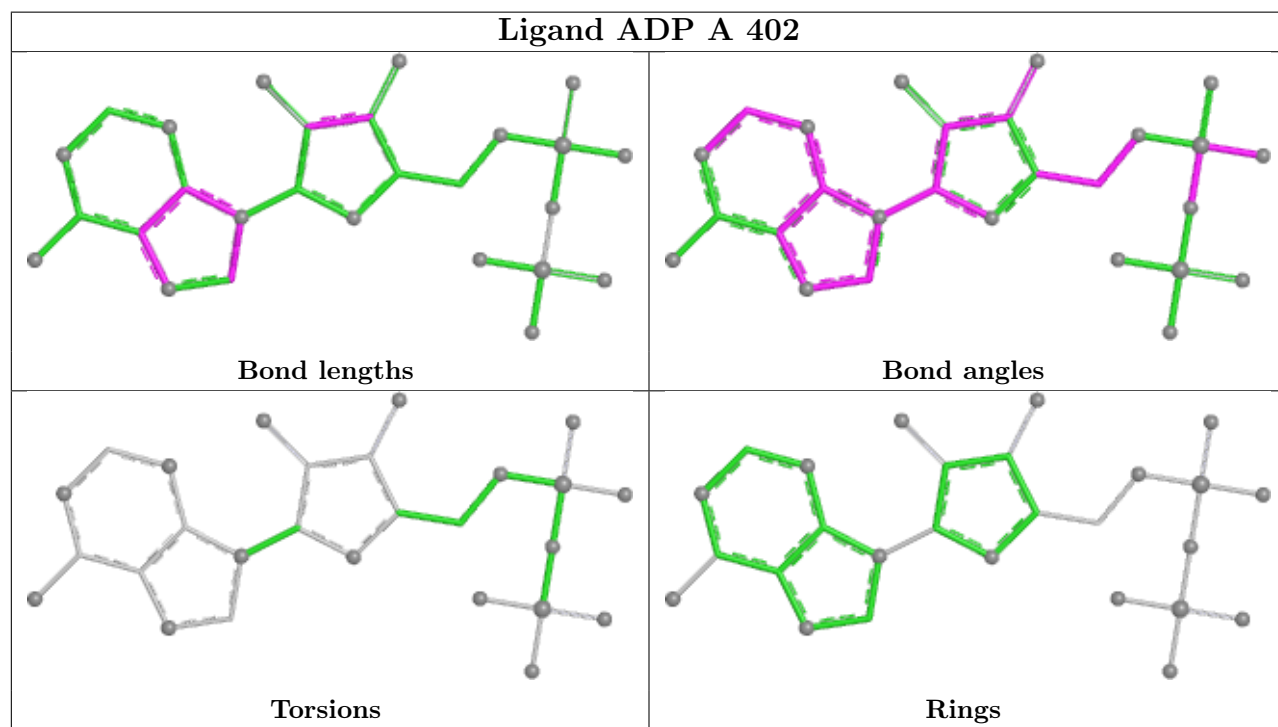
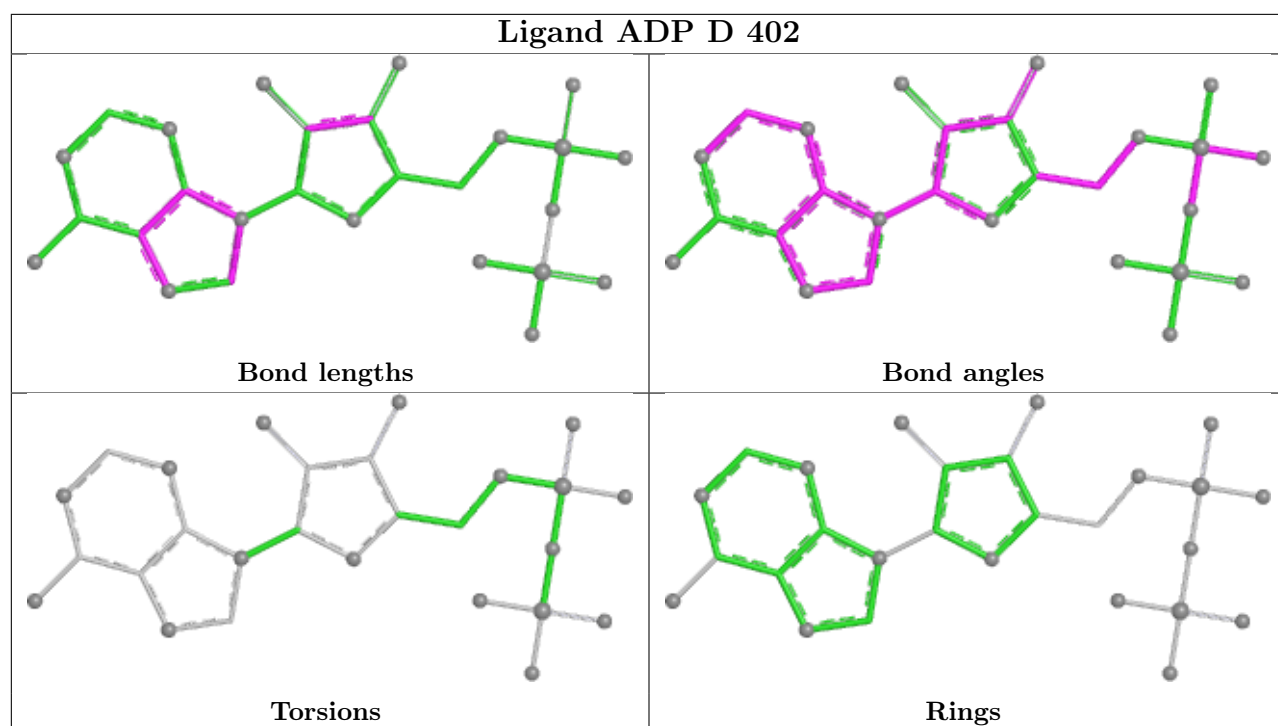
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	402	GH3	4	0
5	O	402	GH3	5	0
6	C	402	ADP	4	0
6	D	402	ADP	4	0
6	A	402	ADP	4	0
5	N	402	GH3	5	0
6	E	402	ADP	4	0
5	L	402	GH3	5	0

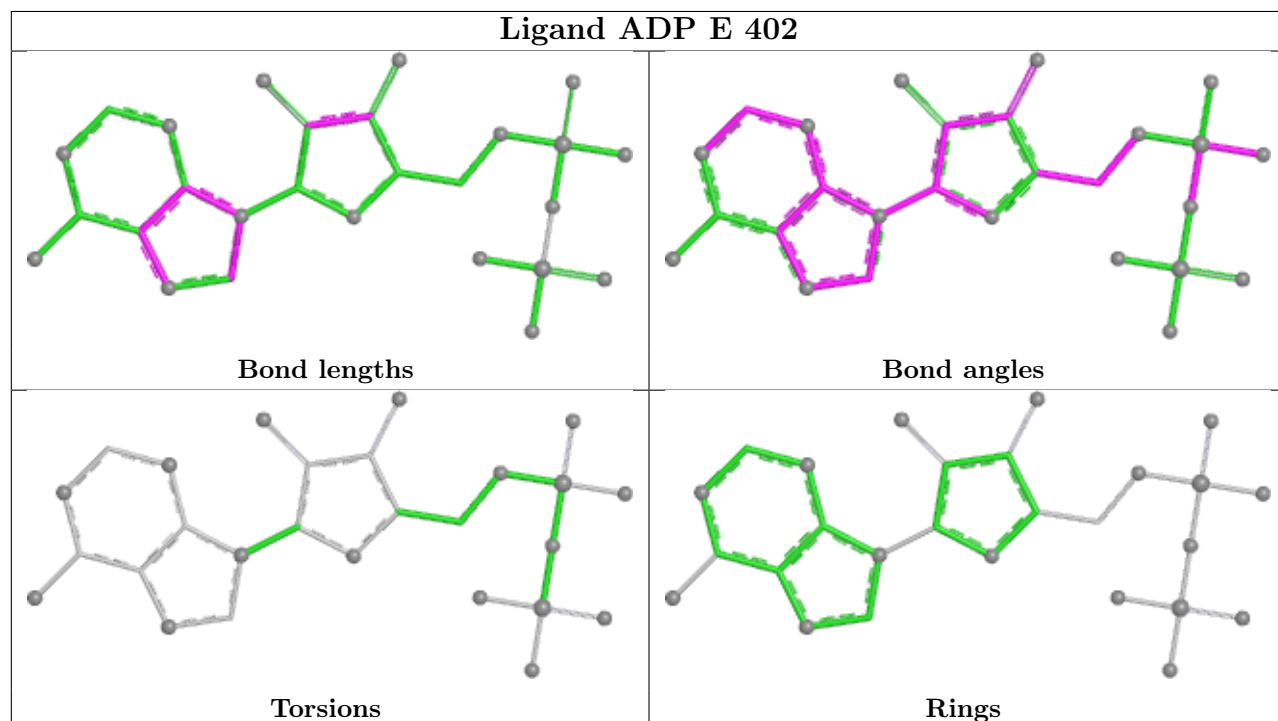
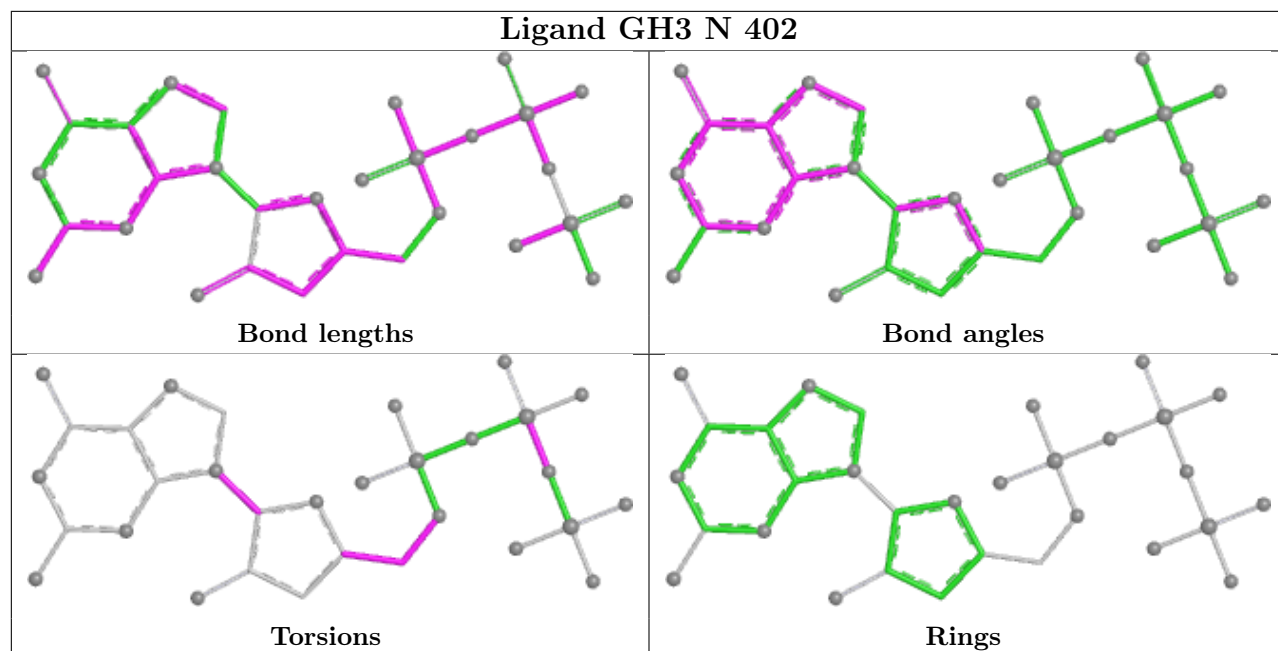
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

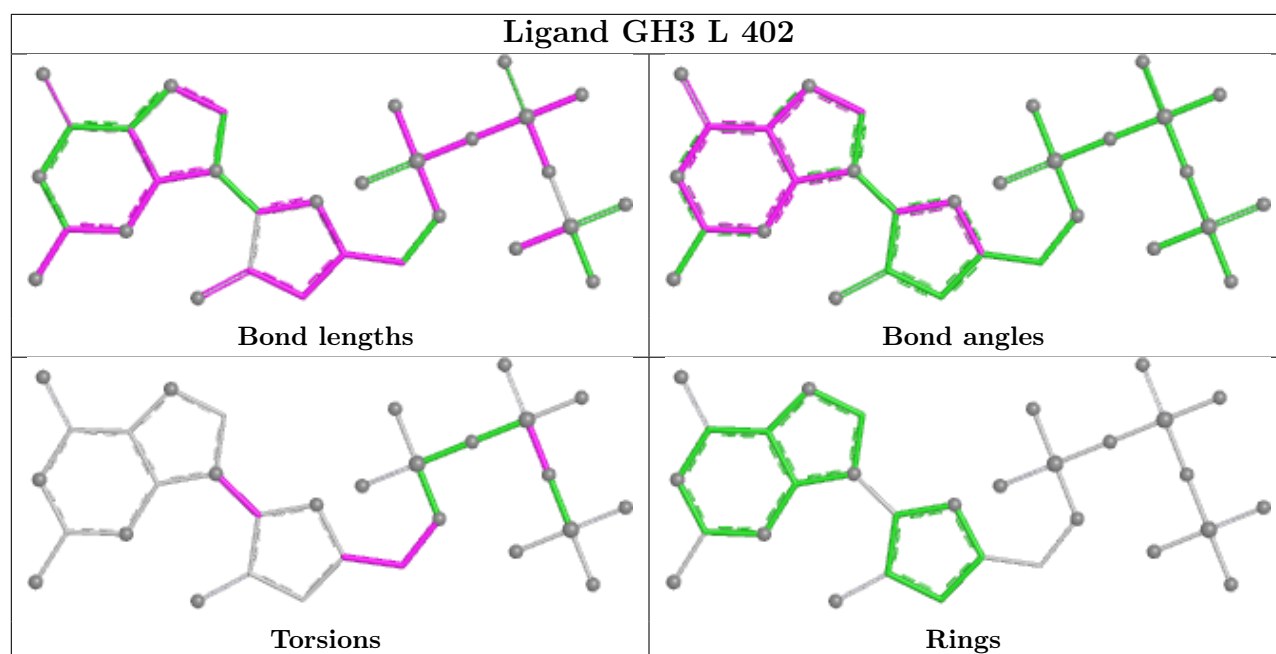












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

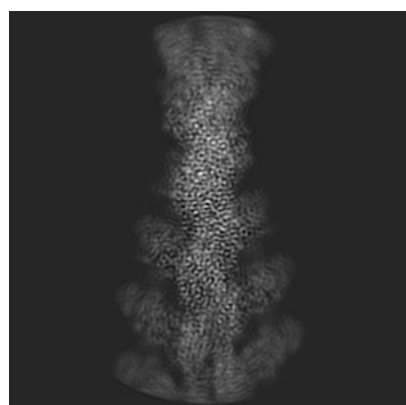
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13158. These allow visual inspection of the internal detail of the map and identification of artifacts.

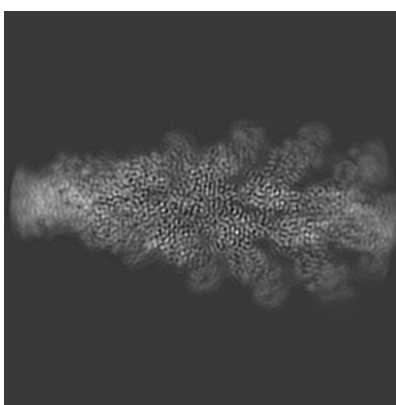
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

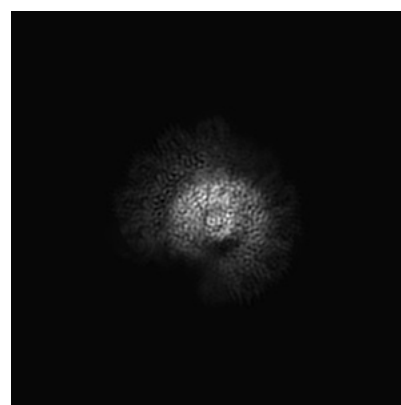
6.1.1 Primary map



X



Y

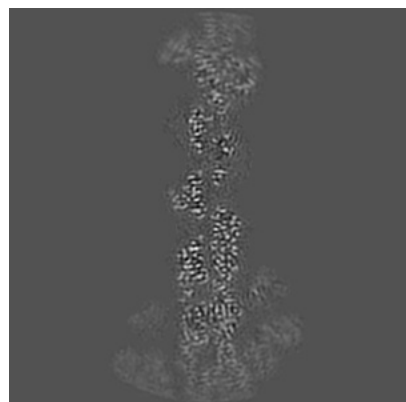


Z

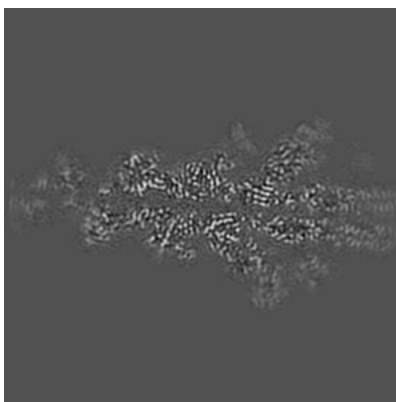
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150



Y Index: 150

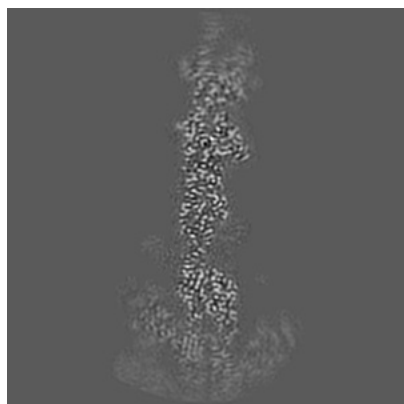


Z Index: 150

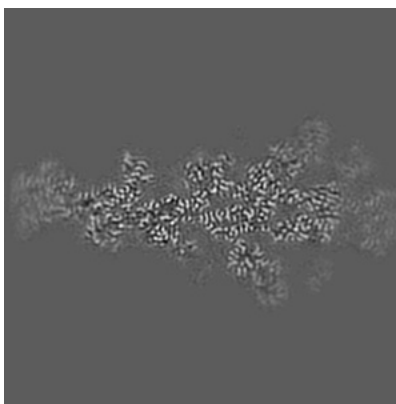
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

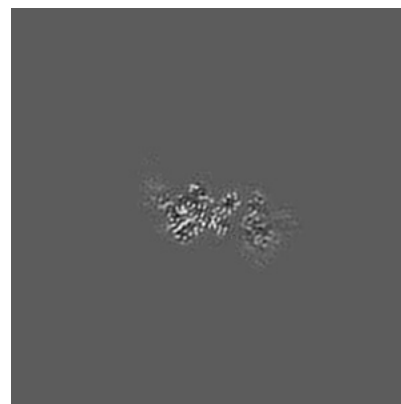
6.3.1 Primary map



X Index: 162



Y Index: 157

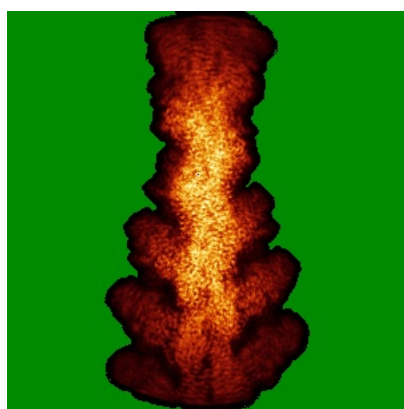


Z Index: 168

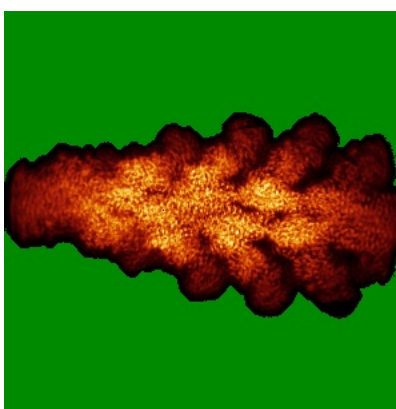
The images above show the largest variance slices of the map in three orthogonal directions.

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

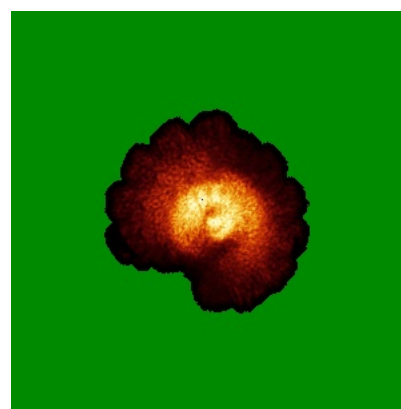
6.4.1 Primary map



X



Y

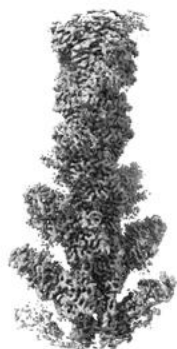


Z

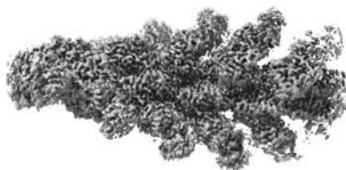
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

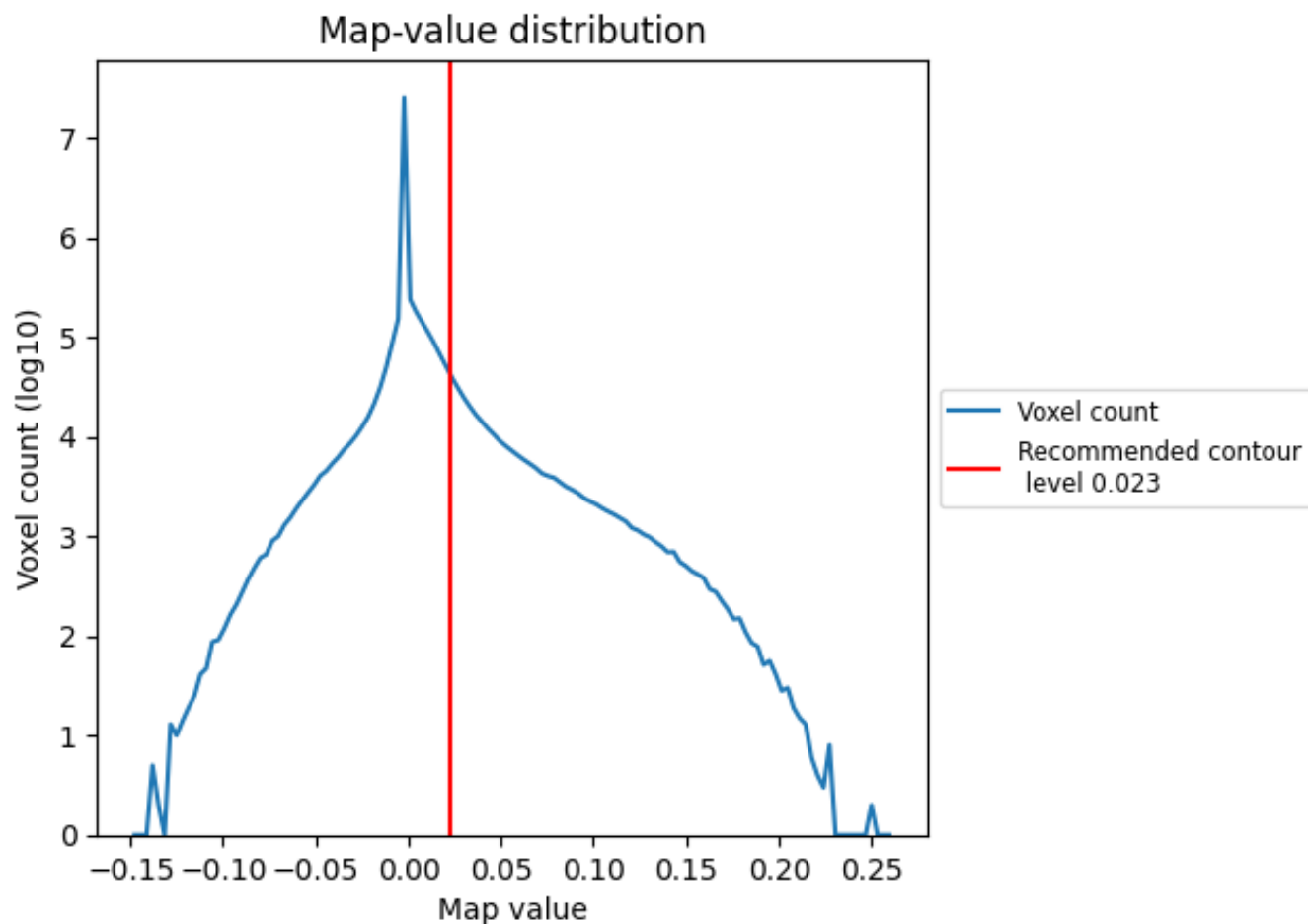
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

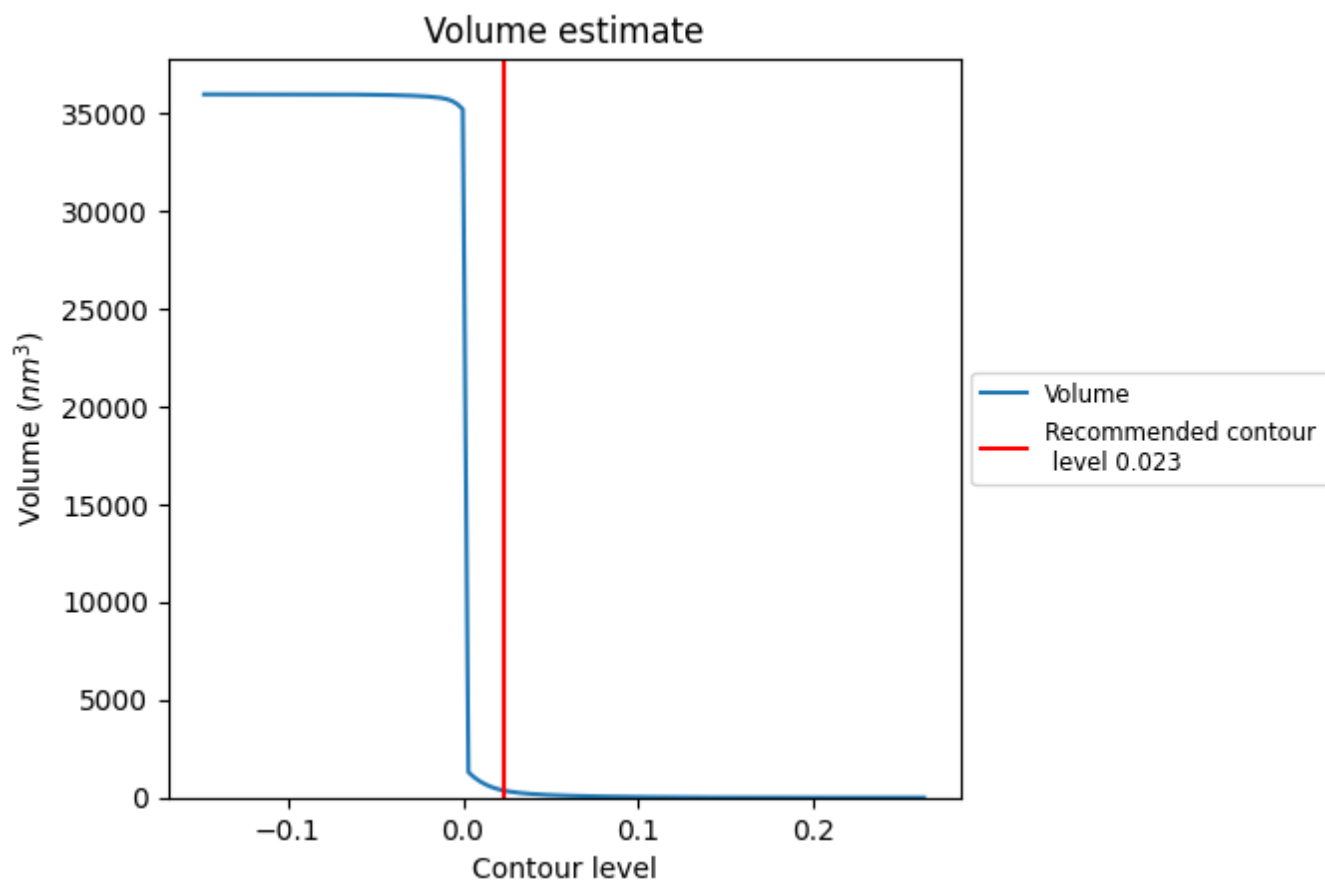
This section contains the results of statistical analysis of the map.

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.

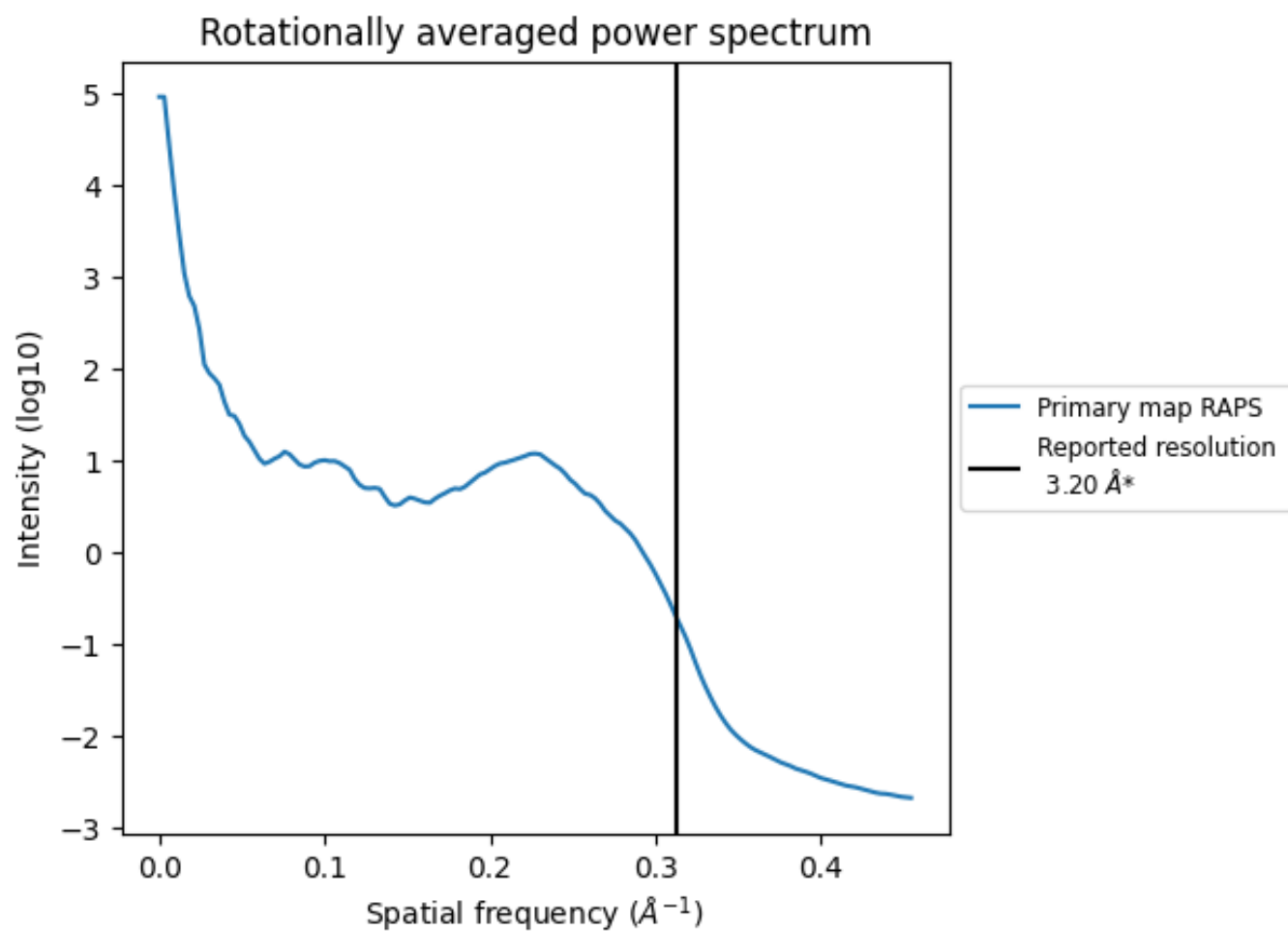
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 366 nm^3 ; this corresponds to an approximate mass of 330 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 ⓘ

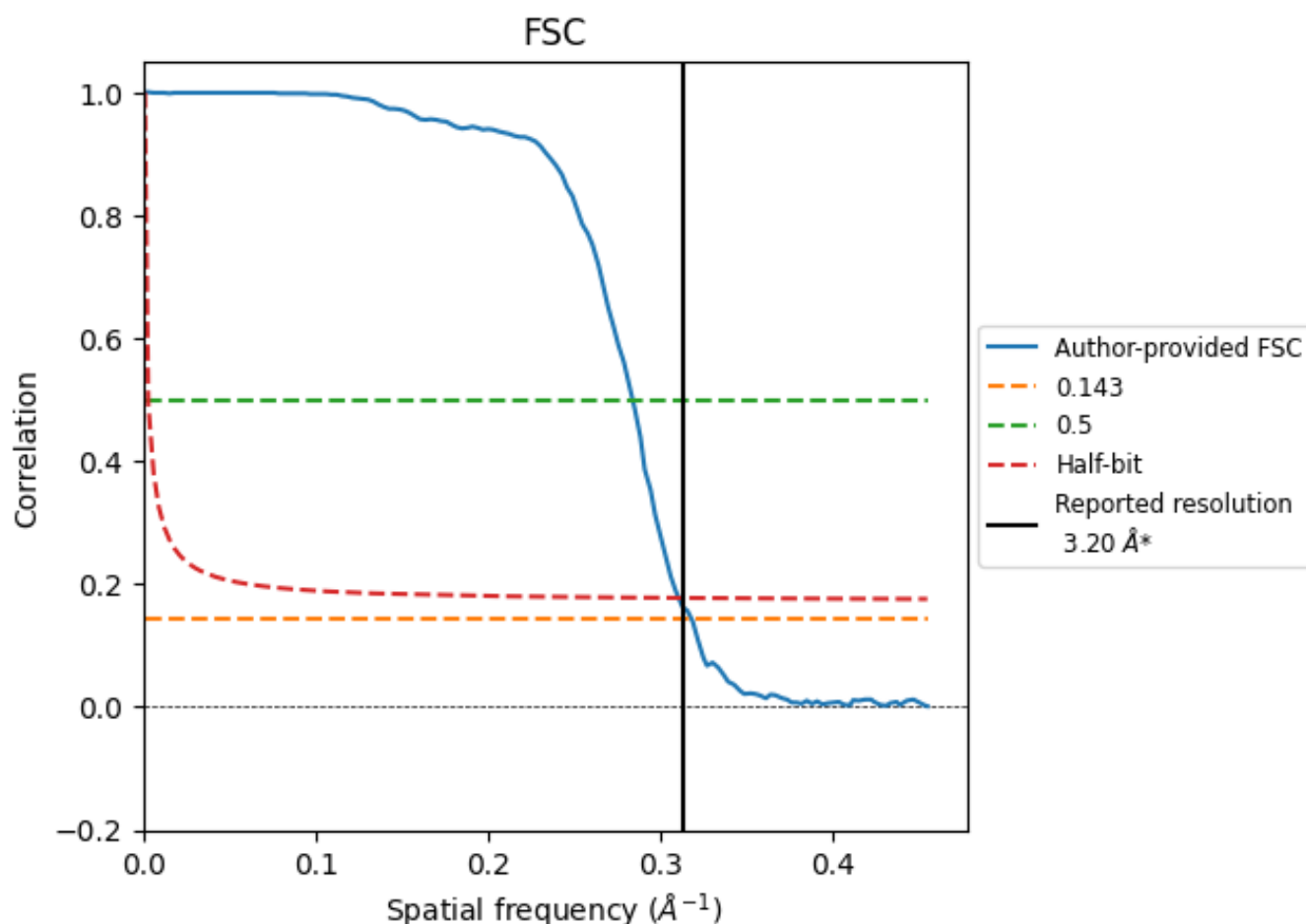


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

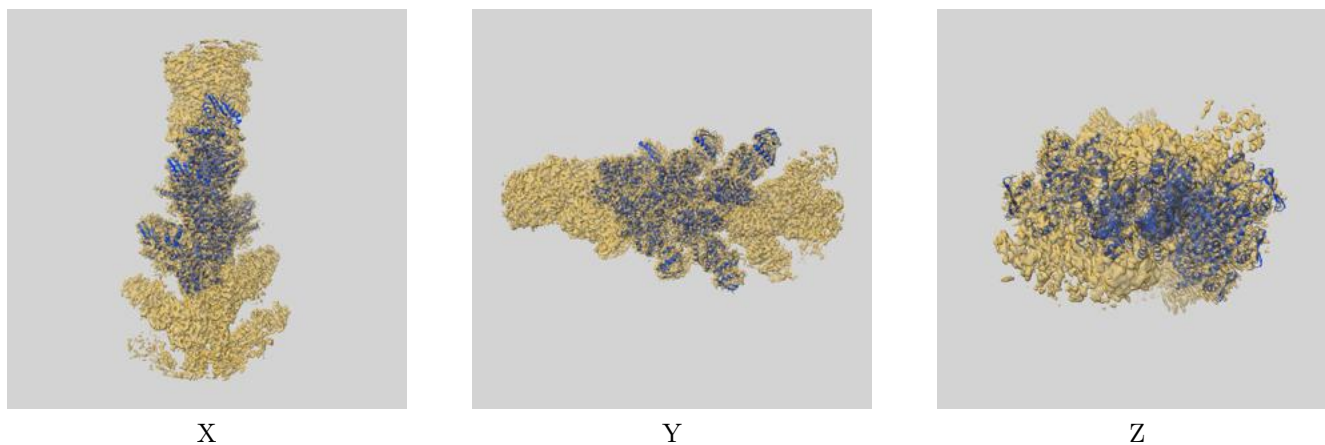
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.53	3.22
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

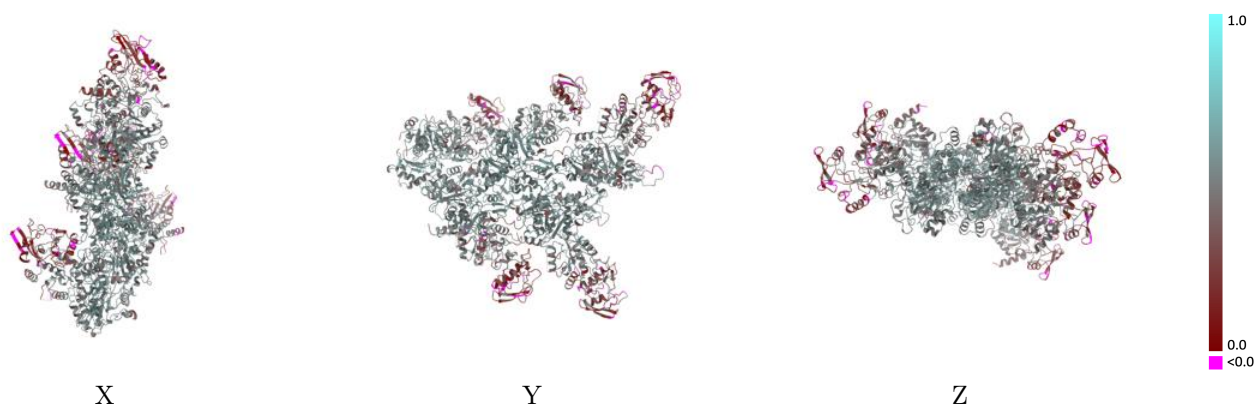
This section contains information regarding the fit between EMDB map EMD-13158 and PDB model 7P1G. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.023 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](#)

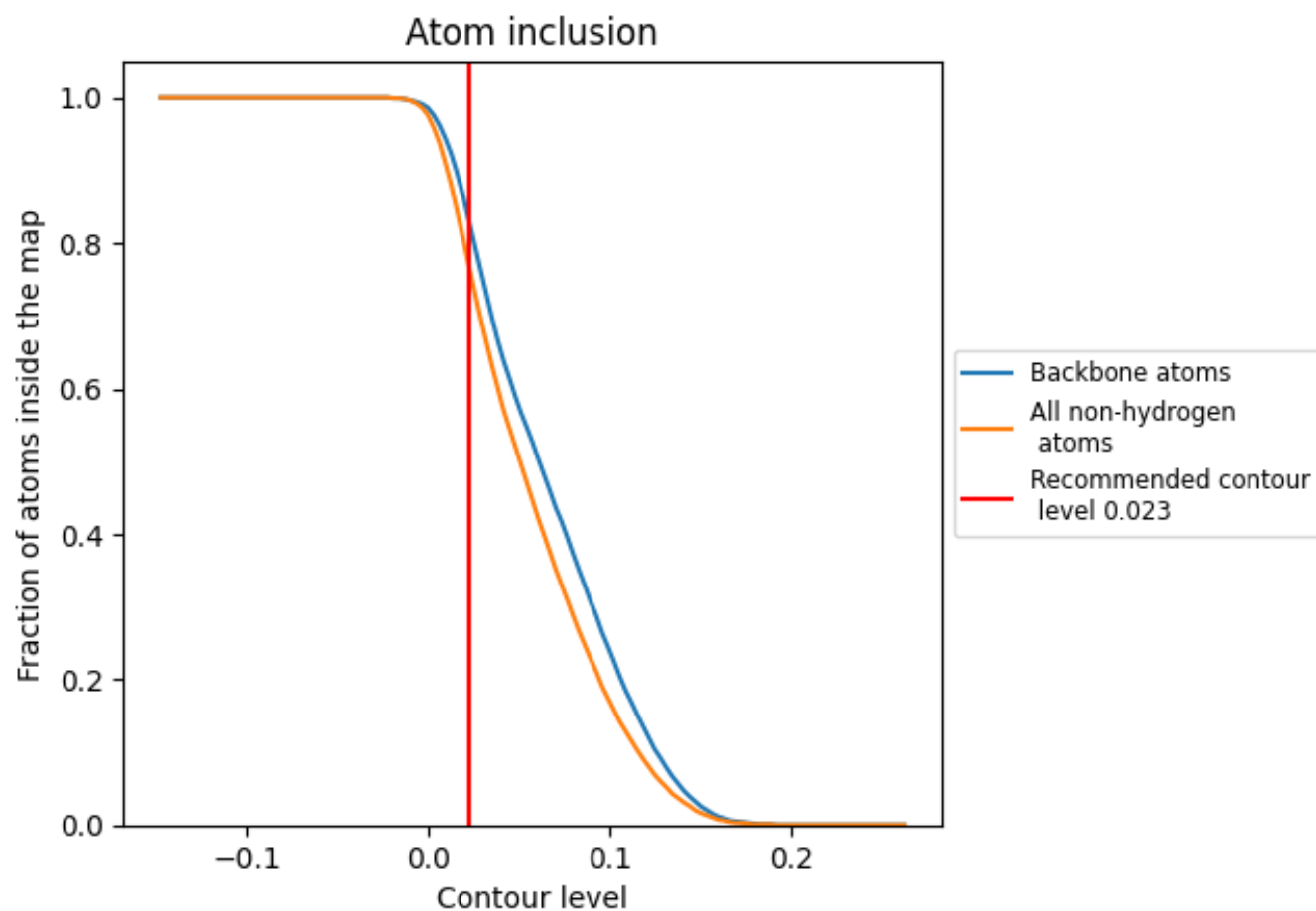


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7630	0.4600
A	0.8740	0.5270
B	0.8790	0.5310
C	0.8950	0.5570
D	0.8690	0.5340
E	0.8660	0.5120
F	0.9260	0.5700
G	0.9820	0.5890
H	0.9820	0.6050
I	0.9440	0.5850
J	0.9440	0.5540
K	0.6420	0.3770
L	0.6350	0.3660
M	0.7040	0.4330
N	0.6520	0.3890
O	0.5500	0.3290

1.0

0.0

<0.0