



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 12:55 PM EDT

PDB ID : 9YNH / pdb_00009ynh
EMDB ID : EMD-73179
Title : Full-length human cytoplasmic dynein-1 in phi-like state bound to dynactin-p150glued and LIS1
Authors : Yang, J.; Rao, Q.; Chai, P.; Zhang, K.
Deposited on : 2025-10-10
Resolution : 5.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

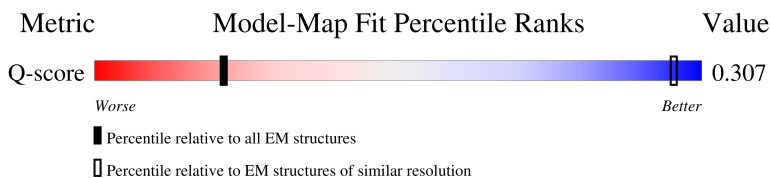
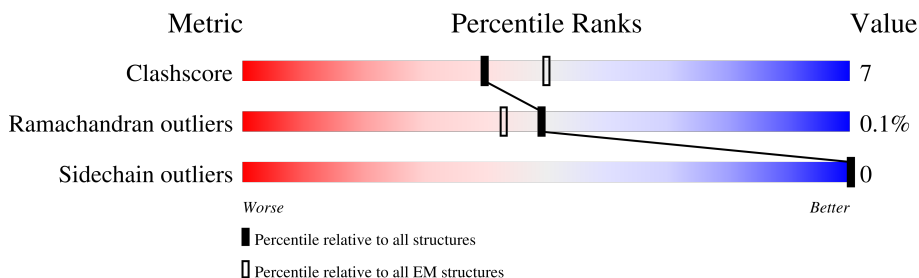
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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	520 (5.00 - 6.00)

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

Mol	Chain	Length	Quality of chain
1	A	4646	
1	B	4646	
2	C	638	
2	D	638	

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Mol	Chain	Length	Quality of chain
2	U	638	
2	V	638	
3	E	492	
3	F	492	
4	G	96	
4	H	96	
5	I	89	
5	J	89	
6	K	113	
6	L	113	
7	O	410	
7	P	410	
8	W	1281	
8	X	1281	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ADP	A	4704	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 62508 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	4355	Total	C	N	O	0	0
			21575	12865	4355	4355		
1	B	4335	Total	C	N	O	0	0
			21479	12809	4335	4335		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	C	394	Total	C	N	O	0	0
			1947	1159	394	394		
2	D	394	Total	C	N	O	0	0
			1947	1159	394	394		
2	U	34	Total	C	N	O	0	0
			170	102	34	34		
2	V	34	Total	C	N	O	0	0
			170	102	34	34		

- Molecule 3 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	311	Total	C	N	O	0	0
			1540	918	311	311		
3	F	311	Total	C	N	O	0	0
			1540	918	311	311		

- Molecule 4 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	93	Total	C	N	O	0	0
			462	276	93	93		
4	H	93	Total	C	N	O	0	0
			462	276	93	93		

- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	I	89	Total	C	N	O	0	0
			441	263	89	89		
5	J	89	Total	C	N	O	0	0
			441	263	89	89		

- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	113	Total	C	N	O	0	0
			558	332	113	113		
6	L	113	Total	C	N	O	0	0
			558	332	113	113		

- Molecule 7 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	397	Total	C	N	O	0	0
			1963	1169	397	397		
7	P	388	Total	C	N	O	0	0
			1920	1144	388	388		

- Molecule 8 is a protein called Dynactin subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	W	515	Total	C	N	O	0	0
			2554	1524	515	515		
8	X	513	Total	C	N	O	1	0
			2553	1523	515	515		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	118	ARG	LYS	conflict	UNP Q14203
W	124	SER	THR	conflict	UNP Q14203
W	125	ASN	THR	conflict	UNP Q14203
W	134	PRO	LEU	conflict	UNP Q14203
W	200	ALA	VAL	conflict	UNP Q14203
W	207	ALA	VAL	conflict	UNP Q14203
W	631	ASP	GLU	conflict	UNP Q14203
W	742	SER	CYS	conflict	UNP Q14203
W	778	SER	THR	conflict	UNP Q14203

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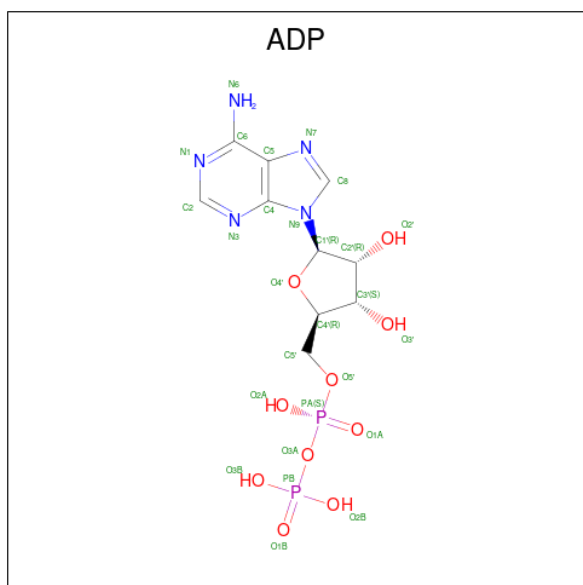
Chain	Residue	Modelled	Actual	Comment	Reference
W	821	ALA	PRO	conflict	UNP Q14203
W	862	PRO	LEU	conflict	UNP Q14203
W	1048	ILE	LEU	conflict	UNP Q14203
W	1072	GLY	ALA	conflict	UNP Q14203
W	1073	ALA	ILE	conflict	UNP Q14203
W	1080	ILE	SER	conflict	UNP Q14203
W	1113	VAL	ILE	conflict	UNP Q14203
W	1125	ALA	SER	conflict	UNP Q14203
W	1136	LEU	-	insertion	UNP Q14203
W	1137	PRO	-	insertion	UNP Q14203
W	1138	PRO	-	insertion	UNP Q14203
W	1147	ALA	PRO	conflict	UNP Q14203
W	1156	ASN	SER	conflict	UNP Q14203
W	1177	SER	THR	conflict	UNP Q14203
W	1189	LEU	MET	conflict	UNP Q14203
W	1193	THR	ALA	conflict	UNP Q14203
W	1202	ILE	VAL	conflict	UNP Q14203
W	1259	LEU	PHE	conflict	UNP Q14203
W	1277	ASP	SER	conflict	UNP Q14203
X	118	ARG	LYS	conflict	UNP Q14203
X	124	SER	THR	conflict	UNP Q14203
X	125	ASN	THR	conflict	UNP Q14203
X	134	PRO	LEU	conflict	UNP Q14203
X	200	ALA	VAL	conflict	UNP Q14203
X	207	ALA	VAL	conflict	UNP Q14203
X	631	ASP	GLU	conflict	UNP Q14203
X	742	SER	CYS	conflict	UNP Q14203
X	778	SER	THR	conflict	UNP Q14203
X	821	ALA	PRO	conflict	UNP Q14203
X	862	PRO	LEU	conflict	UNP Q14203
X	1048	ILE	LEU	conflict	UNP Q14203
X	1072	GLY	ALA	conflict	UNP Q14203
X	1073	ALA	ILE	conflict	UNP Q14203
X	1080	ILE	SER	conflict	UNP Q14203
X	1113	VAL	ILE	conflict	UNP Q14203
X	1125	ALA	SER	conflict	UNP Q14203
X	1136	LEU	-	insertion	UNP Q14203
X	1137	PRO	-	insertion	UNP Q14203
X	1138	PRO	-	insertion	UNP Q14203
X	1147	ALA	PRO	conflict	UNP Q14203
X	1156	ASN	SER	conflict	UNP Q14203
X	1177	SER	THR	conflict	UNP Q14203

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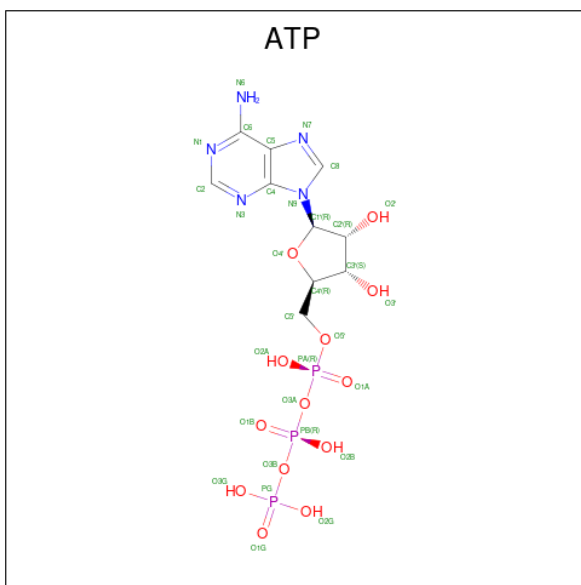
Chain	Residue	Modelled	Actual	Comment	Reference
X	1189	LEU	MET	conflict	UNP Q14203
X	1193	THR	ALA	conflict	UNP Q14203
X	1202	ILE	VAL	conflict	UNP Q14203
X	1259	LEU	PHE	conflict	UNP Q14203
X	1277	ASP	SER	conflict	UNP Q14203

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

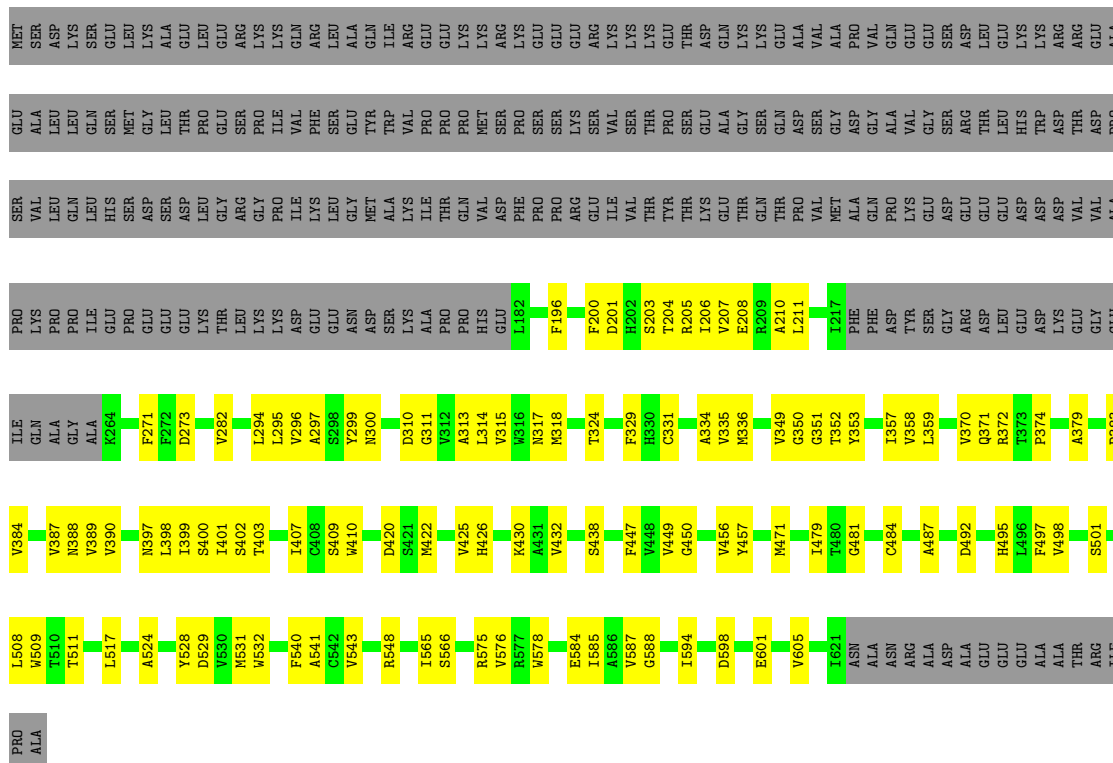
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
11	A	2	Total Mg 2 2	0
11	B	2	Total Mg 2 2	0



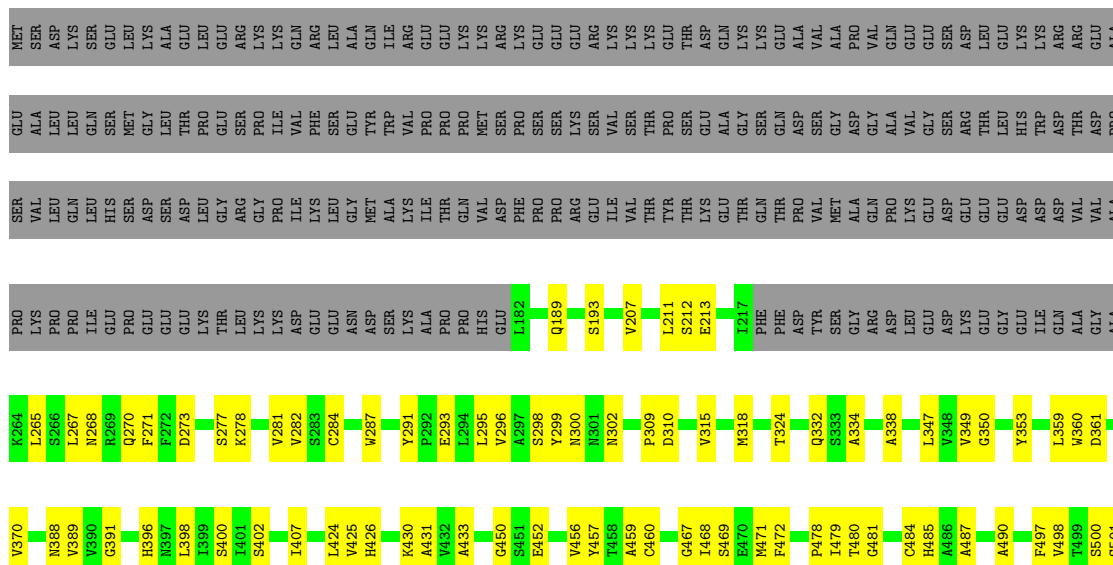
• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

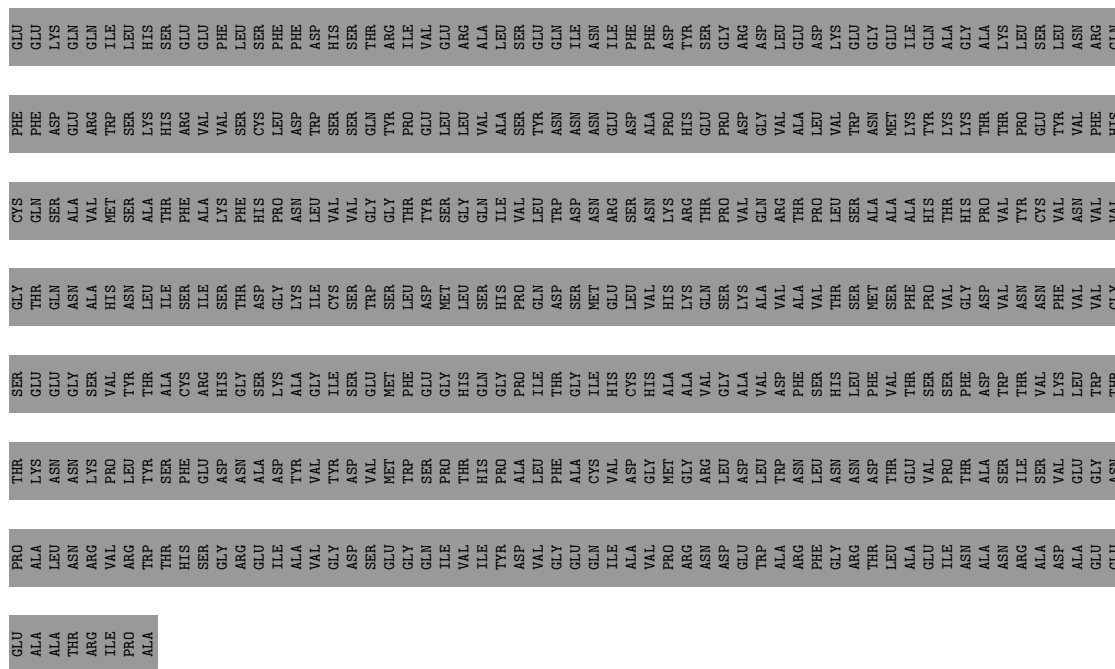
Chain C: 45% 17% 38%



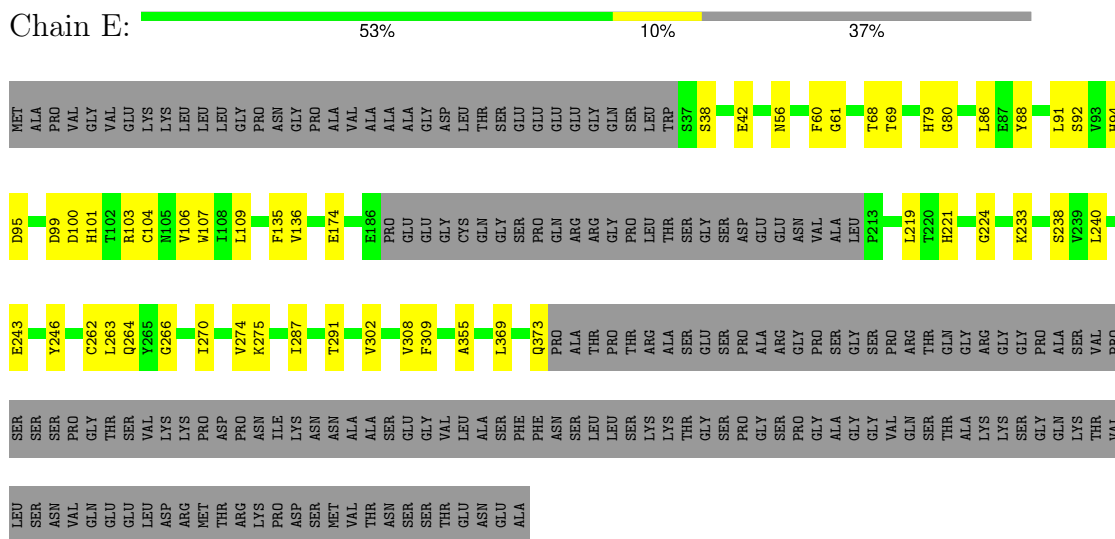
• Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

Chain D: 44% 17% 38%

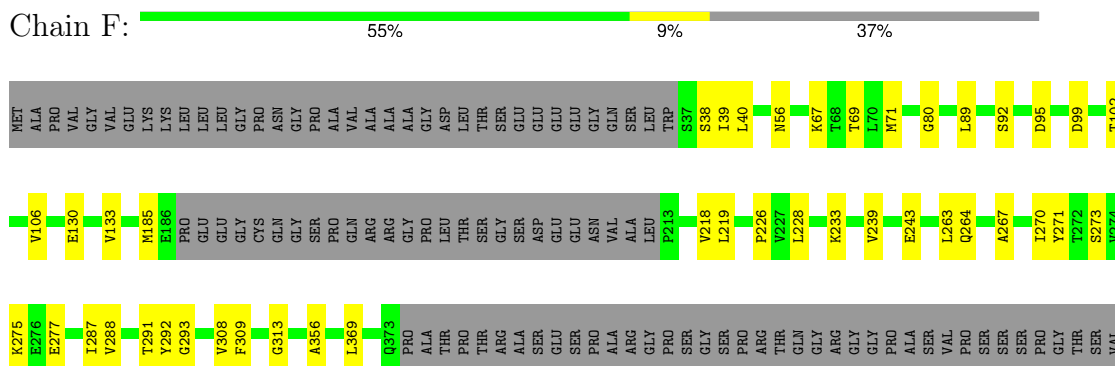


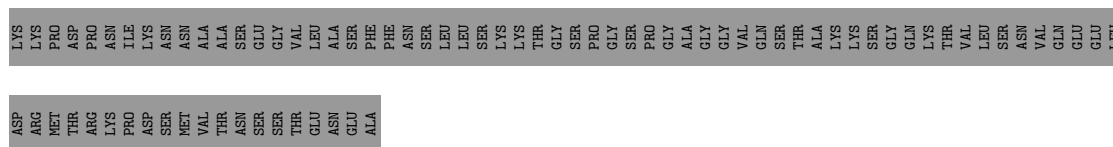


- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2



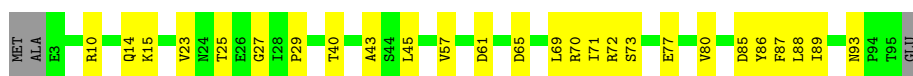
- Molecule 3: Cytoplasmic dynein 1 light intermediate chain 2





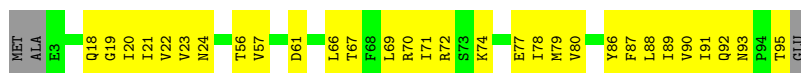
- Molecule 4: Dynein light chain roadblock-type 1

Chain G: 70% 27% .



- Molecule 4: Dynein light chain roadblock-type 1

Chain H: 66% 31% .



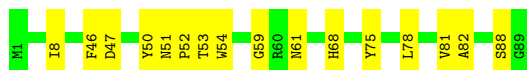
- Molecule 5: Dynein light chain 1, cytoplasmic

Chain I: 64% 34% .



- Molecule 5: Dynein light chain 1, cytoplasmic

Chain J: 82% 18% .



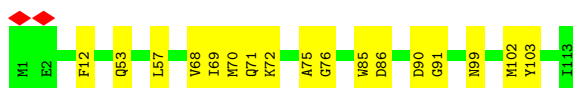
- Molecule 6: Dynein light chain Tctex-type 1

Chain K: 8% 87% 13% .



- Molecule 6: Dynein light chain Tctex-type 1

Chain L: 85% 15% .



- Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta

ASN	SER	LEU	PRO	ARG
SER	ALA	LEU	GLY	LEU
GLN	MET	GLU	ALA	ILE
SER	THR	THR	ALA	SER
LYS	LEU	VAL	VAL	
ARG	HIS	ASN	PRO	
THR	ILE	GLN	THR	
ILE	SER	LEU	ASP	
GLU	GLN	SER	PHE	
GLY	LEU	THR	ALA	
ILE	GLN	THR	THR	
ARG	HIS	PHE	THR	
GLY	GLU	PRO	PHE	
PRO	ASN	VAL	SER	
PRO	PRO	VAL	SER	
SER	VAL	ALA	ALA	
LEU	LEU	PHE	PHE	
GLY	LYS	LEU	LEU	
ILE	GLY	ARG	ARG	
ALA	ALA	SER	ALA	
THR	GLN	SER	LYS	
LEU	MET	PRO	GLU	
VAL	LYS	ALA	GLU	
SER	ALA	ALA	GLN	
GLY	SER	LYS	GLN	
ILE	LEU	SER	ASP	
ALA	ALA	PRO	ASP	
GLY	GLY	SER	THR	
GLU	LEU	ALA	VAL	
GLU	PRO	LEU	TYR	
GLN	PRO	LEU	MET	
GLN	GLN	LEU	GLY	
ARG	ARG	GLU	LYS	
GLY	GLY	VAL	VAL	
ALA	GLY	THR	THR	
ALA	LYS	THR	PHE	
PRO	ALA	GLN	SER	
GLY	GLY	LEU	CYS	
GLN	GLN	LYS	ALA	
PRO	PRO	SER	ALA	
PRO	PRO	LEU	ALA	
GLY	GLY	LEU	GLY	
ILE	ILE	SER	LEU	
VAL	VAL	ASP	GLY	
PRO	PRO	THR	GLN	
GLY	GLY	ILE	ARG	
GLY	SER	GLU	HIS	
GLY	PRO	LYS	ARG	
LEU	LEU	LEU	LEU	
VAL	ALA	VAL	VAL	
LYS	ALA	GLU	THR	
ASP	GLY	VAL	GLN	
LEU	LYS	LEU	GLN	
THR	LYS	GLU	LEU	
LEU	TYR	GLU	THR	
ARG	ARG	THR	HIS	
LEU	LEU	VAL	GLN	
LEU	LYS	SER	LEU	
GLN	THR	THR	HIS	
ASN	GLN	SER	LEU	
ILE	GLN	ASP	HIS	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.798	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	670.09595, 670.09595, 670.09595	wwPDB
Map dimensions	386, 386, 386	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7359998, 1.7359998, 1.7359998	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, MG, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/21569	0.35	2/30067 (0.0%)
1	B	0.20	0/21472	0.35	0/29932
2	C	0.15	0/1945	0.41	0/2706
2	D	0.26	0/1945	0.46	0/2706
2	U	0.06	0/169	0.14	0/235
2	V	0.05	0/169	0.13	0/235
3	E	0.13	0/1538	0.35	0/2141
3	F	0.12	0/1538	0.33	0/2141
4	G	0.19	0/461	0.36	0/642
4	H	0.24	0/461	0.45	0/642
5	I	0.48	0/440	0.77	0/612
5	J	0.43	0/440	0.49	0/612
6	K	0.15	0/557	0.39	0/774
6	L	0.13	0/557	0.38	0/774
7	O	0.11	0/1961	0.28	0/2729
7	P	0.26	0/1917	0.34	0/2667
8	W	0.25	0/2552	0.41	0/3557
8	X	0.24	0/2551	0.45	1/3555 (0.0%)
All	All	0.21	0/62242	0.37	3/86727 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	I	0	1
7	P	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	X	606	VAL	N-CA-C	-5.23	104.55	111.09
1	A	298	LEU	N-CA-C	-5.17	105.54	111.07
1	A	762	LEU	CB-CA-C	-5.13	109.69	115.79

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	52	PRO	Peptide
7	P	98	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21575	0	9567	153	0
1	B	21479	0	9521	135	0
2	C	1947	0	873	63	0
2	D	1947	0	873	63	0
2	U	170	0	73	0	0
2	V	170	0	73	0	0
3	E	1540	0	675	28	0
3	F	1540	0	675	26	0
4	G	462	0	192	21	0
4	H	462	0	192	25	0
5	I	441	0	204	26	0
5	J	441	0	204	12	0
6	K	558	0	261	12	0
6	L	558	0	261	13	0
7	O	1963	0	868	14	0
7	P	1920	0	848	19	0
8	W	2554	0	1213	18	0
8	X	2553	0	1216	39	0
9	A	81	0	36	17	0
9	B	81	0	36	2	0
10	A	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	31	0	12	1	0
11	A	2	0	0	0	0
11	B	2	0	0	0	0
All	All	62508	0	27885	640	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 7.

All (640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HA	1:A:536:LEU:HA	1.36	1.06
1:A:2942:GLY:HA2	9:A:4704:ADP:O1A	1.55	1.05
1:A:2942:GLY:HA2	9:A:4704:ADP:PA	2.01	0.99
3:F:92:SER:HA	3:F:102:THR:O	1.72	0.90
2:C:297:ALA:HB3	2:C:314:LEU:O	1.72	0.90
3:E:233:LYS:H	3:E:274:VAL:H	1.19	0.89
1:A:2942:GLY:CA	9:A:4704:ADP:O1A	2.22	0.88
1:A:2942:GLY:HA3	9:A:4704:ADP:H8	1.44	0.82
4:H:80:VAL:HA	4:H:89:ILE:HA	1.62	0.82
2:D:479:ILE:HA	2:D:501:SER:HA	1.61	0.81
1:B:2229:GLY:HA2	10:B:4702:ATP:H5'1	1.63	0.81
8:W:642:LEU:HA	8:W:647:GLY:HA3	1.63	0.80
2:D:548:ARG:HA	2:D:566:SER:HA	1.62	0.79
2:C:389:VAL:HA	2:C:398:LEU:HA	1.65	0.78
2:D:484:CYS:HA	2:D:497:PHE:HA	1.65	0.78
2:C:531:MET:H	2:C:541:ALA:HB3	1.48	0.78
1:A:2942:GLY:CA	9:A:4704:ADP:PA	2.72	0.77
6:L:12:PHE:H	6:L:91:GLY:H	1.32	0.76
2:C:481:GLY:HA3	2:C:529:ASP:HA	1.68	0.76
4:G:23:VAL:HA	4:G:29:PRO:HA	1.67	0.75
2:C:498:VAL:HA	2:C:508:LEU:HA	1.69	0.75
2:D:425:VAL:H	2:D:468:ILE:H	1.35	0.75
3:E:56:ASN:HA	3:E:106:VAL:HA	1.69	0.75
2:C:532:TRP:HA	2:C:540:PHE:HA	1.68	0.74
1:A:2942:GLY:HA2	9:A:4704:ADP:O5'	1.87	0.74
1:A:464:ASP:HA	1:A:468:LYS:H	1.51	0.74
1:A:654:ILE:HA	2:C:524:ALA:HB1	1.68	0.74
2:C:509:TRP:HA	2:C:517:LEU:H	1.53	0.73
2:C:438:SER:O	2:C:447:PHE:HA	1.89	0.73
4:H:24:ASN:HA	4:H:86:TYR:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:72:ARG:HA	4:H:77:GLU:HA	1.69	0.72
2:C:335:VAL:HA	2:C:352:THR:HA	1.70	0.72
2:C:282:VAL:HA	2:C:299:TYR:HA	1.69	0.71
1:A:228:LYS:CA	1:A:299:LEU:HA	2.21	0.71
1:A:4285:ALA:HB3	1:A:4294:ILE:H	1.55	0.71
3:F:270:ILE:HA	3:F:309:PHE:HA	1.73	0.71
4:G:57:VAL:O	4:G:61:ASP:N	2.24	0.71
8:X:772:GLN:O	8:X:776:GLU:N	2.24	0.71
5:I:77:TYR:HA	5:I:82:ALA:HA	1.71	0.70
1:B:1332:VAL:O	1:B:1335:GLU:N	2.24	0.70
1:A:118:PHE:HA	1:A:137:VAL:HA	1.74	0.70
1:A:747:SER:HA	1:A:768:ALA:HB1	1.74	0.69
2:C:387:VAL:HA	2:C:400:SER:HA	1.73	0.69
1:A:2942:GLY:HA2	9:A:4704:ADP:C5'	2.23	0.69
2:D:481:GLY:HA3	2:D:529:ASP:HA	1.73	0.69
4:H:70:ARG:HA	4:H:79:MET:HA	1.72	0.69
1:B:410:GLU:HA	1:B:467:ARG:HA	1.74	0.69
2:D:480:THR:N	2:D:500:SER:O	2.23	0.69
4:G:80:VAL:HA	4:G:89:ILE:HA	1.74	0.69
6:L:71:GLN:HA	6:L:102:MET:HA	1.73	0.69
1:B:119:ILE:O	1:B:136:ARG:N	2.26	0.69
2:D:424:LEU:HA	2:D:467:GLY:HA2	1.73	0.69
1:B:303:ILE:O	1:B:308:LYS:N	2.24	0.69
4:G:71:ILE:HA	4:H:69:LEU:HA	1.75	0.69
8:W:885:PRO:O	8:W:889:LEU:CB	2.41	0.68
8:X:772:GLN:N	8:X:861:LEU:O	2.23	0.68
1:B:513:ASP:O	1:B:517:ALA:N	2.23	0.68
2:C:450:GLY:HA2	2:C:456:VAL:HA	1.74	0.68
2:C:359:LEU:N	2:C:371:GLN:O	2.24	0.67
1:A:605:GLN:O	1:A:609:ILE:N	2.27	0.67
2:C:295:LEU:H	2:C:317:ASN:HA	1.60	0.67
2:D:273:ASP:HA	2:D:324:THR:HA	1.75	0.67
1:A:65:MET:O	1:A:69:LEU:N	2.26	0.67
2:C:484:CYS:HA	2:C:497:PHE:HA	1.77	0.67
2:C:384:VAL:HA	2:C:402:SER:HA	1.75	0.67
8:X:625:GLN:O	8:X:629:LYS:CB	2.43	0.66
2:D:588:GLY:HA2	2:D:594:ILE:HA	1.77	0.66
5:I:13:MET:N	5:I:73:PHE:O	2.29	0.66
1:A:217:ALA:C	1:A:219:GLN:H	2.03	0.66
1:A:1396:ILE:HA	1:A:1439:LEU:H	1.60	0.66
1:B:303:ILE:O	1:B:307:GLY:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:LEU:O	1:B:573:GLY:N	2.28	0.66
3:F:38:SER:O	3:F:40:LEU:N	2.28	0.66
8:X:566:ALA:O	8:X:570:GLU:N	2.28	0.66
2:C:401:ILE:HA	2:C:407:ILE:HA	1.79	0.65
5:I:73:PHE:HA	5:I:86:PHE:HA	1.78	0.65
1:A:36:LYS:HA	1:A:48:ALA:H	1.62	0.65
1:A:4564:LYS:HA	1:A:4584:ALA:HA	1.78	0.65
3:E:61:GLY:HA3	3:E:136:VAL:H	1.61	0.65
7:O:4:SER:O	7:O:8:ARG:N	2.29	0.64
8:W:596:PHE:O	8:W:603:HIS:N	2.29	0.64
1:A:959:VAL:HA	1:A:1106:VAL:H	1.62	0.64
1:B:666:GLU:O	1:B:670:GLY:N	2.31	0.64
3:E:92:SER:HA	3:E:103:ARG:HA	1.79	0.64
3:E:219:LEU:N	3:E:263:LEU:O	2.28	0.64
2:C:548:ARG:HA	2:C:566:SER:HA	1.77	0.64
6:L:86:ASP:O	6:L:90:ASP:N	2.29	0.64
5:J:78:LEU:H	5:J:82:ALA:HA	1.63	0.64
2:D:268:ASN:N	2:D:596:ILE:O	2.28	0.64
1:A:475:GLN:O	1:A:479:VAL:N	2.24	0.64
1:A:463:LEU:HA	1:A:536:LEU:CA	2.22	0.63
2:C:351:GLY:HA2	2:C:357:ILE:HA	1.78	0.63
4:H:22:VAL:HA	4:H:88:LEU:HA	1.78	0.63
6:L:53:GLN:O	6:L:57:LEU:N	2.30	0.63
6:K:25:ILE:O	6:K:30:GLY:N	2.32	0.63
1:A:476:LEU:O	1:A:480:ILE:N	2.28	0.63
1:B:157:VAL:O	1:B:161:PHE:N	2.31	0.63
2:C:211:LEU:HA	4:G:14:GLN:HA	1.80	0.62
1:A:228:LYS:HA	1:A:299:LEU:HA	1.80	0.62
1:A:294:SER:O	1:A:295:PRO:C	2.42	0.62
1:B:163:SER:O	1:B:167:GLU:N	2.31	0.62
3:F:95:ASP:O	3:F:99:ASP:CA	2.47	0.62
1:A:1238:ASN:O	1:A:1242:LYS:N	2.32	0.62
3:F:95:ASP:O	3:F:99:ASP:N	2.32	0.62
2:D:360:TRP:HA	2:D:370:VAL:H	1.65	0.62
1:A:2942:GLY:C	9:A:4704:ADP:O1A	2.43	0.62
5:I:89:GLY:HA3	5:J:68:HIS:HA	1.82	0.62
1:B:1136:GLY:HA2	1:B:1208:TRP:HA	1.81	0.62
4:G:23:VAL:O	4:G:87:PHE:N	2.26	0.62
7:O:279:VAL:HA	7:O:315:SER:HA	1.81	0.61
2:C:300:ASN:HA	2:C:311:GLY:HA2	1.82	0.61
8:W:594:ASP:O	8:W:598:ARG:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1666:LEU:HA	1:A:1673:VAL:HA	1.82	0.61
2:D:478:PRO:O	2:D:502:PHE:N	2.32	0.61
1:A:2942:GLY:HA2	9:A:4704:ADP:H5'2	1.83	0.61
1:A:4283:LYS:HA	1:A:4295:GLN:HA	1.83	0.61
2:C:334:ALA:O	2:C:353:TYR:N	2.32	0.61
1:A:528:GLU:O	1:A:532:GLU:CB	2.49	0.61
1:A:1274:GLU:O	1:A:1278:GLN:N	2.30	0.61
1:B:4283:LYS:HA	1:B:4295:GLN:HA	1.83	0.61
2:C:487:ALA:HB1	2:C:492:ASP:HA	1.83	0.61
2:D:457:TYR:HA	2:D:471:MET:HA	1.81	0.61
6:K:25:ILE:O	6:K:29:ILE:N	2.34	0.61
8:X:934:GLU:O	8:X:938:ALA:HB2	2.01	0.61
1:A:2942:GLY:CA	9:A:4704:ADP:O5'	2.48	0.60
7:O:237:VAL:HA	7:O:253:SER:HA	1.83	0.60
8:X:576:MET:O	8:X:579:ALA:HB3	2.01	0.60
5:J:54:TRP:HA	5:J:88:SER:H	1.64	0.60
5:I:47:ASP:HA	5:I:52:PRO:N	2.16	0.60
7:P:384:THR:H	7:P:399:SER:HA	1.66	0.60
8:X:575:GLN:O	8:X:579:ALA:N	2.34	0.60
2:D:532:TRP:HA	2:D:540:PHE:HA	1.83	0.60
4:H:77:GLU:N	4:H:92:GLN:O	2.35	0.60
1:B:1665:ILE:O	1:B:1674:LEU:N	2.35	0.60
1:A:406:TYR:HA	1:A:471:ARG:HA	1.83	0.60
5:I:59:GLY:O	5:I:82:ALA:N	2.35	0.60
1:A:474:GLU:O	1:A:478:ALA:N	2.28	0.60
3:F:219:LEU:N	3:F:263:LEU:O	2.35	0.60
4:H:93:ASN:C	4:H:95:THR:H	2.09	0.60
1:A:706:VAL:O	1:A:710:ASN:N	2.30	0.60
2:D:270:GLN:HA	2:D:595:VAL:HA	1.83	0.59
3:E:238:SER:O	3:E:243:GLU:N	2.26	0.59
2:D:347:LEU:HA	2:D:361:ASP:HA	1.84	0.59
4:G:27:GLY:HA2	4:G:43:ALA:HB3	1.84	0.59
4:H:23:VAL:O	4:H:87:PHE:N	2.35	0.59
1:A:723:THR:N	1:A:732:VAL:O	2.30	0.59
2:C:383:PRO:O	2:C:403:THR:N	2.36	0.59
4:H:21:ILE:N	4:H:89:ILE:O	2.36	0.59
2:C:584:GLU:HA	2:C:598:ASP:HA	1.85	0.59
2:D:426:HIS:N	2:D:430:LYS:O	2.35	0.59
2:C:336:MET:N	2:C:351:GLY:O	2.36	0.58
1:A:583:ARG:O	1:A:587:ARG:N	2.36	0.58
1:B:575:ALA:HB3	1:B:581:MET:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:538:ALA:HB1	2:D:555:ASN:H	1.68	0.58
5:I:46:PHE:CB	5:I:56:CYS:H	2.15	0.58
8:X:731:TYR:O	8:X:736:ALA:N	2.28	0.58
2:D:281:VAL:O	2:D:300:ASN:N	2.28	0.58
2:D:509:TRP:HA	2:D:517:LEU:H	1.69	0.58
4:G:69:LEU:HA	4:H:71:ILE:HA	1.85	0.58
6:L:99:ASN:N	6:L:102:MET:O	2.36	0.58
7:P:296:ALA:HB2	7:P:368:LYS:HA	1.85	0.58
1:A:80:GLU:HA	1:A:110:GLY:HA3	1.85	0.58
3:F:228:LEU:HA	3:F:267:ALA:HB1	1.84	0.58
7:P:322:MET:O	7:P:331:LEU:N	2.36	0.58
1:A:1100:LYS:H	1:A:1108:ASP:HA	1.68	0.58
3:F:95:ASP:O	3:F:99:ASP:HA	2.02	0.58
1:B:1347:LYS:HA	1:B:1395:LYS:H	1.69	0.58
1:A:4538:GLU:O	1:A:4595:GLN:N	2.36	0.58
1:B:68:PHE:HA	1:B:75:HIS:HA	1.84	0.58
8:X:849:ALA:O	8:X:853:ALA:N	2.37	0.58
1:B:715:GLY:O	1:B:824:TRP:N	2.32	0.57
2:C:349:VAL:HA	2:C:359:LEU:HA	1.84	0.57
2:C:601:GLU:O	2:C:605:VAL:N	2.35	0.57
3:E:91:LEU:N	3:E:104:CYS:O	2.35	0.57
2:C:399:ILE:HA	2:C:409:SER:HA	1.86	0.57
1:A:83:THR:HA	1:A:99:ILE:HA	1.86	0.57
1:A:2900:PHE:O	1:A:2904:GLU:N	2.33	0.57
7:O:196:SER:H	7:O:211:SER:HA	1.69	0.57
1:A:84:LEU:N	1:A:98:PHE:O	2.37	0.57
1:B:626:GLN:O	1:B:630:SER:N	2.27	0.57
1:A:271:ALA:HB3	1:A:342:ASN:H	1.70	0.57
3:E:68:THR:C	3:E:80:GLY:H	2.13	0.57
8:W:875:GLU:HA	8:W:881:PRO:HA	1.86	0.57
7:O:365:TRP:HA	7:O:373:MET:H	1.69	0.57
1:A:4073:SER:O	1:A:4077:PHE:N	2.33	0.57
1:B:1260:ASP:O	1:B:1264:THR:N	2.38	0.57
2:C:578:TRP:HA	2:C:585:ILE:HA	1.87	0.57
8:X:801:ILE:O	8:X:805:MET:N	2.38	0.57
2:C:359:LEU:O	2:C:370:VAL:N	2.36	0.57
2:C:388:ASN:N	2:C:399:ILE:O	2.34	0.57
3:E:233:LYS:H	3:E:274:VAL:N	1.96	0.57
7:P:342:ARG:H	7:P:357:ALA:HA	1.70	0.56
1:A:464:ASP:C	1:A:466:MET:N	2.62	0.56
1:B:329:VAL:O	1:B:333:ASN:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1724:VAL:O	1:B:1728:GLY:N	2.36	0.56
3:E:270:ILE:HA	3:E:309:PHE:HA	1.87	0.56
1:B:1176:LEU:O	1:B:1181:LYS:N	2.35	0.56
2:D:391:GLY:HA3	2:D:396:HIS:HA	1.88	0.56
6:K:67:CYS:HA	6:K:107:SER:H	1.70	0.56
5:I:46:PHE:O	5:I:51:ASN:N	2.30	0.56
1:A:806:ALA:HB1	3:E:355:ALA:HA	1.86	0.56
1:B:659:THR:O	1:B:663:LYS:N	2.31	0.56
4:G:45:LEU:CB	4:H:56:THR:HA	2.36	0.56
7:P:323:TRP:HA	7:P:331:LEU:H	1.71	0.56
1:A:228:LYS:C	1:A:299:LEU:HA	2.30	0.55
1:B:1143:HIS:CB	1:B:1214:ILE:HA	2.36	0.55
3:E:302:VAL:HA	3:E:308:VAL:HA	1.88	0.55
4:H:20:ILE:HA	4:H:90:VAL:HA	1.88	0.55
4:H:78:ILE:HA	4:H:91:ILE:HA	1.89	0.55
5:I:52:PRO:HA	5:I:53:THR:C	2.32	0.55
1:B:4565:LEU:N	1:B:4583:THR:O	2.40	0.55
4:G:72:ARG:O	4:H:67:THR:N	2.40	0.55
1:B:191:MET:O	1:B:195:HIS:N	2.40	0.55
2:C:206:ILE:O	2:C:210:ALA:N	2.38	0.55
4:G:70:ARG:N	4:H:70:ARG:O	2.39	0.55
3:F:67:LYS:O	3:F:71:MET:CB	2.55	0.55
7:O:293:ILE:O	7:O:297:THR:N	2.38	0.55
8:W:557:ILE:O	8:W:561:GLU:N	2.38	0.55
1:A:36:LYS:HA	1:A:48:ALA:N	2.21	0.55
2:C:310:ASP:N	2:C:331:CYS:O	2.40	0.55
6:K:78:HIS:O	6:L:69:ILE:N	2.40	0.55
1:B:723:THR:O	1:B:732:VAL:N	2.30	0.55
1:A:2590:PRO:HA	1:A:2708:PHE:O	2.07	0.55
1:B:1136:GLY:HA2	1:B:1208:TRP:CA	2.36	0.55
1:B:2664:ASP:HA	1:B:2711:ALA:HB3	1.89	0.55
1:A:723:THR:O	1:A:732:VAL:N	2.38	0.54
8:X:641:GLY:O	8:X:648:GLU:N	2.40	0.54
1:A:578:ALA:O	1:A:583:ARG:N	2.40	0.54
2:D:287:TRP:HA	2:D:295:LEU:HA	1.89	0.54
1:B:1101:GLU:HA	1:B:1106:VAL:HA	1.90	0.54
4:H:18:GLN:N	4:H:91:ILE:O	2.41	0.54
8:X:875:GLU:CB	8:X:883:SER:H	2.20	0.54
1:A:1374:PRO:O	1:A:1378:ARG:N	2.39	0.54
3:F:239:VAL:O	3:F:243:GLU:N	2.40	0.54
7:O:177:TRP:HA	7:O:184:CYS:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1375:ALA:O	1:B:1379:GLN:N	2.36	0.54
1:A:479:VAL:O	1:A:483:VAL:N	2.41	0.54
1:B:1911:GLY:H	9:B:4701:ADP:H5'1	1.72	0.54
2:D:553:ASN:O	2:D:557:ASP:N	2.36	0.54
1:B:4002:LEU:O	1:B:4005:ALA:HB3	2.08	0.54
1:B:1197:LEU:O	1:B:1202:PHE:N	2.41	0.54
3:F:273:SER:O	3:F:277:GLU:N	2.41	0.54
1:B:121:ARG:H	1:B:135:LEU:HA	1.73	0.53
2:D:338:ALA:HA	2:D:350:GLY:HA3	1.90	0.53
7:O:95:ILE:O	7:O:410:ARG:N	2.37	0.53
2:C:398:LEU:N	2:C:410:TRP:O	2.40	0.53
1:A:1430:THR:O	1:A:1434:ILE:N	2.40	0.53
1:A:2659:LEU:O	1:A:2707:GLN:N	2.38	0.53
1:B:804:LEU:O	1:B:894:SER:N	2.41	0.53
8:W:717:VAL:O	8:W:721:THR:N	2.34	0.53
1:B:1375:ALA:C	1:B:1380:TYR:H	2.16	0.53
1:B:256:ILE:O	1:B:260:THR:N	2.38	0.53
1:B:807:GLY:O	1:B:811:GLU:N	2.41	0.53
2:D:388:ASN:H	2:D:400:SER:HA	1.73	0.53
1:B:896:LEU:O	1:B:900:VAL:CB	2.57	0.53
8:W:767:LEU:O	8:W:771:LEU:N	2.42	0.53
1:A:4387:TRP:O	1:A:4391:ILE:N	2.33	0.53
6:K:29:ILE:O	6:K:32:ASN:N	2.42	0.53
2:C:296:VAL:HA	2:C:315:VAL:HA	1.90	0.53
3:F:288:VAL:O	3:F:293:GLY:N	2.41	0.53
4:H:19:GLY:O	4:H:91:ILE:N	2.35	0.53
8:W:873:ALA:O	8:W:877:ILE:N	2.34	0.53
1:B:320:THR:O	1:B:322:LEU:N	2.42	0.53
5:J:47:ASP:CB	5:J:53:THR:HA	2.39	0.53
7:P:366:ASP:N	7:P:371:ARG:O	2.41	0.53
8:X:905:THR:O	8:X:909:GLU:N	2.42	0.53
3:E:287:ILE:O	3:E:291:THR:N	2.41	0.52
1:A:2957:SER:O	1:A:2991:ALA:N	2.38	0.52
2:D:284:CYS:O	2:D:298:SER:N	2.29	0.52
1:A:205:ILE:H	1:A:256:ILE:HA	1.74	0.52
2:D:334:ALA:O	2:D:353:TYR:N	2.40	0.52
3:F:69:THR:HA	3:F:80:GLY:H	1.74	0.52
7:P:238:ARG:H	7:P:253:SER:HA	1.75	0.52
1:A:217:ALA:C	1:A:219:GLN:N	2.63	0.52
1:A:912:GLY:O	1:A:1026:MET:HA	2.09	0.52
5:I:35:GLU:O	5:I:39:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:35:GLU:O	5:I:39:ALA:CB	2.58	0.52
5:I:53:THR:C	5:I:87:LYS:HA	2.35	0.52
2:D:267:LEU:HA	2:D:597:TYR:HA	1.91	0.52
3:F:89:LEU:N	3:F:106:VAL:O	2.43	0.52
5:I:52:PRO:HA	5:I:54:TRP:N	2.25	0.52
1:A:23:ASN:O	1:A:126:ASP:HA	2.10	0.52
1:A:2942:GLY:N	9:A:4704:ADP:PA	2.83	0.52
1:B:1667:ASN:N	1:B:1672:VAL:O	2.39	0.52
1:B:1901:GLY:O	1:B:2037:ARG:N	2.43	0.52
8:X:816:ALA:N	8:X:914:ALA:O	2.43	0.52
1:A:4445:THR:O	1:A:4449:ARG:N	2.30	0.51
5:J:54:TRP:HA	5:J:88:SER:N	2.25	0.51
1:B:1161:ALA:C	1:B:1163:THR:H	2.18	0.51
2:D:490:ALA:HB2	2:D:608:ASN:HA	1.92	0.51
6:L:70:MET:O	6:L:103:TYR:CB	2.59	0.51
8:W:874:SER:HA	8:W:878:TYR:H	1.75	0.51
1:A:2942:GLY:H	9:A:4704:ADP:PA	2.33	0.51
1:B:1082:LEU:O	1:B:1086:ILE:N	2.37	0.51
1:A:120:LYS:HA	1:A:135:LEU:HA	1.91	0.51
1:A:721:GLU:H	1:A:735:LEU:HA	1.76	0.51
3:E:233:LYS:HA	3:E:275:LYS:H	1.76	0.51
8:W:683:LYS:O	8:W:687:SER:N	2.44	0.51
1:A:1151:GLN:O	1:A:1155:GLN:N	2.43	0.51
1:A:1260:ASP:O	1:A:1264:THR:N	2.31	0.51
4:H:77:GLU:O	4:H:92:GLN:N	2.38	0.51
8:X:567:LYS:O	8:X:571:MET:N	2.40	0.51
1:A:485:ARG:O	1:A:512:PHE:N	2.44	0.51
1:A:578:ALA:C	1:A:583:ARG:H	2.19	0.51
1:B:718:PHE:HA	1:B:738:ASN:H	1.76	0.51
8:X:705:LEU:O	8:X:709:ASP:N	2.44	0.51
8:X:875:GLU:O	8:X:880:THR:N	2.44	0.51
1:A:294:SER:O	1:A:297:VAL:N	2.44	0.50
1:B:4285:ALA:O	1:B:4294:ILE:N	2.42	0.50
1:B:806:ALA:HB1	3:F:356:ALA:HB2	1.93	0.50
2:C:207:VAL:O	2:C:211:LEU:N	2.45	0.50
3:F:288:VAL:HA	3:F:292:TYR:H	1.76	0.50
5:I:54:TRP:N	5:I:87:LYS:HA	2.25	0.50
1:A:2600:GLY:HA2	9:A:4703:ADP:H5'1	1.94	0.50
1:B:110:GLY:O	1:B:144:SER:N	2.44	0.50
3:E:240:LEU:O	3:E:246:TYR:N	2.42	0.50
1:B:923:THR:O	1:B:927:LEU:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:495:HIS:O	2:C:511:THR:N	2.44	0.50
4:G:15:LYS:O	4:G:93:ASN:N	2.43	0.50
8:X:600:GLY:O	8:X:683:LYS:HA	2.11	0.50
1:B:4445:THR:O	1:B:4449:ARG:N	2.33	0.50
3:E:69:THR:HA	3:E:79:HIS:HA	1.93	0.50
1:A:991:MET:HA	1:A:995:SER:H	1.77	0.50
1:B:723:THR:N	1:B:732:VAL:O	2.41	0.50
1:B:722:SER:HA	1:B:733:LEU:HA	1.93	0.50
2:C:426:HIS:N	2:C:430:LYS:O	2.44	0.50
3:F:218:VAL:HA	3:F:264:GLN:HA	1.93	0.50
7:P:323:TRP:HA	7:P:330:CYS:HA	1.93	0.50
3:E:262:CYS:O	3:E:266:GLY:N	2.44	0.49
5:I:60:ARG:N	5:J:61:ASN:O	2.45	0.49
8:X:677:CYS:N	8:X:921:PRO:O	2.45	0.49
1:B:441:LYS:O	1:B:445:ASN:N	2.45	0.49
1:B:594:ARG:O	1:B:598:ARG:N	2.45	0.49
2:D:389:VAL:HA	2:D:398:LEU:HA	1.94	0.49
1:A:3511:ALA:O	1:A:3515:ALA:HB2	2.12	0.49
2:C:204:THR:O	2:C:208:GLU:N	2.33	0.49
2:C:350:GLY:O	2:C:358:VAL:N	2.33	0.49
2:C:528:TYR:N	2:C:543:VAL:O	2.28	0.49
3:E:38:SER:O	3:E:42:GLU:N	2.44	0.49
1:A:3928:THR:O	1:A:3932:ALA:N	2.38	0.49
6:K:71:GLN:HA	6:K:102:MET:HA	1.93	0.49
8:X:573:LEU:HA	8:X:577:GLU:H	1.78	0.49
1:A:990:LYS:O	1:A:994:LEU:N	2.28	0.49
1:B:81:ARG:O	1:B:113:SER:HA	2.12	0.49
1:B:4603:SER:O	1:B:4626:ILE:N	2.44	0.49
2:D:502:PHE:O	2:D:526:TYR:N	2.46	0.49
7:P:219:TRP:HA	7:P:226:CYS:HA	1.94	0.49
1:A:529:ASN:O	1:A:533:VAL:N	2.46	0.49
1:B:579:ASN:O	1:B:583:ARG:N	2.36	0.49
1:B:37:LEU:O	1:B:41:LEU:N	2.36	0.49
1:B:716:ARG:HA	1:B:823:VAL:HA	1.95	0.49
1:A:1277:LEU:HA	1:A:1330:LYS:HA	1.95	0.49
2:C:271:PHE:N	2:C:594:ILE:O	2.45	0.49
8:X:778:SER:H	8:X:781:ALA:HB3	1.77	0.49
8:X:922:PRO:O	8:X:926:LEU:N	2.43	0.49
1:B:962:LEU:HA	1:B:971:LEU:HA	1.94	0.48
1:B:1329:LEU:O	1:B:1333:TRP:N	2.45	0.48
2:D:293:GLU:O	2:D:318:MET:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:SER:H	2:D:407:ILE:HA	1.78	0.48
5:I:46:PHE:C	5:I:49:LYS:H	2.20	0.48
1:A:164:TYR:CB	1:B:146:TYR:H	2.27	0.48
1:A:1068:ILE:O	1:A:1072:LEU:N	2.46	0.48
8:X:637:SER:O	8:X:762:VAL:HA	2.13	0.48
1:B:642:PRO:O	1:B:646:GLY:N	2.39	0.48
2:C:407:ILE:N	2:C:422:MET:O	2.36	0.48
7:O:278:VAL:O	7:O:316:ARG:N	2.40	0.48
7:P:99:PRO:C	7:P:101:LYS:H	2.20	0.48
7:O:178:ASP:O	7:O:182:PHE:N	2.47	0.48
8:X:766:ARG:O	8:X:769:ALA:N	2.46	0.48
2:D:309:PRO:HA	2:D:332:GLN:HA	1.96	0.48
4:G:65:ASP:O	4:H:74:LYS:N	2.46	0.48
7:P:340:TRP:O	7:P:358:ASP:N	2.37	0.48
1:B:333:ASN:O	1:B:335:LEU:N	2.47	0.48
8:W:731:TYR:O	8:W:736:ALA:N	2.47	0.48
1:B:1269:GLY:HA3	1:B:1384:GLU:H	1.79	0.48
1:B:1475:LEU:N	1:B:1586:PRO:O	2.46	0.48
2:C:358:VAL:HA	2:C:372:ARG:HA	1.94	0.48
2:D:574:ASN:N	2:D:588:GLY:O	2.47	0.48
1:A:294:SER:O	1:A:298:LEU:N	2.36	0.48
1:A:464:ASP:C	1:A:466:MET:H	2.21	0.48
1:A:4603:SER:O	1:A:4626:ILE:N	2.38	0.48
2:C:457:TYR:HA	2:C:471:MET:HA	1.95	0.48
3:E:95:ASP:N	3:E:100:ASP:O	2.47	0.48
8:X:658:TYR:HA	8:X:755:SER:CB	2.43	0.48
8:X:816:ALA:O	8:X:914:ALA:N	2.45	0.48
1:A:119:ILE:O	1:A:136:ARG:N	2.42	0.47
1:B:58:GLU:O	1:B:62:LEU:N	2.32	0.47
1:B:717:ILE:N	1:B:822:LEU:O	2.29	0.47
5:I:42:ILE:O	5:I:46:PHE:N	2.40	0.47
6:K:79:THR:HA	6:L:68:VAL:HA	1.94	0.47
1:B:4341:SER:O	1:B:4345:LYS:N	2.42	0.47
2:C:425:VAL:HA	2:C:432:VAL:H	1.79	0.47
2:C:576:VAL:HA	2:C:587:VAL:HA	1.95	0.47
2:D:433:ALA:HB3	2:D:452:GLU:H	1.78	0.47
3:F:287:ILE:O	3:F:291:THR:N	2.32	0.47
1:A:2693:TYR:HA	1:A:2700:TRP:HA	1.97	0.47
1:A:2942:GLY:N	9:A:4704:ADP:O5'	2.48	0.47
5:I:60:ARG:HA	5:I:81:VAL:HA	1.96	0.47
8:X:599:PRO:HA	8:X:604:ASP:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1474:GLU:HA	1:B:1587:LEU:HA	1.96	0.47
2:D:539:LEU:HA	2:D:553:ASN:HA	1.96	0.47
4:G:10:ARG:O	4:G:14:GLN:N	2.45	0.47
1:B:721:GLU:O	1:B:734:LYS:N	2.48	0.47
2:D:457:TYR:HA	2:D:472:PHE:H	1.79	0.47
8:X:598:ARG:O	8:X:603:HIS:N	2.48	0.47
8:X:875:GLU:O	8:X:879:GLY:N	2.48	0.47
1:A:117:ALA:N	1:A:138:LEU:O	2.46	0.47
1:A:958:VAL:N	1:A:1104:PRO:O	2.47	0.47
7:O:217:LYS:HA	7:O:229:THR:HA	1.97	0.47
8:W:423:ILE:HA	8:X:423:ILE:HA	1.96	0.47
1:B:1138:ASN:O	1:B:1142:PHE:N	2.47	0.47
2:D:265:LEU:HA	2:D:599:VAL:HA	1.96	0.47
2:D:459:ALA:HA	2:D:468:ILE:HA	1.97	0.47
1:A:716:ARG:HA	1:A:823:VAL:HA	1.97	0.46
1:B:912:GLY:HA2	1:B:1022:ALA:HB1	1.96	0.46
2:D:273:ASP:O	2:D:277:SER:N	2.49	0.46
1:A:477:ARG:O	1:A:481:VAL:N	2.47	0.46
1:A:2641:TYR:HA	1:A:2650:LEU:HA	1.96	0.46
2:C:196:PHE:O	2:C:200:PHE:N	2.48	0.46
7:P:24:TYR:O	7:P:28:TYR:N	2.47	0.46
1:A:4565:LEU:N	1:A:4583:THR:O	2.48	0.46
1:B:1141:GLU:O	1:B:1145:GLN:N	2.41	0.46
1:B:1177:LYS:C	8:X:909:GLU:HA	2.41	0.46
1:B:1375:ALA:O	1:B:1380:TYR:N	2.43	0.46
1:B:2942:GLY:HA3	9:B:4704:ADP:C8	2.51	0.46
3:E:88:TYR:HA	3:E:107:TRP:HA	1.98	0.46
5:I:5:LYS:C	5:I:78:LEU:HA	2.41	0.46
8:W:670:TYR:HA	8:W:735:LEU:O	2.16	0.46
1:B:2616:GLU:O	1:B:2660:VAL:N	2.47	0.46
4:G:73:SER:HA	4:H:67:THR:H	1.80	0.46
7:P:153:VAL:HA	7:P:169:SER:HA	1.98	0.46
2:D:460:CYS:H	2:D:469:SER:H	1.63	0.46
6:K:76:GLY:O	6:K:78:HIS:N	2.46	0.46
8:X:642:LEU:HA	8:X:647:GLY:C	2.40	0.46
1:A:3071:SER:O	1:A:3075:LEU:N	2.40	0.46
1:B:1018:PHE:O	1:B:1020:ARG:N	2.44	0.46
7:O:24:TYR:O	7:O:28:TYR:N	2.46	0.45
1:B:568:LEU:C	1:B:573:GLY:H	2.24	0.45
1:B:717:ILE:HA	1:B:824:TRP:HA	1.98	0.45
1:B:1332:VAL:O	1:B:1334:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:O	1:A:73:GLN:N	2.47	0.45
1:A:964:ILE:HA	1:A:969:ILE:HA	1.99	0.45
1:B:1801:PRO:O	1:B:1805:ARG:N	2.40	0.45
1:B:2185:VAL:O	1:B:2189:MET:N	2.49	0.45
4:G:27:GLY:C	4:G:40:THR:HA	2.41	0.45
1:A:2229:GLY:HA2	10:A:4702:ATP:O5'	2.16	0.45
1:B:635:MET:O	1:B:639:ARG:N	2.44	0.45
1:B:4007:MET:O	1:B:4011:THR:N	2.47	0.45
8:W:770:PHE:CB	8:W:848:ALA:HB1	2.47	0.45
1:B:3928:THR:O	1:B:3932:ALA:N	2.39	0.45
2:C:313:ALA:H	2:C:329:PHE:H	1.64	0.45
5:I:9:LYS:H	5:I:76:PHE:HA	1.82	0.45
1:A:1911:GLY:HA3	9:A:4701:ADP:H8	1.82	0.45
1:A:3570:ASP:O	1:A:3574:THR:N	2.41	0.45
2:D:450:GLY:HA2	2:D:456:VAL:HA	1.99	0.45
5:I:28:ALA:O	5:I:32:TYR:N	2.50	0.45
1:B:4087:ALA:O	1:B:4091:GLY:N	2.48	0.45
2:C:548:ARG:HA	2:C:565:ILE:O	2.16	0.45
8:X:599:PRO:C	8:X:601:GLY:H	2.24	0.45
2:C:388:ASN:O	2:C:399:ILE:N	2.39	0.45
2:D:189:GLN:O	2:D:193:SER:N	2.50	0.45
2:D:291:TYR:O	2:D:293:GLU:N	2.46	0.45
8:W:867:GLU:HA	8:W:885:PRO:CB	2.47	0.45
8:X:600:GLY:H	8:X:604:ASP:CB	2.30	0.45
1:A:40:LEU:HA	1:A:45:GLY:N	2.32	0.45
4:G:73:SER:HA	4:H:66:LEU:HA	1.99	0.45
7:P:237:VAL:HA	7:P:253:SER:HA	1.98	0.45
8:W:679:VAL:O	8:W:683:LYS:CB	2.65	0.45
1:A:536:LEU:O	1:A:537:ASP:C	2.60	0.44
4:G:86:TYR:O	4:G:88:LEU:N	2.50	0.44
1:A:117:ALA:N	1:A:140:LEU:H	2.15	0.44
1:A:917:ALA:C	1:A:950:GLY:HA2	2.43	0.44
3:E:86:LEU:HA	3:E:109:LEU:HA	1.98	0.44
2:D:296:VAL:HA	2:D:315:VAL:HA	1.99	0.44
6:K:71:GLN:H	6:L:75:ALA:HB1	1.83	0.44
1:A:37:LEU:O	1:A:41:LEU:N	2.46	0.44
1:A:1473:TYR:O	1:A:1588:VAL:N	2.42	0.44
1:B:568:LEU:HA	1:B:572:LEU:H	1.82	0.44
1:B:802:SER:O	1:B:806:ALA:N	2.47	0.44
1:B:1666:LEU:HA	1:B:1673:VAL:HA	1.98	0.44
1:B:2901:TYR:HA	1:B:2905:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:567:VAL:O	2:D:570:ASN:N	2.50	0.44
7:P:365:TRP:HA	7:P:372:CYS:HA	1.98	0.44
1:A:597:ILE:O	1:A:601:ILE:N	2.47	0.44
2:D:498:VAL:HA	2:D:508:LEU:HA	2.00	0.44
3:F:233:LYS:HA	3:F:275:LYS:H	1.82	0.44
1:A:2592:VAL:O	1:A:2733:VAL:HA	2.17	0.44
1:B:997:PRO:HA	1:B:1018:PHE:HA	2.00	0.44
1:B:3958:GLY:O	1:B:3962:ASP:N	2.48	0.44
2:C:374:PRO:O	2:C:379:ALA:HB3	2.16	0.44
2:D:282:VAL:O	2:D:575:ARG:N	2.51	0.44
5:I:17:MET:CA	5:I:50:TYR:HA	2.47	0.44
7:P:309:PRO:O	7:P:325:VAL:N	2.48	0.44
8:W:732:SER:HA	8:W:736:ALA:HB3	2.00	0.44
1:A:4546:THR:H	1:A:4588:THR:HA	1.83	0.43
5:I:9:LYS:N	5:I:75:TYR:O	2.51	0.43
1:A:657:GLN:HA	1:A:660:ALA:HB3	2.00	0.43
1:B:1347:LYS:HA	1:B:1395:LYS:N	2.31	0.43
2:D:487:ALA:HB2	2:D:534:PRO:C	2.42	0.43
2:D:547:GLY:O	2:D:567:VAL:N	2.50	0.43
3:F:56:ASN:N	3:F:130:GLU:O	2.47	0.43
7:O:344:VAL:HA	7:O:355:SER:HA	2.00	0.43
1:A:775:TYR:O	1:A:779:ILE:CB	2.67	0.43
1:A:1013:THR:O	1:A:1017:LYS:N	2.38	0.43
1:A:1672:VAL:HA	1:A:1691:SER:HA	2.00	0.43
1:B:1384:GLU:O	1:B:1388:ARG:N	2.26	0.43
1:B:1409:LYS:O	1:B:1413:TRP:N	2.39	0.43
2:C:390:VAL:N	2:C:397:ASN:O	2.42	0.43
7:P:178:ASP:O	7:P:182:PHE:N	2.51	0.43
1:B:721:GLU:H	1:B:735:LEU:HA	1.83	0.43
2:D:302:ASN:N	2:D:310:ASP:O	2.51	0.43
3:F:271:TYR:N	3:F:308:VAL:O	2.51	0.43
1:B:718:PHE:HA	1:B:737:VAL:HA	2.01	0.43
1:B:1254:THR:HA	1:B:1290:LEU:CB	2.49	0.43
1:B:2221:MET:N	1:B:2360:GLY:O	2.36	0.43
2:D:271:PHE:N	2:D:594:ILE:O	2.39	0.43
2:D:349:VAL:HA	2:D:359:LEU:HA	1.99	0.43
1:A:630:SER:O	1:A:634:LYS:N	2.50	0.43
1:A:3037:ALA:O	1:A:3041:GLY:N	2.51	0.43
2:D:425:VAL:HA	2:D:431:ALA:HA	2.00	0.43
7:P:324:ASP:N	7:P:329:MET:O	2.51	0.43
1:A:1075:ASP:CB	1:A:1079:TRP:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:LEU:O	1:A:1201:ARG:N	2.52	0.43
1:A:1431:LEU:HA	1:A:1435:TRP:H	1.84	0.43
1:A:2942:GLY:N	9:A:4704:ADP:O3A	2.52	0.43
1:B:485:ARG:O	1:B:486:PRO:C	2.61	0.43
5:J:8:ILE:HA	5:J:75:TYR:O	2.18	0.43
1:A:588:PHE:O	1:A:590:ALA:N	2.52	0.43
1:A:722:SER:HA	1:A:733:LEU:HA	2.00	0.43
1:A:4564:LYS:N	1:A:4643:LEU:O	2.51	0.43
1:B:480:ILE:HA	1:B:484:LEU:H	1.84	0.43
2:C:203:SER:O	2:C:207:VAL:N	2.36	0.43
5:I:4:ARG:O	5:I:26:THR:HA	2.19	0.43
6:L:72:LYS:H	6:L:102:MET:CA	2.32	0.43
1:A:2942:GLY:CA	9:A:4704:ADP:C5'	2.94	0.42
1:B:374:ILE:HA	1:B:377:ALA:HB3	2.00	0.42
5:J:59:GLY:O	5:J:81:VAL:HA	2.19	0.42
6:K:62:LYS:HA	6:L:85:TRP:HA	2.01	0.42
1:A:268:SER:O	1:B:176:ASP:HA	2.19	0.42
1:B:331:ASP:O	1:B:371:LYS:N	2.27	0.42
1:B:333:ASN:O	1:B:336:MET:N	2.45	0.42
1:B:373:PRO:O	1:B:377:ALA:N	2.41	0.42
2:C:449:VAL:O	2:C:457:TYR:N	2.50	0.42
1:A:1671:SER:O	1:A:1692:ILE:N	2.30	0.42
1:B:1666:LEU:HA	1:B:1674:LEU:H	1.84	0.42
3:F:69:THR:HA	3:F:80:GLY:N	2.34	0.42
1:A:441:LYS:O	1:A:445:ASN:N	2.53	0.42
1:A:925:VAL:HA	1:A:930:ALA:H	1.85	0.42
1:A:1869:GLY:HA3	1:A:1924:GLY:C	2.44	0.42
1:B:1197:LEU:O	1:B:1201:ARG:N	2.52	0.42
1:B:2776:PHE:O	1:B:2780:SER:N	2.49	0.42
2:C:201:ASP:O	2:C:205:ARG:N	2.35	0.42
7:P:99:PRO:C	7:P:101:LYS:N	2.77	0.42
8:X:561:GLU:O	8:X:564:ALA:HB3	2.19	0.42
1:A:2659:LEU:N	1:A:2705:ARG:O	2.37	0.42
3:E:94:HIS:HA	3:E:101:HIS:HA	2.02	0.42
3:F:133:VAL:N	3:F:226:PRO:O	2.53	0.42
1:A:464:ASP:O	1:A:466:MET:N	2.52	0.42
1:B:4538:GLU:O	1:B:4595:GLN:N	2.43	0.42
7:O:262:VAL:N	7:O:267:GLU:O	2.36	0.42
1:B:3650:ASN:C	1:B:3652:GLU:N	2.76	0.42
1:B:3950:LYS:HA	1:B:3953:ALA:HB3	2.02	0.42
1:A:179:ALA:HA	1:B:193:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1665:ILE:O	1:A:1674:LEU:N	2.53	0.42
1:B:165:ILE:HA	1:B:171:ALA:H	1.84	0.42
1:B:1088:LYS:O	1:B:1092:THR:CB	2.68	0.42
6:L:72:LYS:H	6:L:102:MET:HA	1.84	0.42
1:A:717:ILE:HA	1:A:738:ASN:H	1.85	0.42
1:A:828:LYS:O	1:A:832:TYR:N	2.34	0.42
1:A:1110:GLY:HA2	1:A:1113:GLN:CB	2.50	0.42
1:A:1186:GLN:HA	1:A:1189:LEU:CB	2.50	0.42
1:B:1143:HIS:CA	1:B:1214:ILE:HA	2.50	0.42
1:B:1210:TYR:O	1:B:1213:ASN:N	2.48	0.42
2:C:575:ARG:O	2:C:588:GLY:N	2.37	0.42
2:D:273:ASP:O	2:D:278:LYS:N	2.52	0.42
8:X:672:HIS:O	8:X:676:GLN:N	2.53	0.42
1:A:222:GLU:C	1:A:224:GLY:H	2.28	0.41
5:I:17:MET:HA	5:I:50:TYR:HA	2.02	0.41
8:X:906:ALA:O	8:X:911:GLU:N	2.52	0.41
1:A:207:LEU:O	1:A:209:ILE:N	2.53	0.41
1:A:228:LYS:H	1:A:231:ASP:CB	2.33	0.41
1:A:236:VAL:HA	1:A:303:ILE:HA	2.03	0.41
1:A:463:LEU:O	1:A:467:ARG:N	2.36	0.41
4:G:73:SER:H	4:G:77:GLU:HA	1.84	0.41
1:A:1076:LEU:O	1:A:1190:TYR:HA	2.20	0.41
1:B:2594:CYS:HA	1:B:2712:CYS:O	2.21	0.41
2:C:409:SER:N	2:C:420:ASP:O	2.49	0.41
2:D:212:SER:O	2:D:213:GLU:C	2.63	0.41
3:E:60:PHE:H	3:E:135:PHE:HA	1.85	0.41
5:J:46:PHE:O	5:J:50:TYR:N	2.54	0.41
2:D:207:VAL:O	2:D:211:LEU:N	2.53	0.41
3:E:174:GLU:HA	3:E:224:GLY:HA3	2.03	0.41
5:J:47:ASP:HA	5:J:52:PRO:HA	2.00	0.41
1:A:752:ASN:O	1:A:756:LEU:N	2.36	0.41
2:D:485:HIS:HA	2:D:532:TRP:CB	2.50	0.41
1:A:1847:ASP:N	1:A:1856:GLN:O	2.53	0.41
2:C:479:ILE:HA	2:C:501:SER:HA	2.02	0.41
2:D:540:PHE:O	2:D:551:LEU:HA	2.20	0.41
6:K:98:GLU:HA	6:K:103:TYR:HA	2.03	0.41
8:X:678:SER:O	8:X:681:VAL:N	2.54	0.41
1:A:2639:CYS:HA	1:A:2653:VAL:H	1.86	0.41
1:B:821:ALA:HB2	3:F:369:LEU:CB	2.50	0.41
3:F:185:MET:HA	3:F:313:GLY:HA3	2.02	0.41
8:X:906:ALA:O	8:X:910:GLY:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:369:LEU:O	3:E:373:GLN:N	2.41	0.41
1:A:94:GLU:H	1:A:212:MET:HA	1.86	0.41
1:A:229:VAL:O	1:A:233:GLY:N	2.54	0.41
1:A:1112:VAL:O	1:A:1116:VAL:N	2.25	0.41
1:B:1345:GLN:HA	1:B:1348:GLU:C	2.45	0.41
1:B:2504:GLY:O	1:B:2735:TYR:N	2.52	0.41
2:C:294:LEU:HA	2:C:318:MET:H	1.84	0.41
2:D:282:VAL:HA	2:D:299:TYR:HA	2.02	0.41
4:H:93:ASN:C	4:H:95:THR:N	2.75	0.41
5:J:47:ASP:O	5:J:52:PRO:N	2.54	0.41
5:J:78:LEU:N	5:J:82:ALA:HA	2.33	0.41
3:E:221:HIS:N	3:E:264:GLN:O	2.54	0.41
1:A:716:ARG:HA	1:A:823:VAL:CA	2.50	0.40
1:B:657:GLN:HA	1:B:660:ALA:HB3	2.03	0.40
1:B:706:VAL:O	1:B:710:ASN:N	2.43	0.40
1:B:806:ALA:O	3:F:356:ALA:HA	2.21	0.40
1:B:4557:SER:HA	1:B:4591:ARG:HA	2.02	0.40
3:E:95:ASP:O	3:E:99:ASP:N	2.54	0.40
4:G:25:THR:N	4:G:85:ASP:O	2.54	0.40
1:A:2951:ALA:O	1:A:2955:GLY:N	2.54	0.40
1:A:3037:ALA:HB1	1:A:3042:LEU:O	2.20	0.40
1:B:526:ALA:HA	1:B:553:TYR:HA	2.03	0.40
1:B:1674:LEU:O	1:B:1686:PHE:N	2.48	0.40
2:C:273:ASP:HA	2:C:324:THR:HA	2.04	0.40
2:D:500:SER:HA	2:D:506:VAL:HA	2.04	0.40
1:B:1430:THR:O	1:B:1434:ILE:N	2.40	0.40
2:D:531:MET:O	2:D:541:ALA:HB3	2.21	0.40
4:G:69:LEU:HA	4:H:72:ARG:H	1.87	0.40
6:K:36:HIS:H	6:L:76:GLY:HA3	1.85	0.40
1:A:1163:THR:O	1:A:1167:VAL:CB	2.69	0.40
1:B:145:PRO:O	1:B:149:LEU:CB	2.69	0.40
4:H:57:VAL:O	4:H:61:ASP:C	2.64	0.40
1:B:1137:SER:O	1:B:1141:GLU:N	2.55	0.40
1:B:3626:ALA:O	1:B:3630:GLY:N	2.55	0.40
3:E:68:THR:O	3:E:80:GLY:N	2.44	0.40
5:I:46:PHE:O	5:I:49:LYS:N	2.49	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4343/4646 (94%)	4106 (94%)	225 (5%)	12 (0%)	36	72
1	B	4321/4646 (93%)	4112 (95%)	206 (5%)	3 (0%)	48	83
2	C	390/638 (61%)	332 (85%)	58 (15%)	0	100	100
2	D	390/638 (61%)	330 (85%)	60 (15%)	0	100	100
2	U	32/638 (5%)	32 (100%)	0	0	100	100
2	V	32/638 (5%)	32 (100%)	0	0	100	100
3	E	307/492 (62%)	282 (92%)	25 (8%)	0	100	100
3	F	307/492 (62%)	272 (89%)	34 (11%)	1 (0%)	36	72
4	G	91/96 (95%)	75 (82%)	16 (18%)	0	100	100
4	H	91/96 (95%)	75 (82%)	16 (18%)	0	100	100
5	I	87/89 (98%)	74 (85%)	12 (14%)	1 (1%)	11	45
5	J	87/89 (98%)	77 (88%)	9 (10%)	1 (1%)	11	45
6	K	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
6	L	111/113 (98%)	98 (88%)	13 (12%)	0	100	100
7	O	393/410 (96%)	371 (94%)	22 (6%)	0	100	100
7	P	382/410 (93%)	361 (94%)	21 (6%)	0	100	100
8	W	511/1281 (40%)	486 (95%)	25 (5%)	0	100	100
8	X	510/1281 (40%)	483 (95%)	27 (5%)	0	100	100
All	All	12496/16806 (74%)	11696 (94%)	782 (6%)	18 (0%)	49	83

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	PRO
1	A	1349	GLN
1	A	1352	VAL
1	B	973	PRO

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Mol	Chain	Res	Type
1	B	1333	TRP
3	F	39	ILE
1	A	206	SER
1	A	208	PRO
1	A	295	PRO
1	B	1393	TYR
1	A	222	GLU
1	A	223	ARG
1	A	465	GLN
1	A	218	LYS
1	A	537	ASP
5	I	51	ASN
5	J	51	ASN
1	A	205	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	X	1/1078 (0%)	1 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
10	ATP	B	4702	11	32,33,33	0.56	0	48,52,52	0.59	0
9	ADP	B	4701	11	28,29,29	0.45	0	43,45,45	0.48	0
10	ATP	A	4702	11	32,33,33	0.56	0	48,52,52	0.67	0
9	ADP	A	4701	11	28,29,29	0.46	0	43,45,45	0.52	0
9	ADP	B	4703	-	28,29,29	0.45	0	43,45,45	0.48	0
9	ADP	A	4703	-	28,29,29	0.45	0	43,45,45	0.49	0
9	ADP	B	4704	-	28,29,29	0.46	0	43,45,45	0.49	0
9	ADP	A	4704	-	28,29,29	0.47	0	43,45,45	0.49	0

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
10	ATP	B	4702	11	-	0/22/38/38	0/3/3/3
9	ADP	B	4701	11	-	2/16/32/32	0/3/3/3
10	ATP	A	4702	11	-	1/22/38/38	0/3/3/3
9	ADP	A	4701	11	-	3/16/32/32	0/3/3/3
9	ADP	B	4703	-	-	0/16/32/32	0/3/3/3
9	ADP	A	4703	-	-	0/16/32/32	0/3/3/3
9	ADP	B	4704	-	-	0/16/32/32	0/3/3/3
9	ADP	A	4704	-	-	0/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

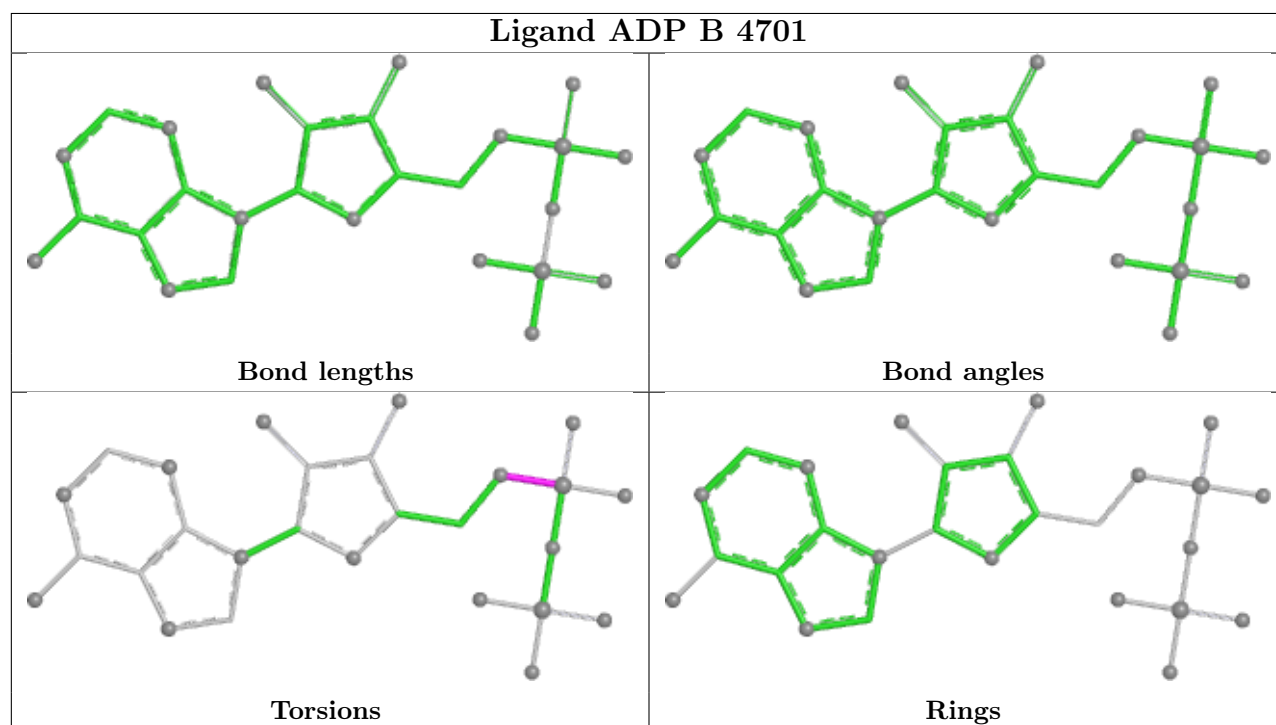
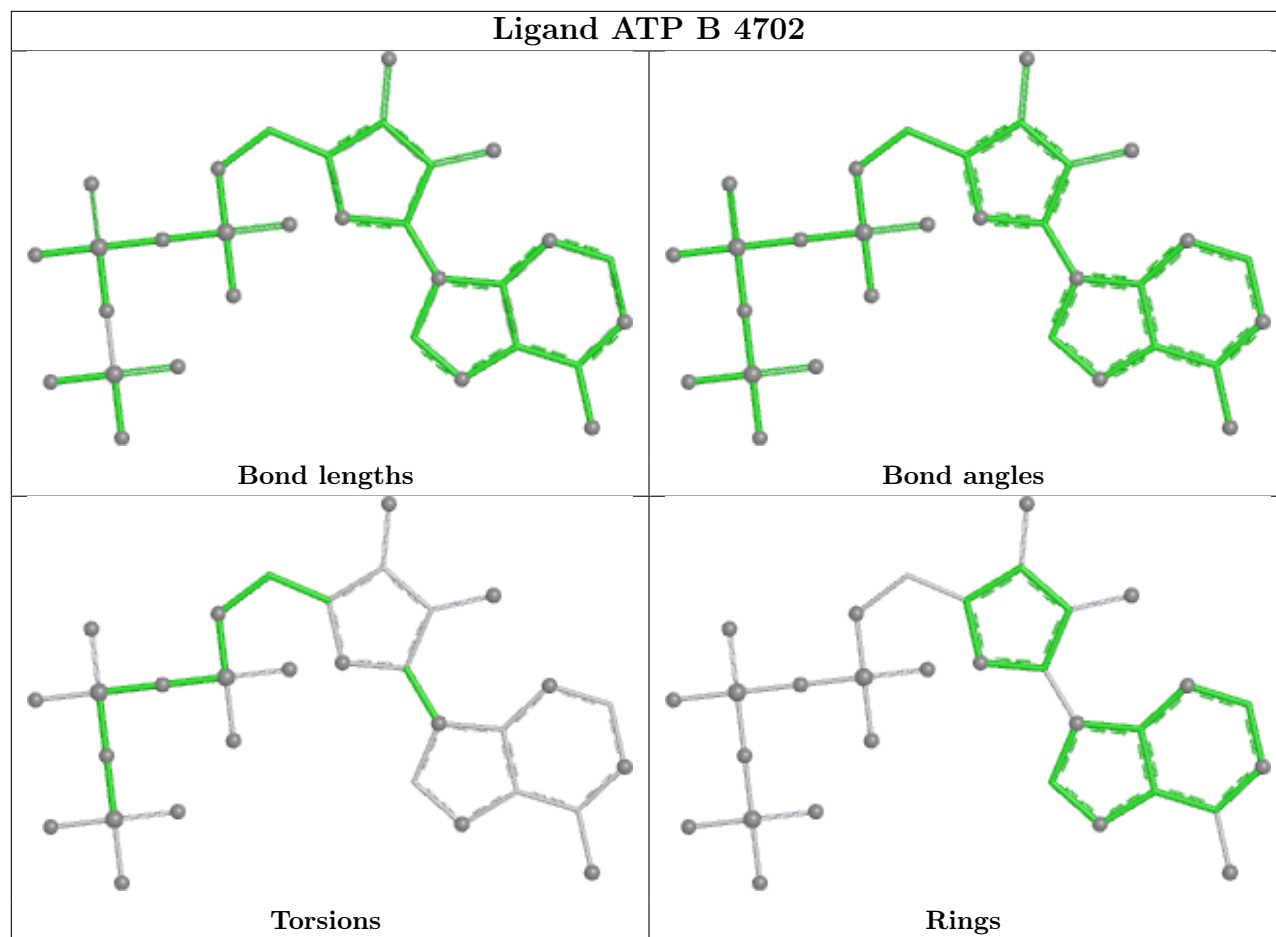
Mol	Chain	Res	Type	Atoms
9	A	4701	ADP	C5'-O5'-PA-O1A
9	B	4701	ADP	C5'-O5'-PA-O2A
9	B	4701	ADP	C5'-O5'-PA-O3A
9	A	4701	ADP	C3'-C4'-C5'-O5'
9	A	4701	ADP	O4'-C4'-C5'-O5'
10	A	4702	ATP	PA-O3A-PB-O2B

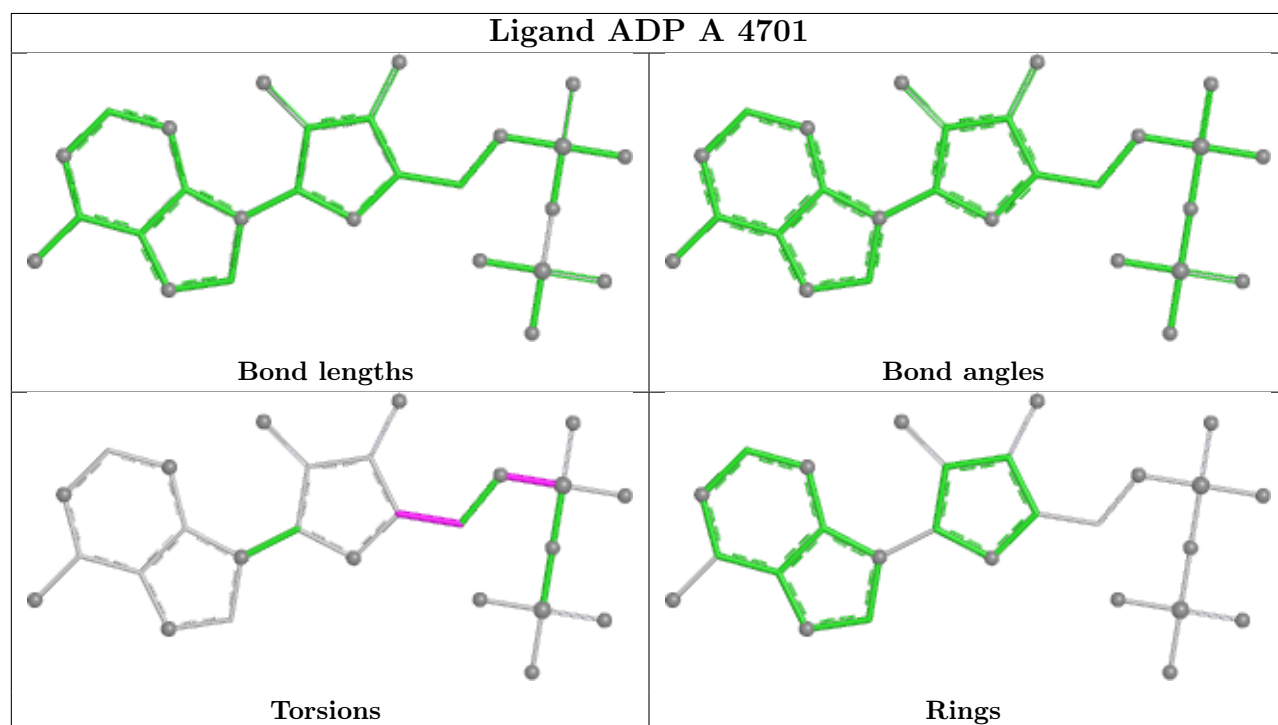
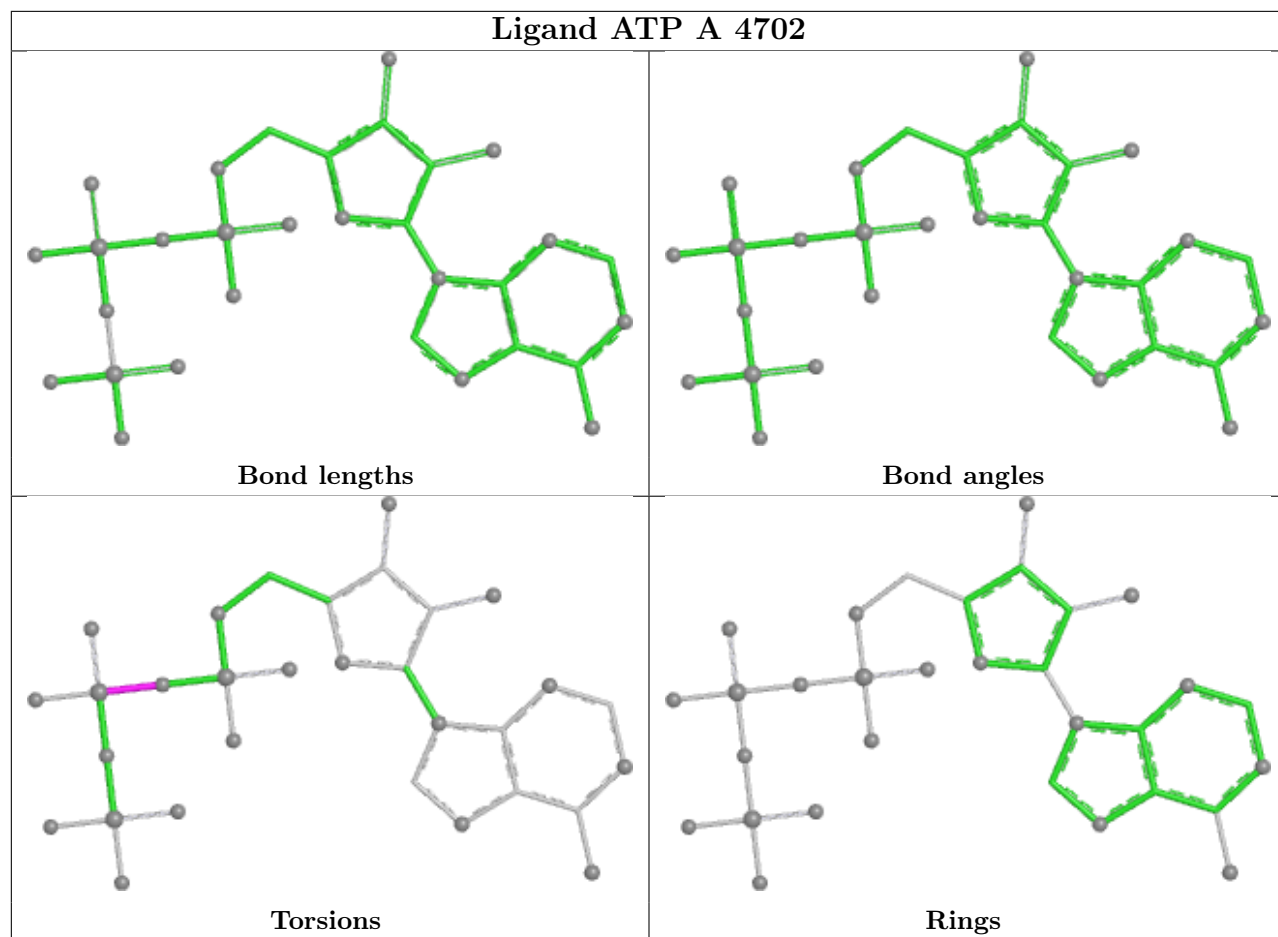
There are no ring outliers.

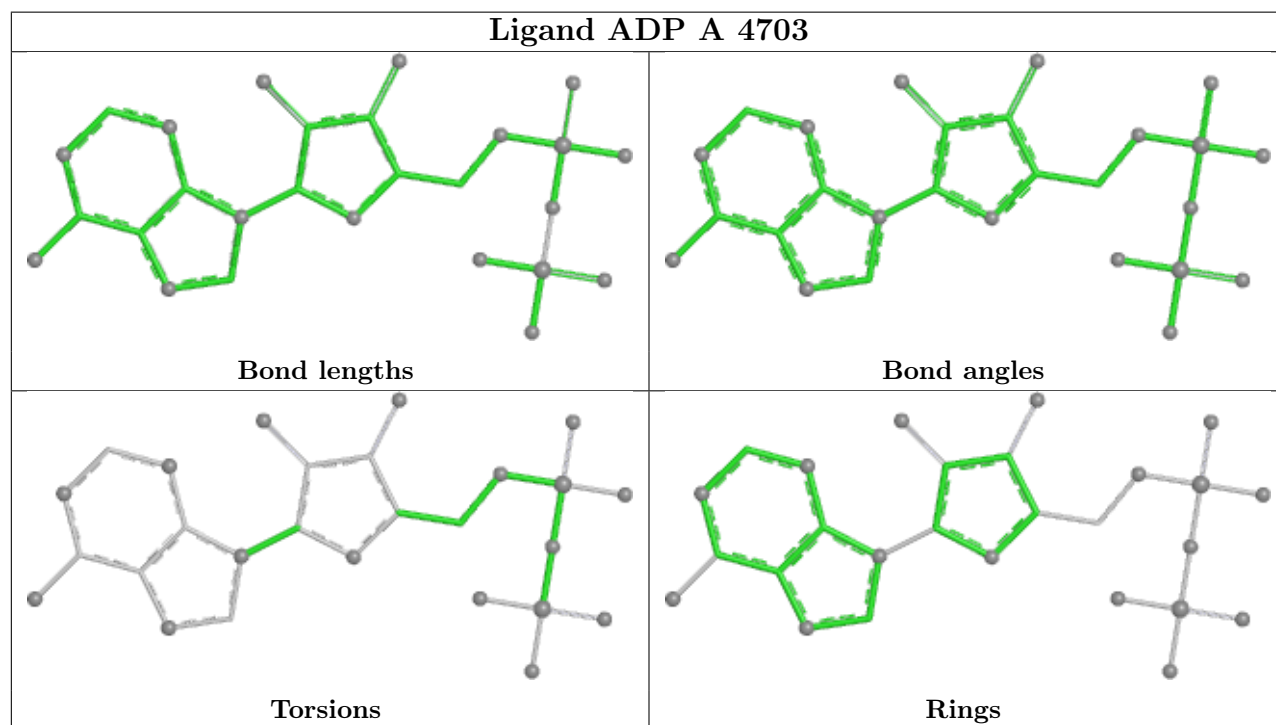
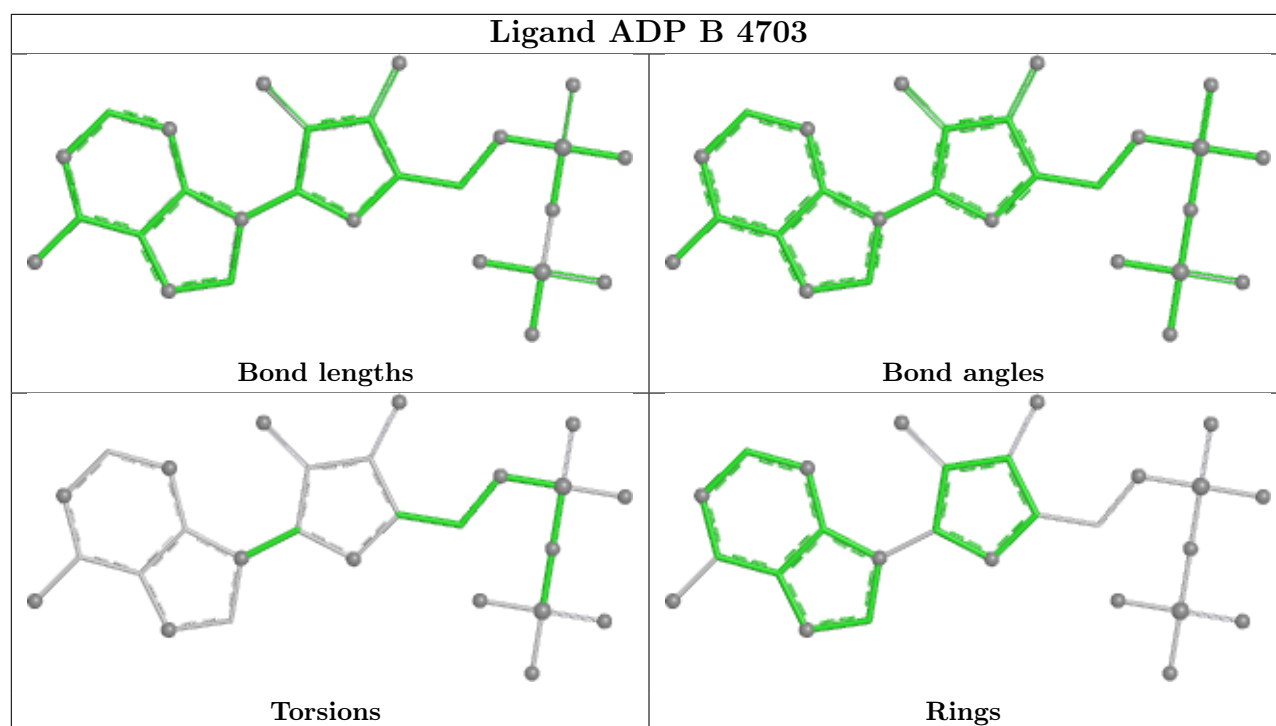
7 monomers are involved in 21 short contacts:

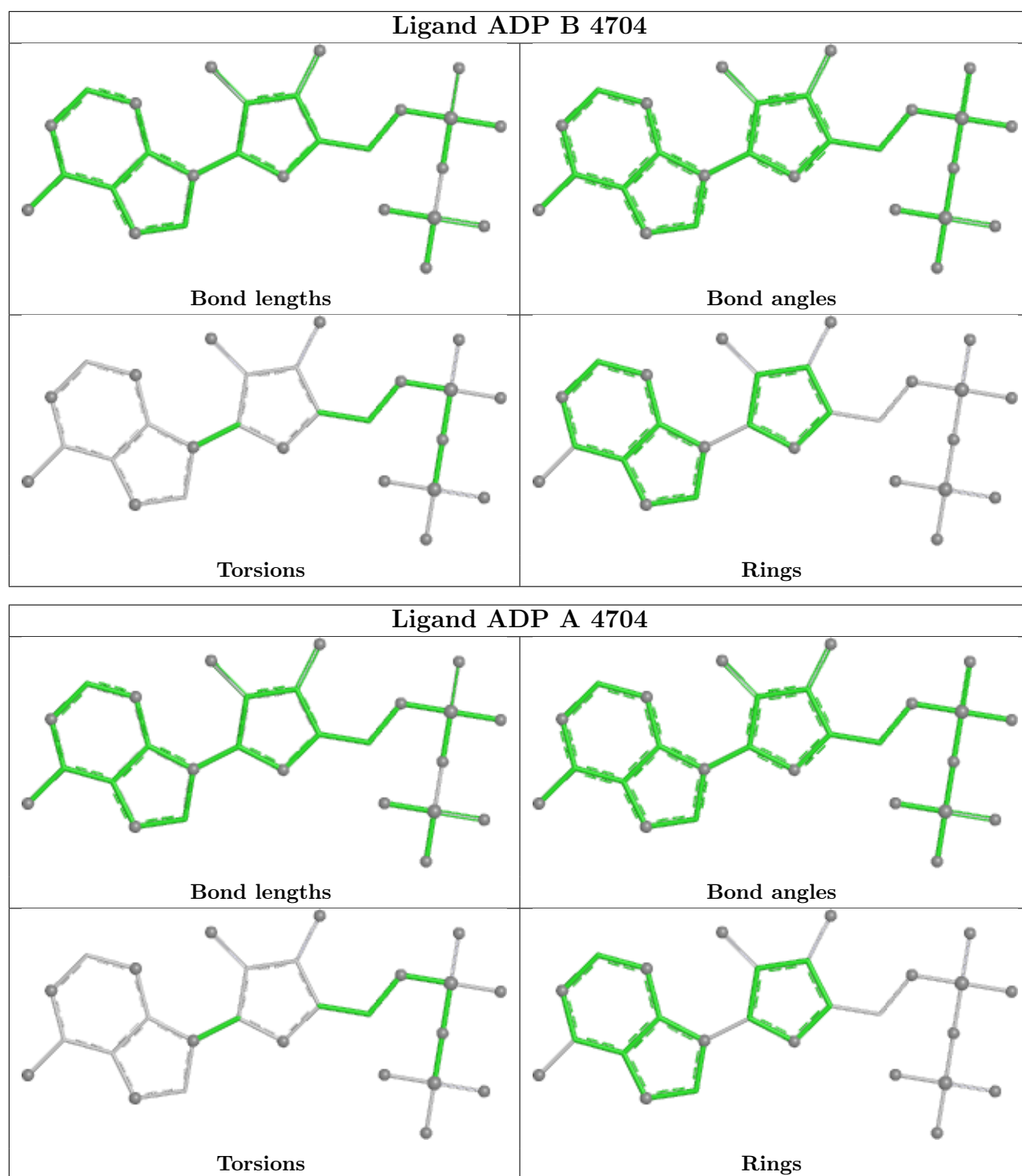
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	4702	ATP	1	0
9	B	4701	ADP	1	0
10	A	4702	ATP	1	0
9	A	4701	ADP	1	0
9	A	4703	ADP	1	0
9	B	4704	ADP	1	0
9	A	4704	ADP	15	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

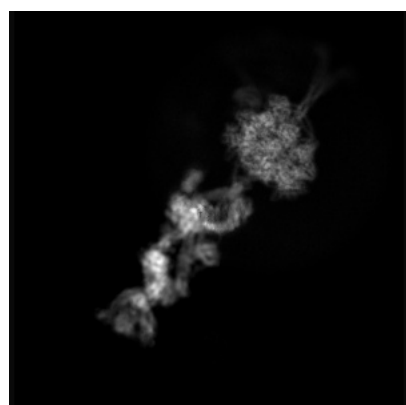
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73179. These allow visual inspection of the internal detail of the map and identification of artifacts.

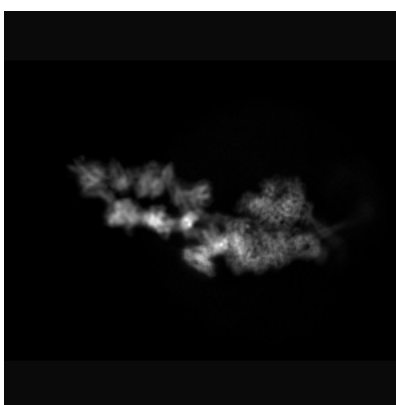
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

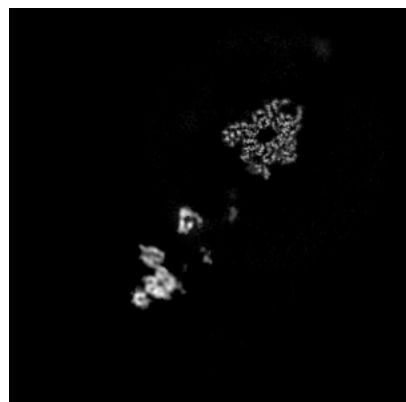


Z

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

6.2 Central slices [i](#)

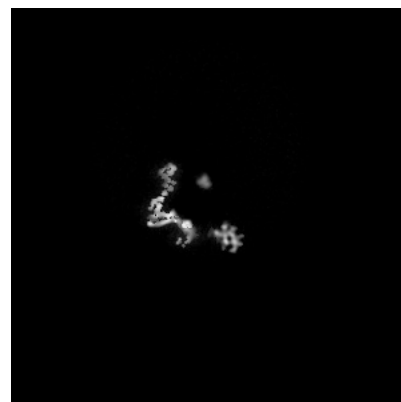
6.2.1 Primary map



X Index: 193



Y Index: 193

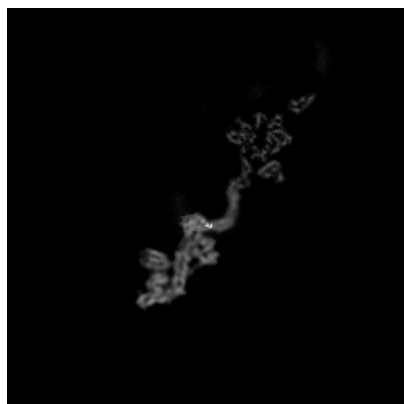


Z Index: 193

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

6.3 Largest variance slices [i](#)

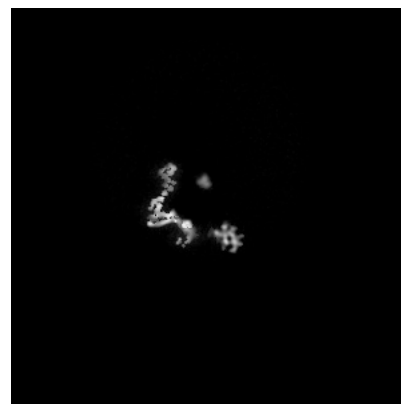
6.3.1 Primary map



X Index: 183



Y Index: 140

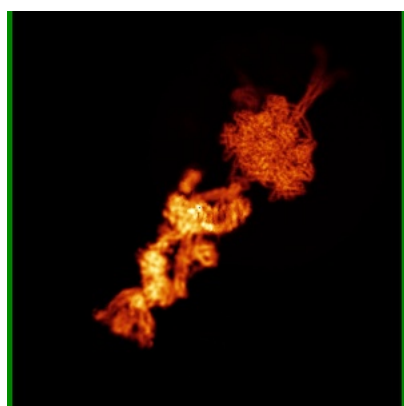


Z Index: 193

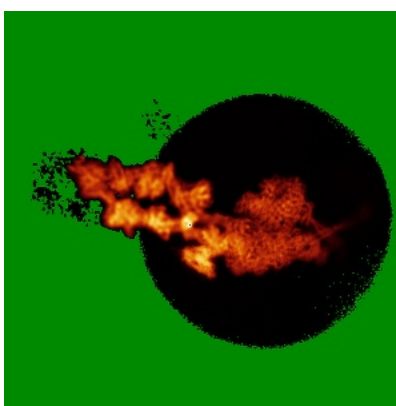
The images above show the largest variance slices of the map in three orthogonal directions.

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

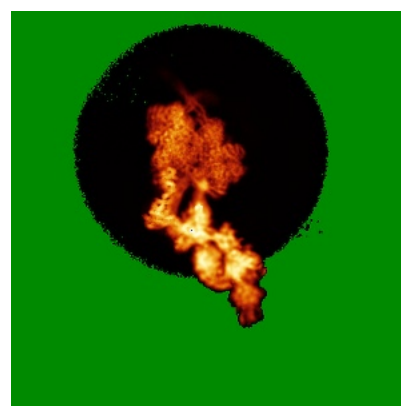
6.4.1 Primary map



X



Y

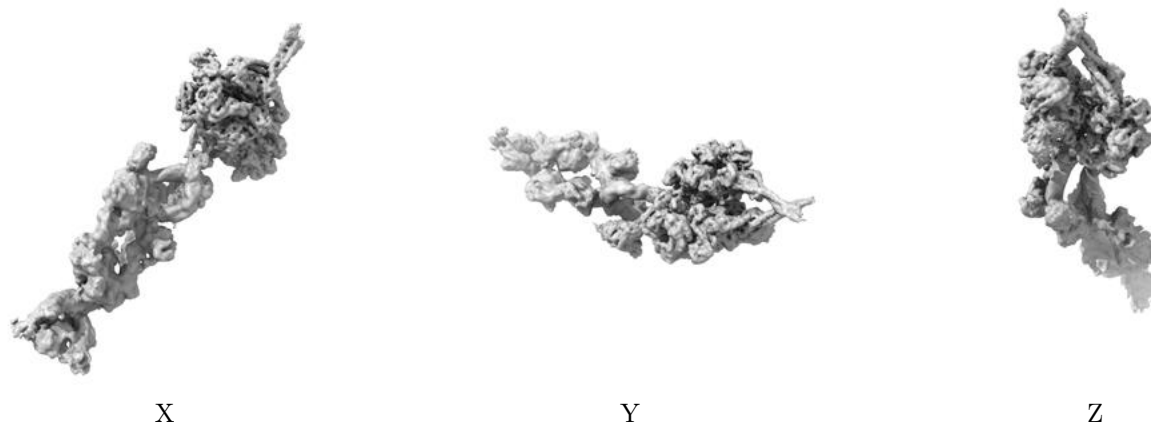


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

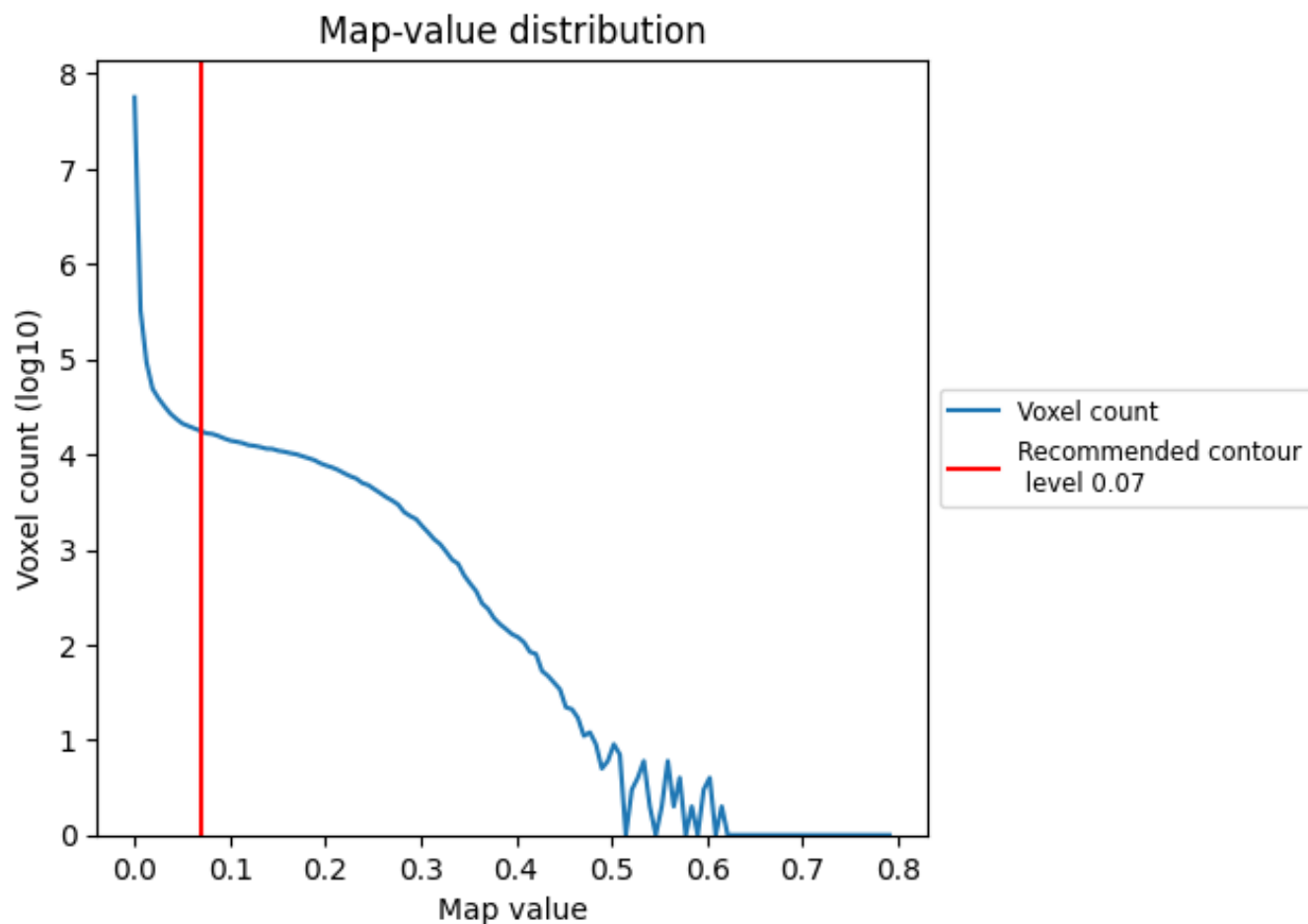
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

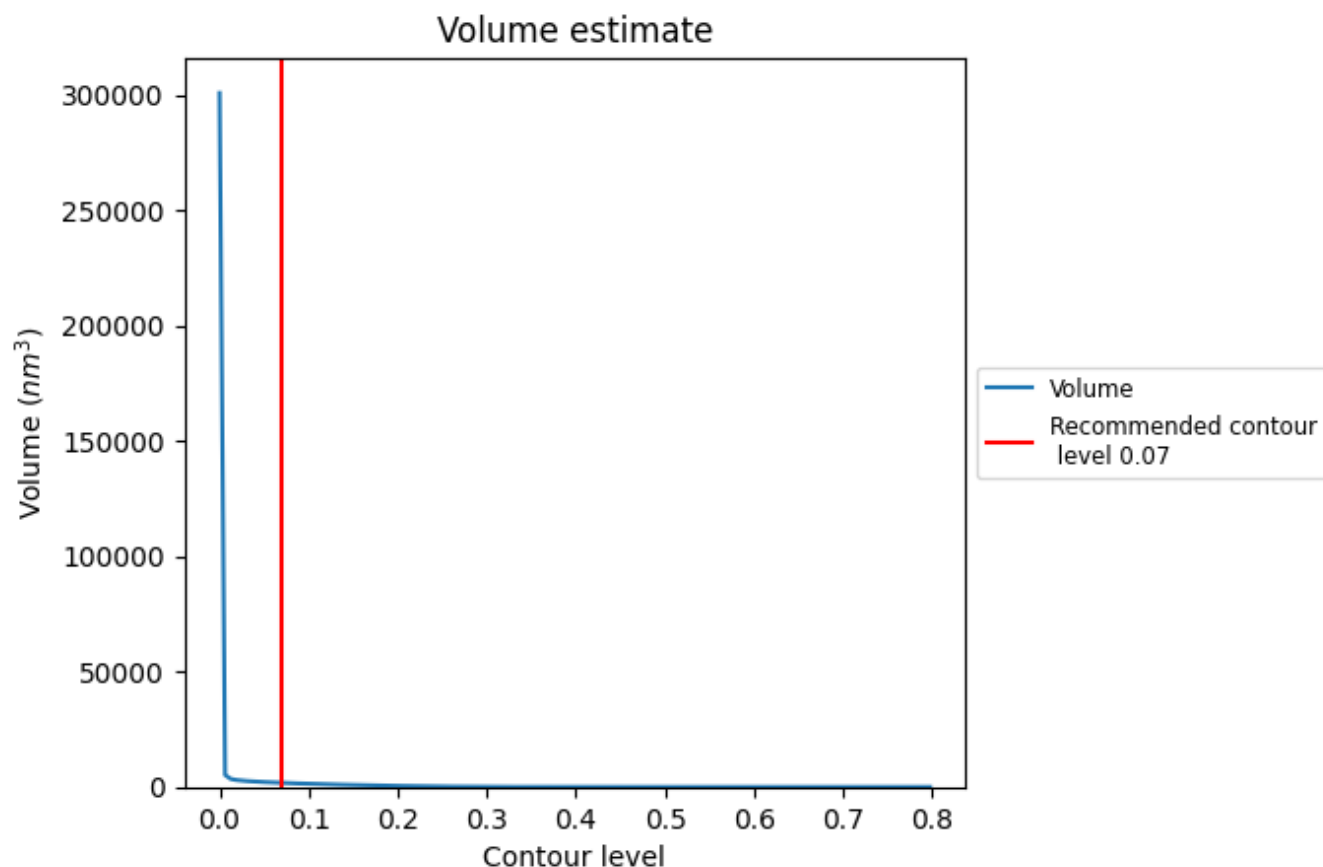
This section contains the results of statistical analysis of the map.

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.

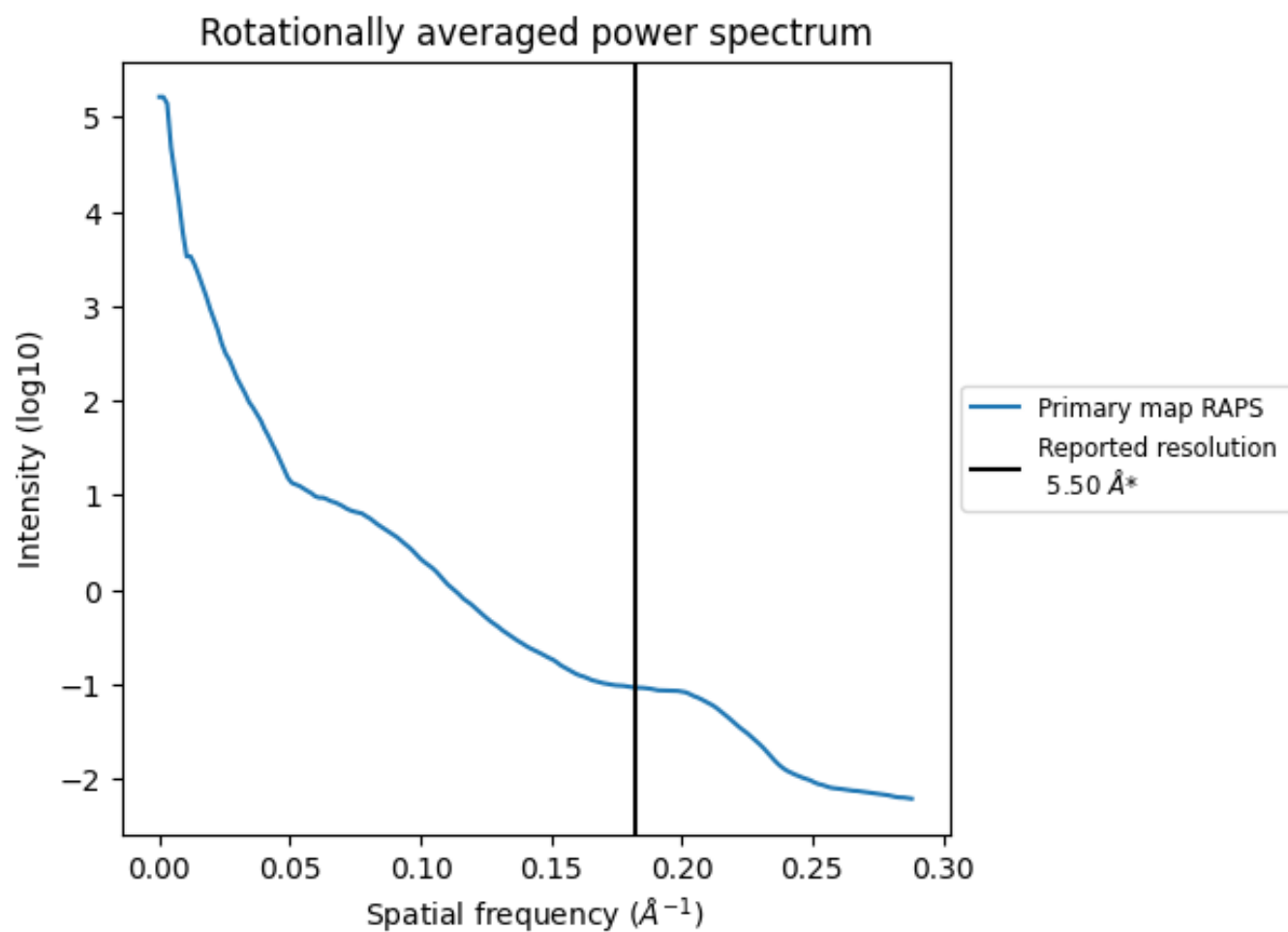
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1788 nm^3 ; this corresponds to an approximate mass of 1615 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 0.182 Å⁻¹

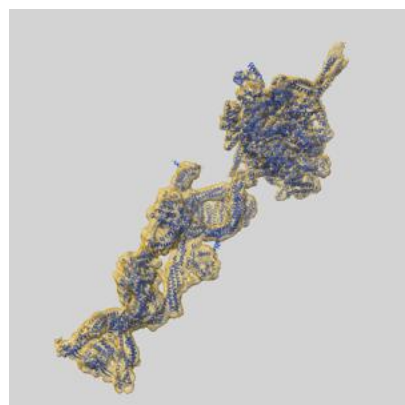
8 Fourier-Shell correlation ⓘ

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

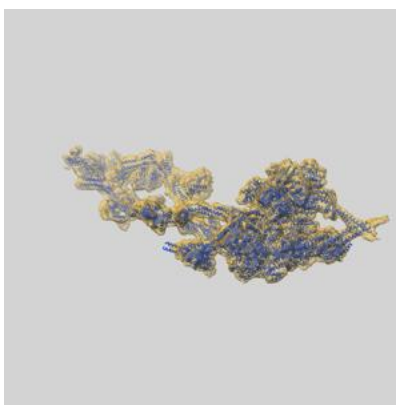
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73179 and PDB model 9YNH. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

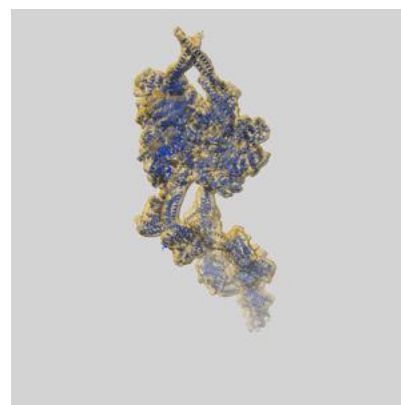
9.1 Map-model overlay [i](#)



X



Y



Z

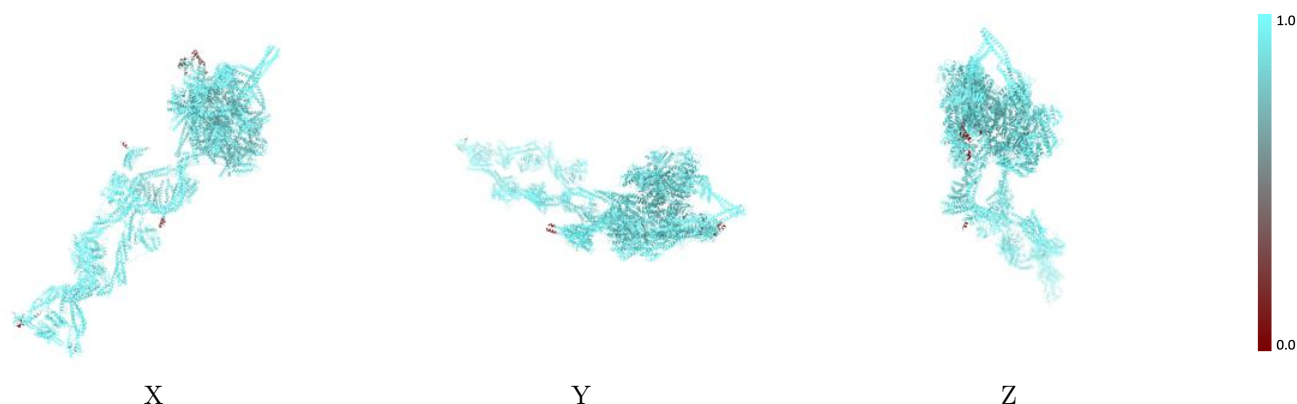
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



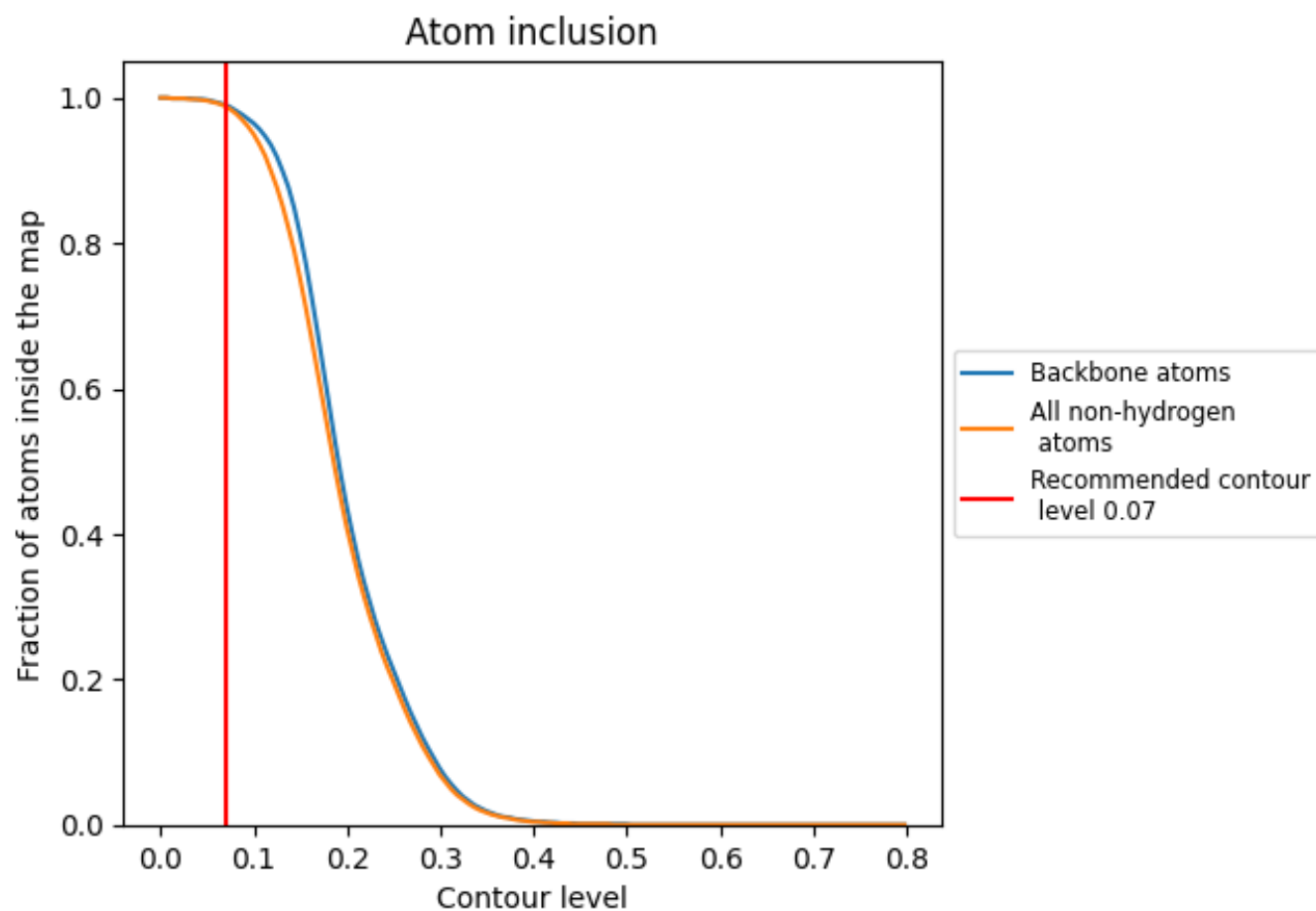
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).







































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.3070
A	 0.9940	 0.3280
B	 0.9980	 0.3340
C	 1.0000	 0.1850
D	 1.0000	 0.1860
E	 1.0000	 0.2470
F	 1.0000	 0.2390
G	 1.0000	 0.1940
H	 1.0000	 0.2020
I	 1.0000	 0.1830
J	 1.0000	 0.1890
K	 0.9250	 0.1380
L	 0.9820	 0.1440
O	 0.9600	 0.4050
P	 0.9350	 0.3590
U	 0.9230	 0.2810
V	 0.8820	 0.3030
W	 0.9260	 0.2470
X	 0.9580	 0.2680

