



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:20 PM UTC

PDB ID : 6F1U / pdb_00006f1u
EMDB ID : EMD-4169
Title : N terminal region of dynein tail domains in complex with dynactin filament and BICDR-1
Authors : Urnavicius, L.; Lau, C.K.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.; Yildiz, A.; Carter, A.P.
Deposited on : 2017-11-23
Resolution : 3.40 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:

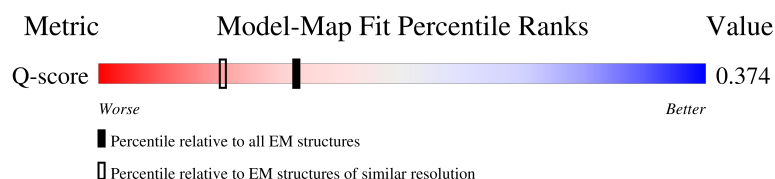
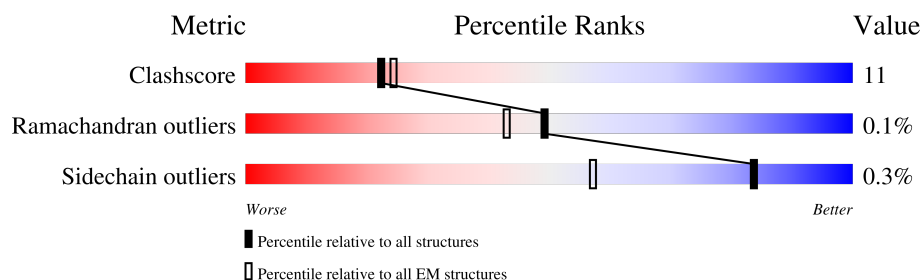
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

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	B	376	
1	D	376	
1	F	376	
2	K	286	

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Mol	Chain	Length	Quality of chain
3	L	271	
4	c	50	
5	d	26	
6	f	1186	
6	m	1186	
6	n	1186	
7	h	612	
8	X	577	
8	x	577	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28866 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	D	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		
1	F	370	Total	C	N	O	S	0	0
			2956	1892	509	545	10		

- Molecule 2 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	278	Total	C	N	O	S	0	0
			2264	1428	396	434	6		

- Molecule 3 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	269	Total	C	N	O	S	0	0
			2122	1323	370	418	11		

- Molecule 4 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	37	Total	C	N	O	S	0	0
			256	159	42	54	1		

- Molecule 5 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	d	24	Total	C	N	O	0	0
			188	118	29	41		

- Molecule 6 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	596	Total	C	N	O	S	0	0
			4902	3107	894	886	15		
6	m	396	Total	C	N	O	S	0	0
			3288	2080	601	597	10		
6	n	341	Total	C	N	O	S	0	0
			2815	1777	512	517	9		

- Molecule 7 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	358	Total	C	N	O	S	0	0
			2801	1767	490	529	15		

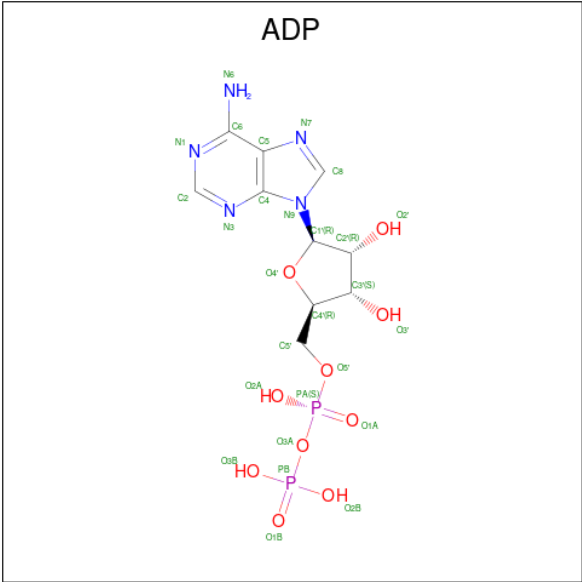
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409

- Molecule 8 is a protein called BICD family-like cargo adapter 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	79	Total	C	N	O	S	0	0
			688	413	134	140	1		
8	x	67	Total	C	N	O	S	0	0
			593	358	115	119	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

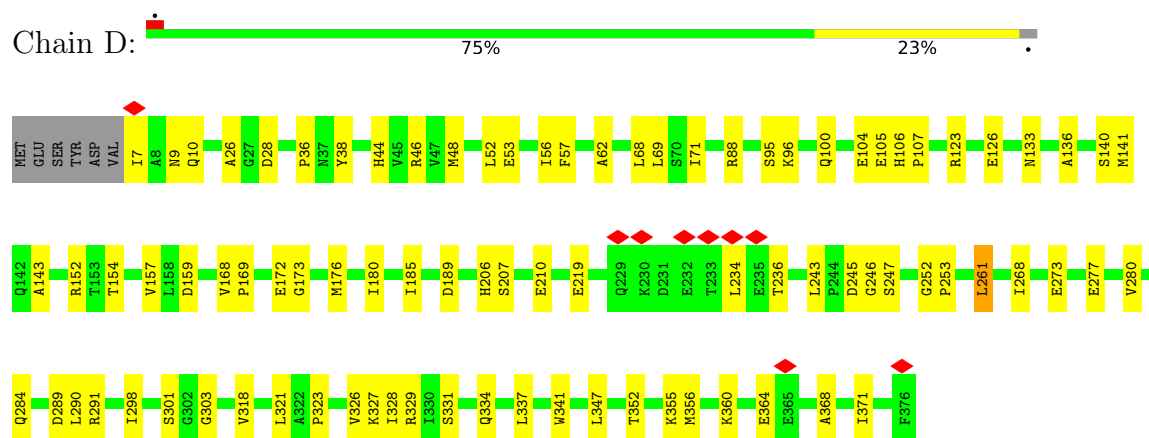
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

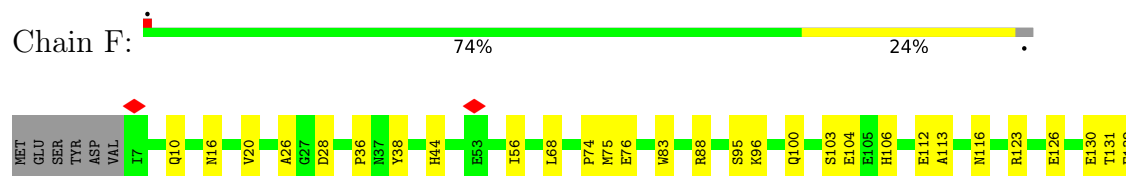
- Molecule 1: ARP1 actin related protein 1 homolog A

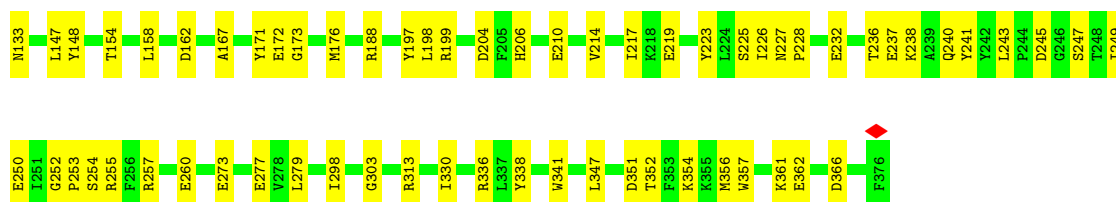


- Molecule 1: ARP1 actin related protein 1 homolog A

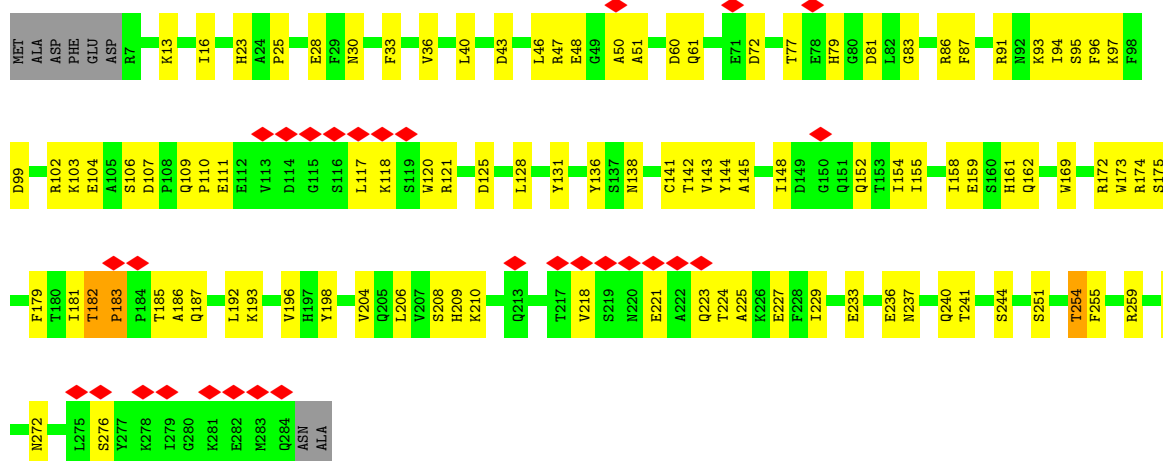


- Molecule 1: ARP1 actin related protein 1 homolog A

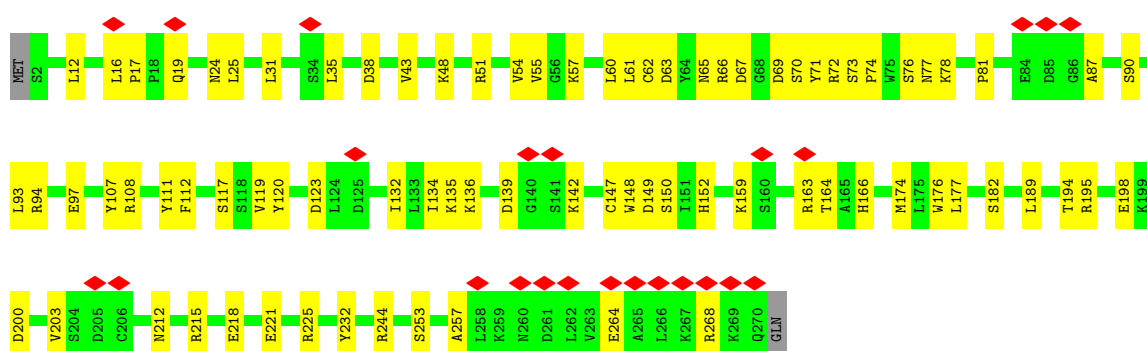




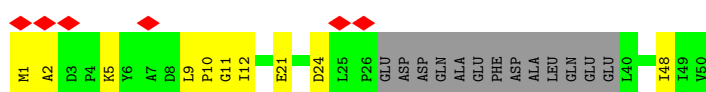
• Molecule 2: Capping protein (Actin filament) muscle Z-line, alpha 1



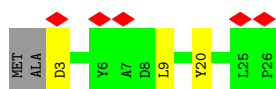
• Molecule 3: F-actin capping protein beta subunit



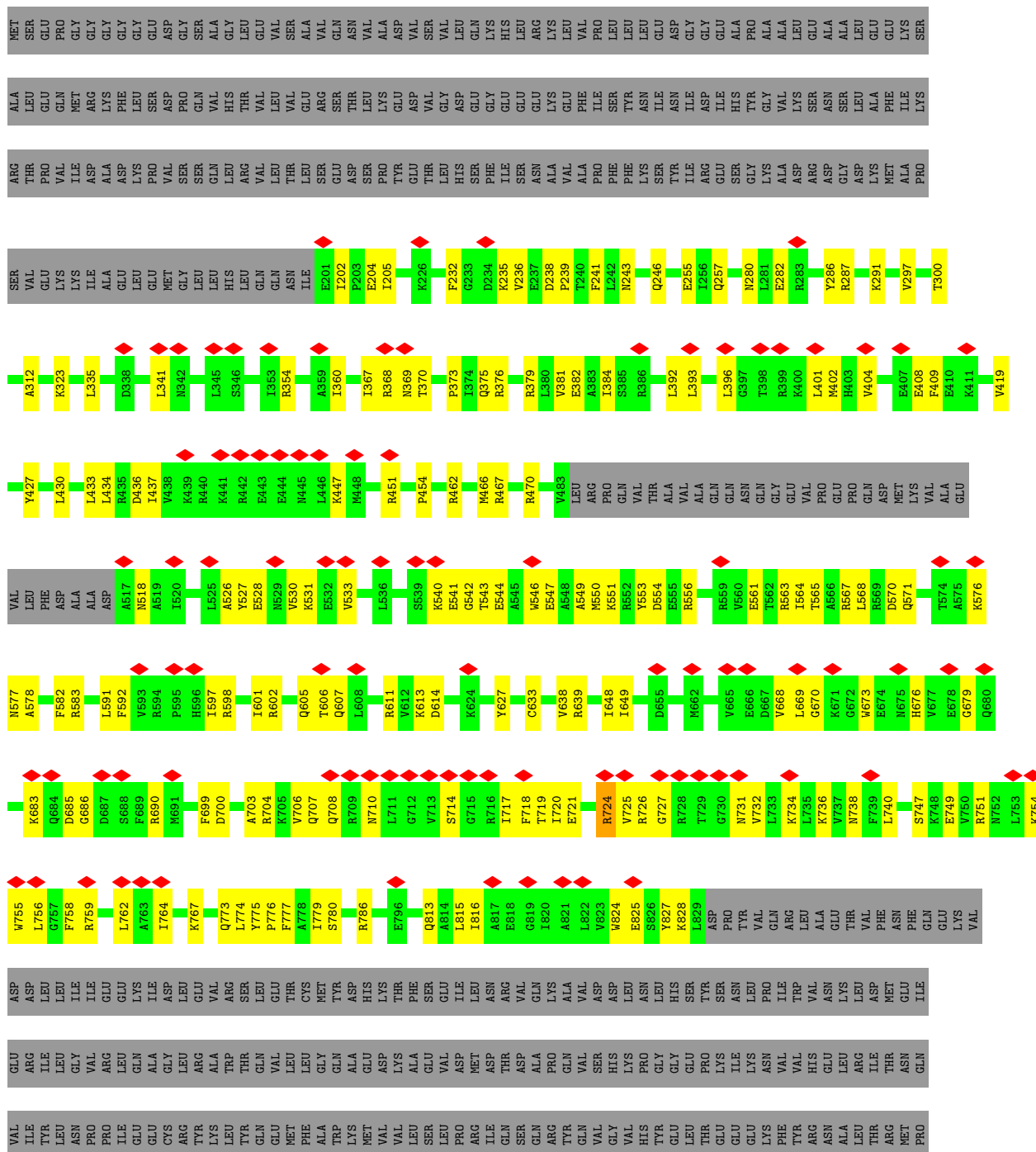
• Molecule 4: Dynactin subunit 2



• Molecule 5: Dynactin subunit 2



Chain f:



- Molecule 6: Cytoplasmic dynein 1 heavy chain 1



ARG	THR	PRO	VAL	ILE	ASP	ALA	ASP	LYS	PRO	GLY	SER	SER	GLN	LEU	ARG	VAL	VAL	LEU	THR	LEU	SER	GLU	ASP	SER	SER	PRO	TYR	GLU	THR	LEU	LEU	HIS	SER	PHE	ILE	SER	ASN	ALA	VAL	ALA	PRO	PHE	PHE	LYS	TYR	ILE	ARG	GLU	SER	SER	GLY	LYS	ALA	ASP	ARG	ASP	GLY	LYS	ASP	LYS	MET	ALA	PRO
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SER	VAL	GLU	LYS	ILE	ALA	GLU	LEU	GLU	MET	GLY	LEU	LEU	HIS	LEU	GLN	ASN	ILE	E201	E204	D238	P239	T240	F241	T242	N243	K252	E255	K258	D263	R264	P266	A267	S268	G269	T270	A271	L272	Q273	E274	T275	S276	F277	G278	L279	N280	R287	V297
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[illegible]

	LEU	PHE	ASP	ALA	ALA	ASP	A517	A518	A519	V523	A526	V527	E528	N529	V530	K531	E532	V533	D534	G535	L536	D537	V538	S539	G542	T543	E544	A545	M546	N550	K551	R552	V553	D554	E555	R556	V557	D558	R559	V560	L568	L572	N577	A578	N579	E580	F581	V582	R583	S586	R587	F588
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M589	A590	L591	R594	L601	L608	K613	L616	E617	S618	L619	K627	P628	SER	GLN	ALA	CYS	LYS	MET	SER	HIS	VAL	ASP	ARG	ARG	GLN	LEU	THR	TYR	MET	LYS	ARG	VAL
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GLU	ASP	VAL	LEU	GLY	LYS	TRP	GLY	GLU	ASN	HIS	VAL	GLU	GLY	GLN	LYS	LEU	LYS	GLN	ASP	GLY	ASP	SER	PHE	ARG	MET	LYS	LEU	THR	GLU	GLN	ILE	PHE	ASP	ASP	TRP	ALA	ARG	LYS	VAL	GLN	GLN	ARG	ASN	LEU	GLY	VAL	SER	PHE	ILE	THR	THR	GLU	SER	THR	ARG	VAL
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ARG	ARG	GLY	GLY	THR	GLY	ASN	VAL	LEU	LYS	LYS	LYS	VAL	ASN	PRE	LEU	PRO	GLU	ILE	ILE	THR	LEU	SER	LYS	GLU	VAL	ARG	ASN	LYS	LYS	TRP	LEU	GLY	PHE	ARG	VAL	PRO	LEU	ALA	ILE	ILE	VAL	ASN	LYS	LYS	ALA	HIS	GLN	ALA	ALA	ASN	GLN	LEU	TVR	PRO	PHE	ALA	ALA	ILE	ILE	LEU	LEU	GLU	SER	VAL
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ARG	THR	THR	GLU	ARG	ARG	THR	CYS	GLU	GLY	LYS	VAL	GLU	ARG	ASN	THR	ILE	SER	LEU	LEU	VAL	ALA	GLY	LYS	GLU	VAL	GLN	ALA	ALA	LEU	ILE	ALA	GLU	GLY	ILE	ALA	LEU	VAL	TRP	GLU	SER	SER	TYR	LYS	ASP	LEU	ASP	PRO	THR	VAL	VAL	GLN	ARG	LEU	ALA	GLU	THR	VAL	PHE	ASN	PHE	GLN	GLU
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[illegible]

GLU	ILE	GLU	ARG	ILE	LEU	GLY	VAL	ARG	ANG	GLN	ALA	GLY	LEU	ARG	ALA	ALA	THR	GLN	VAL	LEU	LEU	GLY	GLN	ALA	ALA	GLU	ASP	ASP	ASP	ASP	THR	THR	ASP	ALA	PRO	PRO	GLN	VAL	VAL	SER	SER	HIS	LYS	HIS	LYS	PRO	GLY	GLY	GLU	PRO	GLU	LYS	LYS	ILE	LYS	ASN	VAL	VAL	HIS	HIS	GLU	LEU	ARG	ILE	THR
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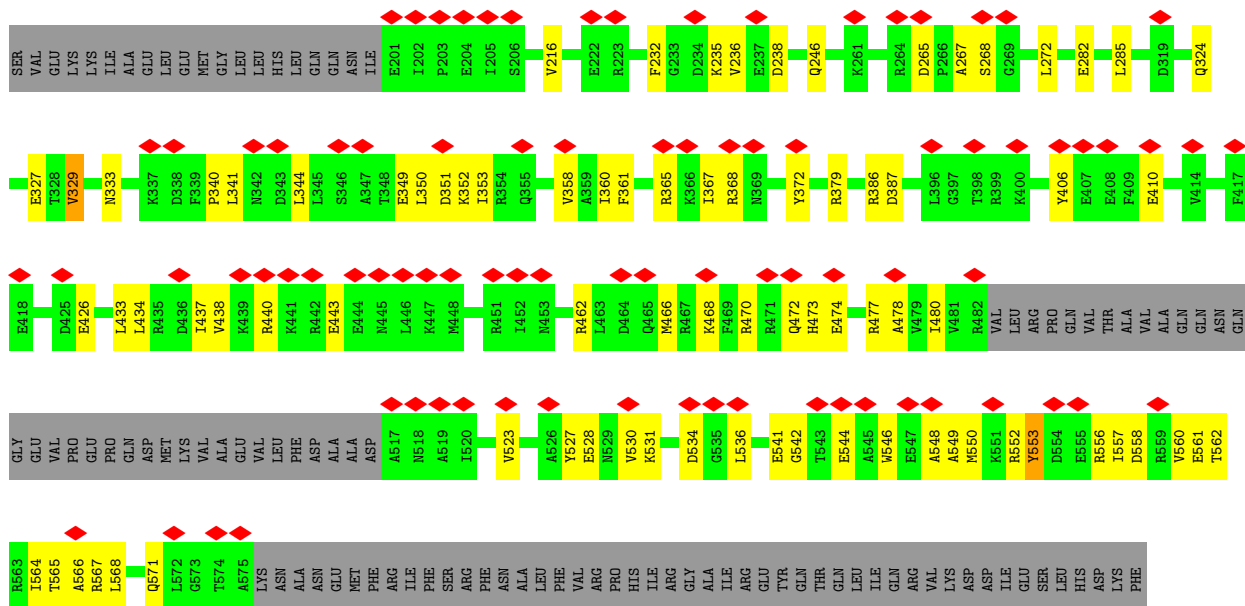
ASN	GLN	VAL	ILE	TYR	LEU	ASN	PRO	PRO	ILE	GLU	CYS	ARG	TYR	LYS	TYR	GLN	GLU	MET	PHE	ALA	TRP	LYS	MET	VAL	VAL	LEU	SER	LEU	PRO	ARG	ILE	GLN	SER	SER	GLN	ARG	TYR	GLN	VAL	GLY	VAL	VAL	HIS	TYR	GLU	TYR	LEU	THR	THR	GLU	GLU	LYS	PHE	ARG	TYR	ASN	ALA	LEU	THR	ARG
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ILE	SER	LYS	SER	ARG	GLN	GLU	LEU	GLU	GLN	HIS	SER	SER	VAL	ASP	THR	ALA	THR	SER	SER	ASP	ALA	VAL	THR	PHE	ILE	THR	TYR	VAL	GLN	SER	SER	LEU	LYS	ARG	LYS	ILE	LYS	GLN	PHE	GLU	LYS	GLN
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- Molecule 6: Cytoplasmic dynein 1 heavy chain 1



ARG	THR	PRO	THR	VAL	ILE	ASP	ASP	ALA	LYS	PRO	PRO	VAL	VAL	SER	SER	GLN	LEU	LEU	ARG	VAL	VAL	LEU	THR	THR	LEU	SER	SER	GLU	GLU	ASP	SER	SER	PRO	PRO	TYR	TYR	GLU	GLU	LEU	LEU	HIS	SER	ASP	ILE	ILE	SER	SER	ASN	ALA	ALA	VAL	VAL	PRO	PRO	PHE	PHE	PHE	LYS	LYS	TYR	TYR	ILE	ILE	ARG	GLU	GLU	SER	SER	GLY	GLY	LYS	ALA	ASP	ASP	ARG	ARG	ASP	ASP	GLY	GLY	LYS	LYS	MET	PRO	ALA	PRO
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LEU	GLU	THR	CYS	MET	TYR	ASP	HIS	LYS	THR	PHI	SER	GLU	ILE	LEU	ASN	ARG	VAL	GLN	LYS	ALA	VAL	ASP	ASP	LEU	ASN	LEU	HIS	SER	TYR	SER	ASN	LEU	PRO	ILE	ILE	TRP	VAL	ASN	LYS	GLU	LEU	ILE	ARG	GLY	VAL	ARG	LEU	GLN	ALA	GLY	LEU	ARG	ALA	THR	THR
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LYS	LYS
CYS	CYS
LYS	LYS
MET	MET
GLY	ASP
MET	MET
MET	MET
SER	SER
LEU	LEU
ASN	ASN
SER	SER
THR	GLN
ALA	LEU
ASP	LEU
GLY	ASP
LYS	ALA
ARG	ILE
LEU	GLN
PHE	GLN
SER	LYS
PHE	LEU
PHE	ASN
ARG	LEU
LYS	SER
ILE	GLN
	GLN
	LEU
	GLU
	ALA
	TRP
	GLN
	ASP
	ASP
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	205611	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 ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.145	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	804.0, 804.0, 804.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	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

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	B	0.82	0/3025	0.89	1/4085 (0.0%)
1	D	0.83	0/3025	0.90	0/4085
1	F	0.86	0/3025	0.97	2/4085 (0.0%)
2	K	0.63	0/2316	0.91	5/3135 (0.2%)
3	L	0.62	0/2156	0.88	2/2906 (0.1%)
4	c	0.53	0/260	0.84	0/356
5	d	0.68	0/193	0.84	0/265
6	f	0.52	0/4986	0.93	2/6718 (0.0%)
6	m	0.63	0/3344	1.00	7/4504 (0.2%)
6	n	0.46	0/2860	0.95	5/3854 (0.1%)
7	h	0.65	0/2880	1.02	8/3927 (0.2%)
8	X	0.42	0/695	0.78	0/926
8	x	0.42	0/600	0.81	0/798
All	All	0.67	0/29365	0.93	32/39644 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	n	553	TYR	CA-CB-CG	-7.47	100.46	113.90
2	K	182	THR	N-CA-C	-7.22	93.07	108.66
1	F	336	ARG	CB-CG-CD	-6.54	96.26	111.30
1	B	38	TYR	CA-CB-CG	6.46	125.52	113.90
6	n	480	ILE	CA-C-N	6.20	129.28	120.53
6	n	480	ILE	C-N-CA	6.20	129.28	120.53
6	m	601	ILE	CG1-CB-CG2	-5.89	93.04	110.70
2	K	183	PRO	N-CA-C	5.80	117.78	110.70
7	h	490	PRO	CA-C-N	5.80	132.62	121.54
7	h	490	PRO	C-N-CA	5.80	132.62	121.54
6	m	536	LEU	CA-C-N	5.55	132.14	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	m	536	LEU	C-N-CA	5.55	132.14	121.54
6	m	625	VAL	N-CA-C	-5.54	101.67	109.21
6	n	536	LEU	CA-C-N	5.50	132.04	121.54
6	n	536	LEU	C-N-CA	5.50	132.04	121.54
6	m	528	GLU	CA-CB-CG	-5.47	103.15	114.10
3	L	123	ASP	CA-C-N	5.32	131.70	121.54
3	L	123	ASP	C-N-CA	5.32	131.70	121.54
1	F	227	ASN	N-CA-C	-5.30	97.67	108.12
7	h	557	ARG	CA-C-N	5.20	133.27	122.41
7	h	557	ARG	C-N-CA	5.20	133.27	122.41
6	f	724	ARG	CA-C-N	5.18	129.88	121.95
6	f	724	ARG	C-N-CA	5.18	129.88	121.95
7	h	463	GLY	N-CA-C	-5.15	100.97	113.18
2	K	148	ILE	CA-C-N	5.11	131.30	121.54
2	K	148	ILE	C-N-CA	5.11	131.30	121.54
7	h	506	TRP	CA-CB-CG	5.09	123.28	113.60
2	K	83	GLY	N-CA-C	5.08	125.21	113.18
7	h	366	THR	CA-C-N	5.03	128.36	120.82
7	h	366	THR	C-N-CA	5.03	128.36	120.82
6	m	534	ASP	CA-C-N	5.02	131.25	121.41
6	m	534	ASP	C-N-CA	5.02	131.25	121.41

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	B	2956	0	2950	54	0
1	D	2956	0	2950	55	0
1	F	2956	0	2948	57	0
2	K	2264	0	2186	80	0
3	L	2122	0	2113	59	0
4	c	256	0	210	8	0
5	d	188	0	172	4	0
6	f	4902	0	5030	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	m	3288	0	3355	82	0
6	n	2815	0	2878	60	0
7	h	2801	0	2665	101	0
8	X	688	0	653	12	0
8	x	593	0	566	14	0
9	B	27	0	12	0	0
9	D	27	0	12	2	0
9	F	27	0	11	3	0
All	All	28866	0	28711	658	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 11.

All (658) 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)
6:n:556:ARG:O	6:n:560:VAL:HG23	1.53	1.09
6:m:530:VAL:O	6:m:534:ASP:HB2	1.57	1.05
6:m:542:GLY:O	6:m:546:TRP:HB3	1.58	1.03
2:K:46:LEU:O	2:K:50:ALA:HB3	1.69	0.92
6:n:542:GLY:O	6:n:546:TRP:HB3	1.72	0.89
2:K:43:ASP:O	2:K:47:ARG:HB2	1.73	0.88
7:h:522:ARG:NH1	7:h:524:ASP:OD2	2.07	0.87
1:D:206:HIS:N	1:D:210:GLU:OE2	2.08	0.86
3:L:264:GLU:O	3:L:268:ARG:HB2	1.76	0.85
1:D:38:TYR:OH	1:D:62:ALA:O	1.95	0.84
6:n:556:ARG:O	6:n:560:VAL:CG2	2.25	0.83
6:f:239:PRO:O	6:f:243:ASN:HB2	1.82	0.80
6:f:543:THR:O	6:f:547:GLU:HB3	1.82	0.79
7:h:526:TRP:HB3	7:h:536:THR:H	1.50	0.77
1:D:152:ARG:HH22	1:D:329:ARG:HH12	1.34	0.75
6:m:462:ARG:HE	6:m:537:ASP:HB2	1.51	0.74
7:h:430:VAL:HB	7:h:446:PHE:CE1	2.22	0.74
7:h:305:CYS:SG	7:h:306:GLN:N	2.60	0.74
1:F:228:PRO:O	1:F:232:GLU:HB2	1.89	0.72
7:h:331:ILE:H	7:h:347:THR:HB	1.55	0.71
1:B:112:GLU:OE2	1:B:116:ASN:ND2	2.18	0.70
6:n:406:TYR:O	6:n:410:GLU:HB2	1.90	0.70
3:L:61:LEU:HA	3:L:65:ASN:HD21	1.55	0.70
6:m:401:LEU:HD11	6:m:413:MET:HE2	1.74	0.70
6:n:232:PHE:HB3	6:n:235:LYS:HB3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:718:PHE:HA	6:f:824:TRP:HB2	1.74	0.69
7:h:240:SER:HB2	7:h:572:ASP:HB3	1.75	0.69
1:F:351:ASP:OD2	6:f:257:GLN:NE2	2.26	0.68
6:f:202:ILE:HG21	6:f:280:ASN:HB3	1.75	0.68
7:h:426:GLU:HG3	7:h:427:GLU:HG2	1.75	0.68
1:B:239:ALA:HB3	1:B:255:ARG:HH12	1.59	0.68
2:K:16:ILE:HG21	3:L:31:LEU:HD11	1.75	0.68
7:h:462:VAL:HB	7:h:465:VAL:HB	1.75	0.67
1:B:152:ARG:HH22	1:B:329:ARG:HH12	1.42	0.67
6:m:586:SER:HA	6:m:589:ASN:HD21	1.59	0.67
2:K:121:ARG:O	2:K:125:ASP:HB2	1.94	0.67
2:K:204:VAL:HG21	3:L:232:TYR:HB3	1.76	0.66
1:B:243:LEU:HD12	1:B:247:SER:HB2	1.76	0.66
6:m:334:PRO:HG2	6:m:370:THR:HG22	1.76	0.66
7:h:449:HIS:HB2	7:h:477:ASP:OD2	1.95	0.66
1:D:104:GLU:HG2	1:D:133:ASN:HB2	1.77	0.66
7:h:429:SER:H	7:h:447:GLU:HG2	1.61	0.65
1:B:82:ASP:OD2	1:B:85:ASP:N	2.17	0.65
6:f:382:GLU:HG3	6:f:454:PRO:HB3	1.78	0.65
7:h:258:CYS:HA	7:h:549:ARG:HG3	1.78	0.65
6:m:335:LEU:HB2	6:m:370:THR:HG21	1.79	0.65
6:f:282:GLU:O	6:f:286:TYR:HB2	1.97	0.65
1:B:104:GLU:OE2	1:B:133:ASN:HB2	1.97	0.65
2:K:169:TRP:HB3	2:K:198:TYR:HD1	1.62	0.64
7:h:351:ALA:O	7:h:380:LYS:NZ	2.30	0.64
7:h:462:VAL:HA	7:h:511:PRO:HG3	1.79	0.64
6:f:409:PHE:HZ	6:f:467:ARG:HA	1.63	0.64
2:K:47:ARG:O	2:K:51:ALA:HB2	1.98	0.64
6:f:668:VAL:HG12	6:f:669:LEU:HD12	1.81	0.63
1:D:368:ALA:HA	1:D:371:ILE:HD12	1.80	0.63
8:X:191:LEU:HB2	8:x:191:LEU:HD13	1.78	0.63
2:K:223:GLN:O	2:K:227:GLU:HB2	1.99	0.63
2:K:158:ILE:HB	2:K:175:SER:HB3	1.80	0.63
6:f:205:ILE:O	6:f:291:LYS:NZ	2.32	0.63
6:f:526:ALA:HB2	6:f:556:ARG:HG2	1.79	0.63
7:h:252:LYS:O	7:h:276:ASN:ND2	2.31	0.62
7:h:471:PHE:HA	7:h:506:TRP:HH2	1.64	0.62
1:F:112:GLU:HG2	1:F:116:ASN:HD22	1.63	0.62
3:L:51:ARG:NH1	3:L:57:LYS:O	2.32	0.62
3:L:148:TRP:NE1	3:L:150:SER:OG	2.32	0.62
1:F:238:LYS:HG2	1:F:252:GLY:HA2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:401:LEU:HA	6:f:404:VAL:HG12	1.82	0.62
1:D:140:SER:OG	1:D:141:MET:N	2.33	0.61
6:f:638:VAL:HG21	7:h:255:VAL:HG11	1.81	0.61
1:D:133:ASN:HD21	6:f:368:ARG:HH21	1.49	0.61
1:B:165:THR:HG23	1:B:183:ILE:HG13	1.83	0.61
1:B:245:ASP:OD2	1:B:247:SER:OG	2.13	0.61
7:h:243:ARG:NH1	7:h:292:MET:SD	2.74	0.61
1:D:7:ILE:HD11	1:D:105:GLU:HG2	1.82	0.60
1:B:368:ALA:HA	1:B:371:ILE:HD12	1.83	0.60
6:m:588:PHE:HB3	6:m:591:LEU:HB2	1.83	0.60
1:D:303:GLY:HA3	9:D:800:ADP:H5'2	1.83	0.60
1:F:10:GLN:O	1:F:106:HIS:ND1	2.34	0.60
1:D:96:LYS:O	1:D:100:GLN:NE2	2.35	0.59
1:B:225:SER:HB2	1:B:231:ASP:OD2	2.02	0.59
1:B:366:ASP:HB2	1:B:370:SER:HB3	1.84	0.59
2:K:40:LEU:HD23	2:K:46:LEU:HB3	1.84	0.59
6:m:205:ILE:HG21	6:m:255:GLU:HB3	1.84	0.59
1:D:337:LEU:HD12	4:c:11:GLY:HA3	1.84	0.59
6:m:551:LYS:HG3	6:m:555:GLU:OE2	2.02	0.59
1:F:104:GLU:HG2	1:F:133:ASN:HB2	1.83	0.59
6:n:557:ILE:O	6:n:561:GLU:N	2.31	0.59
6:n:474:GLU:O	6:n:478:ALA:HB3	2.02	0.59
6:n:541:GLU:HA	6:n:544:GLU:HB3	1.85	0.59
8:X:187:GLN:OE1	8:x:188:GLN:NE2	2.33	0.59
7:h:342:THR:HG23	7:h:346:ARG:HH21	1.66	0.58
1:B:113:ALA:HB3	1:B:116:ASN:HD21	1.68	0.58
3:L:212:ASN:OD1	3:L:215:ARG:NH2	2.36	0.58
6:m:470:ARG:O	6:m:474:GLU:HB3	2.03	0.58
8:x:143:ASP:O	8:x:147:HIS:ND1	2.35	0.58
1:B:28:ASP:HB2	1:B:341:TRP:HH2	1.68	0.58
2:K:174:ARG:HH12	2:K:193:LYS:HE3	1.68	0.58
3:L:166:HIS:NE2	3:L:198:GLU:OE2	2.37	0.58
6:f:530:VAL:HA	6:f:533:VAL:HG22	1.84	0.58
1:F:206:HIS:N	1:F:210:GLU:OE1	2.35	0.58
6:f:613:LYS:NZ	6:f:685:ASP:OD2	2.30	0.58
1:D:234:LEU:HD12	1:D:236:THR:HG22	1.86	0.58
6:f:239:PRO:O	6:f:243:ASN:CB	2.51	0.57
6:f:639:ARG:NH2	7:h:548:ASN:OD1	2.26	0.57
6:f:751:ARG:O	6:f:755:TRP:CB	2.52	0.57
6:m:413:MET:HE1	6:m:463:LEU:HD22	1.86	0.57
6:n:468:LYS:O	6:n:472:GLN:NE2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:184:LEU:HA	8:x:184:LEU:HD13	1.85	0.57
1:D:154:THR:HG22	1:D:172:GLU:H	1.68	0.57
2:K:210:LYS:NZ	3:L:182:SER:O	2.38	0.57
1:F:352:THR:O	1:F:356:MET:HB2	2.04	0.57
7:h:345:GLN:HE21	7:h:389:LEU:HB3	1.69	0.57
1:B:126:GLU:O	1:B:130:GLU:HB2	2.04	0.57
7:h:522:ARG:HA	7:h:540:SER:HA	1.86	0.57
6:f:649:ILE:HD13	7:h:452:PRO:HG3	1.86	0.57
2:K:86:ARG:NH2	2:K:107:ASP:OD2	2.30	0.57
2:K:117:LEU:HB2	2:K:145:ALA:HB1	1.87	0.57
7:h:529:ASN:HB3	7:h:585:TRP:HB2	1.87	0.56
2:K:255:PHE:O	2:K:259:ARG:N	2.38	0.56
3:L:67:ASP:OD2	3:L:87:ALA:N	2.37	0.56
6:f:576:LYS:O	6:f:611:ARG:NE	2.39	0.56
1:B:154:THR:HG22	1:B:172:GLU:H	1.70	0.56
2:K:25:PRO:HG2	2:K:28:GLU:HB2	1.88	0.56
6:n:558:ASP:O	6:n:562:THR:N	2.39	0.56
7:h:546:ALA:HB3	7:h:564:SER:HB3	1.88	0.56
1:F:28:ASP:HB2	1:F:341:TRP:HH2	1.71	0.56
2:K:138:ASN:ND2	2:K:162:GLN:OE1	2.39	0.56
7:h:275:ASN:ND2	7:h:277:GLU:OE2	2.39	0.56
6:m:458:LYS:HE2	6:m:539:SER:HB3	1.87	0.56
1:D:329:ARG:HG2	4:c:21:GLU:HG2	1.88	0.56
8:X:197:GLU:HA	8:X:200:ARG:HD2	1.88	0.56
1:F:162:ASP:OD1	9:F:800:ADP:O3'	2.22	0.55
6:f:466:MET:HG2	6:f:546:TRP:HZ2	1.70	0.55
3:L:76:SER:O	3:L:78:LYS:NZ	2.36	0.55
6:f:583:ARG:HH12	7:h:534:VAL:HG13	1.71	0.55
6:n:473:HIS:CE1	6:n:477:ARG:HE	2.25	0.55
7:h:260:ASP:OD2	7:h:313:THR:OG1	2.16	0.55
7:h:431:TYR:HE1	7:h:445:MET:HG2	1.71	0.55
6:f:335:LEU:HB2	6:f:370:THR:HG21	1.88	0.55
6:f:707:GLN:HG3	6:f:764:ILE:HD11	1.87	0.55
6:n:546:TRP:O	6:n:550:MET:CB	2.53	0.55
7:h:249:ARG:O	7:h:252:LYS:NZ	2.39	0.55
6:f:762:LEU:HD13	8:X:172:GLU:OE2	2.07	0.55
6:f:341:LEU:HA	6:f:360:ILE:HD11	1.88	0.55
7:h:481:LYS:HE2	7:h:493:SER:HB2	1.88	0.55
8:X:142:THR:HA	8:X:145:LEU:HD12	1.89	0.55
2:K:23:HIS:HB3	3:L:17:PRO:HG2	1.88	0.55
6:f:543:THR:O	6:f:547:GLU:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:724:ARG:HD3	6:f:734:LYS:HB2	1.89	0.55
6:m:378:LEU:HB3	6:m:452:ILE:HD11	1.89	0.55
6:n:561:GLU:O	6:n:561:GLU:HG2	2.06	0.55
1:F:16:ASN:HB3	1:F:75:MET:HE1	1.88	0.54
1:F:56:ILE:HD13	1:F:88:ARG:HD3	1.88	0.54
3:L:132:ILE:HB	3:L:152:HIS:HB2	1.87	0.54
1:D:334:GLN:HB3	4:c:12:ILE:HG23	1.89	0.54
7:h:358:VAL:HA	7:h:376:SER:HA	1.89	0.54
7:h:510:HIS:HB2	7:h:578:ALA:HA	1.90	0.54
1:B:76:GLU:O	1:B:81:LYS:NZ	2.39	0.54
6:m:616:ILE:O	6:m:620:HIS:ND1	2.40	0.54
7:h:260:ASP:OD1	7:h:261:TRP:N	2.41	0.54
6:f:598:ARG:HA	6:f:601:ILE:HB	1.89	0.54
6:f:706:VAL:HA	6:f:710:ASN:HB2	1.88	0.54
6:m:358:VAL:HA	6:m:426:GLU:OE2	2.08	0.54
7:h:452:PRO:HG2	7:h:476:PHE:HD2	1.72	0.54
1:B:18:SER:O	1:B:188:ARG:NH2	2.41	0.54
1:D:10:GLN:NE2	1:D:26:ALA:O	2.41	0.54
6:f:567:ARG:HD3	6:f:570:ASP:OD2	2.07	0.54
7:h:526:TRP:HB3	7:h:535:PRO:HA	1.90	0.54
3:L:163:ARG:HB3	3:L:203:VAL:HB	1.89	0.54
1:F:279:LEU:HD21	1:F:298:ILE:HD13	1.90	0.54
6:n:349:GLU:OE1	6:n:352:LYS:NZ	2.38	0.54
6:f:591:LEU:HD13	6:f:597:ILE:HG12	1.90	0.54
6:m:341:LEU:HA	6:m:360:ILE:HD11	1.89	0.54
1:D:46:ARG:NH1	1:D:52:LEU:O	2.41	0.53
3:L:253:SER:O	3:L:257:ALA:HB2	2.08	0.53
7:h:240:SER:N	7:h:572:ASP:O	2.39	0.53
1:F:95:SER:OG	1:F:96:LYS:N	2.41	0.53
3:L:90:SER:HB2	3:L:93:LEU:HB2	1.90	0.53
6:f:561:GLU:HA	6:f:564:ILE:HB	1.91	0.53
6:m:546:TRP:NE1	6:m:550:MET:SD	2.82	0.53
1:F:243:LEU:HD12	1:F:247:SER:HB2	1.90	0.53
2:K:46:LEU:O	2:K:50:ALA:CB	2.50	0.53
7:h:481:LYS:HD3	7:h:490:PRO:HD2	1.89	0.53
6:m:469:PHE:HB2	6:m:550:MET:HE1	1.90	0.53
8:x:142:THR:HA	8:x:145:LEU:HD12	1.90	0.53
2:K:218:VAL:HA	2:K:224:THR:HG21	1.91	0.53
2:K:240:GLN:NE2	3:L:244:ARG:O	2.41	0.53
6:f:751:ARG:O	6:f:755:TRP:HB3	2.09	0.53
1:D:28:ASP:HB2	1:D:341:TRP:HH2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:773:GLN:NE2	8:X:161:ASN:OD1	2.42	0.52
7:h:254:ARG:HG2	7:h:276:ASN:HB2	1.91	0.52
7:h:548:ASN:N	7:h:562:GLY:O	2.42	0.52
1:B:73:TYR:OH	1:B:212:GLU:OE2	2.26	0.52
6:m:350:LEU:HD23	6:m:353:ILE:HD12	1.91	0.52
1:B:327:LYS:HG3	4:c:48:ILE:HA	1.91	0.52
1:D:243:LEU:HD12	1:D:247:SER:HB2	1.90	0.52
1:F:330:ILE:HB	5:d:20:TYR:HB2	1.91	0.52
6:m:572:LEU:HD11	6:m:581:MET:HG3	1.90	0.52
6:n:530:VAL:HB	6:n:553:TYR:HD1	1.74	0.52
1:D:57:PHE:HD2	1:D:69:LEU:HD21	1.75	0.52
3:L:166:HIS:ND1	3:L:200:ASP:OD1	2.33	0.52
1:F:351:ASP:OD1	1:F:354:LYS:NZ	2.39	0.52
2:K:94:ILE:HA	2:K:111:GLU:H	1.72	0.52
7:h:419:ASN:HB2	7:h:435:ARG:HB2	1.92	0.52
2:K:95:SER:N	2:K:109:GLN:O	2.36	0.52
2:K:182:THR:OG1	2:K:185:THR:O	2.27	0.52
6:n:546:TRP:O	6:n:550:MET:HB3	2.10	0.52
1:D:123:ARG:NH1	1:D:126:GLU:OE1	2.42	0.52
6:f:404:VAL:HG11	6:f:408:GLU:HB2	1.92	0.52
2:K:61:GLN:OE1	2:K:172:ARG:NH2	2.43	0.52
6:m:543:THR:OG1	6:m:544:GLU:N	2.43	0.52
7:h:425:SER:OG	7:h:426:GLU:N	2.42	0.52
6:f:714:SER:HB2	6:f:767:LYS:HB3	1.92	0.52
3:L:135:LYS:NZ	3:L:147:CYS:SG	2.83	0.51
5:d:3:ASP:OD1	5:d:3:ASP:N	2.41	0.51
6:f:749:GLU:OE2	6:f:764:ILE:HG22	2.09	0.51
3:L:90:SER:O	3:L:94:ARG:N	2.42	0.51
6:f:369:ASN:OD1	6:f:369:ASN:N	2.41	0.51
6:n:530:VAL:HG21	6:n:556:ARG:HG3	1.91	0.51
7:h:303:PHE:HB3	7:h:334:TRP:CE2	2.45	0.51
1:B:122:GLU:HG2	1:B:368:ALA:HB1	1.93	0.51
3:L:48:LYS:HB2	3:L:61:LEU:HB2	1.92	0.51
6:m:204:GLU:OE2	6:m:287:ARG:NH1	2.43	0.51
1:B:287:ASP:OD1	2:K:266:ARG:NE	2.44	0.51
2:K:118:LYS:HB3	2:K:121:ARG:HH21	1.75	0.51
2:K:141:CYS:SG	2:K:142:THR:N	2.84	0.51
6:f:427:TYR:HA	6:f:430:LEU:HD12	1.92	0.51
6:m:438:VAL:O	6:m:442:ARG:N	2.44	0.51
6:n:344:LEU:HD21	6:n:387:ASP:HB3	1.91	0.51
7:h:481:LYS:NZ	7:h:490:PRO:O	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:m:452:ILE:HG22	6:m:454:PRO:HD3	1.91	0.51
2:K:183:PRO:HA	2:K:218:VAL:HB	1.93	0.51
1:F:240:GLN:HG2	1:F:250:GLU:OE2	2.11	0.51
6:f:518:ASN:HB3	6:f:563:ARG:HH12	1.76	0.51
1:F:158:LEU:HD23	1:F:167:ALA:HB2	1.92	0.50
8:x:196:ARG:HB3	8:x:200:ARG:HH12	1.76	0.50
6:f:375:GLN:OE1	6:f:379:ARG:NH1	2.44	0.50
6:m:620:HIS:O	6:m:624:LYS:HB2	2.11	0.50
1:B:228:PRO:HD3	1:B:313:ARG:HH12	1.77	0.50
1:F:38:TYR:HA	1:F:74:PRO:HD3	1.93	0.50
6:m:470:ARG:O	6:m:474:GLU:CB	2.58	0.50
6:f:726:ARG:N	6:f:732:VAL:O	2.44	0.50
6:m:626:GLN:HB3	6:m:628:PRO:HD2	1.93	0.50
6:n:267:ALA:O	6:n:386:ARG:NH2	2.44	0.50
6:n:470:ARG:O	6:n:474:GLU:HB2	2.11	0.50
6:f:205:ILE:HG21	6:f:255:GLU:HB3	1.92	0.50
6:f:568:LEU:HD11	6:f:597:ILE:HG13	1.93	0.50
6:f:727:GLY:HA2	6:f:731:ASN:HD22	1.77	0.50
8:x:186:ARG:O	8:x:190:HIS:ND1	2.35	0.50
1:B:263:PHE:HD2	1:B:313:ARG:HE	1.59	0.50
6:m:333:ASN:O	6:m:337:LYS:N	2.44	0.50
1:F:273:GLU:HB3	1:F:277:GLU:HB2	1.94	0.50
2:K:251:SER:O	3:L:225:ARG:NH2	2.44	0.50
1:F:223:TYR:HE1	1:F:255:ARG:HG3	1.76	0.50
6:f:717:ILE:HG21	6:f:774:LEU:HD13	1.94	0.50
6:n:523:VAL:O	6:n:527:TYR:HB2	2.12	0.50
7:h:239:LEU:HD12	7:h:539:ILE:HB	1.94	0.50
3:L:119:VAL:HG22	3:L:132:ILE:HG12	1.93	0.50
6:n:235:LYS:HA	6:n:238:ASP:OD2	2.12	0.49
1:D:169:PRO:HB2	1:D:176:MET:HE3	1.95	0.49
6:f:719:THR:O	6:f:738:ASN:ND2	2.45	0.49
2:K:117:LEU:HD23	2:K:181:ILE:HD12	1.93	0.49
3:L:70:SER:HA	3:L:81:PRO:HD2	1.94	0.49
7:h:558:GLU:HG2	7:h:572:ASP:HB2	1.93	0.49
6:f:754:LYS:HD3	7:h:426:GLU:OE2	2.13	0.49
6:f:775:TYR:CZ	6:f:779:ILE:HD11	2.48	0.49
6:f:777:PHE:O	6:f:780:SER:OG	2.30	0.49
7:h:531:ASP:OD2	7:h:536:THR:OG1	2.30	0.49
6:f:542:GLY:O	6:f:546:TRP:HB2	2.13	0.49
6:m:530:VAL:O	6:m:534:ASP:CB	2.46	0.49
7:h:459:HIS:HE1	7:h:470:LEU:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:143:VAL:HG13	2:K:154:ILE:HG23	1.94	0.49
6:f:611:ARG:HA	6:f:614:ASP:OD2	2.12	0.49
1:F:44:HIS:HD2	1:F:68:LEU:HD12	1.77	0.48
6:f:246:GLN:HG3	6:f:312:ALA:HB2	1.95	0.48
6:f:541:GLU:HB3	6:f:544:GLU:HB3	1.94	0.48
7:h:327:TYR:HA	7:h:357:PRO:HB3	1.95	0.48
6:f:373:PRO:HB2	6:f:376:ARG:HB2	1.95	0.48
6:n:350:LEU:HD23	6:n:353:ILE:HD12	1.95	0.48
6:n:474:GLU:O	6:n:478:ALA:CB	2.61	0.48
1:F:214:VAL:HA	1:F:217:ILE:HD12	1.94	0.48
2:K:254:THR:HG22	3:L:177:LEU:HD22	1.96	0.48
6:n:462:ARG:NH2	6:n:534:ASP:OD1	2.47	0.48
6:m:474:GLU:HG2	6:m:477:ARG:HH21	1.78	0.48
6:n:282:GLU:HG2	6:n:329:VAL:HG13	1.94	0.48
7:h:434:CYS:HB2	7:h:440:ALA:HA	1.96	0.48
1:B:287:ASP:OD2	2:K:266:ARG:HG3	2.13	0.48
1:F:225:SER:OG	1:F:226:ILE:N	2.45	0.48
2:K:47:ARG:O	2:K:51:ALA:CB	2.62	0.48
6:m:438:VAL:HA	6:m:441:LYS:HB3	1.95	0.48
6:m:475:GLN:OE1	6:m:594:ARG:NH2	2.46	0.48
6:m:617:GLU:HA	6:m:620:HIS:HD1	1.78	0.48
2:K:77:THR:HB	2:K:144:TYR:CE2	2.49	0.48
2:K:272:ASN:O	2:K:276:SER:OG	2.27	0.48
6:m:264:ARG:HD2	6:m:274:GLU:HG2	1.95	0.48
7:h:313:THR:OG1	7:h:314:PHE:N	2.43	0.48
1:B:179:SER:OG	1:B:285:LYS:O	2.23	0.48
2:K:117:LEU:HD21	2:K:152:GLN:HB3	1.95	0.48
6:f:232:PHE:HB3	6:f:235:LYS:HB2	1.95	0.48
6:m:579:ASN:HA	6:m:582:PHE:HD2	1.79	0.48
6:n:272:LEU:HD13	6:n:341:LEU:HD22	1.94	0.48
6:n:365:ARG:HG3	6:n:433:LEU:HD11	1.94	0.48
1:B:238:LYS:HG2	1:B:252:GLY:HA2	1.95	0.48
1:D:261:LEU:HD21	1:D:268:ILE:HB	1.95	0.48
1:F:76:GLU:HG2	1:F:188:ARG:HH12	1.79	0.48
3:L:73:SER:O	3:L:77:ASN:N	2.43	0.48
6:f:759:ARG:NH1	8:X:175:THR:OG1	2.36	0.48
6:f:776:PRO:HA	6:f:779:ILE:HD12	1.96	0.48
1:D:323:PRO:HG2	1:D:326:VAL:HG21	1.95	0.48
1:F:154:THR:HG22	1:F:172:GLU:H	1.78	0.48
1:D:347:LEU:HD11	1:D:356:MET:HE1	1.94	0.47
6:n:564:ILE:HA	6:n:567:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:43:ASP:O	2:K:47:ARG:CB	2.55	0.47
6:f:433:LEU:HA	6:f:436:ASP:OD2	2.14	0.47
7:h:573:VAL:HB	7:h:576:GLN:HB2	1.96	0.47
6:f:367:ILE:HD12	6:f:433:LEU:HD22	1.95	0.47
6:n:324:GLN:HA	6:n:327:GLU:HG2	1.96	0.47
6:n:527:TYR:HA	6:n:553:TYR:CE1	2.50	0.47
6:f:434:LEU:HA	6:f:437:ILE:HD12	1.96	0.47
7:h:452:PRO:HG2	7:h:476:PHE:CD2	2.49	0.47
7:h:524:ASP:HA	7:h:538:SER:HB2	1.96	0.47
1:F:75:MET:O	1:F:188:ARG:NH2	2.47	0.47
1:F:83:TRP:CE2	1:F:123:ARG:HG2	2.50	0.47
3:L:25:LEU:HD13	3:L:43:VAL:HG11	1.95	0.47
6:m:375:GLN:HE21	6:m:379:ARG:HH22	1.63	0.47
6:m:408:GLU:HA	6:m:411:LYS:HE2	1.95	0.47
1:B:189:ASP:OD2	1:B:261:LEU:HD21	2.15	0.47
1:F:236:THR:OG1	1:F:237:GLU:N	2.48	0.47
6:n:267:ALA:HB2	6:n:379:ARG:HD3	1.96	0.47
1:F:113:ALA:HB3	1:F:116:ASN:HD21	1.80	0.47
3:L:108:ARG:HD3	3:L:117:SER:HB3	1.96	0.47
6:m:553:TYR:CE2	6:m:557:ILE:HD11	2.49	0.47
6:n:367:ILE:HB	6:n:372:TYR:HB2	1.96	0.47
7:h:256:VAL:HG23	7:h:566:GLY:HA2	1.97	0.47
7:h:470:LEU:HB3	7:h:482:LEU:HD11	1.95	0.47
1:B:15:ASP:OD2	1:B:340:THR:OG1	2.31	0.47
6:n:564:ILE:HG13	6:n:565:THR:N	2.28	0.47
6:m:526:ALA:HA	6:m:529:ASN:HD22	1.80	0.47
6:n:265:ASP:HB3	6:n:268:SER:HB2	1.96	0.47
7:h:272:SER:HB3	7:h:312:ALA:HB3	1.96	0.47
7:h:409:THR:N	7:h:424:GLY:O	2.48	0.47
1:F:10:GLN:NE2	1:F:26:ALA:O	2.36	0.47
6:f:381:VAL:HA	6:f:384:ILE:HD12	1.96	0.46
6:f:676:HIS:HB3	6:f:679:GLY:H	1.80	0.46
1:B:232:GLU:OE2	1:B:257:ARG:NH2	2.48	0.46
1:D:143:ALA:HA	1:D:157:VAL:HG11	1.97	0.46
1:D:168:VAL:HG22	1:D:180:ILE:HG12	1.97	0.46
2:K:185:THR:HG22	2:K:187:GLN:HG3	1.98	0.46
1:D:68:LEU:HD12	1:F:171:TYR:HD2	1.81	0.46
6:n:528:GLU:HA	6:n:531:LYS:HG2	1.97	0.46
7:h:366:THR:H	7:h:369:ALA:HB3	1.80	0.46
3:L:264:GLU:O	3:L:268:ARG:CB	2.57	0.46
6:f:547:GLU:HG2	6:f:551:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:n:285:LEU:HD12	6:n:329:VAL:HG21	1.98	0.46
8:X:198:LYS:NZ	8:x:195:ASP:OD1	2.43	0.46
1:B:113:ALA:O	1:B:116:ASN:ND2	2.48	0.46
1:F:103:SER:HB2	1:F:132:PHE:HB3	1.98	0.46
2:K:72:ASP:HB3	2:K:91:ARG:HH11	1.81	0.46
6:f:724:ARG:HB2	6:f:734:LYS:H	1.81	0.46
1:D:280:VAL:HG11	1:D:321:LEU:HB3	1.97	0.46
1:F:361:LYS:HE2	1:F:361:LYS:HB2	1.77	0.46
2:K:13:LYS:HB3	2:K:40:LEU:HD11	1.96	0.46
6:f:751:ARG:O	6:f:755:TRP:HB2	2.16	0.46
6:f:825:GLU:HG3	6:f:828:LYS:H	1.79	0.46
2:K:60:ASP:OD1	2:K:61:GLN:N	2.49	0.46
2:K:121:ARG:HE	2:K:121:ARG:HB3	1.57	0.46
3:L:60:LEU:O	3:L:65:ASN:ND2	2.49	0.46
7:h:288:LEU:HD22	7:h:299:PRO:HB2	1.98	0.46
1:B:318:VAL:HG12	1:B:328:ILE:HD13	1.98	0.46
2:K:81:ASP:HA	2:K:87:PHE:HA	1.97	0.46
3:L:139:ASP:HB2	3:L:142:LYS:HB2	1.98	0.46
1:D:352:THR:HA	1:D:355:LYS:HE2	1.98	0.46
3:L:16:LEU:HD11	3:L:24:ASN:HB3	1.97	0.45
3:L:74:PRO:HD3	3:L:120:TYR:HE1	1.81	0.45
4:c:1:MET:N	6:m:307:GLY:O	2.49	0.45
6:f:648:ILE:HD12	6:f:699:PHE:HE1	1.81	0.45
6:f:786:ARG:HE	7:h:306:GLN:NE2	2.13	0.45
1:D:207:SER:N	1:D:210:GLU:OE2	2.37	0.45
3:L:136:LYS:O	3:L:148:TRP:N	2.45	0.45
6:f:540:LYS:HG3	6:f:541:GLU:HG2	1.98	0.45
6:n:216:VAL:HG21	6:n:232:PHE:HE1	1.80	0.45
6:n:361:PHE:HB2	6:n:426:GLU:OE2	2.17	0.45
2:K:99:ASP:HB3	2:K:102:ARG:HB3	1.97	0.45
1:B:8:ALA:HB3	1:B:107:PRO:HD3	1.97	0.45
1:B:121:ARG:NH1	1:B:375:THR:OG1	2.49	0.45
6:m:266:PRO:HA	6:m:274:GLU:OE2	2.16	0.45
7:h:521:GLY:O	7:h:541:VAL:N	2.39	0.45
8:x:175:THR:HA	8:x:178:LYS:HD2	1.99	0.45
2:K:121:ARG:O	2:K:125:ASP:CB	2.60	0.45
3:L:194:THR:O	3:L:195:ARG:NH2	2.45	0.45
6:f:756:LEU:HD23	6:f:758:PHE:HE1	1.80	0.45
6:f:815:LEU:HA	6:f:815:LEU:HD23	1.79	0.45
6:m:466:MET:HE3	6:m:534:ASP:OD2	2.17	0.45
7:h:481:LYS:NZ	7:h:491:LEU:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:MET:HG2	1:B:376:PHE:HE1	1.80	0.45
6:f:550:MET:O	6:f:554:ASP:HB2	2.16	0.45
6:m:268:SER:OG	6:m:269:GLY:N	2.49	0.45
6:m:268:SER:HA	6:m:386:ARG:HH12	1.81	0.45
2:K:121:ARG:HB2	2:K:145:ALA:HB2	1.98	0.45
6:f:759:ARG:HA	6:f:759:ARG:HD3	1.76	0.45
6:m:272:LEU:HB2	6:m:341:LEU:HD11	1.98	0.45
6:n:368:ARG:HG3	6:n:437:ILE:HG12	1.98	0.45
7:h:258:CYS:O	7:h:272:SER:OG	2.33	0.45
7:h:400:HIS:CG	7:h:401:LYS:H	2.34	0.45
1:B:147:LEU:HA	1:B:147:LEU:HD23	1.81	0.45
1:B:323:PRO:HG2	1:B:326:VAL:HG21	1.97	0.45
2:K:97:LYS:O	2:K:106:SER:N	2.45	0.45
6:m:475:GLN:O	6:m:479:VAL:HG23	2.17	0.45
7:h:383:SER:O	7:h:393:GLN:N	2.50	0.45
7:h:414:PRO:HD3	7:h:421:PHE:HA	1.97	0.45
1:B:52:LEU:HA	1:B:52:LEU:HD23	1.76	0.45
2:K:154:ILE:O	2:K:179:PHE:N	2.49	0.45
2:K:196:VAL:HB	2:K:206:LEU:HB3	1.99	0.45
3:L:134:ILE:HB	3:L:150:SER:HB2	1.98	0.45
6:n:282:GLU:OE2	6:n:333:ASN:HA	2.17	0.45
6:n:434:LEU:HA	6:n:437:ILE:HD12	1.98	0.45
1:B:74:PRO:HB3	1:B:85:ASP:HB2	1.98	0.45
1:B:130:GLU:O	6:m:368:ARG:NH2	2.40	0.45
1:D:56:ILE:HD13	1:D:88:ARG:HD3	2.00	0.45
3:L:35:LEU:HA	3:L:38:ASP:OD2	2.16	0.45
3:L:67:ASP:CG	3:L:87:ALA:H	2.23	0.45
6:f:577:ASN:OD1	6:f:578:ALA:N	2.49	0.45
6:m:278:TRP:HB2	6:m:336:MET:HG2	1.99	0.45
1:B:48:MET:HB3	1:D:173:GLY:HA2	1.97	0.44
7:h:307:SER:OG	7:h:308:ALA:N	2.50	0.44
2:K:102:ARG:NE	2:K:104:GLU:OE1	2.50	0.44
2:K:136:TYR:CZ	3:L:244:ARG:HD2	2.52	0.44
6:m:474:GLU:HA	6:m:477:ARG:HE	1.82	0.44
7:h:475:SER:OG	7:h:476:PHE:N	2.48	0.44
2:K:224:THR:HA	2:K:227:GLU:HB3	1.99	0.44
1:D:53:GLU:OE1	6:f:323:LYS:NZ	2.44	0.44
1:D:298:ILE:O	1:D:331:SER:N	2.49	0.44
2:K:128:LEU:HD12	2:K:131:TYR:HB3	1.98	0.44
3:L:61:LEU:HD22	3:L:71:TYR:CG	2.53	0.44
6:m:276:SER:O	6:m:280:ASN:ND2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:285:GLY:HA3	7:h:309:VAL:H	1.82	0.44
7:h:333:LEU:HD12	7:h:333:LEU:HA	1.77	0.44
1:D:360:LYS:HE2	1:D:364:GLU:OE2	2.18	0.44
6:f:568:LEU:HA	6:f:571:GLN:HG2	1.99	0.44
7:h:518:ASP:OD2	7:h:520:MET:HB2	2.17	0.44
1:B:20:VAL:O	1:B:22:LYS:NZ	2.48	0.44
1:F:254:SER:HA	1:F:257:ARG:HB2	2.00	0.44
6:f:549:ALA:O	6:f:553:TYR:CB	2.66	0.44
7:h:535:PRO:HB2	7:h:538:SER:HB3	2.00	0.44
1:B:263:PHE:HE1	1:B:275:ILE:HB	1.83	0.44
1:D:9:ASN:O	1:D:106:HIS:ND1	2.37	0.44
1:F:131:THR:OG1	1:F:132:PHE:N	2.51	0.44
1:F:253:PRO:HG2	1:F:257:ARG:HH12	1.82	0.44
2:K:30:ASN:OD1	2:K:103:LYS:NZ	2.50	0.44
2:K:154:ILE:HD13	2:K:154:ILE:HA	1.85	0.44
3:L:19:GLN:HG3	3:L:176:TRP:CZ3	2.53	0.44
6:m:616:ILE:HG22	6:m:620:HIS:CE1	2.52	0.44
6:n:565:THR:OG1	6:n:566:ALA:N	2.50	0.44
1:F:241:TYR:HD2	1:F:249:ILE:HD11	1.82	0.44
2:K:109:GLN:HA	2:K:110:PRO:HD3	1.91	0.44
2:K:136:TYR:OH	2:K:173:TRP:NE1	2.51	0.44
3:L:60:LEU:O	3:L:120:TYR:OH	2.34	0.44
6:f:392:LEU:HD23	6:f:392:LEU:HA	1.86	0.44
6:n:358:VAL:HA	6:n:426:GLU:OE2	2.18	0.44
1:F:147:LEU:HD23	1:F:147:LEU:HA	1.80	0.44
1:F:303:GLY:N	9:F:800:ADP:O2A	2.37	0.44
2:K:241:THR:O	2:K:244:SER:OG	2.29	0.44
6:f:720:ILE:HG22	6:f:721:GLU:OE2	2.18	0.44
7:h:340:LYS:HD3	7:h:344:VAL:HG12	1.99	0.44
7:h:343:PRO:HG2	7:h:346:ARG:HE	1.83	0.44
7:h:510:HIS:HD2	7:h:579:VAL:H	1.66	0.44
2:K:79:HIS:CD2	2:K:155:ILE:HG21	2.53	0.43
6:f:528:GLU:O	6:f:531:LYS:HG2	2.17	0.43
7:h:245:PHE:CD2	7:h:570:ILE:HD11	2.54	0.43
7:h:572:ASP:OD1	7:h:573:VAL:N	2.50	0.43
1:B:10:GLN:OE1	6:n:246:GLN:NE2	2.47	0.43
1:B:197:TYR:HD1	1:B:197:TYR:HA	1.67	0.43
1:B:226:ILE:O	1:B:313:ARG:NH1	2.50	0.43
6:f:592:PHE:O	6:f:598:ARG:NH2	2.52	0.43
6:m:619:LEU:HA	6:m:619:LEU:HD23	1.75	0.43
6:n:564:ILE:O	6:n:568:LEU:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:360:CYS:HB2	7:h:410:SER:HA	1.99	0.43
6:f:700:ASP:O	6:f:704:ARG:HB2	2.19	0.43
6:f:786:ARG:HH11	7:h:306:GLN:HE21	1.66	0.43
1:F:126:GLU:O	1:F:130:GLU:HB2	2.19	0.43
3:L:159:LYS:HD2	3:L:164:THR:HG23	1.99	0.43
6:f:393:LEU:HA	6:f:396:LEU:HB3	2.00	0.43
6:n:232:PHE:HB2	6:n:236:VAL:HG23	2.01	0.43
1:B:128:PHE:O	1:B:133:ASN:N	2.52	0.43
1:D:44:HIS:CG	1:F:176:MET:HG2	2.54	0.43
6:f:565:THR:HA	6:f:568:LEU:HD12	2.01	0.43
6:f:724:ARG:HH12	6:f:726:ARG:HD3	1.83	0.43
7:h:254:ARG:O	7:h:566:GLY:N	2.51	0.43
1:F:75:MET:HE3	1:F:75:MET:HB2	1.89	0.43
1:F:354:LYS:HG2	1:F:357:TRP:CH2	2.54	0.43
7:h:315:ALA:HB3	7:h:318:HIS:HB2	1.99	0.43
4:c:2:ALA:HB1	4:c:5:LYS:HD3	2.01	0.43
7:h:256:VAL:O	7:h:548:ASN:ND2	2.52	0.43
1:D:219:GLU:OE2	9:D:800:ADP:H2'	2.18	0.43
2:K:47:ARG:HE	2:K:48:GLU:HG3	1.84	0.43
6:n:340:PRO:HG2	6:n:360:ILE:HG12	2.01	0.43
2:K:159:GLU:OE2	2:K:161:HIS:HB3	2.18	0.43
6:f:549:ALA:O	6:f:553:TYR:HB2	2.19	0.43
6:m:304:LEU:HD23	6:m:304:LEU:HA	1.87	0.43
7:h:480:VAL:O	7:h:494:PHE:N	2.52	0.43
1:F:362:GLU:OE2	1:F:366:ASP:OD2	2.38	0.42
6:f:238:ASP:HB2	6:f:241:PHE:HB3	2.01	0.42
7:h:479:THR:HA	7:h:495:GLU:HA	2.00	0.42
6:n:548:ALA:O	6:n:552:ARG:HB2	2.17	0.42
1:B:305:THR:O	1:B:336:ARG:NH1	2.52	0.42
1:D:159:ASP:HB3	1:D:301:SER:HB3	2.01	0.42
1:D:273:GLU:HB3	1:D:277:GLU:HB2	2.01	0.42
1:F:198:LEU:HD23	1:F:198:LEU:HA	1.83	0.42
2:K:225:ALA:O	2:K:229:ILE:HG12	2.20	0.42
6:f:561:GLU:O	6:f:565:THR:OG1	2.25	0.42
6:n:349:GLU:HG2	6:n:351:ASP:H	1.84	0.42
7:h:259:LEU:HD23	7:h:271:ALA:HA	2.01	0.42
7:h:459:HIS:CE1	7:h:470:LEU:HB2	2.54	0.42
1:F:96:LYS:HA	1:F:100:GLN:HG2	2.01	0.42
1:F:197:TYR:HD1	1:F:197:TYR:HA	1.66	0.42
2:K:13:LYS:HZ2	3:L:31:LEU:HA	1.84	0.42
2:K:159:GLU:OE2	2:K:172:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:m:465:GLN:HB2	6:m:546:TRP:HH2	1.83	0.42
6:m:473:HIS:NE2	6:m:523:VAL:HG12	2.35	0.42
6:m:476:LEU:HD23	6:m:476:LEU:HA	1.89	0.42
6:m:581:MET:HE2	6:m:608:LEU:HG	2.02	0.42
2:K:13:LYS:HD3	2:K:16:ILE:HD12	2.02	0.42
3:L:72:ARG:NH2	3:L:97:GLU:OE2	2.52	0.42
3:L:112:PHE:O	3:L:136:LYS:NZ	2.46	0.42
7:h:419:ASN:HB2	7:h:435:ARG:HD3	2.01	0.42
8:x:191:LEU:HA	8:x:191:LEU:HD23	1.83	0.42
1:B:66:ARG:HD2	1:D:289:ASP:OD2	2.19	0.42
1:D:252:GLY:HA3	1:D:253:PRO:HD3	1.87	0.42
6:f:724:ARG:HB3	6:f:725:VAL:H	1.58	0.42
6:m:519:ALA:O	6:m:523:VAL:HG23	2.19	0.42
6:n:523:VAL:HG22	6:n:560:VAL:CG1	2.50	0.42
7:h:336:ASN:OD1	7:h:337:ARG:N	2.53	0.42
7:h:470:LEU:HD23	7:h:482:LEU:HD11	2.01	0.42
1:F:260:GLU:OE2	1:F:313:ARG:NH1	2.52	0.42
2:K:33:PHE:HA	2:K:36:VAL:HG12	2.02	0.42
3:L:136:LYS:HB3	3:L:148:TRP:HB3	2.01	0.42
6:f:602:ARG:HA	6:f:605:GLN:CD	2.44	0.42
6:f:736:LYS:HZ3	6:f:740:LEU:HD11	1.84	0.42
8:X:188:GLN:NE2	8:x:187:GLN:OE1	2.35	0.42
1:F:338:TYR:CE2	5:d:9:LEU:HD13	2.55	0.42
6:m:448:MET:HB2	6:m:450:TRP:CE2	2.55	0.42
7:h:356:HIS:HB2	7:h:378:ASP:HB2	2.02	0.42
8:X:148:LEU:O	8:x:152:LYS:NZ	2.49	0.42
2:K:97:LYS:HB3	2:K:106:SER:HB2	2.02	0.42
2:K:192:LEU:HD21	2:K:236:GLU:HG2	2.01	0.42
2:K:208:SER:OG	2:K:209:HIS:N	2.53	0.42
6:f:232:PHE:HB2	6:f:236:VAL:HG23	2.02	0.42
6:f:567:ARG:HA	6:f:570:ASP:HB2	2.02	0.42
7:h:250:TRP:HB2	7:h:288:LEU:HD11	2.01	0.42
1:B:205:PHE:HB3	1:B:210:GLU:HG2	2.02	0.42
1:F:20:VAL:HA	1:F:36:PRO:HA	2.02	0.42
1:F:223:TYR:CE1	1:F:255:ARG:HG3	2.55	0.42
3:L:12:LEU:HA	3:L:12:LEU:HD12	1.86	0.42
3:L:142:LYS:HA	3:L:142:LYS:HD2	1.84	0.42
6:f:606:THR:OG1	6:f:607:GLN:N	2.51	0.42
6:f:686:GLY:O	6:f:690:ARG:HG2	2.20	0.42
6:f:703:ALA:O	6:f:707:GLN:HB2	2.20	0.42
6:n:546:TRP:HA	6:n:549:ALA:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:HD23	1:D:290:LEU:HA	1.84	0.41
6:f:627:TYR:O	6:f:633:CYS:HB2	2.20	0.41
6:f:827:TYR:CD1	8:X:149:GLU:HB3	2.55	0.41
6:m:255:GLU:HA	6:m:258:LYS:HD2	2.02	0.41
6:m:469:PHE:HZ	6:m:527:TYR:HA	1.85	0.41
6:n:564:ILE:CG1	6:n:565:THR:N	2.83	0.41
7:h:316:LYS:HG3	7:h:317:PHE:CD2	2.55	0.41
3:L:60:LEU:HD23	3:L:60:LEU:HA	1.86	0.41
6:f:409:PHE:CD1	6:f:470:ARG:HD3	2.55	0.41
6:m:435:ARG:HG3	8:x:165:GLU:OE2	2.20	0.41
7:h:477:ASP:OD1	7:h:477:ASP:N	2.52	0.41
1:D:159:ASP:OD1	1:D:159:ASP:N	2.50	0.41
1:D:245:ASP:OD1	1:D:246:GLY:N	2.53	0.41
6:f:670:GLY:O	6:f:673:TRP:NE1	2.48	0.41
6:m:238:ASP:HB2	6:m:241:PHE:HB3	2.02	0.41
6:m:613:LYS:HE3	6:m:613:LYS:HB2	1.91	0.41
6:n:438:VAL:HG13	6:n:443:GLU:OE2	2.20	0.41
1:D:38:TYR:HB2	1:D:71:ILE:HG23	2.02	0.41
1:F:219:GLU:HG2	9:F:800:ADP:C4	2.55	0.41
3:L:54:VAL:HG23	3:L:55:VAL:HG23	2.02	0.41
1:B:236:THR:HG23	1:B:238:LYS:H	1.85	0.41
2:K:93:LYS:HE2	2:K:93:LYS:HB2	1.89	0.41
6:f:204:GLU:OE1	6:f:287:ARG:NH1	2.53	0.41
6:f:402:MET:O	6:f:527:TYR:OH	2.25	0.41
6:f:813:GLN:HA	6:f:816:ILE:HB	2.02	0.41
6:m:403:HIS:HA	6:m:531:LYS:NZ	2.35	0.41
6:m:454:PRO:O	6:m:457:ARG:HG2	2.21	0.41
6:m:473:HIS:CE1	6:m:477:ARG:HG2	2.54	0.41
6:n:443:GLU:OE1	6:n:443:GLU:N	2.52	0.41
6:n:567:ARG:O	6:n:571:GLN:HG2	2.20	0.41
7:h:456:ILE:HG13	7:h:473:THR:HG22	2.02	0.41
1:D:36:PRO:HB2	1:D:38:TYR:CE2	2.56	0.41
3:L:111:TYR:OH	3:L:218:GLU:OE2	2.38	0.41
6:f:297:VAL:O	6:f:300:THR:OG1	2.38	0.41
6:m:542:GLY:O	6:m:546:TRP:CB	2.49	0.41
2:K:87:PHE:HB2	2:K:96:PHE:CZ	2.56	0.41
3:L:66:ARG:NH2	3:L:69:ASP:OD1	2.53	0.41
6:m:523:VAL:HG22	6:m:560:VAL:HG21	2.02	0.41
1:B:13:VAL:HG22	1:B:109:LEU:HD23	2.02	0.41
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.91	0.41
1:D:107:PRO:HB3	1:D:136:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:447:LYS:HA	6:f:447:LYS:HD3	1.83	0.41
6:f:747:SER:O	6:f:751:ARG:HD3	2.21	0.41
1:B:270:GLU:HG2	1:B:272:SER:H	1.86	0.41
1:D:185:ILE:HA	1:D:189:ASP:OD2	2.21	0.41
1:D:284:GLN:O	1:D:291:ARG:NH2	2.54	0.41
1:D:318:VAL:HG12	1:D:328:ILE:HD13	2.02	0.41
1:F:199:ARG:HG2	1:F:204:ASP:HA	2.03	0.41
2:K:272:ASN:O	2:K:276:SER:CB	2.69	0.41
3:L:107:TYR:OH	3:L:221:GLU:OE1	2.33	0.41
6:f:354:ARG:HB2	6:f:419:VAL:HG22	2.02	0.41
6:f:373:PRO:HG2	6:f:376:ARG:HD3	2.02	0.41
6:f:607:GLN:HB3	6:f:611:ARG:NH1	2.36	0.41
6:f:726:ARG:NH2	6:f:727:GLY:O	2.54	0.41
6:m:264:ARG:HH22	6:m:273:GLN:HB3	1.86	0.41
6:m:454:PRO:HB2	6:m:456:HIS:CE1	2.55	0.41
6:m:583:ARG:HD3	6:m:583:ARG:HA	1.75	0.41
6:n:556:ARG:HA	6:n:556:ARG:HD2	1.82	0.41
7:h:380:LYS:HA	7:h:397:GLU:HA	2.02	0.41
7:h:481:LYS:HA	7:h:493:SER:HA	2.02	0.41
7:h:510:HIS:CD2	7:h:579:VAL:H	2.38	0.41
1:D:327:LYS:NZ	4:c:24:ASP:OD1	2.44	0.41
2:K:233:GLU:O	2:K:237:ASN:ND2	2.53	0.41
4:c:9:LEU:HA	4:c:10:PRO:HD3	1.86	0.41
6:f:704:ARG:O	6:f:708:GLN:HG2	2.21	0.41
6:m:239:PRO:O	6:m:243:ASN:HB2	2.21	0.41
6:m:438:VAL:HG21	6:m:450:TRP:HZ2	1.86	0.41
6:m:577:ASN:OD1	6:m:578:ALA:N	2.53	0.41
3:L:149:ASP:HB2	3:L:174:MET:HB2	2.03	0.40
6:f:683:LYS:HE2	6:f:683:LYS:HB3	1.75	0.40
6:m:568:LEU:HD23	6:m:568:LEU:HA	1.70	0.40
6:n:561:GLU:HG3	6:n:564:ILE:HD13	2.03	0.40
1:B:224:LEU:HD23	1:B:224:LEU:HA	1.86	0.40
2:K:240:GLN:OE1	3:L:244:ARG:NH1	2.54	0.40
3:L:62:CYS:SG	3:L:63:ASP:N	2.94	0.40
3:L:177:LEU:HD12	3:L:189:LEU:HD23	2.03	0.40
6:f:451:ARG:HD3	6:f:451:ARG:HA	1.84	0.40
6:m:267:ALA:HA	6:m:379:ARG:HB3	2.04	0.40
6:n:368:ARG:O	6:n:440:ARG:NH1	2.55	0.40
7:h:398:LEU:HD23	7:h:398:LEU:HA	1.89	0.40
2:K:40:LEU:HB3	2:K:46:LEU:HD23	2.04	0.40
2:K:223:GLN:O	2:K:227:GLU:CB	2.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:462:ARG:HH12	6:f:542:GLY:HA2	1.85	0.40
6:f:578:ALA:O	6:f:582:PHE:HB2	2.21	0.40
6:m:588:PHE:HD1	6:m:591:LEU:HD12	1.86	0.40
7:h:411:MET:HE1	7:h:413:PHE:CE2	2.56	0.40
1:D:48:MET:HB3	1:F:173:GLY:HA2	2.03	0.40
2:K:186:ALA:HB2	2:K:218:VAL:HG23	2.04	0.40
5:d:20:TYR:HD1	5:d:20:TYR:HA	1.73	0.40
6:m:473:HIS:NE2	6:m:527:TYR:HB2	2.35	0.40
6:n:466:MET:O	6:n:470:ARG:HG2	2.22	0.40
1:D:95:SER:OG	1:D:96:LYS:N	2.55	0.40
1:F:148:TYR:CE2	1:F:347:LEU:HB2	2.57	0.40
2:K:120:TRP:CH2	2:K:221:GLU:HA	2.55	0.40
3:L:70:SER:OG	3:L:81:PRO:O	2.30	0.40
6:f:726:ARG:HD2	6:f:726:ARG:HA	1.80	0.40
6:m:252:TRP:CZ3	6:m:297:VAL:HG13	2.57	0.40
6:m:271:ALA:O	6:m:275:ILE:HG12	2.22	0.40
7:h:460:ALA:H	7:h:508:PRO:HB3	1.87	0.40
8:x:194:ALA:O	8:x:198:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	368/376 (98%)	338 (92%)	30 (8%)	0	100	100
1	D	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
1	F	368/376 (98%)	332 (90%)	36 (10%)	0	100	100
2	K	276/286 (96%)	244 (88%)	32 (12%)	0	100	100
3	L	267/271 (98%)	233 (87%)	34 (13%)	0	100	100
4	c	33/50 (66%)	26 (79%)	7 (21%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	22/26 (85%)	16 (73%)	6 (27%)	0	100	100
6	f	592/1186 (50%)	538 (91%)	54 (9%)	0	100	100
6	m	392/1186 (33%)	361 (92%)	30 (8%)	1 (0%)	36	65
6	n	337/1186 (28%)	304 (90%)	33 (10%)	0	100	100
7	h	356/612 (58%)	299 (84%)	54 (15%)	3 (1%)	16	44
8	X	77/577 (13%)	74 (96%)	3 (4%)	0	100	100
8	x	65/577 (11%)	65 (100%)	0	0	100	100
All	All	3521/7085 (50%)	3162 (90%)	355 (10%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	h	491	LEU
6	m	455	ALA
7	h	511	PRO
7	h	490	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	318/324 (98%)	315 (99%)	3 (1%)	70	76
1	D	318/324 (98%)	317 (100%)	1 (0%)	86	84
1	F	318/324 (98%)	317 (100%)	1 (0%)	86	84
2	K	247/254 (97%)	246 (100%)	1 (0%)	84	83
3	L	238/240 (99%)	238 (100%)	0	100	100
4	c	22/44 (50%)	22 (100%)	0	100	100
5	d	21/22 (96%)	21 (100%)	0	100	100
6	f	534/1056 (51%)	534 (100%)	0	100	100
6	m	358/1056 (34%)	357 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	n	307/1056 (29%)	306 (100%)	1 (0%)	86	84
7	h	307/531 (58%)	306 (100%)	1 (0%)	86	84
8	X	74/503 (15%)	74 (100%)	0	100	100
8	x	64/503 (13%)	64 (100%)	0	100	100
All	All	3126/6237 (50%)	3117 (100%)	9 (0%)	84	84

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	TYR
1	B	197	TYR
1	B	245	ASP
1	D	261	LEU
1	F	245	ASP
2	K	254	THR
6	m	438	VAL
6	n	329	VAL
7	h	472	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	133	ASN
1	D	10	GLN
1	D	65	HIS
1	D	133	ASN
1	F	9	ASN
1	F	44	HIS
1	F	65	HIS
1	F	297	ASN
2	K	58	ASN
2	K	100	HIS
2	K	147	ASN
2	K	167	ASN
2	K	248	GLN
3	L	20	GLN
3	L	229	ASN
6	f	215	ASN
6	f	653	GLN
6	f	708	GLN

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Mol	Chain	Res	Type
6	f	731	ASN
6	f	772	ASN
6	f	773	GLN
6	m	280	ASN
6	m	391	GLN
6	m	472	GLN
6	m	524	ASN
6	m	529	ASN
6	m	589	ASN
6	n	243	ASN
6	n	529	ASN
6	n	571	GLN
7	h	264	GLN
7	h	276	ASN
7	h	306	GLN
7	h	320	ASN
7	h	330	GLN
7	h	345	GLN
7	h	371	ASN
7	h	497	ASN
7	h	544	ASN
8	X	161	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	ADP	D	800	-	28,29,29	1.54	3 (10%)	43,45,45	1.65	7 (16%)
9	ADP	B	800	-	28,29,29	1.53	5 (17%)	43,45,45	1.99	13 (30%)
9	ADP	F	800	-	28,29,29	1.66	5 (17%)	43,45,45	1.88	11 (25%)

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
9	ADP	D	800	-	-	4/16/32/32	0/3/3/3
9	ADP	B	800	-	-	3/16/32/32	0/3/3/3
9	ADP	F	800	-	-	4/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	800	ADP	C4-N9	-4.24	1.28	1.37
9	D	800	ADP	C5-N7	-3.65	1.32	1.39
9	D	800	ADP	C5-C4	3.61	1.45	1.39
9	F	800	ADP	C5-N7	-3.45	1.32	1.39
9	B	800	ADP	C5-N7	-3.38	1.32	1.39
9	B	800	ADP	C5-C4	3.31	1.45	1.39
9	B	800	ADP	C4-N9	-3.18	1.31	1.37
9	D	800	ADP	C4-N9	-3.14	1.31	1.37
9	F	800	ADP	C8-N9	-2.97	1.32	1.37
9	F	800	ADP	C5-C4	2.96	1.44	1.39
9	B	800	ADP	C8-N9	-2.62	1.33	1.37
9	F	800	ADP	PA-O3A	-2.53	1.56	1.59
9	B	800	ADP	PA-O3A	-2.38	1.56	1.59

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	800	ADP	C5-C4-N3	-5.88	118.62	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	800	ADP	C5-C4-N3	-5.55	119.07	126.72
9	F	800	ADP	C5-C4-N3	-4.76	120.16	126.72
9	B	800	ADP	N3-C4-N9	4.50	134.83	127.17
9	D	800	ADP	N3-C4-N9	4.02	134.00	127.17
9	F	800	ADP	C4-C5-N7	-3.79	106.24	110.58
9	B	800	ADP	C2-N3-C4	3.65	120.74	111.83
9	F	800	ADP	C4-N9-C8	3.62	109.54	105.74
9	F	800	ADP	N3-C4-N9	3.43	133.00	127.17
9	F	800	ADP	C2'-C1'-N9	-3.41	104.83	113.30
9	B	800	ADP	C4-C5-N7	-3.31	106.80	110.58
9	F	800	ADP	C2-N3-C4	3.23	119.72	111.83
9	F	800	ADP	N3-C2-N1	-3.06	123.96	128.58
9	B	800	ADP	N3-C2-N1	-3.00	124.03	128.58
9	D	800	ADP	C2-N3-C4	3.00	119.16	111.83
9	B	800	ADP	C2'-C1'-N9	-2.89	106.13	113.30
9	B	800	ADP	C4-N9-C8	2.77	108.65	105.74
9	F	800	ADP	N9-C8-N7	-2.72	110.07	113.94
9	D	800	ADP	C3'-C2'-C1'	2.69	106.56	101.46
9	B	800	ADP	C3'-C2'-C1'	2.61	106.40	101.46
9	D	800	ADP	O2'-C2'-C3'	-2.50	103.79	111.82
9	B	800	ADP	O2A-PA-O1A	2.49	124.03	112.44
9	F	800	ADP	C5-N7-C8	2.46	107.31	103.45
9	D	800	ADP	C4-C5-N7	-2.39	107.86	110.58
9	F	800	ADP	C6-C5-N7	2.38	136.67	132.09
9	B	800	ADP	C5-N7-C8	2.29	107.04	103.45
9	B	800	ADP	C2'-C3'-C4'	2.27	107.00	102.61
9	F	800	ADP	O3B-PB-O1B	2.25	119.61	110.83
9	B	800	ADP	N9-C8-N7	-2.11	110.95	113.94
9	B	800	ADP	O3B-PB-O2B	2.08	115.59	107.80
9	D	800	ADP	O2A-PA-O1A	2.03	121.87	112.44

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	800	ADP	C5'-O5'-PA-O1A
9	D	800	ADP	C5'-O5'-PA-O3A
9	F	800	ADP	C5'-O5'-PA-O2A
9	F	800	ADP	C5'-O5'-PA-O3A
9	B	800	ADP	C3'-C4'-C5'-O5'
9	F	800	ADP	C3'-C4'-C5'-O5'
9	D	800	ADP	O4'-C4'-C5'-O5'

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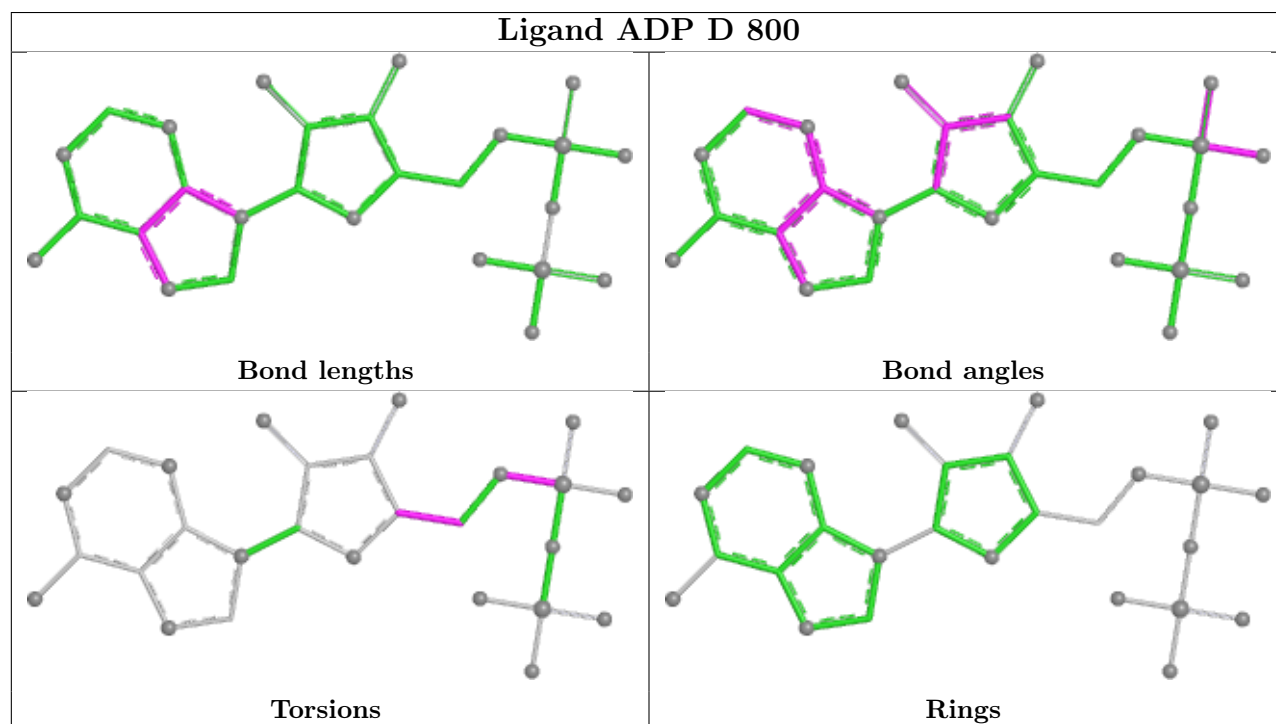
Mol	Chain	Res	Type	Atoms
9	F	800	ADP	O4'-C4'-C5'-O5'
9	D	800	ADP	C3'-C4'-C5'-O5'
9	B	800	ADP	O4'-C4'-C5'-O5'
9	B	800	ADP	C5'-O5'-PA-O1A

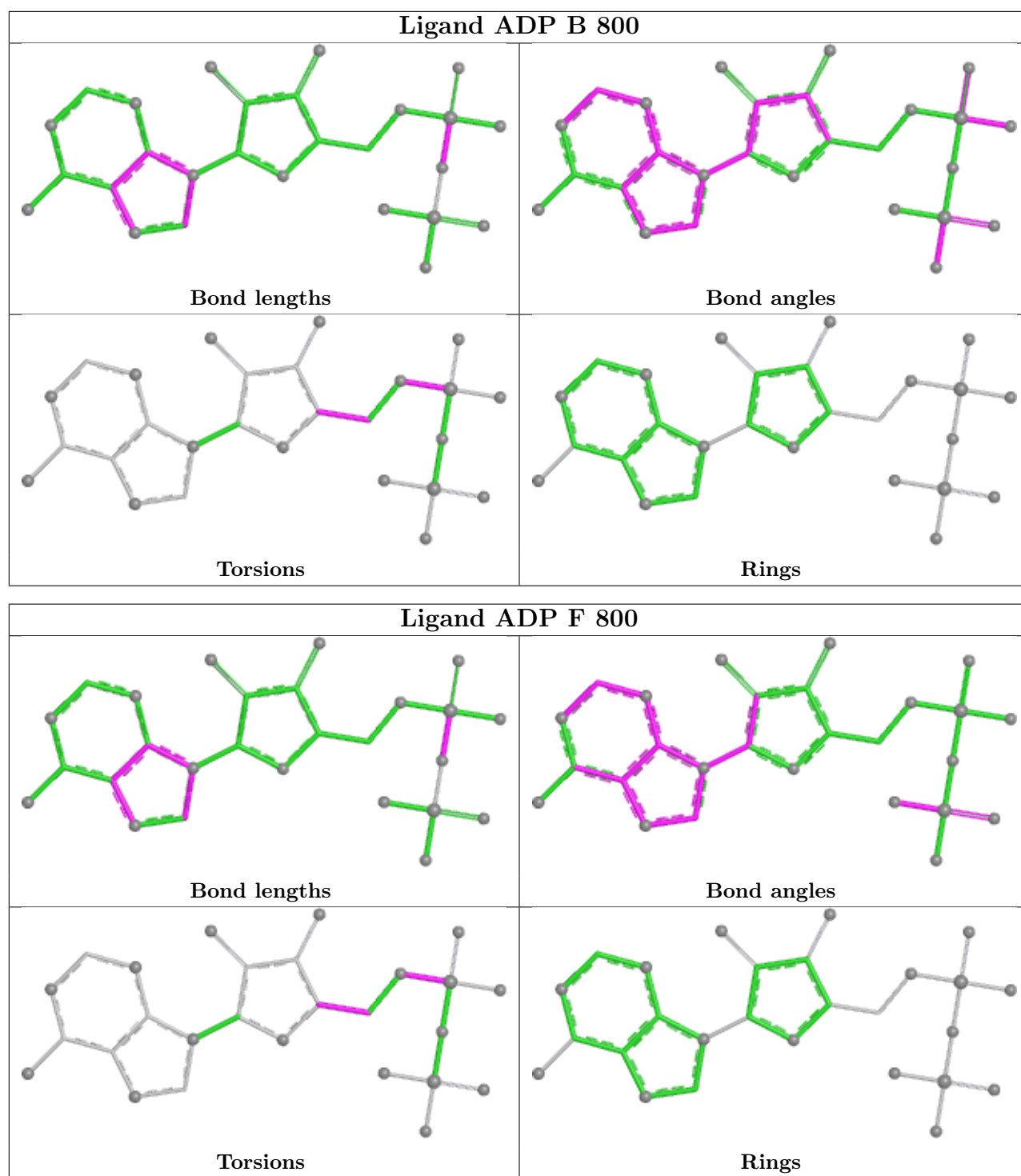
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	800	ADP	2	0
9	F	800	ADP	3	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.

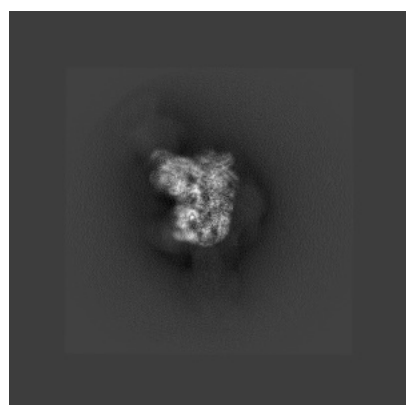
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4169. These allow visual inspection of the internal detail of the map and identification of artifacts.

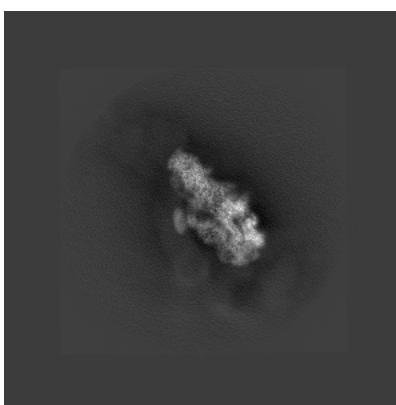
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

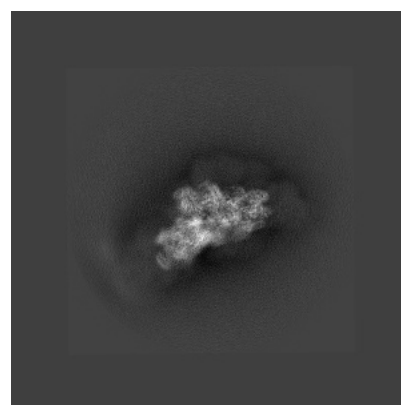
6.1.1 Primary map



X



Y

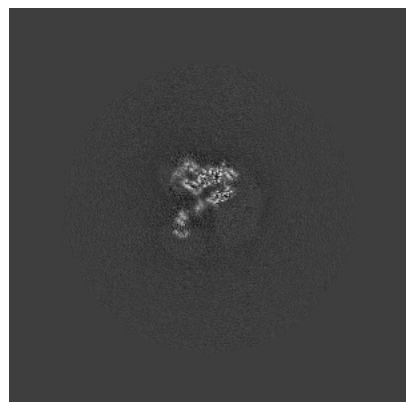


Z

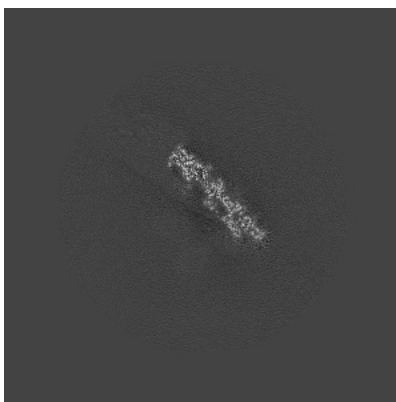
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300



Y Index: 300

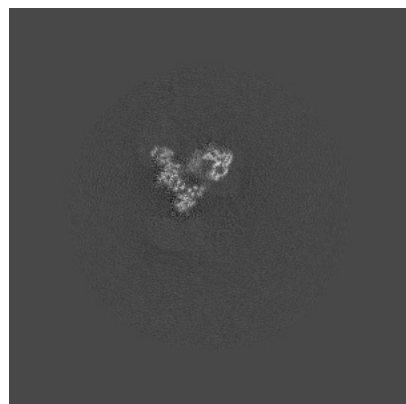


Z Index: 300

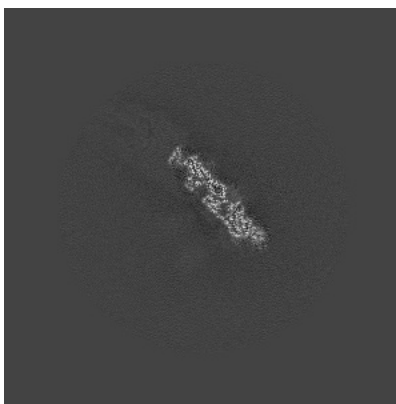
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

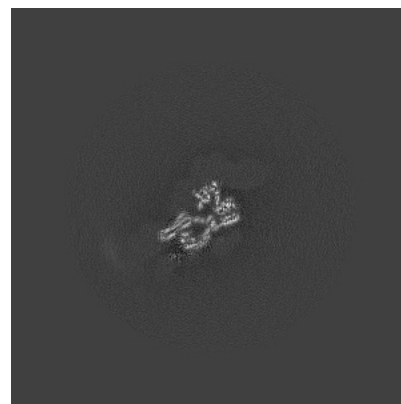
6.3.1 Primary map



X Index: 257



Y Index: 305

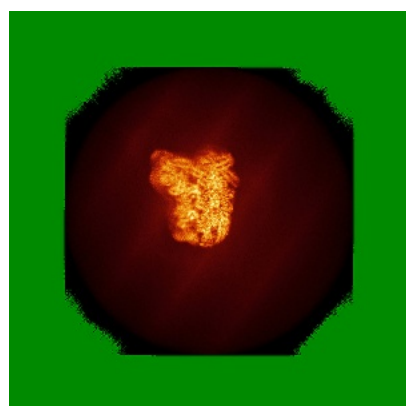


Z Index: 328

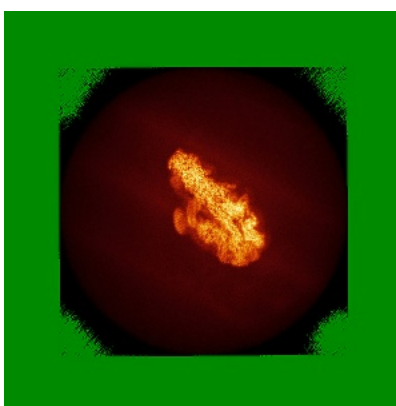
The images above show the largest variance slices of the map in three orthogonal directions.

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

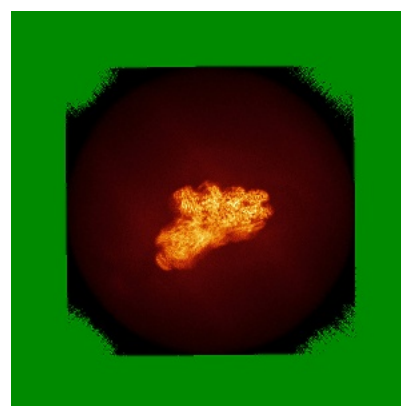
6.4.1 Primary map



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

This section was not generated.

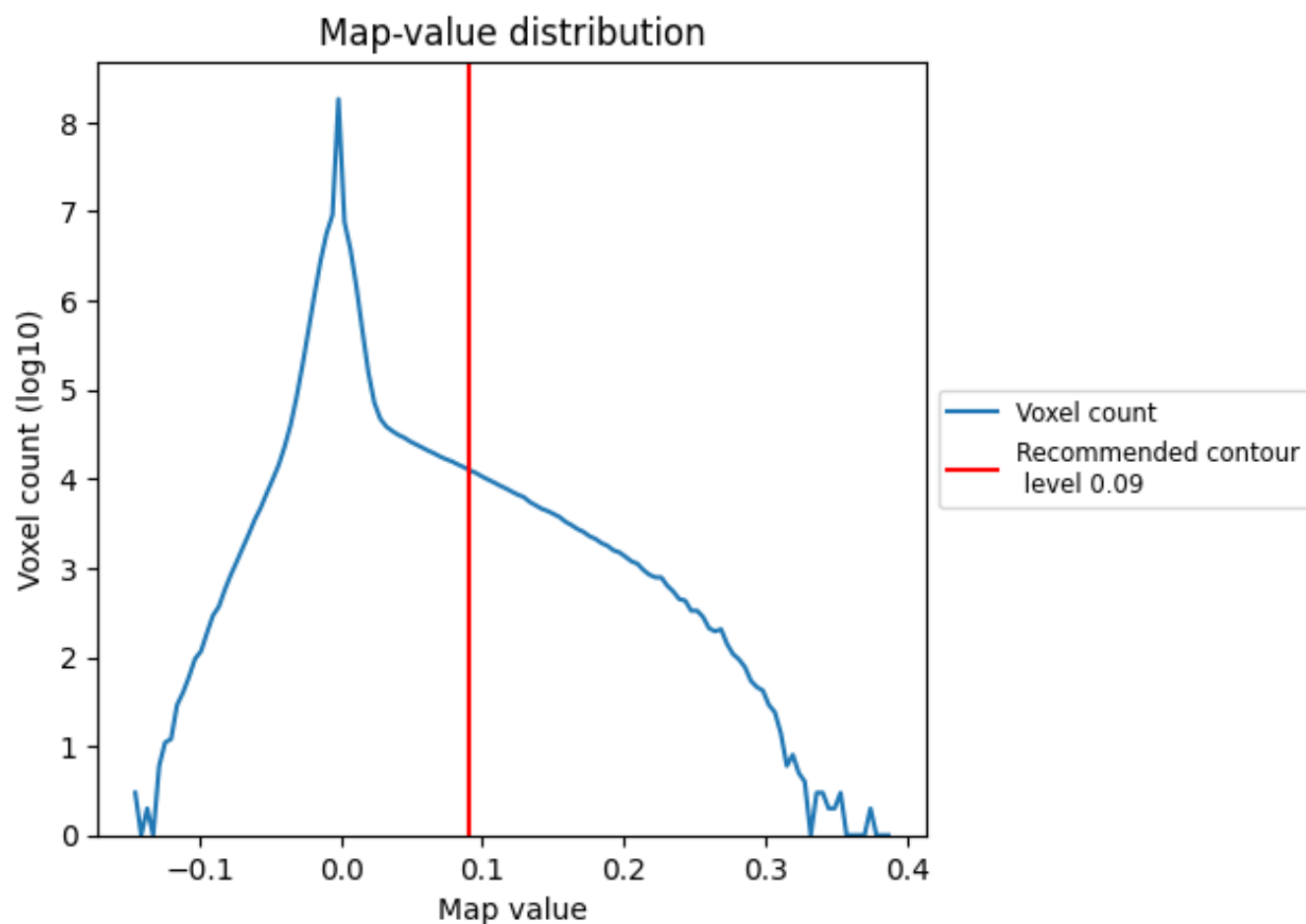
6.6 Mask visualisation

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

7 Map analysis [i](#)

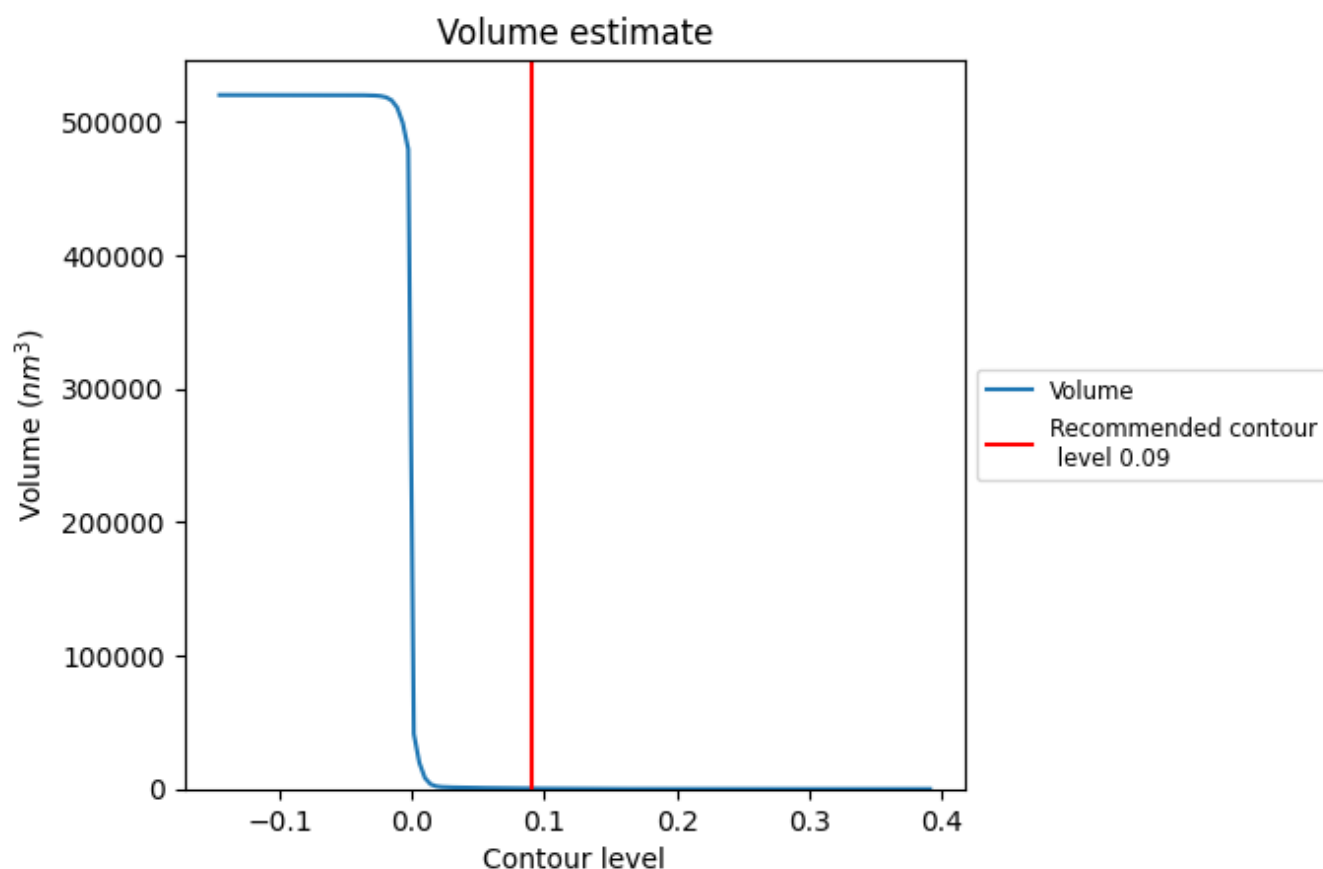
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

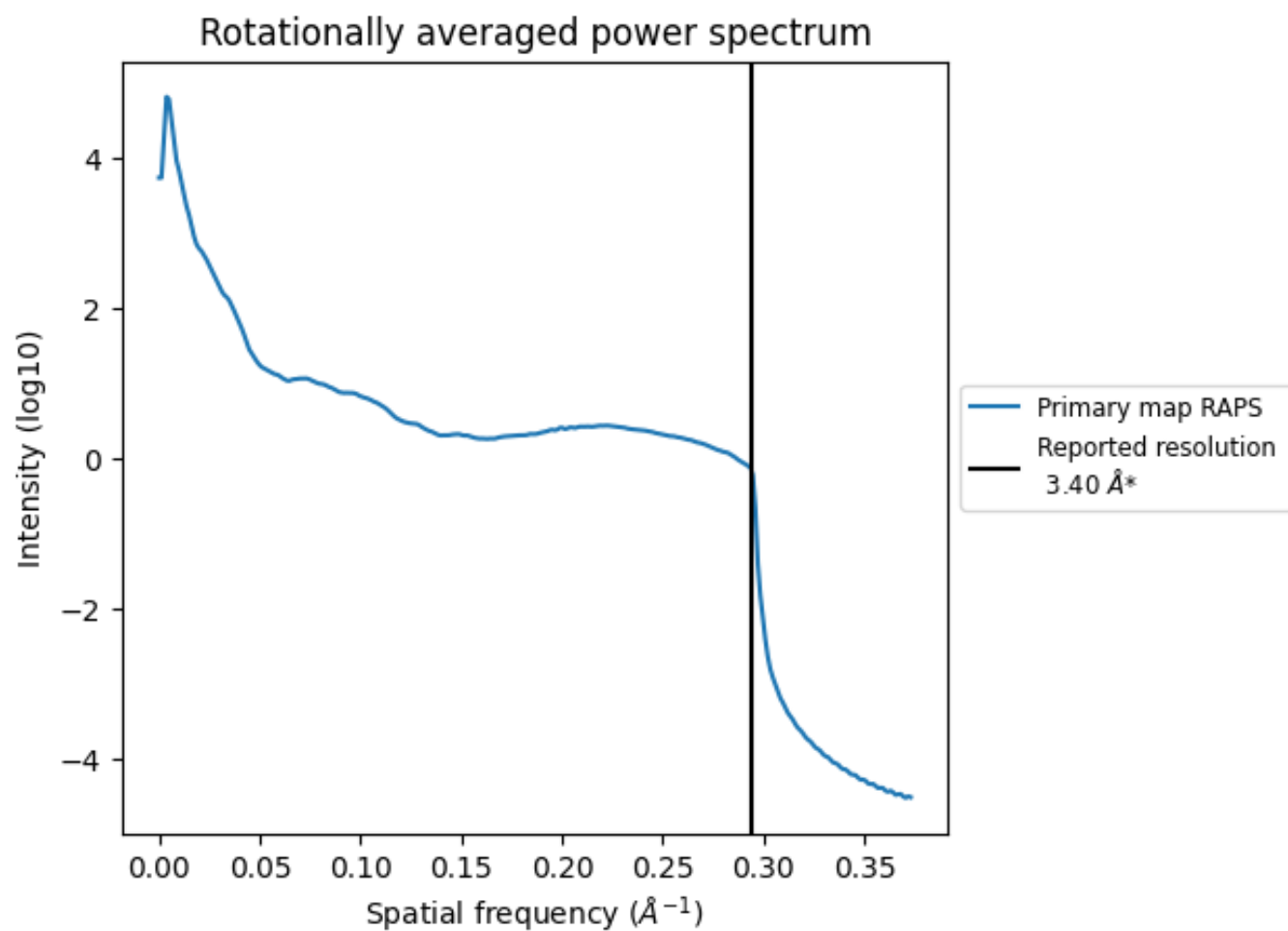
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 373 nm^3 ; this corresponds to an approximate mass of 337 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 0.294 Å⁻¹

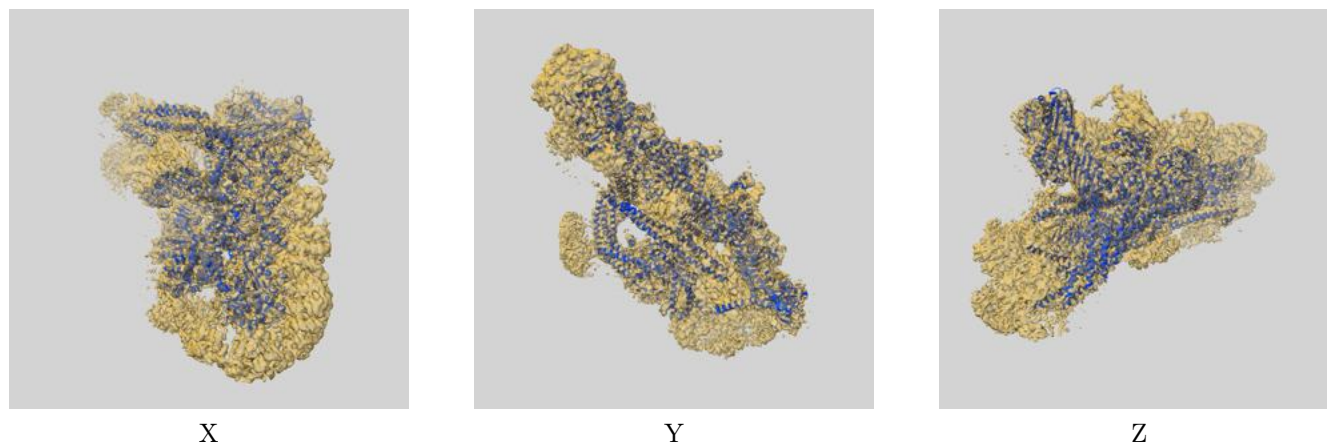
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

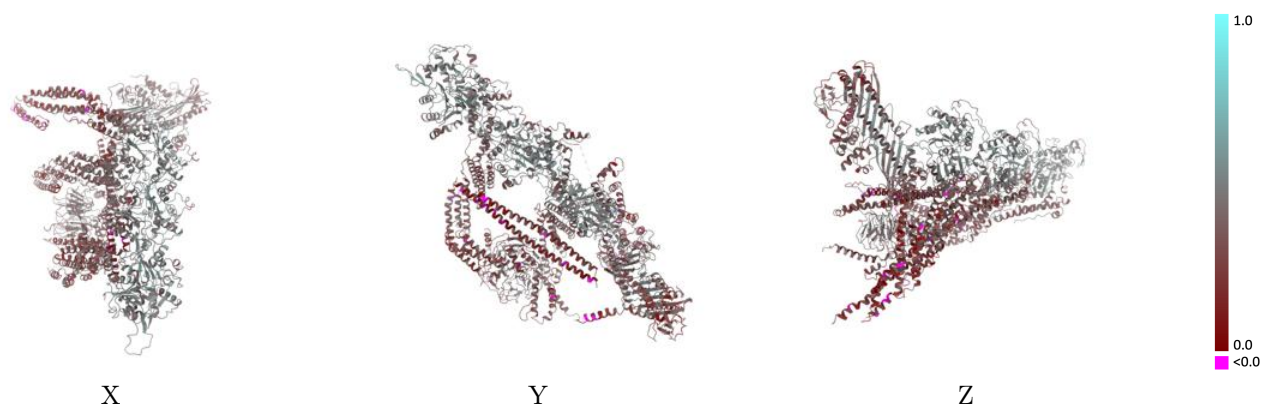
This section contains information regarding the fit between EMDB map EMD-4169 and PDB model 6F1U. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



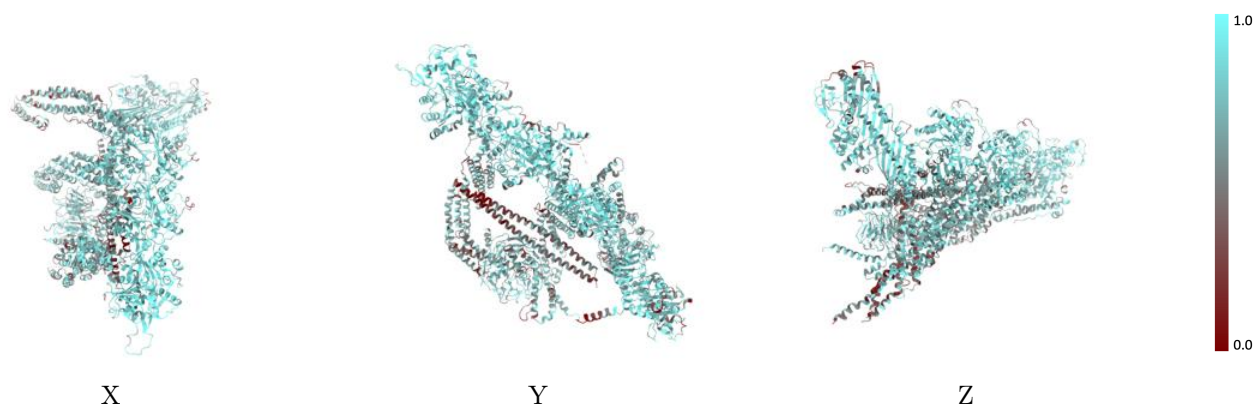
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



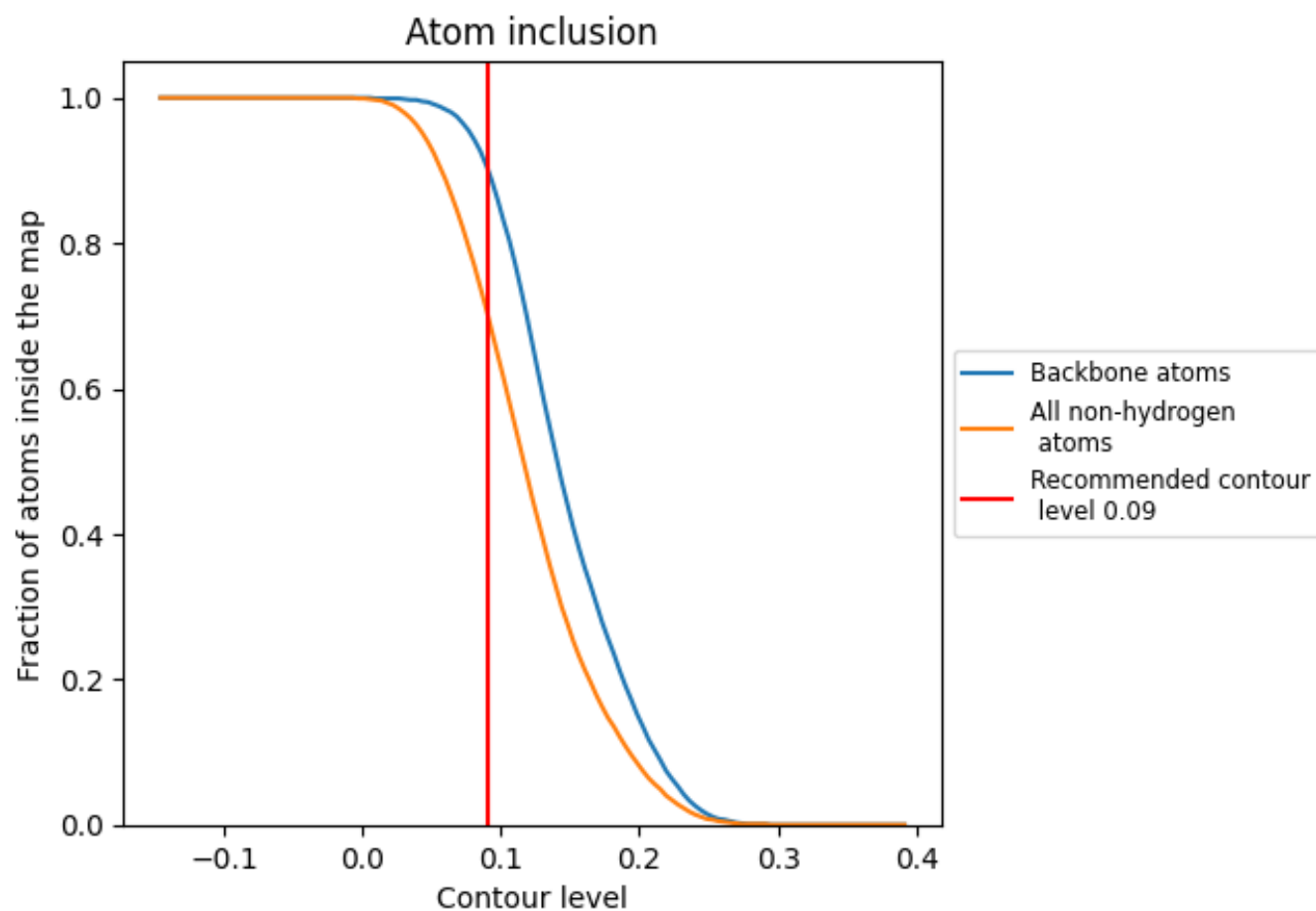
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 71% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7060	0.3740
B	0.8100	0.4770
D	0.8200	0.4800
F	0.8410	0.4820
K	0.7310	0.3700
L	0.7320	0.3990
X	0.3900	0.1670
c	0.6590	0.4530
d	0.6200	0.4340
f	0.6160	0.3080
h	0.7370	0.3720
m	0.7040	0.3490
n	0.5710	0.2440
x	0.4080	0.2140

1.0

0.0

<0.0