Full wwPDB EM Validation Report ⓘ

May 18, 2025 – 12:31 AM JST

PDB ID	:	9IS8 / pdb_00009is8
EMDB ID	:	EMD-60834
Title	:	Cryo-EM structure of AKT1-AtKC1(G315D)
Authors	:	Dongliang, L.; Zijie, Z.; Yannan, Q.; Yuyue, T.; Huaizong, S.
Deposited on	:	2024-07-17
Resolution	:	2.77 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:

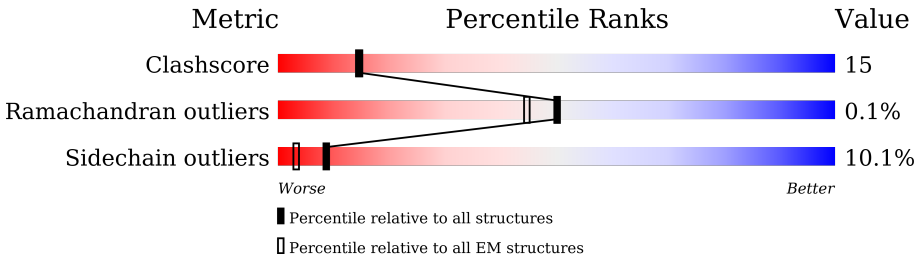
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	885	9% 33% 15% · 50%
1	C	885	10% 33% 15% · 50%
1	D	885	15% 30% 18% · 50%
2	B	710	15% 41% 22% · 33%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14809 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 Potassium channel AKT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	441	Total 3599	C 2341	N 608	O 630	S 20	0	0
1	C	441	Total 3599	C 2341	N 608	O 630	S 20	0	0
1	D	440	Total 3591	C 2335	N 607	O 629	S 20	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	858	LEU	-	expression tag	UNP Q38998
A	859	GLU	-	expression tag	UNP Q38998
A	860	GLY	-	expression tag	UNP Q38998
A	861	SER	-	expression tag	UNP Q38998
A	862	ASP	-	expression tag	UNP Q38998
A	863	GLU	-	expression tag	UNP Q38998
A	864	VAL	-	expression tag	UNP Q38998
A	865	ASP	-	expression tag	UNP Q38998
A	866	ALA	-	expression tag	UNP Q38998
A	867	GLY	-	expression tag	UNP Q38998
A	868	SER	-	expression tag	UNP Q38998
A	869	ALA	-	expression tag	UNP Q38998
A	870	ALA	-	expression tag	UNP Q38998
A	871	ALA	-	expression tag	UNP Q38998
A	872	SER	-	expression tag	UNP Q38998
A	873	GLY	-	expression tag	UNP Q38998
A	874	GLY	-	expression tag	UNP Q38998
A	875	SER	-	expression tag	UNP Q38998
A	876	GLY	-	expression tag	UNP Q38998
A	877	SER	-	expression tag	UNP Q38998
A	878	ASP	-	expression tag	UNP Q38998
A	879	TYR	-	expression tag	UNP Q38998
A	880	LYS	-	expression tag	UNP Q38998
A	881	ASP	-	expression tag	UNP Q38998

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Chain	Residue	Modelled	Actual	Comment	Reference
A	882	ASP	-	expression tag	UNP Q38998
A	883	ASP	-	expression tag	UNP Q38998
A	884	ASP	-	expression tag	UNP Q38998
A	885	LYS	-	expression tag	UNP Q38998
C	858	LEU	-	expression tag	UNP Q38998
C	859	GLU	-	expression tag	UNP Q38998
C	860	GLY	-	expression tag	UNP Q38998
C	861	SER	-	expression tag	UNP Q38998
C	862	ASP	-	expression tag	UNP Q38998
C	863	GLU	-	expression tag	UNP Q38998
C	864	VAL	-	expression tag	UNP Q38998
C	865	ASP	-	expression tag	UNP Q38998
C	866	ALA	-	expression tag	UNP Q38998
C	867	GLY	-	expression tag	UNP Q38998
C	868	SER	-	expression tag	UNP Q38998
C	869	ALA	-	expression tag	UNP Q38998
C	870	ALA	-	expression tag	UNP Q38998
C	871	ALA	-	expression tag	UNP Q38998
C	872	SER	-	expression tag	UNP Q38998
C	873	GLY	-	expression tag	UNP Q38998
C	874	GLY	-	expression tag	UNP Q38998
C	875	SER	-	expression tag	UNP Q38998
C	876	GLY	-	expression tag	UNP Q38998
C	877	SER	-	expression tag	UNP Q38998
C	878	ASP	-	expression tag	UNP Q38998
C	879	TYR	-	expression tag	UNP Q38998
C	880	LYS	-	expression tag	UNP Q38998
C	881	ASP	-	expression tag	UNP Q38998
C	882	ASP	-	expression tag	UNP Q38998
C	883	ASP	-	expression tag	UNP Q38998
C	884	ASP	-	expression tag	UNP Q38998
C	885	LYS	-	expression tag	UNP Q38998
D	858	LEU	-	expression tag	UNP Q38998
D	859	GLU	-	expression tag	UNP Q38998
D	860	GLY	-	expression tag	UNP Q38998
D	861	SER	-	expression tag	UNP Q38998
D	862	ASP	-	expression tag	UNP Q38998
D	863	GLU	-	expression tag	UNP Q38998
D	864	VAL	-	expression tag	UNP Q38998
D	865	ASP	-	expression tag	UNP Q38998
D	866	ALA	-	expression tag	UNP Q38998
D	867	GLY	-	expression tag	UNP Q38998

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Chain	Residue	Modelled	Actual	Comment	Reference
D	868	SER	-	expression tag	UNP Q38998
D	869	ALA	-	expression tag	UNP Q38998
D	870	ALA	-	expression tag	UNP Q38998
D	871	ALA	-	expression tag	UNP Q38998
D	872	SER	-	expression tag	UNP Q38998
D	873	GLY	-	expression tag	UNP Q38998
D	874	GLY	-	expression tag	UNP Q38998
D	875	SER	-	expression tag	UNP Q38998
D	876	GLY	-	expression tag	UNP Q38998
D	877	SER	-	expression tag	UNP Q38998
D	878	ASP	-	expression tag	UNP Q38998
D	879	TYR	-	expression tag	UNP Q38998
D	880	LYS	-	expression tag	UNP Q38998
D	881	ASP	-	expression tag	UNP Q38998
D	882	ASP	-	expression tag	UNP Q38998
D	883	ASP	-	expression tag	UNP Q38998
D	884	ASP	-	expression tag	UNP Q38998
D	885	LYS	-	expression tag	UNP Q38998

- Molecule 2 is a protein called Potassium channel KAT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	474	Total	C	N	O	S	0	0
			3861	2533	636	676	16		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	315	ASP	GLY	engineered mutation	UNP P92960
B	663	LEU	-	expression tag	UNP P92960
B	664	GLU	-	expression tag	UNP P92960
B	665	GLY	-	expression tag	UNP P92960
B	666	SER	-	expression tag	UNP P92960
B	667	ASP	-	expression tag	UNP P92960
B	668	GLU	-	expression tag	UNP P92960
B	669	VAL	-	expression tag	UNP P92960
B	670	ASP	-	expression tag	UNP P92960
B	671	ALA	-	expression tag	UNP P92960
B	672	GLY	-	expression tag	UNP P92960
B	673	SER	-	expression tag	UNP P92960
B	674	ALA	-	expression tag	UNP P92960
B	675	ALA	-	expression tag	UNP P92960

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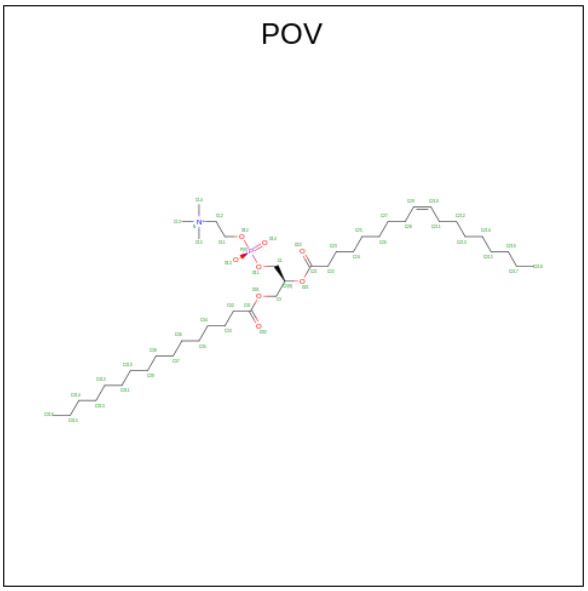
Chain	Residue	Modelled	Actual	Comment	Reference
B	676	ALA	-	expression tag	UNP P92960
B	677	SER	-	expression tag	UNP P92960
B	678	GLY	-	expression tag	UNP P92960
B	679	GLY	-	expression tag	UNP P92960
B	680	SER	-	expression tag	UNP P92960
B	681	GLY	-	expression tag	UNP P92960
B	682	SER	-	expression tag	UNP P92960
B	683	TRP	-	expression tag	UNP P92960
B	684	SER	-	expression tag	UNP P92960
B	685	HIS	-	expression tag	UNP P92960
B	686	PRO	-	expression tag	UNP P92960
B	687	GLN	-	expression tag	UNP P92960
B	688	PHE	-	expression tag	UNP P92960
B	689	GLU	-	expression tag	UNP P92960
B	690	LYS	-	expression tag	UNP P92960
B	691	GLY	-	expression tag	UNP P92960
B	692	GLY	-	expression tag	UNP P92960
B	693	GLY	-	expression tag	UNP P92960
B	694	ALA	-	expression tag	UNP P92960
B	695	ARG	-	expression tag	UNP P92960
B	696	GLY	-	expression tag	UNP P92960
B	697	GLY	-	expression tag	UNP P92960
B	698	SER	-	expression tag	UNP P92960
B	699	GLY	-	expression tag	UNP P92960
B	700	GLY	-	expression tag	UNP P92960
B	701	GLY	-	expression tag	UNP P92960
B	702	SER	-	expression tag	UNP P92960
B	703	TRP	-	expression tag	UNP P92960
B	704	SER	-	expression tag	UNP P92960
B	705	HIS	-	expression tag	UNP P92960
B	706	PRO	-	expression tag	UNP P92960
B	707	GLN	-	expression tag	UNP P92960
B	708	PHE	-	expression tag	UNP P92960
B	709	GLU	-	expression tag	UNP P92960
B	710	LYS	-	expression tag	UNP P92960

- Molecule 3 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	P	0
			39	30	8	1	
3	B	1	Total	C	O	P	0
			39	30	8	1	
3	C	1	Total	C	O	P	0
			39	30	8	1	
3	D	1	Total	C	O	P	0
			39	30	8	1	

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

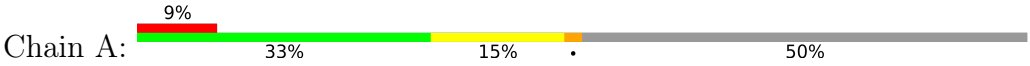
Mol	Chain	Residues	Atoms		AltConf
4	C	2	Total	K	0
			2	2	
4	D	1	Total	K	0
			1	1	

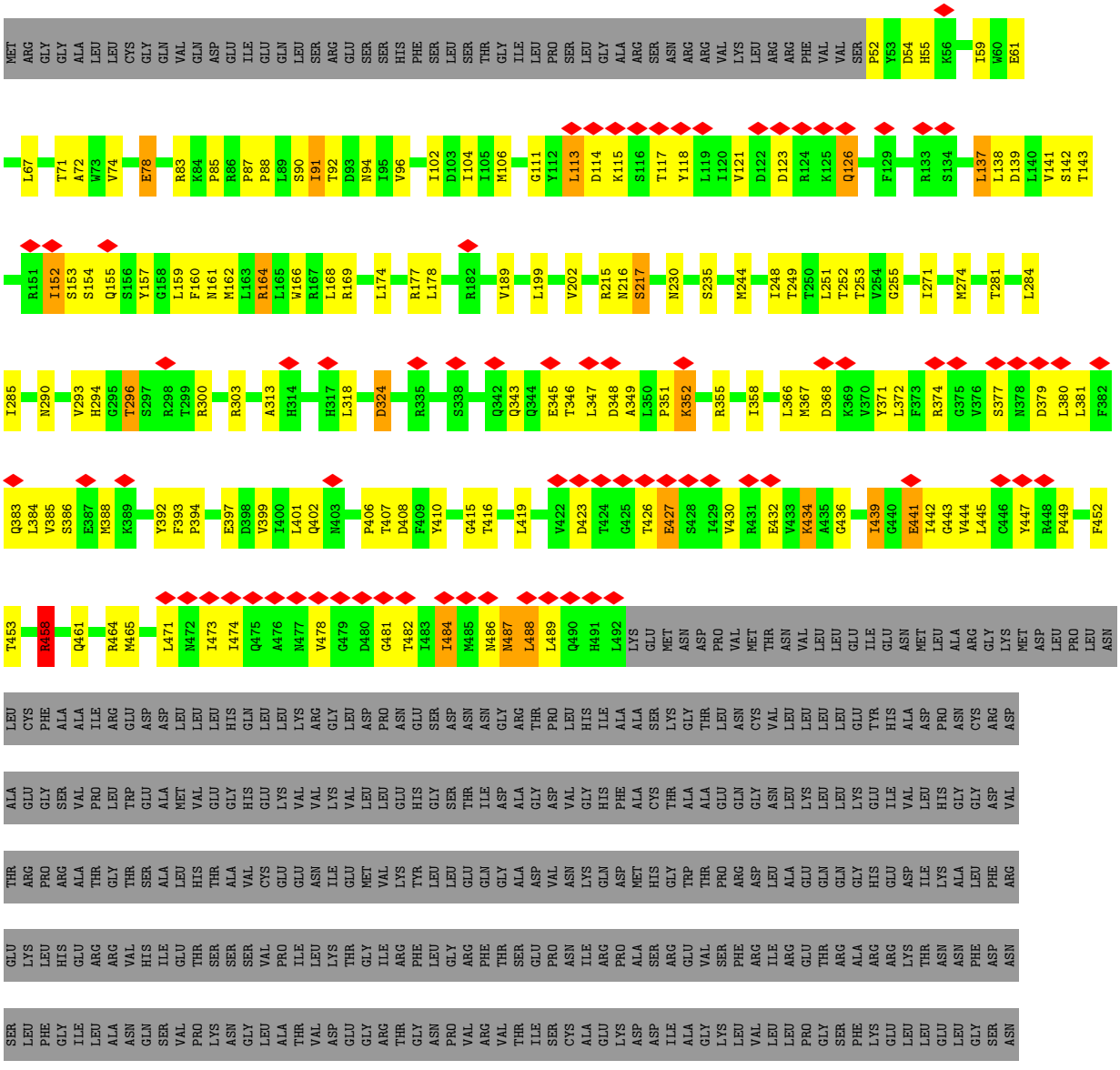
3 Residue-property plots (i)

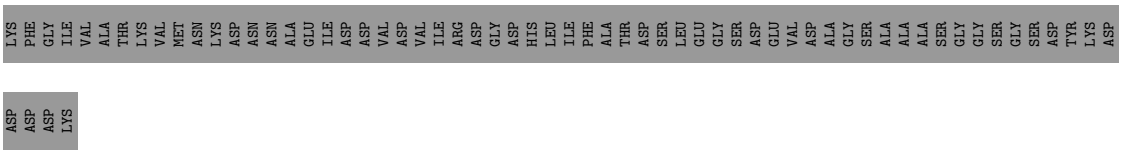
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Potassium channel AKT1

Chain A:

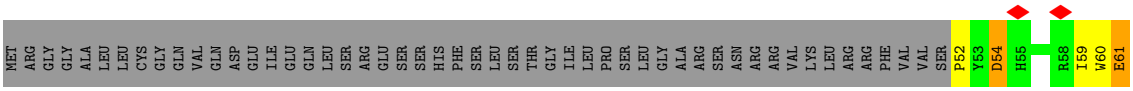


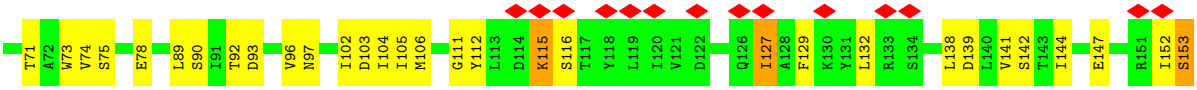


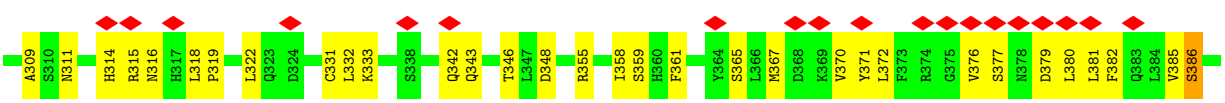


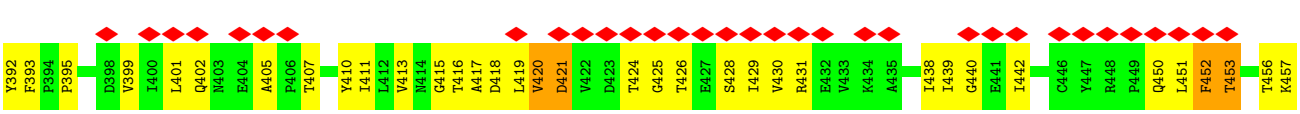
• Molecule 1: Potassium channel AKT1

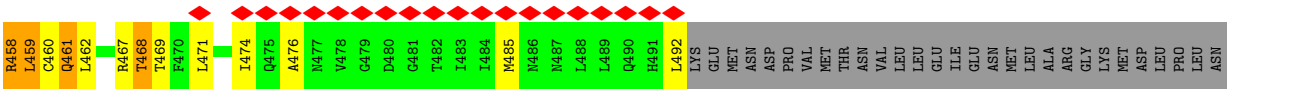
Chain C:

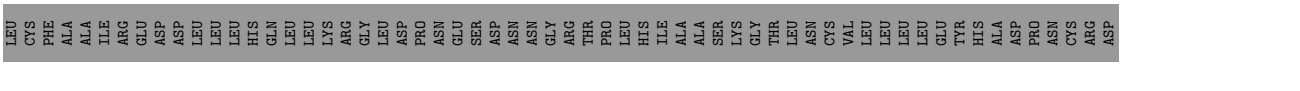


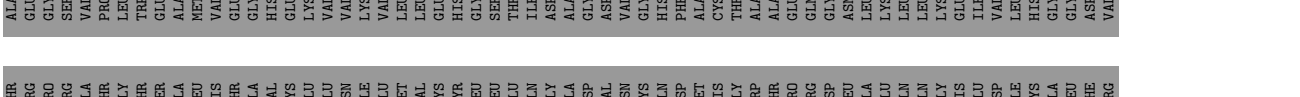


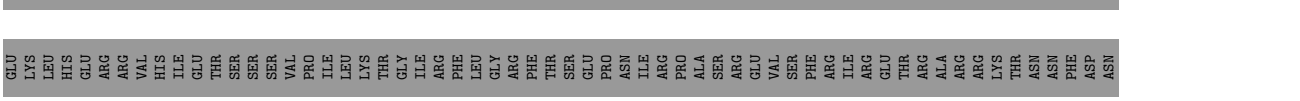


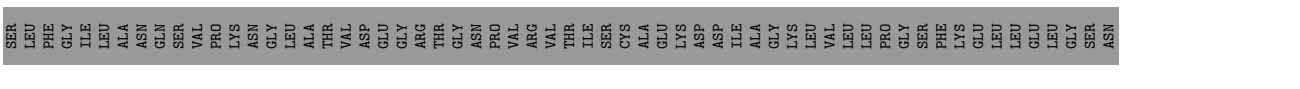


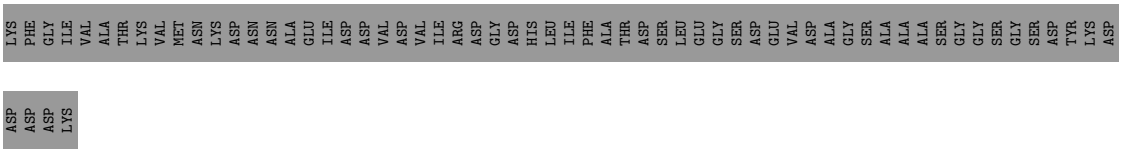






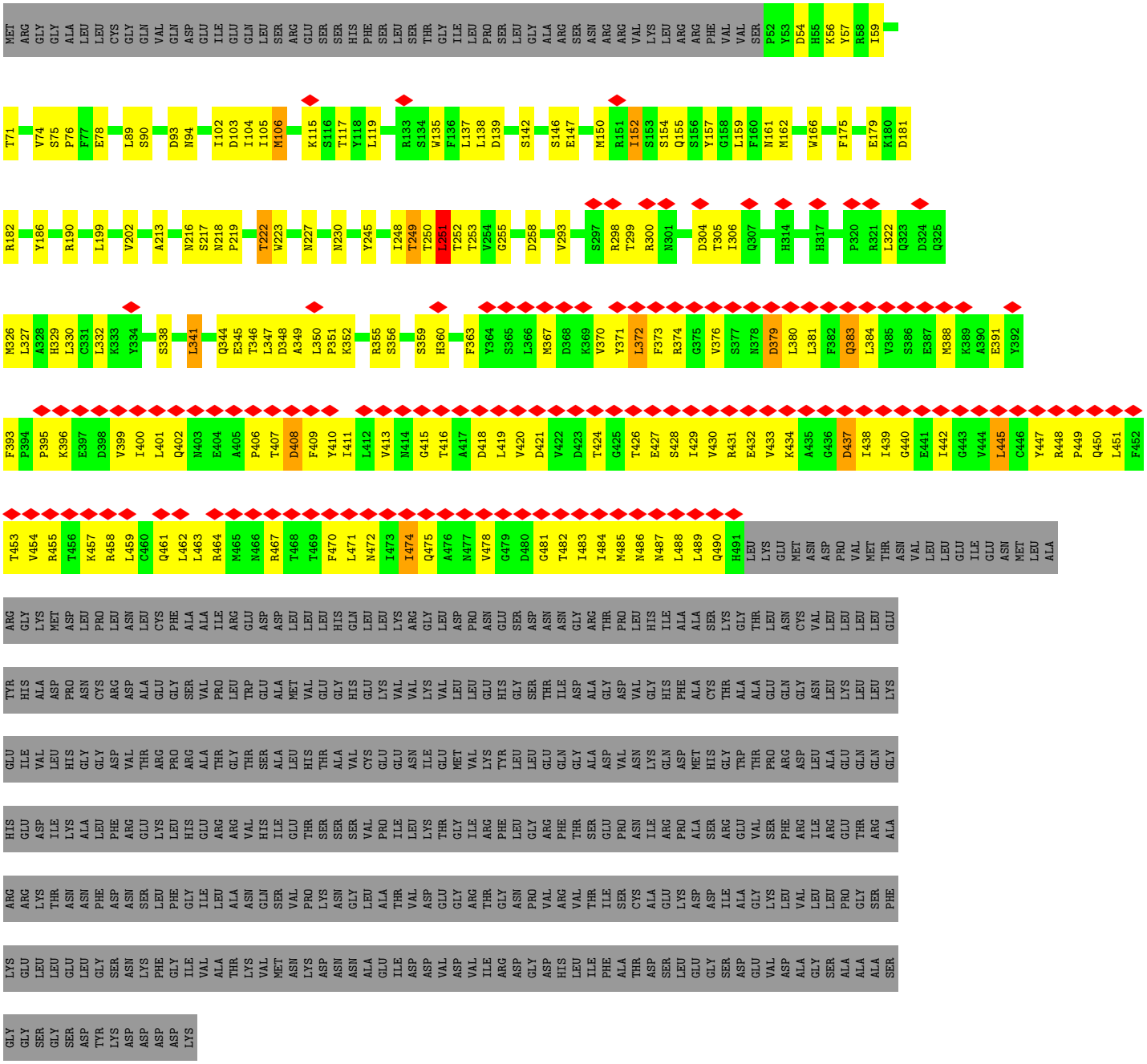






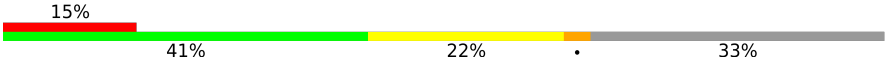
• Molecule 1: Potassium channel AKT1

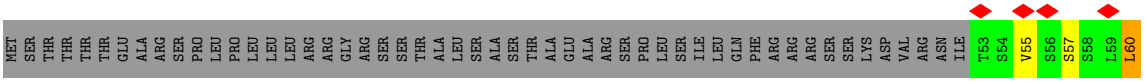
Chain D:

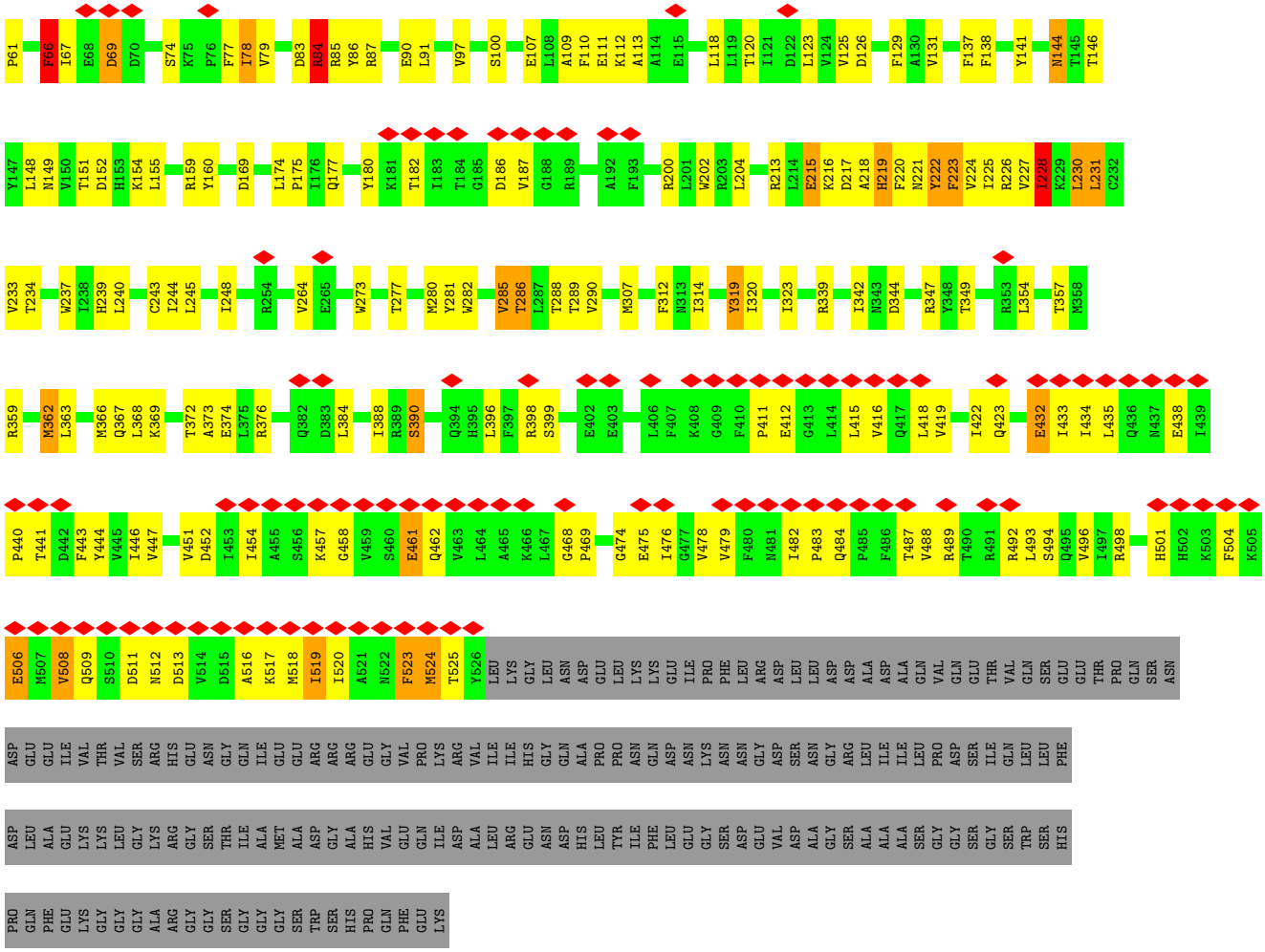


• Molecule 2: Potassium channel KAT3

Chain B:






P61 F66 I67 E68 D69 D70 S74 K75 P76 F77 I78 V79 D83 R84 R85 Y86 R87 E90 L91 V97 S100 E107 L108 A109 F110 E111 K112 A113 A114 E115 L118 L119 T120 I121 D122 L123 V124 V125 D126 F129 A130 V131 F137 F138 Y141 N144 T145 T146
Y147 L148 N149 V150 T151 D152 H153 K154 L155 R159 Y160 D169 L174 P175 I176 Q177 Y180 K181 T182 I183 T184 G185 D186 V187 G188 R189 A192 F193 R200 L201 W202 R203 L204 R213 L214 E215 K216 D217 A218 H219 F220 N221 Y222 F223 V224 I225 R226 V227 I228 K229 L230 L231 C232
V233 T234 W237 I238 H239 L240 C243 I244 L245 I248 R254 V264 E265 W273 T277 M280 Y281 W282 V285 T286 L287 T288 T289 V290 M307 F312 N313 I314 Y319 I320 I323 R339 I342 M343 D344 R347 Y348 T349 R353 L354 T357 M358
R359 M362 L363 M366 Q367 L368 K369 T372 A373 E374 L375 R376 Q382 D383 L384 I388 R389 S390 Q394 H395 L396 F397 R398 S399 E402 E403 L406 F407 K408 G409 F410 P411 E412 G413 L414 L415 V416 Q417 L418 V419 I422 Q423 E432 I433 I434 L435 Q436 N437 E438 I439
P440 T441 D442 F443 Y444 V445 I446 V447 V451 D452 I453 I454 A455 S456 K457 G458 V459 S460 E461 Q462 V463 L464 A465 K466 L467 G468 P469 G474 E475 I476 G477 V478 V479 F480 N481 I482 P483 Q484 P485 F486 T487 V488 R489 T490 R491 R492 L493 S494 Q495 V496 I497 R498 H501 H502 K503 F504 K505
E506 M507 V508 Q509 S510 D511 N512 D513 V514 D515 A516 K517 M518 I519 I520 A521 N522 F523 M524 T525 Y526 LEU LYS GLY LEU ASN ASP GLU LEU LYS LYS GLU ILE PRO PHE LEU ARG ASP LEU LEU ASP ASP ALA ASP ALA GLN VAL GLN GLU THR VAL GLN SER GLU GLU THR PRO GLN SER ASN
ASP GLU GLU ILE VAL THR VAL SER ARG HIS GLU ASN GLY GLN ILE GLU GLU ARG ARG GLU GLY VAL PRO LYS ARG VAL ILE ILE HIS GLY GLN ALA PRO PRO ASN GLN ASP ASN LYS ASN ASN GLY ASP SER ASN GLY ARG LEU ILE ILE LEU PRO ASP SER ILE GLN LEU LEU PHE
ASP LEU ALA GLU LYS LYS LEU GLY LYS ARG GLY SER THR ILE ALA MET ALA ASP GLY ALA HIS VAL GLU GLN ILE ASP ALA LEU ARG GLU ASN ASP HIS LEU TYR ILE PHE LEU GLU GLY SER ASP GLU VAL ASP ALA GLY SER ALA ALA ALA SER GLY GLY SER GLY SER TRP SER HIS
PRO GLN PHE GLU LYS GLY GLY GLY ALA ARG GLY GLY SER GLY GLY GLY SER TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	649659	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	8.860	Depositor
Minimum map value	-5.951	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.160	Depositor
Recommended contour level	0.642	Depositor
Map size (Å)	258.552, 258.552, 258.552	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0773, 1.0773, 1.0773	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.43	1/3689 (0.0%)	0.53	1/5010 (0.0%)
1	C	0.38	0/3689	0.54	1/5010 (0.0%)
1	D	0.43	3/3681 (0.1%)	0.55	4/4999 (0.1%)
2	B	0.59	6/3958 (0.2%)	0.77	12/5368 (0.2%)
All	All	0.47	10/15017 (0.1%)	0.61	18/20387 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	458	ARG	C-O	-10.47	1.12	1.23
2	B	215	GLU	C-O	-7.36	1.13	1.23
2	B	217	ASP	C-O	-7.34	1.15	1.23
1	D	250	THR	C-O	-6.93	1.14	1.23
1	D	251	LEU	C-O	-6.07	1.17	1.24
1	D	253	THR	C-O	-5.95	1.16	1.24
2	B	320	ILE	C-O	-5.93	1.17	1.24
2	B	218	ALA	C-O	-5.59	1.16	1.24
2	B	216	LYS	C-O	-5.39	1.16	1.23
2	B	228	ILE	C-O	-5.01	1.18	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	222	TYR	CB-CA-C	-9.63	95.68	110.90
1	A	78	GLU	CB-CA-C	-9.26	96.27	110.90
1	D	250	THR	CA-CB-OG1	-8.60	96.70	109.60
2	B	216	LYS	N-CA-C	-7.21	105.02	113.88
2	B	217	ASP	CA-C-O	-6.59	113.23	120.81
2	B	234	THR	CA-CB-OG1	-6.41	99.98	109.60
2	B	319	TYR	CB-CA-C	-6.30	100.95	110.90
2	B	227	VAL	CA-C-O	-5.77	114.95	120.95
2	B	125	VAL	N-CA-C	-5.67	107.29	112.96
2	B	223	PHE	N-CA-C	-5.55	105.23	112.23
2	B	66	PHE	CA-CB-CG	5.48	119.28	113.80
1	C	189	VAL	N-CA-C	-5.22	108.42	113.53
1	D	252	THR	CA-CB-OG1	-5.21	101.79	109.60
2	B	84	ARG	CA-C-O	-5.16	115.58	120.90
2	B	215	GLU	CB-CA-C	-5.11	101.56	110.09
1	D	252	THR	CA-C-N	5.09	131.27	121.54
1	D	252	THR	C-N-CA	5.09	131.27	121.54
2	B	66	PHE	N-CA-CB	-5.01	102.39	109.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	303	ARG	Sidechain

5.2 Too-close contacts (i)

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	3599	0	3614	93	0
1	C	3599	0	3614	130	0
1	D	3591	0	3602	125	0
2	B	3861	0	3907	130	0
3	A	39	0	52	0	0
3	B	39	0	52	0	0
3	C	39	0	52	9	0
3	D	39	0	52	3	0
4	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
All	All	14809	0	14945	448	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (448) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:VAL:HG11	2:B:523:PHE:CE2	1.49	1.47
2:B:479:VAL:CG1	2:B:523:PHE:HE2	1.61	1.13
1:C:458:ARG:HG2	1:D:117:THR:HG21	1.26	1.12
1:A:458:ARG:HH21	1:A:458:ARG:HB3	1.24	1.01
1:C:395:PRO:HB3	1:C:458:ARG:O	1.64	0.96
1:C:458:ARG:HG2	1:D:117:THR:CG2	1.97	0.94
2:B:479:VAL:CG1	2:B:523:PHE:CE2	2.42	0.94
1:C:415:GLY:HA3	1:C:460:CYS:HB3	1.53	0.91
1:C:303:ARG:HH21	1:D:186:TYR:HB2	1.34	0.90
1:C:458:ARG:HB3	1:C:458:ARG:HH21	1.35	0.90
2:B:479:VAL:HG11	2:B:523:PHE:HE2	0.77	0.90
1:C:193:LYS:HE2	3:C:901:POV:H3	1.55	0.87
1:C:458:ARG:HH21	1:C:458:ARG:CB	1.89	0.85
1:A:458:ARG:HB3	1:A:458:ARG:NH2	1.91	0.85
1:C:395:PRO:CB	1:C:458:ARG:O	2.25	0.84
2:B:479:VAL:HG21	2:B:523:PHE:CZ	2.14	0.82
1:A:274:MET:HE1	1:D:249:THR:HG22	1.61	0.81
2:B:228:ILE:O	2:B:228:ILE:HD12	1.80	0.81
1:D:202:VAL:HG23	1:D:251:LEU:HD12	1.62	0.81
1:C:190:ARG:HG2	1:C:190:ARG:HH11	1.45	0.80
1:A:458:ARG:HH21	1:A:458:ARG:CB	1.95	0.79
1:C:416:THR:HG22	1:C:458:ARG:HD3	1.61	0.79
2:B:446:ILE:HG22	2:B:496:VAL:HG12	1.64	0.79
1:D:448:ARG:HH22	1:D:451:LEU:HB2	1.47	0.78
1:C:413:VAL:CG2	1:C:461:GLN:HG2	2.15	0.76
2:B:349:THR:HG22	2:B:354:LEU:HD12	1.68	0.75
1:C:395:PRO:CA	1:C:458:ARG:O	2.35	0.74
1:C:193:LYS:HE3	3:C:901:POV:H32	1.67	0.74
1:C:303:ARG:NH1	1:D:182:ARG:HA	2.03	0.74
1:D:399:VAL:HG23	1:D:400:ILE:HG13	1.70	0.73
1:A:366:LEU:HD11	1:A:436:GLY:HA2	1.68	0.73
2:B:457:LYS:HZ3	2:B:462:GLN:HB2	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ASP:HB2	1:C:343:GLN:HE22	1.53	0.72
1:A:293:VAL:O	1:D:300:ARG:NH2	2.21	0.72
1:A:74:VAL:O	1:A:78:GLU:HG2	1.89	0.71
2:B:339:ARG:NH2	1:C:181:ASP:O	2.24	0.70
1:D:426:THR:HG22	1:D:427:GLU:H	1.55	0.70
1:C:459:LEU:HD23	1:C:459:LEU:O	1.92	0.70
1:A:248:ILE:HD12	2:B:307:MET:HB2	1.72	0.70
2:B:239:HIS:HA	2:B:280:MET:HE1	1.72	0.70
2:B:231:LEU:C	2:B:231:LEU:HD23	2.16	0.70
2:B:504:PHE:O	2:B:508:VAL:HG12	1.91	0.69
2:B:126:ASP:OD2	2:B:200:ARG:NH2	2.26	0.69
1:C:413:VAL:CG2	1:C:461:GLN:CG	2.70	0.68
1:D:332:LEU:HD21	1:D:459:LEU:HD21	1.76	0.68
1:A:367:MET:HG3	1:A:385:VAL:HG12	1.77	0.67
1:C:193:LYS:CE	3:C:901:POV:H32	2.24	0.67
1:D:251:LEU:HD23	1:D:251:LEU:O	1.94	0.67
2:B:285:VAL:HG12	1:C:274:MET:HE1	1.77	0.67
1:C:147:GLU:N	1:C:147:GLU:OE2	2.27	0.67
1:C:416:THR:HG22	1:C:458:ARG:CD	2.26	0.66
1:D:372:LEU:HD11	1:D:484:ILE:HG23	1.77	0.66
1:D:408:ASP:N	1:D:408:ASP:OD1	2.29	0.66
2:B:146:THR:HG22	2:B:148:LEU:HG	1.78	0.66
1:C:410:TYR:HB2	1:C:439:ILE:HD11	1.77	0.66
1:D:440:GLY:O	1:D:450:GLN:NE2	2.29	0.66
2:B:458:GLY:HA2	1:C:476:ALA:HB1	1.78	0.65
1:A:121:VAL:HG12	1:A:123:ASP:H	1.60	0.65
2:B:90:GLU:OE2	2:B:213:ARG:NH2	2.22	0.65
1:A:216:ASN:ND2	1:A:217:SER:O	2.29	0.65
1:A:300:ARG:HD3	2:B:222:TYR:CE2	2.32	0.65
2:B:524:MET:HE3	2:B:524:MET:HA	1.77	0.65
1:D:418:ASP:HA	1:D:432:GLU:HA	1.79	0.65
2:B:519:ILE:O	2:B:523:PHE:HB2	1.96	0.65
1:D:202:VAL:CG2	1:D:251:LEU:HD12	2.27	0.64
1:A:61:GLU:OE1	1:A:177:ARG:NH2	2.31	0.63
2:B:440:PRO:HD3	2:B:483:PRO:HA	1.81	0.63
1:C:418:ASP:OD2	1:C:457:LYS:NZ	2.31	0.63
2:B:237:TRP:HH2	2:B:312:PHE:HB2	1.64	0.63
1:C:190:ARG:HG2	1:C:190:ARG:NH1	2.09	0.63
2:B:282:TRP:O	2:B:286:THR:HG23	1.99	0.63
1:D:447:TYR:HD1	1:D:467:ARG:HH12	1.46	0.63
1:A:324:ASP:N	1:A:324:ASP:OD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:LEU:HD12	1:C:452:PHE:HB2	1.81	0.62
1:A:416:THR:HG22	1:A:434:LYS:HA	1.82	0.62
1:D:181:ASP:OD1	1:D:182:ARG:N	2.34	0.61
1:C:371:TYR:HE2	1:C:438:ILE:HD11	1.65	0.61
2:B:84:ARG:O	2:B:86:TYR:N	2.33	0.61
1:D:416:THR:HB	1:D:457:LYS:HE3	1.82	0.61
1:C:181:ASP:OD1	1:C:183:ASN:N	2.30	0.60
1:D:304:ASP:OD1	1:D:305:THR:N	2.35	0.60
2:B:476:ILE:HD12	2:B:476:ILE:H	1.66	0.60
1:C:440:GLY:HA2	1:C:450:GLN:HE22	1.66	0.60
2:B:416:VAL:HA	2:B:419:VAL:HG12	1.84	0.60
2:B:368:LEU:HD12	2:B:493:LEU:HD12	1.84	0.59
1:C:425:GLY:O	1:C:426:THR:OG1	2.19	0.59
1:D:445:LEU:HD21	1:D:470:PHE:HE2	1.67	0.59
2:B:281:TYR:O	2:B:285:VAL:HG13	2.03	0.59
2:B:432:GLU:HA	2:B:489:ARG:HA	1.84	0.59
1:D:481:GLY:O	1:D:482:THR:OG1	2.19	0.59
1:A:142:SER:O	1:A:164:ARG:NH1	2.36	0.59
1:C:60:TRP:NE1	1:C:103:ASP:OD2	2.31	0.59
1:D:216:ASN:ND2	1:D:218:ASN:O	2.36	0.58
1:D:433:VAL:HG23	1:D:437:ASP:HB2	1.85	0.58
1:C:73:TRP:HD1	3:C:901:POV:H315	1.68	0.58
1:A:383:GLN:O	1:A:386:SER:OG	2.20	0.58
1:C:348:ASP:O	1:C:355:ARG:NH1	2.37	0.58
1:C:376:VAL:HG11	1:C:380:LEU:HD22	1.86	0.57
1:D:416:THR:HG22	1:D:434:LYS:HE2	1.85	0.57
1:C:303:ARG:HH11	1:D:182:ARG:HA	1.69	0.57
2:B:423:GLN:HE22	2:B:498:ARG:HG2	1.69	0.57
1:C:458:ARG:CG	1:D:117:THR:CG2	2.80	0.57
2:B:228:ILE:HD12	2:B:228:ILE:C	2.29	0.57
2:B:288:THR:O	2:B:289:THR:OG1	2.22	0.57
1:C:458:ARG:HH21	1:C:458:ARG:CG	2.15	0.57
2:B:347:ARG:NH2	1:C:343:GLN:OE1	2.38	0.57
1:A:123:ASP:HB3	1:A:126:GLN:HB2	1.88	0.56
1:D:406:PRO:HG2	1:D:467:ARG:HH11	1.68	0.56
1:D:147:GLU:OE1	1:D:147:GLU:N	2.38	0.56
2:B:186:ASP:OD1	2:B:187:VAL:N	2.39	0.56
1:C:402:GLN:H	1:C:453:THR:HG23	1.71	0.56
1:A:91:ILE:HD12	1:A:92:THR:H	1.70	0.56
1:D:379:ASP:OD1	1:D:379:ASP:N	2.31	0.55
1:C:181:ASP:OD1	1:C:182:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:MET:HA	2:B:524:MET:CE	2.35	0.55
1:C:246:TRP:O	1:C:250:THR:HG22	2.07	0.55
1:D:388:MET:HE3	1:D:463:LEU:HD23	1.87	0.55
1:D:471:LEU:HA	1:D:474:ILE:HD12	1.87	0.55
1:A:139:ASP:OD1	1:A:169:ARG:NH2	2.40	0.55
2:B:344:ASP:N	2:B:344:ASP:OD1	2.37	0.55
2:B:113:ALA:HB1	2:B:118:LEU:HD13	1.89	0.54
1:D:485:MET:HA	1:D:488:LEU:HB3	1.89	0.54
1:C:413:VAL:HG22	1:C:461:GLN:O	2.08	0.54
1:C:52:PRO:HB3	1:C:111:GLY:HA3	1.88	0.54
1:A:313:ALA:HA	1:A:318:LEU:HD12	1.90	0.54
2:B:149:ASN:O	2:B:151:THR:OG1	2.24	0.54
1:C:420:VAL:HG13	1:C:453:THR:HB	1.89	0.54
1:A:458:ARG:HG2	2:B:146:THR:HG23	1.89	0.54
1:D:157:TYR:O	1:D:161:ASN:ND2	2.41	0.54
1:D:483:ILE:HA	1:D:486:ASN:HB2	1.87	0.54
1:C:228:VAL:HG21	1:C:238:MET:HE1	1.89	0.53
1:C:413:VAL:HG22	1:C:461:GLN:CG	2.36	0.53
1:C:139:ASP:OD1	1:C:166:TRP:NE1	2.21	0.53
1:C:458:ARG:HB3	1:C:458:ARG:NH2	2.14	0.53
1:D:411:ILE:O	1:D:463:LEU:N	2.42	0.53
1:D:117:THR:O	1:D:119:LEU:N	2.42	0.53
1:C:159:LEU:HD12	1:C:159:LEU:H	1.73	0.53
1:C:311:ASN:HB3	1:C:315:ARG:HH12	1.74	0.53
1:A:371:TYR:OH	1:A:441:GLU:OE1	2.27	0.53
1:D:371:TYR:OH	1:D:488:LEU:O	2.27	0.53
1:C:190:ARG:NH1	1:C:190:ARG:CG	2.72	0.52
1:C:331:CYS:SG	1:C:332:LEU:N	2.82	0.52
1:D:75:SER:HB2	1:D:76:PRO:HD3	1.90	0.52
1:D:407:THR:O	1:D:467:ARG:N	2.40	0.52
1:D:472:ASN:O	1:D:475:GLN:NE2	2.41	0.52
2:B:237:TRP:CD1	2:B:240:LEU:HD23	2.45	0.52
1:D:350:LEU:HG	1:D:351:PRO:HD3	1.92	0.52
2:B:219:HIS:C	2:B:219:HIS:CD2	2.88	0.52
1:C:112:TYR:HB2	1:C:127:ILE:HD13	1.92	0.52
1:C:115:LYS:O	1:C:115:LYS:NZ	2.29	0.52
1:C:319:PRO:HD2	1:C:322:LEU:HD21	1.90	0.52
1:C:419:LEU:HD23	1:C:431:ARG:HD2	1.90	0.52
2:B:146:THR:O	2:B:148:LEU:N	2.41	0.52
1:D:396:LYS:HG3	1:D:455:ARG:HD2	1.92	0.52
1:A:426:THR:OG1	1:A:427:GLU:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ILE:O	1:A:488:LEU:HD12	2.09	0.51
2:B:519:ILE:HD12	2:B:520:ILE:H	1.74	0.51
1:D:395:PRO:HG3	1:D:458:ARG:HA	1.92	0.51
1:A:358:ILE:HD12	1:A:358:ILE:H	1.74	0.51
2:B:474:GLY:O	2:B:484:GLN:NE2	2.40	0.51
1:C:413:VAL:HG22	1:C:461:GLN:HG2	1.92	0.51
1:C:471:LEU:HA	1:C:474:ILE:HG22	1.92	0.51
2:B:443:PHE:CD1	2:B:478:VAL:HG11	2.46	0.51
1:A:72:ALA:HB2	1:A:168:LEU:HD11	1.93	0.51
1:A:402:GLN:N	1:A:453:THR:OG1	2.44	0.51
2:B:137:PHE:HE1	2:B:160:TYR:HD2	1.59	0.51
2:B:435:LEU:HD23	2:B:438:GLU:OE1	2.11	0.51
1:D:344:GLN:HA	1:D:347:LEU:HD13	1.91	0.51
1:C:392:TYR:CE1	1:C:461:GLN:HB3	2.46	0.51
1:D:93:ASP:OD1	1:D:94:ASN:N	2.44	0.51
1:D:421:ASP:OD2	1:D:430:VAL:HG13	2.11	0.51
1:A:114:ASP:OD1	1:A:115:LYS:N	2.44	0.51
1:A:345:GLU:OE1	1:A:345:GLU:N	2.33	0.51
2:B:169:ASP:OD1	2:B:202:TRP:NE1	2.35	0.51
1:C:54:ASP:OD1	1:C:54:ASP:N	2.42	0.51
1:C:193:LYS:HE2	3:C:901:POV:C3	2.34	0.51
2:B:84:ARG:C	2:B:86:TYR:H	2.17	0.50
2:B:230:LEU:HD21	2:B:319:TYR:CD2	2.46	0.50
2:B:435:LEU:HA	2:B:487:THR:HG23	1.93	0.50
2:B:69:ASP:OD1	2:B:69:ASP:N	2.43	0.50
1:C:311:ASN:HB3	1:C:315:ARG:NH1	2.25	0.50
1:D:251:LEU:HD23	1:D:251:LEU:C	2.36	0.50
1:A:152:ILE:HG13	1:A:153:SER:N	2.25	0.50
1:C:485:MET:HE3	1:C:485:MET:O	2.12	0.50
1:D:74:VAL:O	1:D:78:GLU:HG2	2.11	0.50
1:C:60:TRP:HD1	1:C:61:GLU:OE1	1.94	0.50
3:D:901:POV:H1	3:D:901:POV:O22	2.12	0.50
2:B:231:LEU:C	2:B:231:LEU:CD2	2.84	0.50
1:C:248:ILE:O	1:C:252:THR:OG1	2.27	0.50
1:D:175:PHE:O	1:D:179:GLU:HG2	2.11	0.50
1:D:415:GLY:HA2	1:D:458:ARG:NE	2.26	0.50
1:D:420:VAL:HG13	1:D:453:THR:HG23	1.94	0.50
1:C:303:ARG:HH21	1:D:186:TYR:CB	2.15	0.50
1:C:309:ALA:HB2	1:D:345:GLU:HG3	1.94	0.50
1:D:348:ASP:C	1:D:350:LEU:H	2.18	0.50
1:D:413:VAL:HG12	1:D:461:GLN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:THR:O	1:C:253:THR:OG1	2.27	0.50
1:C:395:PRO:HB3	1:C:458:ARG:C	2.35	0.50
1:A:230:ASN:OD1	1:A:230:ASN:N	2.42	0.49
1:A:300:ARG:HD3	2:B:222:TYR:CD2	2.46	0.49
1:A:394:PRO:HG2	1:A:397:GLU:HG3	1.94	0.49
2:B:57:SER:O	2:B:61:PRO:HD2	2.12	0.49
2:B:77:PHE:O	2:B:78:ILE:HG12	2.10	0.49
1:D:78:GLU:OE1	1:D:157:TYR:OH	2.27	0.49
1:D:190:ARG:NH2	3:D:901:POV:O12	2.45	0.49
1:C:244:MET:HE1	3:C:901:POV:H31H	1.93	0.49
1:A:444:VAL:HG12	1:A:445:LEU:HD23	1.95	0.49
1:C:104:ILE:HD11	1:C:139:ASP:O	2.12	0.49
1:A:202:VAL:HG12	1:A:244:MET:HE3	1.94	0.49
1:A:343:GLN:O	1:A:346:THR:HG22	2.13	0.49
1:C:348:ASP:HA	1:C:355:ARG:HD3	1.93	0.49
1:C:458:ARG:HB3	1:D:117:THR:HG23	1.95	0.49
1:D:251:LEU:C	1:D:251:LEU:CD2	2.85	0.49
1:D:352:LYS:HA	1:D:355:ARG:HG2	1.95	0.49
2:B:221:ASN:HB3	2:B:224:VAL:HB	1.95	0.49
1:D:245:TYR:O	1:D:249:THR:HG23	2.12	0.49
1:A:244:MET:O	1:A:248:ILE:HG13	2.11	0.49
1:A:381:LEU:O	1:A:385:VAL:HG13	2.13	0.49
1:C:395:PRO:HA	1:C:458:ARG:O	2.10	0.49
1:A:67:LEU:HD13	1:A:96:VAL:HG13	1.94	0.48
2:B:87:ARG:HA	2:B:90:GLU:HG2	1.94	0.48
1:D:56:LYS:O	1:D:59:ILE:HG13	2.13	0.48
1:A:85:PRO:HG3	1:A:157:TYR:CE1	2.48	0.48
2:B:137:PHE:CE1	2:B:160:TYR:HD2	2.32	0.48
2:B:524:MET:SD	2:B:524:MET:N	2.87	0.48
1:C:74:VAL:O	1:C:78:GLU:HG3	2.14	0.48
1:C:421:ASP:N	1:C:428:SER:O	2.30	0.48
1:D:376:VAL:HG12	1:D:380:LEU:HD21	1.94	0.48
2:B:362:MET:SD	1:C:358:ILE:HD11	2.53	0.48
2:B:516:ALA:N	2:B:518:MET:SD	2.79	0.48
1:C:73:TRP:CD1	3:C:901:POV:H315	2.48	0.48
1:C:280:LEU:HA	3:C:901:POV:H25	1.95	0.48
1:C:303:ARG:NH1	1:D:181:ASP:O	2.46	0.48
1:D:218:ASN:HD22	1:D:219:PRO:HD2	1.78	0.48
2:B:230:LEU:CD2	2:B:323:ILE:HG13	2.43	0.48
1:A:458:ARG:HG2	2:B:146:THR:CG2	2.44	0.48
1:C:152:ILE:HD12	1:C:153:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:LEU:HD23	2:B:323:ILE:HG13	1.95	0.48
1:A:78:GLU:HA	1:A:78:GLU:OE1	2.13	0.48
1:C:154:SER:OG	1:C:155:GLN:N	2.47	0.48
1:D:393:PHE:CD1	1:D:462:LEU:HD12	2.49	0.48
1:A:303:ARG:NH2	2:B:220:PHE:O	2.40	0.47
1:A:352:LYS:HA	1:A:355:ARG:HB3	1.96	0.47
1:A:408:ASP:OD2	1:A:464:ARG:HD3	2.14	0.47
2:B:479:VAL:CG2	2:B:523:PHE:CZ	2.92	0.47
1:D:348:ASP:OD1	1:D:348:ASP:N	2.47	0.47
1:A:392:TYR:CE1	1:A:461:GLN:HB2	2.50	0.47
1:D:380:LEU:HD12	1:D:384:LEU:HD23	1.96	0.47
1:A:90:SER:O	1:A:94:ASN:ND2	2.46	0.47
1:A:379:ASP:N	1:A:379:ASP:OD1	2.46	0.47
2:B:440:PRO:HB3	2:B:484:GLN:HG2	1.96	0.47
2:B:519:ILE:HD12	2:B:520:ILE:N	2.30	0.47
1:C:303:ARG:NH2	1:D:186:TYR:HB2	2.15	0.47
1:A:252:THR:O	1:A:253:THR:OG1	2.26	0.47
2:B:411:PRO:HG2	2:B:512:ASN:ND2	2.29	0.47
2:B:418:LEU:O	2:B:422:ILE:HG23	2.15	0.47
1:C:216:ASN:ND2	1:C:218:ASN:H	2.12	0.47
1:D:154:SER:OG	1:D:155:GLN:N	2.47	0.47
2:B:223:PHE:HA	2:B:226:ARG:HG3	1.96	0.47
2:B:506:GLU:HA	2:B:509:GLN:NE2	2.29	0.47
1:D:402:GLN:HG3	1:D:451:LEU:HA	1.97	0.47
1:C:102:ILE:O	1:C:105:ILE:HG13	2.14	0.47
2:B:84:ARG:C	2:B:86:TYR:N	2.73	0.47
1:A:415:GLY:HA2	1:A:458:ARG:HD3	1.96	0.46
2:B:461:GLU:O	2:B:462:GLN:NE2	2.48	0.46
1:C:458:ARG:CG	1:C:458:ARG:NH2	2.72	0.46
1:C:411:ILE:HG12	1:C:438:ILE:HG22	1.98	0.46
1:C:413:VAL:HG21	1:C:461:GLN:OE1	2.15	0.46
2:B:144:ASN:C	2:B:146:THR:H	2.24	0.46
1:A:290:ASN:OD1	1:D:293:VAL:HG22	2.16	0.46
1:D:154:SER:O	1:D:155:GLN:HG2	2.15	0.46
1:D:448:ARG:HG2	1:D:449:PRO:HD2	1.95	0.46
1:C:183:ASN:N	1:C:183:ASN:OD1	2.48	0.46
1:D:439:ILE:HD12	1:D:454:VAL:HG11	1.97	0.46
1:A:393:PHE:CE2	1:A:399:VAL:HG12	2.51	0.46
2:B:219:HIS:CD2	2:B:219:HIS:O	2.68	0.46
1:D:347:LEU:O	1:D:350:LEU:HB3	2.16	0.46
1:D:434:LYS:HA	1:D:434:LYS:HD3	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ASP:O	1:C:97:ASN:ND2	2.48	0.46
1:D:249:THR:O	1:D:255:GLY:N	2.47	0.46
1:C:451:LEU:H	1:C:451:LEU:HD12	1.81	0.46
2:B:475:GLU:HA	2:B:478:VAL:HG12	1.98	0.46
2:B:492:ARG:O	2:B:494:SER:OG	2.29	0.46
1:D:298:ARG:HD2	1:D:299:THR:N	2.30	0.46
1:D:367:MET:HB3	1:D:381:LEU:HD11	1.97	0.46
1:A:388:MET:HG3	1:A:465:MET:HE3	1.97	0.46
2:B:482:ILE:HD12	2:B:483:PRO:O	2.16	0.46
1:C:370:VAL:HG12	1:C:372:LEU:H	1.80	0.46
2:B:215:GLU:HG2	2:B:222:TYR:HE1	1.81	0.45
2:B:411:PRO:HG2	2:B:512:ASN:HD21	1.81	0.45
1:C:257:GLY:O	1:C:260:HIS:ND1	2.43	0.45
1:C:442:ILE:HG21	1:C:451:LEU:HD21	1.98	0.45
1:D:349:ALA:C	1:D:351:PRO:HD2	2.42	0.45
1:A:137:LEU:HD13	1:A:137:LEU:HA	1.83	0.45
2:B:344:ASP:HB2	1:C:343:GLN:NE2	2.28	0.45
1:D:485:MET:HE2	1:D:485:MET:H	1.82	0.45
2:B:517:LYS:N	2:B:517:LYS:HE2	2.31	0.45
1:C:424:THR:OG1	1:C:425:GLY:N	2.49	0.45
1:A:166:TRP:CZ2	1:A:169:ARG:HD3	2.51	0.45
1:A:471:LEU:O	1:A:474:ILE:HG22	2.15	0.45
2:B:60:LEU:HD23	2:B:60:LEU:HA	1.62	0.45
1:C:442:ILE:HB	1:C:451:LEU:HD11	1.98	0.45
1:A:348:ASP:OD1	1:A:349:ALA:N	2.49	0.45
2:B:222:TYR:O	2:B:222:TYR:CD1	2.70	0.45
2:B:342:ILE:HG23	2:B:363:LEU:HD22	1.97	0.45
2:B:452:ASP:OD1	2:B:452:ASP:N	2.50	0.45
1:C:413:VAL:HG22	1:C:461:GLN:HG3	1.98	0.45
1:A:343:GLN:HB2	1:A:346:THR:HG22	1.99	0.45
2:B:83:ASP:OD1	2:B:84:ARG:N	2.50	0.45
1:D:104:ILE:HD11	1:D:139:ASP:O	2.17	0.45
1:A:482:THR:O	1:A:486:ASN:ND2	2.32	0.45
1:C:348:ASP:HA	1:C:355:ARG:HH11	1.81	0.45
1:D:150:MET:SD	1:D:157:TYR:HB2	2.57	0.45
1:D:117:THR:HG22	1:D:119:LEU:HG	1.98	0.44
1:C:417:ALA:HB2	1:C:456:THR:HA	1.98	0.44
1:D:370:VAL:HG21	1:D:373:PHE:HD2	1.82	0.44
1:D:396:LYS:HB2	1:D:396:LYS:HE2	1.70	0.44
2:B:506:GLU:HA	2:B:509:GLN:HE21	1.83	0.44
1:C:420:VAL:HA	1:C:429:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LYS:HD2	1:D:115:LYS:C	2.43	0.44
1:A:83:ARG:HH12	1:A:215:ARG:HG3	1.82	0.44
1:A:368:ASP:O	1:A:374:ARG:NH2	2.50	0.44
1:A:379:ASP:OD1	1:A:380:LEU:HD12	2.17	0.44
2:B:398:ARG:HH22	2:B:415:LEU:HB3	1.83	0.44
1:D:374:ARG:O	1:D:374:ARG:NE	2.51	0.44
1:D:103:ASP:HA	1:D:106:MET:HG2	1.99	0.44
2:B:446:ILE:HD11	2:B:468:GLY:O	2.17	0.44
1:C:333:LYS:NZ	1:C:342:GLN:HE22	2.16	0.44
1:C:138:LEU:HD23	1:C:138:LEU:HA	1.84	0.43
1:C:190:ARG:HA	1:C:190:ARG:HD3	1.62	0.43
1:A:249:THR:HG22	1:A:255:GLY:H	1.83	0.43
1:A:294:HIS:C	1:A:296:THR:H	2.26	0.43
1:D:139:ASP:OD1	1:D:166:TRP:NE1	2.39	0.43
1:D:258:ASP:OD1	1:D:258:ASP:N	2.50	0.43
1:D:330:LEU:HD23	1:D:330:LEU:HA	1.86	0.43
1:A:113:LEU:HD12	1:A:113:LEU:O	2.18	0.43
1:A:160:PHE:C	1:A:162:MET:H	2.27	0.43
2:B:373:ALA:HA	2:B:376:ARG:HH21	1.83	0.43
2:B:434:ILE:HD13	2:B:434:ILE:HA	1.87	0.43
2:B:110:PHE:O	2:B:112:LYS:N	2.52	0.43
1:C:196:CYS:HB3	3:C:901:POV:H38A	2.00	0.43
1:A:54:ASP:OD1	1:A:54:ASP:N	2.42	0.43
1:A:281:THR:O	1:A:285:ILE:HG13	2.18	0.43
1:A:401:LEU:H	1:A:401:LEU:HD23	1.84	0.43
1:C:381:LEU:O	1:C:385:VAL:HG12	2.19	0.43
2:B:349:THR:HG21	2:B:359:ARG:HG3	2.01	0.43
2:B:366:MET:HE3	2:B:367:GLN:HG2	2.01	0.43
2:B:398:ARG:HH12	2:B:412:GLU:HG3	1.83	0.43
1:C:314:HIS:C	1:C:316:ASN:H	2.26	0.43
1:C:393:PHE:CE2	1:C:399:VAL:HG22	2.54	0.43
1:C:430:VAL:O	1:C:431:ARG:HB2	2.17	0.43
1:D:371:TYR:HD2	1:D:438:ILE:HD11	1.84	0.43
1:D:400:ILE:O	1:D:453:THR:HA	2.19	0.43
1:A:478:VAL:O	1:A:481:GLY:N	2.42	0.43
1:C:230:ASN:OD1	1:C:230:ASN:N	2.51	0.43
1:D:56:LYS:HG3	1:D:57:TYR:N	2.34	0.43
1:D:419:LEU:HD12	1:D:419:LEU:HA	1.86	0.43
3:D:901:POV:C1	3:D:901:POV:C31	2.97	0.43
2:B:215:GLU:HG2	2:B:222:TYR:CE1	2.54	0.43
1:C:372:LEU:HA	1:C:372:LEU:HD23	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ASN:OD1	1:D:227:ASN:N	2.52	0.43
1:D:448:ARG:NH2	1:D:449:PRO:O	2.52	0.43
1:C:141:VAL:HA	1:C:144:ILE:HG13	2.01	0.42
1:C:382:PHE:O	1:C:386:SER:OG	2.37	0.42
1:A:271:ILE:HG23	1:D:248:ILE:HD12	2.01	0.42
2:B:79:VAL:HG12	2:B:138:PHE:O	2.19	0.42
1:A:87:PRO:HG2	1:A:88:PRO:HD3	2.01	0.42
2:B:66:PHE:CD1	2:B:66:PHE:C	2.97	0.42
1:C:405:ALA:O	1:C:407:THR:HG23	2.20	0.42
2:B:517:LYS:HA	2:B:520:ILE:HB	2.01	0.42
1:D:410:TYR:CE1	1:D:464:ARG:HB2	2.55	0.42
1:C:458:ARG:CB	1:D:117:THR:HG23	2.49	0.42
1:D:137:LEU:HD23	1:D:138:LEU:H	1.85	0.42
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.85	0.42
1:A:442:ILE:HG13	1:A:443:GLY:N	2.34	0.42
2:B:444:TYR:HD2	2:B:496:VAL:HB	1.83	0.42
2:B:511:ASP:OD1	2:B:511:ASP:N	2.51	0.42
1:C:401:LEU:HA	1:C:453:THR:CG2	2.50	0.42
1:D:409:PHE:HE1	1:D:438:ILE:HB	1.84	0.42
2:B:244:ILE:O	2:B:248:ILE:HG13	2.20	0.42
2:B:290:VAL:HG22	1:C:253:THR:HA	2.01	0.42
1:D:338:SER:HA	1:D:341:LEU:HD22	2.01	0.42
2:B:97:VAL:HG23	2:B:129:PHE:HZ	1.84	0.42
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.91	0.41
1:A:384:LEU:HD23	1:A:465:MET:HE1	2.02	0.41
1:A:473:ILE:HD12	1:A:473:ILE:HA	1.92	0.41
1:D:162:MET:HE3	1:D:162:MET:HB3	1.96	0.41
1:D:352:LYS:O	1:D:356:SER:HB3	2.19	0.41
1:A:347:LEU:HD12	1:A:347:LEU:HA	1.77	0.41
2:B:141:TYR:CE2	2:B:159:ARG:HD3	2.56	0.41
2:B:152:ASP:OD1	2:B:155:LEU:HB2	2.20	0.41
2:B:273:TRP:O	2:B:277:THR:OG1	2.26	0.41
2:B:523:PHE:HD1	2:B:523:PHE:HA	1.70	0.41
1:A:419:LEU:HD23	1:A:452:PHE:HB2	2.02	0.41
1:D:213:ALA:HB2	1:D:223:TRP:NE1	2.34	0.41
1:A:114:ASP:O	1:A:118:TYR:N	2.49	0.41
2:B:231:LEU:HD23	2:B:231:LEU:O	2.18	0.41
1:C:202:VAL:HG13	1:C:247:SER:OG	2.21	0.41
1:C:401:LEU:HA	1:C:453:THR:HG22	2.03	0.41
1:D:326:MET:HG3	1:D:327:LEU:N	2.35	0.41
1:D:401:LEU:HD23	1:D:402:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:OE2	1:A:432:GLU:N	2.54	0.41
1:C:421:ASP:OD1	1:C:430:VAL:HG12	2.21	0.41
1:A:410:TYR:HB2	1:A:439:ILE:HD11	2.03	0.41
2:B:109:ALA:HB2	2:B:243:CYS:HB3	2.02	0.41
2:B:354:LEU:HA	1:C:361:PHE:CE2	2.56	0.41
2:B:369:LYS:HE2	2:B:369:LYS:HB3	1.95	0.41
1:C:318:LEU:HD22	1:C:322:LEU:HD11	2.03	0.41
1:C:468:THR:OG1	1:C:469:THR:N	2.53	0.41
1:D:199:LEU:HD23	1:D:199:LEU:HA	1.87	0.41
1:A:52:PRO:HG3	1:A:111:GLY:H	1.86	0.41
1:A:137:LEU:O	1:A:141:VAL:HG12	2.19	0.41
1:A:374:ARG:HA	1:A:374:ARG:HD3	1.57	0.41
2:B:396:LEU:HD23	2:B:396:LEU:HA	1.86	0.41
1:C:92:THR:O	1:C:96:VAL:HG23	2.21	0.41
1:A:139:ASP:CG	1:A:169:ARG:HH22	2.29	0.41
1:A:379:ASP:O	1:A:383:GLN:HG2	2.20	0.41
2:B:154:LYS:H	2:B:154:LYS:HG2	1.65	0.41
2:B:174:LEU:HA	2:B:175:PRO:HD3	1.95	0.41
2:B:174:LEU:HA	2:B:174:LEU:HD12	1.86	0.41
2:B:237:TRP:CH2	2:B:312:PHE:HB2	2.51	0.41
2:B:390:SER:O	2:B:390:SER:OG	2.30	0.41
2:B:446:ILE:HD12	2:B:469:PRO:HA	2.02	0.41
2:B:512:ASN:OD1	2:B:513:ASP:N	2.54	0.41
1:C:442:ILE:HD13	1:C:442:ILE:HA	1.87	0.41
1:D:218:ASN:HD22	1:D:219:PRO:CD	2.34	0.41
1:D:380:LEU:HA	1:D:383:GLN:HE21	1.85	0.41
1:A:406:PRO:HD3	1:A:449:PRO:HA	2.02	0.41
2:B:369:LYS:HA	2:B:372:THR:HG22	2.03	0.41
1:D:54:ASP:OD1	1:D:54:ASP:N	2.52	0.41
1:D:428:SER:OG	1:D:429:ILE:N	2.54	0.41
1:A:55:HIS:O	1:A:59:ILE:HG13	2.21	0.40
1:A:351:PRO:HD3	1:D:329:HIS:NE2	2.36	0.40
1:D:152:ILE:HD13	1:D:152:ILE:HA	1.82	0.40
1:D:230:ASN:OD1	1:D:230:ASN:N	2.46	0.40
1:A:154:SER:OG	1:A:155:GLN:N	2.54	0.40
1:A:484:ILE:HA	1:A:487:ASN:OD1	2.21	0.40
1:D:219:PRO:O	1:D:222:THR:OG1	2.37	0.40
1:D:360:HIS:ND1	1:D:360:HIS:C	2.78	0.40
2:B:478:VAL:HG23	2:B:501:HIS:HB2	2.03	0.40
1:C:175:PHE:O	1:C:179:GLU:HG2	2.21	0.40
1:C:392:TYR:CE2	1:C:461:GLN:NE2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:GLY:HA2	1:D:458:ARG:HE	1.86	0.40
1:D:420:VAL:HG21	1:D:455:ARG:NH2	2.36	0.40
1:D:431:ARG:HG3	1:D:432:GLU:N	2.35	0.40
2:B:67:ILE:HD13	2:B:67:ILE:HA	1.93	0.40
2:B:441:THR:O	2:B:501:HIS:N	2.48	0.40
1:C:407:THR:O	1:C:467:ARG:HB2	2.21	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	A	439/885 (50%)	396 (90%)	43 (10%)	0	100	100
1	C	439/885 (50%)	393 (90%)	46 (10%)	0	100	100
1	D	438/885 (50%)	403 (92%)	35 (8%)	0	100	100
2	B	472/710 (66%)	429 (91%)	41 (9%)	2 (0%)	30	58
All	All	1788/3365 (53%)	1621 (91%)	165 (9%)	2 (0%)	50	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ARG
2	B	60	LEU

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	
1	A	392/766 (51%)	353 (90%)	39 (10%)	6	18
1	C	392/766 (51%)	354 (90%)	38 (10%)	6	19
1	D	391/766 (51%)	356 (91%)	35 (9%)	8	22
2	B	420/615 (68%)	371 (88%)	49 (12%)	4	13
All	All	1595/2913 (55%)	1434 (90%)	161 (10%)	9	17

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	91	ILE
1	A	102	ILE
1	A	104	ILE
1	A	106	MET
1	A	113	LEU
1	A	117	THR
1	A	126	GLN
1	A	137	LEU
1	A	143	THR
1	A	152	ILE
1	A	159	LEU
1	A	161	ASN
1	A	164	ARG
1	A	174	LEU
1	A	178	LEU
1	A	189	VAL
1	A	217	SER
1	A	235	SER
1	A	251	LEU
1	A	284	LEU
1	A	296	THR
1	A	324	ASP
1	A	352	LYS
1	A	372	LEU
1	A	377	SER
1	A	407	THR
1	A	423	ASP
1	A	427	GLU
1	A	430	VAL

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Mol	Chain	Res	Type
1	A	434	LYS
1	A	439	ILE
1	A	441	GLU
1	A	447	TYR
1	A	458	ARG
1	A	484	ILE
1	A	487	ASN
1	A	488	LEU
1	A	489	LEU
2	B	55	VAL
2	B	66	PHE
2	B	69	ASP
2	B	74	SER
2	B	78	ILE
2	B	84	ARG
2	B	91	LEU
2	B	100	SER
2	B	107	GLU
2	B	111	GLU
2	B	120	THR
2	B	123	LEU
2	B	131	VAL
2	B	144	ASN
2	B	177	GLN
2	B	180	TYR
2	B	182	THR
2	B	204	LEU
2	B	219	HIS
2	B	225	ILE
2	B	228	ILE
2	B	230	LEU
2	B	231	LEU
2	B	233	VAL
2	B	245	LEU
2	B	264	VAL
2	B	285	VAL
2	B	286	THR
2	B	314	ILE
2	B	357	THR
2	B	362	MET
2	B	374	GLU
2	B	384	LEU

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Mol	Chain	Res	Type
2	B	388	ILE
2	B	390	SER
2	B	399	SER
2	B	432	GLU
2	B	433	ILE
2	B	447	VAL
2	B	451	VAL
2	B	454	ILE
2	B	461	GLU
2	B	488	VAL
2	B	506	GLU
2	B	508	VAL
2	B	519	ILE
2	B	523	PHE
2	B	524	MET
2	B	525	THR
1	C	54	ASP
1	C	59	ILE
1	C	61	GLU
1	C	71	THR
1	C	75	SER
1	C	89	LEU
1	C	90	SER
1	C	106	MET
1	C	115	LYS
1	C	116	SER
1	C	127	ILE
1	C	129	PHE
1	C	132	LEU
1	C	142	SER
1	C	153	SER
1	C	169	ARG
1	C	174	LEU
1	C	178	LEU
1	C	183	ASN
1	C	190	ARG
1	C	291	LEU
1	C	346	THR
1	C	359	SER
1	C	365	SER
1	C	367	MET
1	C	377	SER

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Mol	Chain	Res	Type
1	C	379	ASP
1	C	386	SER
1	C	420	VAL
1	C	421	ASP
1	C	452	PHE
1	C	453	THR
1	C	458	ARG
1	C	459	LEU
1	C	461	GLN
1	C	462	LEU
1	C	468	THR
1	C	492	LEU
1	D	71	THR
1	D	89	LEU
1	D	90	SER
1	D	102	ILE
1	D	105	ILE
1	D	106	MET
1	D	135	TRP
1	D	142	SER
1	D	146	SER
1	D	152	ILE
1	D	159	LEU
1	D	217	SER
1	D	222	THR
1	D	249	THR
1	D	251	LEU
1	D	306	ILE
1	D	322	LEU
1	D	341	LEU
1	D	346	THR
1	D	359	SER
1	D	363	PHE
1	D	372	LEU
1	D	379	ASP
1	D	383	GLN
1	D	391	GLU
1	D	408	ASP
1	D	424	THR
1	D	437	ASP
1	D	442	ILE
1	D	445	LEU

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Mol	Chain	Res	Type
1	D	474	ILE
1	D	478	VAL
1	D	487	ASN
1	D	489	LEU
1	D	490	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	ASN
1	A	323	GLN
1	A	402	GLN
2	B	81	HIS
2	B	149	ASN
2	B	153	HIS
2	B	219	HIS
2	B	251	HIS
2	B	330	HIS
2	B	361	GLN
2	B	421	GLN
2	B	423	GLN
2	B	495	GLN
2	B	522	ASN
1	C	94	ASN
1	C	185	ASN
1	C	216	ASN
1	C	227	ASN
1	C	290	ASN
1	C	301	ASN
1	C	307	GLN
1	C	342	GLN
1	C	378	ASN
1	C	383	GLN
1	C	414	ASN
1	C	450	GLN
1	D	185	ASN
1	D	218	ASN
1	D	277	ASN
1	D	294	HIS
1	D	314	HIS
1	D	383	GLN
1	D	487	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	POV	B	801	-	38,38,51	0.53	0	42,43,59	0.70	2 (4%)
3	POV	A	901	-	38,38,51	1.27	6 (15%)	42,43,59	1.24	6 (14%)
3	POV	C	901	-	38,38,51	1.04	1 (2%)	42,43,59	1.38	5 (11%)
3	POV	D	901	-	38,38,51	0.54	0	42,43,59	0.87	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	POV	B	801	-	-	21/40/40/55	-
3	POV	A	901	-	-	21/40/40/55	-
3	POV	C	901	-	-	19/40/40/55	-
3	POV	D	901	-	-	25/40/40/55	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	POV	O22-C21	-3.13	1.13	1.22
3	A	901	POV	C313-C312	-3.01	1.34	1.51
3	A	901	POV	C27-C28	-2.92	1.40	1.52
3	A	901	POV	O22-C21	-2.77	1.14	1.22
3	A	901	POV	C23-C22	-2.44	1.43	1.52
3	A	901	POV	C22-C21	-2.08	1.44	1.50
3	A	901	POV	C36-C35	-2.05	1.40	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	901	POV	O21-C21-C22	5.29	122.89	111.50
3	D	901	POV	O21-C21-C22	3.35	118.72	111.50
3	A	901	POV	O11-P-O14	3.35	115.87	106.47
3	A	901	POV	O21-C21-C22	3.28	118.58	111.50
3	A	901	POV	O12-P-O11	-2.76	99.38	106.73
3	D	901	POV	O13-P-O14	2.46	120.31	110.68
3	C	901	POV	O11-P-O14	2.46	113.37	106.47
3	C	901	POV	O22-C21-C22	-2.31	114.72	123.73
3	A	901	POV	O13-P-O14	2.28	119.59	110.68
3	A	901	POV	C3-C2-C1	2.27	117.16	111.79
3	C	901	POV	O12-P-O14	-2.25	101.86	110.68
3	D	901	POV	O13-P-O11	2.25	112.72	106.73
3	C	901	POV	O13-P-O14	2.25	119.48	110.68
3	B	801	POV	O13-P-O14	2.18	119.22	110.68
3	A	901	POV	C2-O21-C21	2.10	122.97	117.79
3	B	801	POV	O12-P-O11	-2.04	101.30	106.73

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	POV	C1-O11-P-O12
3	A	901	POV	C1-O11-P-O13
3	A	901	POV	C1-O11-P-O14
3	B	801	POV	C1-O11-P-O12
3	B	801	POV	C1-O11-P-O13
3	B	801	POV	C1-O11-P-O14
3	B	801	POV	C211-C210-C29-C28
3	B	801	POV	C22-C21-O21-C2
3	C	901	POV	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
3	C	901	POV	C1-O11-P-O13
3	C	901	POV	C1-O11-P-O14
3	C	901	POV	C2-C1-O11-P
3	C	901	POV	C32-C31-O31-C3
3	D	901	POV	C1-O11-P-O12
3	D	901	POV	C1-O11-P-O13
3	D	901	POV	C1-O11-P-O14
3	C	901	POV	O32-C31-O31-C3
3	D	901	POV	O32-C31-O31-C3
3	B	801	POV	O22-C21-O21-C2
3	D	901	POV	C2-C3-O31-C31
3	D	901	POV	C32-C31-O31-C3
3	B	801	POV	C32-C33-C34-C35
3	B	801	POV	C34-C35-C36-C37
3	D	901	POV	C22-C21-O21-C2
3	A	901	POV	C21-C22-C23-C24
3	C	901	POV	C31-C32-C33-C34
3	D	901	POV	C31-C32-C33-C34
3	D	901	POV	O22-C21-O21-C2
3	A	901	POV	C39-C310-C311-C312
3	A	901	POV	C23-C24-C25-C26
3	D	901	POV	C311-C310-C39-C38
3	D	901	POV	C23-C24-C25-C26
3	D	901	POV	C32-C33-C34-C35
3	A	901	POV	C32-C33-C34-C35
3	B	801	POV	C36-C37-C38-C39
3	C	901	POV	C33-C34-C35-C36
3	D	901	POV	C24-C25-C26-C27
3	A	901	POV	C36-C37-C38-C39
3	C	901	POV	C311-C312-C313-C314
3	D	901	POV	C34-C35-C36-C37
3	D	901	POV	C35-C36-C37-C38
3	A	901	POV	O22-C21-O21-C2
3	B	801	POV	C22-C23-C24-C25
3	A	901	POV	C33-C34-C35-C36
3	D	901	POV	C26-C27-C28-C29
3	C	901	POV	C37-C38-C39-C310
3	C	901	POV	C24-C25-C26-C27
3	A	901	POV	C22-C21-O21-C2
3	C	901	POV	C22-C21-O21-C2
3	B	801	POV	C37-C38-C39-C310
3	C	901	POV	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
3	B	801	POV	C311-C310-C39-C38
3	D	901	POV	C310-C311-C312-C313
3	D	901	POV	C311-C312-C313-C314
3	D	901	POV	O11-C1-C2-C3
3	B	801	POV	C24-C25-C26-C27
3	A	901	POV	C1-C2-O21-C21
3	A	901	POV	C310-C311-C312-C313
3	A	901	POV	C34-C35-C36-C37
3	B	801	POV	O21-C2-C3-O31
3	D	901	POV	C37-C38-C39-C310
3	B	801	POV	O11-C1-C2-C3
3	A	901	POV	C31-C32-C33-C34
3	A	901	POV	C2-C1-O11-P
3	B	801	POV	C1-C2-C3-O31
3	D	901	POV	O11-C1-C2-O21
3	D	901	POV	C25-C26-C27-C28
3	C	901	POV	C22-C23-C24-C25
3	D	901	POV	C211-C210-C29-C28
3	A	901	POV	C25-C26-C27-C28
3	C	901	POV	C23-C24-C25-C26
3	B	801	POV	C1-C2-O21-C21
3	B	801	POV	C3-C2-O21-C21
3	C	901	POV	C1-C2-O21-C21
3	B	801	POV	C25-C26-C27-C28
3	A	901	POV	C22-C23-C24-C25
3	D	901	POV	C27-C28-C29-C210
3	A	901	POV	O21-C2-C3-O31
3	C	901	POV	C1-C2-C3-O31
3	D	901	POV	C1-C2-O21-C21
3	B	801	POV	C311-C312-C313-C314
3	C	901	POV	C39-C310-C311-C312
3	B	801	POV	C27-C28-C29-C210
3	C	901	POV	C27-C28-C29-C210
3	A	901	POV	C1-C2-C3-O31
3	A	901	POV	C311-C310-C39-C38

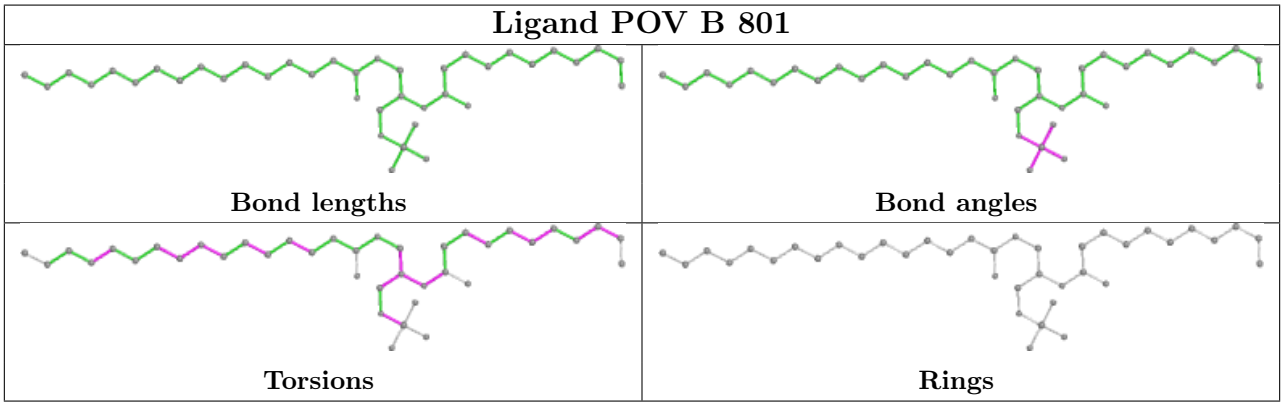
There are no ring outliers.

2 monomers are involved in 12 short contacts:

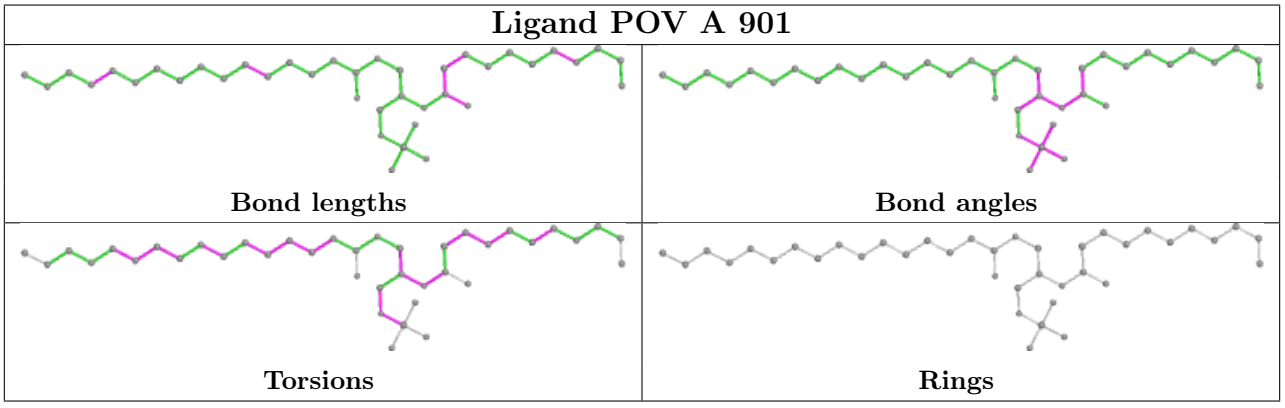
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	POV	9	0
3	D	901	POV	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

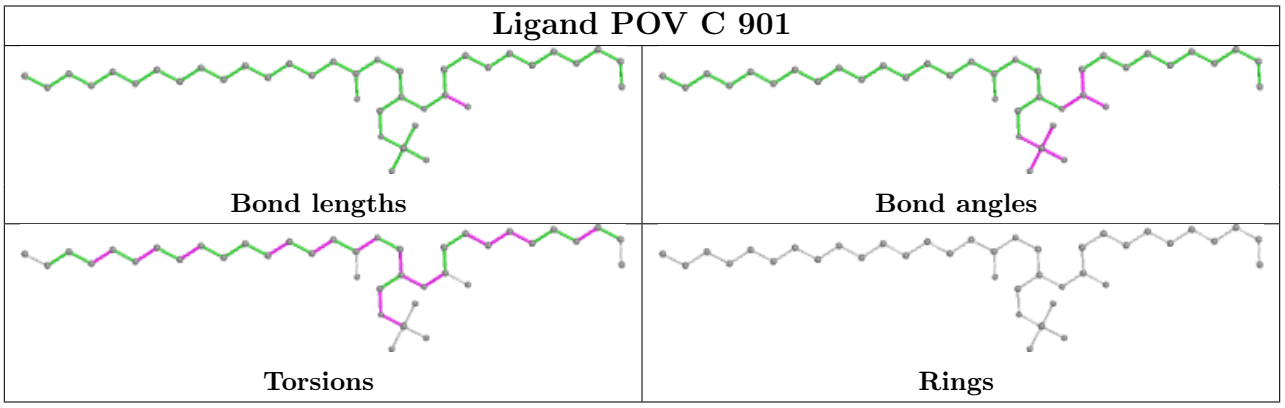
Ligand POV B 801

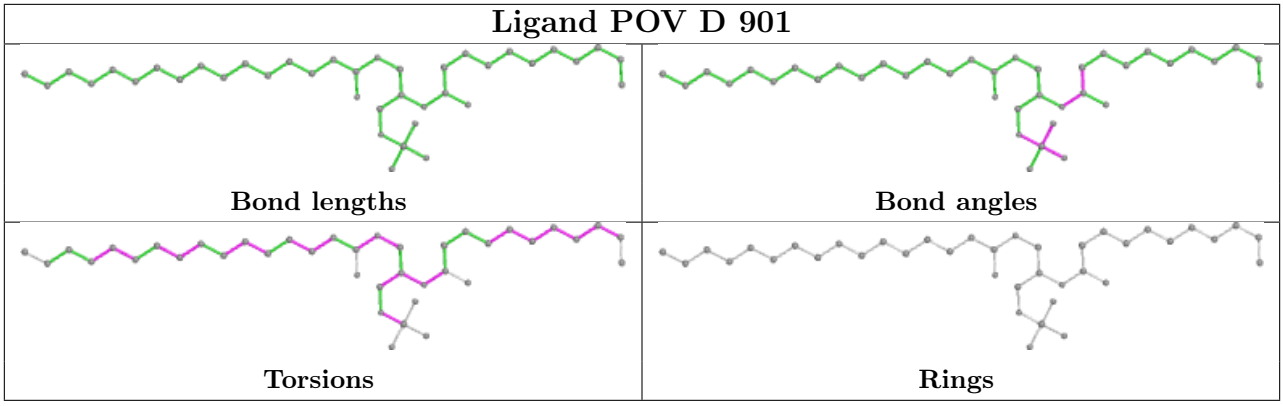


Ligand POV A 901



Ligand POV C 901





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.

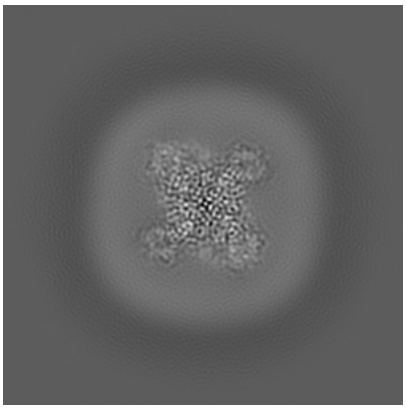
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60834. These allow visual inspection of the internal detail of the map and identification of artifacts.

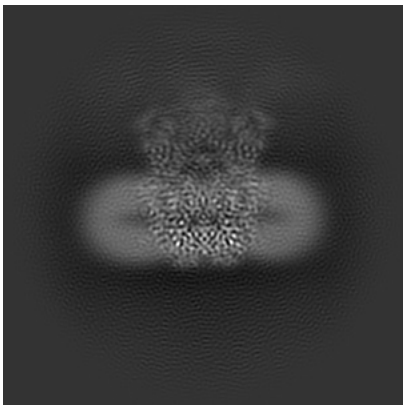
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

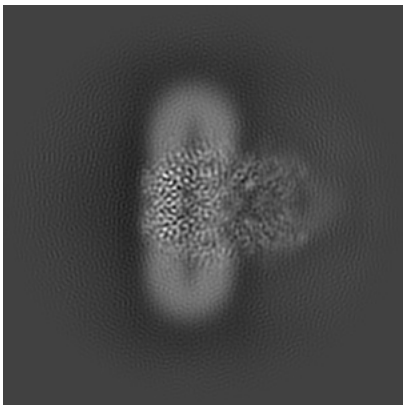
6.1.1 Primary map



X

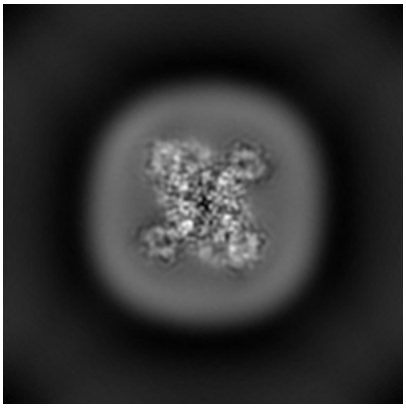


Y

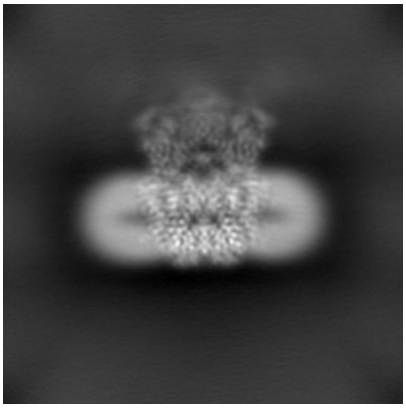


Z

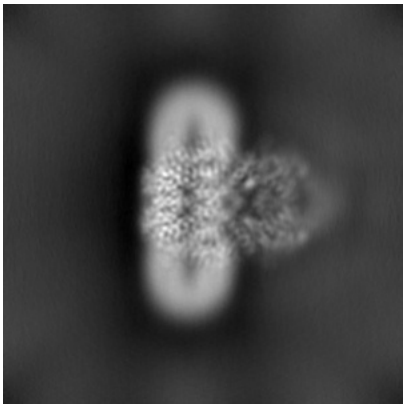
6.1.2 Raw map



X



Y

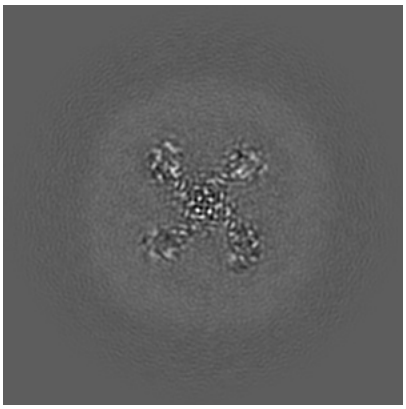


Z

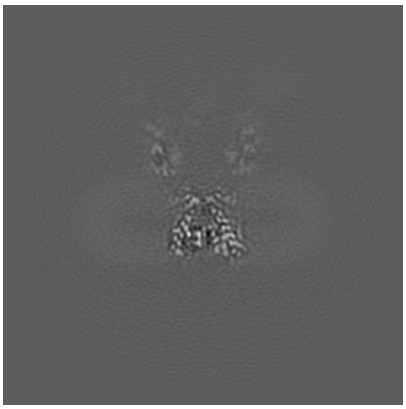
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

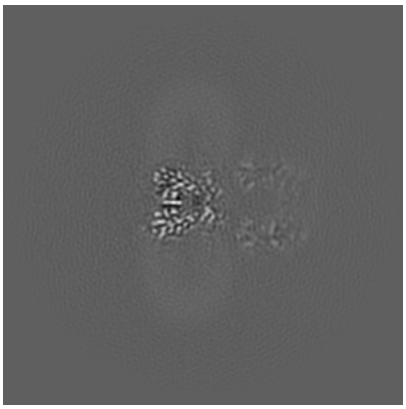
6.2.1 Primary map



X Index: 120

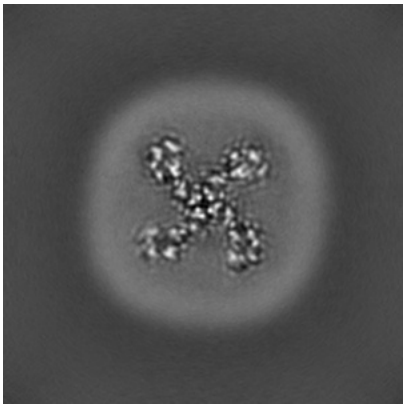


Y Index: 120

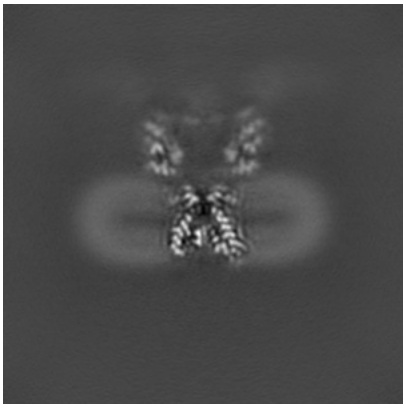


Z Index: 120

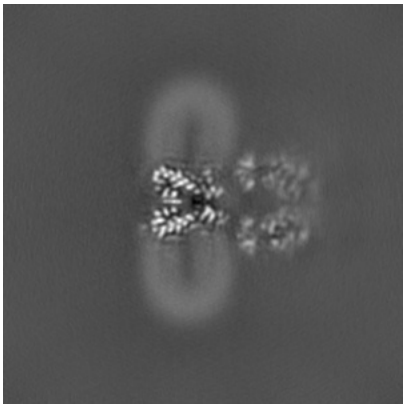
6.2.2 Raw map



X Index: 120



Y Index: 120

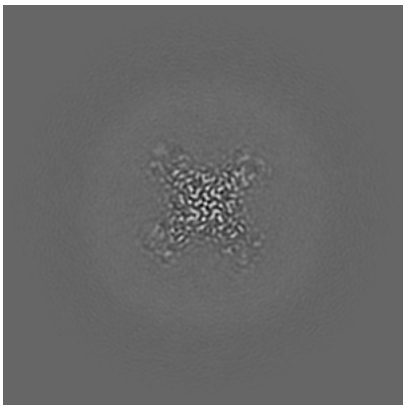


Z Index: 120

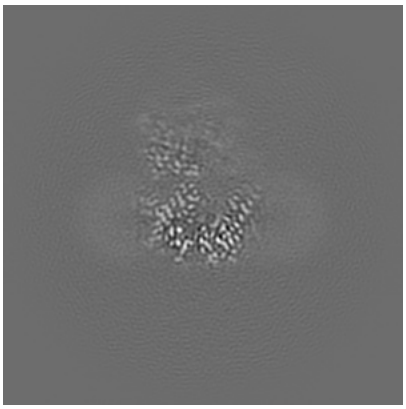
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

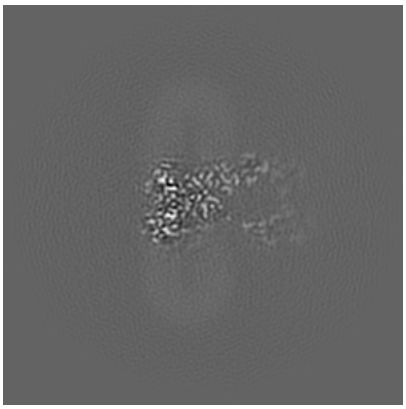
6.3.1 Primary map



X Index: 102

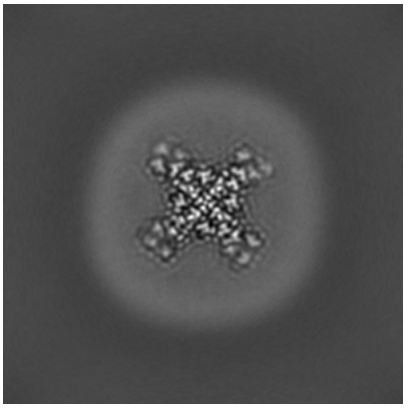


Y Index: 137

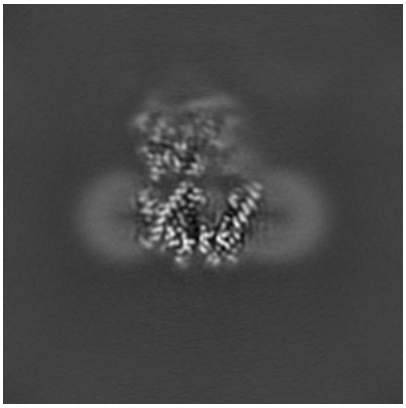


Z Index: 112

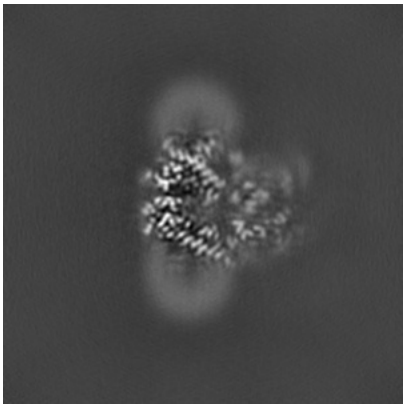
6.3.2 Raw map



X Index: 101



Y Index: 138

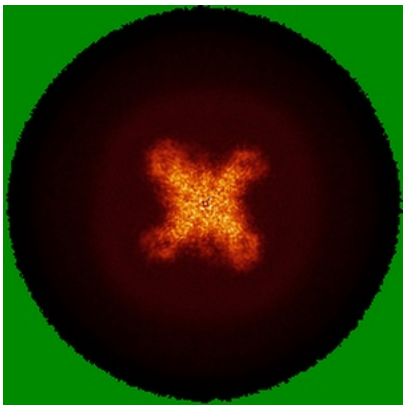


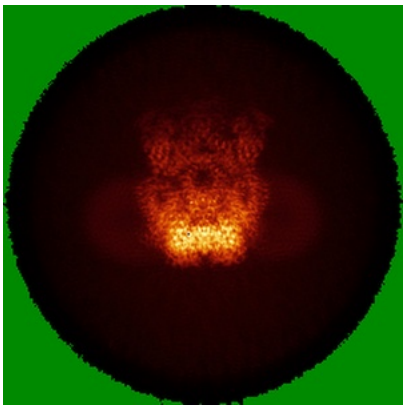
Z Index: 137

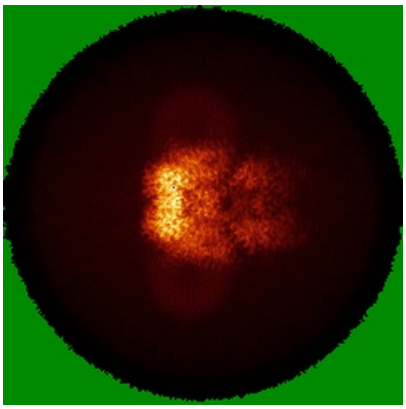
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

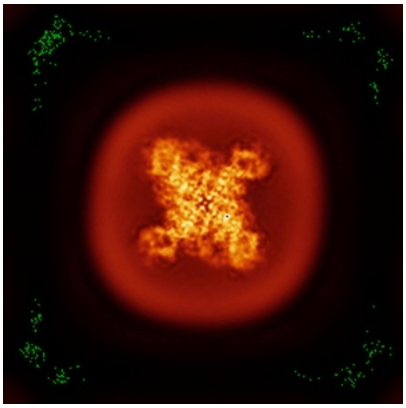
6.4.1 Primary map

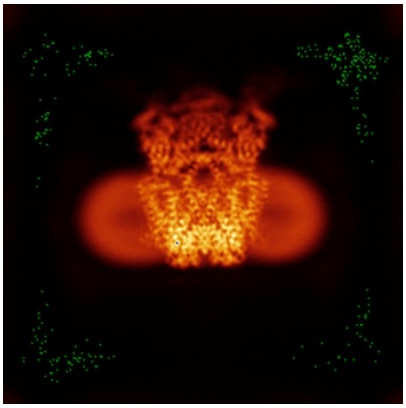

X

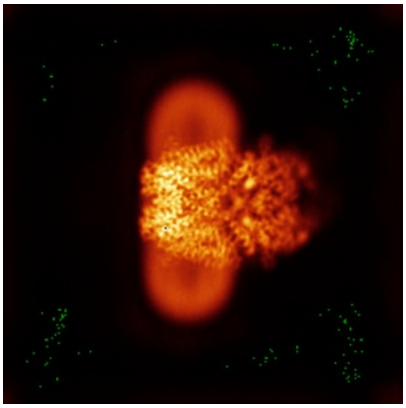

Y


Z

6.4.2 Raw map


X


Y


Z

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

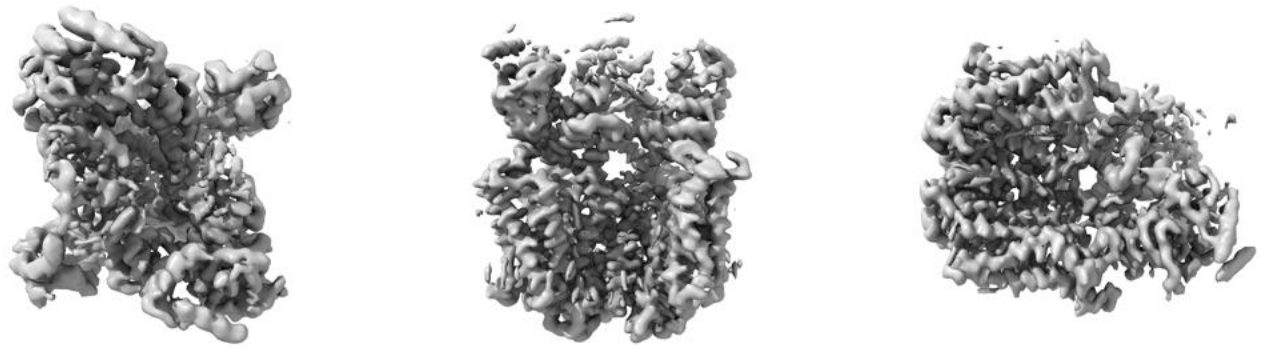
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.642. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

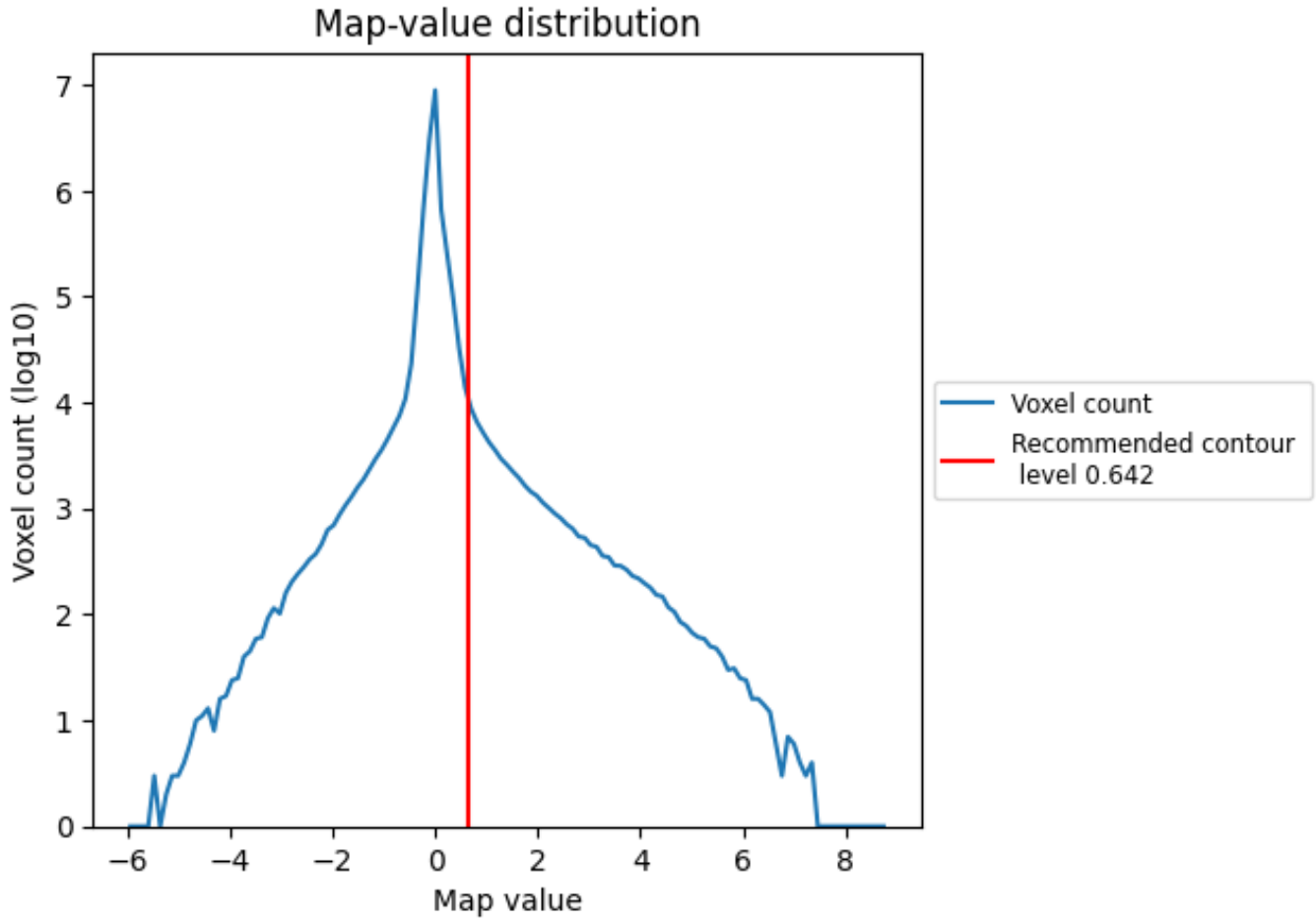
6.6 Mask visualisation (i)

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

7 Map analysis

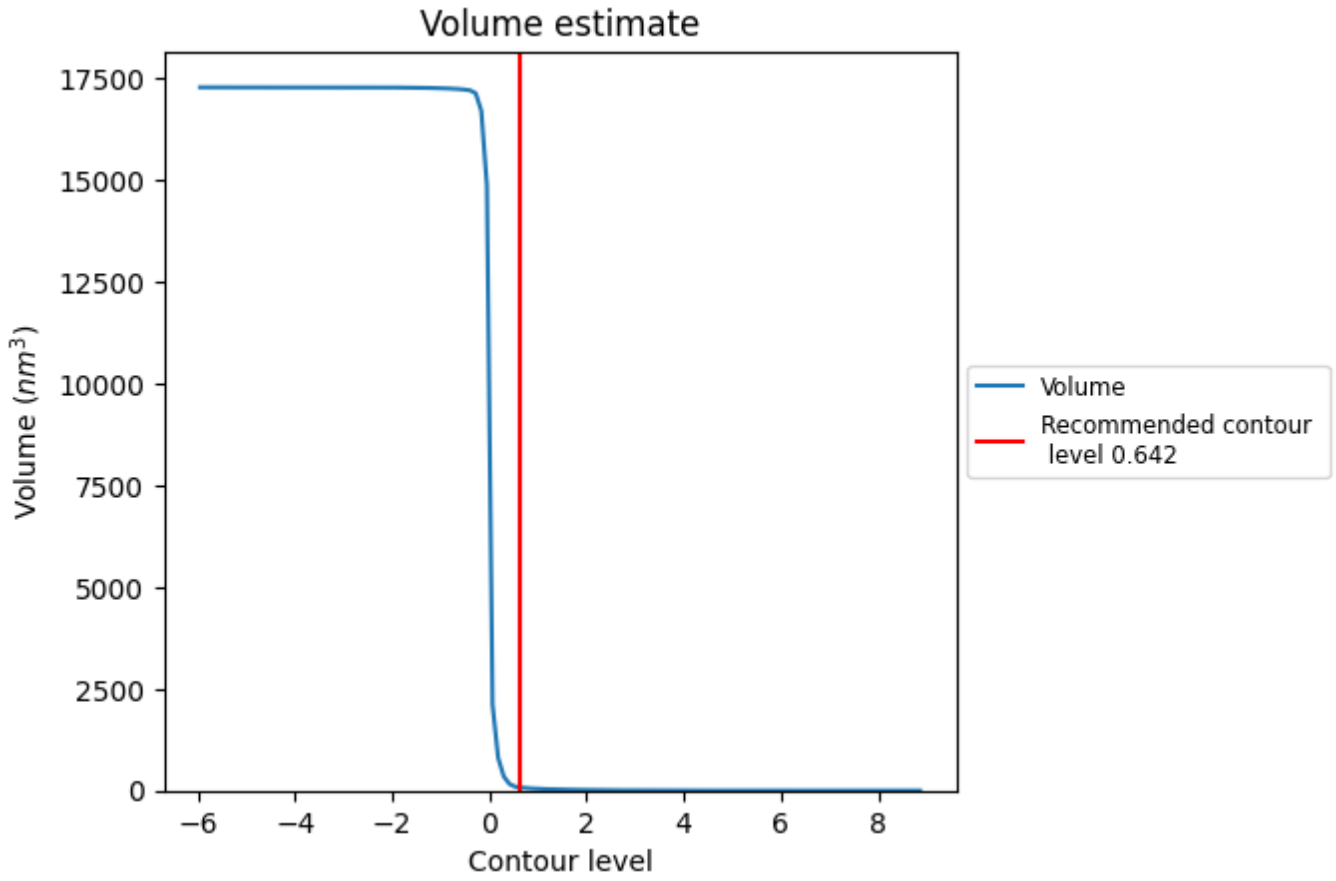
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

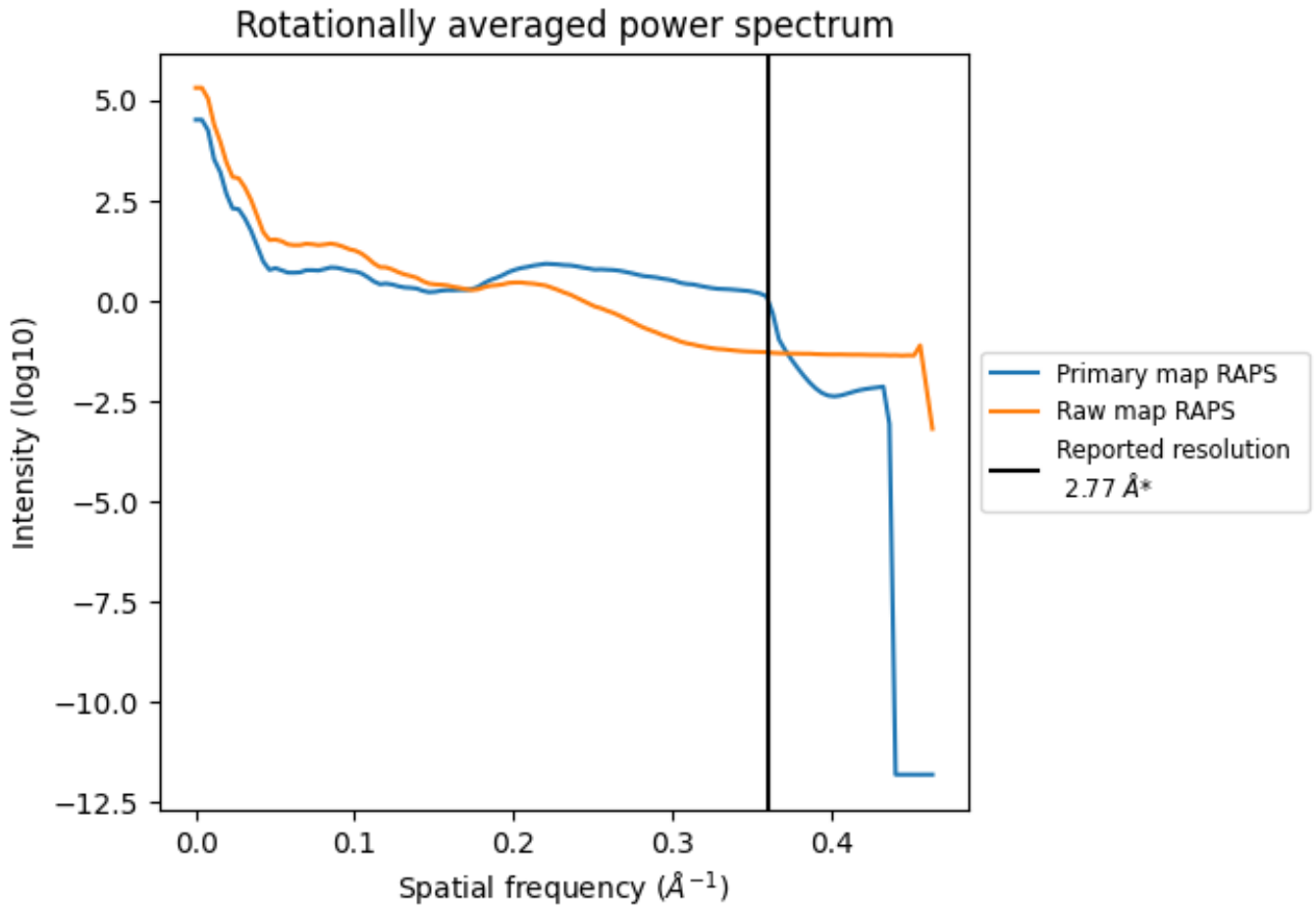
7.2 Volume estimate (i)



The volume at the recommended contour level is 74 nm^3; this corresponds to an approximate mass of 67 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

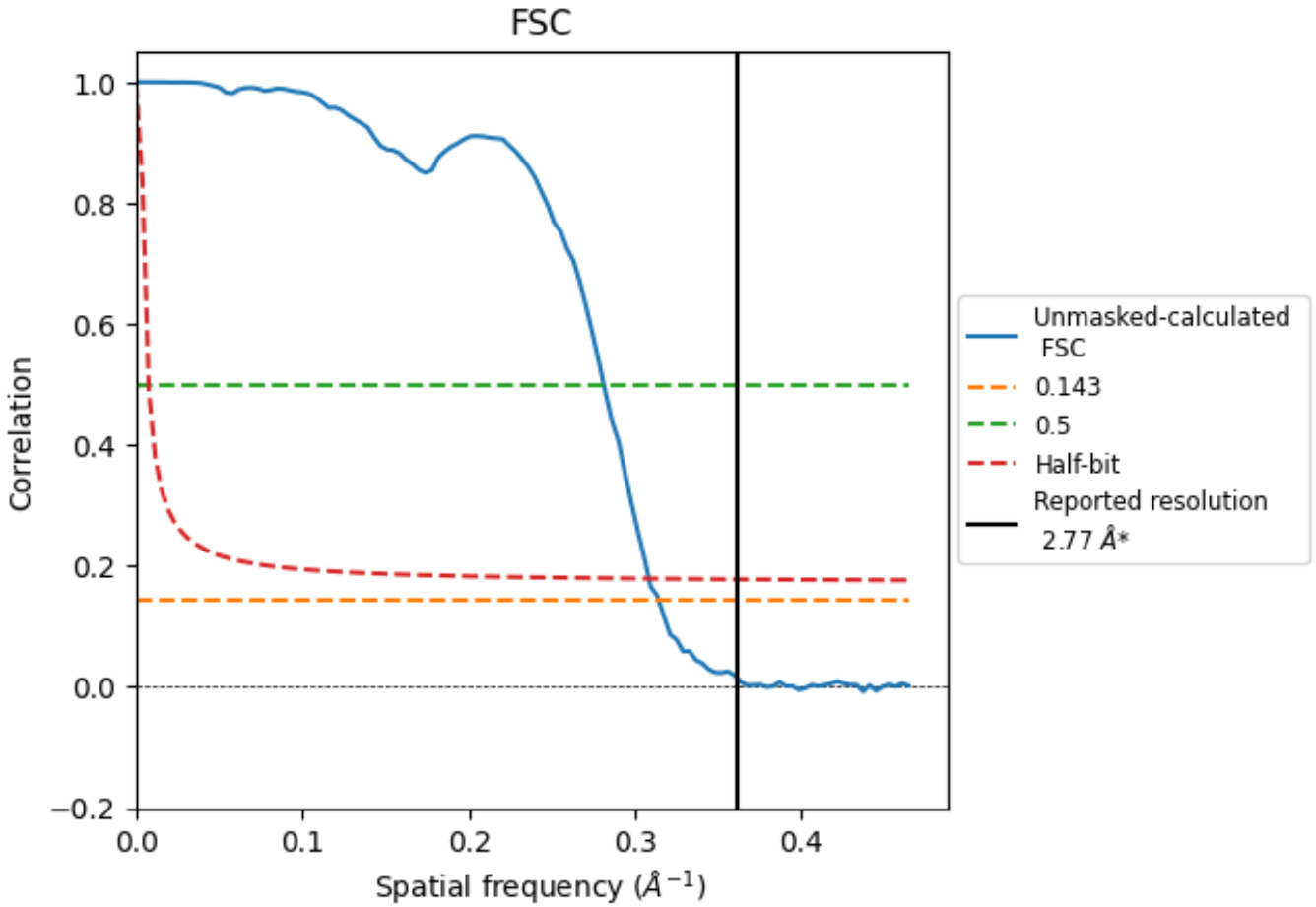


*Reported resolution corresponds to spatial frequency of 0.361 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.361 Å^{-1}

8.2 Resolution estimates (i)

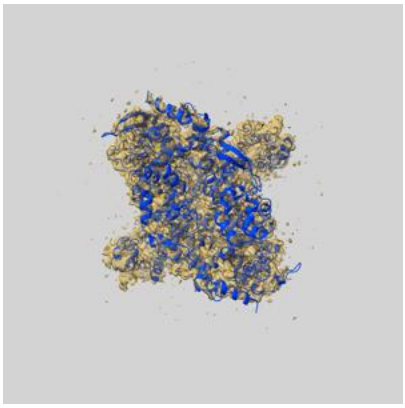
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.56	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.77 by more than 10 %

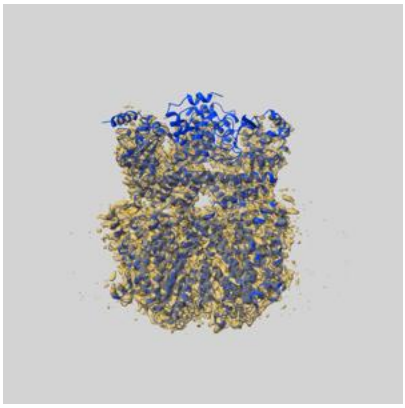
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60834 and PDB model 9IS8. Per-residue inclusion information can be found in section 3 on page 8.

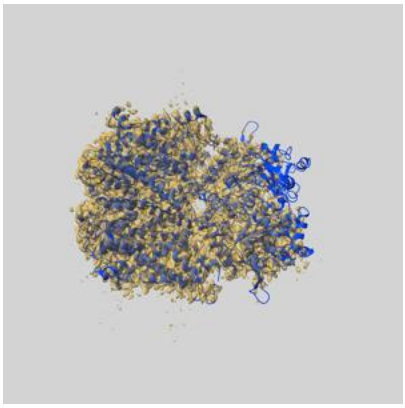
9.1 Map-model overlay



X



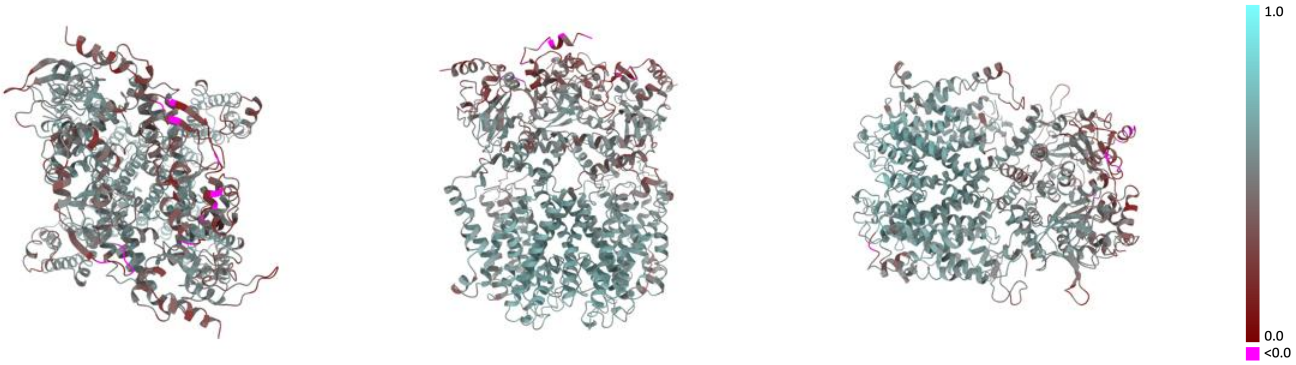
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.642 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.

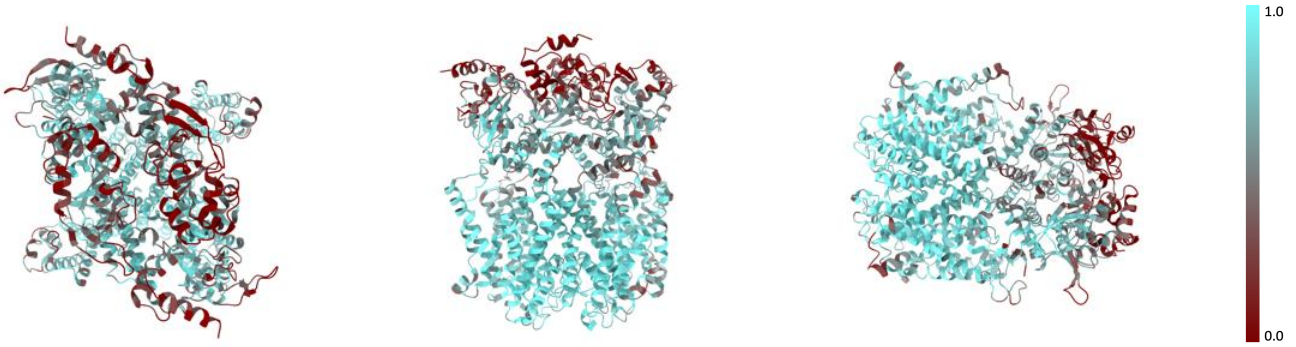
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

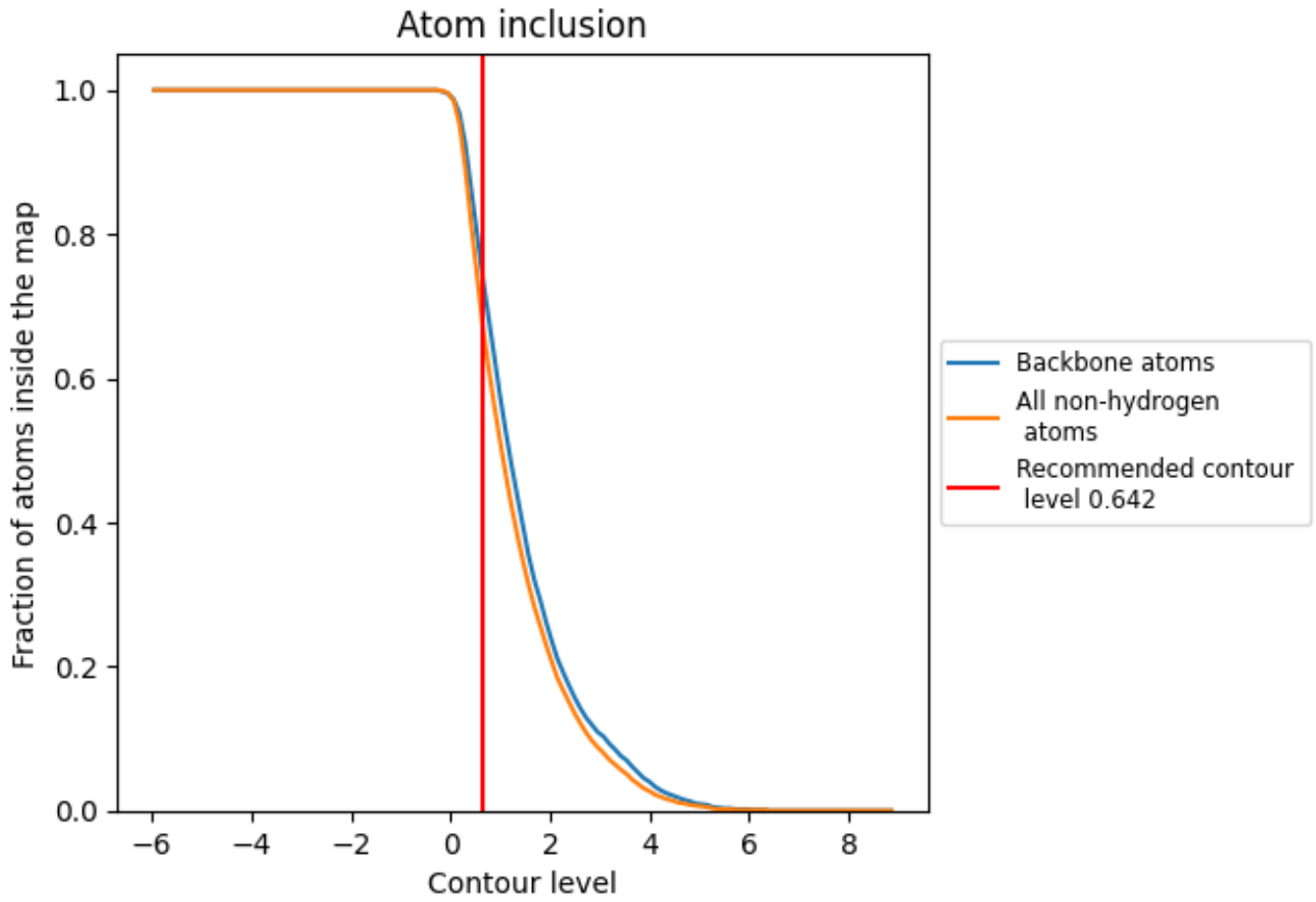
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.642).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 68% 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 (0.642) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.5160
A	0.7140	0.5290
B	0.6800	0.5250
C	0.7020	0.5200
D	0.6120	0.4880