



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:32 PM UTC

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.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

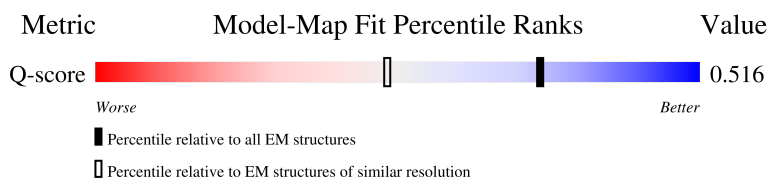
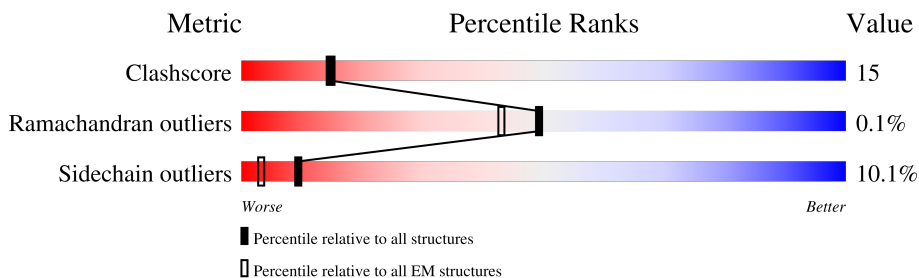
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10695 (2.27 - 3.27)

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

Mol	Chain	Length	Quality of chain
1	A	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

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	C	N	O	S	0	0
			3599	2341	608	630	20		
1	C	441	Total	C	N	O	S	0	0
			3599	2341	608	630	20		
1	D	440	Total	C	N	O	S	0	0
			3591	2335	607	629	20		

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:

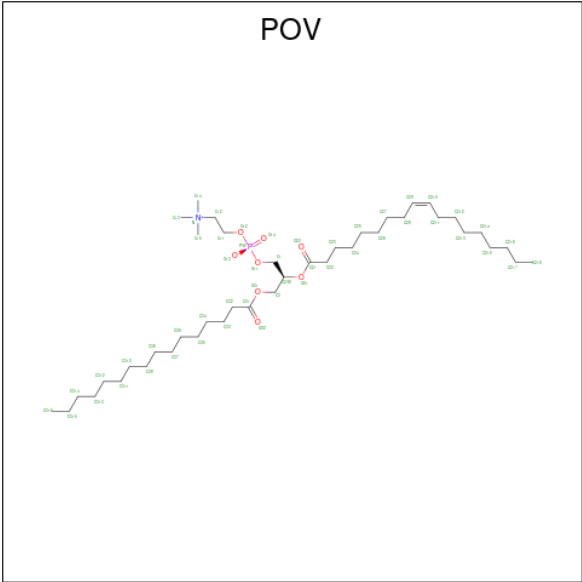
Chain	Residue	Modelled	Actual	Comment	Reference
B	315	ASP	GLY	engineered mutation	UNP P92960
B	663	LEU	-	expression tag	UNP P92960
B	664	GLU	-	expression tag	UNP P92960
B	665	GLY	-	expression tag	UNP P92960
B	666	SER	-	expression tag	UNP P92960
B	667	ASP	-	expression tag	UNP P92960
B	668	GLU	-	expression 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

Continued on next page...

Continued from previous page...

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: C₄₂H₈₂NO₈P).



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	

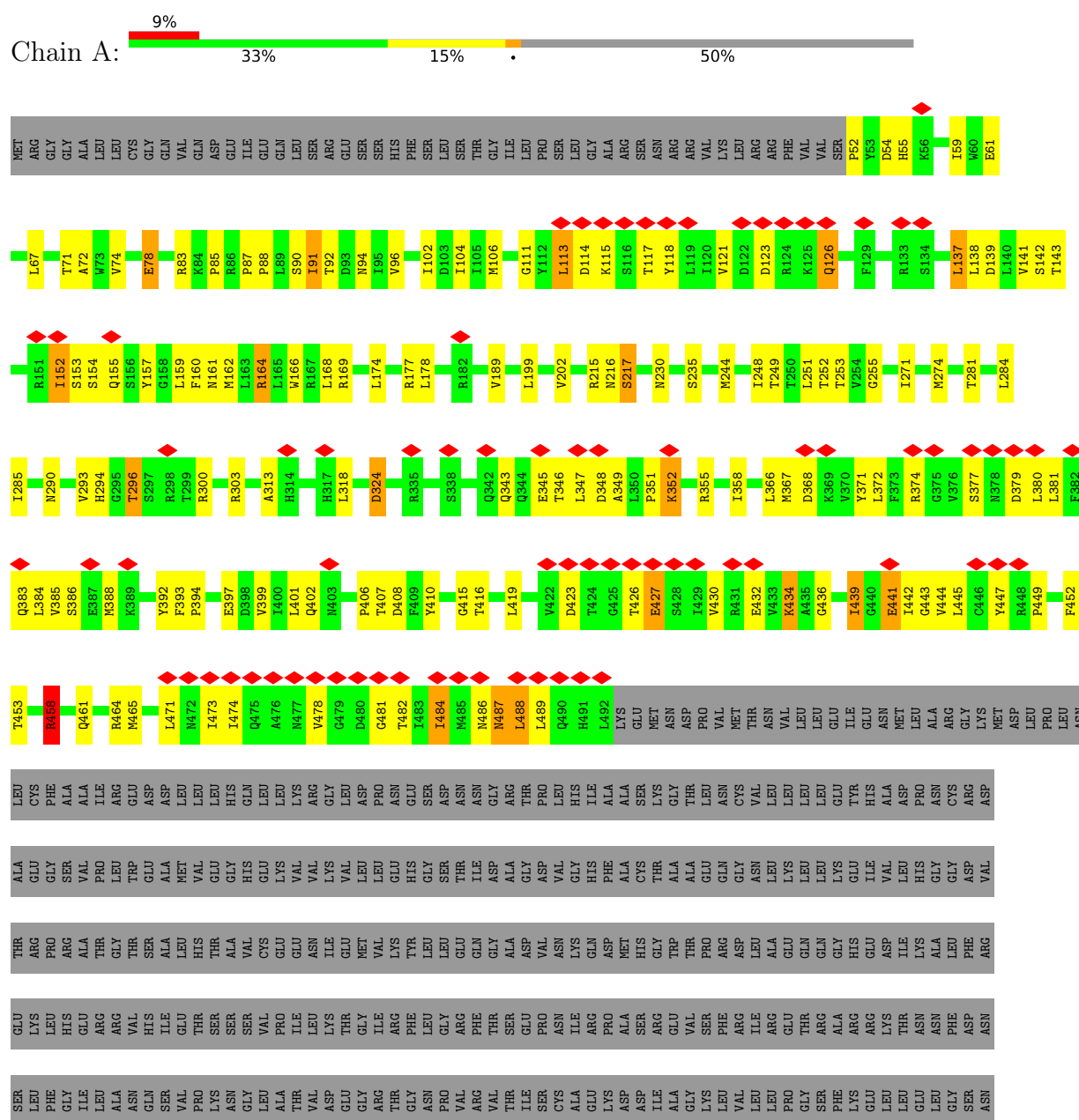
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

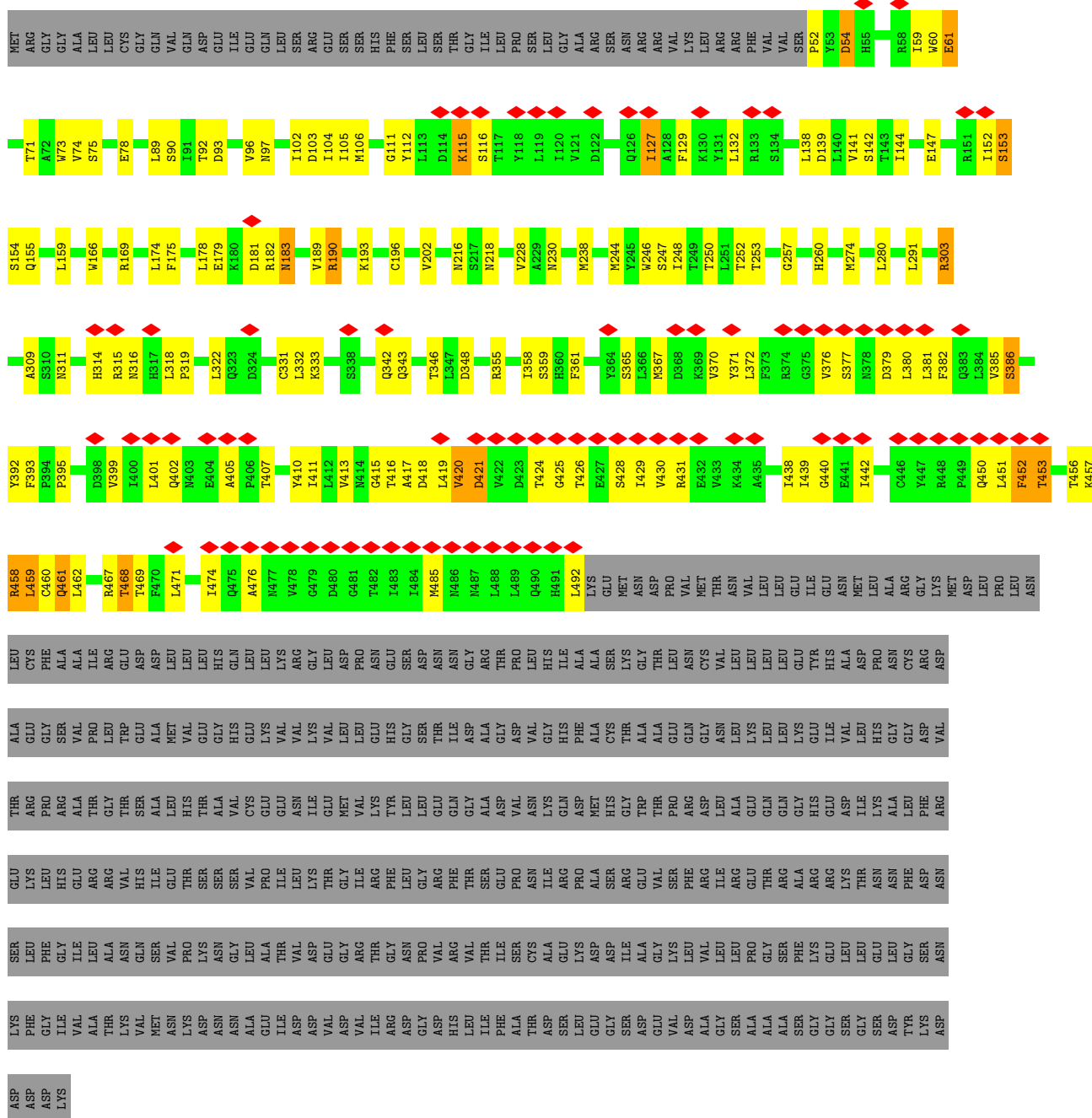
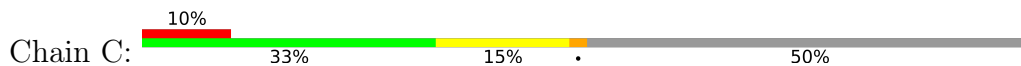
3 Residue-property plots

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.

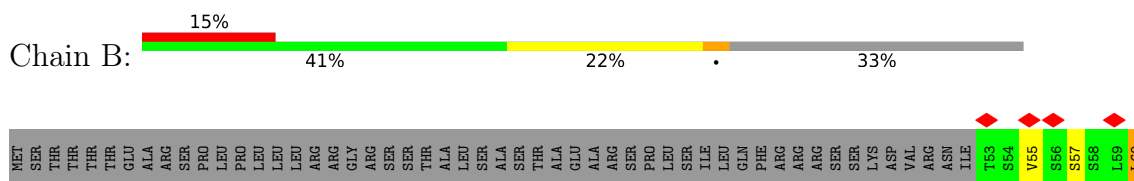
• Molecule 1: Potassium channel AKT1



- Molecule 1: Potassium channel AKT1



- Molecule 1: Potassium channel AKT1



P61	Y147	V233	R359	P440	E506	ASP	ASP	PRO
F66	L148	T234	M362	T441	M507	GLU	LEU	GLN
I67	N149	T237	L363	D442	V508	GLU	ALA	PHE
E68	V150	W238	M366	F443	Q509	VAL	LYS	LYS
D69	T151	H239	Q367	Y444	S510	THR	LEU	GLY
D70	D152	L240	L368	I445	D511	VAL	GLY	GLY
K154	H153	L243	K369	V446	N512	SER	GLY	ALA
S74	L155	C243	T372	V447	D513	ARG	LYS	ALA
K75	R159	L244	A373	V451	V514	HIS	ARG	ARG
P76	Y160	L245	E374	D452	D515	GLU	GLU	GLY
I78	D169	I248	L375	I453	A516	GLY	THR	GLY
V79	L174	R254	R376	I454	K517	ILE	ILE	ILE
D83	P175	V264	Q382	A455	M518	GLU	ALA	GLY
R84	I176	E265	L384	S456	V519	ARG	ALA	ASP
R85	Q177	W273	D383	K457	T520	ARG	GLY	TRP
Y86	Y180	T277	L388	G458	A521	ARG	ALA	SER
R87	K181	M280	R389	V459	N522	GLU	HIS	HIS
E90	T182	Y281	S390	S460	M524	GLY	VAL	PRO
L91	I183	W282	Q394	E461	T525	VAL	GLU	PHE
V97	T184	G185	H395	Q462	W526	PRO	GLN	GLU
S100	G186	V285	L396	V463		LYS	ILE	LYS
E107	D186	T286	F397	L464		ARG	ALA	ASP
L108	G188	L287	R398	A465		ILE	LEU	ALA
A109	R189	T288	S399	K466		ILE	GLU	ARG
F110	A192	T289	E402	L467		GLY	LEU	HIS
E111	F193	V290	E403	G468		GLN	ASN	ASP
K112	R200	M307	L406	P469		ALA	ASP	ASP
A113	L201	F312	F407	G474		PRO	LEU	LEU
E115	W202	N313	K408	E475		ASN	ILE	ILE
L118	R203	I314	G409	I476		LYS	GLN	LYS
L119	L204	Y319	F410	G477		ILE	ASP	GLU
T120	R213	I320	P411	V478		ASP	ASN	ASN
I121	L214	I323	E412	V479		GLY	LEU	ASP
D122	E215	R339	G413	F480		ASP	ASP	VAL
L123	K216	T342	L414	N481		SER	LEU	ASP
V124	D217	N343	L415	I482		ASN	ALA	ALA
D126	A218	D344	V416	Q483		ASP	GLY	GLY
F129	H219	R347	Q417	Q484		ALA	LEU	SER
A130	F220	Y348	L418	F486		ILE	ILE	ALA
V131	N221	T349	V419	T487		ILE	ALA	ALA
F137	F223	R353	I422	V488		PRO	GLN	SER
F138	I225	L354	Q423	R489		THR	VAL	GLY
Y141	R226	T357	E432	T490		VAL	GLY	SER
W144	V227	M358	I433	R491		GLN	ILE	GLY
T145	I228	T357	I434	R492		LEU	GLN	THR
T146	K229	T357	L435	S494		LEU	LEU	TRP
	L230		Q436	Q495		PHE	LEU	HIS
	L231		I436	V496				
	C232		I439	R498				
				H501				
				H502				
				K503				
				F504				
				K505				

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 [i](#)

5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	57
All	All	1788/3365 (53%)	1621 (91%)	165 (9%)	2 (0%)	49	75

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%)	7	22
1	C	392/766 (51%)	354 (90%)	38 (10%)	8	23
1	D	391/766 (51%)	356 (91%)	35 (9%)	9	26
2	B	420/615 (68%)	371 (88%)	49 (12%)	5	15
All	All	1595/2913 (55%)	1434 (90%)	161 (10%)	9	21

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	0.57	0	41,43,59	0.71	2 (4%)
3	POV	C	901	-	38,38,51	1.10	2 (5%)	41,43,59	1.38	5 (12%)
3	POV	D	901	-	38,38,51	0.57	0	41,43,59	0.89	3 (7%)
3	POV	A	901	-	38,38,51	1.35	7 (18%)	41,43,59	1.27	6 (14%)

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	C	901	-	-	19/40/40/55	-
3	POV	D	901	-	-	26/40/40/55	-
3	POV	A	901	-	-	21/40/40/55	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	POV	C313-C312	-3.44	1.34	1.51
3	C	901	POV	O22-C21	-3.10	1.13	1.22
3	A	901	POV	C27-C28	-2.76	1.40	1.52
3	A	901	POV	O22-C21	-2.75	1.14	1.22
3	A	901	POV	C23-C22	-2.46	1.43	1.52
3	A	901	POV	C36-C35	-2.36	1.40	1.51
3	A	901	POV	C22-C21	-2.10	1.44	1.50
3	A	901	POV	C314-C313	-2.08	1.41	1.51
3	C	901	POV	C32-C31	2.01	1.56	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	POV	O21-C21-C22	5.28	122.89	111.48
3	A	901	POV	O11-P-O14	3.49	115.87	106.44
3	D	901	POV	O21-C21-C22	3.35	118.72	111.48
3	A	901	POV	O21-C21-C22	3.28	118.58	111.48
3	A	901	POV	O12-P-O11	-2.79	99.38	106.67
3	C	901	POV	O11-P-O14	2.56	113.37	106.44
3	D	901	POV	O13-P-O14	2.43	120.31	110.83
3	D	901	POV	O13-P-O11	2.32	112.72	106.67
3	C	901	POV	O22-C21-C22	-2.32	114.72	123.78
3	A	901	POV	C3-C2-C1	2.31	117.16	111.78
3	C	901	POV	O12-P-O14	-2.30	101.86	110.83
3	A	901	POV	O13-P-O14	2.25	119.59	110.83
3	C	901	POV	O13-P-O14	2.22	119.48	110.83
3	A	901	POV	C2-O21-C21	2.16	122.97	117.80
3	B	801	POV	O13-P-O14	2.15	119.22	110.83
3	B	801	POV	O12-P-O11	-2.06	101.30	106.67

There are no chirality outliers.

All (87) 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

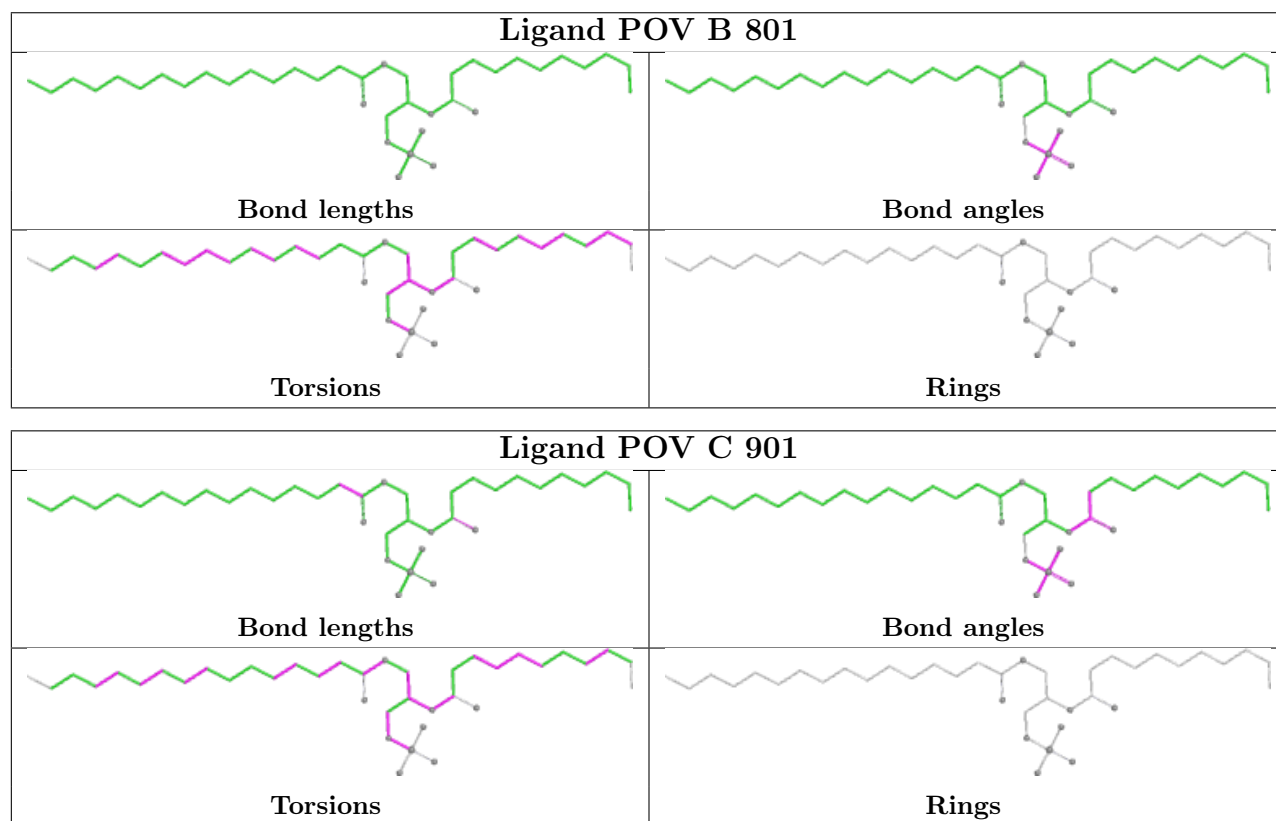
Mol	Chain	Res	Type	Atoms
3	B	801	POV	C311-C310-C39-C38
3	C	901	POV	O22-C21-O21-C2
3	C	901	POV	C24-C25-C26-C27
3	B	801	POV	C37-C38-C39-C310
3	A	901	POV	C1-C2-O21-C21
3	D	901	POV	C310-C311-C312-C313
3	D	901	POV	C311-C312-C313-C314
3	B	801	POV	C24-C25-C26-C27
3	B	801	POV	O21-C2-C3-O31
3	D	901	POV	C37-C38-C39-C310
3	A	901	POV	C34-C35-C36-C37
3	A	901	POV	C310-C311-C312-C313
3	A	901	POV	C2-C1-O11-P
3	B	801	POV	O11-C1-C2-C3
3	D	901	POV	C211-C210-C29-C28
3	B	801	POV	C1-C2-C3-O31
3	D	901	POV	O11-C1-C2-O21
3	A	901	POV	C31-C32-C33-C34
3	D	901	POV	C25-C26-C27-C28
3	C	901	POV	C22-C23-C24-C25
3	C	901	POV	C23-C24-C25-C26
3	A	901	POV	C25-C26-C27-C28
3	D	901	POV	C27-C28-C29-C210
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	A	901	POV	O21-C2-C3-O31
3	D	901	POV	C1-C2-O21-C21
3	C	901	POV	C39-C310-C311-C312
3	B	801	POV	C311-C312-C313-C314
3	C	901	POV	C1-C2-C3-O31
3	C	901	POV	C27-C28-C29-C210
3	B	801	POV	C27-C28-C29-C210
3	A	901	POV	C1-C2-C3-O31
3	A	901	POV	C311-C310-C39-C38
3	D	901	POV	O21-C2-C3-O31

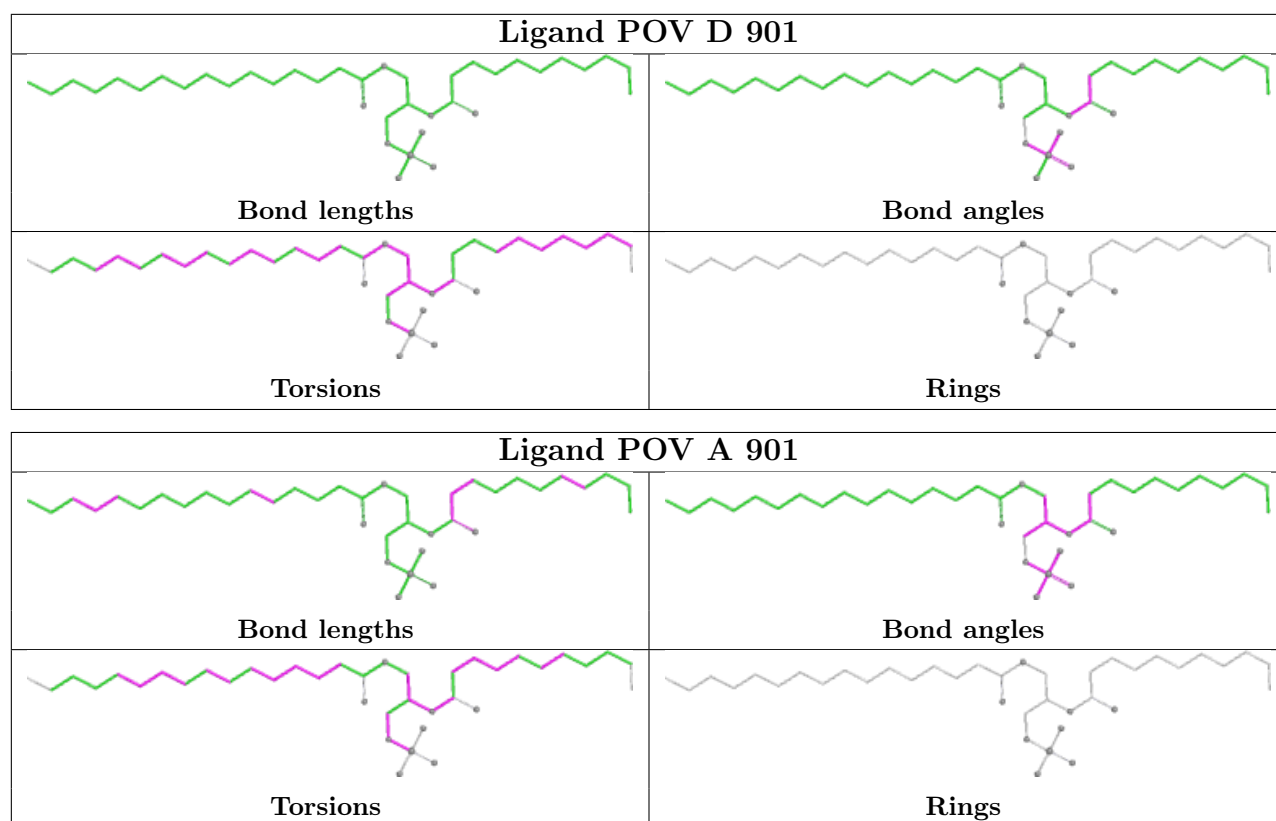
There are no ring outliers.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

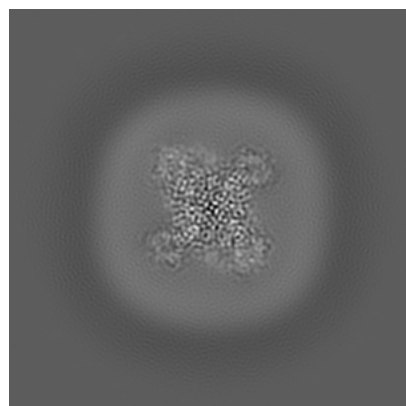
6 Map visualisation [i](#)

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

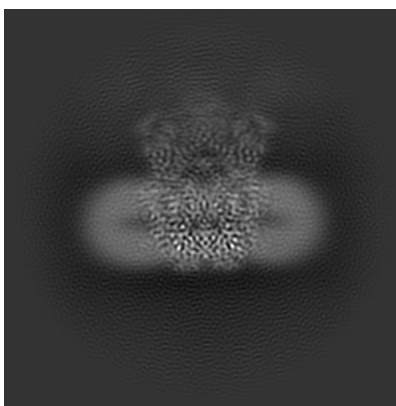
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

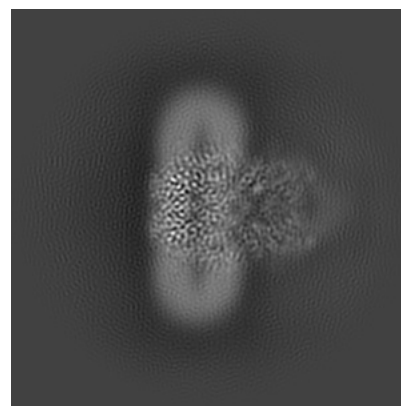
6.1.1 Primary map



X

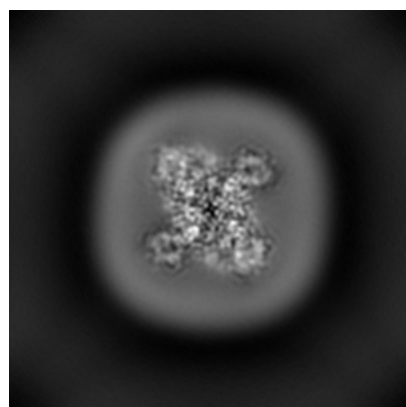


Y

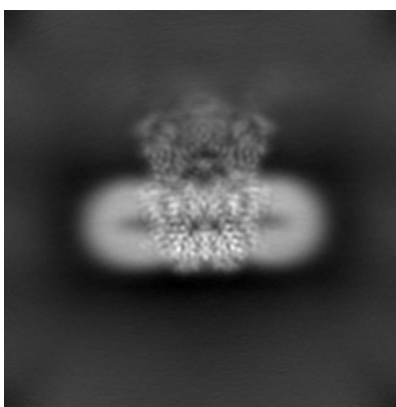


Z

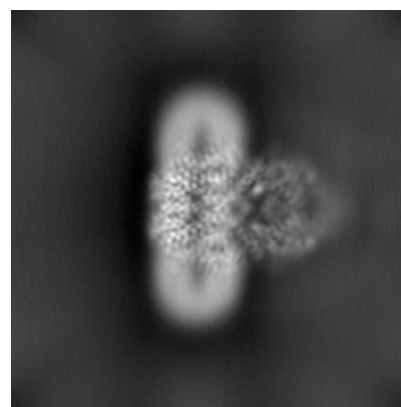
6.1.2 Raw map



X



Y

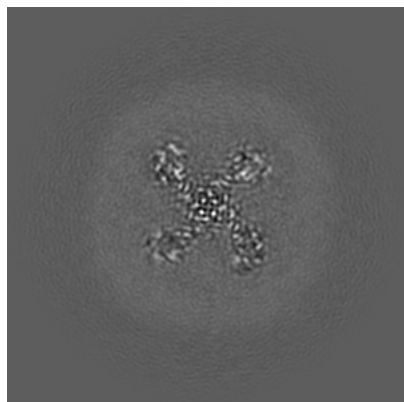


Z

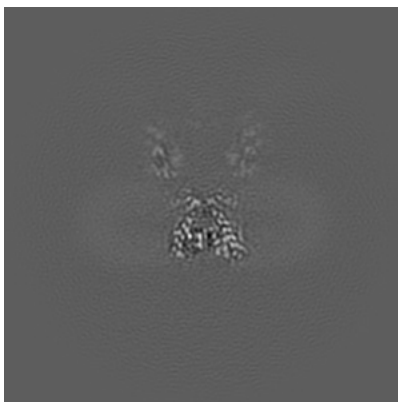
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

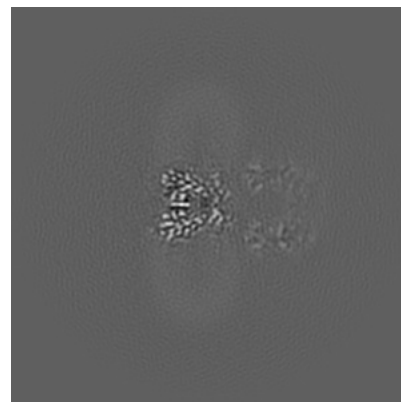
6.2.1 Primary map



X Index: 120

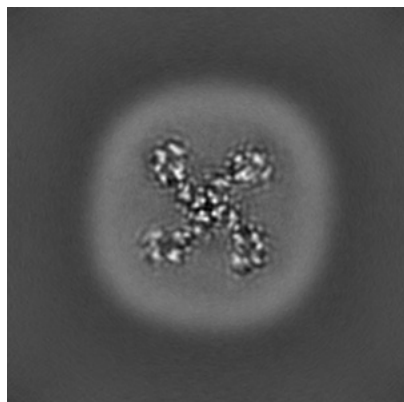


Y Index: 120

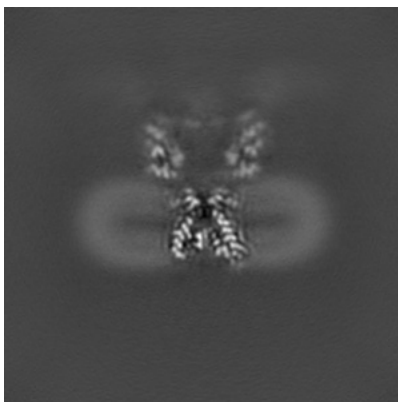


Z Index: 120

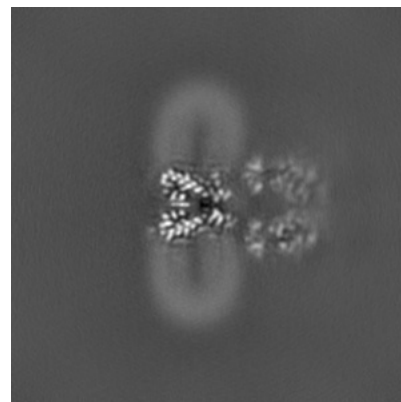
6.2.2 Raw map



X Index: 120



Y Index: 120

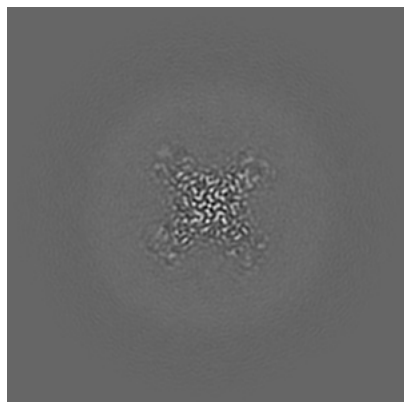


Z Index: 120

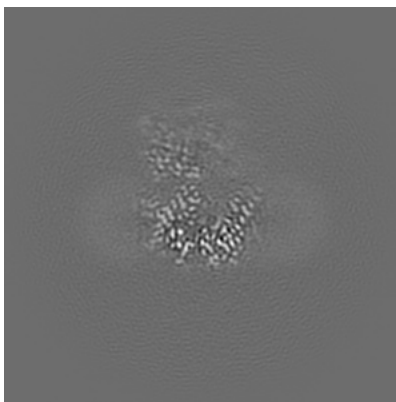
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

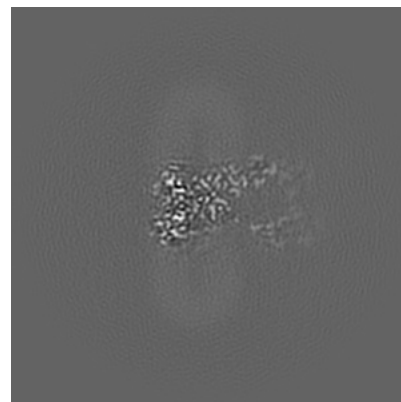
6.3.1 Primary map



X Index: 102

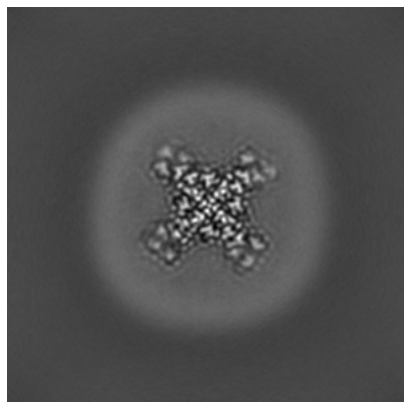


Y Index: 137

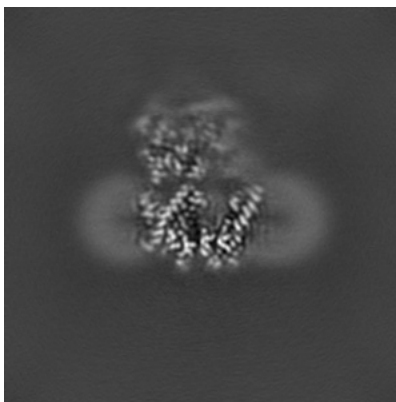


Z Index: 112

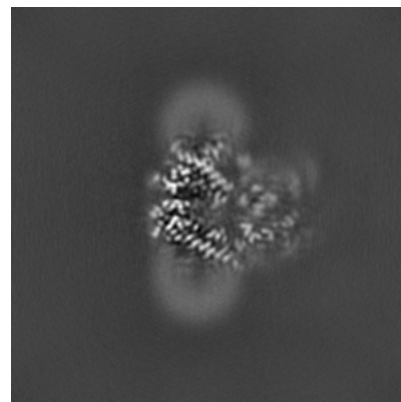
6.3.2 Raw map



X Index: 101



Y Index: 138

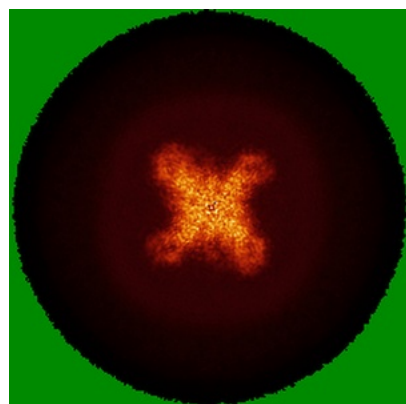


Z Index: 137

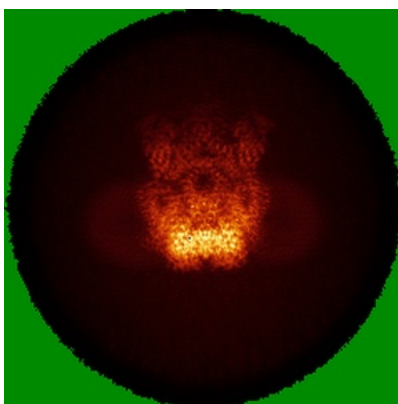
The images above show the largest variance slices of the map in three orthogonal directions.

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

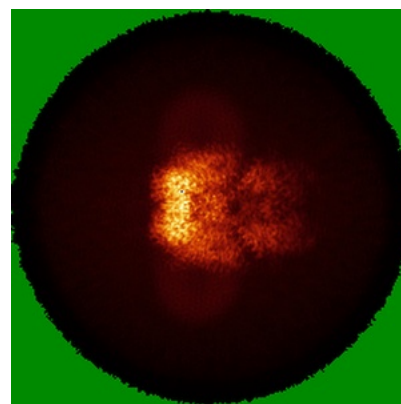
6.4.1 Primary map



X

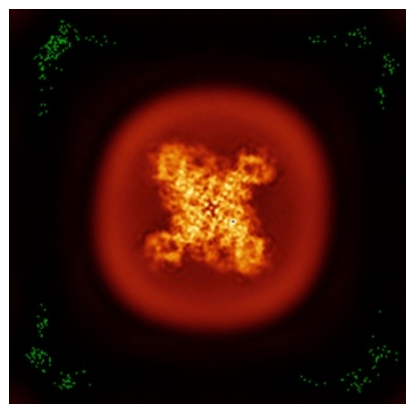


Y

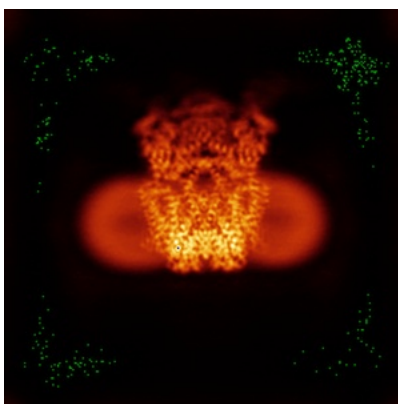


Z

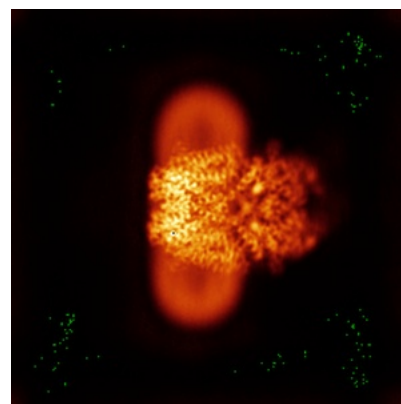
6.4.2 Raw map



X



Y

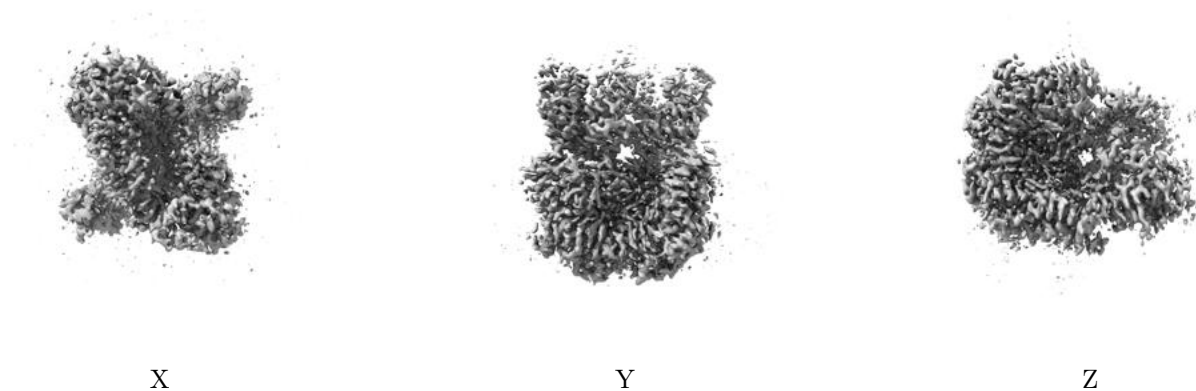


Z

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.

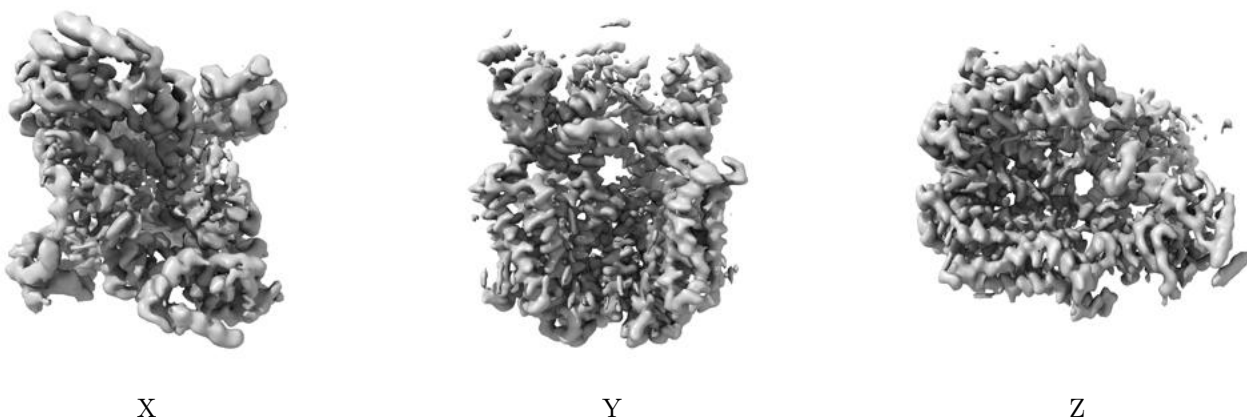
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

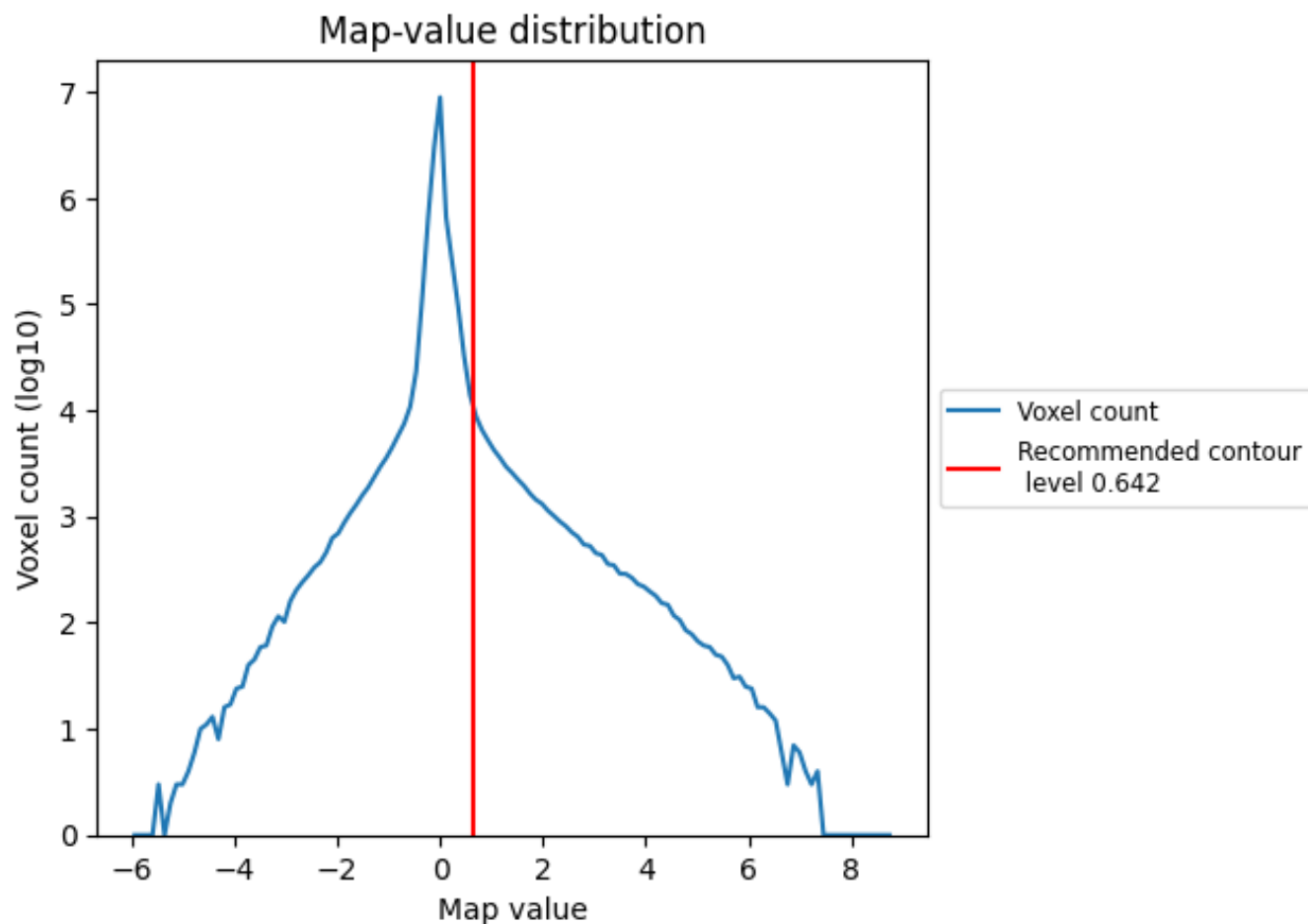
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

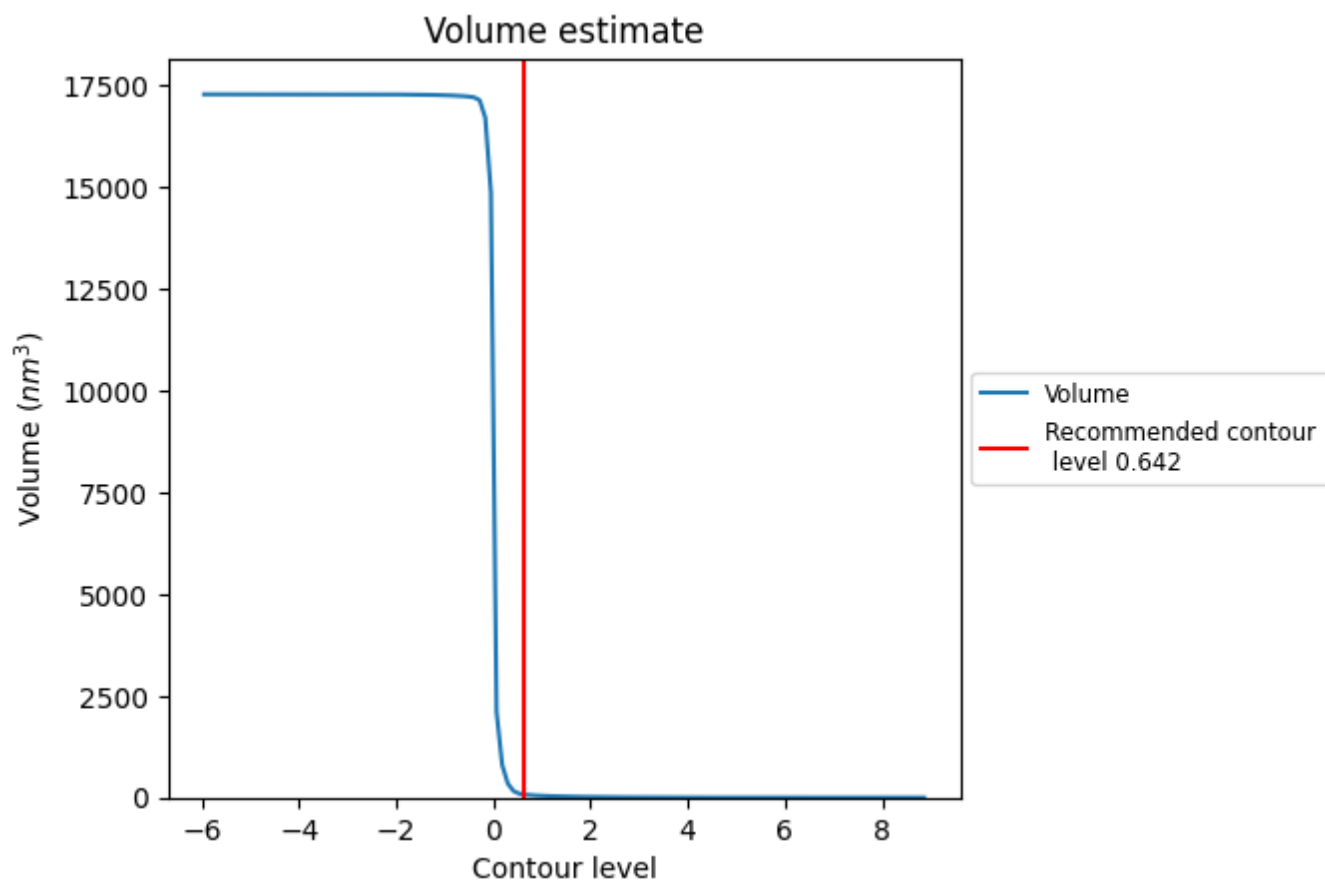
This section contains the results of statistical analysis of the map.

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.

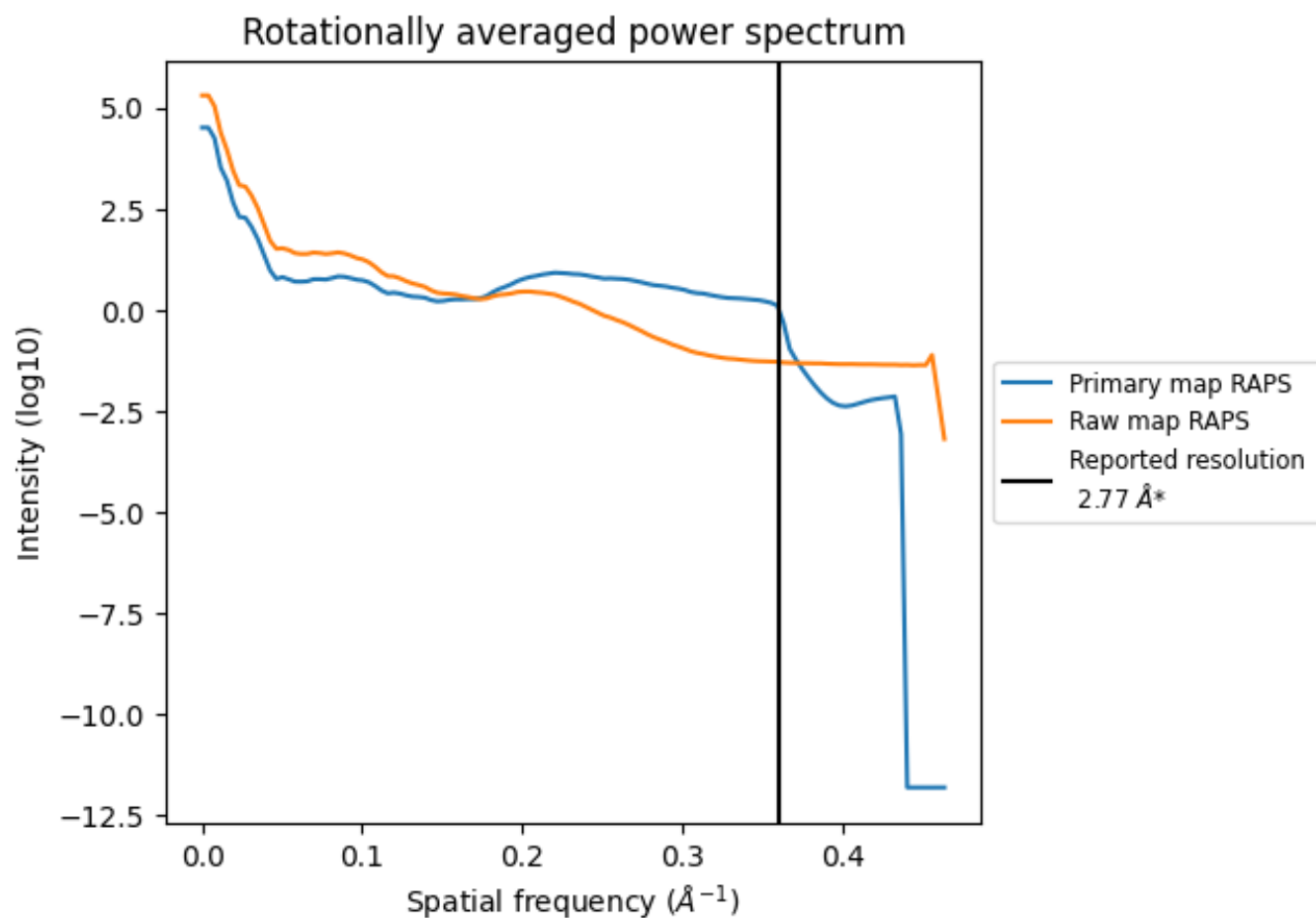
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ

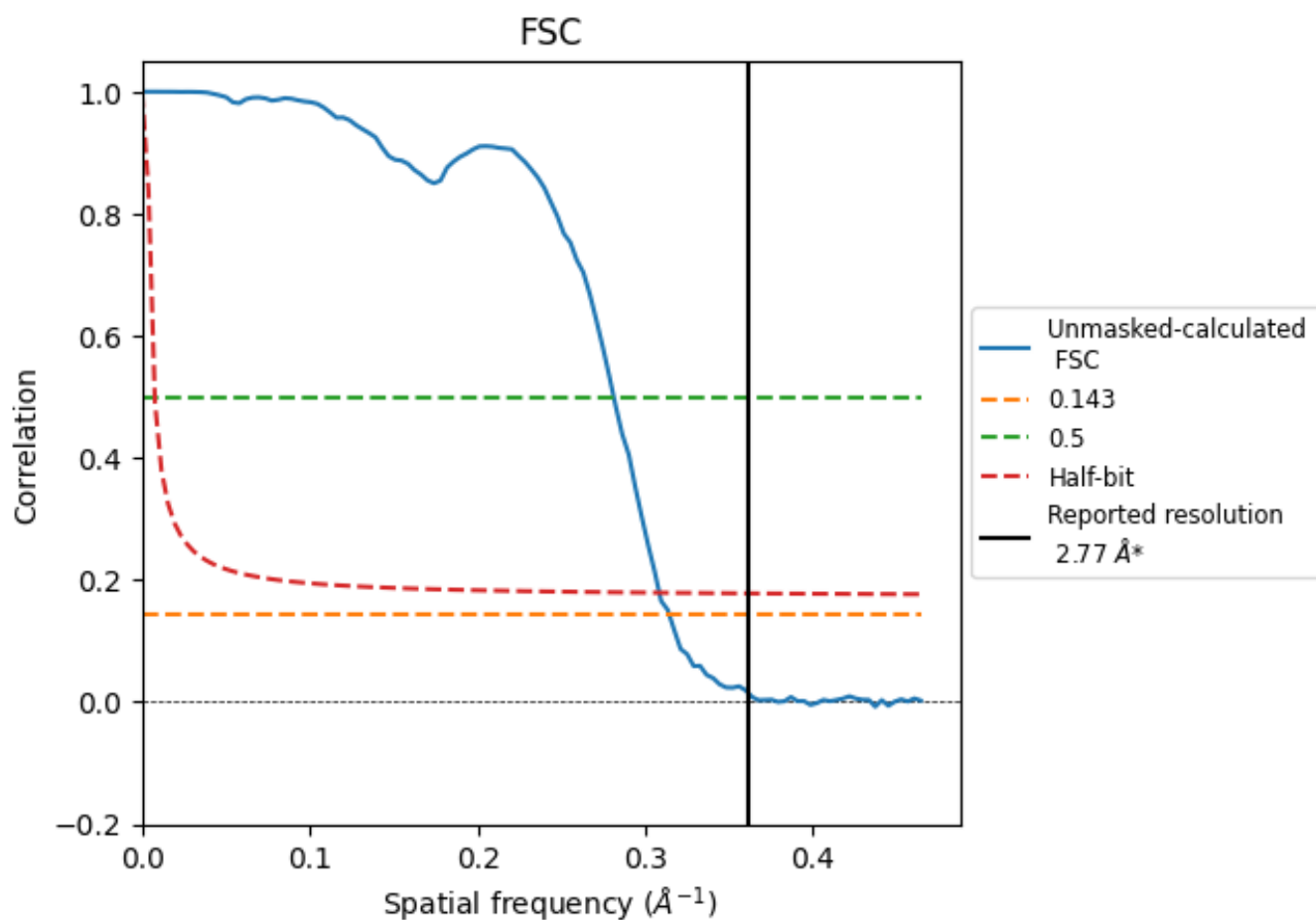


*Reported resolution corresponds to spatial frequency of 0.361 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.361 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

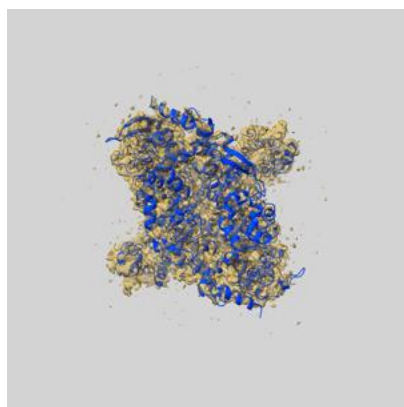
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.56	3.24

*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 %

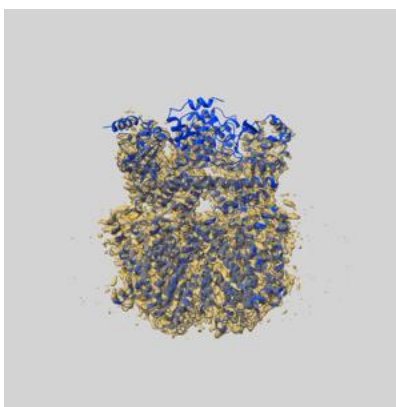
9 Map-model fit [i](#)

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](#).

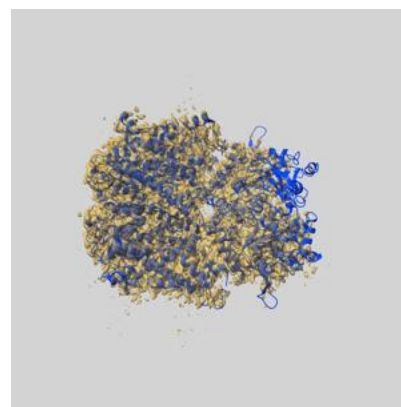
9.1 Map-model overlay [i](#)



X



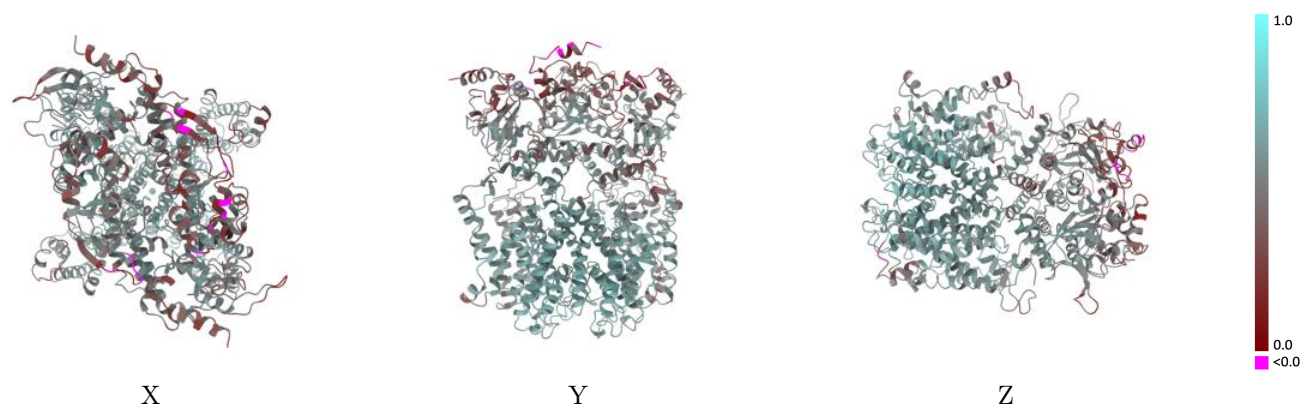
Y



Z

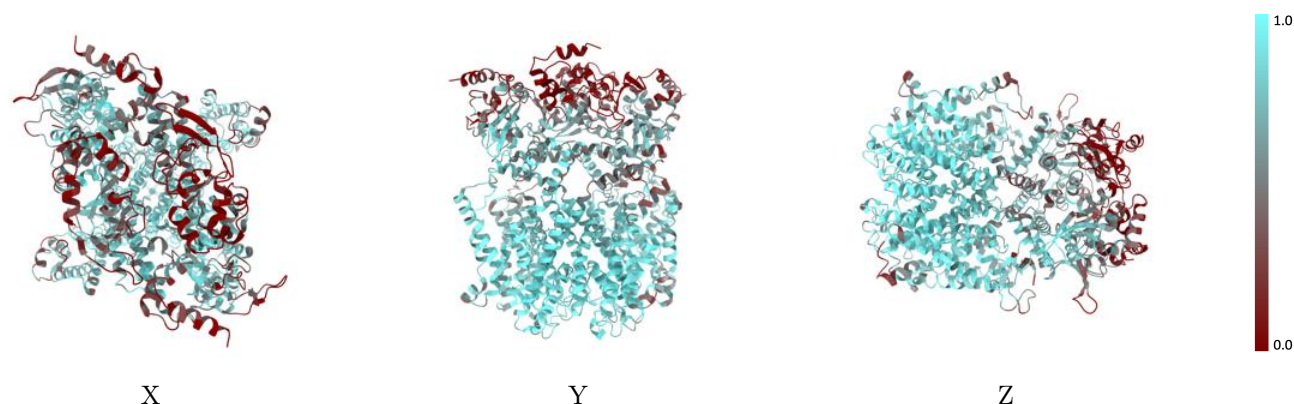
The images above show the 3D surface view of the map at the recommended contour level 0.642 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



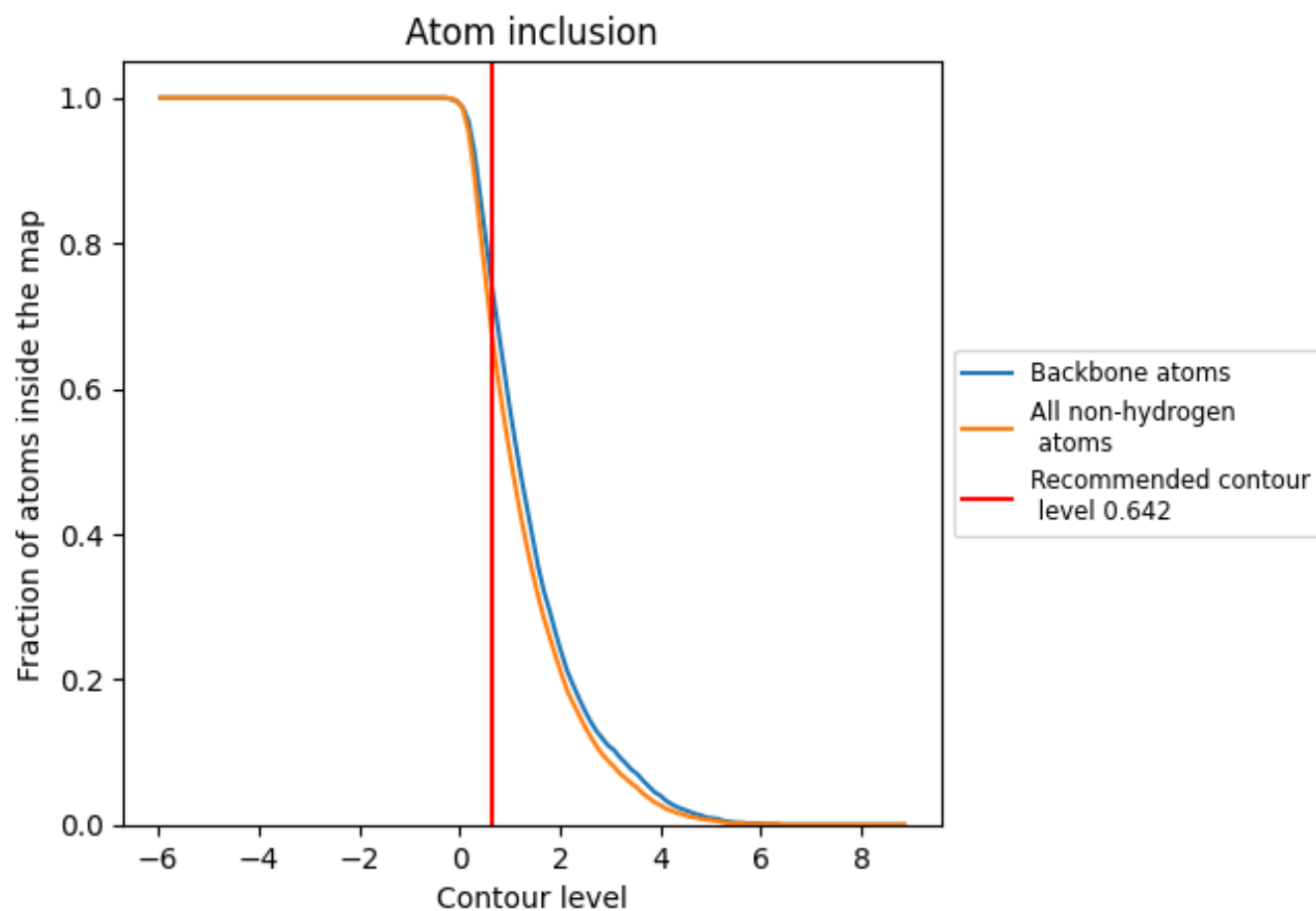
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.642).

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

