Full wwPDB EM Validation Report (i)

Nov 8, 2022 – 08:52 AM EST

PDB ID	:	6DVZ
EMDB ID	:	EMD-8921
Title	:	Cryo-EM structure of mouse TRPV3-Y564A in complex with 2-Aminoethoxy diphenyl borate (2-APB)
Authors	:	Singh, A.K.; McGoldrick, L.L.; Sobolevsky, A.I.
Deposited on	:	2018-06-25
Resolution	:	4.24 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 (i) 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 (i)) were used in the production of this report:

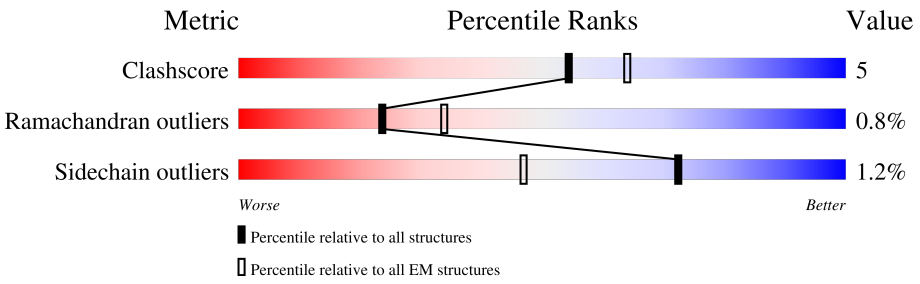
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.24 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	791	44% 67% 14% • 19%
1	B	791	44% 67% 14% • 19%
1	C	791	44% 66% 14% • 19%
1	D	791	44% 67% 14% • 19%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20976 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.

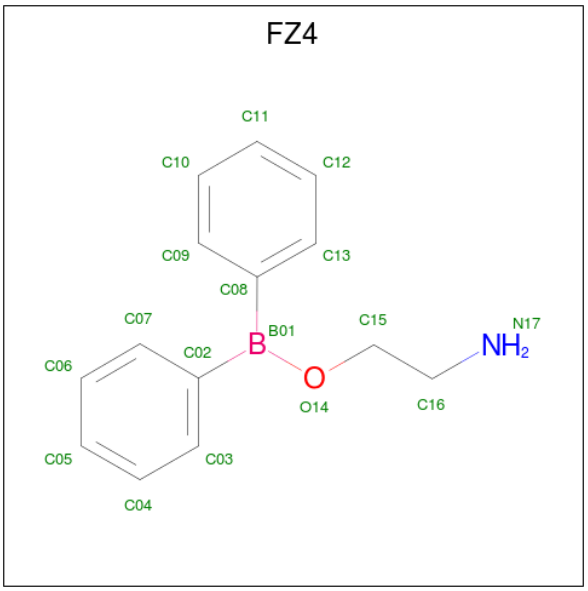
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	643	5193	3372	860	930	31	0	0
1	B	643	5193	3372	860	930	31	0	0
1	C	643	5193	3372	860	930	31	0	0
1	D	643	5193	3372	860	930	31	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8K424
A	2	GLY	-	expression tag	UNP Q8K424
A	564	ALA	TYR	engineered mutation	UNP Q8K424
B	1	MET	-	initiating methionine	UNP Q8K424
B	2	GLY	-	expression tag	UNP Q8K424
B	564	ALA	TYR	engineered mutation	UNP Q8K424
C	1	MET	-	initiating methionine	UNP Q8K424
C	2	GLY	-	expression tag	UNP Q8K424
C	564	ALA	TYR	engineered mutation	UNP Q8K424
D	1	MET	-	initiating methionine	UNP Q8K424
D	2	GLY	-	expression tag	UNP Q8K424
D	564	ALA	TYR	engineered mutation	UNP Q8K424

- Molecule 2 is 2-aminoethyl diphenylborinate (three-letter code: FZ4) (formula: $C_{14}H_{16}BNO$).



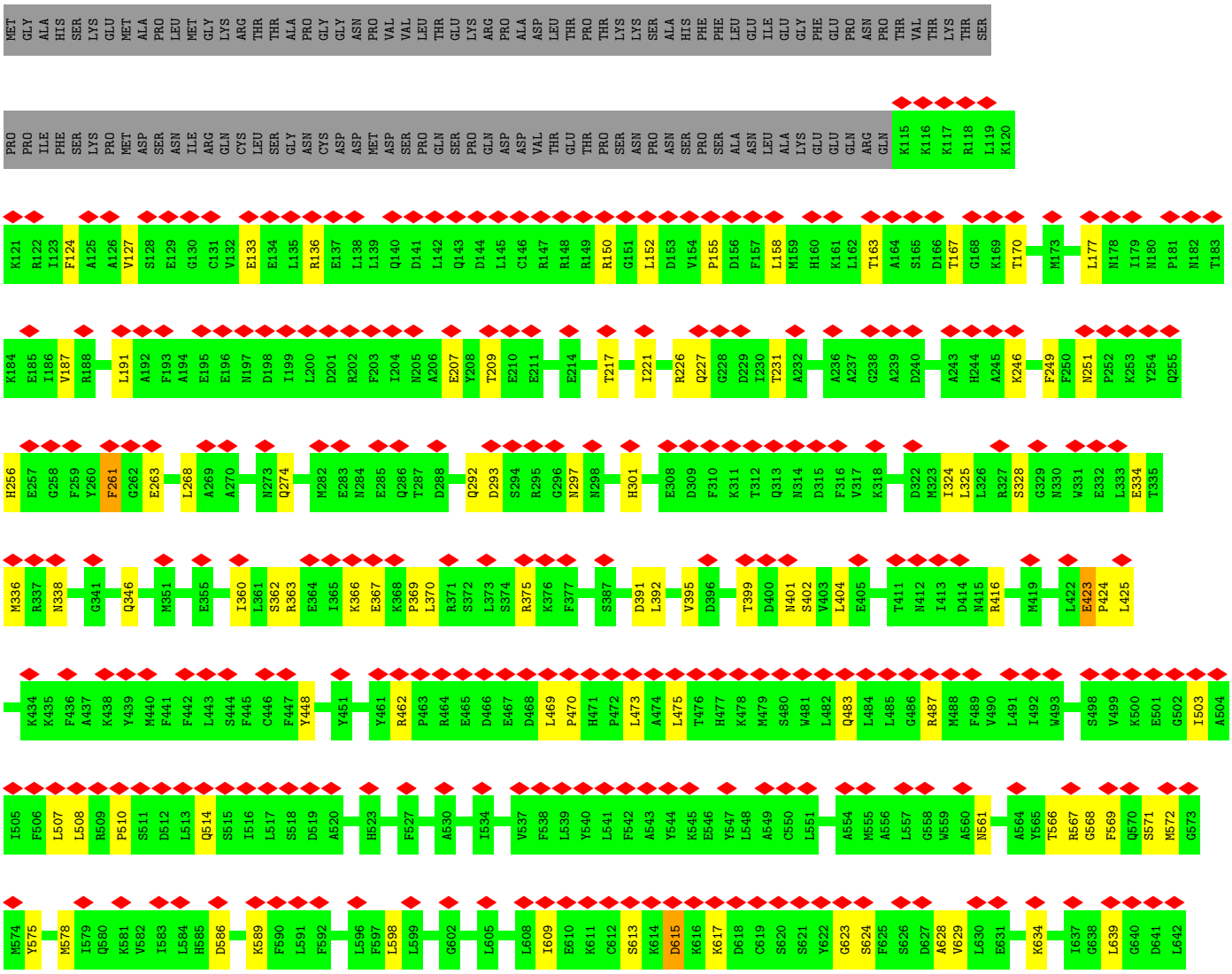
Mol	Chain	Residues	Atoms					AltConf
			Total	B	C	N	O	
2	A	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	A	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	A	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	B	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	B	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	B	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	C	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	C	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	C	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	D	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	D	1	51	3	42	3	3	0
			Total	B	C	N	O	
2	D	1	51	3	42	3	3	0

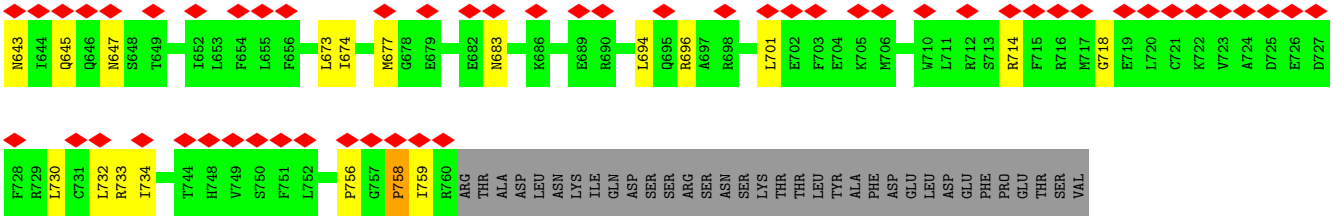
3 Residue-property plots (i)

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: Transient receptor potential cation channel subfamily V member 3

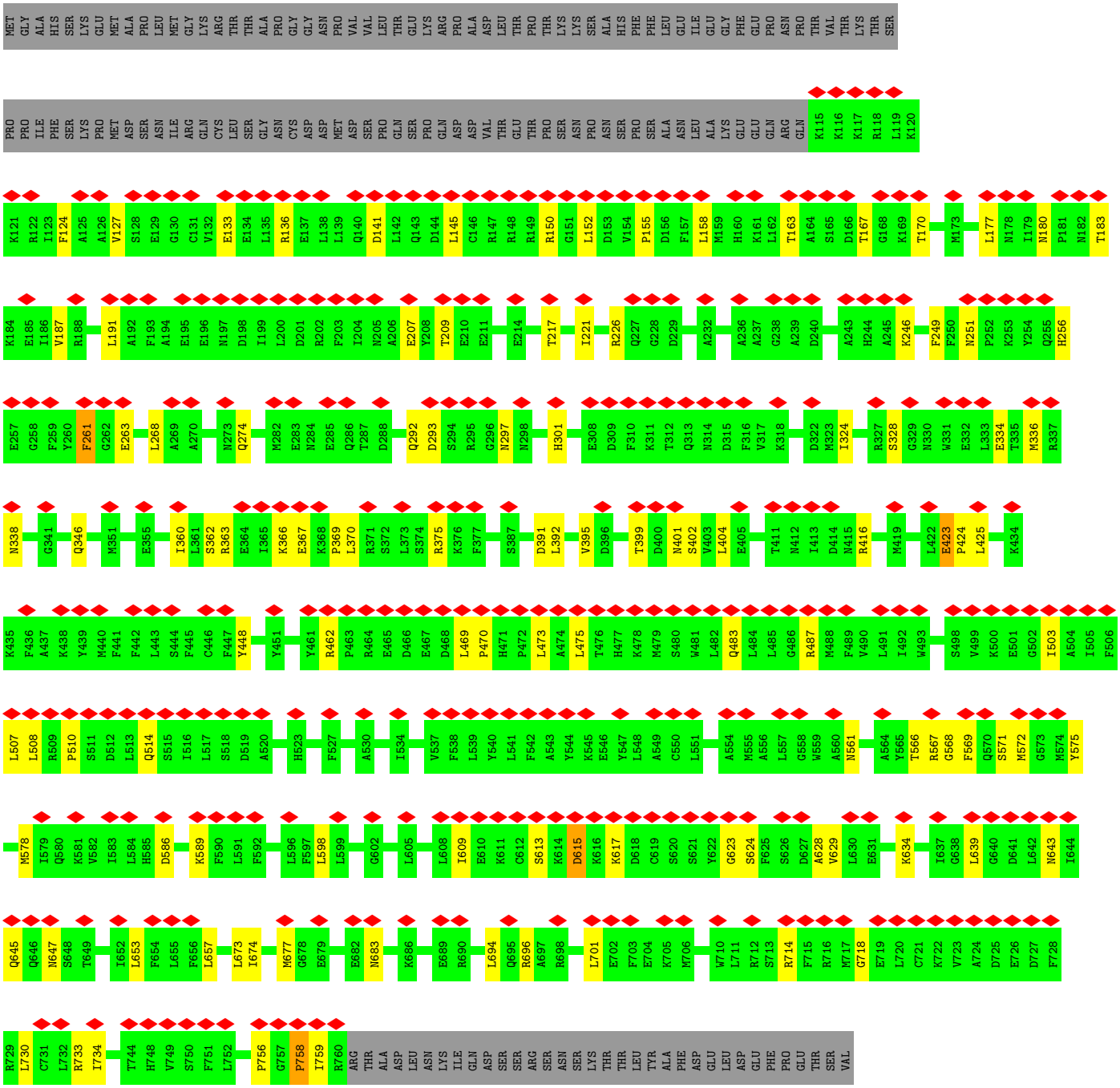
Chain A:





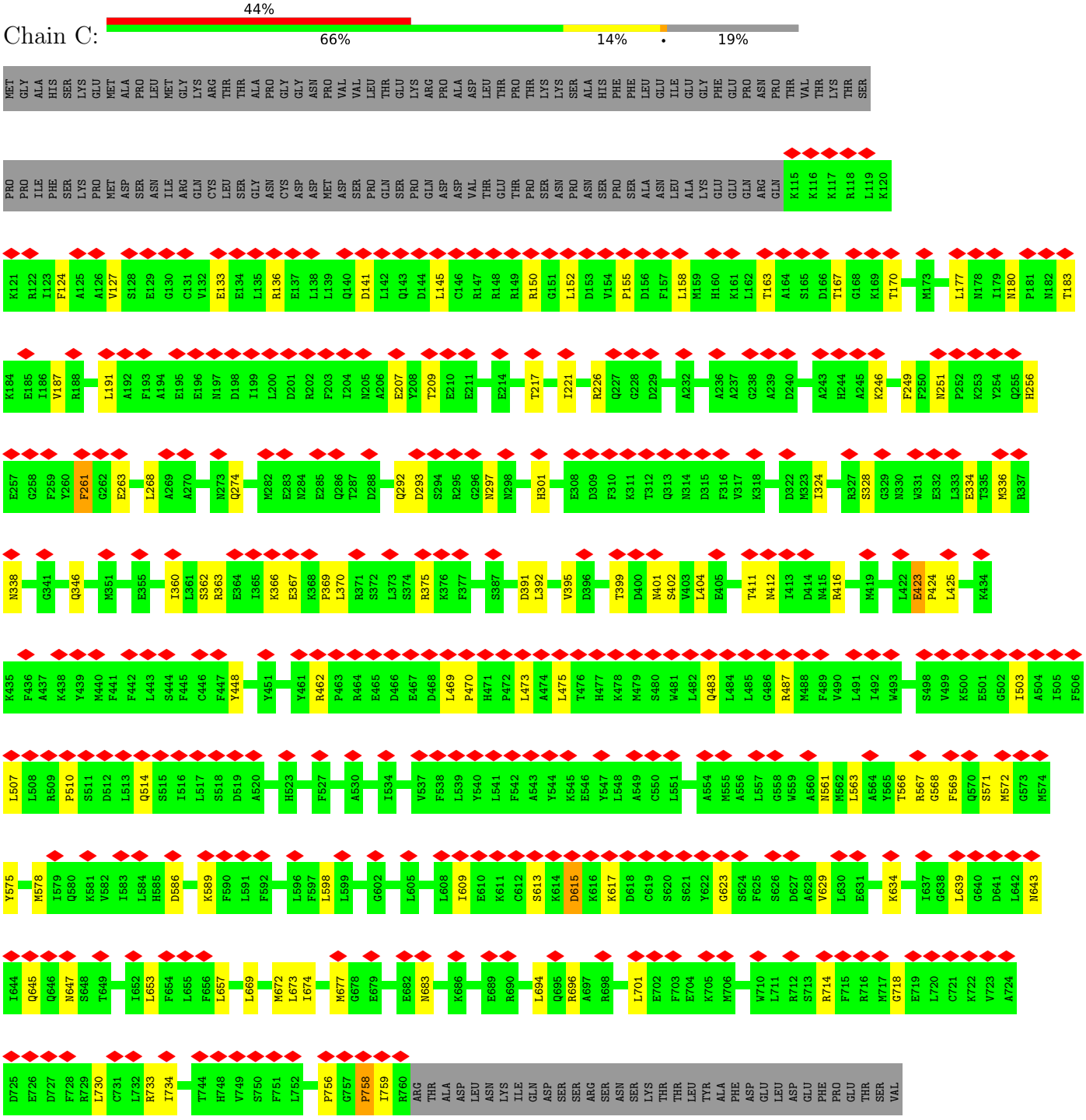
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain B:



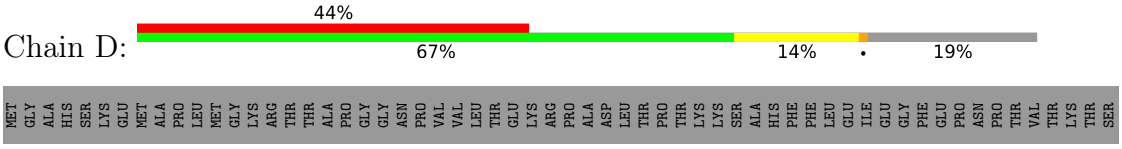
• Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 3

Chain D:



PRO PRO ILE PHE SER LYS PRO MET ASP SER ASN ILE ARG GLN CYS LEU SER GLY ASN CYS ASP ASP MET ASP SER PRO GLN SER PRO GLN ASP ASP VAL THR GLU THR PRO SER ASN PRO ASN SER PRO SER ALA ASN LEU ALA LYS GLU GLU GLN ARG GLN K115 K116 K117 R118 L119 K120

K121 R122 I123 F124 A125 A126 V127 S128 E129 G130 C131 V132 E133 E134 L135 R136 E137 L138 L139 Q140 D141 L142 Q143 D144 L145 C146 R147 R148 R149 R150 G151 L152 D153 V154 P155 D156 F157 L158 M159 H160 K161 L162 T163 A164 S165 D166 T167 G168 K169 T170 M173 L177 N178 T179 N180 P181 N182 T183

K184 E185 I186 V187 R188 L191 A192 F193 A194 E195 E196 N197 D198 I199 L200 D201 R202 F203 I204 N205 A206 E207 Y208 T209 E210 E211 E214 T217 A218 L219 N220 I221 R226 Q227 G228 D229 A232 A236 A237 G238 A239 D240 A243 H244 A245 K246 F249 F250 N251 P252 K253 Y254

Q255 H256 E257 G258 F259 Y260 F261 G262 E263 L268 A269 A270 N273 Q274 M282 E283 N284 E285 Q286 T287 D288 Q292 D293 S294 R295 G296 N297 N298 H301 E308 D309 F310 K311 T312 Q313 N314 D315 F316 V317 K318 D322 M323 I324 L325 L326 R327 S328 G329 N330 W331 E332 L333 E334

T335 M336 R337 N338 G341 Q346 M351 E355 I360 L361 S362 R363 E364 I365 K366 E367 K368 P369 L370 R371 S372 L373 S374 R375 K376 F377 S387 D391 L392 V395 D396 T399 D400 N401 S402 V403 L404 E405 T411 N412 I413 D414 N415 R416 M419 L422 E423 P424

L425 K434 K435 F436 A437 K438 Y439 M440 F441 F442 L443 S444 F445 C446 F447 Y448 Y451 Y461 R462 P463 R464 E465 D466 E467 D468 L469 P470 H471 P472 L473 A474 L475 T476 H477 K478 M479 S480 W481 L482 Q483 L484 L485 G486 R487 M488 F489 V490 L491 I492 W493 S498 V499 K500 E501 G502 I503

A504 I505 F506 L507 L508 R509 P510 S511 D512 L513 Q514 S515 I516 L517 S518 D519 A520 H523 F527 A530 I534 V537 F538 L539 Y540 L541 F542 A543 Y544 K545 E546 Y547 L548 A549 C550 L551 A554 M555 A556 L557 G558 W559 A560 N561 A564 Y565 T566 R567 G568 F569 Q570 S571 M572

G573 M574 Y575 M578 I579 Q580 K581 V582 I583 L584 H585 D586 K589 F590 L591 F592 L596 F597 L598 L599 G602 L605 L608 I609 E610 K611 C612 S613 K614 D615 K616 K617 D618 C619 S620 S621 Y622 G623 S624 F625 S626 D627 A628 V629 L630 E631 K634 I637 G638 L639 G640 D641

L642 N643 I644 Q645 Q646 N647 S648 T649 I652 L653 F654 L655 F656 L657 L669 M672 L673 I674 M677 G678 E679 E682 N683 K686 E689 R690 L694 Q695 R696 A697 R698 L701 E702 F703 E704 K705 M706 W710 L711 R712 S713 R714 F715 R716 M717 G718 E719 L720 C721 K722

V723 A724 D725 E726 D727 F728 R729 L730 C731 L732 R733 I734 T744 H748 V749 S750 F751 L752 P756 G757 P758 I759 R760 ARG THR ALA ASP LEU ASN LYS ILE GLN ASP SER SER ARG SER ASN SER LYS THR THR LEU TYR ALA PHE ASP GLU LEU ASP GLU PHE PRO GLU THR SER VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28075	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 ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.139	Depositor
Minimum map value	-0.084	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.057	Depositor
Map size (Å)	233.19998, 233.19998, 233.19998	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: FZ4

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	0/5301	0.67	4/7171 (0.1%)
1	B	0.43	0/5301	0.67	4/7171 (0.1%)
1	C	0.43	0/5301	0.67	4/7171 (0.1%)
1	D	0.43	0/5301	0.67	4/7171 (0.1%)
All	All	0.43	0/21204	0.67	16/28684 (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	A	0	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	615	ASP	CB-CG-OD1	6.67	124.31	118.30
1	D	615	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	615	ASP	CB-CG-OD1	6.63	124.27	118.30
1	C	615	ASP	CB-CG-OD1	6.63	124.27	118.30
1	C	758	PRO	N-CA-CB	6.59	111.21	103.30
1	A	758	PRO	N-CA-CB	6.58	111.20	103.30
1	D	758	PRO	N-CA-CB	6.58	111.20	103.30
1	B	758	PRO	N-CA-CB	6.56	111.17	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	756	PRO	N-CA-CB	6.23	110.78	103.30
1	A	756	PRO	N-CA-CB	6.20	110.74	103.30
1	B	756	PRO	N-CA-CB	6.20	110.74	103.30
1	C	756	PRO	N-CA-CB	6.20	110.74	103.30
1	C	152	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	152	LEU	CA-CB-CG	5.84	128.74	115.30
1	D	152	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	152	LEU	CA-CB-CG	5.83	128.70	115.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	PHE	Peptide
1	A	261	PHE	Peptide
1	A	423	GLU	Peptide
1	A	469	LEU	Peptide
1	A	733	ARG	Peptide
1	B	249	PHE	Peptide
1	B	261	PHE	Peptide
1	B	423	GLU	Peptide
1	B	469	LEU	Peptide
1	B	733	ARG	Peptide
1	C	249	PHE	Peptide
1	C	261	PHE	Peptide
1	C	423	GLU	Peptide
1	C	469	LEU	Peptide
1	C	733	ARG	Peptide
1	D	249	PHE	Peptide
1	D	261	PHE	Peptide
1	D	423	GLU	Peptide
1	D	469	LEU	Peptide
1	D	733	ARG	Peptide

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	5193	0	5243	57	0
1	B	5193	0	5243	56	0
1	C	5193	0	5243	58	0
1	D	5193	0	5243	57	0
2	A	51	0	0	1	0
2	B	51	0	0	1	0
2	C	51	0	0	1	0
2	D	51	0	0	1	0
All	All	20976	0	20972	228	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 5.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:GLY:HA2	1:A:730:LEU:HB2	1.78	0.66
1:D:718:GLY:HA2	1:D:730:LEU:HB2	1.78	0.66
1:B:718:GLY:HA2	1:B:730:LEU:HB2	1.78	0.65
1:C:718:GLY:HA2	1:C:730:LEU:HB2	1.78	0.64
1:A:483:GLN:HG3	1:A:487:ARG:HH11	1.63	0.63
1:D:483:GLN:HG3	1:D:487:ARG:HH11	1.63	0.62
1:C:483:GLN:HG3	1:C:487:ARG:HH11	1.63	0.62
1:B:483:GLN:HG3	1:B:487:ARG:HH11	1.63	0.62
1:A:367:GLU:HB3	1:A:370:LEU:HB2	1.82	0.61
1:B:367:GLU:HG3	1:B:369:PRO:HD2	1.83	0.61
1:B:367:GLU:HB3	1:B:370:LEU:HB2	1.82	0.61
1:A:367:GLU:HG3	1:A:369:PRO:HD2	1.83	0.60
1:C:367:GLU:HG3	1:C:369:PRO:HD2	1.83	0.60
1:D:367:GLU:HB3	1:D:370:LEU:HB2	1.82	0.60
1:C:367:GLU:HB3	1:C:370:LEU:HB2	1.82	0.59
1:C:510:PRO:O	1:C:514:GLN:NE2	2.36	0.59
1:D:367:GLU:HG3	1:D:369:PRO:HD2	1.83	0.59
1:A:510:PRO:O	1:A:514:GLN:NE2	2.35	0.59
1:D:163:THR:HG22	1:D:170:THR:HA	1.84	0.59
1:B:510:PRO:O	1:B:514:GLN:NE2	2.36	0.59
1:D:510:PRO:O	1:D:514:GLN:NE2	2.35	0.58
1:A:163:THR:HG22	1:A:170:THR:HA	1.84	0.58
1:C:163:THR:HG22	1:C:170:THR:HA	1.85	0.58
1:A:346:GLN:NE2	1:A:401:ASN:O	2.37	0.58
1:D:346:GLN:NE2	1:D:401:ASN:O	2.37	0.58
1:C:251:ASN:ND2	1:C:256:HIS:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:GLN:NE2	1:C:401:ASN:O	2.37	0.58
1:B:251:ASN:ND2	1:B:256:HIS:O	2.37	0.57
1:B:163:THR:HG22	1:B:170:THR:HA	1.84	0.57
1:B:346:GLN:NE2	1:B:401:ASN:O	2.37	0.57
1:A:251:ASN:ND2	1:A:256:HIS:O	2.37	0.57
2:D:801:FZ4:C03	2:D:801:FZ4:C08	2.83	0.57
1:D:251:ASN:ND2	1:D:256:HIS:O	2.37	0.56
1:A:448:TYR:OH	1:A:561:ASN:ND2	2.39	0.56
2:A:801:FZ4:C03	2:A:801:FZ4:C08	2.83	0.56
2:B:801:FZ4:C03	2:B:801:FZ4:C08	2.83	0.56
1:C:334:GLU:OE2	1:C:363:ARG:NH1	2.39	0.55
1:D:448:TYR:OH	1:D:561:ASN:ND2	2.39	0.55
1:C:448:TYR:OH	1:C:561:ASN:ND2	2.39	0.55
1:A:334:GLU:OE2	1:A:363:ARG:NH1	2.39	0.55
1:B:334:GLU:OE2	1:B:363:ARG:NH1	2.39	0.55
1:B:416:ARG:HD2	1:B:694:LEU:HD21	1.89	0.54
1:B:448:TYR:OH	1:B:561:ASN:ND2	2.39	0.54
1:D:334:GLU:OE2	1:D:363:ARG:NH1	2.39	0.54
1:A:416:ARG:HD2	1:A:694:LEU:HD21	1.89	0.54
1:A:674:ILE:HA	1:A:677:MET:HB3	1.90	0.54
2:C:801:FZ4:C03	2:C:801:FZ4:C08	2.83	0.54
1:C:416:ARG:HD2	1:C:694:LEU:HD21	1.89	0.54
1:D:674:ILE:HA	1:D:677:MET:HB3	1.90	0.54
1:C:674:ILE:HA	1:C:677:MET:HB3	1.90	0.54
1:B:674:ILE:HA	1:B:677:MET:HB3	1.90	0.53
1:C:261:PHE:HB2	1:C:263:GLU:H	1.73	0.53
1:D:416:ARG:HD2	1:D:694:LEU:HD21	1.89	0.53
1:D:261:PHE:HB2	1:D:263:GLU:H	1.73	0.53
1:B:392:LEU:HD12	1:B:395:VAL:HB	1.91	0.53
1:B:261:PHE:HB2	1:B:263:GLU:H	1.73	0.53
1:C:392:LEU:HD12	1:C:395:VAL:HB	1.91	0.53
1:D:292:GLN:NE2	1:D:336:MET:SD	2.76	0.53
1:D:226:ARG:HG2	1:D:274:GLN:HE21	1.74	0.52
1:A:261:PHE:HB2	1:A:263:GLU:H	1.73	0.52
1:B:292:GLN:NE2	1:B:336:MET:SD	2.76	0.52
1:B:375:ARG:NH1	1:B:391:ASP:OD2	2.43	0.52
1:C:375:ARG:NH1	1:C:391:ASP:OD2	2.43	0.52
1:D:392:LEU:HD12	1:D:395:VAL:HB	1.91	0.52
1:A:167:THR:O	1:A:209:THR:OG1	2.27	0.52
1:A:226:ARG:HG2	1:A:274:GLN:HE21	1.74	0.52
1:B:226:ARG:HG2	1:B:274:GLN:HE21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:643:ASN:HA	1:D:645:GLN:HE22	1.75	0.52
1:A:392:LEU:HD12	1:A:395:VAL:HB	1.91	0.52
1:B:643:ASN:HA	1:B:645:GLN:HE22	1.75	0.51
1:C:643:ASN:HA	1:C:645:GLN:HE22	1.75	0.51
1:D:167:THR:O	1:D:209:THR:OG1	2.27	0.51
1:D:360:ILE:O	1:D:363:ARG:NH2	2.44	0.51
1:A:360:ILE:O	1:A:363:ARG:NH2	2.44	0.51
1:A:643:ASN:HA	1:A:645:GLN:HE22	1.75	0.51
1:C:226:ARG:HG2	1:C:274:GLN:HE21	1.74	0.51
1:C:292:GLN:NE2	1:C:336:MET:SD	2.76	0.51
1:D:375:ARG:NH1	1:D:391:ASP:OD2	2.43	0.51
1:A:292:GLN:NE2	1:A:336:MET:SD	2.76	0.51
1:B:598:LEU:HD11	1:B:629:VAL:HG13	1.93	0.51
1:C:360:ILE:O	1:C:363:ARG:NH2	2.44	0.51
1:C:598:LEU:HD11	1:C:629:VAL:HG13	1.93	0.51
1:A:375:ARG:NH1	1:A:391:ASP:OD2	2.43	0.50
1:B:360:ILE:O	1:B:363:ARG:NH2	2.44	0.50
1:B:167:THR:O	1:B:209:THR:OG1	2.27	0.50
1:D:598:LEU:HD11	1:D:629:VAL:HG13	1.93	0.50
1:A:598:LEU:HD11	1:A:629:VAL:HG13	1.93	0.50
1:C:167:THR:O	1:C:209:THR:OG1	2.27	0.49
1:D:133:GLU:OE2	1:D:136:ARG:NH2	2.46	0.49
1:B:399:THR:O	1:B:402:SER:OG	2.30	0.48
1:D:423:GLU:O	1:D:425:LEU:N	2.46	0.48
1:B:423:GLU:O	1:B:425:LEU:N	2.46	0.48
1:D:293:ASP:HB3	1:D:297:ASN:H	1.79	0.48
1:A:133:GLU:OE2	1:A:136:ARG:NH2	2.46	0.48
1:B:609:ILE:HD13	1:B:623:GLY:HA2	1.96	0.48
1:C:133:GLU:OE2	1:C:136:ARG:NH2	2.46	0.48
1:C:423:GLU:O	1:C:425:LEU:N	2.46	0.48
1:B:293:ASP:HB3	1:B:297:ASN:H	1.79	0.48
1:A:423:GLU:O	1:A:425:LEU:N	2.46	0.48
1:C:293:ASP:HB3	1:C:297:ASN:H	1.78	0.48
1:B:133:GLU:OE2	1:B:136:ARG:NH2	2.46	0.48
1:C:609:ILE:HD13	1:C:623:GLY:HA2	1.96	0.48
1:C:399:THR:O	1:C:402:SER:OG	2.30	0.48
1:A:293:ASP:HB3	1:A:297:ASN:H	1.78	0.47
1:C:367:GLU:HG2	1:C:370:LEU:HD12	1.96	0.47
1:D:367:GLU:HG2	1:D:370:LEU:HD12	1.96	0.47
1:D:609:ILE:HD13	1:D:623:GLY:HA2	1.96	0.47
1:C:613:SER:HB3	1:C:617:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:VAL:O	1:B:191:LEU:N	2.42	0.47
1:B:367:GLU:HG2	1:B:370:LEU:HD12	1.96	0.47
1:D:187:VAL:O	1:D:191:LEU:N	2.42	0.47
1:D:613:SER:HB3	1:D:617:LYS:HA	1.97	0.47
1:A:613:SER:HB3	1:A:617:LYS:HA	1.97	0.47
1:B:613:SER:HB3	1:B:617:LYS:HA	1.97	0.47
1:A:367:GLU:HG2	1:A:370:LEU:HD12	1.96	0.46
1:A:568:GLY:O	1:A:696:ARG:NH2	2.49	0.46
1:A:609:ILE:HD13	1:A:623:GLY:HA2	1.96	0.46
1:C:568:GLY:O	1:C:696:ARG:NH2	2.49	0.46
1:B:566:THR:HB	1:B:572:MET:HB3	1.97	0.46
1:A:566:THR:HB	1:A:572:MET:HB3	1.97	0.46
1:B:568:GLY:O	1:B:696:ARG:NH2	2.49	0.46
1:C:207:GLU:HB3	1:C:217:THR:HG22	1.98	0.46
1:D:207:GLU:HB3	1:D:217:THR:HG22	1.98	0.46
1:D:566:THR:HB	1:D:572:MET:HB3	1.97	0.46
1:D:568:GLY:O	1:D:696:ARG:NH2	2.49	0.46
1:A:187:VAL:O	1:A:191:LEU:N	2.42	0.45
1:C:566:THR:HB	1:C:572:MET:HB3	1.97	0.45
1:A:634:LYS:HB3	1:A:639:LEU:HB2	1.97	0.45
1:B:207:GLU:HB3	1:B:217:THR:HG22	1.98	0.45
1:B:567:ARG:O	1:B:569:PHE:N	2.50	0.45
1:C:634:LYS:HB3	1:C:639:LEU:HB2	1.97	0.45
1:D:634:LYS:HB3	1:D:639:LEU:HB2	1.97	0.45
1:A:575:TYR:HA	1:A:578:MET:HE2	1.98	0.45
1:B:324:ILE:O	1:B:328:SER:N	2.50	0.45
1:C:653:LEU:O	1:C:657:LEU:N	2.36	0.45
1:D:567:ARG:O	1:D:569:PHE:N	2.50	0.45
1:B:124:PHE:HA	1:B:127:VAL:HB	1.98	0.45
1:B:634:LYS:HB3	1:B:639:LEU:HB2	1.97	0.45
1:D:324:ILE:O	1:D:328:SER:N	2.50	0.45
1:A:567:ARG:O	1:A:569:PHE:N	2.50	0.45
1:A:399:THR:O	1:A:402:SER:OG	2.30	0.45
1:A:124:PHE:HA	1:A:127:VAL:HB	1.99	0.44
1:A:207:GLU:HB3	1:A:217:THR:HG22	1.98	0.44
1:A:261:PHE:HD1	1:A:268:LEU:HD13	1.83	0.44
1:C:124:PHE:HA	1:C:127:VAL:HB	1.99	0.44
1:B:575:TYR:HA	1:B:578:MET:HE2	2.00	0.44
1:C:567:ARG:O	1:C:569:PHE:N	2.50	0.44
1:D:261:PHE:HD1	1:D:268:LEU:HD13	1.83	0.44
1:C:324:ILE:O	1:C:328:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:TYR:HA	1:C:578:MET:HE2	2.00	0.44
1:D:399:THR:O	1:D:402:SER:OG	2.30	0.44
1:B:141:ASP:O	1:B:145:LEU:N	2.47	0.44
1:C:673:LEU:O	1:C:677:MET:N	2.40	0.43
1:D:124:PHE:HA	1:D:127:VAL:HB	1.99	0.43
1:C:261:PHE:HD1	1:C:268:LEU:HD13	1.83	0.43
1:A:324:ILE:O	1:A:328:SER:N	2.50	0.43
1:B:624:SER:O	1:B:628:ALA:N	2.48	0.43
1:B:261:PHE:HD1	1:B:268:LEU:HD13	1.83	0.43
1:A:673:LEU:O	1:A:677:MET:N	2.41	0.43
1:D:624:SER:O	1:D:628:ALA:N	2.48	0.43
1:A:227:GLN:O	1:A:231:THR:OG1	2.29	0.43
1:B:226:ARG:HG2	1:B:274:GLN:NE2	2.34	0.43
1:C:404:LEU:HG	1:C:701:LEU:HD11	2.01	0.43
1:D:375:ARG:HB3	1:D:391:ASP:HB2	2.01	0.43
1:A:375:ARG:HB3	1:A:391:ASP:HB2	2.01	0.43
1:C:155:PRO:HA	1:C:158:LEU:HD12	2.01	0.43
1:A:155:PRO:HA	1:A:158:LEU:HD12	2.01	0.42
1:C:177:LEU:HG	1:C:221:ILE:HD11	2.01	0.42
1:C:226:ARG:HG2	1:C:274:GLN:NE2	2.34	0.42
1:B:673:LEU:O	1:B:677:MET:N	2.41	0.42
1:D:155:PRO:HA	1:D:158:LEU:HD12	2.01	0.42
1:B:177:LEU:HG	1:B:221:ILE:HD11	2.01	0.42
1:A:589:LYS:HE2	1:B:571:SER:HB2	2.02	0.42
1:A:624:SER:O	1:A:628:ALA:N	2.48	0.42
1:D:362:SER:OG	1:D:363:ARG:N	2.53	0.42
1:D:732:LEU:HD23	1:D:732:LEU:HA	1.89	0.42
1:B:375:ARG:HB3	1:B:391:ASP:HB2	2.01	0.42
1:C:180:ASN:OD1	1:C:183:THR:OG1	2.27	0.42
1:D:177:LEU:HG	1:D:221:ILE:HD11	2.01	0.42
1:A:362:SER:OG	1:A:363:ARG:N	2.53	0.42
1:B:404:LEU:HG	1:B:701:LEU:HD11	2.01	0.42
1:B:589:LYS:HE2	1:C:571:SER:HB2	2.02	0.42
1:D:673:LEU:O	1:D:677:MET:N	2.40	0.42
1:B:155:PRO:HA	1:B:158:LEU:HD12	2.01	0.42
1:C:187:VAL:O	1:C:191:LEU:N	2.42	0.42
1:C:362:SER:OG	1:C:363:ARG:N	2.53	0.42
1:A:177:LEU:HG	1:A:221:ILE:HD11	2.01	0.42
1:D:180:ASN:OD1	1:D:183:THR:OG1	2.26	0.42
1:D:575:TYR:HA	1:D:578:MET:HE2	2.02	0.42
1:B:653:LEU:O	1:B:657:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ARG:HB3	1:C:391:ASP:HB2	2.01	0.41
1:D:226:ARG:HG2	1:D:274:GLN:NE2	2.34	0.41
1:A:404:LEU:HG	1:A:701:LEU:HD11	2.01	0.41
1:D:404:LEU:HG	1:D:701:LEU:HD11	2.01	0.41
1:C:589:LYS:HE2	1:D:571:SER:HB2	2.02	0.41
1:C:669:LEU:HD23	1:C:669:LEU:HA	1.86	0.41
1:A:226:ARG:HG2	1:A:274:GLN:NE2	2.34	0.41
1:B:734:ILE:HD11	1:B:759:ILE:HA	2.03	0.41
1:A:508:LEU:HD13	1:A:508:LEU:HA	1.93	0.41
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.89	0.41
1:B:503:ILE:HG22	1:B:507:LEU:HG	2.03	0.41
1:D:503:ILE:HG22	1:D:507:LEU:HG	2.03	0.41
1:D:653:LEU:O	1:D:657:LEU:N	2.36	0.41
1:A:301:HIS:HE1	1:A:338:ASN:HB3	1.86	0.41
1:A:503:ILE:HG22	1:A:507:LEU:HG	2.03	0.41
1:A:571:SER:HB2	1:D:589:LYS:HE2	2.02	0.41
1:B:180:ASN:OD1	1:B:183:THR:OG1	2.27	0.41
1:B:301:HIS:HE1	1:B:338:ASN:HB3	1.86	0.41
1:B:362:SER:OG	1:B:363:ARG:N	2.53	0.41
1:B:473:LEU:HD11	1:B:475:LEU:HD23	2.03	0.41
1:C:141:ASP:O	1:C:145:LEU:N	2.47	0.41
1:C:734:ILE:HD11	1:C:759:ILE:HA	2.03	0.41
1:D:669:LEU:HA	1:D:672:MET:HB3	2.03	0.41
1:D:411:THR:OG1	1:D:412:ASN:N	2.54	0.41
1:A:473:LEU:HD11	1:A:475:LEU:HD23	2.03	0.40
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.92	0.40
1:D:473:LEU:HD11	1:D:475:LEU:HD23	2.03	0.40
1:A:734:ILE:HD11	1:A:759:ILE:HA	2.03	0.40
1:C:301:HIS:HE1	1:C:338:ASN:HB3	1.86	0.40
1:C:473:LEU:HD11	1:C:475:LEU:HD23	2.03	0.40
1:C:503:ILE:HG22	1:C:507:LEU:HG	2.03	0.40
1:C:563:LEU:O	1:C:566:THR:OG1	2.32	0.40
1:D:325:LEU:HD23	1:D:325:LEU:HA	1.90	0.40
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.90	0.40
1:A:701:LEU:HD23	1:A:701:LEU:HA	1.90	0.40
1:B:508:LEU:HD13	1:B:508:LEU:HA	1.93	0.40
1:C:669:LEU:HA	1:C:672:MET:HB3	2.03	0.40
1:C:411:THR:OG1	1:C:412:ASN:N	2.54	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	639/791 (81%)	528 (83%)	106 (17%)	5 (1%)	19	60
1	B	639/791 (81%)	528 (83%)	106 (17%)	5 (1%)	19	60
1	C	639/791 (81%)	528 (83%)	106 (17%)	5 (1%)	19	60
1	D	639/791 (81%)	527 (82%)	107 (17%)	5 (1%)	19	60
All	All	2556/3164 (81%)	2111 (83%)	425 (17%)	20 (1%)	24	60

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	PRO
1	B	758	PRO
1	C	758	PRO
1	D	758	PRO
1	A	586	ASP
1	A	615	ASP
1	B	586	ASP
1	B	615	ASP
1	C	586	ASP
1	C	615	ASP
1	D	586	ASP
1	D	615	ASP
1	A	424	PRO
1	B	424	PRO
1	C	424	PRO
1	D	424	PRO
1	A	470	PRO
1	B	470	PRO
1	C	470	PRO
1	D	470	PRO

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	561/706 (80%)	554 (99%)	7 (1%)	71	84
1	B	561/706 (80%)	554 (99%)	7 (1%)	71	84
1	C	561/706 (80%)	554 (99%)	7 (1%)	71	84
1	D	561/706 (80%)	554 (99%)	7 (1%)	71	84
All	All	2244/2824 (80%)	2216 (99%)	28 (1%)	72	84

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	A	246	LYS
1	A	366	LYS
1	A	462	ARG
1	A	647	ASN
1	A	683	ASN
1	A	714	ARG
1	B	150	ARG
1	B	246	LYS
1	B	366	LYS
1	B	462	ARG
1	B	647	ASN
1	B	683	ASN
1	B	714	ARG
1	C	150	ARG
1	C	246	LYS
1	C	366	LYS
1	C	462	ARG
1	C	647	ASN
1	C	683	ASN
1	C	714	ARG
1	D	150	ARG
1	D	246	LYS
1	D	366	LYS

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Mol	Chain	Res	Type
1	D	462	ARG
1	D	647	ASN
1	D	683	ASN
1	D	714	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	645	GLN
1	A	647	ASN
1	A	671	ASN
1	A	683	ASN
1	B	178	ASN
1	B	645	GLN
1	B	647	ASN
1	B	671	ASN
1	B	683	ASN
1	C	178	ASN
1	C	645	GLN
1	C	647	ASN
1	C	671	ASN
1	C	683	ASN
1	D	178	ASN
1	D	645	GLN
1	D	647	ASN
1	D	671	ASN
1	D	683	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FZ4	A	801	1	16,18,18	0.89	1 (6%)	17,22,22	1.73	4 (23%)
2	FZ4	D	801	1	16,18,18	0.88	1 (6%)	17,22,22	1.73	4 (23%)
2	FZ4	B	801	1	16,18,18	0.90	1 (6%)	17,22,22	1.73	4 (23%)
2	FZ4	D	803	1	16,18,18	0.70	0	17,22,22	1.57	3 (17%)
2	FZ4	C	801	1	16,18,18	0.89	1 (6%)	17,22,22	1.72	4 (23%)
2	FZ4	B	802	-	16,18,18	0.66	0	17,22,22	1.62	4 (23%)
2	FZ4	A	803	1	16,18,18	0.71	0	17,22,22	1.59	3 (17%)
2	FZ4	C	802	-	16,18,18	0.66	0	17,22,22	1.62	5 (29%)
2	FZ4	B	803	1	16,18,18	0.70	0	17,22,22	1.59	3 (17%)
2	FZ4	D	802	-	16,18,18	0.67	0	17,22,22	1.62	5 (29%)
2	FZ4	A	802	-	16,18,18	0.68	0	17,22,22	1.62	4 (23%)
2	FZ4	C	803	1	16,18,18	0.70	0	17,22,22	1.58	3 (17%)

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
2	FZ4	A	801	1	-	6/12/12/12	0/2/2/2
2	FZ4	D	801	1	-	6/12/12/12	0/2/2/2
2	FZ4	B	801	1	-	6/12/12/12	0/2/2/2
2	FZ4	D	803	1	-	7/12/12/12	0/2/2/2
2	FZ4	C	801	1	-	6/12/12/12	0/2/2/2
2	FZ4	B	802	-	-	3/12/12/12	0/2/2/2
2	FZ4	A	803	1	-	7/12/12/12	0/2/2/2
2	FZ4	C	802	-	-	3/12/12/12	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FZ4	B	803	1	-	7/12/12/12	0/2/2/2
2	FZ4	D	802	-	-	3/12/12/12	0/2/2/2
2	FZ4	A	802	-	-	3/12/12/12	0/2/2/2
2	FZ4	C	803	1	-	7/12/12/12	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FZ4	C03-C02	-2.32	1.37	1.40
2	A	801	FZ4	C03-C02	-2.25	1.37	1.40
2	C	801	FZ4	C03-C02	-2.23	1.37	1.40
2	D	801	FZ4	C03-C02	-2.22	1.37	1.40

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	802	FZ4	C07-C02-C03	3.88	121.22	116.88
2	D	802	FZ4	C07-C02-C03	3.87	121.21	116.88
2	D	801	FZ4	B01-C02-C03	-3.85	115.10	121.49
2	B	802	FZ4	C07-C02-C03	3.84	121.18	116.88
2	A	801	FZ4	B01-C02-C03	-3.84	115.12	121.49
2	A	802	FZ4	C07-C02-C03	3.84	121.17	116.88
2	B	801	FZ4	B01-C02-C03	-3.82	115.15	121.49
2	C	801	FZ4	B01-C02-C03	-3.82	115.15	121.49
2	A	803	FZ4	C13-C08-C09	3.44	120.73	116.88
2	C	803	FZ4	C13-C08-C09	3.41	120.70	116.88
2	D	803	FZ4	C13-C08-C09	3.39	120.67	116.88
2	B	803	FZ4	C13-C08-C09	3.38	120.66	116.88
2	B	801	FZ4	C07-C02-C03	3.13	120.38	116.88
2	B	803	FZ4	C07-C02-C03	3.10	120.35	116.88
2	A	801	FZ4	C07-C02-C03	3.10	120.34	116.88
2	D	801	FZ4	C07-C02-C03	3.09	120.34	116.88
2	C	801	FZ4	C07-C02-C03	3.06	120.30	116.88
2	A	803	FZ4	C07-C02-C03	3.06	120.30	116.88
2	C	803	FZ4	C07-C02-C03	3.03	120.27	116.88
2	D	803	FZ4	C07-C02-C03	2.99	120.22	116.88
2	A	802	FZ4	C13-C08-C09	2.75	119.96	116.88
2	B	802	FZ4	C13-C08-C09	2.72	119.92	116.88
2	D	802	FZ4	C13-C08-C09	2.69	119.89	116.88
2	C	802	FZ4	C13-C08-C09	2.68	119.88	116.88
2	D	802	FZ4	C04-C03-C02	-2.54	119.05	121.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	802	FZ4	C04-C03-C02	-2.54	119.06	121.57
2	C	802	FZ4	C04-C03-C02	-2.54	119.06	121.57
2	B	802	FZ4	C04-C03-C02	-2.52	119.07	121.57
2	A	803	FZ4	C10-C09-C08	-2.43	119.16	121.57
2	D	803	FZ4	C10-C09-C08	-2.41	119.18	121.57
2	B	803	FZ4	C10-C09-C08	-2.40	119.19	121.57
2	C	803	FZ4	C10-C09-C08	-2.40	119.19	121.57
2	D	801	FZ4	C04-C03-C02	-2.37	119.22	121.57
2	B	801	FZ4	C04-C03-C02	-2.34	119.25	121.57
2	A	801	FZ4	C04-C03-C02	-2.34	119.25	121.57
2	C	801	FZ4	C04-C03-C02	-2.31	119.28	121.57
2	B	802	FZ4	C10-C09-C08	-2.22	119.37	121.57
2	A	802	FZ4	C10-C09-C08	-2.22	119.37	121.57
2	D	802	FZ4	C10-C09-C08	-2.19	119.40	121.57
2	C	802	FZ4	C10-C09-C08	-2.17	119.42	121.57
2	A	801	FZ4	C13-C08-C09	2.07	119.20	116.88
2	B	801	FZ4	C13-C08-C09	2.07	119.20	116.88
2	C	801	FZ4	C13-C08-C09	2.07	119.20	116.88
2	D	801	FZ4	C13-C08-C09	2.07	119.20	116.88
2	C	802	FZ4	C06-C07-C02	-2.04	119.55	121.57
2	D	802	FZ4	C06-C07-C02	-2.02	119.57	121.57

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FZ4	C02-B01-O14-C15
2	A	801	FZ4	C08-B01-O14-C15
2	A	802	FZ4	C08-B01-O14-C15
2	A	802	FZ4	O14-C15-C16-N17
2	A	803	FZ4	C02-B01-O14-C15
2	A	803	FZ4	C08-B01-O14-C15
2	A	803	FZ4	O14-C15-C16-N17
2	B	801	FZ4	C02-B01-O14-C15
2	B	801	FZ4	C08-B01-O14-C15
2	B	802	FZ4	C08-B01-O14-C15
2	B	802	FZ4	O14-C15-C16-N17
2	B	803	FZ4	C02-B01-O14-C15
2	B	803	FZ4	C08-B01-O14-C15
2	B	803	FZ4	O14-C15-C16-N17
2	C	801	FZ4	C02-B01-O14-C15
2	C	801	FZ4	C08-B01-O14-C15

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Mol	Chain	Res	Type	Atoms
2	C	802	FZ4	C08-B01-O14-C15
2	C	802	FZ4	O14-C15-C16-N17
2	C	803	FZ4	C02-B01-O14-C15
2	C	803	FZ4	C08-B01-O14-C15
2	C	803	FZ4	O14-C15-C16-N17
2	D	801	FZ4	C02-B01-O14-C15
2	D	801	FZ4	C08-B01-O14-C15
2	D	802	FZ4	C08-B01-O14-C15
2	D	802	FZ4	O14-C15-C16-N17
2	D	803	FZ4	C02-B01-O14-C15
2	D	803	FZ4	C08-B01-O14-C15
2	D	803	FZ4	O14-C15-C16-N17
2	A	801	FZ4	O14-B01-C08-C09
2	A	801	FZ4	O14-B01-C08-C13
2	A	803	FZ4	O14-B01-C02-C03
2	A	803	FZ4	O14-B01-C02-C07
2	B	801	FZ4	O14-B01-C08-C09
2	B	801	FZ4	O14-B01-C08-C13
2	B	803	FZ4	O14-B01-C02-C03
2	B	803	FZ4	O14-B01-C02-C07
2	C	801	FZ4	O14-B01-C08-C09
2	C	801	FZ4	O14-B01-C08-C13
2	C	803	FZ4	O14-B01-C02-C03
2	C	803	FZ4	O14-B01-C02-C07
2	D	801	FZ4	O14-B01-C08-C09
2	D	801	FZ4	O14-B01-C08-C13
2	D	803	FZ4	O14-B01-C02-C03
2	D	803	FZ4	O14-B01-C02-C07
2	A	801	FZ4	C02-B01-C08-C13
2	B	801	FZ4	C02-B01-C08-C13
2	C	801	FZ4	C02-B01-C08-C13
2	D	801	FZ4	C02-B01-C08-C13
2	A	802	FZ4	O14-B01-C08-C09
2	B	802	FZ4	O14-B01-C08-C09
2	C	802	FZ4	O14-B01-C08-C09
2	D	802	FZ4	O14-B01-C08-C09
2	A	801	FZ4	C02-B01-C08-C09
2	A	803	FZ4	C08-B01-C02-C03
2	A	803	FZ4	C08-B01-C02-C07
2	B	801	FZ4	C02-B01-C08-C09
2	B	803	FZ4	C08-B01-C02-C03
2	B	803	FZ4	C08-B01-C02-C07

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Mol	Chain	Res	Type	Atoms
2	C	801	FZ4	C02-B01-C08-C09
2	C	803	FZ4	C08-B01-C02-C03
2	C	803	FZ4	C08-B01-C02-C07
2	D	801	FZ4	C02-B01-C08-C09
2	D	803	FZ4	C08-B01-C02-C03
2	D	803	FZ4	C08-B01-C02-C07

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FZ4	1	0
2	D	801	FZ4	1	0
2	B	801	FZ4	1	0
2	C	801	FZ4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	744:THR	C	748:HIS	N	35.64
1	B	744:THR	C	748:HIS	N	35.64
1	C	744:THR	C	748:HIS	N	35.64
1	D	744:THR	C	748:HIS	N	35.64

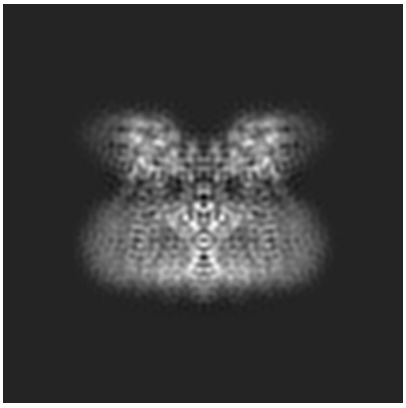
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8921. These allow visual inspection of the internal detail of the map and identification of artifacts.

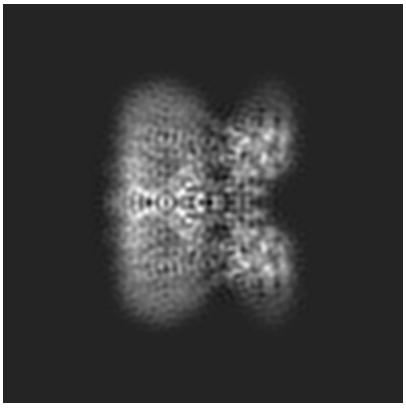
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

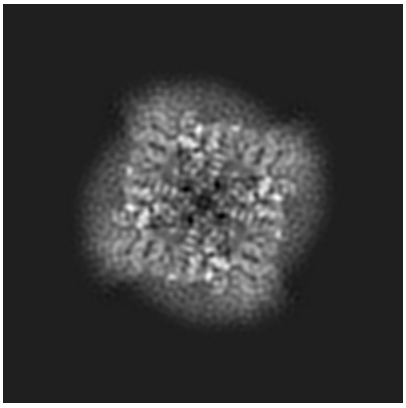
6.1.1 Primary map



X



Y

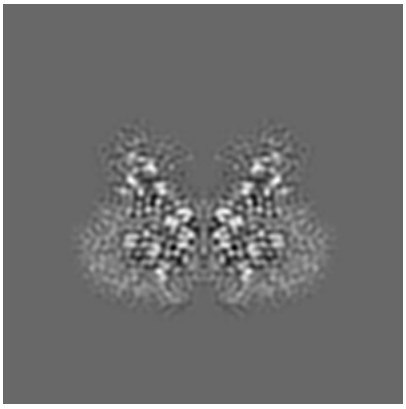


Z

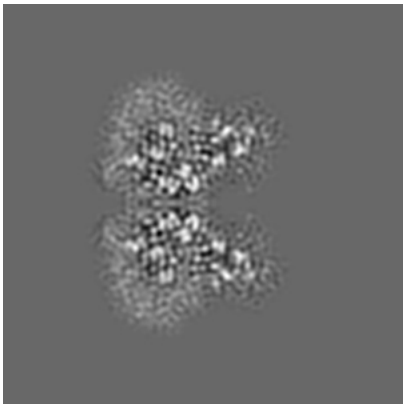
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 110



Y Index: 110

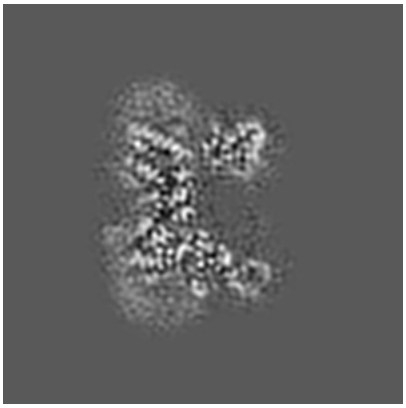
Z Index: 110

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

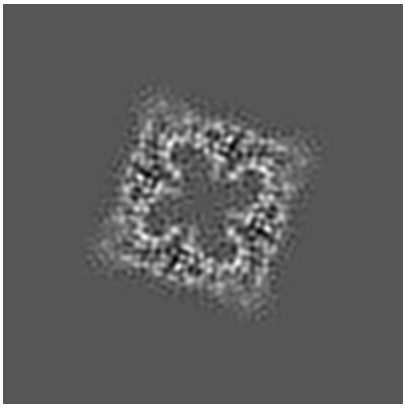
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 104



Y Index: 104

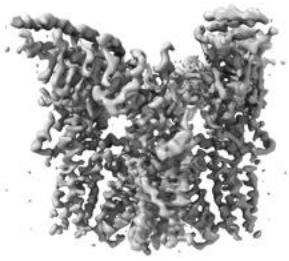


Z Index: 134

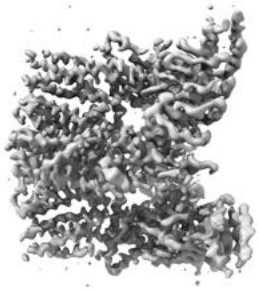
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

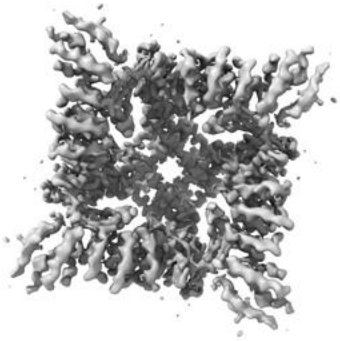
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.057. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

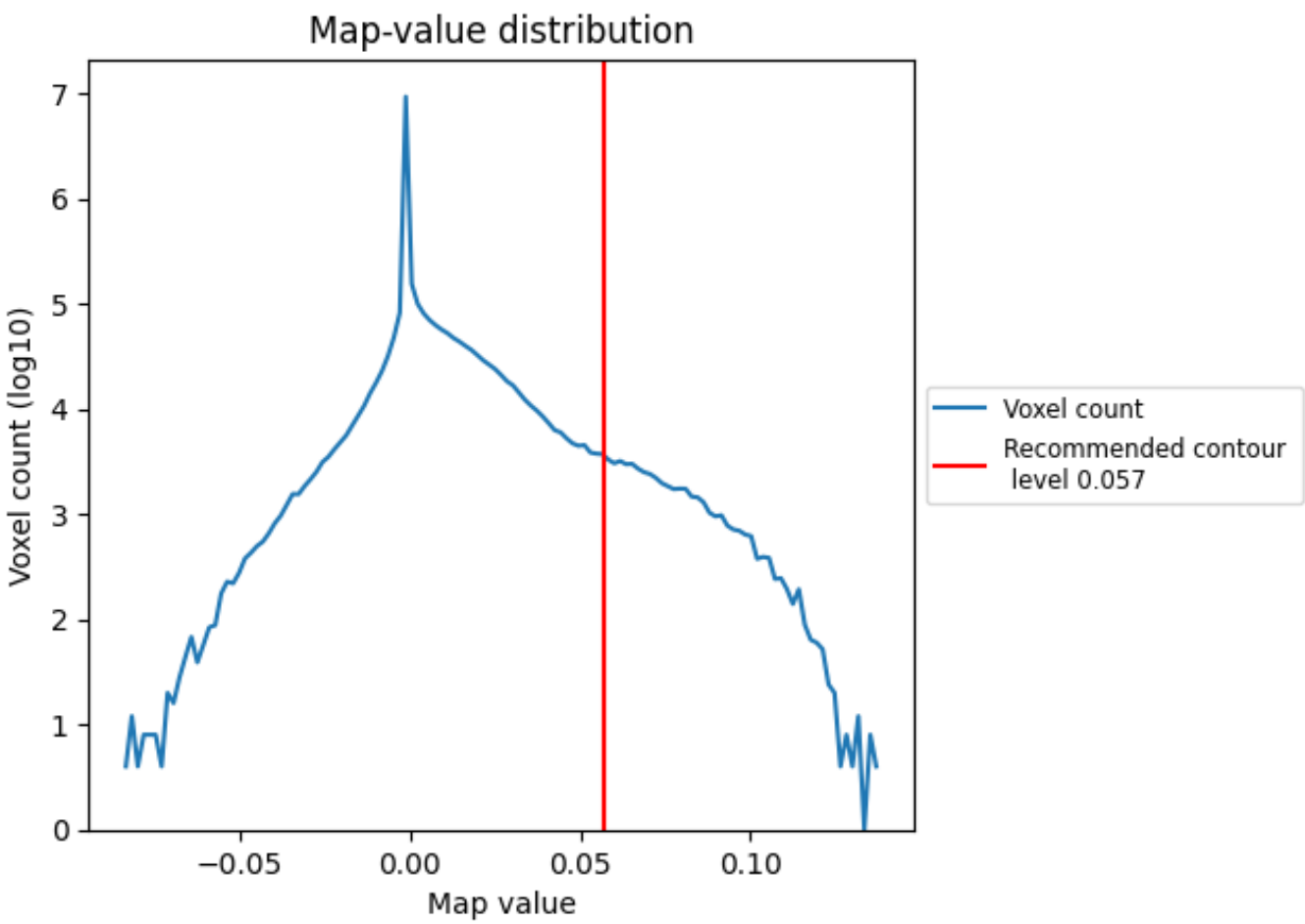
6.5 Mask visualisation (i)

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

7 Map analysis (i)

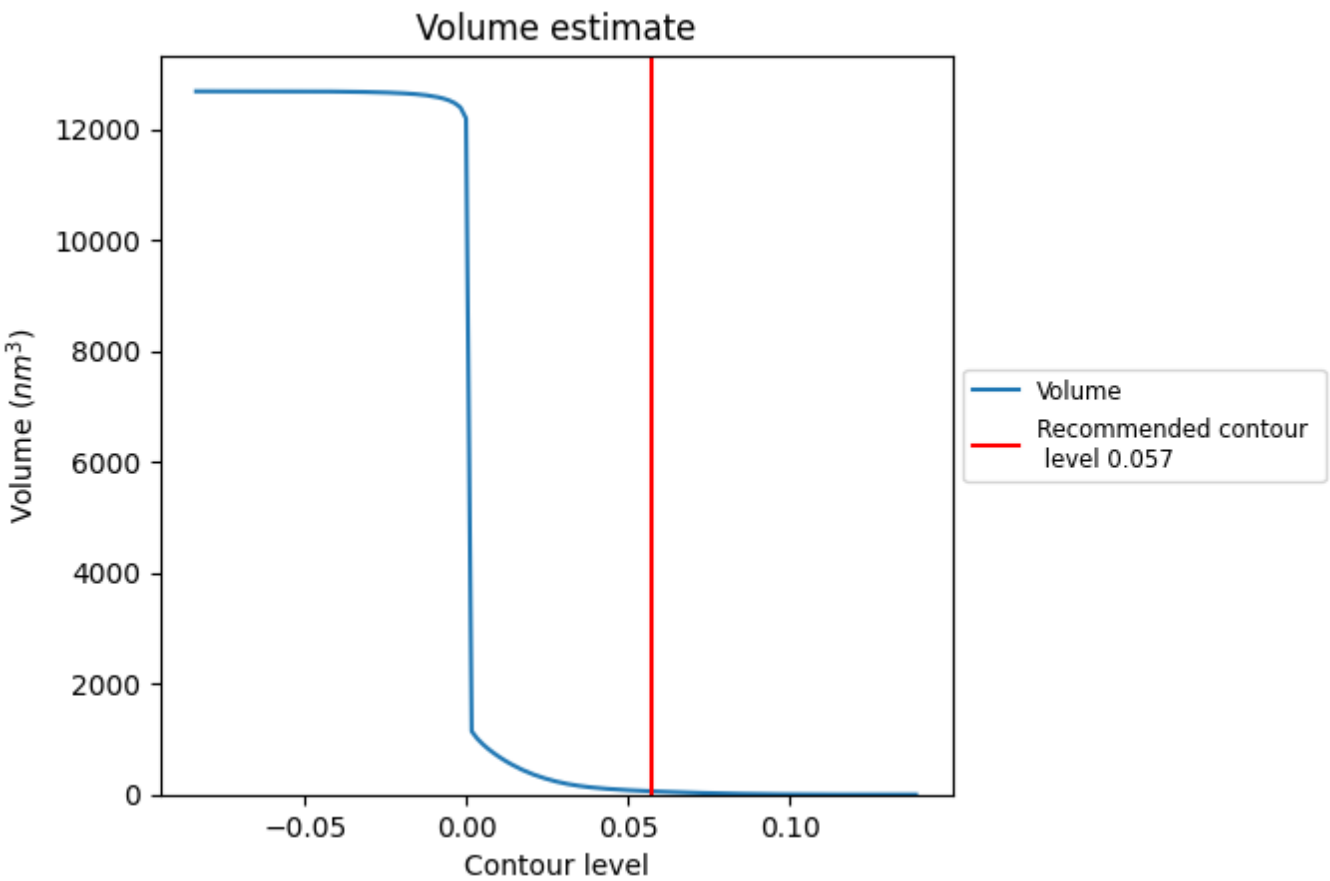
This section contains the results of statistical analysis of the map.

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.

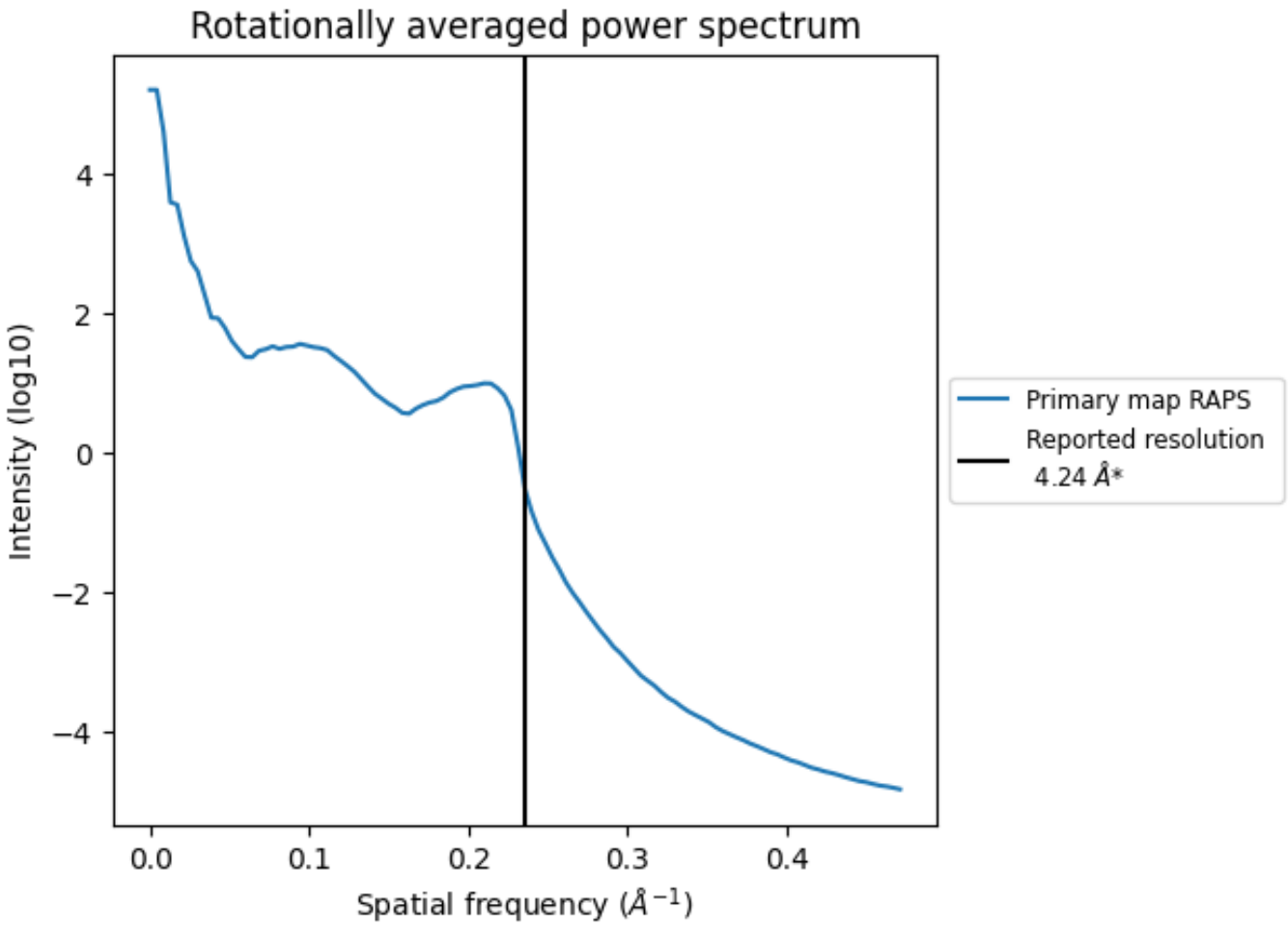
7.2 Volume estimate (i)



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 54 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 0.236 Å^{-1}

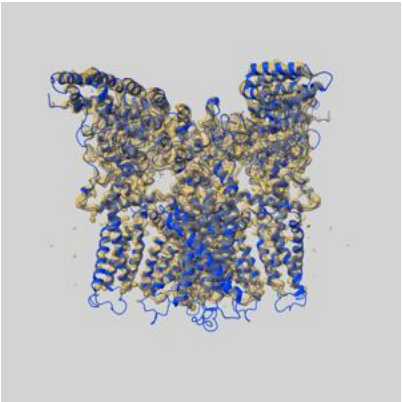
8 Fourier-Shell correlation (i)

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

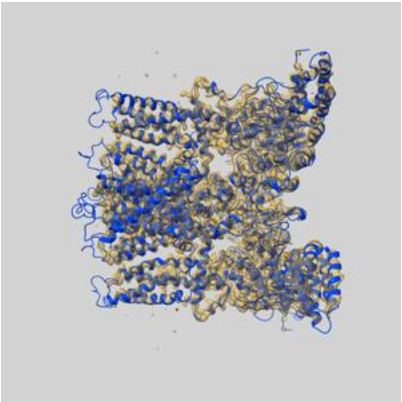
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-8921 and PDB model 6DVZ. Per-residue inclusion information can be found in section 3 on page 5.

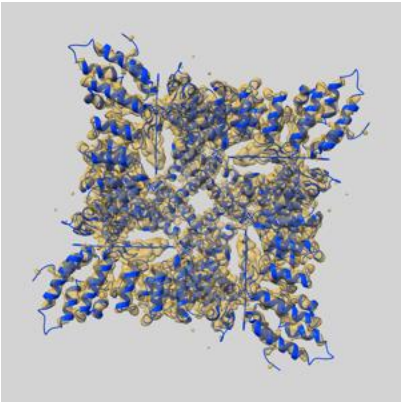
9.1 Map-model overlay (i)



X



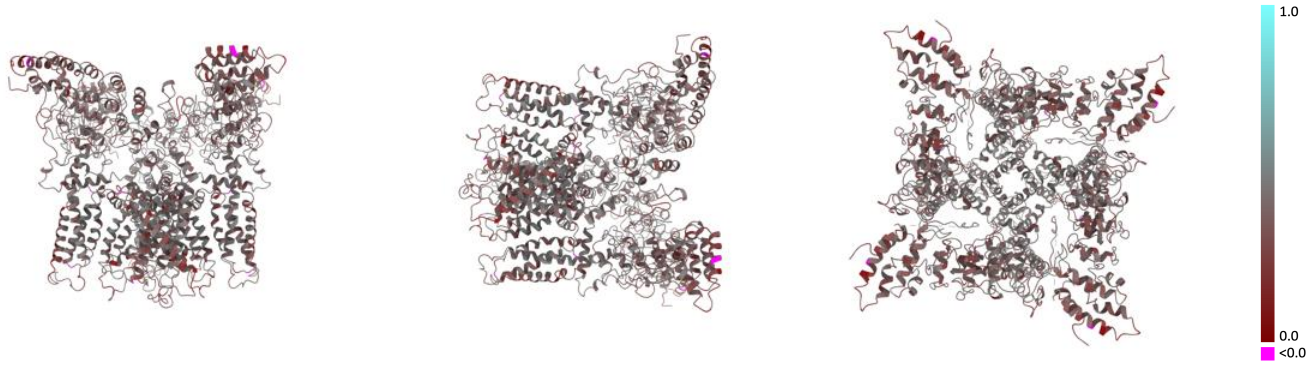
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.057 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.

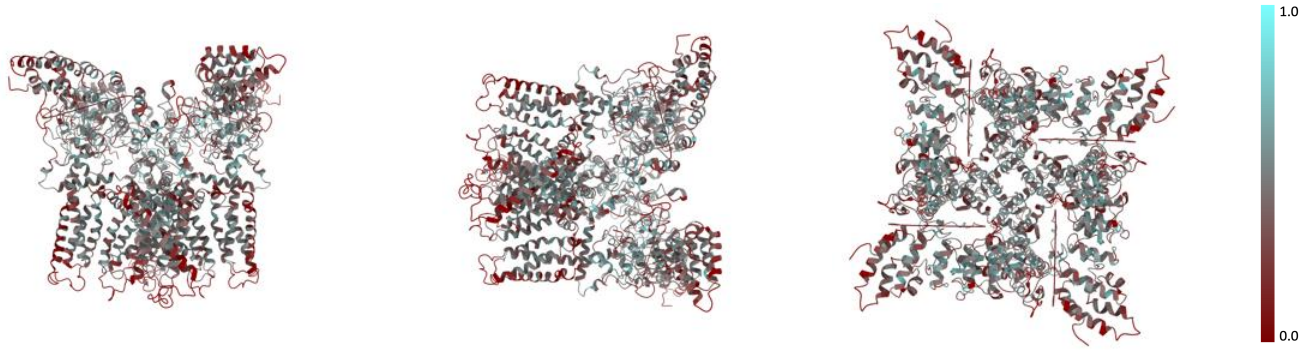
9.2 Q-score mapped to coordinate model (i)



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.

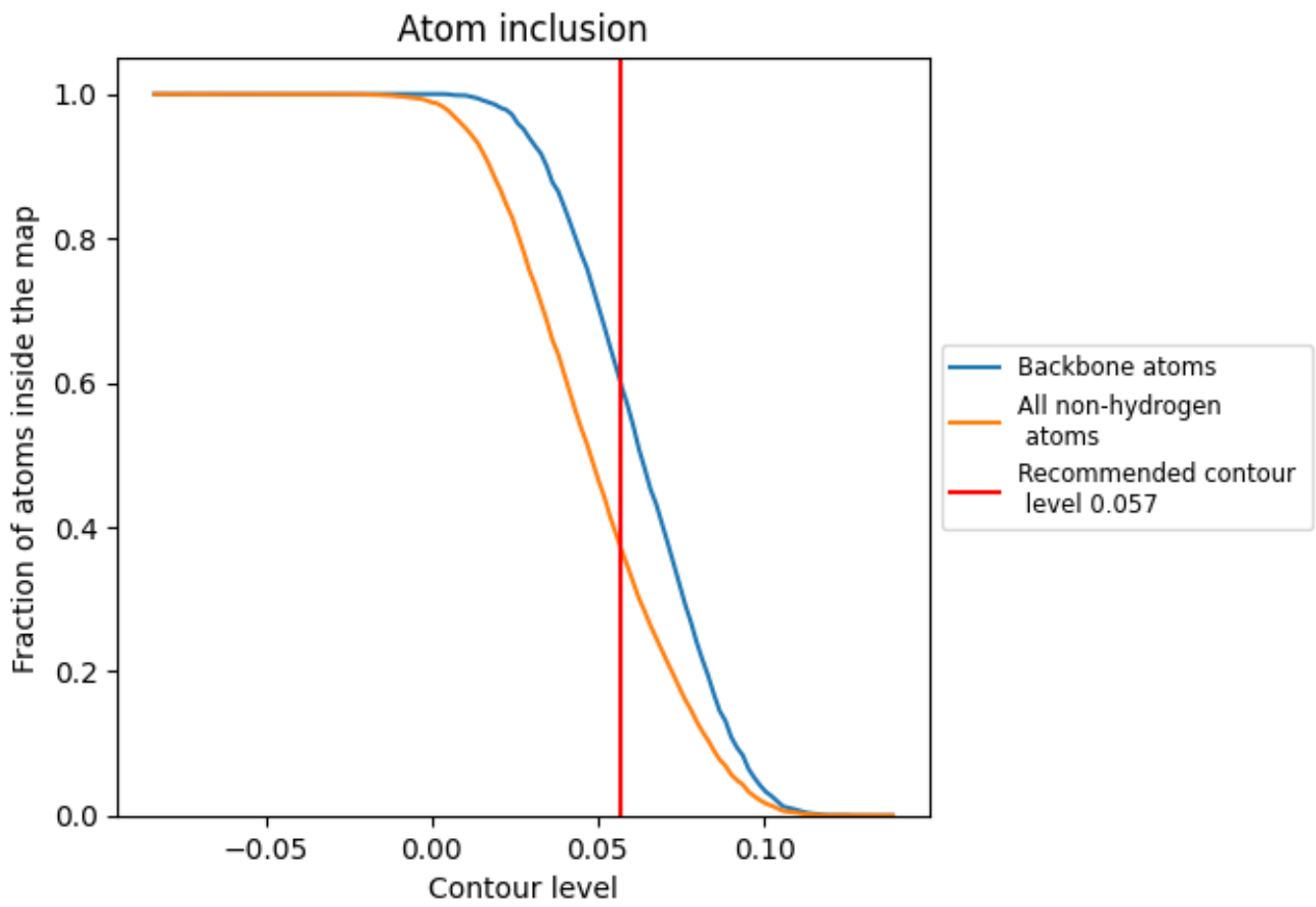
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.057).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 37% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.057) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3706	0.3870
A	0.3705	0.3850
B	0.3705	0.3870
C	0.3705	0.3880
D	0.3707	0.3860