Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 09:38 AM EST

PDB ID	:	6D7T
EMDB ID	:	EMD-7825
Title	:	Cryo-EM structure of human TRPV6-Y467A in complex with 2-Aminoethoxydiphenyl borate (2-APB)
Authors	:	Singh, A.K.; Saotome, K.; McGoldrick, L.L.; Sobolevsky, A.I.
Deposited on	:	2018-04-25
Resolution	:	4.44 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:

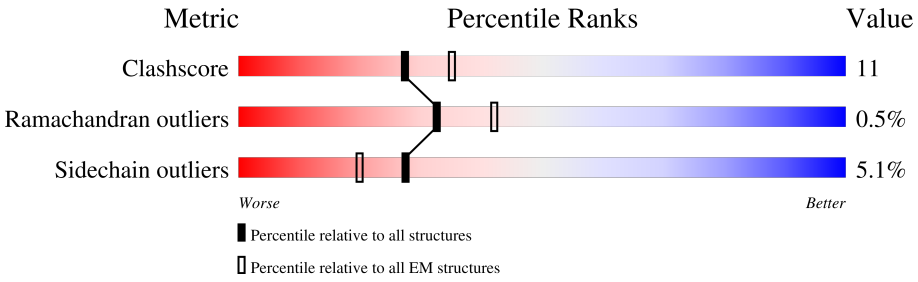
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 4.44 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	742	33% 57% 23% · 18%
1	B	742	33% 57% 23% · 18%
1	C	742	33% 56% 24% · 18%
1	D	742	32% 57% 23% · 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19654 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 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		
1	B	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		
1	C	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		
1	D	611	Total	C	N	O	S	0	0
			4896	3162	830	864	40		

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	ALA	TYR	engineered mutation	UNP Q9H1D0
A	726	LEU	-	expression tag	UNP Q9H1D0
A	727	VAL	-	expression tag	UNP Q9H1D0
A	728	PRO	-	expression tag	UNP Q9H1D0
A	729	ARG	-	expression tag	UNP Q9H1D0
A	730	GLY	-	expression tag	UNP Q9H1D0
A	731	SER	-	expression tag	UNP Q9H1D0
A	732	ALA	-	expression tag	UNP Q9H1D0
A	733	ALA	-	expression tag	UNP Q9H1D0
A	734	ALA	-	expression tag	UNP Q9H1D0
A	735	TRP	-	expression tag	UNP Q9H1D0
A	736	SER	-	expression tag	UNP Q9H1D0
A	737	HIS	-	expression tag	UNP Q9H1D0
A	738	PRO	-	expression tag	UNP Q9H1D0
A	739	GLN	-	expression tag	UNP Q9H1D0
A	740	PHE	-	expression tag	UNP Q9H1D0
A	741	GLU	-	expression tag	UNP Q9H1D0
A	742	LYS	-	expression tag	UNP Q9H1D0
B	467	ALA	TYR	engineered mutation	UNP Q9H1D0
B	726	LEU	-	expression tag	UNP Q9H1D0
B	727	VAL	-	expression tag	UNP Q9H1D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	728	PRO	-	expression tag	UNP Q9H1D0
B	729	ARG	-	expression tag	UNP Q9H1D0
B	730	GLY	-	expression tag	UNP Q9H1D0
B	731	SER	-	expression tag	UNP Q9H1D0
B	732	ALA	-	expression tag	UNP Q9H1D0
B	733	ALA	-	expression tag	UNP Q9H1D0
B	734	ALA	-	expression tag	UNP Q9H1D0
B	735	TRP	-	expression tag	UNP Q9H1D0
B	736	SER	-	expression tag	UNP Q9H1D0
B	737	HIS	-	expression tag	UNP Q9H1D0
B	738	PRO	-	expression tag	UNP Q9H1D0
B	739	GLN	-	expression tag	UNP Q9H1D0
B	740	PHE	-	expression tag	UNP Q9H1D0
B	741	GLU	-	expression tag	UNP Q9H1D0
B	742	LYS	-	expression tag	UNP Q9H1D0
C	467	ALA	TYR	engineered mutation	UNP Q9H1D0
C	726	LEU	-	expression tag	UNP Q9H1D0
C	727	VAL	-	expression tag	UNP Q9H1D0
C	728	PRO	-	expression tag	UNP Q9H1D0
C	729	ARG	-	expression tag	UNP Q9H1D0
C	730	GLY	-	expression tag	UNP Q9H1D0
C	731	SER	-	expression tag	UNP Q9H1D0
C	732	ALA	-	expression tag	UNP Q9H1D0
C	733	ALA	-	expression tag	UNP Q9H1D0
C	734	ALA	-	expression tag	UNP Q9H1D0
C	735	TRP	-	expression tag	UNP Q9H1D0
C	736	SER	-	expression tag	UNP Q9H1D0
C	737	HIS	-	expression tag	UNP Q9H1D0
C	738	PRO	-	expression tag	UNP Q9H1D0
C	739	GLN	-	expression tag	UNP Q9H1D0
C	740	PHE	-	expression tag	UNP Q9H1D0
C	741	GLU	-	expression tag	UNP Q9H1D0
C	742	LYS	-	expression tag	UNP Q9H1D0
D	467	ALA	TYR	engineered mutation	UNP Q9H1D0
D	726	LEU	-	expression tag	UNP Q9H1D0
D	727	VAL	-	expression tag	UNP Q9H1D0
D	728	PRO	-	expression tag	UNP Q9H1D0
D	729	ARG	-	expression tag	UNP Q9H1D0
D	730	GLY	-	expression tag	UNP Q9H1D0
D	731	SER	-	expression tag	UNP Q9H1D0
D	732	ALA	-	expression tag	UNP Q9H1D0
D	733	ALA	-	expression tag	UNP Q9H1D0

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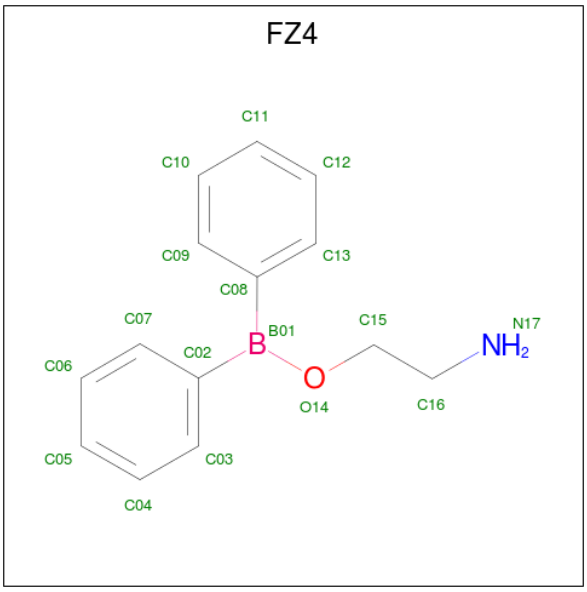
Chain	Residue	Modelled	Actual	Comment	Reference
D	734	ALA	-	expression tag	UNP Q9H1D0
D	735	TRP	-	expression tag	UNP Q9H1D0
D	736	SER	-	expression tag	UNP Q9H1D0
D	737	HIS	-	expression tag	UNP Q9H1D0
D	738	PRO	-	expression tag	UNP Q9H1D0
D	739	GLN	-	expression tag	UNP Q9H1D0
D	740	PHE	-	expression tag	UNP Q9H1D0
D	741	GLU	-	expression tag	UNP Q9H1D0
D	742	LYS	-	expression tag	UNP Q9H1D0

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



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	B	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	C	1	Total	B	C	N	O	0
			17	1	14	1	1	
2	D	1	Total	B	C	N	O	0
			17	1	14	1	1	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

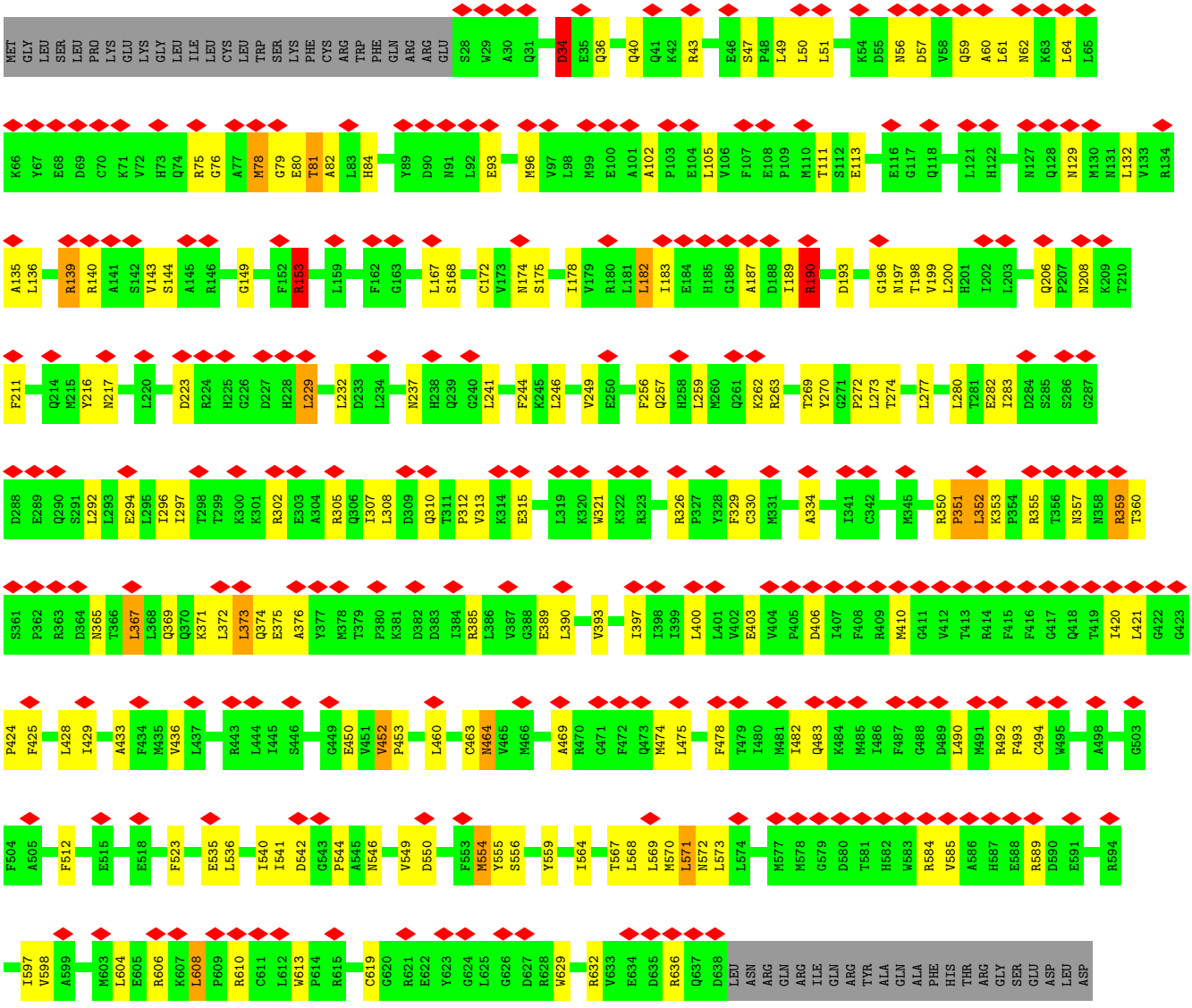
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	

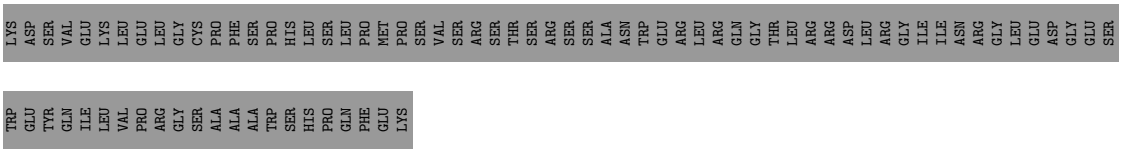
3 Residue-property plots (i)

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 6

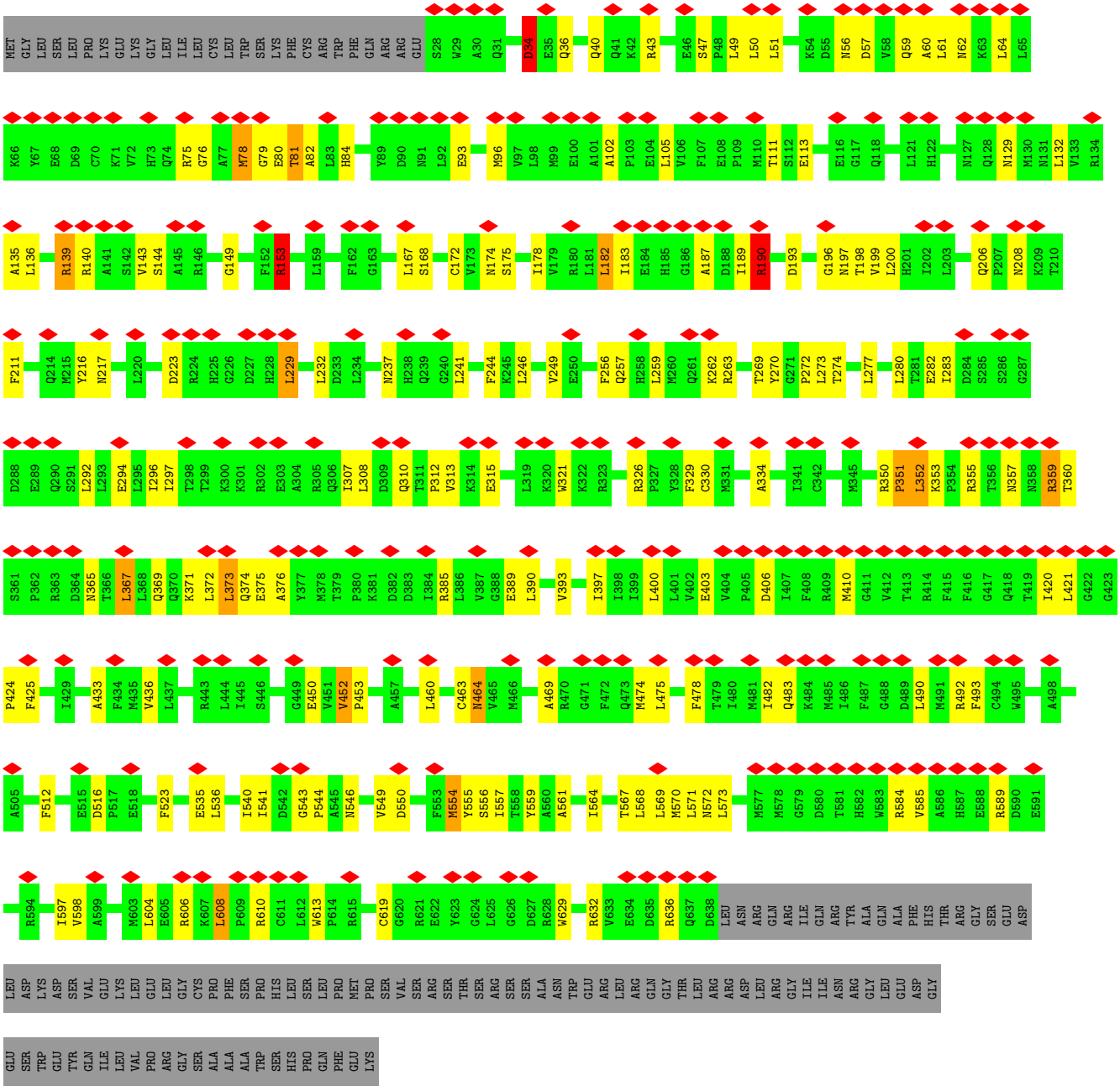
Chain A:





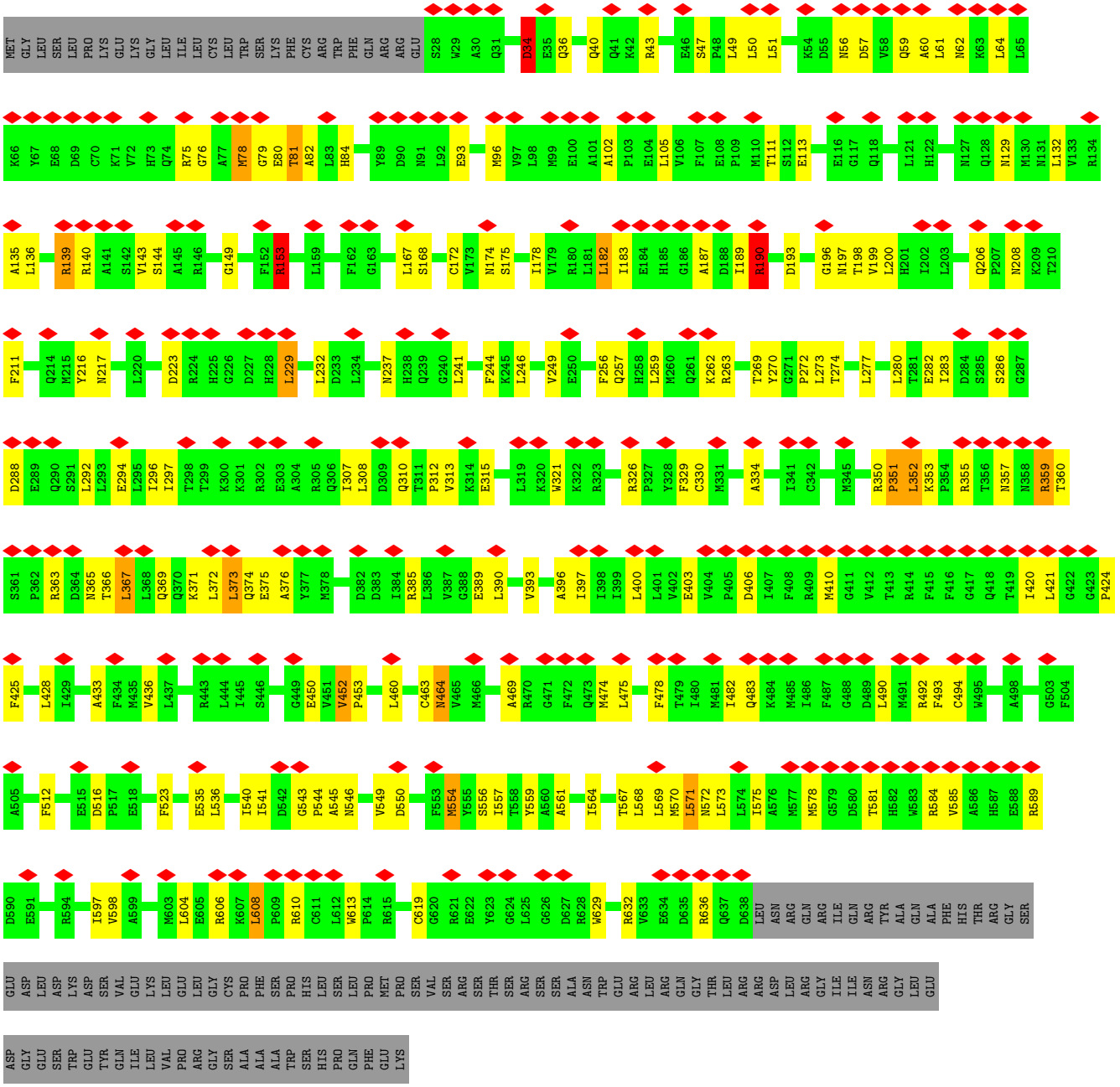
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain B:



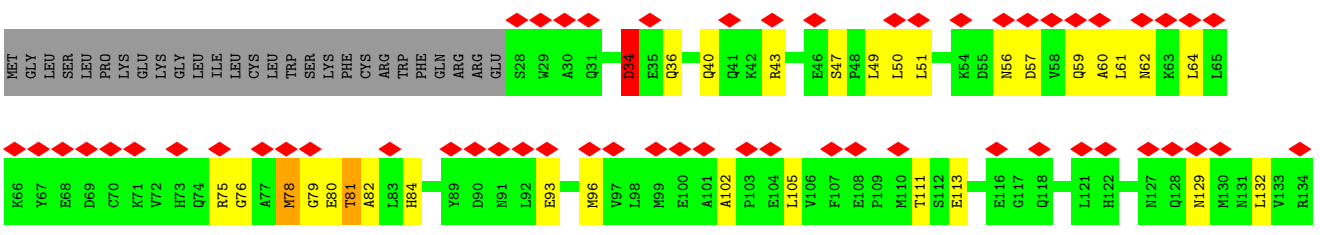
• Molecule 1: Transient receptor potential cation channel subfamily V member 6

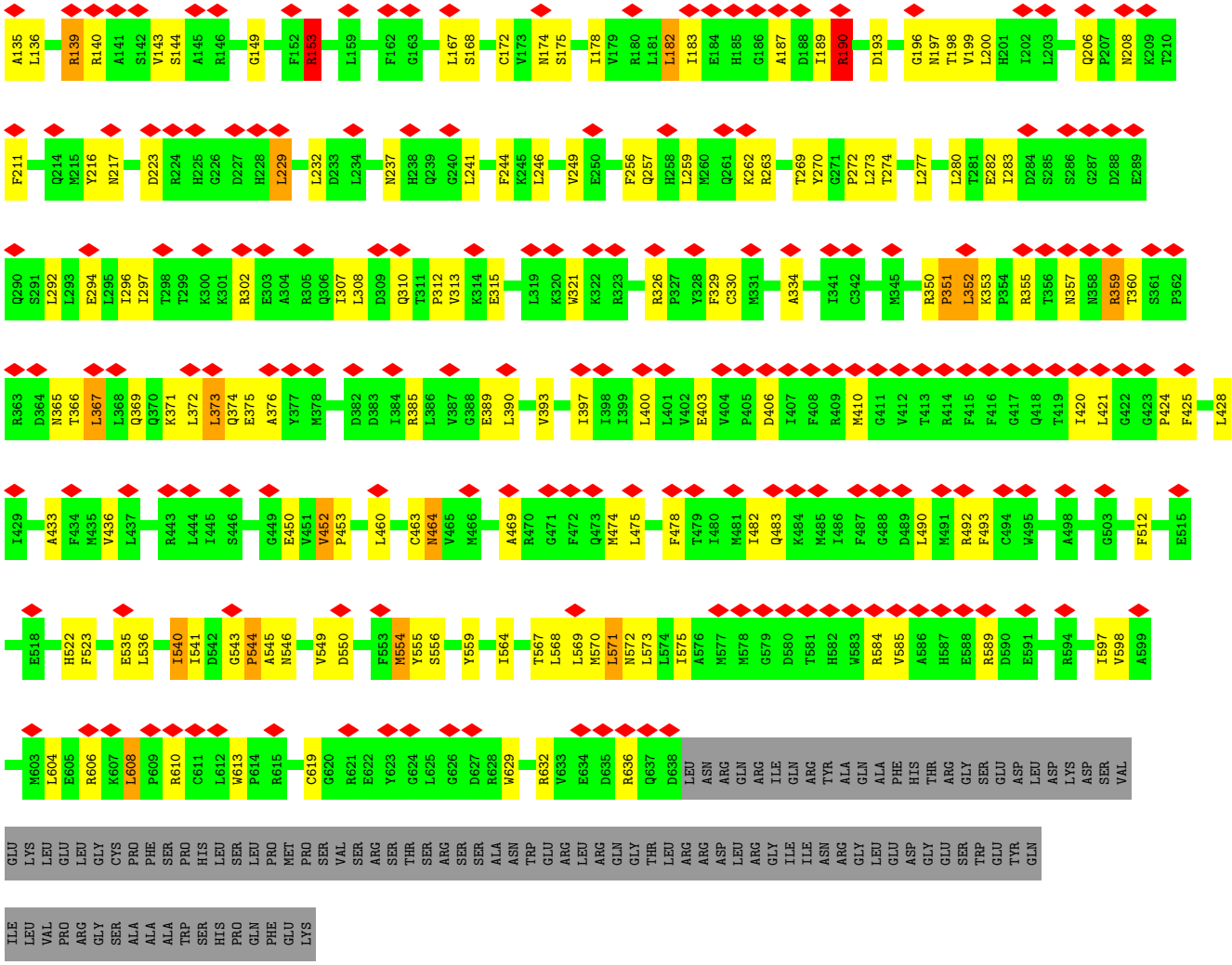
Chain C:



• Molecule 1: Transient receptor potential cation channel subfamily V member 6

Chain D:




A135 L136 R139 R140 A141 S142 V143 S144 A145 R146 G149 F152 R153 L159 F162 G163 L167 S168 C172 V173 N174 S175 I178 V179 R180 L181 L182 I183 E184 H185 G186 A187 D188 I189 R190 D193 G196 N197 T198 V199 L200 H201 I202 L203 Q206 P207 N208 K209 T210
F211 Q214 M215 Y216 N217 D223 R224 H225 G226 D227 H228 L229 L232 D233 L234 N237 H238 Q239 G240 L241 F244 K245 L246 V249 E250 F256 Q257 H258 L259 M260 Q261 K262 R263 T269 Y270 G271 P272 L273 T274 L277 L280 T281 E282 I283 D284 S285 S286 G287 D288 E289
Q290 S291 L292 L293 E294 L295 T296 I297 T298 T299 K300 K301 R302 E303 A304 R305 Q306 I307 L308 D309 Q310 T311 P312 V313 K314 E315 L319 K320 W321 K322 R323 R326 P327 Y328 F329 C330 M331 A334 I341 C342 M345 R350 P351 L352 K353 P354 R355 T356 N357 N358 R359 T360 S361 P362
R363 D364 N365 T366 L367 L368 Q369 Q370 K371 L372 L373 Q374 E375 A376 Y377 M378 D382 D383 I384 R385 L386 V387 G388 E389 L390 V393 I397 I398 I399 L400 L401 V402 E403 V404 P405 D406 I407 F408 R409 M410 G411 V412 T413 R414 F415 F416 G417 Q418 T419 I420 L421 G422 G423 P424 F425 L428
I429 A433 F434 M435 V436 L437 R443 L444 I445 S446 G449 E450 V451 V452 P453 L460 C463 N464 V465 M466 A469 R470 G471 F472 Q473 M474 L475 F478 T479 I480 M481 I482 Q483 K484 M485 I486 F487 G488 D489 L490 M491 R492 F493 C494 W495 A498 G503 F512 E515
E518 H522 F523 E535 L536 I540 I541 D542 G543 P544 A545 N546 V549 D550 F553 M554 Y555 S556 Y559 I564 T567 L568 L569 M570 L571 N572 L573 L574 I575 A576 M577 M578 G579 D580 T581 H582 W583 R584 V585 A586 H587 E588 R589 D590 E591 R594 I597 V598 A599
M603 L604 E605 R606 K607 L608 P609 R610 C611 L612 W613 P614 R615 C619 G620 R621 E622 Y623 G624 L625 G626 D627 R628 W629 R632 V633 E634 D635 R636 Q637 D638
LEU ASN ARG GLN ARG ILE GLN ARG TYR ALA GLN ALA PHE HIS THR ARG GLY SER GLU ASP LEU ASP LYS ASP SER VAL
GLU LYS LEU GLU LEU GLY CYS PRO PHE SER PRO HIS LEU SER LEU PRO MET PRO SER VAL SER ARG SER THR SER ARG SER SER ALA ASN TRP GLU ARG LEU ARG ARG GLN GLY THR LEU ARG ARG ASP LEU ARG GLY ILE ILE ASN ARG GLY LEU GLU ASP GLY GLU SER TRP GLU TYR GLN
ILE LEU VAL PRO ARG GLY SER ALA ALA ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77460	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	43.0	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	0.200	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0669	Depositor
Map size (Å)	248.88, 248.88, 248.88	wwPDB
Map dimensions	204, 204, 204	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.48	1/5008 (0.0%)	0.79	15/6795 (0.2%)
1	B	0.48	1/5008 (0.0%)	0.79	15/6795 (0.2%)
1	C	0.49	1/5008 (0.0%)	0.78	15/6795 (0.2%)
1	D	0.54	2/5008 (0.0%)	0.80	19/6795 (0.3%)
All	All	0.50	5/20032 (0.0%)	0.79	64/27180 (0.2%)

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	3
1	B	0	3
1	C	0	4
1	D	0	4
All	All	0	14

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	544	PRO	C-N	17.00	1.73	1.34
1	C	540	ILE	C-N	-10.15	1.10	1.34
1	D	540	ILE	C-N	9.40	1.55	1.34
1	A	540	ILE	C-N	7.56	1.51	1.34
1	B	540	ILE	C-N	7.56	1.51	1.34

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	ARG	NE-CZ-NH2	10.29	125.44	120.30
1	D	190	ARG	NE-CZ-NH2	10.27	125.44	120.30
1	A	190	ARG	NE-CZ-NH2	10.23	125.41	120.30
1	C	190	ARG	NE-CZ-NH2	10.23	125.41	120.30
1	D	372	LEU	CA-CB-CG	8.06	133.84	115.30
1	C	372	LEU	CA-CB-CG	8.04	133.80	115.30
1	B	372	LEU	CA-CB-CG	8.04	133.79	115.30
1	A	372	LEU	CA-CB-CG	8.04	133.78	115.30
1	C	229	LEU	CA-CB-CG	7.83	133.31	115.30
1	D	229	LEU	CA-CB-CG	7.82	133.28	115.30
1	B	229	LEU	CA-CB-CG	7.81	133.27	115.30
1	A	229	LEU	CA-CB-CG	7.81	133.26	115.30
1	D	540	ILE	C-N-CA	-7.63	102.63	121.70
1	D	544	PRO	O-C-N	-7.58	110.57	122.70
1	A	153	ARG	CG-CD-NE	7.41	127.36	111.80
1	B	153	ARG	CG-CD-NE	7.40	127.35	111.80
1	D	153	ARG	CG-CD-NE	7.40	127.34	111.80
1	C	153	ARG	CG-CD-NE	7.38	127.29	111.80
1	D	367	LEU	CA-CB-CG	7.24	131.96	115.30
1	C	367	LEU	CA-CB-CG	7.24	131.96	115.30
1	B	367	LEU	CA-CB-CG	7.24	131.94	115.30
1	A	367	LEU	CA-CB-CG	7.23	131.93	115.30
1	A	608	LEU	CA-CB-CG	7.09	131.60	115.30
1	C	608	LEU	CA-CB-CG	7.07	131.57	115.30
1	B	608	LEU	CA-CB-CG	7.07	131.55	115.30
1	D	608	LEU	CA-CB-CG	7.06	131.53	115.30
1	B	190	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	C	190	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	A	190	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	D	190	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	D	540	ILE	CA-C-N	-6.64	102.58	117.20
1	A	352	LEU	CA-CB-CG	6.39	130.00	115.30
1	B	352	LEU	CA-CB-CG	6.38	129.98	115.30
1	C	352	LEU	CA-CB-CG	6.38	129.98	115.30
1	D	352	LEU	CA-CB-CG	6.38	129.97	115.30
1	C	190	ARG	CD-NE-CZ	6.33	132.46	123.60
1	A	190	ARG	CD-NE-CZ	6.32	132.44	123.60
1	B	190	ARG	CD-NE-CZ	6.29	132.40	123.60
1	D	190	ARG	CD-NE-CZ	6.29	132.40	123.60
1	C	34	ASP	CB-CG-OD1	6.26	123.94	118.30
1	B	34	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	34	ASP	CB-CG-OD1	6.24	123.91	118.30
1	D	34	ASP	CB-CG-OD1	6.20	123.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	540	ILE	O-C-N	6.13	132.50	122.70
1	D	153	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	B	153	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	A	153	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	C	153	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	D	190	ARG	CG-CD-NE	5.94	124.28	111.80
1	B	190	ARG	CG-CD-NE	5.94	124.28	111.80
1	A	190	ARG	CG-CD-NE	5.92	124.22	111.80
1	C	190	ARG	CG-CD-NE	5.91	124.20	111.80
1	C	153	ARG	CD-NE-CZ	5.22	130.91	123.60
1	B	153	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	153	ARG	CD-NE-CZ	5.16	130.83	123.60
1	D	153	ARG	CD-NE-CZ	5.16	130.83	123.60
1	A	229	LEU	CB-CG-CD1	5.09	119.65	111.00
1	B	229	LEU	CB-CG-CD1	5.08	119.63	111.00
1	B	315	GLU	CA-CB-CG	5.07	124.56	113.40
1	D	315	GLU	CA-CB-CG	5.07	124.56	113.40
1	A	315	GLU	CA-CB-CG	5.07	124.56	113.40
1	C	315	GLU	CA-CB-CG	5.06	124.53	113.40
1	D	229	LEU	CB-CG-CD1	5.05	119.59	111.00
1	C	229	LEU	CB-CG-CD1	5.04	119.57	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASN	Peptide
1	A	223	ASP	Peptide
1	A	351	PRO	Peptide
1	B	129	ASN	Peptide
1	B	223	ASP	Peptide
1	B	351	PRO	Peptide
1	C	129	ASN	Peptide
1	C	223	ASP	Peptide
1	C	351	PRO	Peptide
1	C	544	PRO	Mainchain
1	D	129	ASN	Peptide
1	D	223	ASP	Peptide
1	D	351	PRO	Peptide
1	D	540	ILE	Mainchain

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	4896	0	4954	110	0
1	B	4896	0	4954	109	0
1	C	4896	0	4953	119	0
1	D	4896	0	4953	123	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
2	C	17	0	0	0	0
2	D	17	0	0	0	0
3	A	2	0	0	0	0
All	All	19654	0	19814	428	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (428) 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:D:544:PRO:C	1:D:545:ALA:N	1.73	1.42
1:D:535:GLU:OE1	1:D:541:ILE:HB	1.54	1.06
1:D:535:GLU:CD	1:D:541:ILE:HB	1.93	0.88
1:B:535:GLU:HG3	1:C:559:TYR:HE2	1.58	0.68
1:A:535:GLU:HG3	1:B:559:TYR:HE2	1.58	0.68
1:D:535:GLU:OE2	1:D:541:ILE:N	2.27	0.68
1:A:374:GLN:HG3	1:A:375:GLU:HG2	1.76	0.68
1:C:40:GLN:NE2	1:C:78:MET:SD	2.66	0.68
1:A:40:GLN:NE2	1:A:78:MET:SD	2.66	0.68
1:D:40:GLN:NE2	1:D:78:MET:SD	2.66	0.68
1:D:263:ARG:NH2	1:D:282:GLU:OE2	2.28	0.67
1:A:263:ARG:NH2	1:A:282:GLU:OE2	2.28	0.67
1:D:374:GLN:HG3	1:D:375:GLU:HG2	1.76	0.67
1:A:559:TYR:HE2	1:D:535:GLU:HG3	1.59	0.67
1:B:40:GLN:NE2	1:B:78:MET:SD	2.66	0.67
1:D:57:ASP:HB3	1:D:60:ALA:HB3	1.77	0.67
1:B:263:ARG:NH2	1:B:282:GLU:OE2	2.27	0.66
1:C:263:ARG:NH2	1:C:282:GLU:OE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASP:HB3	1:A:60:ALA:HB3	1.77	0.66
1:C:57:ASP:HB3	1:C:60:ALA:HB3	1.77	0.66
1:B:56:ASN:ND2	1:B:93:GLU:OE2	2.29	0.66
1:B:374:GLN:HG3	1:B:375:GLU:HG2	1.76	0.65
1:C:535:GLU:HG3	1:D:559:TYR:HE2	1.61	0.65
1:C:374:GLN:HG3	1:C:375:GLU:HG2	1.76	0.65
1:D:56:ASN:ND2	1:D:93:GLU:OE2	2.30	0.65
1:D:360:THR:HG1	1:D:366:THR:HG1	1.44	0.65
1:A:56:ASN:ND2	1:A:93:GLU:OE2	2.29	0.65
1:B:57:ASP:HB3	1:B:60:ALA:HB3	1.77	0.65
1:C:56:ASN:ND2	1:C:93:GLU:OE2	2.30	0.64
1:C:353:LYS:HB3	1:C:373:LEU:HG	1.80	0.64
1:C:360:THR:HG1	1:C:366:THR:HG1	1.46	0.63
1:B:353:LYS:HB3	1:B:373:LEU:HG	1.80	0.63
1:D:149:GLY:O	1:D:153:ARG:NH2	2.32	0.63
1:D:175:SER:HB3	1:D:178:ILE:HD13	1.80	0.63
1:B:175:SER:HB3	1:B:178:ILE:HD13	1.80	0.63
1:C:149:GLY:O	1:C:153:ARG:NH2	2.32	0.62
1:B:149:GLY:O	1:B:153:ARG:NH2	2.32	0.62
1:B:297:ILE:HD11	1:B:598:VAL:HG23	1.81	0.62
1:C:175:SER:HB3	1:C:178:ILE:HD13	1.80	0.62
1:A:149:GLY:O	1:A:153:ARG:NH2	2.32	0.62
1:A:297:ILE:HD11	1:A:598:VAL:HG23	1.82	0.62
1:A:353:LYS:HB3	1:A:373:LEU:HG	1.80	0.62
1:C:297:ILE:HD11	1:C:598:VAL:HG23	1.82	0.62
1:D:353:LYS:HB3	1:D:373:LEU:HG	1.80	0.62
1:D:297:ILE:HD11	1:D:598:VAL:HG23	1.81	0.62
1:B:490:LEU:HD13	1:C:568:LEU:HD12	1.82	0.62
1:A:175:SER:HB3	1:A:178:ILE:HD13	1.80	0.61
1:C:554:MET:SD	1:C:554:MET:N	2.74	0.60
1:A:36:GLN:NE2	1:A:113:GLU:OE2	2.35	0.60
1:B:554:MET:SD	1:B:554:MET:N	2.74	0.60
1:C:277:LEU:HD23	1:C:632:ARG:HB3	1.84	0.60
1:B:36:GLN:NE2	1:B:113:GLU:OE2	2.35	0.60
1:D:277:LEU:HD23	1:D:632:ARG:HB3	1.84	0.60
1:A:554:MET:SD	1:A:554:MET:N	2.74	0.60
1:B:478:PHE:O	1:B:482:ILE:N	2.35	0.59
1:C:190:ARG:HG3	1:C:232:LEU:HD12	1.85	0.59
1:D:478:PHE:O	1:D:482:ILE:N	2.35	0.59
1:D:522:HIS:ND1	1:D:544:PRO:HB3	2.16	0.59
1:D:190:ARG:HG3	1:D:232:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:GLN:NE2	1:C:113:GLU:OE2	2.35	0.59
1:D:36:GLN:NE2	1:D:113:GLU:OE2	2.35	0.59
1:D:554:MET:N	1:D:554:MET:SD	2.74	0.59
1:B:280:LEU:HD12	1:B:283:ILE:HB	1.85	0.59
1:A:280:LEU:HD12	1:A:283:ILE:HB	1.85	0.59
1:B:174:ASN:ND2	1:B:211:PHE:O	2.36	0.59
1:C:280:LEU:HD12	1:C:283:ILE:HB	1.85	0.59
1:D:174:ASN:ND2	1:D:211:PHE:O	2.36	0.59
1:B:76:GLY:H	1:B:80:GLU:H	1.51	0.58
1:C:452:VAL:HG13	1:C:453:PRO:HD3	1.85	0.58
1:A:277:LEU:HD23	1:A:632:ARG:HB3	1.84	0.58
1:B:190:ARG:HG3	1:B:232:LEU:HD12	1.84	0.58
1:C:174:ASN:ND2	1:C:211:PHE:O	2.36	0.58
1:A:174:ASN:ND2	1:A:211:PHE:O	2.36	0.58
1:A:490:LEU:HD13	1:B:568:LEU:HD12	1.84	0.58
1:B:452:VAL:HG13	1:B:453:PRO:HD3	1.85	0.58
1:A:190:ARG:HG3	1:A:232:LEU:HD12	1.85	0.58
1:B:277:LEU:HD23	1:B:632:ARG:HB3	1.84	0.58
1:A:452:VAL:HG13	1:A:453:PRO:HD3	1.85	0.58
1:C:76:GLY:H	1:C:80:GLU:H	1.51	0.58
1:A:549:VAL:HG21	1:D:367:LEU:HD13	1.85	0.58
1:D:280:LEU:HD12	1:D:283:ILE:HB	1.85	0.58
1:D:452:VAL:HG13	1:D:453:PRO:HD3	1.85	0.58
1:D:351:PRO:HB3	1:D:373:LEU:HB2	1.86	0.57
1:A:568:LEU:HD12	1:D:490:LEU:HD13	1.85	0.57
1:A:76:GLY:H	1:A:80:GLU:H	1.51	0.57
1:C:172:CYS:SG	1:C:206:GLN:NE2	2.77	0.57
1:C:478:PHE:O	1:C:482:ILE:N	2.35	0.57
1:A:172:CYS:SG	1:A:206:GLN:NE2	2.77	0.57
1:B:172:CYS:SG	1:B:206:GLN:NE2	2.77	0.57
1:A:478:PHE:O	1:A:482:ILE:N	2.35	0.57
1:C:490:LEU:HD13	1:D:568:LEU:HD12	1.87	0.57
1:D:172:CYS:SG	1:D:206:GLN:NE2	2.77	0.57
1:B:351:PRO:HB3	1:B:373:LEU:HB2	1.86	0.57
1:D:76:GLY:H	1:D:80:GLU:H	1.51	0.56
1:A:351:PRO:HB3	1:A:373:LEU:HB2	1.86	0.56
1:C:193:ASP:OD1	1:C:197:ASN:N	2.38	0.56
1:C:351:PRO:HB3	1:C:373:LEU:HB2	1.86	0.56
1:D:272:PRO:HB2	1:D:636:ARG:HG3	1.88	0.56
1:D:546:ASN:HD22	1:D:549:VAL:HG22	1.70	0.56
1:A:272:PRO:HB2	1:A:636:ARG:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:536:LEU:HD11	1:D:544:PRO:HD2	1.88	0.56
1:B:193:ASP:OD1	1:B:197:ASN:N	2.38	0.56
1:B:237:ASN:OD1	1:B:241:LEU:N	2.38	0.56
1:B:469:ALA:HB1	1:B:475:LEU:HG	1.88	0.56
1:D:544:PRO:O	1:D:555:TYR:OH	2.16	0.56
1:A:350:ARG:NH2	1:A:450:GLU:OE1	2.39	0.56
1:A:546:ASN:HD22	1:A:549:VAL:HG22	1.70	0.56
1:B:350:ARG:NH2	1:B:450:GLU:OE1	2.39	0.56
1:A:193:ASP:OD1	1:A:197:ASN:N	2.38	0.56
1:A:469:ALA:HB1	1:A:475:LEU:HG	1.88	0.56
1:B:367:LEU:HD13	1:C:549:VAL:HG21	1.87	0.56
1:D:350:ARG:NH2	1:D:450:GLU:OE1	2.39	0.56
1:A:367:LEU:HD13	1:B:549:VAL:HG21	1.87	0.55
1:B:482:ILE:HD13	1:C:572:ASN:HD22	1.72	0.55
1:C:350:ARG:NH2	1:C:450:GLU:OE1	2.39	0.55
1:D:193:ASP:OD1	1:D:197:ASN:N	2.38	0.55
1:C:81:THR:OG1	1:C:82:ALA:N	2.39	0.55
1:C:272:PRO:HB2	1:C:636:ARG:HG3	1.88	0.55
1:C:367:LEU:HD13	1:D:549:VAL:HG21	1.87	0.55
1:D:237:ASN:OD1	1:D:241:LEU:N	2.38	0.55
1:A:81:THR:OG1	1:A:82:ALA:N	2.39	0.55
1:C:469:ALA:HB1	1:C:475:LEU:HG	1.88	0.55
1:C:546:ASN:HD22	1:C:549:VAL:HG22	1.70	0.55
1:B:272:PRO:HB2	1:B:636:ARG:HG3	1.88	0.54
1:B:546:ASN:HD22	1:B:549:VAL:HG22	1.70	0.54
1:D:102:ALA:HB1	1:D:105:LEU:HD13	1.90	0.54
1:D:469:ALA:HB1	1:D:475:LEU:HG	1.88	0.54
1:C:237:ASN:OD1	1:C:241:LEU:N	2.38	0.54
1:A:357:ASN:H	1:A:371:LYS:HZ3	1.55	0.54
1:A:237:ASN:OD1	1:A:241:LEU:N	2.38	0.54
1:A:102:ALA:HB1	1:A:105:LEU:HD13	1.90	0.54
1:B:102:ALA:HB1	1:B:105:LEU:HD13	1.90	0.54
1:A:482:ILE:HD13	1:B:572:ASN:HD22	1.73	0.54
1:C:102:ALA:HB1	1:C:105:LEU:HD13	1.90	0.54
1:C:482:ILE:HD13	1:D:572:ASN:HD22	1.72	0.54
1:A:355:ARG:HH22	1:A:360:THR:HB	1.73	0.53
1:B:355:ARG:HH22	1:B:360:THR:HB	1.73	0.53
1:D:244:PHE:HA	1:D:259:LEU:HD21	1.91	0.53
1:A:572:ASN:HD22	1:D:482:ILE:HD13	1.73	0.53
1:C:355:ARG:HH22	1:C:360:THR:HB	1.73	0.53
1:B:81:THR:OG1	1:B:82:ALA:N	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:THR:HG23	1:B:200:LEU:H	1.74	0.53
1:D:355:ARG:HH22	1:D:360:THR:HB	1.73	0.53
1:C:198:THR:HG23	1:C:200:LEU:H	1.74	0.53
1:D:81:THR:OG1	1:D:82:ALA:N	2.39	0.53
1:B:365:ASN:HB2	1:C:550:ASP:H	1.73	0.53
1:C:244:PHE:HA	1:C:259:LEU:HD21	1.91	0.52
1:D:198:THR:HG23	1:D:200:LEU:H	1.74	0.52
1:B:257:GLN:NE2	1:B:310:GLN:OE1	2.35	0.52
1:D:143:VAL:HG21	1:D:187:ALA:HA	1.91	0.52
1:A:244:PHE:HA	1:A:259:LEU:HD21	1.91	0.52
1:A:168:SER:HA	1:A:199:VAL:HG23	1.92	0.52
1:A:198:THR:HG23	1:A:200:LEU:H	1.74	0.52
1:D:357:ASN:H	1:D:371:LYS:HZ3	1.58	0.52
1:A:143:VAL:HG21	1:A:187:ALA:HA	1.91	0.52
1:A:460:LEU:HA	1:A:463:CYS:HB3	1.92	0.52
1:B:143:VAL:HG21	1:B:187:ALA:HA	1.91	0.52
1:D:168:SER:HA	1:D:199:VAL:HG23	1.92	0.52
1:D:512:PHE:HD2	1:D:523:PHE:HD2	1.57	0.52
1:A:326:ARG:HA	1:A:329:PHE:HB3	1.93	0.51
1:B:244:PHE:HA	1:B:259:LEU:HD21	1.91	0.51
1:C:257:GLN:NE2	1:C:310:GLN:OE1	2.35	0.51
1:A:512:PHE:HD2	1:A:523:PHE:HD2	1.57	0.51
1:B:357:ASN:H	1:B:371:LYS:HZ3	1.57	0.51
1:C:143:VAL:HG21	1:C:187:ALA:HA	1.91	0.51
1:B:460:LEU:HA	1:B:463:CYS:HB3	1.92	0.51
1:C:168:SER:HA	1:C:199:VAL:HG23	1.92	0.51
1:A:294:GLU:OE1	1:A:606:ARG:NH2	2.43	0.51
1:A:365:ASN:HB2	1:B:550:ASP:H	1.76	0.51
1:B:326:ARG:HA	1:B:329:PHE:HB3	1.93	0.51
1:D:200:LEU:HD11	1:D:216:TYR:HE1	1.76	0.51
1:A:200:LEU:HD11	1:A:216:TYR:HE1	1.76	0.51
1:C:460:LEU:HA	1:C:463:CYS:HB3	1.92	0.51
1:D:294:GLU:OE1	1:D:606:ARG:NH2	2.43	0.51
1:B:294:GLU:OE1	1:B:606:ARG:NH2	2.43	0.51
1:B:168:SER:HA	1:B:199:VAL:HG23	1.92	0.51
1:C:326:ARG:HA	1:C:329:PHE:HB3	1.92	0.51
1:D:40:GLN:NE2	1:D:80:GLU:OE2	2.44	0.50
1:D:535:GLU:OE2	1:D:541:ILE:CA	2.59	0.50
1:B:200:LEU:HD11	1:B:216:TYR:HE1	1.76	0.50
1:B:351:PRO:HD3	1:B:385:ARG:HH12	1.77	0.50
1:B:512:PHE:HD2	1:B:523:PHE:HD2	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:PHE:HD2	1:C:523:PHE:HD2	1.57	0.50
1:D:351:PRO:HD3	1:D:385:ARG:HH12	1.77	0.50
1:A:40:GLN:NE2	1:A:80:GLU:OE2	2.44	0.50
1:B:40:GLN:NE2	1:B:80:GLU:OE2	2.44	0.50
1:C:200:LEU:HD11	1:C:216:TYR:HE1	1.76	0.50
1:D:460:LEU:HA	1:D:463:CYS:HB3	1.92	0.50
1:C:294:GLU:OE1	1:C:606:ARG:NH2	2.43	0.50
1:A:351:PRO:HD3	1:A:385:ARG:HH12	1.77	0.50
1:C:198:THR:OG1	1:C:199:VAL:N	2.45	0.50
1:B:198:THR:OG1	1:B:199:VAL:N	2.45	0.49
1:C:385:ARG:O	1:C:389:GLU:N	2.45	0.49
1:D:326:ARG:HA	1:D:329:PHE:HB3	1.92	0.49
1:C:40:GLN:NE2	1:C:80:GLU:OE2	2.44	0.49
1:C:351:PRO:HD3	1:C:385:ARG:HH12	1.77	0.49
1:D:385:ARG:O	1:D:389:GLU:N	2.45	0.49
1:A:34:ASP:HB2	1:D:632:ARG:HD3	1.93	0.49
1:D:198:THR:OG1	1:D:199:VAL:N	2.45	0.49
1:D:257:GLN:NE2	1:D:310:GLN:OE1	2.35	0.49
1:A:198:THR:OG1	1:A:199:VAL:N	2.45	0.49
1:C:632:ARG:HD3	1:D:34:ASP:HB2	1.92	0.49
1:D:535:GLU:OE2	1:D:541:ILE:HB	2.12	0.49
1:A:550:ASP:H	1:D:365:ASN:HB2	1.76	0.49
1:C:390:LEU:HA	1:C:393:VAL:HG12	1.95	0.49
1:A:385:ARG:O	1:A:389:GLU:N	2.45	0.49
1:D:390:LEU:HA	1:D:393:VAL:HG12	1.95	0.49
1:A:390:LEU:HA	1:A:393:VAL:HG12	1.95	0.48
1:B:385:ARG:O	1:B:389:GLU:N	2.45	0.48
1:A:632:ARG:HD3	1:B:34:ASP:HB2	1.95	0.48
1:C:357:ASN:H	1:C:371:LYS:HZ3	1.61	0.48
1:D:167:LEU:HD11	1:D:189:ILE:HA	1.96	0.48
1:A:167:LEU:HD11	1:A:189:ILE:HA	1.96	0.48
1:C:365:ASN:HB2	1:D:550:ASP:H	1.78	0.48
1:B:390:LEU:HA	1:B:393:VAL:HG12	1.95	0.48
1:C:269:THR:HG22	1:C:274:THR:HG23	1.96	0.48
1:A:257:GLN:NE2	1:A:310:GLN:OE1	2.35	0.48
1:A:269:THR:HG22	1:A:274:THR:HG23	1.96	0.48
1:A:355:ARG:HD3	1:A:369:GLN:HA	1.96	0.48
1:B:167:LEU:HD11	1:B:189:ILE:HA	1.96	0.48
1:C:355:ARG:HD3	1:C:369:GLN:HA	1.96	0.48
1:D:355:ARG:HD3	1:D:369:GLN:HA	1.96	0.48
1:C:167:LEU:HD11	1:C:189:ILE:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:HA	1:D:64:LEU:HD13	1.97	0.47
1:D:373:LEU:HD13	1:D:376:ALA:HB3	1.96	0.47
1:A:49:LEU:HA	1:A:64:LEU:HD13	1.97	0.47
1:C:36:GLN:HE21	1:C:78:MET:HB3	1.80	0.47
1:A:373:LEU:HD13	1:A:376:ALA:HB3	1.96	0.47
1:D:246:LEU:HA	1:D:249:VAL:HG12	1.97	0.47
1:A:36:GLN:HE21	1:A:78:MET:HB3	1.79	0.47
1:B:246:LEU:HA	1:B:249:VAL:HG12	1.97	0.47
1:D:36:GLN:HE21	1:D:78:MET:HB3	1.79	0.47
1:A:246:LEU:HA	1:A:249:VAL:HG12	1.97	0.47
1:B:47:SER:HB2	1:B:50:LEU:HB2	1.97	0.47
1:B:269:THR:HG22	1:B:274:THR:HG23	1.96	0.47
1:B:355:ARG:HD3	1:B:369:GLN:HA	1.96	0.47
1:B:373:LEU:HD13	1:B:376:ALA:HB3	1.96	0.47
1:B:632:ARG:HD3	1:C:34:ASP:HB2	1.95	0.47
1:C:246:LEU:HA	1:C:249:VAL:HG12	1.97	0.47
1:C:474:MET:HG3	1:D:492:ARG:HG3	1.96	0.47
1:A:47:SER:HB2	1:A:50:LEU:HB2	1.97	0.47
1:B:139:ARG:HA	1:B:139:ARG:HD3	1.67	0.47
1:B:81:THR:HG23	1:B:84:HIS:HD1	1.80	0.47
1:C:47:SER:HB2	1:C:50:LEU:HB2	1.97	0.47
1:D:536:LEU:HD11	1:D:544:PRO:CD	2.45	0.47
1:C:43:ARG:NH1	1:C:75:ARG:O	2.49	0.46
1:A:43:ARG:NH1	1:A:75:ARG:O	2.48	0.46
1:B:36:GLN:HE21	1:B:78:MET:HB3	1.79	0.46
1:C:373:LEU:HD13	1:C:376:ALA:HB3	1.96	0.46
1:D:397:ILE:HA	1:D:400:LEU:HB2	1.97	0.46
1:D:43:ARG:NH1	1:D:75:ARG:O	2.48	0.46
1:A:397:ILE:HA	1:A:400:LEU:HB2	1.97	0.46
1:A:493:PHE:CG	1:A:573:LEU:HD13	2.51	0.46
1:B:49:LEU:HA	1:B:64:LEU:HD13	1.97	0.46
1:C:81:THR:HG23	1:C:84:HIS:HD1	1.80	0.46
1:D:269:THR:HG22	1:D:274:THR:HG23	1.96	0.46
1:C:49:LEU:HA	1:C:64:LEU:HD13	1.97	0.46
1:D:433:ALA:HA	1:D:436:VAL:HG12	1.97	0.46
1:A:420:ILE:O	1:A:483:GLN:NE2	2.49	0.46
1:B:43:ARG:NH1	1:B:75:ARG:O	2.49	0.46
1:B:397:ILE:HA	1:B:400:LEU:HB2	1.97	0.46
1:D:139:ARG:HA	1:D:139:ARG:HD3	1.67	0.46
1:B:420:ILE:O	1:B:483:GLN:NE2	2.49	0.46
1:C:321:TRP:CE2	1:C:597:ILE:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:522:HIS:CE1	1:D:544:PRO:HB3	2.51	0.46
1:A:564:ILE:HA	1:A:567:THR:HG22	1.98	0.46
1:A:610:ARG:NH1	1:A:613:TRP:O	2.49	0.46
1:B:321:TRP:CE2	1:B:597:ILE:HD11	2.51	0.46
1:B:564:ILE:HA	1:B:567:THR:HG22	1.98	0.46
1:B:569:LEU:O	1:B:573:LEU:N	2.45	0.46
1:C:564:ILE:HA	1:C:567:THR:HG22	1.98	0.46
1:D:47:SER:HB2	1:D:50:LEU:HB2	1.97	0.46
1:D:321:TRP:CE2	1:D:597:ILE:HD11	2.51	0.46
1:D:564:ILE:HA	1:D:567:THR:HG22	1.98	0.46
1:A:59:GLN:HA	1:A:62:ASN:HD22	1.81	0.46
1:B:312:PRO:HG2	1:B:313:VAL:HG23	1.98	0.46
1:D:59:GLN:HA	1:D:62:ASN:HD22	1.81	0.46
1:C:139:ARG:HA	1:C:139:ARG:HD3	1.67	0.45
1:C:312:PRO:HG2	1:C:313:VAL:HG23	1.98	0.45
1:C:610:ARG:NH1	1:C:613:TRP:O	2.49	0.45
1:A:81:THR:HG23	1:A:84:HIS:HD1	1.80	0.45
1:A:321:TRP:CE2	1:A:597:ILE:HD11	2.51	0.45
1:A:433:ALA:HA	1:A:436:VAL:HG12	1.97	0.45
1:B:493:PHE:CG	1:B:573:LEU:HD13	2.51	0.45
1:D:420:ILE:O	1:D:483:GLN:NE2	2.49	0.45
1:D:610:ARG:NH1	1:D:613:TRP:O	2.49	0.45
1:B:610:ARG:NH1	1:B:613:TRP:O	2.49	0.45
1:C:493:PHE:CG	1:C:573:LEU:HD13	2.51	0.45
1:D:493:PHE:CG	1:D:573:LEU:HD13	2.51	0.45
1:C:59:GLN:HA	1:C:62:ASN:HD22	1.81	0.45
1:C:397:ILE:HA	1:C:400:LEU:HB2	1.97	0.45
1:C:420:ILE:O	1:C:483:GLN:NE2	2.49	0.45
1:A:312:PRO:HG2	1:A:313:VAL:HG23	1.98	0.45
1:C:569:LEU:O	1:C:573:LEU:N	2.45	0.45
1:D:81:THR:HG23	1:D:84:HIS:HD1	1.80	0.45
1:D:307:ILE:HD12	1:D:307:ILE:HA	1.88	0.45
1:B:433:ALA:HA	1:B:436:VAL:HG12	1.97	0.45
1:D:312:PRO:HG2	1:D:313:VAL:HG23	1.98	0.45
1:B:59:GLN:HA	1:B:62:ASN:HD22	1.81	0.45
1:A:492:ARG:HG3	1:D:474:MET:HG3	1.98	0.45
1:A:542:ASP:O	1:D:541:ILE:HA	2.16	0.45
1:B:182:LEU:H	1:B:182:LEU:HG	1.51	0.45
1:C:217:ASN:OD1	1:C:217:ASN:N	2.50	0.45
1:D:217:ASN:OD1	1:D:217:ASN:N	2.50	0.45
1:C:433:ALA:HA	1:C:436:VAL:HG12	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:PRO:HG2	1:B:555:TYR:OH	2.17	0.44
1:C:270:TYR:HB3	1:C:273:LEU:HG	1.99	0.44
1:D:302:ARG:HA	1:D:302:ARG:HD3	1.73	0.44
1:B:270:TYR:HB3	1:B:273:LEU:HG	1.99	0.44
1:B:420:ILE:HA	1:B:424:PRO:HB3	1.99	0.44
1:B:619:CYS:SG	1:B:629:TRP:NE1	2.91	0.44
1:A:569:LEU:O	1:A:573:LEU:N	2.46	0.44
1:D:420:ILE:HA	1:D:424:PRO:HB3	1.99	0.44
1:A:474:MET:HG3	1:B:492:ARG:HG3	1.99	0.44
1:A:619:CYS:SG	1:A:629:TRP:NE1	2.91	0.44
1:B:217:ASN:N	1:B:217:ASN:OD1	2.50	0.44
1:A:544:PRO:HG2	1:A:555:TYR:OH	2.17	0.44
1:C:357:ASN:HB2	1:C:371:LYS:HZ3	1.83	0.44
1:C:619:CYS:SG	1:C:629:TRP:NE1	2.91	0.44
1:A:270:TYR:HB3	1:A:273:LEU:HG	1.99	0.44
1:A:535:GLU:OE1	1:A:541:ILE:HB	2.18	0.44
1:A:302:ARG:HA	1:A:302:ARG:HD3	1.73	0.43
1:A:420:ILE:HA	1:A:424:PRO:HB3	1.99	0.43
1:A:571:LEU:HD13	1:A:571:LEU:HA	1.83	0.43
1:C:193:ASP:OD1	1:C:196:GLY:N	2.51	0.43
1:A:217:ASN:OD1	1:A:217:ASN:N	2.50	0.43
1:B:535:GLU:OE1	1:B:541:ILE:HB	2.18	0.43
1:B:570:MET:HA	1:B:573:LEU:HB3	2.00	0.43
1:D:270:TYR:HB3	1:D:273:LEU:HG	1.99	0.43
1:D:570:MET:HA	1:D:573:LEU:HB3	2.01	0.43
1:B:132:LEU:HA	1:B:135:ALA:HB3	2.01	0.43
1:D:132:LEU:HA	1:D:135:ALA:HB3	2.01	0.43
1:A:193:ASP:OD1	1:A:196:GLY:N	2.51	0.43
1:B:403:GLU:HA	1:B:406:ASP:HB3	2.00	0.43
1:D:193:ASP:OD1	1:D:196:GLY:N	2.51	0.43
1:D:536:LEU:CD1	1:D:544:PRO:HD3	2.48	0.43
1:D:571:LEU:HD13	1:D:571:LEU:HA	1.84	0.43
1:D:619:CYS:SG	1:D:629:TRP:NE1	2.91	0.43
1:A:403:GLU:HA	1:A:406:ASP:HB3	2.00	0.43
1:A:570:MET:HA	1:A:573:LEU:HB3	2.01	0.43
1:A:132:LEU:HA	1:A:135:ALA:HB3	2.01	0.43
1:C:330:CYS:O	1:C:334:ALA:N	2.51	0.43
1:B:193:ASP:OD1	1:B:196:GLY:N	2.51	0.43
1:C:132:LEU:HA	1:C:135:ALA:HB3	2.01	0.43
1:D:403:GLU:HA	1:D:406:ASP:HB3	2.00	0.43
1:C:420:ILE:HA	1:C:424:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:MET:HA	1:C:573:LEU:HB3	2.00	0.43
1:A:536:LEU:HD11	1:A:559:TYR:HE1	1.83	0.42
1:B:330:CYS:O	1:B:334:ALA:N	2.51	0.42
1:C:403:GLU:HA	1:C:406:ASP:HB3	2.00	0.42
1:C:575:ILE:HD11	1:C:578:MET:HE1	2.01	0.42
1:D:543:GLY:HA3	1:D:559:TYR:OH	2.19	0.42
1:B:474:MET:HG3	1:C:492:ARG:HG3	2.01	0.42
1:C:474:MET:O	1:D:492:ARG:NH1	2.46	0.42
1:B:425:PHE:HB3	1:B:464:ASN:HD21	1.85	0.42
1:C:182:LEU:H	1:C:182:LEU:HG	1.52	0.42
1:C:536:LEU:HD11	1:C:559:TYR:HE1	1.83	0.42
1:D:536:LEU:HD11	1:D:559:TYR:HE1	1.83	0.42
1:A:283:ILE:HG23	1:A:292:LEU:HD23	2.02	0.42
1:A:425:PHE:HB3	1:A:464:ASN:HD21	1.85	0.42
1:C:200:LEU:HD22	1:C:200:LEU:HA	1.89	0.42
1:C:283:ILE:HG23	1:C:292:LEU:HD23	2.02	0.42
1:D:619:CYS:HG	1:D:629:TRP:HE1	1.64	0.42
1:B:536:LEU:HD11	1:B:559:TYR:HE1	1.83	0.42
1:A:79:GLY:HA3	1:A:111:THR:OG1	2.20	0.42
1:C:425:PHE:HB3	1:C:464:ASN:HD21	1.85	0.42
1:D:425:PHE:HB3	1:D:464:ASN:HD21	1.85	0.42
1:D:536:LEU:HD12	1:D:544:PRO:HD3	2.02	0.42
1:C:296:ILE:HG12	1:C:307:ILE:HG21	2.02	0.42
1:D:283:ILE:HG23	1:D:292:LEU:HD23	2.02	0.42
1:D:330:CYS:O	1:D:334:ALA:N	2.51	0.42
1:B:283:ILE:HG23	1:B:292:LEU:HD23	2.02	0.41
1:D:569:LEU:O	1:D:573:LEU:N	2.46	0.41
1:C:396:ALA:O	1:C:400:LEU:N	2.53	0.41
1:D:256:PHE:CG	1:D:307:ILE:HD11	2.55	0.41
1:D:296:ILE:HG12	1:D:307:ILE:HG21	2.02	0.41
1:B:256:PHE:CG	1:B:307:ILE:HD11	2.55	0.41
1:C:256:PHE:CG	1:C:307:ILE:HD11	2.55	0.41
1:B:367:LEU:HG	1:C:516:ASP:HB3	2.01	0.41
1:C:359:ARG:H	1:C:359:ARG:HD3	1.86	0.41
1:C:581:THR:HG21	1:D:575:ILE:HG12	2.02	0.41
1:D:79:GLY:HA3	1:D:111:THR:OG1	2.20	0.41
1:C:286:SER:O	1:C:288:ASP:N	2.49	0.41
1:C:571:LEU:HD13	1:C:571:LEU:HA	1.84	0.41
1:D:57:ASP:O	1:D:61:LEU:N	2.54	0.41
1:D:359:ARG:H	1:D:359:ARG:HD3	1.86	0.41
1:A:57:ASP:O	1:A:61:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ILE:O	1:B:561:ALA:N	2.45	0.41
1:C:57:ASP:O	1:C:61:LEU:N	2.54	0.41
1:D:308:LEU:HD21	1:D:598:VAL:HG21	2.02	0.41
1:A:256:PHE:CG	1:A:307:ILE:HD11	2.55	0.41
1:A:139:ARG:HA	1:A:139:ARG:HD3	1.67	0.41
1:A:330:CYS:O	1:A:334:ALA:N	2.51	0.41
1:B:79:GLY:HA3	1:B:111:THR:OG1	2.20	0.41
1:C:557:ILE:O	1:C:561:ALA:N	2.46	0.41
1:A:296:ILE:HG12	1:A:307:ILE:HG21	2.02	0.41
1:A:359:ARG:H	1:A:359:ARG:HD3	1.86	0.41
1:A:367:LEU:HG	1:B:516:ASP:HB3	2.03	0.41
1:A:429:ILE:HD12	1:A:429:ILE:HA	1.97	0.41
1:B:57:ASP:O	1:B:61:LEU:N	2.54	0.41
1:B:296:ILE:HG12	1:B:307:ILE:HG21	2.03	0.41
1:B:307:ILE:HD12	1:B:307:ILE:HA	1.88	0.41
1:B:308:LEU:HD21	1:B:598:VAL:HG21	2.02	0.41
1:B:543:GLY:CA	1:B:559:TYR:OH	2.69	0.41
1:C:79:GLY:HA3	1:C:111:THR:OG1	2.20	0.41
1:C:308:LEU:HD21	1:C:598:VAL:HG21	2.02	0.41
1:C:321:TRP:CZ2	1:C:326:ARG:HB3	2.56	0.41
1:C:610:ARG:HA	1:C:610:ARG:HD2	1.94	0.41
1:D:182:LEU:HD12	1:D:183:ILE:HG23	2.03	0.41
1:D:428:LEU:HD12	1:D:460:LEU:HB2	2.03	0.41
1:B:359:ARG:H	1:B:359:ARG:HD3	1.86	0.41
1:C:490:LEU:O	1:C:494:CYS:N	2.52	0.41
1:B:321:TRP:CZ2	1:B:326:ARG:HB3	2.56	0.40
1:C:541:ILE:HG23	1:C:543:GLY:H	1.86	0.40
1:A:182:LEU:HD12	1:A:183:ILE:HG23	2.03	0.40
1:A:321:TRP:CZ2	1:A:326:ARG:HB3	2.56	0.40
1:A:428:LEU:HD12	1:A:460:LEU:HB2	2.03	0.40
1:B:182:LEU:HD12	1:B:183:ILE:HG23	2.03	0.40
1:B:541:ILE:HG23	1:B:543:GLY:H	1.86	0.40
1:C:81:THR:HG23	1:C:84:HIS:ND1	2.36	0.40
1:C:428:LEU:HD12	1:C:460:LEU:HB2	2.03	0.40
1:D:321:TRP:CZ2	1:D:326:ARG:HB3	2.56	0.40
1:A:302:ARG:HB3	1:A:305:ARG:HH21	1.86	0.40
1:A:490:LEU:O	1:A:494:CYS:N	2.52	0.40
1:A:308:LEU:HD21	1:A:598:VAL:HG21	2.02	0.40
1:C:182:LEU:HD12	1:C:183:ILE:HG23	2.03	0.40
1:C:50:LEU:HD13	1:C:50:LEU:HA	1.97	0.40
1:C:363:ARG:HD3	1:C:365:ASN:ND2	2.37	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	609/742 (82%)	541 (89%)	65 (11%)	3 (0%)	29	68
1	B	609/742 (82%)	540 (89%)	66 (11%)	3 (0%)	29	68
1	C	609/742 (82%)	541 (89%)	64 (10%)	4 (1%)	22	62
1	D	609/742 (82%)	540 (89%)	66 (11%)	3 (0%)	29	68
All	All	2436/2968 (82%)	2162 (89%)	261 (11%)	13 (0%)	32	68

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	VAL
1	B	585	VAL
1	C	585	VAL
1	D	585	VAL
1	C	545	ALA
1	A	373	LEU
1	A	584	ARG
1	B	373	LEU
1	C	373	LEU
1	D	373	LEU
1	B	584	ARG
1	C	584	ARG
1	D	584	ARG

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	529/645 (82%)	502 (95%)	27 (5%)	24	50
1	B	529/645 (82%)	502 (95%)	27 (5%)	24	50
1	C	529/645 (82%)	502 (95%)	27 (5%)	24	50
1	D	529/645 (82%)	502 (95%)	27 (5%)	24	50
All	All	2116/2580 (82%)	2008 (95%)	108 (5%)	27	50

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	51	LEU
1	A	78	MET
1	A	81	THR
1	A	96	MET
1	A	136	LEU
1	A	139	ARG
1	A	140	ARG
1	A	144	SER
1	A	153	ARG
1	A	182	LEU
1	A	190	ARG
1	A	208	ASN
1	A	229	LEU
1	A	262	LYS
1	A	352	LEU
1	A	359	ARG
1	A	410	MET
1	A	421	LEU
1	A	452	VAL
1	A	464	ASN
1	A	554	MET
1	A	556	SER
1	A	571	LEU
1	A	589	ARG
1	A	604	LEU
1	A	608	LEU
1	B	34	ASP
1	B	51	LEU
1	B	78	MET

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Mol	Chain	Res	Type
1	B	81	THR
1	B	96	MET
1	B	136	LEU
1	B	139	ARG
1	B	140	ARG
1	B	144	SER
1	B	153	ARG
1	B	182	LEU
1	B	190	ARG
1	B	208	ASN
1	B	229	LEU
1	B	262	LYS
1	B	352	LEU
1	B	359	ARG
1	B	410	MET
1	B	421	LEU
1	B	452	VAL
1	B	464	ASN
1	B	554	MET
1	B	556	SER
1	B	571	LEU
1	B	589	ARG
1	B	604	LEU
1	B	608	LEU
1	C	34	ASP
1	C	51	LEU
1	C	78	MET
1	C	81	THR
1	C	96	MET
1	C	136	LEU
1	C	139	ARG
1	C	140	ARG
1	C	144	SER
1	C	153	ARG
1	C	182	LEU
1	C	190	ARG
1	C	208	ASN
1	C	229	LEU
1	C	262	LYS
1	C	352	LEU
1	C	359	ARG
1	C	410	MET

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Mol	Chain	Res	Type
1	C	421	LEU
1	C	452	VAL
1	C	464	ASN
1	C	554	MET
1	C	556	SER
1	C	571	LEU
1	C	589	ARG
1	C	604	LEU
1	C	608	LEU
1	D	34	ASP
1	D	51	LEU
1	D	78	MET
1	D	81	THR
1	D	96	MET
1	D	136	LEU
1	D	139	ARG
1	D	140	ARG
1	D	144	SER
1	D	153	ARG
1	D	182	LEU
1	D	190	ARG
1	D	208	ASN
1	D	229	LEU
1	D	262	LYS
1	D	352	LEU
1	D	359	ARG
1	D	410	MET
1	D	421	LEU
1	D	452	VAL
1	D	464	ASN
1	D	554	MET
1	D	556	SER
1	D	571	LEU
1	D	589	ARG
1	D	604	LEU
1	D	608	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	GLN
1	A	208	ASN

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Mol	Chain	Res	Type
1	A	464	ASN
1	A	546	ASN
1	B	206	GLN
1	B	208	ASN
1	B	464	ASN
1	B	546	ASN
1	C	206	GLN
1	C	208	ASN
1	C	464	ASN
1	C	522	HIS
1	C	546	ASN
1	D	206	GLN
1	D	208	ASN
1	D	464	ASN
1	D	546	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)

Of 6 ligands modelled in this entry, 2 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	$\#\|Z\|>2$
2	FZ4	B	801	1	16,18,18	0.74	0	17,22,22	1.50	2 (11%)
2	FZ4	C	801	1	16,18,18	0.75	0	17,22,22	1.52	2 (11%)
2	FZ4	D	801	1	16,18,18	0.76	0	17,22,22	1.51	2 (11%)
2	FZ4	A	801	1	16,18,18	0.75	0	17,22,22	1.51	2 (11%)

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	B	801	1	-	7/12/12/12	0/2/2/2
2	FZ4	C	801	1	-	7/12/12/12	0/2/2/2
2	FZ4	D	801	1	-	7/12/12/12	0/2/2/2
2	FZ4	A	801	1	-	7/12/12/12	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	FZ4	C13-C08-C09	3.24	120.51	116.88
2	D	801	FZ4	C13-C08-C09	3.23	120.49	116.88
2	A	801	FZ4	C13-C08-C09	3.22	120.48	116.88
2	B	801	FZ4	C13-C08-C09	3.22	120.48	116.88
2	D	801	FZ4	C07-C02-C03	3.20	120.46	116.88
2	C	801	FZ4	C07-C02-C03	3.19	120.45	116.88
2	A	801	FZ4	C07-C02-C03	3.18	120.43	116.88
2	B	801	FZ4	C07-C02-C03	3.16	120.41	116.88

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FZ4	O14-B01-C02-C03
2	A	801	FZ4	O14-B01-C02-C07
2	A	801	FZ4	C02-B01-O14-C15
2	A	801	FZ4	C08-B01-O14-C15
2	A	801	FZ4	O14-C15-C16-N17
2	B	801	FZ4	O14-B01-C02-C03

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

There are no ring outliers.

No monomer is involved in short contacts.

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	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	544:PRO	C	545:ALA	N	1.73
1	C	540:ILE	C	541:ILE	N	1.10

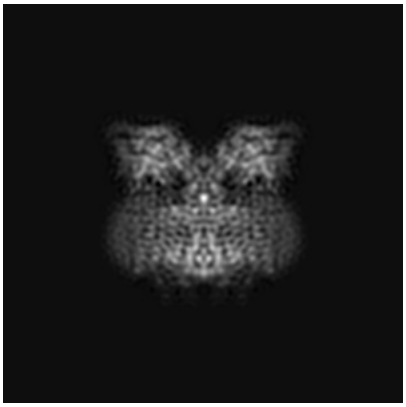
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-7825. These allow visual inspection of the internal detail of the map and identification of artifacts.

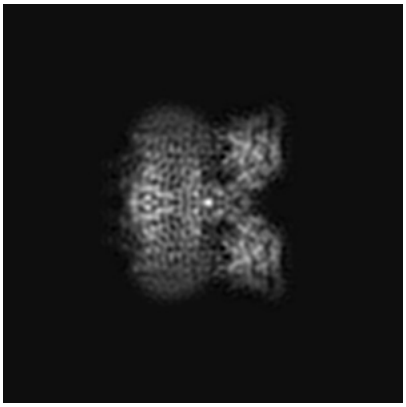
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

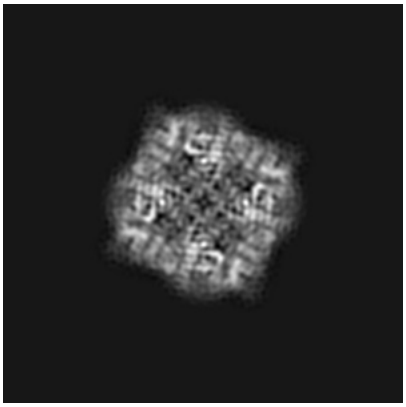
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices

6.2.1 Primary map

X Index: 102

Y Index: 102

Z Index: 102

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

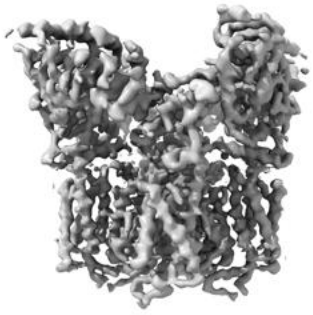
Y Index: 102

Z Index: 122

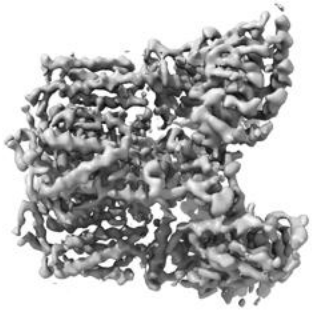
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

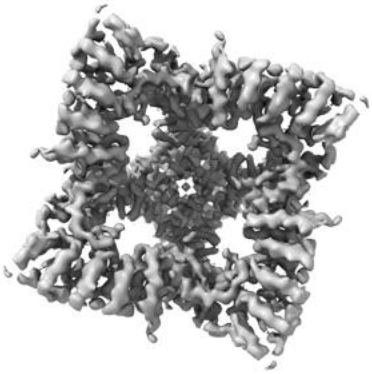
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0669. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

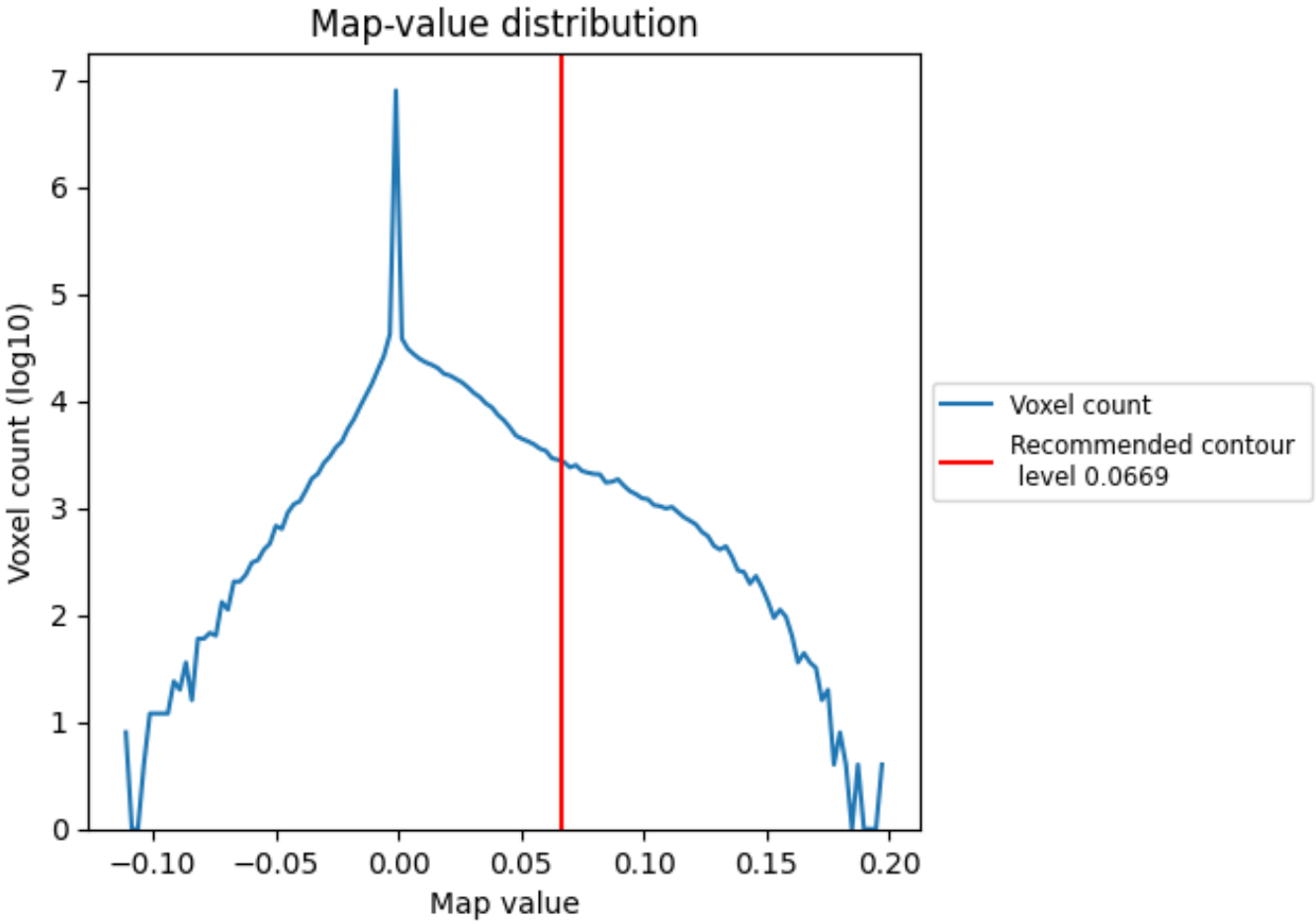
6.5 Mask visualisation (i)

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

7 Map analysis

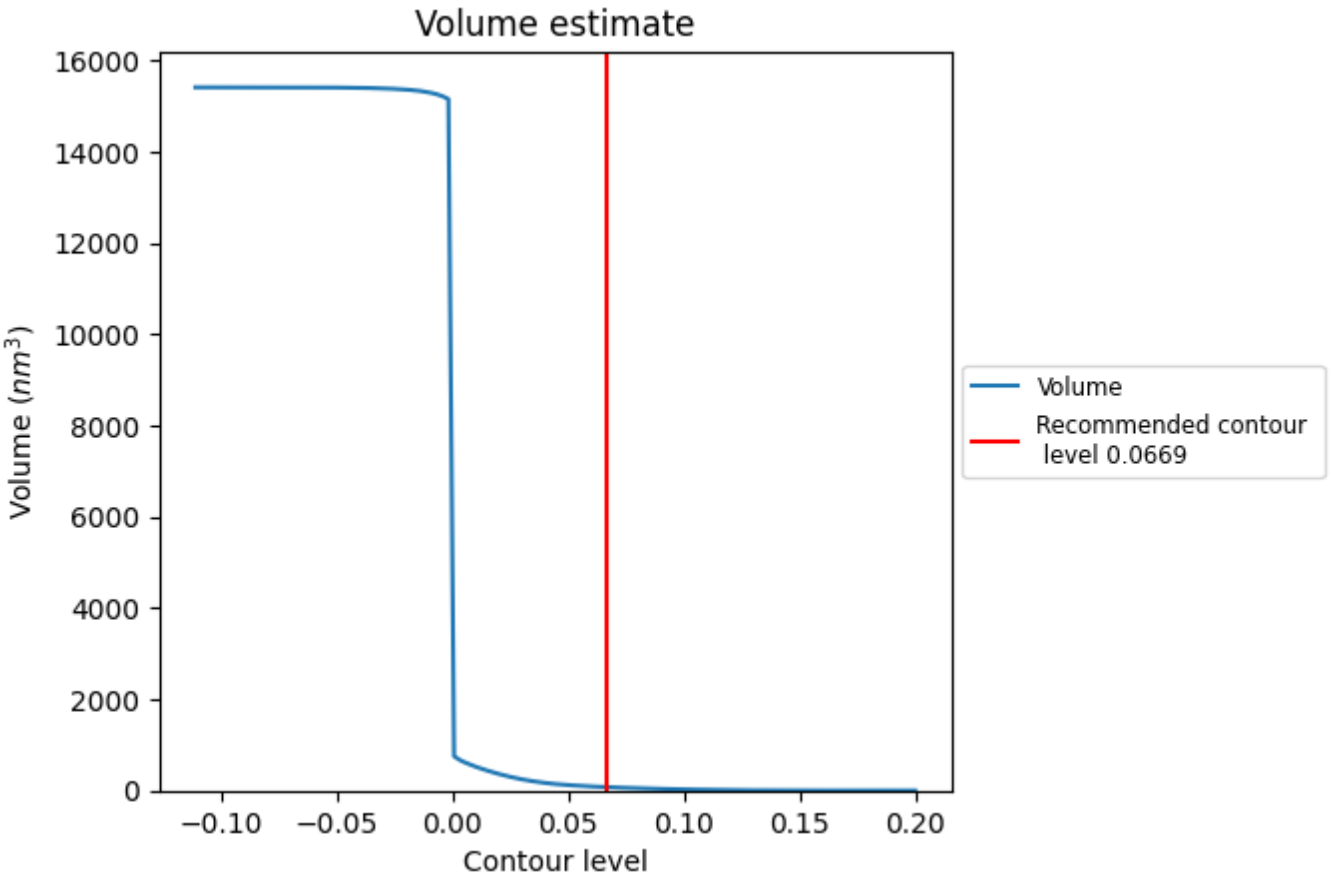
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

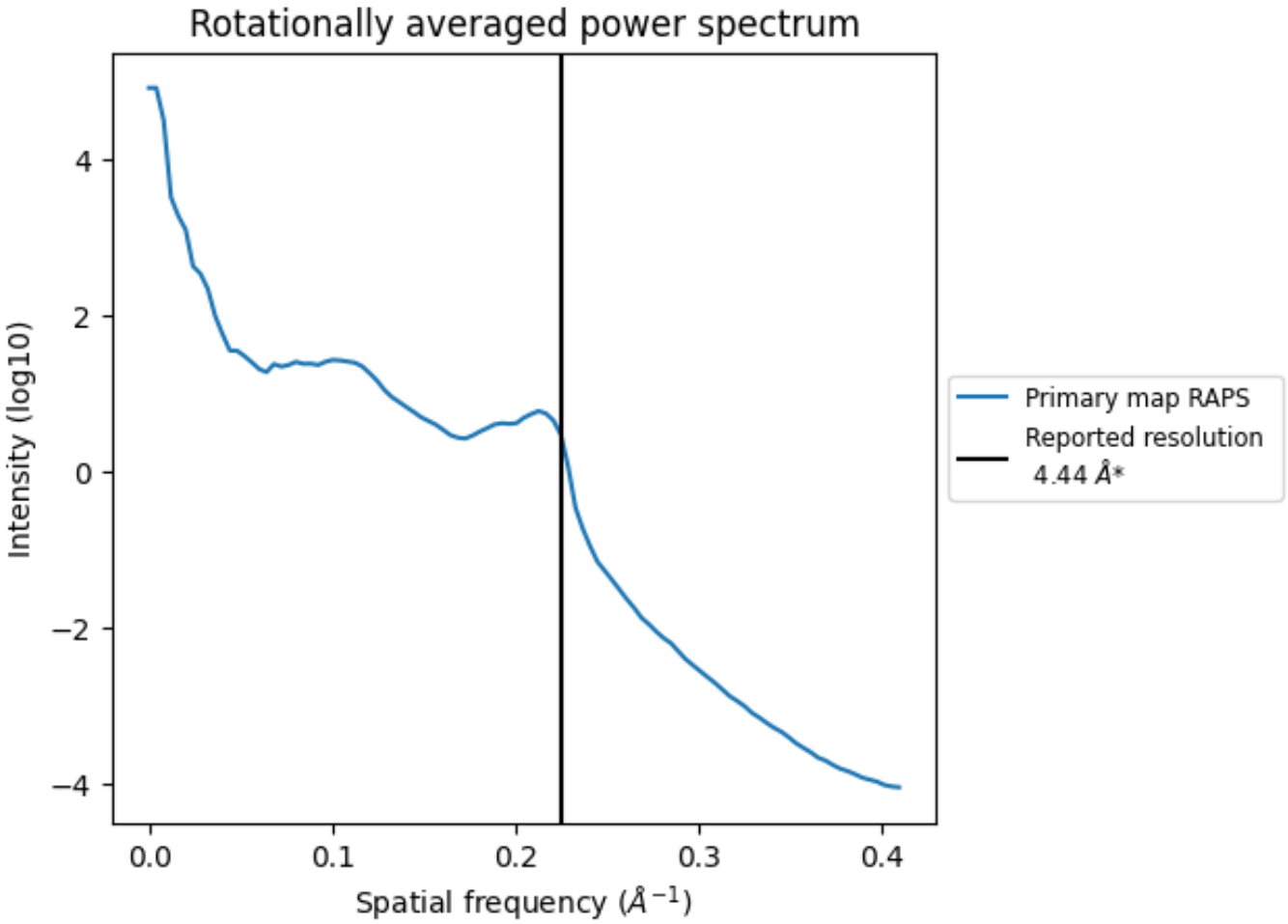
7.2 Volume estimate



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

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.225 $Å^{-1}$

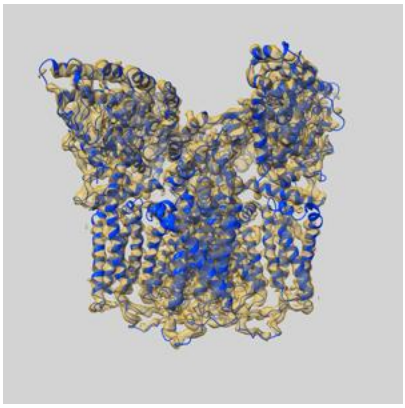
8 Fourier-Shell correlation

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

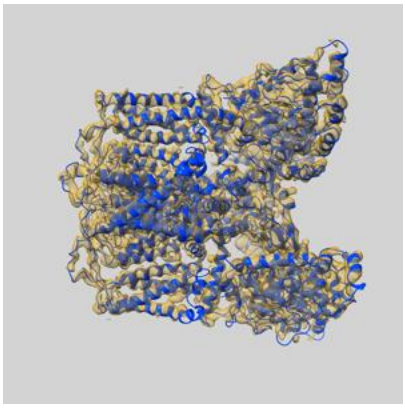
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-7825 and PDB model 6D7T. Per-residue inclusion information can be found in section 3 on page 7.

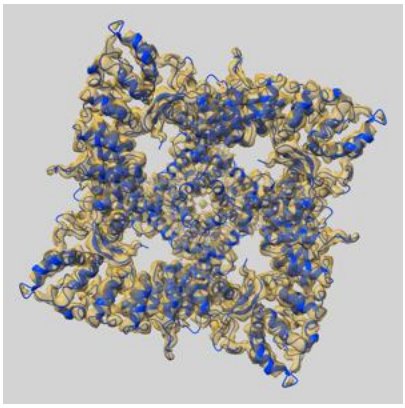
9.1 Map-model overlay



X



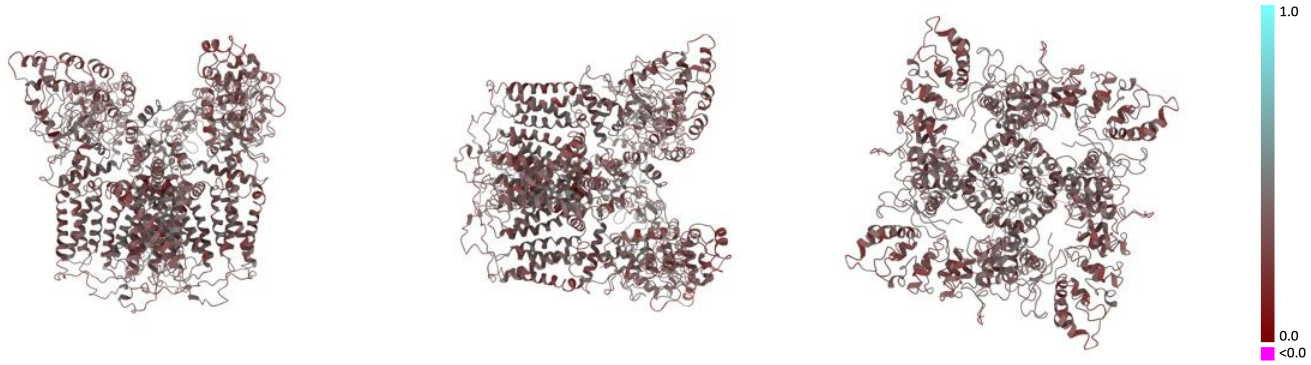
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0669 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.

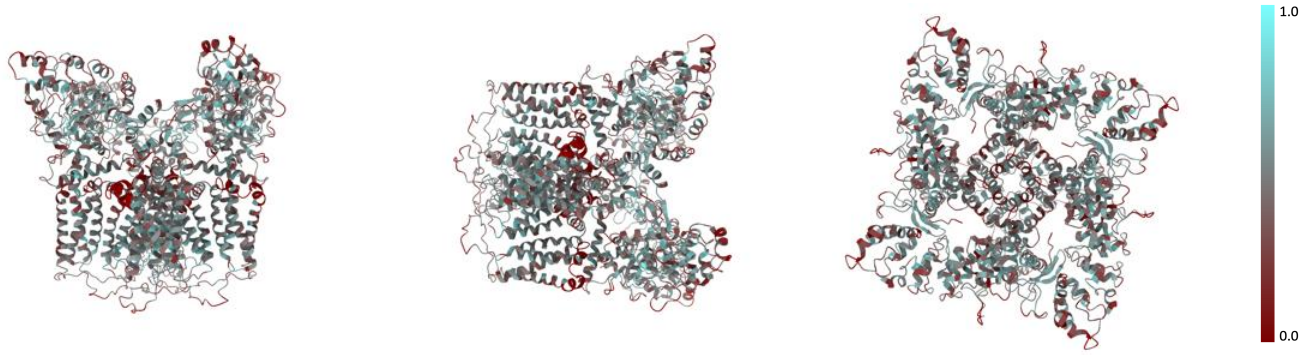
9.2 Q-score mapped to coordinate model (i)



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.

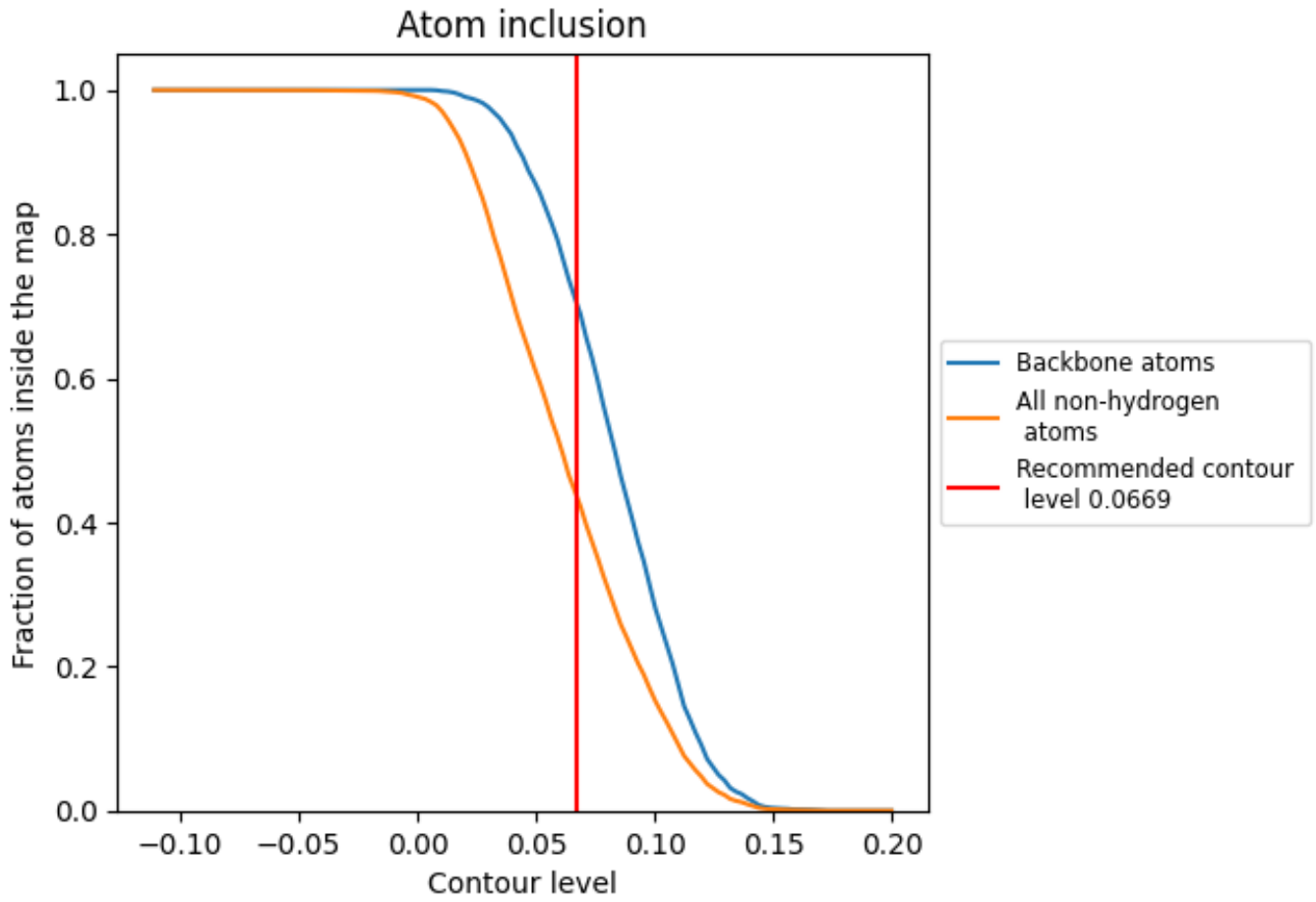
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0669).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 44% 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 (0.0669) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4379	0.3540
A	0.4375	0.3540
B	0.4381	0.3540
C	0.4389	0.3530
D	0.4371	0.3540