Full wwPDB EM Validation Report (i)

May 19, 2024 – 11:12 AM EDT

PDB ID	:	7MDM
EMDB ID	:	EMD-23775
Title	:	Structure of human p97 ATPase L464P mutant
Authors	:	Zhang, X.; Gui, L.; Li, S.; Nandi, P.; Columbres, R.C.; Wong, D.E.; Moen, D.R.; Lin, H.J.; Chiu, P.-L.; Chou, T.-F.
Deposited on	:	2021-04-05
Resolution	:	4.86 Å(reported)
Based on initial model	:	5FTK

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 (1)) were used in the production of this report:

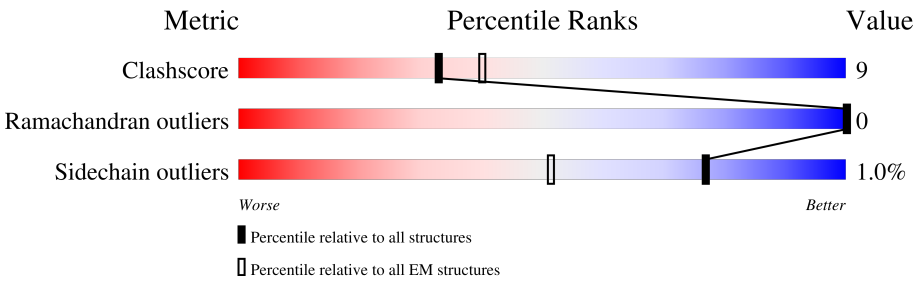
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.86 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	806	8% 67% 19% 13%
1	B	806	8% 65% 21% 13%
1	C	806	11% 65% 22% 13%
1	D	806	11% 67% 20% 13%
1	E	806	30% 65% 22% 13%
1	F	806	10% 49% 17% 33%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31986 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.

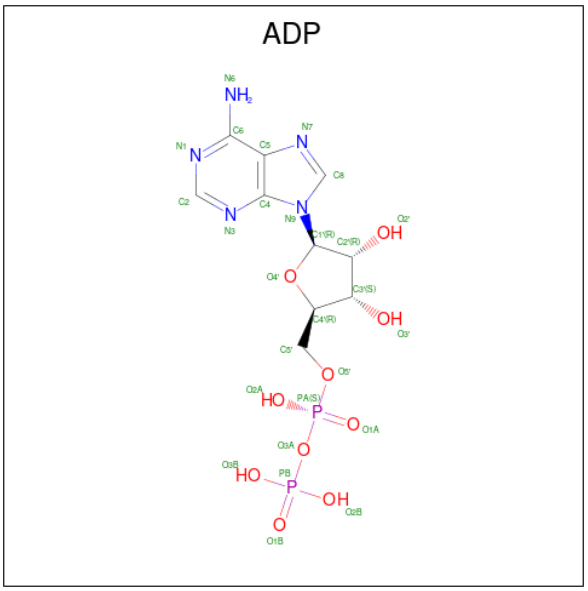
- Molecule 1 is a protein called Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	701	5513	3476	964	1043	30	0	0
1	C	703	5527	3485	967	1045	30	0	0
1	D	703	5527	3485	967	1045	30	0	0
1	E	704	5532	3488	968	1046	30	0	0
1	A	701	5513	3476	964	1043	30	0	0
1	F	539	4212	2653	737	800	22	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	464	PRO	LEU	engineered mutation	UNP P55072
C	464	PRO	LEU	engineered mutation	UNP P55072
D	464	PRO	LEU	engineered mutation	UNP P55072
E	464	PRO	LEU	engineered mutation	UNP P55072
A	464	PRO	LEU	engineered mutation	UNP P55072
F	464	PRO	LEU	engineered mutation	UNP P55072

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



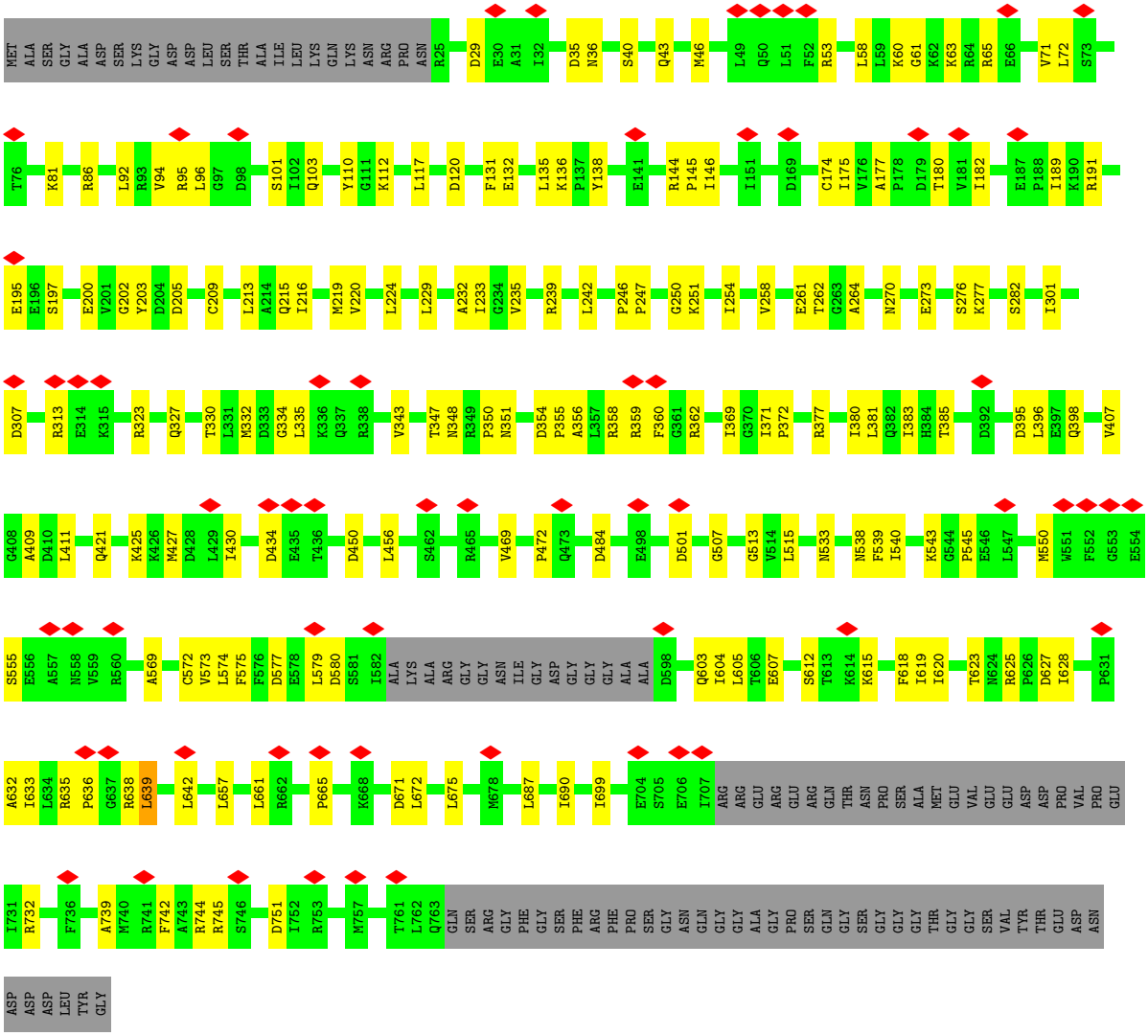
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

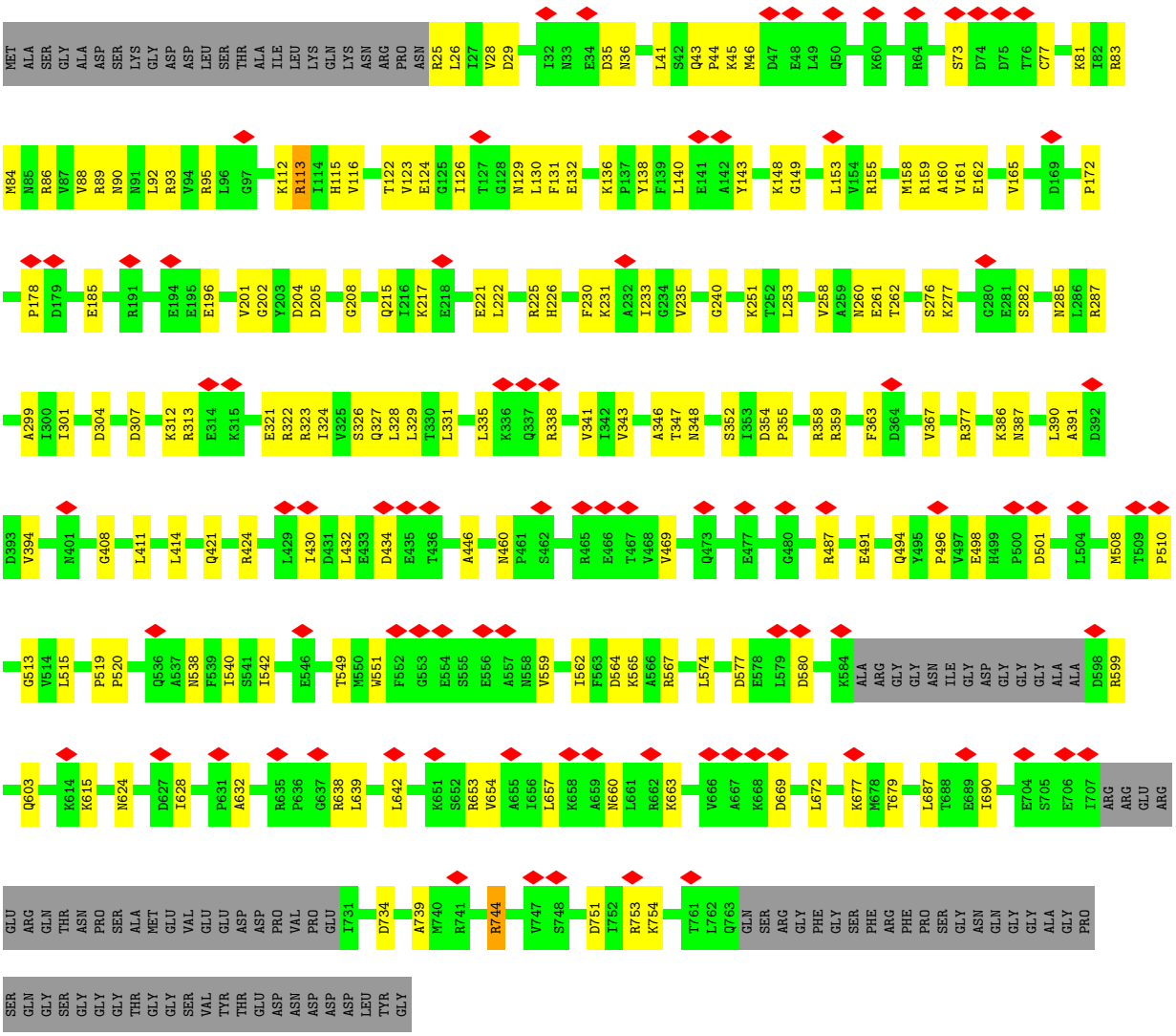
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain B: 8% 65% 21% 13%



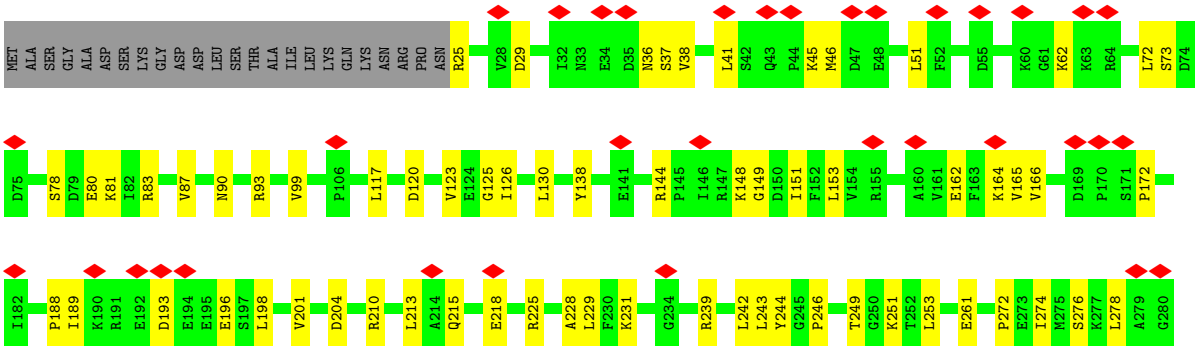
• Molecule 1: Transitional endoplasmic reticulum ATPase

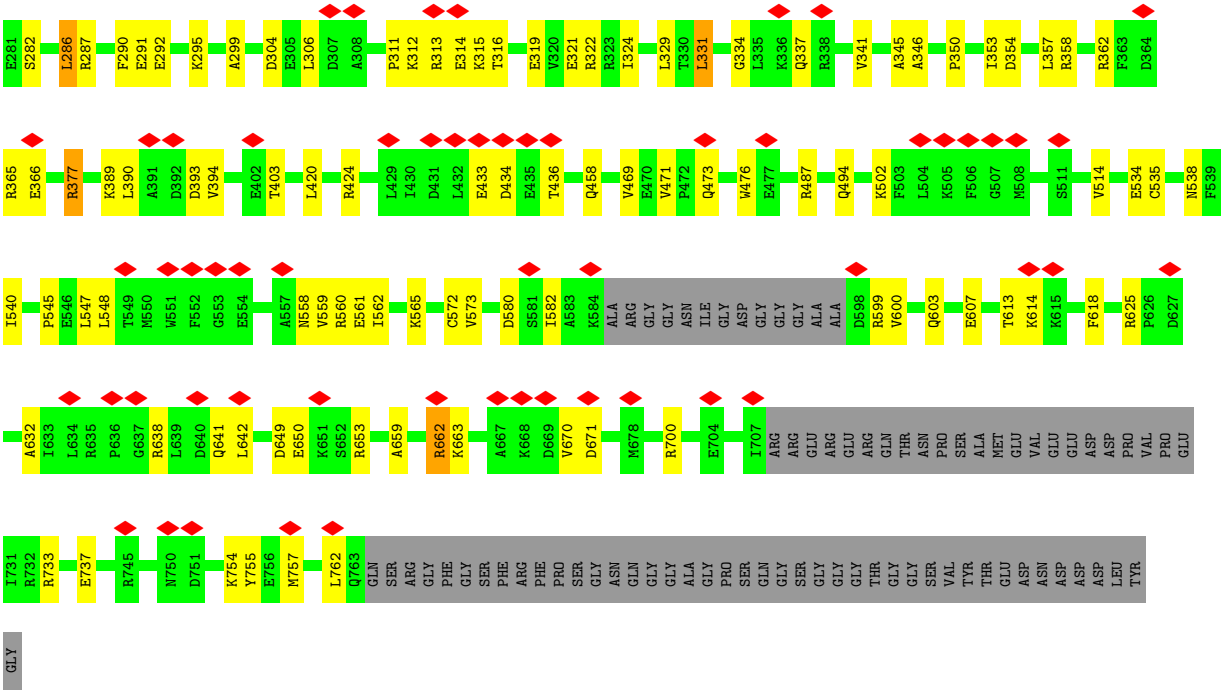
Chain C:



• Molecule 1: Transitional endoplasmic reticulum ATPase

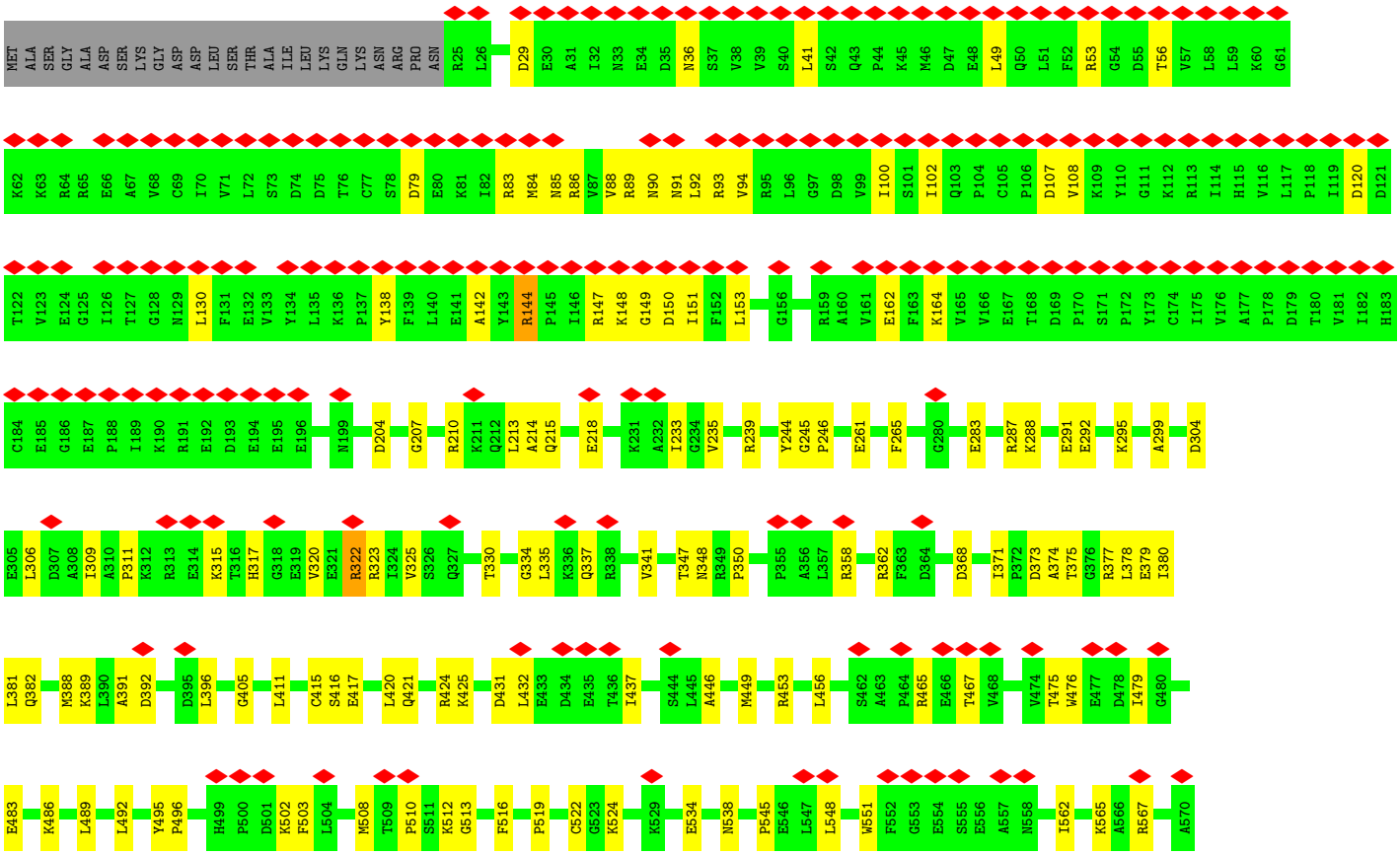
Chain D:

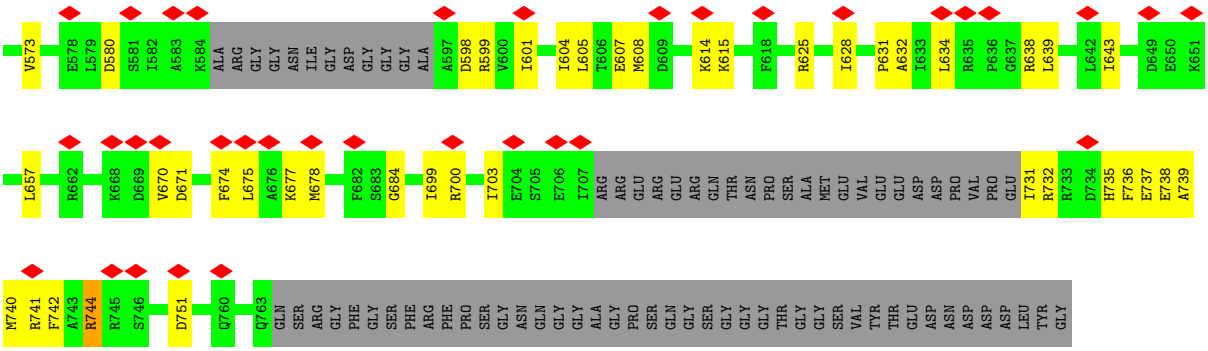




- Molecule 1: Transitional endoplasmic reticulum ATPase

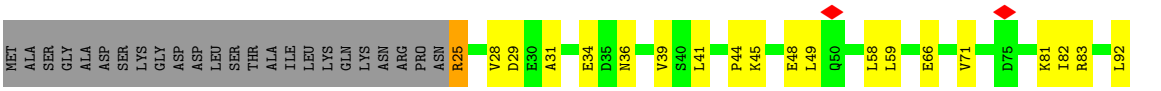
Chain E:

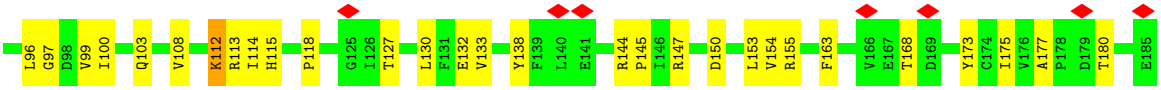


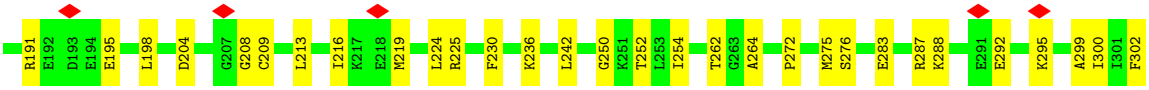


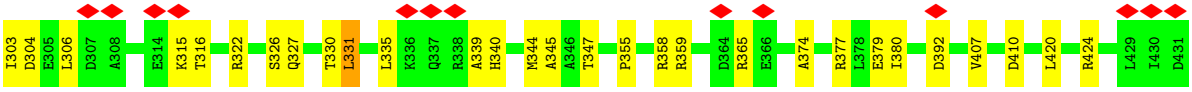
• Molecule 1: Transitional endoplasmic reticulum ATPase

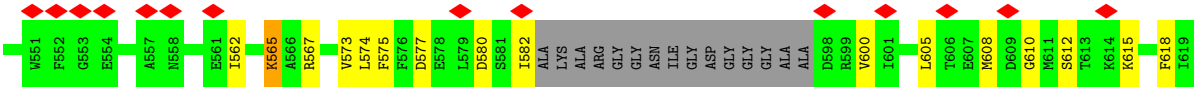
Chain A:

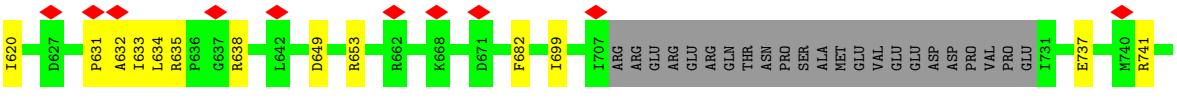






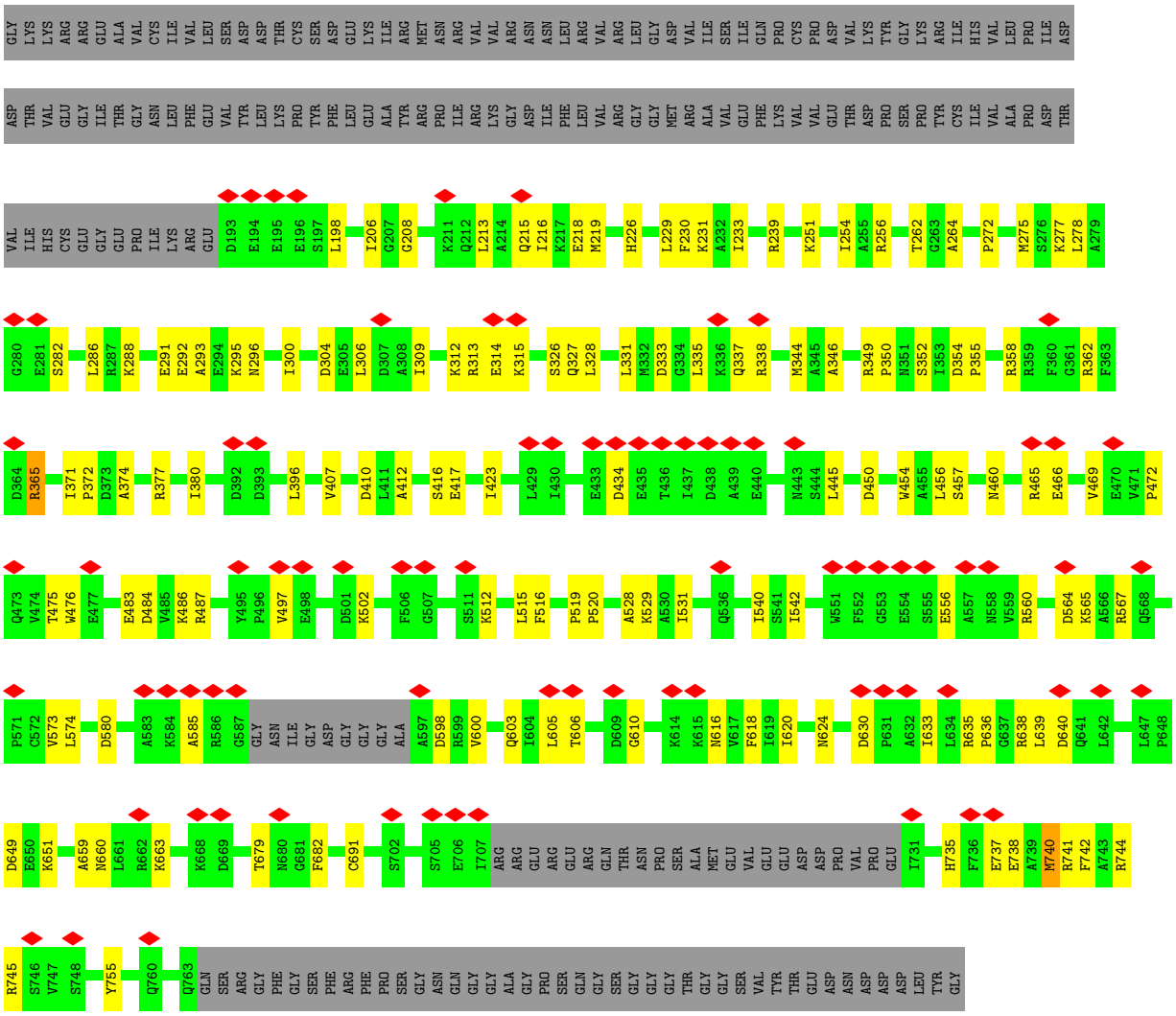






• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:


GLY LYS LYS ARG ARG GLU ALA VAL CYS ILE VAL LEU SER ASP ASP THR CYS SER ASP GLU LYS ILE ARG MET ASN ARG VAL VAL ARG ASN ASN LEU ARG VAL ARG LEU GLY ASP VAL ILE SER ILE GLN PRO CYS PRO ASP VAL LYS TYR GLY LYS ARG ILE HIS VAL LEU PRO ILE ASP
ASP THR VAL GLU GLY ILE THR GLY ASN LEU PHE GLU VAL TYR LEU LYS PRO TYR PHE LEU GLU ALA TYR ARG PRO ILE ARG LYS GLY ASP ILE PHE LEU VAL ARG GLY GLY MET ARG ALA VAL GLU PHE LYS VAL VAL GLU THR ASP PRO SER PRO TYR CYS ILE VAL ALA PRO ASP THR
VAL ILE HIS CYS GLU GLY GLU PRO ILE LYS ARG GLU D193 E194 E195 E196 S197 L198 I206 G207 G208 K211 Q212 L213 A214 Q215 I216 K217 E218 M219 H226 L229 F230 K231 A232 I233 R239 K251 I254 A255 R256 T262 G263 A264 P272 M275 S276 K277 L278 A279
G280 E281 S282 L286 R287 K288 E291 E292 A293 E294 K295 N296 I300 D304 E305 L306 D307 A308 I309 K312 R313 E314 K315 S326 Q327 L328 L331 M332 D333 G334 L335 K336 Q337 R338 M344 A345 A346 R349 P350 N351 S352 I353 D354 P355 R358 R359 F360 G361 R362 F363
D364 R365 I371 P372 D373 A374 R377 I380 D392 D393 L396 V407 D410 L411 A412 S416 E417 I423 L429 I430 E433 D434 E435 T436 I437 D438 A439 E440 N443 S444 L445 D450 W454 A455 L456 S457 N460 R465 E466 V469 E470 V471 P472
Q473 V474 T475 W476 E477 E483 D484 V485 K486 R487 Y495 P496 V497 E498 D501 K502 F506 G507 S511 K512 L515 F516 P519 P520 A528 K529 A530 I531 Q536 I540 S541 I542 W551 F552 G553 E554 S555 E556 A557 N558 V559 R560 D564 K565 A566 R567 Q568
P571 C572 V573 L574 D580 A583 K584 A585 R586 G587 GLY ASN ILE GLY ASP GLY GLY GLY ALA A597 D598 R599 V600 Q603 I604 L605 T606 D609 G610 K614 K615 N616 V617 F618 I619 I620 N624 D630 P631 A632 I633 L634 R635 P636 G637 R638 L639 D640 Q641 L642 L647 P648
D649 E650 K651 A659 N660 L661 R662 K663 K668 D669 T679 N680 G681 F682 C691 S702 S705 E706 I707 ARG ARG GLU ARG GLU ARG GLN THR ASN PRO SER ALA MET GLU VAL GLU GLU ASP ASP PRO VAL PRO GLU I731 H735 F736 E737 E738 A739 M740 R741 F742 A743 R744
R745 S746 V747 S748 Y755 Q760 Q763 GLN SER ARG GLY PHE GLY SER PHE ARG PHE PRO SER GLY ASN GLN GLY GLY ALA GLY PRO SER GLN GLY SER GLY GLY GLY THR GLY GLY SER VAL TYR THR GLU ASP ASN ASP ASP ASP LEU TYR GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81865	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 ($e^-/Å^2$)	64.8	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	2.354	Depositor
Minimum map value	-1.033	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.56, 1.56, 1.56	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: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.31	0/5603	0.66	4/7567 (0.1%)
1	B	0.30	0/5603	0.60	2/7567 (0.0%)
1	C	0.30	0/5617	0.62	1/7585 (0.0%)
1	D	0.32	0/5617	0.69	3/7585 (0.0%)
1	E	0.31	0/5622	0.65	3/7592 (0.0%)
1	F	0.30	0/4280	0.64	4/5776 (0.1%)
All	All	0.31	0/32342	0.64	17/43672 (0.0%)

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	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	LEU	CA-CB-CG	6.44	130.11	115.30
1	F	396	LEU	CA-CB-CG	6.38	129.96	115.30
1	D	151	ILE	CG1-CB-CG2	-6.34	97.46	111.40
1	F	740	MET	CB-CG-SD	6.30	131.29	112.40
1	E	432	LEU	CA-CB-CG	6.06	129.23	115.30
1	B	639	LEU	CA-CB-CG	5.88	128.83	115.30
1	E	378	LEU	CA-CB-CG	5.85	128.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	326	SER	C-N-CA	5.69	135.92	121.70
1	A	303	ILE	CG1-CB-CG2	-5.62	99.04	111.40
1	A	49	LEU	CA-CB-CG	5.42	127.78	115.30
1	C	335	LEU	CA-CB-CG	5.21	127.27	115.30
1	A	326	SER	C-N-CA	5.16	134.60	121.70
1	E	130	LEU	CA-CB-CG	5.08	126.98	115.30
1	F	585	ALA	C-N-CA	5.05	134.32	121.70
1	D	757	MET	CB-CG-SD	5.03	127.49	112.40
1	B	661	LEU	CA-CB-CG	5.00	126.81	115.30
1	D	286	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	331	LEU	Peptide
1	B	95	ARG	Peptide
1	D	331	LEU	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	5513	0	5587	95	0
1	B	5513	0	5587	109	0
1	C	5527	0	5605	113	0
1	D	5527	0	5605	107	0
1	E	5532	0	5610	112	0
1	F	4212	0	4253	88	0
2	A	27	0	12	1	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
All	All	31986	0	32319	593	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 9.

All (593) 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:599:ARG:HB3	1:D:603:GLN:HE22	1.50	0.76
1:F:208:GLY:HA3	2:F:901:ADP:HN62	1.60	0.67
1:C:251:LYS:HD3	1:C:346:ALA:HB1	1.77	0.66
1:D:538:ASN:H	1:D:572:CYS:HA	1.61	0.66
1:D:274:ILE:HD11	1:D:286:LEU:HB3	1.78	0.65
1:A:300:ILE:HD11	1:A:344:MET:HG2	1.79	0.64
1:A:480:GLY:HA3	1:A:486:LYS:HA	1.79	0.63
1:F:660:ASN:ND2	1:F:691:CYS:SG	2.72	0.62
1:D:319:GLU:HA	1:D:322:ARG:HD3	1.80	0.62
1:F:226:HIS:HB3	1:F:229:LEU:HB2	1.81	0.62
1:A:31:ALA:HA	1:A:83:ARG:HE	1.64	0.62
1:D:502:LYS:HB3	1:E:699:ILE:HD12	1.80	0.61
1:C:690:ILE:HB	1:C:744:ARG:HH21	1.65	0.61
1:F:198:LEU:HD12	1:F:256:ARG:HE	1.66	0.61
1:C:26:LEU:HD11	1:C:45:LYS:HE3	1.81	0.60
1:E:625:ARG:HD2	1:E:628:ILE:HB	1.84	0.60
1:F:573:VAL:HG23	1:F:618:PHE:HB3	1.84	0.60
1:D:210:ARG:HA	1:D:213:LEU:HB2	1.83	0.60
1:D:316:THR:OG1	1:D:322:ARG:NH1	2.35	0.59
1:A:115:HIS:H	1:A:168:THR:HG22	1.66	0.59
1:A:39:VAL:HB	1:A:71:VAL:HA	1.84	0.59
1:A:573:VAL:HG23	1:A:618:PHE:HB3	1.83	0.59
1:F:313:ARG:HH11	1:F:315:LYS:HB3	1.67	0.59
1:B:135:LEU:HD13	1:B:182:ILE:HD13	1.85	0.58
1:C:43:GLN:HG2	1:C:44:PRO:HD3	1.86	0.58
1:E:615:LYS:NZ	1:F:456:LEU:O	2.35	0.58
1:A:424:ARG:NH1	1:F:218:GLU:OE2	2.36	0.58
1:A:44:PRO:O	1:A:48:GLU:HB3	2.04	0.58
1:B:672:LEU:HA	1:B:675:LEU:HD12	1.85	0.58
1:C:240:GLY:HA3	1:C:363:PHE:HA	1.85	0.58
1:A:108:VAL:HG11	1:A:173:TYR:HB2	1.86	0.58
1:D:312:LYS:HB2	1:D:354:ASP:HA	1.86	0.57
1:E:233:ILE:HG23	1:E:235:VAL:H	1.69	0.57
1:A:540:ILE:HB	1:A:574:LEU:HA	1.86	0.57
1:B:313:ARG:NH2	1:B:351:ASN:O	2.37	0.57
1:D:659:ALA:O	1:D:662:ARG:NH1	2.38	0.57
1:B:61:GLY:HA3	1:B:65:ARG:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:HE	1:B:146:ILE:HD11	1.67	0.57
1:D:573:VAL:HG23	1:D:618:PHE:HB3	1.86	0.57
1:B:239:ARG:NH1	1:B:332:MET:O	2.38	0.57
1:D:311:PRO:HG2	1:D:315:LYS:HG2	1.86	0.57
1:E:510:PRO:HB2	1:E:512:LYS:HE3	1.87	0.57
1:D:90:ASN:HB3	1:D:198:LEU:HD11	1.86	0.56
1:E:417:GLU:HA	1:E:420:LEU:HB2	1.86	0.56
1:E:678:MET:HG3	1:E:740:MET:HB3	1.88	0.56
1:D:321:GLU:HA	1:D:324:ILE:HG12	1.88	0.56
1:E:551:TRP:HZ3	1:E:599:ARG:H	1.53	0.56
1:F:327:GLN:O	1:F:331:LEU:HB2	2.05	0.56
1:B:262:THR:HG23	1:B:264:ALA:H	1.71	0.56
1:F:740:MET:SD	1:F:741:ARG:NH1	2.78	0.56
1:D:599:ARG:O	1:D:603:GLN:NE2	2.38	0.56
1:A:288:LYS:O	1:A:292:GLU:HB3	2.05	0.56
1:B:350:PRO:O	1:B:358:ARG:NH2	2.39	0.56
1:B:174:CYS:SG	1:B:175:ILE:N	2.78	0.56
1:B:359:ARG:NH2	1:B:360:PHE:O	2.39	0.56
1:C:313:ARG:NH1	1:C:352:SER:O	2.39	0.56
1:A:58:LEU:HB2	1:A:103:GLN:HB3	1.88	0.56
1:A:377:ARG:HA	1:A:380:ILE:HG22	1.88	0.56
1:C:225:ARG:NH2	1:C:261:GLU:O	2.38	0.55
1:E:142:ALA:HB3	1:E:144:ARG:HH11	1.71	0.55
1:C:323:ARG:HH22	1:D:278:LEU:HD22	1.71	0.55
1:F:219:MET:HB2	1:F:365:ARG:HH21	1.71	0.55
1:A:230:PHE:HB3	1:A:340:HIS:HE1	1.71	0.55
1:A:29:ASP:N	1:A:82:ILE:O	2.40	0.55
1:F:300:ILE:HD11	1:F:344:MET:HB2	1.89	0.55
1:E:421:GLN:O	1:E:425:LYS:NZ	2.40	0.55
1:C:131:PHE:HE2	1:C:185:GLU:H	1.54	0.55
1:E:739:ALA:O	1:E:744:ARG:NH1	2.39	0.55
1:B:53:ARG:NH1	1:B:71:VAL:O	2.40	0.54
1:C:95:ARG:HB2	1:C:225:ARG:HH22	1.73	0.54
1:F:737:GLU:OE2	1:F:741:ARG:NH1	2.40	0.54
1:B:40:SER:HA	1:B:72:LEU:HB3	1.90	0.54
1:B:327:GLN:NE2	1:C:276:SER:O	2.41	0.54
1:A:209:CYS:SG	2:A:901:ADP:N6	2.81	0.54
1:B:63:LYS:O	1:B:65:ARG:NH1	2.40	0.54
1:B:330:THR:O	1:B:334:GLY:N	2.38	0.54
1:B:407:VAL:HG12	1:B:409:ALA:H	1.73	0.54
1:E:388:MET:HG3	1:E:415:CYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:TRP:HA	1:E:479:ILE:HG22	1.90	0.54
1:A:699:ILE:HG23	1:F:502:LYS:HB3	1.90	0.54
1:C:599:ARG:HB3	1:C:603:GLN:HE22	1.71	0.54
1:F:327:GLN:HB2	1:F:331:LEU:HD23	1.89	0.54
1:B:573:VAL:HG23	1:B:618:PHE:HB3	1.90	0.54
1:E:138:TYR:O	1:E:144:ARG:NH1	2.40	0.54
1:D:476:TRP:HD1	1:D:534:GLU:HG3	1.73	0.54
1:B:635:ARG:HD3	1:B:636:PRO:HD2	1.90	0.53
1:F:659:ALA:O	1:F:663:LYS:NZ	2.41	0.53
1:B:215:GLN:O	1:B:219:MET:HB2	2.09	0.53
1:D:123:VAL:HG23	1:D:126:ILE:HB	1.90	0.53
1:F:239:ARG:NH1	1:F:333:ASP:OD1	2.41	0.53
1:E:580:ASP:OD1	1:E:580:ASP:N	2.40	0.53
1:F:377:ARG:HA	1:F:380:ILE:HG12	1.91	0.53
1:B:232:ALA:O	1:C:159:ARG:NH1	2.41	0.53
1:C:287:ARG:NH1	1:C:327:GLN:OE1	2.40	0.53
1:D:494:GLN:NE2	1:D:535:CYS:SG	2.82	0.53
1:A:147:ARG:HB3	1:A:150:ASP:HB3	1.91	0.53
1:A:632:ALA:O	1:A:638:ARG:NH2	2.39	0.53
1:C:577:ASP:OD1	1:C:577:ASP:N	2.42	0.53
1:C:391:ALA:HB2	1:C:446:ALA:HB1	1.89	0.53
1:D:471:VAL:O	1:D:473:GLN:NE2	2.41	0.53
1:F:362:ARG:O	1:F:362:ARG:NH1	2.36	0.53
1:E:210:ARG:HA	1:E:213:LEU:HB2	1.90	0.53
1:F:277:LYS:HB2	1:F:282:SER:HB2	1.90	0.53
1:F:560:ARG:NH1	1:F:606:THR:OG1	2.42	0.53
1:C:28:VAL:O	1:C:81:LYS:NZ	2.41	0.53
1:B:110:TYR:HB3	1:B:177:ALA:HB2	1.91	0.53
1:B:203:TYR:HE1	1:B:258:VAL:HG12	1.74	0.53
1:E:94:VAL:HG21	1:E:100:ILE:HD11	1.90	0.52
1:F:306:LEU:HA	1:F:309:ILE:HG22	1.90	0.52
1:C:513:GLY:HA3	1:C:639:LEU:HA	1.91	0.52
1:C:88:VAL:O	1:C:92:LEU:HB2	2.09	0.52
1:C:202:GLY:H	1:C:205:ASP:HB2	1.74	0.52
1:A:472:PRO:HB2	1:A:533:ASN:HB2	1.90	0.52
1:C:149:GLY:H	1:C:165:VAL:HB	1.75	0.52
1:D:239:ARG:NH1	1:D:337:GLN:OE1	2.43	0.52
1:B:538:ASN:H	1:B:572:CYS:HA	1.75	0.52
1:A:420:LEU:O	1:A:424:ARG:HB2	2.09	0.52
1:D:90:ASN:O	1:D:93:ARG:NH1	2.43	0.52
1:D:350:PRO:O	1:D:358:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:598:ASP:HB3	1:E:601:ILE:HG12	1.92	0.52
1:B:36:ASN:ND2	1:B:138:TYR:OH	2.37	0.52
1:B:58:LEU:HB2	1:B:103:GLN:HB2	1.92	0.52
1:B:191:ARG:NH2	1:B:195:GLU:OE2	2.43	0.52
2:B:901:ADP:O2B	1:A:359:ARG:NH1	2.41	0.52
1:C:653:ARG:NH1	1:C:679:THR:O	2.43	0.52
1:D:274:ILE:O	1:D:282:SER:OG	2.27	0.52
1:E:36:ASN:HA	1:E:85:ASN:HD21	1.75	0.52
1:E:347:THR:OG1	1:E:348:ASN:N	2.42	0.52
1:B:513:GLY:HA3	1:B:639:LEU:HA	1.90	0.52
1:F:292:GLU:O	1:F:296:ASN:ND2	2.43	0.52
1:E:147:ARG:NH1	1:E:148:LYS:O	2.43	0.52
1:A:242:LEU:HD11	1:A:347:THR:HG22	1.92	0.52
1:C:115:HIS:NE2	1:C:185:GLU:OE1	2.43	0.51
1:D:117:LEU:HB3	1:D:164:LYS:HB3	1.92	0.51
1:D:313:ARG:HG3	1:D:315:LYS:H	1.75	0.51
1:A:272:PRO:HA	1:A:275:MET:HG2	1.91	0.51
1:B:145:PRO:HA	1:B:175:ILE:HA	1.91	0.51
1:E:90:ASN:O	1:E:93:ARG:NH1	2.42	0.51
1:A:456:LEU:HD12	1:A:460:ASN:HD21	1.75	0.51
1:F:355:PRO:HA	1:F:358:ARG:HB2	1.92	0.51
1:B:543:LYS:HG3	1:B:545:PRO:HD2	1.91	0.51
1:E:379:GLU:HA	1:E:382:GLN:HB2	1.92	0.51
1:D:547:LEU:HD22	1:D:559:VAL:HG22	1.91	0.51
1:F:293:ALA:HA	1:F:296:ASN:HD22	1.74	0.51
1:B:323:ARG:NH1	1:C:277:LYS:O	2.43	0.51
1:E:631:PRO:HB2	1:E:634:LEU:HB2	1.92	0.51
1:B:751:ASP:OD1	1:B:751:ASP:N	2.42	0.51
1:D:733:ARG:NH2	1:D:737:GLU:OE1	2.44	0.51
1:F:407:VAL:HG13	1:F:410:ASP:H	1.75	0.51
1:E:742:PHE:HD2	1:E:744:ARG:HD2	1.76	0.51
1:B:657:LEU:HG	1:B:687:LEU:HD13	1.92	0.51
1:E:311:PRO:HG2	1:E:315:LYS:HG2	1.93	0.51
1:E:322:ARG:HA	1:E:325:VAL:HG22	1.92	0.51
1:E:453:ARG:HA	1:E:456:LEU:HG	1.93	0.51
1:F:231:LYS:O	1:F:338:ARG:NH1	2.44	0.51
1:D:314:GLU:OE2	1:E:317:HIS:NE2	2.44	0.50
1:E:522:CYS:HA	1:E:684:GLY:H	1.74	0.50
1:C:559:VAL:HA	1:C:562:ILE:HG12	1.93	0.50
1:D:99:VAL:HG21	1:E:431:ASP:HB3	1.94	0.50
1:D:514:VAL:HG23	1:D:641:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ASP:HA	1:B:383:ILE:HG12	1.93	0.50
1:A:177:ALA:HB3	1:A:180:THR:HG23	1.93	0.50
1:C:90:ASN:O	1:C:93:ARG:NH1	2.44	0.50
1:C:158:MET:HA	1:C:387:ASN:HB3	1.93	0.50
1:C:615:LYS:NZ	1:D:458:GLN:O	2.44	0.50
1:E:41:LEU:HD13	1:E:53:ARG:HH12	1.76	0.50
1:E:245:GLY:N	1:E:348:ASN:O	2.40	0.50
1:A:112:LYS:HD2	1:A:113:ARG:HB2	1.94	0.50
1:F:213:LEU:HD23	1:F:216:ILE:HD11	1.92	0.50
1:F:598:ASP:N	1:F:598:ASP:OD1	2.44	0.50
1:C:204:ASP:OD1	1:C:204:ASP:N	2.44	0.50
1:E:283:GLU:O	1:E:287:ARG:NH1	2.45	0.50
1:E:350:PRO:O	1:E:358:ARG:NH2	2.45	0.50
1:B:742:PHE:O	1:B:745:ARG:NH1	2.45	0.50
1:C:508:MET:HB3	1:D:663:LYS:HD2	1.93	0.50
1:D:329:LEU:HD22	1:D:362:ARG:HD3	1.93	0.50
1:C:208:GLY:H	2:C:901:ADP:HN62	1.60	0.50
1:F:272:PRO:HA	1:F:275:MET:HG2	1.92	0.50
1:B:209:CYS:HB2	1:B:369:ILE:HG13	1.94	0.50
1:B:665:PRO:O	1:B:732:ARG:NH2	2.43	0.50
1:C:95:ARG:NH2	1:C:196:GLU:OE2	2.44	0.50
1:F:636:PRO:HA	1:F:640:ASP:HA	1.94	0.50
1:D:331:LEU:HD13	1:D:334:GLY:HA3	1.94	0.49
1:E:86:ARG:HA	1:E:89:ARG:HB2	1.93	0.49
1:B:699:ILE:HD11	1:A:502:LYS:HB3	1.94	0.49
1:B:507:GLY:O	1:C:663:LYS:NZ	2.44	0.49
1:D:632:ALA:O	1:D:638:ARG:NH1	2.46	0.49
1:C:551:TRP:HE1	1:C:599:ARG:HB2	1.78	0.49
1:D:287:ARG:O	1:D:290:PHE:N	2.45	0.49
1:D:306:LEU:HD11	1:D:345:ALA:HB1	1.94	0.49
1:D:357:LEU:HA	1:D:362:ARG:HD2	1.95	0.49
1:E:380:ILE:HG22	1:E:411:LEU:HD11	1.94	0.49
1:E:391:ALA:HB2	1:E:446:ALA:HB1	1.93	0.49
1:C:29:ASP:HB2	1:C:81:LYS:HG3	1.94	0.49
1:E:496:PRO:HG3	1:E:502:LYS:HE3	1.94	0.49
1:E:513:GLY:HA3	1:E:639:LEU:HB3	1.93	0.49
1:E:615:LYS:NZ	1:F:460:ASN:OD1	2.45	0.49
1:C:95:ARG:NH1	1:C:260:ASN:O	2.44	0.49
1:C:301:ILE:HG13	1:C:343:VAL:HA	1.94	0.49
1:D:37:SER:HB3	1:D:144:ARG:HH22	1.77	0.49
1:D:469:VAL:HG22	1:D:540:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:OD1	1:A:204:ASP:N	2.42	0.49
1:B:270:ASN:HD22	1:B:273:GLU:HB3	1.77	0.49
1:D:228:ALA:HA	1:D:231:LYS:HG2	1.94	0.49
1:F:349:ARG:HE	1:F:350:PRO:HD2	1.77	0.49
1:B:632:ALA:O	1:B:638:ARG:NH1	2.44	0.49
1:E:204:ASP:OD1	1:E:204:ASP:N	2.45	0.49
1:A:28:VAL:HB	1:A:97:GLY:H	1.76	0.49
1:A:97:GLY:O	1:A:225:ARG:NH2	2.46	0.49
1:A:519:PRO:O	1:A:524:LYS:NZ	2.41	0.49
1:B:456:LEU:O	1:A:615:LYS:NZ	2.45	0.49
1:B:671:ASP:N	1:B:671:ASP:OD1	2.45	0.49
1:D:304:ASP:HA	1:D:346:ALA:HB3	1.95	0.49
1:D:390:LEU:HD12	1:D:394:VAL:HG11	1.95	0.49
1:B:625:ARG:NH2	1:B:627:ASP:OD2	2.45	0.49
1:D:204:ASP:OD1	1:D:204:ASP:N	2.45	0.49
1:E:731:ILE:O	1:E:735:HIS:ND1	2.46	0.49
1:A:315:LYS:HD2	1:F:314:GLU:HG3	1.94	0.49
1:E:421:GLN:HA	1:E:424:ARG:HE	1.77	0.48
1:E:605:LEU:HA	1:E:608:MET:HG2	1.95	0.48
1:C:323:ARG:HH12	1:D:278:LEU:HD13	1.77	0.48
1:D:243:LEU:HB3	1:D:251:LYS:HG2	1.95	0.48
1:E:304:ASP:OD1	1:E:304:ASP:N	2.46	0.48
1:F:483:GLU:HA	1:F:486:LYS:HB2	1.95	0.48
1:B:43:GLN:HA	1:B:46:MET:HG3	1.96	0.48
1:B:277:LYS:HB2	1:B:282:SER:HB3	1.95	0.48
1:B:327:GLN:HA	1:B:330:THR:HB	1.96	0.48
1:C:143:TYR:HE1	1:C:178:PRO:HD3	1.78	0.48
1:C:434:ASP:OD1	1:C:434:ASP:N	2.46	0.48
1:D:80:GLU:HG2	1:D:81:LYS:HD3	1.96	0.48
1:D:125:GLY:O	1:D:436:THR:OG1	2.31	0.48
1:E:153:LEU:HB3	1:E:162:GLU:HG3	1.93	0.48
1:A:145:PRO:HA	1:A:175:ILE:HA	1.93	0.48
1:A:59:LEU:HD13	1:A:100:ILE:HG21	1.95	0.48
1:A:264:ALA:HB1	1:A:299:ALA:HA	1.96	0.48
1:C:43:GLN:HA	1:C:46:MET:HG2	1.94	0.48
1:C:307:ASP:H	1:C:347:THR:HG21	1.77	0.48
1:F:239:ARG:HH21	1:F:335:LEU:HB3	1.77	0.48
1:B:515:LEU:HG	1:B:642:LEU:HD23	1.96	0.48
1:C:520:PRO:HG3	1:C:624:ASN:HB3	1.95	0.48
1:D:153:LEU:HA	1:D:162:GLU:HA	1.96	0.48
1:D:291:GLU:O	1:D:295:LYS:NZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:483:GLU:HA	1:E:486:LYS:HB2	1.96	0.48
1:A:516:PHE:HE2	1:A:620:ILE:HB	1.79	0.48
1:F:649:ASP:OD2	1:F:651:LYS:NZ	2.43	0.48
1:B:270:ASN:HD21	1:A:330:THR:HG21	1.79	0.48
1:B:574:LEU:HD22	1:B:619:ILE:HG23	1.96	0.48
1:D:117:LEU:HD21	1:D:189:ILE:HG13	1.96	0.48
1:E:56:THR:HG21	1:E:108:VAL:HG21	1.96	0.48
1:E:288:LYS:O	1:E:292:GLU:HB2	2.14	0.48
1:B:690:ILE:HG23	1:B:739:ALA:HB1	1.96	0.47
1:C:657:LEU:HA	1:C:660:ASN:HB2	1.96	0.47
1:A:29:ASP:HB2	1:A:81:LYS:HG3	1.96	0.47
1:B:250:GLY:O	1:B:254:ILE:N	2.46	0.47
1:C:669:ASP:OD1	1:C:669:ASP:N	2.46	0.47
1:D:148:LYS:H	1:D:172:PRO:HB3	1.79	0.47
1:E:657:LEU:HD13	1:E:675:LEU:HD12	1.96	0.47
1:A:34:GLU:OE1	1:A:155:ARG:NH2	2.47	0.47
1:C:304:ASP:N	1:C:304:ASP:OD1	2.45	0.47
1:C:41:LEU:HB3	1:C:73:SER:HA	1.96	0.47
1:C:148:LYS:H	1:C:172:PRO:HB3	1.79	0.47
1:E:79:ASP:OD1	1:E:79:ASP:N	2.42	0.47
1:E:567:ARG:NH2	1:E:607:GLU:O	2.46	0.47
1:B:120:ASP:N	1:B:120:ASP:OD1	2.45	0.47
1:E:246:PRO:HG3	1:E:371:ILE:HG13	1.96	0.47
1:A:242:LEU:HA	1:A:345:ALA:HB3	1.97	0.47
1:D:558:ASN:HA	1:D:561:GLU:HG2	1.96	0.47
1:E:374:ALA:HA	1:E:377:ARG:HG2	1.96	0.47
1:E:489:LEU:HA	1:E:492:LEU:HB2	1.97	0.47
1:A:25:ARG:HA	1:A:99:VAL:HG13	1.97	0.47
1:B:472:PRO:HB2	1:B:533:ASN:HB2	1.96	0.47
1:B:575:PHE:HA	1:B:620:ILE:HB	1.96	0.47
1:C:86:ARG:HG2	1:C:89:ARG:HH21	1.79	0.47
1:C:126:ILE:HG21	1:C:130:LEU:HB3	1.96	0.47
1:A:407:VAL:HG13	1:A:410:ASP:H	1.80	0.47
1:A:577:ASP:OD1	1:A:577:ASP:N	2.47	0.47
1:F:472:PRO:HB3	1:F:529:LYS:HG3	1.96	0.47
1:B:434:ASP:OD1	1:B:434:ASP:N	2.48	0.47
1:E:519:PRO:O	1:E:524:LYS:NZ	2.48	0.47
1:F:497:VAL:HG12	1:F:616:ASN:HB3	1.96	0.47
1:D:41:LEU:HB3	1:D:73:SER:HA	1.96	0.47
1:D:246:PRO:O	1:D:249:THR:OG1	2.30	0.47
1:D:545:PRO:HA	1:D:548:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:VAL:O	1:E:92:LEU:HB2	2.15	0.47
1:E:265:PHE:H	1:E:299:ALA:HA	1.79	0.47
1:A:25:ARG:N	1:A:100:ILE:O	2.48	0.47
1:A:514:VAL:HG12	1:A:620:ILE:HG22	1.97	0.47
1:B:605:LEU:HD21	1:B:633:ILE:HG22	1.96	0.47
1:C:355:PRO:HA	1:C:358:ARG:HB2	1.96	0.47
1:E:737:GLU:O	1:E:741:ARG:HB2	2.15	0.47
1:F:567:ARG:NH1	1:F:610:GLY:O	2.47	0.47
1:C:129:ASN:ND2	1:C:132:GLU:OE1	2.48	0.46
1:C:226:HIS:ND1	1:D:433:GLU:OE1	2.41	0.46
1:F:239:ARG:NH2	1:F:335:LEU:O	2.48	0.46
1:B:579:LEU:HG	1:B:623:THR:HB	1.96	0.46
1:C:487:ARG:HH21	1:C:491:GLU:HG3	1.80	0.46
1:F:630:ASP:OD1	1:F:630:ASP:N	2.45	0.46
1:D:117:LEU:HB2	1:D:166:VAL:HG23	1.96	0.46
1:E:335:LEU:HG	1:E:337:GLN:H	1.80	0.46
1:A:250:GLY:O	1:A:254:ILE:N	2.45	0.46
1:A:316:THR:OG1	1:A:322:ARG:NH1	2.47	0.46
1:C:136:LYS:HA	1:C:140:LEU:HD23	1.98	0.46
1:E:86:ARG:NE	1:E:261:GLU:OE2	2.48	0.46
1:C:36:ASN:ND2	1:C:138:TYR:OH	2.40	0.46
1:C:231:LYS:O	1:C:338:ARG:NH2	2.49	0.46
1:D:228:ALA:HB3	1:E:437:ILE:HG12	1.97	0.46
1:D:393:ASP:OD1	1:D:393:ASP:N	2.48	0.46
1:A:114:ILE:HG12	1:A:180:THR:HB	1.97	0.46
1:A:491:GLU:HA	1:A:495:TYR:HD2	1.80	0.46
1:F:484:ASP:OD1	1:F:484:ASP:N	2.48	0.46
1:F:742:PHE:O	1:F:745:ARG:NH1	2.49	0.46
1:C:390:LEU:HD13	1:C:394:VAL:HB	1.96	0.46
1:C:408:GLY:HA2	1:C:411:LEU:HD12	1.98	0.46
1:C:562:ILE:HA	1:C:565:LYS:HG2	1.97	0.46
1:D:754:LYS:HB3	1:D:754:LYS:HE2	1.77	0.46
1:E:306:LEU:HA	1:E:309:ILE:HG12	1.97	0.46
1:A:304:ASP:OD1	1:A:304:ASP:N	2.48	0.46
1:F:262:THR:HG23	1:F:264:ALA:H	1.81	0.46
1:B:131:PHE:HD2	1:B:182:ILE:HD12	1.80	0.46
1:B:550:MET:SD	1:B:555:SER:OG	2.70	0.46
1:C:562:ILE:HG22	1:C:565:LYS:HE2	1.98	0.46
1:D:670:VAL:HG23	1:D:733:ARG:HH11	1.81	0.46
1:A:213:LEU:HA	1:A:216:ILE:HG12	1.98	0.46
1:A:306:LEU:HB2	1:A:347:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:PRO:HB3	1:B:348:ASN:HD21	1.80	0.46
1:C:496:PRO:HB3	1:C:510:PRO:HG3	1.97	0.46
1:C:312:LYS:HD3	1:C:322:ARG:HH21	1.81	0.46
1:E:601:ILE:HD12	1:E:632:ALA:HB2	1.98	0.46
1:E:751:ASP:OD1	1:E:751:ASP:N	2.40	0.46
1:B:112:LYS:HA	1:B:180:THR:HG22	1.98	0.45
1:B:307:ASP:N	1:B:307:ASP:OD1	2.44	0.45
1:C:519:PRO:HA	1:C:520:PRO:HD3	1.87	0.45
1:E:149:GLY:HA2	1:E:164:LYS:HZ3	1.81	0.45
1:E:738:GLU:HA	1:E:741:ARG:HB3	1.97	0.45
1:B:450:ASP:OD1	1:B:450:ASP:N	2.43	0.45
1:B:484:ASP:N	1:B:484:ASP:OD1	2.43	0.45
1:E:29:ASP:HB2	1:E:83:ARG:HA	1.98	0.45
1:F:312:LYS:HB2	1:F:354:ASP:HA	1.98	0.45
1:F:469:VAL:HG12	1:F:540:ILE:HB	1.98	0.45
1:F:580:ASP:OD1	1:F:580:ASP:N	2.48	0.45
1:A:649:ASP:O	1:A:653:ARG:N	2.49	0.45
1:B:577:ASP:N	1:B:577:ASP:OD1	2.48	0.45
1:C:113:ARG:HH12	1:C:115:HIS:HB3	1.80	0.45
1:C:580:ASP:HB2	1:C:628:ILE:HD11	1.98	0.45
1:C:632:ALA:O	1:C:638:ARG:NH1	2.50	0.45
1:E:416:SER:OG	1:E:417:GLU:N	2.49	0.45
1:A:59:LEU:HB3	1:A:92:LEU:HD11	1.98	0.45
1:B:29:ASP:HB2	1:B:81:LYS:HG2	1.98	0.45
1:D:215:GLN:HA	1:D:218:GLU:HB3	1.99	0.45
1:E:207:GLY:H	1:E:380:ILE:HD11	1.82	0.45
1:E:291:GLU:O	1:E:295:LYS:NZ	2.42	0.45
1:B:229:LEU:O	1:B:233:ILE:N	2.50	0.45
1:D:62:LYS:HB2	1:D:93:ARG:HB2	1.99	0.45
1:D:650:GLU:OE1	1:D:653:ARG:NH2	2.45	0.45
1:B:92:LEU:HB3	1:B:94:VAL:HG13	1.98	0.45
1:C:494:GLN:O	1:C:498:GLU:N	2.44	0.45
1:D:613:THR:OG1	1:D:614:LYS:NZ	2.50	0.45
1:A:335:LEU:HA	1:A:339:ALA:HB3	1.98	0.45
1:A:631:PRO:HA	1:A:634:LEU:HD23	1.98	0.45
1:F:288:LYS:HA	1:F:291:GLU:HG3	1.98	0.45
1:F:556:GLU:HG2	1:F:600:VAL:HB	1.99	0.45
1:D:93:ARG:NH1	1:D:196:GLU:OE1	2.49	0.45
1:D:272:PRO:O	1:D:276:SER:HB3	2.17	0.45
1:E:49:LEU:HD13	1:E:102:ILE:HG21	1.99	0.45
1:A:216:ILE:HA	1:A:219:MET:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:735:HIS:ND1	1:F:738:GLU:OE2	2.46	0.45
1:C:28:VAL:HG23	1:C:84:MET:HB2	1.98	0.45
1:A:737:GLU:O	1:A:741:ARG:HB2	2.17	0.45
1:B:224:LEU:HD13	1:B:262:THR:HB	1.98	0.45
1:B:232:ALA:HA	1:C:124:GLU:HG2	1.98	0.45
1:C:153:LEU:HA	1:C:162:GLU:HA	1.99	0.45
1:C:329:LEU:HD12	1:C:359:ARG:HH22	1.81	0.45
1:C:414:LEU:HD11	1:C:460:ASN:HB3	1.99	0.45
1:D:193:ASP:OD1	1:D:193:ASP:N	2.50	0.45
1:A:653:ARG:NH1	1:A:682:PHE:O	2.43	0.45
1:D:36:ASN:ND2	1:D:138:TYR:OH	2.50	0.44
1:D:671:ASP:OD1	1:D:671:ASP:N	2.46	0.44
1:E:306:LEU:HG	1:E:347:THR:HB	1.98	0.44
1:B:354:ASP:O	1:B:358:ARG:NH1	2.49	0.44
1:B:421:GLN:O	1:B:425:LYS:N	2.50	0.44
1:C:515:LEU:HB2	1:C:642:LEU:HA	1.99	0.44
1:E:671:ASP:OD1	1:E:671:ASP:N	2.50	0.44
1:C:734:ASP:OD1	1:C:734:ASP:N	2.49	0.44
1:D:225:ARG:NH2	1:D:261:GLU:O	2.46	0.44
1:E:467:THR:HG21	1:E:562:ILE:HD13	1.99	0.44
1:A:283:GLU:OE2	1:A:287:ARG:NH1	2.45	0.44
1:A:374:ALA:HA	1:A:377:ARG:HB2	1.99	0.44
1:A:580:ASP:OD1	1:A:580:ASP:N	2.45	0.44
1:A:612:SER:HB3	1:A:615:LYS:HB2	1.99	0.44
1:C:123:VAL:HG23	1:C:126:ILE:HD12	2.00	0.44
1:E:91:ASN:HB3	1:E:151:ILE:HG22	1.99	0.44
1:A:127:THR:OG1	1:A:437:ILE:O	2.35	0.44
1:B:427:MET:H	1:B:430:ILE:HG12	1.81	0.44
1:C:231:LYS:HA	1:C:231:LYS:HD3	1.85	0.44
1:F:416:SER:OG	1:F:417:GLU:N	2.50	0.44
1:F:416:SER:OG	1:F:417:GLU:OE1	2.35	0.44
1:C:542:ILE:HG22	1:C:574:LEU:HD11	2.00	0.44
1:D:149:GLY:H	1:D:165:VAL:HB	1.82	0.44
1:B:233:ILE:HA	1:C:159:ARG:HH12	1.83	0.44
1:C:258:VAL:O	1:C:262:THR:OG1	2.30	0.44
1:F:434:ASP:OD1	1:F:434:ASP:N	2.49	0.44
1:B:117:LEU:HD23	1:B:189:ILE:HB	2.00	0.44
1:A:582:ILE:HG21	1:A:600:VAL:HB	2.00	0.44
1:C:153:LEU:HD12	1:C:162:GLU:HB2	1.99	0.44
1:C:155:ARG:HD3	1:C:386:LYS:HD3	2.00	0.44
1:D:46:MET:HA	1:D:51:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:VAL:HG21	1:A:531:ILE:HG23	2.00	0.44
1:C:217:LYS:O	1:C:221:GLU:HB2	2.18	0.43
1:C:299:ALA:HB3	1:C:341:VAL:HG12	1.99	0.43
1:C:326:SER:HB3	1:D:276:SER:HA	2.00	0.43
1:C:687:LEU:HA	1:C:690:ILE:HG12	2.00	0.43
1:E:368:ASP:OD1	1:E:368:ASP:N	2.51	0.43
1:F:216:ILE:HA	1:F:219:MET:HG2	2.00	0.43
1:B:538:ASN:HD22	1:B:569:ALA:HB1	1.83	0.43
1:C:122:THR:HB	1:C:161:VAL:HA	2.00	0.43
1:D:164:LYS:HD3	1:D:164:LYS:HA	1.80	0.43
1:F:735:HIS:HA	1:F:738:GLU:HG2	2.00	0.43
1:D:29:ASP:HB2	1:D:83:ARG:HA	1.99	0.43
1:D:36:ASN:HB2	1:D:87:VAL:HG21	1.99	0.43
1:D:560:ARG:HH21	1:D:607:GLU:HG3	1.82	0.43
1:E:700:ARG:HA	1:E:703:ILE:HD12	2.00	0.43
1:A:545:PRO:HA	1:A:548:LEU:HB2	2.00	0.43
1:F:251:LYS:HD2	1:F:346:ALA:HB1	1.99	0.43
1:F:423:ILE:HG22	1:F:445:LEU:HD22	2.00	0.43
1:B:354:ASP:HA	1:B:355:PRO:HD3	1.88	0.43
1:B:356:ALA:O	1:B:362:ARG:NH1	2.50	0.43
1:E:614:LYS:HD3	1:F:456:LEU:HD21	2.00	0.43
1:C:277:LYS:HE2	1:C:282:SER:HA	2.00	0.43
1:C:421:GLN:HA	1:C:424:ARG:HE	1.83	0.43
1:A:138:TYR:HB2	1:A:154:VAL:HG21	2.00	0.43
1:F:335:LEU:HD23	1:F:337:GLN:H	1.84	0.43
1:B:381:LEU:O	1:B:385:THR:N	2.52	0.43
1:A:355:PRO:HA	1:A:358:ARG:HB2	2.01	0.43
1:B:395:ASP:H	1:B:398:GLN:HE22	1.67	0.43
1:B:501:ASP:OD1	1:B:501:ASP:N	2.52	0.43
1:E:503:PHE:HD1	1:E:508:MET:HB3	1.83	0.43
1:A:236:LYS:HD3	1:A:236:LYS:HA	1.86	0.43
1:A:327:GLN:O	1:A:331:LEU:HB2	2.19	0.43
1:F:560:ARG:NH1	1:F:603:GLN:O	2.52	0.43
1:C:321:GLU:HA	1:C:324:ILE:HG12	2.00	0.43
1:C:328:LEU:HD23	1:C:331:LEU:HD21	1.99	0.43
1:D:649:ASP:OD1	1:D:649:ASP:N	2.48	0.43
1:E:670:VAL:HG21	1:E:736:PHE:HD1	1.82	0.43
1:A:633:ILE:HG13	1:A:634:LEU:HD22	2.01	0.43
1:C:430:ILE:HD12	1:C:432:LEU:HD12	2.01	0.43
1:A:252:THR:HG22	1:A:302:PHE:HE2	1.83	0.43
1:B:580:ASP:HB2	1:B:628:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:VAL:HG11	1:D:420:LEU:HD21	2.00	0.43
1:E:239:ARG:NH2	1:E:335:LEU:O	2.40	0.43
1:E:320:VAL:HG12	1:E:323:ARG:HD2	1.99	0.43
1:E:604:ILE:HD12	1:E:604:ILE:HA	1.94	0.43
1:A:41:LEU:HD13	1:A:45:LYS:HB2	2.01	0.43
1:F:516:PHE:HE2	1:F:620:ILE:HB	1.83	0.43
1:B:472:PRO:HG3	1:B:539:PHE:HB2	2.01	0.42
1:E:392:ASP:N	1:E:392:ASP:OD1	2.47	0.42
1:E:405:GLY:O	1:E:465:ARG:NH1	2.52	0.42
1:F:206:ILE:HG12	1:F:254:ILE:HD11	2.01	0.42
1:F:312:LYS:N	1:F:352:SER:O	2.51	0.42
1:F:515:LEU:HD21	1:F:639:LEU:HD22	2.01	0.42
1:E:299:ALA:H	1:E:341:VAL:HG12	1.83	0.42
1:F:304:ASP:OD1	1:F:304:ASP:N	2.52	0.42
1:C:540:ILE:HG23	1:C:574:LEU:HA	2.01	0.42
1:D:580:ASP:OD1	1:D:580:ASP:N	2.52	0.42
1:A:272:PRO:O	1:A:276:SER:HB3	2.19	0.42
1:F:230:PHE:HA	1:F:233:ILE:HG12	2.01	0.42
1:C:222:LEU:HD22	1:D:424:ARG:HB3	2.02	0.42
1:D:562:ILE:HA	1:D:565:LYS:HG2	2.01	0.42
1:E:150:ASP:OD1	1:E:150:ASP:N	2.52	0.42
1:A:191:ARG:NH2	1:A:195:GLU:OE1	2.52	0.42
1:F:450:ASP:OD1	1:F:450:ASP:N	2.53	0.42
1:F:519:PRO:HA	1:F:520:PRO:HD3	1.89	0.42
1:C:469:VAL:HB	1:C:538:ASN:HD21	1.85	0.42
1:C:739:ALA:O	1:C:744:ARG:NH1	2.38	0.42
1:D:37:SER:O	1:D:37:SER:OG	2.34	0.42
1:E:239:ARG:NH2	1:E:337:GLN:OE1	2.51	0.42
1:E:449:MET:HB3	1:E:453:ARG:HH12	1.84	0.42
1:B:35:ASP:N	1:B:35:ASP:OD1	2.45	0.42
1:C:35:ASP:OD1	1:C:35:ASP:N	2.51	0.42
1:E:323:ARG:HH22	1:F:278:LEU:HA	1.83	0.42
1:A:45:LYS:HD3	1:A:45:LYS:HA	1.85	0.42
1:B:96:LEU:HD12	1:B:261:GLU:HA	2.01	0.42
1:C:751:ASP:OD1	1:C:754:LYS:NZ	2.43	0.42
1:D:25:ARG:HA	1:D:99:VAL:HG13	2.00	0.42
1:E:92:LEU:HD23	1:E:92:LEU:HA	1.94	0.42
1:E:516:PHE:HE1	1:E:643:ILE:HD11	1.84	0.42
1:A:28:VAL:HG12	1:A:96:LEU:HD13	2.02	0.42
1:A:331:LEU:HD23	1:A:331:LEU:HA	1.83	0.42
1:B:197:SER:HB2	1:B:200:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:ILE:HG23	1:B:411:LEU:HD22	2.02	0.42
1:C:153:LEU:HD21	1:C:160:ALA:HB1	2.01	0.42
1:D:582:ILE:HG21	1:D:600:VAL:HB	2.01	0.42
1:B:242:LEU:HD11	1:B:347:THR:HG22	2.01	0.42
1:D:239:ARG:N	1:D:365:ARG:HH22	2.18	0.42
1:E:214:ALA:O	1:E:218:GLU:HB2	2.19	0.42
1:E:381:LEU:HD13	1:E:396:LEU:HD12	2.02	0.42
1:B:239:ARG:HD2	1:B:335:LEU:HD23	2.01	0.42
1:B:381:LEU:HD22	1:B:396:LEU:HD13	2.00	0.42
1:D:229:LEU:HD12	1:E:437:ILE:HG21	2.02	0.42
1:E:330:THR:O	1:E:334:GLY:N	2.53	0.42
1:E:380:ILE:HD13	1:E:380:ILE:HA	1.88	0.42
1:E:731:ILE:HG13	1:E:732:ARG:HG2	2.01	0.42
1:B:219:MET:HG3	1:B:220:VAL:HG13	2.01	0.41
1:D:377:ARG:NH1	1:D:403:THR:O	2.53	0.41
1:E:545:PRO:HA	1:E:548:LEU:HG	2.01	0.41
1:A:153:LEU:HD11	1:A:198:LEU:HD22	2.00	0.41
1:D:434:ASP:N	1:D:434:ASP:OD1	2.53	0.41
1:F:371:ILE:HD12	1:F:372:PRO:HD2	2.02	0.41
1:F:475:THR:OG1	1:F:476:TRP:N	2.48	0.41
1:B:60:LYS:HE2	1:B:101:SER:HB3	2.02	0.41
1:B:273:GLU:HA	1:B:276:SER:HB3	2.02	0.41
1:C:116:VAL:HG12	1:C:165:VAL:HA	2.02	0.41
1:D:153:LEU:HD12	1:D:162:GLU:HB3	2.03	0.41
1:A:118:PRO:HB3	1:A:163:PHE:HD1	1.85	0.41
1:A:575:PHE:HA	1:A:620:ILE:HG13	2.01	0.41
1:F:374:ALA:HA	1:F:377:ARG:HB2	2.02	0.41
1:B:301:ILE:HG13	1:B:343:VAL:HA	2.01	0.41
1:B:603:GLN:HE21	1:C:549:THR:HG23	1.86	0.41
1:D:201:VAL:HG21	1:D:253:LEU:HG	2.01	0.41
1:E:107:ASP:OD1	1:E:107:ASP:N	2.50	0.41
1:E:120:ASP:OD1	1:E:120:ASP:N	2.52	0.41
1:E:244:TYR:H	1:E:368:ASP:HA	1.85	0.41
1:E:373:ASP:OD2	1:E:375:THR:OG1	2.38	0.41
1:A:392:ASP:N	1:A:392:ASP:OD1	2.52	0.41
1:A:567:ARG:NH1	1:A:610:GLY:O	2.47	0.41
1:F:286:LEU:HD21	1:F:328:LEU:HB2	2.01	0.41
1:B:371:ILE:HD12	1:B:372:PRO:HD2	2.02	0.41
1:C:201:VAL:HG11	1:C:253:LEU:HD13	2.01	0.41
1:C:501:ASP:OD1	1:C:501:ASP:N	2.51	0.41
1:D:126:ILE:HG22	1:D:130:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:TYR:CG	1:D:350:PRO:HB3	2.56	0.41
1:B:146:ILE:N	1:B:174:CYS:O	2.46	0.41
1:D:38:VAL:HB	1:D:72:LEU:HD23	2.03	0.41
1:D:120:ASP:HA	1:D:188:PRO:HB2	2.03	0.41
1:E:495:TYR:HD2	1:E:502:LYS:HD3	1.86	0.41
1:C:654:VAL:HG22	1:C:672:LEU:HB3	2.02	0.41
1:E:674:PHE:HD1	1:E:677:LYS:HZ2	1.68	0.41
1:F:528:ALA:HA	1:F:531:ILE:HG22	2.03	0.41
1:B:246:PRO:O	1:B:251:LYS:NZ	2.41	0.41
1:C:564:ASP:HA	1:C:567:ARG:HD3	2.02	0.41
1:D:78:SER:HB2	1:D:81:LYS:HE2	2.03	0.41
1:D:299:ALA:HB3	1:D:341:VAL:HG12	2.03	0.41
1:D:625:ARG:NH2	1:D:755:TYR:OH	2.54	0.41
1:F:313:ARG:HD2	1:F:315:LYS:HB3	2.03	0.41
1:F:374:ALA:HA	1:F:377:ARG:HE	1.86	0.41
1:B:327:GLN:HE21	1:C:276:SER:HA	1.86	0.41
1:B:377:ARG:HA	1:B:380:ILE:HG22	2.03	0.41
1:C:77:CYS:HB3	1:C:83:ARG:HD3	2.02	0.41
1:A:36:ASN:OD1	1:A:144:ARG:NH1	2.46	0.41
1:A:132:GLU:HG2	1:A:133:VAL:HG23	2.01	0.41
1:A:208:GLY:HA2	1:A:379:GLU:HG2	2.03	0.41
1:A:485:VAL:O	1:A:489:LEU:HB2	2.20	0.41
1:F:412:ALA:O	1:F:416:SER:HB3	2.21	0.41
1:F:454:TRP:O	1:F:457:SER:OG	2.33	0.41
1:B:233:ILE:HG22	1:B:235:VAL:H	1.86	0.41
1:A:635:ARG:HB2	1:A:638:ARG:HH21	1.85	0.41
1:B:213:LEU:HA	1:B:216:ILE:HG12	2.03	0.40
1:C:86:ARG:HA	1:C:89:ARG:HB2	2.02	0.40
1:C:348:ASN:OD1	1:C:348:ASN:N	2.53	0.40
1:D:45:LYS:O	1:D:45:LYS:NZ	2.36	0.40
1:D:242:LEU:HB2	1:D:366:GLU:HG3	2.02	0.40
1:E:475:THR:OG1	1:E:534:GLU:OE2	2.39	0.40
1:F:465:ARG:HD2	1:F:465:ARG:HA	1.92	0.40
1:B:202:GLY:N	1:B:205:ASP:OD2	2.51	0.40
1:B:469:VAL:HG22	1:B:540:ILE:HD13	2.03	0.40
1:D:117:LEU:N	1:D:164:LYS:O	2.54	0.40
1:D:642:LEU:HD13	1:D:762:LEU:HD13	2.03	0.40
1:E:538:ASN:O	1:E:573:VAL:N	2.54	0.40
1:F:466:GLU:OE2	1:F:565:LYS:NZ	2.41	0.40
1:B:86:ARG:NH2	1:B:200:GLU:O	2.55	0.40
1:B:132:GLU:O	1:B:136:LYS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASP:N	1:B:580:ASP:OD1	2.47	0.40
1:C:230:PHE:HA	1:C:233:ILE:HG22	2.04	0.40
1:D:41:LEU:HD21	1:D:46:MET:HB3	2.03	0.40
1:D:292:GLU:HA	1:D:295:LYS:HG2	2.02	0.40
1:A:562:ILE:HA	1:A:565:LYS:HG3	2.02	0.40
1:F:542:ILE:HD13	1:F:574:LEU:HG	2.03	0.40
1:B:604:ILE:HA	1:B:607:GLU:HG3	2.04	0.40
1:D:353:ILE:O	1:D:358:ARG:NH1	2.54	0.40
1:E:29:ASP:O	1:E:89:ARG:NH2	2.54	0.40
1:E:373:ASP:OD1	1:E:373:ASP:N	2.49	0.40
1:E:389:LYS:HA	1:E:389:LYS:HD2	1.73	0.40
1:A:66:GLU:O	1:A:147:ARG:NE	2.54	0.40
1:F:215:GLN:HA	1:F:218:GLU:HB3	2.03	0.40
1:F:635:ARG:HB2	1:F:638:ARG:HE	1.87	0.40
1:F:679:THR:HG22	1:F:682:PHE:HD2	1.87	0.40
1:B:612:SER:HB3	1:B:615:LYS:HB2	2.03	0.40
1:C:215:GLN:HE22	1:C:367:VAL:HG21	1.87	0.40
1:C:312:LYS:HB2	1:C:354:ASP:HB3	2.03	0.40
1:A:224:LEU:HD13	1:A:262:THR:HG21	2.04	0.40
1:A:605:LEU:HA	1:A:608:MET:HG2	2.02	0.40
1:F:564:ASP:HA	1:F:567:ARG:HB2	2.04	0.40
1:F:605:LEU:HD21	1:F:633:ILE:HB	2.04	0.40
1:F:624:ASN:O	1:F:755:TYR:OH	2.33	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	695/806 (86%)	626 (90%)	69 (10%)	0	100	100
1	B	695/806 (86%)	654 (94%)	41 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	697/806 (86%)	643 (92%)	54 (8%)	0	100	100
1	D	697/806 (86%)	639 (92%)	58 (8%)	0	100	100
1	E	698/806 (87%)	641 (92%)	57 (8%)	0	100	100
1	F	533/806 (66%)	493 (92%)	40 (8%)	0	100	100
All	All	4015/4836 (83%)	3696 (92%)	319 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	603/678 (89%)	597 (99%)	6 (1%)	76	86
1	B	603/678 (89%)	602 (100%)	1 (0%)	93	96
1	C	604/678 (89%)	596 (99%)	8 (1%)	69	82
1	D	604/678 (89%)	599 (99%)	5 (1%)	81	89
1	E	604/678 (89%)	596 (99%)	8 (1%)	69	82
1	F	452/678 (67%)	447 (99%)	5 (1%)	73	85
All	All	3470/4068 (85%)	3437 (99%)	33 (1%)	77	86

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	744	ARG
1	C	25	ARG
1	C	112	LYS
1	C	113	ARG
1	C	285	ASN
1	C	377	ARG
1	C	677	LYS
1	C	744	ARG
1	C	753	ARG

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Mol	Chain	Res	Type
1	D	377	ARG
1	D	389	LYS
1	D	487	ARG
1	D	662	ARG
1	D	700	ARG
1	E	84	MET
1	E	144	ARG
1	E	215	GLN
1	E	322	ARG
1	E	362	ARG
1	E	565	LYS
1	E	638	ARG
1	E	744	ARG
1	A	25	ARG
1	A	112	LYS
1	A	295	LYS
1	A	365	ARG
1	A	565	LYS
1	A	744	ARG
1	F	295	LYS
1	F	365	ARG
1	F	487	ARG
1	F	512	LYS
1	F	744	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	270	ASN
1	B	327	GLN
1	C	285	ASN
1	D	494	GLN
1	D	603	GLN
1	F	296	ASN
1	F	317	HIS
1	F	660	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)

6 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	ADP	B	901	-	24,29,29	0.92	1 (4%)	29,45,45	1.38	3 (10%)
2	ADP	A	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.37	4 (13%)
2	ADP	C	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.37	3 (10%)
2	ADP	D	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
2	ADP	E	901	-	24,29,29	0.94	1 (4%)	29,45,45	1.44	4 (13%)
2	ADP	F	901	-	24,29,29	0.99	1 (4%)	29,45,45	1.43	5 (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	ADP	B	901	-	-	3/12/32/32	0/3/3/3
2	ADP	A	901	-	-	5/12/32/32	0/3/3/3
2	ADP	C	901	-	-	6/12/32/32	0/3/3/3
2	ADP	D	901	-	-	4/12/32/32	0/3/3/3
2	ADP	E	901	-	-	5/12/32/32	0/3/3/3
2	ADP	F	901	-	-	2/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ADP	C5-C4	2.54	1.47	1.40
2	F	901	ADP	C5-C4	2.53	1.47	1.40
2	B	901	ADP	C5-C4	2.48	1.47	1.40
2	D	901	ADP	C5-C4	2.48	1.47	1.40
2	C	901	ADP	C5-C4	2.47	1.47	1.40
2	E	901	ADP	C5-C4	2.44	1.47	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	ADP	C3'-C2'-C1'	3.99	106.98	100.98
2	C	901	ADP	C3'-C2'-C1'	3.88	106.82	100.98
2	B	901	ADP	C3'-C2'-C1'	3.63	106.45	100.98
2	F	901	ADP	C3'-C2'-C1'	3.53	106.29	100.98
2	E	901	ADP	N3-C2-N1	-3.37	123.41	128.68
2	B	901	ADP	N3-C2-N1	-3.30	123.52	128.68
2	A	901	ADP	N3-C2-N1	-3.29	123.54	128.68
2	D	901	ADP	PA-O3A-PB	-3.28	121.59	132.83
2	E	901	ADP	PA-O3A-PB	-3.27	121.61	132.83
2	D	901	ADP	N3-C2-N1	-3.20	123.67	128.68
2	A	901	ADP	C3'-C2'-C1'	3.18	105.77	100.98
2	F	901	ADP	N3-C2-N1	-3.10	123.84	128.68
2	E	901	ADP	C3'-C2'-C1'	3.09	105.64	100.98
2	C	901	ADP	N3-C2-N1	-3.07	123.88	128.68
2	F	901	ADP	PA-O3A-PB	-3.02	122.47	132.83
2	A	901	ADP	C4-C5-N7	-2.61	106.68	109.40
2	E	901	ADP	C4-C5-N7	-2.58	106.71	109.40
2	B	901	ADP	C4-C5-N7	-2.52	106.77	109.40
2	C	901	ADP	C4-C5-N7	-2.39	106.91	109.40
2	A	901	ADP	PA-O3A-PB	-2.32	124.88	132.83
2	D	901	ADP	C4-C5-N7	-2.23	107.07	109.40
2	F	901	ADP	C4-C5-N7	-2.10	107.21	109.40
2	F	901	ADP	O3B-PB-O2B	2.01	115.33	107.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	ADP	C5'-O5'-PA-O3A
2	C	901	ADP	PA-O3A-PB-O2B
2	D	901	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
2	E	901	ADP	C5'-O5'-PA-O1A
2	E	901	ADP	C5'-O5'-PA-O2A
2	A	901	ADP	C5'-O5'-PA-O1A
2	A	901	ADP	C5'-O5'-PA-O2A
2	A	901	ADP	C5'-O5'-PA-O3A
2	A	901	ADP	O4'-C4'-C5'-O5'
2	C	901	ADP	C5'-O5'-PA-O3A
2	F	901	ADP	PB-O3A-PA-O1A
2	B	901	ADP	C5'-O5'-PA-O1A
2	B	901	ADP	C5'-O5'-PA-O2A
2	D	901	ADP	C5'-O5'-PA-O1A
2	C	901	ADP	PA-O3A-PB-O1B
2	E	901	ADP	O4'-C4'-C5'-O5'
2	F	901	ADP	O4'-C4'-C5'-O5'
2	E	901	ADP	C5'-O5'-PA-O3A
2	D	901	ADP	O4'-C4'-C5'-O5'
2	E	901	ADP	PB-O3A-PA-O2A
2	C	901	ADP	C5'-O5'-PA-O1A
2	C	901	ADP	C5'-O5'-PA-O2A
2	D	901	ADP	C5'-O5'-PA-O2A
2	C	901	ADP	O4'-C4'-C5'-O5'
2	A	901	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

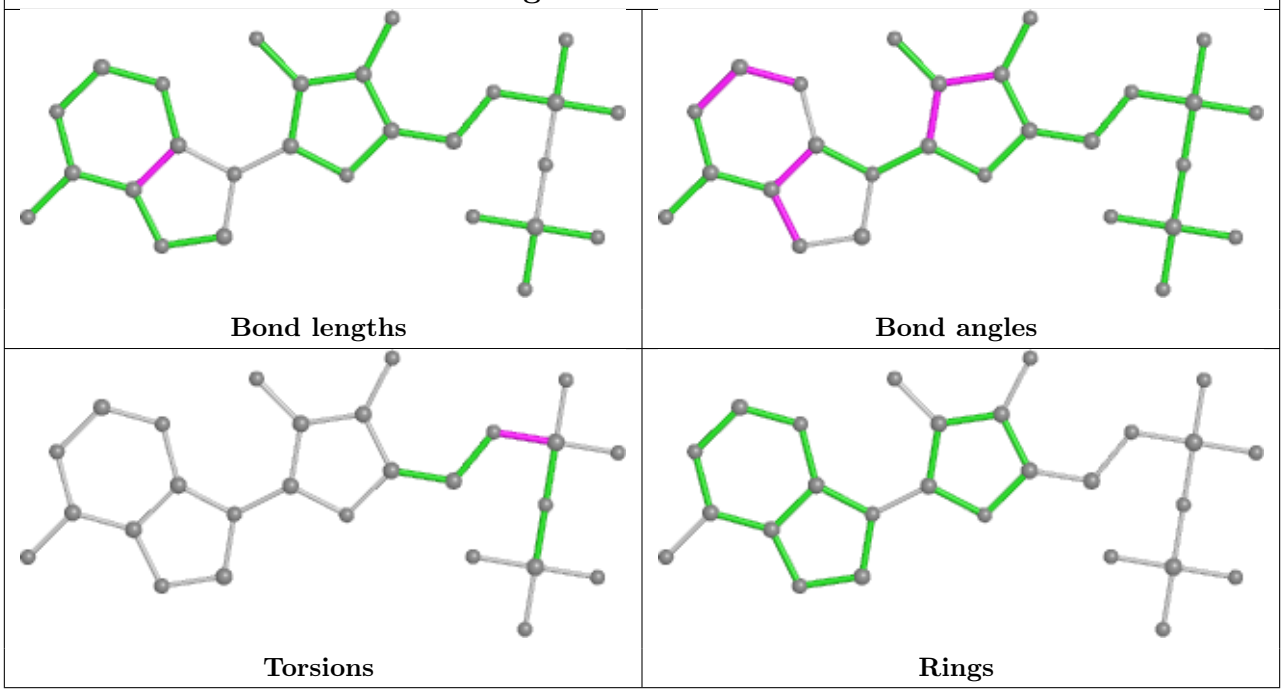
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	ADP	1	0
2	A	901	ADP	1	0
2	C	901	ADP	1	0
2	F	901	ADP	1	0

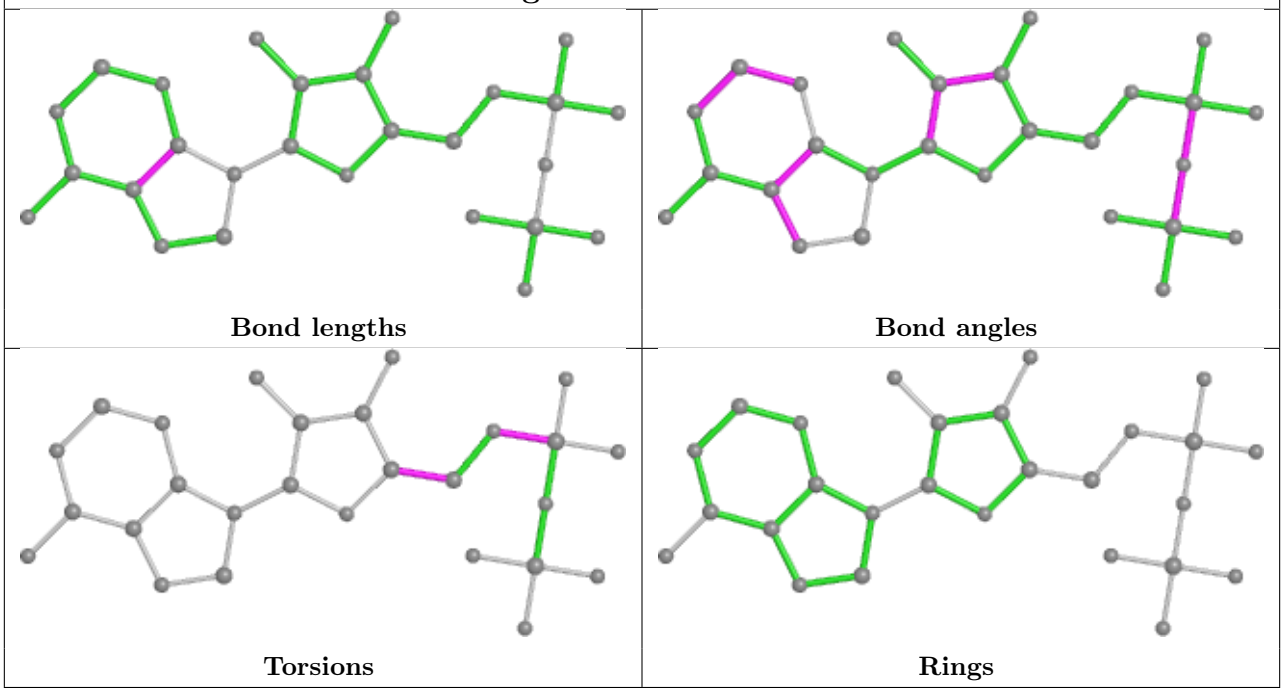
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

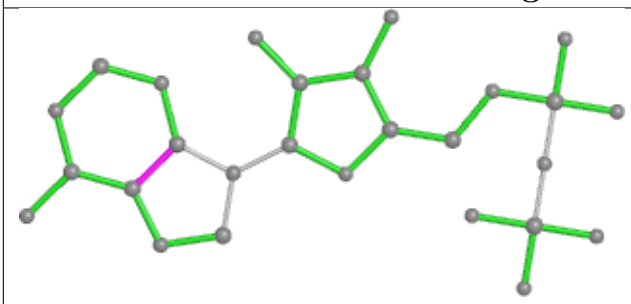
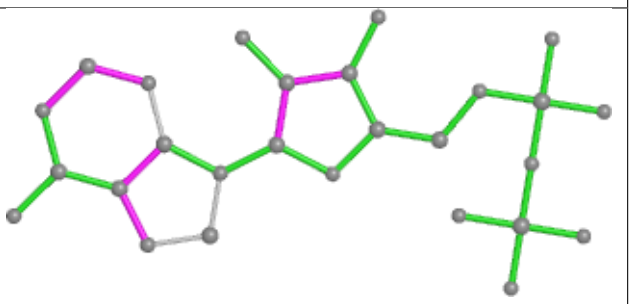
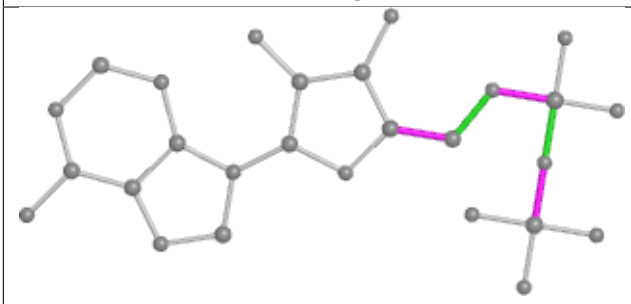
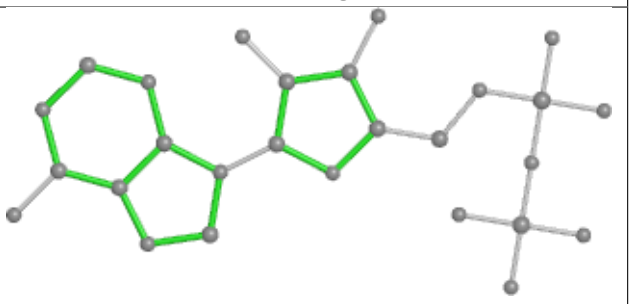
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

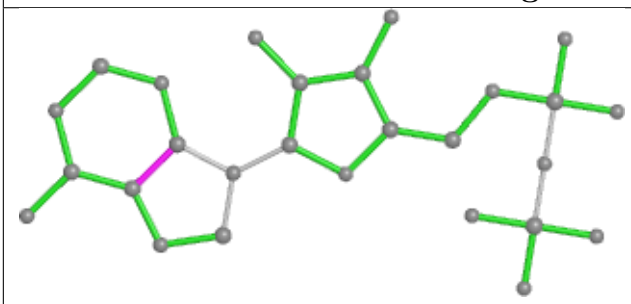
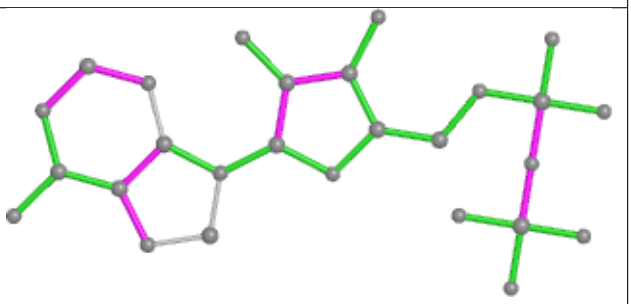
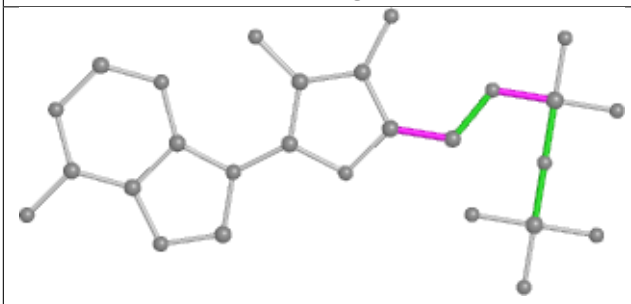
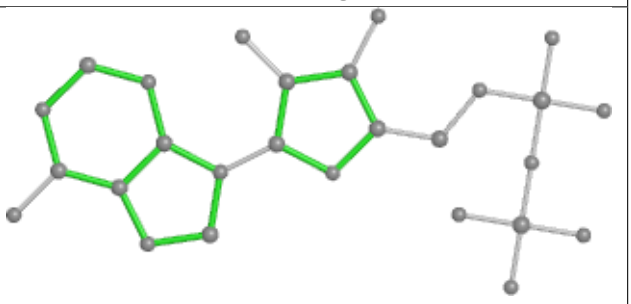
Ligand ADP B 901



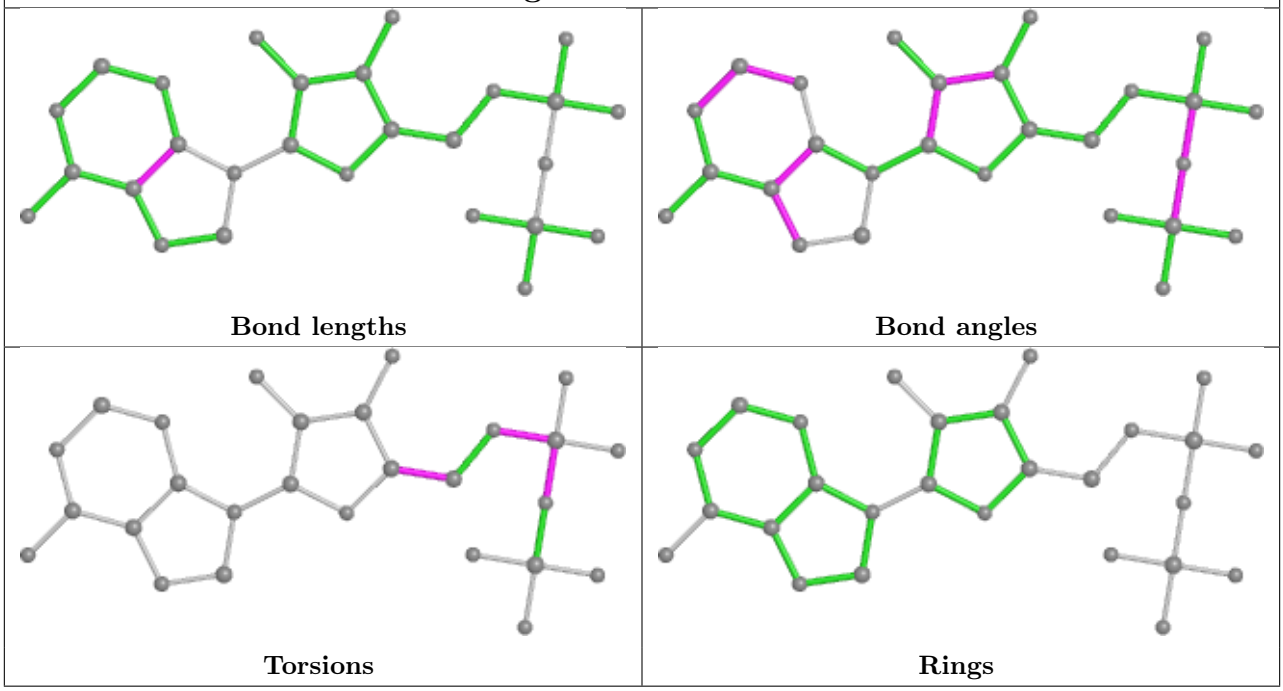
Ligand ADP A 901



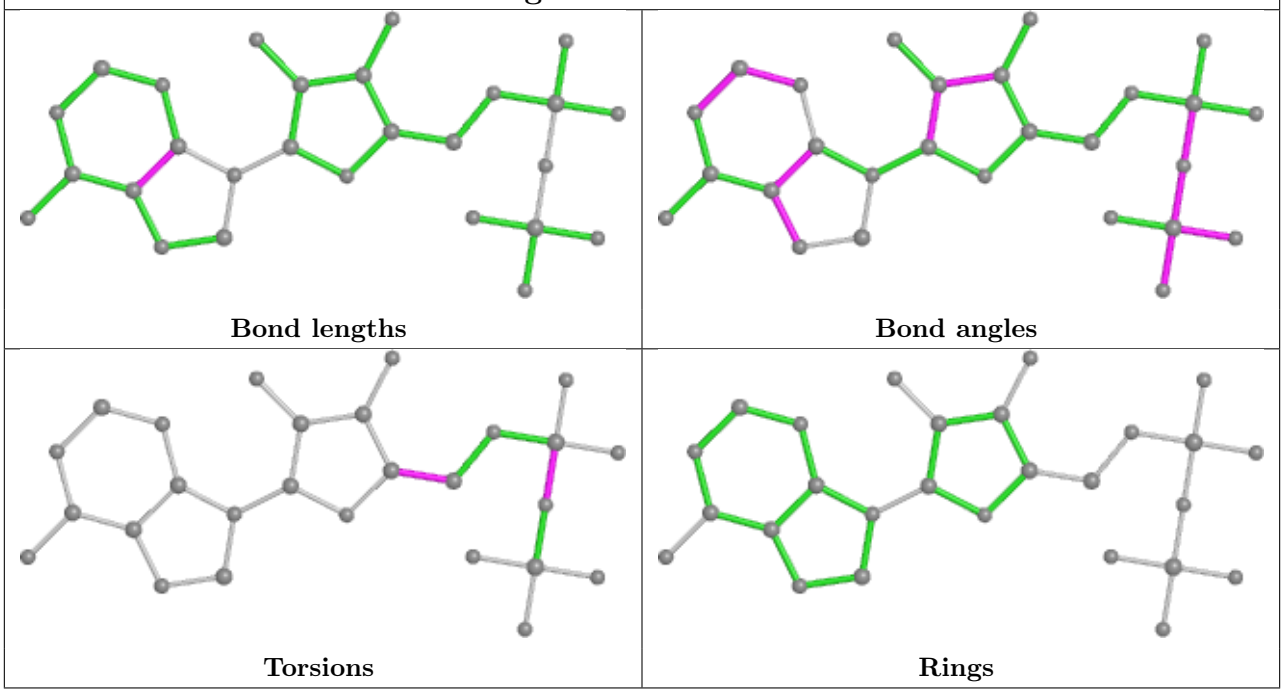
Ligand ADP C 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP E 901



Ligand ADP F 901



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

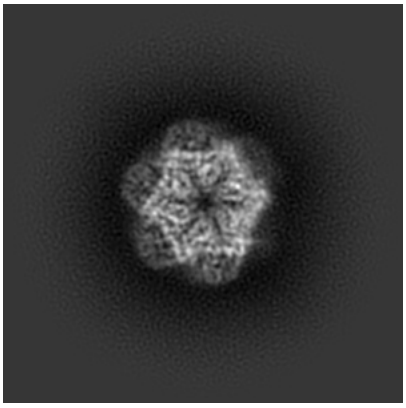
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23775. These allow visual inspection of the internal detail of the map and identification of artifacts.

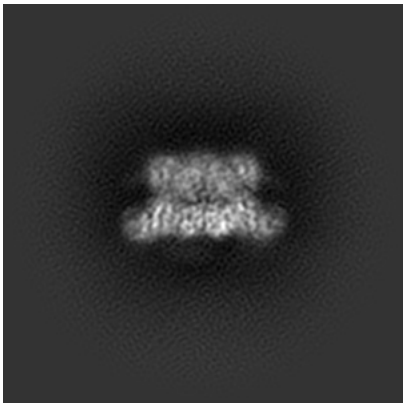
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



X



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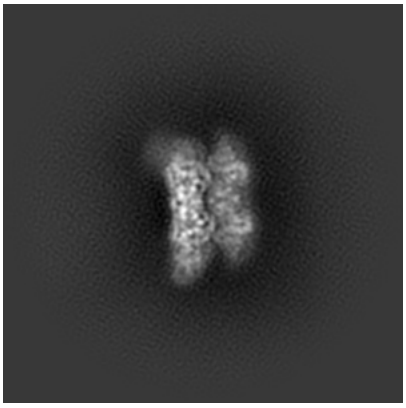
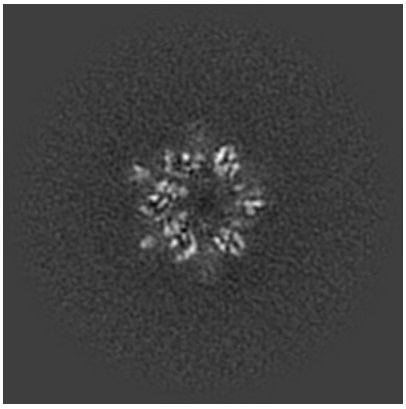


Z

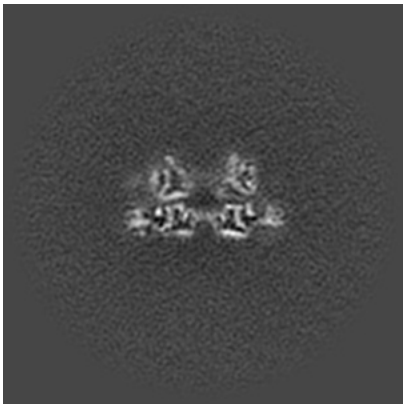
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

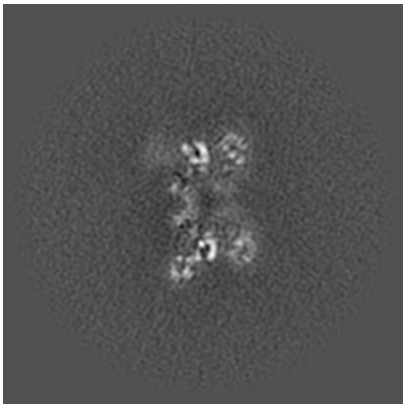
6.2.1 Primary map



X Index: 120



Y Index: 120

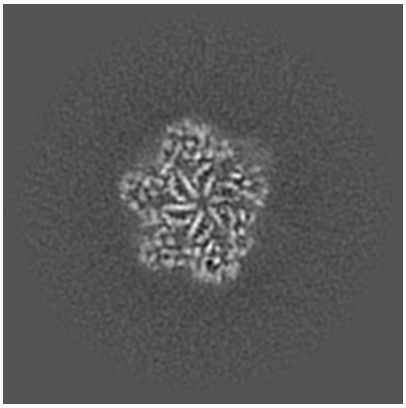


Z Index: 120

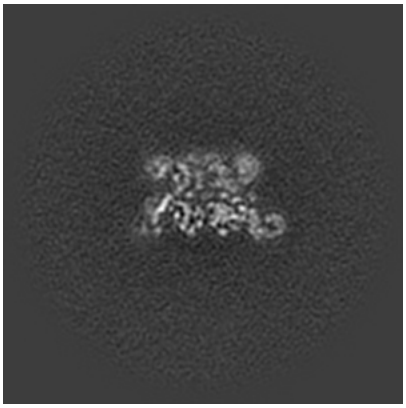
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

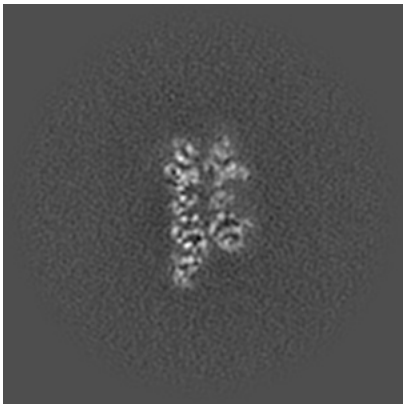
6.3.1 Primary map



X Index: 108



Y Index: 103

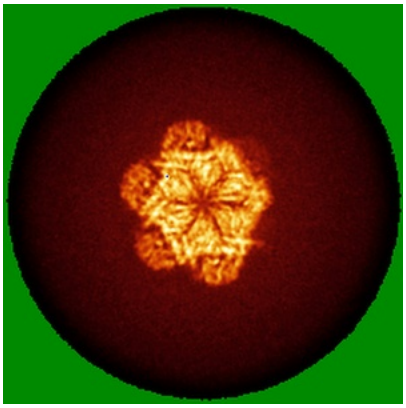


Z Index: 131

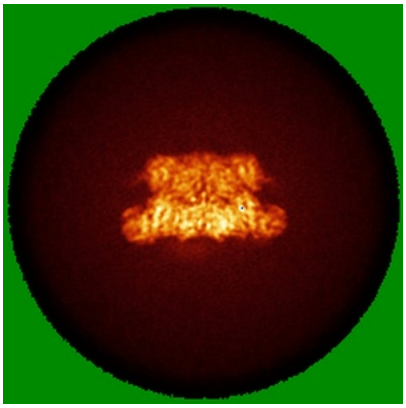
The images above show the largest variance slices of the map in three orthogonal directions.

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

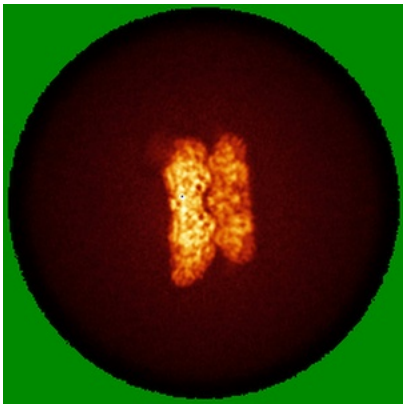
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

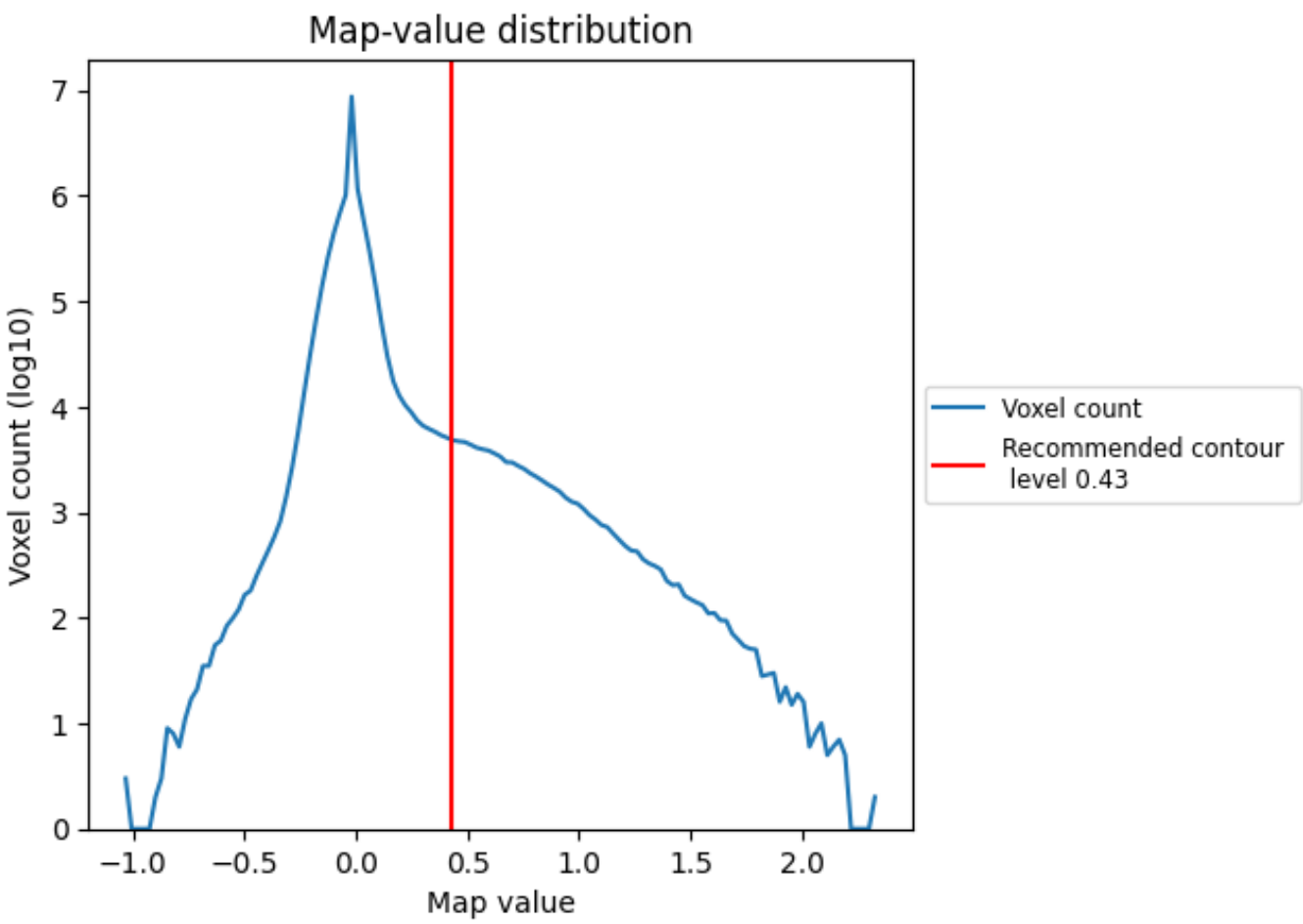
6.6 Mask visualisation (i)

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

7 Map analysis (i)

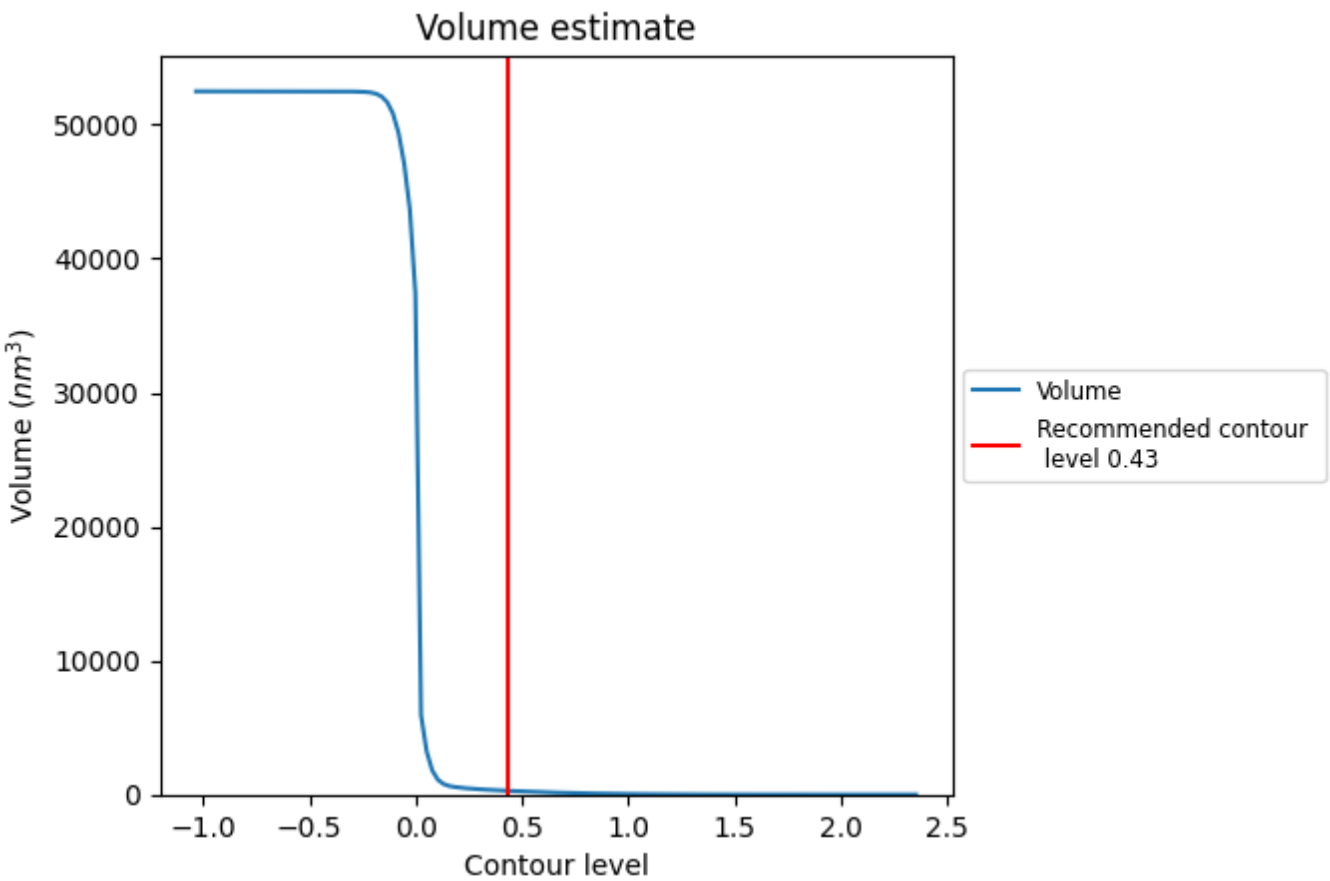
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

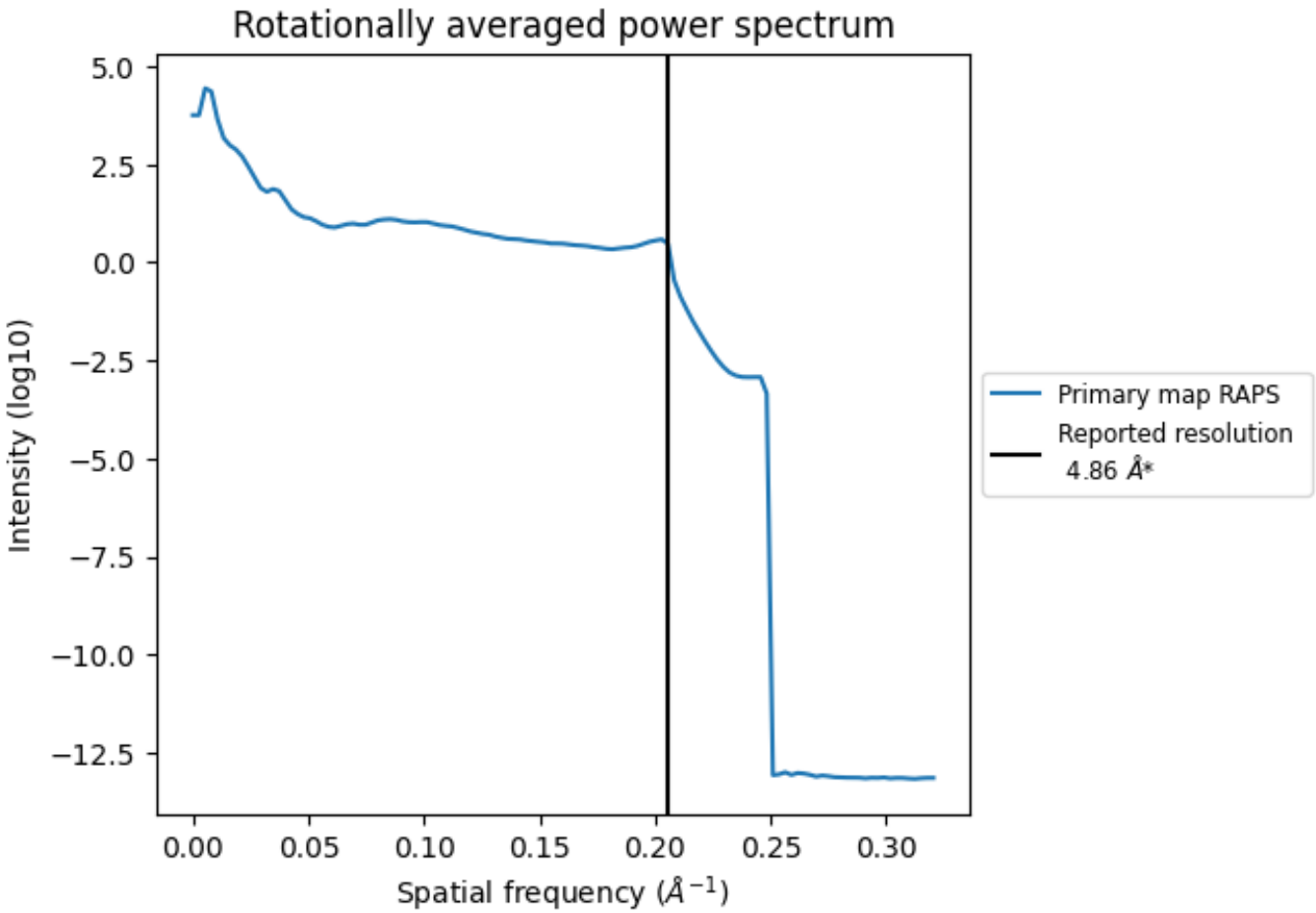
7.2 Volume estimate (i)



The volume at the recommended contour level is 286 nm^3; this corresponds to an approximate mass of 258 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 0.206 Å^{-1}

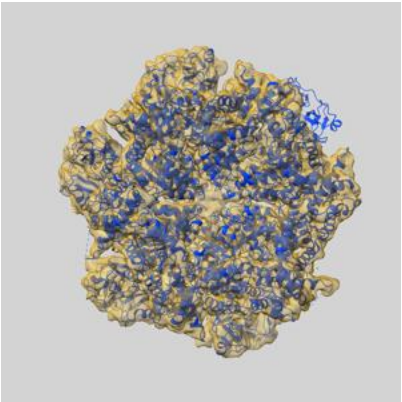
8 Fourier-Shell correlation (i)

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

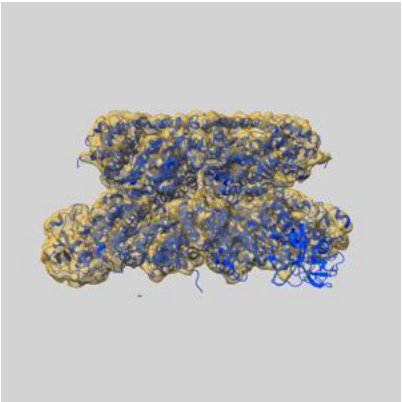
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23775 and PDB model 7MDM. Per-residue inclusion information can be found in section 3 on page 5.

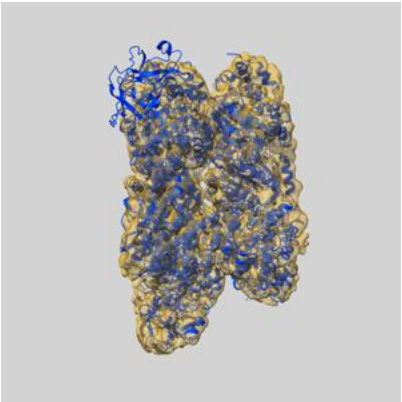
9.1 Map-model overlay (i)



X



Y



Z

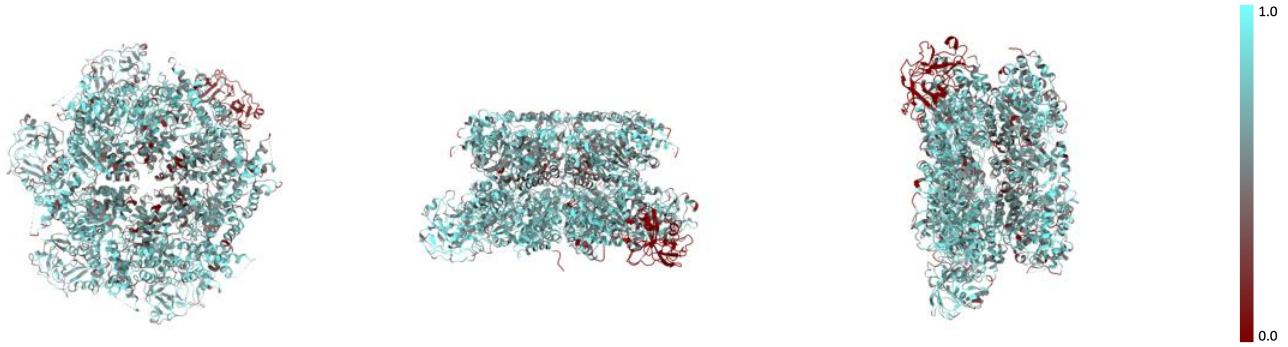
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

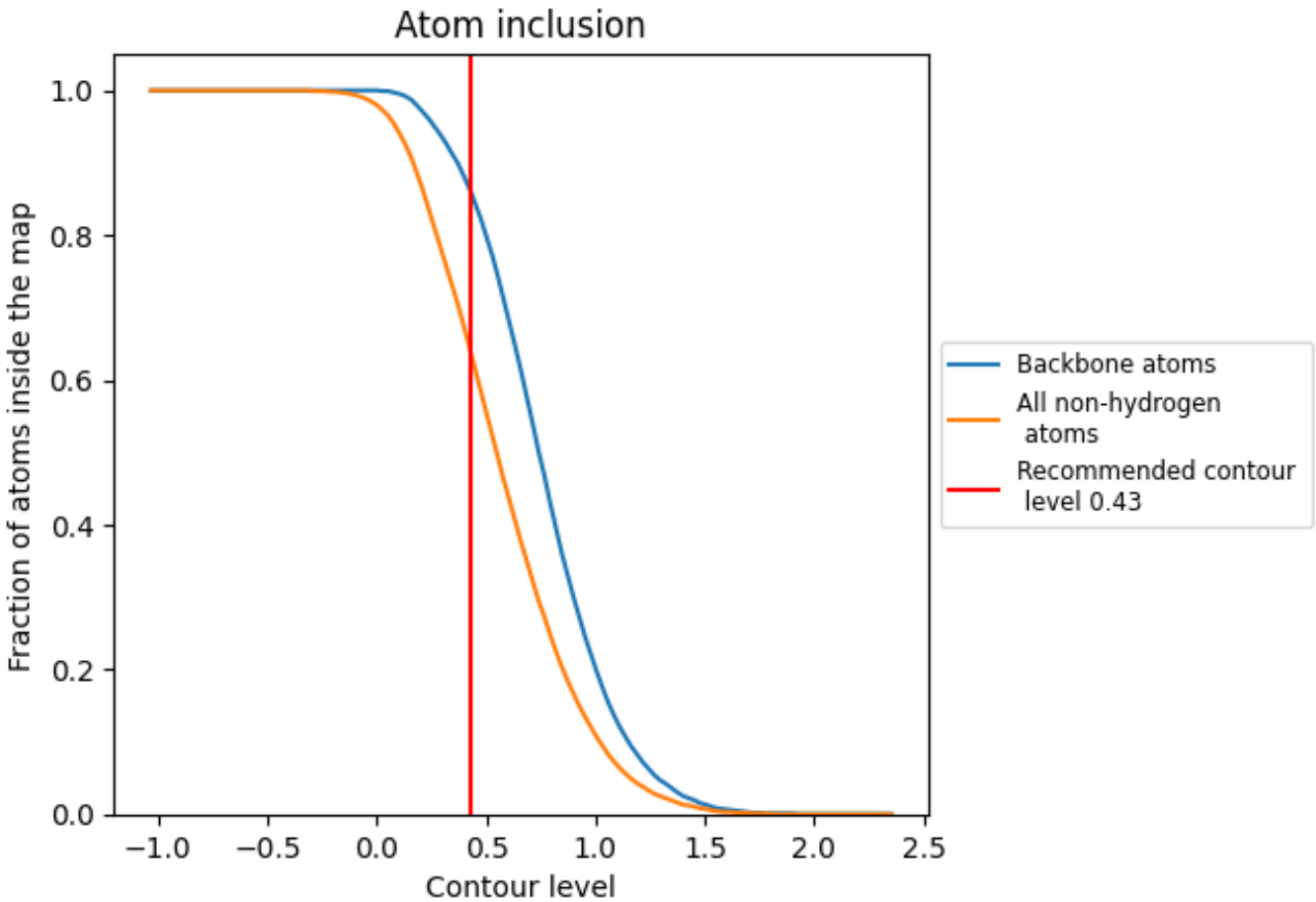
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.43).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 64% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6380	0.1840
A	0.6900	0.1900
B	0.6780	0.1970
C	0.6680	0.1870
D	0.6540	0.1880
E	0.5060	0.1630
F	0.6300	0.1810