Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 09:12 PM UTC

PDB ID	:	9CLM / pdb_00009clm
EMDB ID	:	EMD-45682
Title	:	Transferrin Binding Protein A in complex with transferrin binding protein B and two molecules of transferrin
Authors	:	Dubey, S.; Noinaj, N.
Deposited on	:	2024-07-11
Resolution	:	4.30 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*
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https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

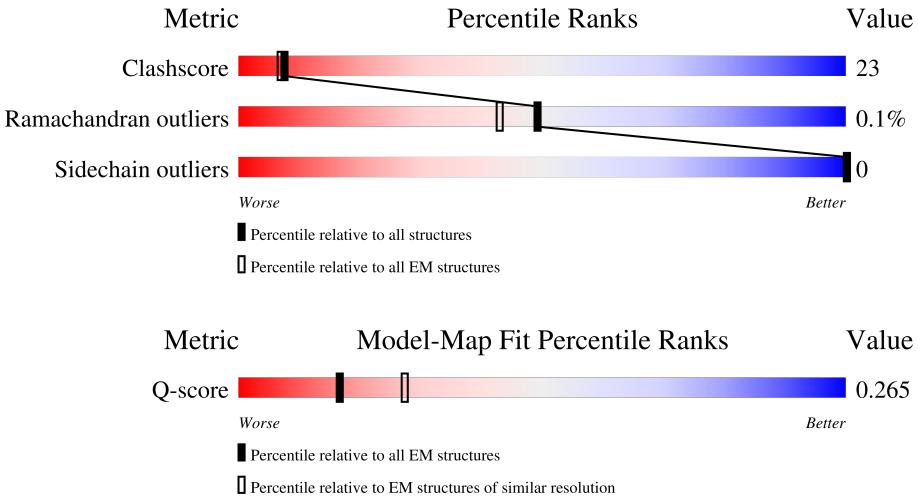
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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	939	6% 54% 38% 7%
2	B	712	42% 42% 16%
3	F	698	20% 54% 42%
3	G	698	6% 55% 41%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCT	F	701	-	-	X	-
4	BCT	G	701	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21972 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 Transferrin Binding Protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	870	6869	4289	1264	1305	11	0	0

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP A0A0E3X1L2
A	-22	SER	-	expression tag	UNP A0A0E3X1L2
A	-21	ASN	-	expression tag	UNP A0A0E3X1L2
A	-20	HIS	-	expression tag	UNP A0A0E3X1L2
A	-19	HIS	-	expression tag	UNP A0A0E3X1L2
A	-18	HIS	-	expression tag	UNP A0A0E3X1L2
A	-17	HIS	-	expression tag	UNP A0A0E3X1L2
A	-16	HIS	-	expression tag	UNP A0A0E3X1L2
A	-15	HIS	-	expression tag	UNP A0A0E3X1L2
A	-14	HIS	-	expression tag	UNP A0A0E3X1L2
A	-13	HIS	-	expression tag	UNP A0A0E3X1L2
A	-12	HIS	-	expression tag	UNP A0A0E3X1L2
A	-11	HIS	-	expression tag	UNP A0A0E3X1L2
A	-10	GLU	-	expression tag	UNP A0A0E3X1L2
A	-9	ASN	-	expression tag	UNP A0A0E3X1L2
A	-8	LEU	-	expression tag	UNP A0A0E3X1L2
A	-7	TYR	-	expression tag	UNP A0A0E3X1L2
A	-6	PHE	-	expression tag	UNP A0A0E3X1L2
A	-5	GLN	-	expression tag	UNP A0A0E3X1L2
A	-4	GLY	-	expression tag	UNP A0A0E3X1L2
A	-3	ALA	-	expression tag	UNP A0A0E3X1L2
A	-2	MET	-	expression tag	UNP A0A0E3X1L2
A	-1	ASP	-	expression tag	UNP A0A0E3X1L2
A	0	ILE	-	expression tag	UNP A0A0E3X1L2
A	22	ALA	VAL	conflict	UNP A0A0E3X1L2
A	222	ARG	HIS	conflict	UNP A0A0E3X1L2
A	226	HIS	ARG	conflict	UNP A0A0E3X1L2
A	235	ALA	ASP	conflict	UNP A0A0E3X1L2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ALA	VAL	conflict	UNP A0A0E3X1L2
A	250	ASP	GLU	conflict	UNP A0A0E3X1L2
A	252	GLY	SER	conflict	UNP A0A0E3X1L2
A	254	LYS	ASN	conflict	UNP A0A0E3X1L2
A	261	GLU	LYS	conflict	UNP A0A0E3X1L2
A	268	GLY	SER	conflict	UNP A0A0E3X1L2
A	269	HIS	TYR	conflict	UNP A0A0E3X1L2
A	271	LYS	THR	conflict	UNP A0A0E3X1L2
A	283	GLU	LYS	conflict	UNP A0A0E3X1L2
A	285	LYS	GLU	conflict	UNP A0A0E3X1L2
A	333	ARG	HIS	conflict	UNP A0A0E3X1L2
A	358	GLN	SER	conflict	UNP A0A0E3X1L2
A	365	ARG	PRO	conflict	UNP A0A0E3X1L2
A	382	SER	ASN	conflict	UNP A0A0E3X1L2
A	386	ASN	GLY	conflict	UNP A0A0E3X1L2
A	388	PRO	LEU	conflict	UNP A0A0E3X1L2
A	478	LYS	ARG	conflict	UNP A0A0E3X1L2
A	503	TYR	PHE	conflict	UNP A0A0E3X1L2
A	519	SER	HIS	conflict	UNP A0A0E3X1L2
A	526	LEU	SER	conflict	UNP A0A0E3X1L2
A	527	LYS	ASN	conflict	UNP A0A0E3X1L2
A	537	THR	ILE	conflict	UNP A0A0E3X1L2
A	542	ARG	SER	conflict	UNP A0A0E3X1L2
A	544	LYS	THR	conflict	UNP A0A0E3X1L2
A	545	ASN	SER	conflict	UNP A0A0E3X1L2
A	550	SER	THR	conflict	UNP A0A0E3X1L2
A	559	ARG	GLY	conflict	UNP A0A0E3X1L2
A	563	LEU	ARG	conflict	UNP A0A0E3X1L2
A	564	PHE	LEU	conflict	UNP A0A0E3X1L2
A	635	ALA	THR	conflict	UNP A0A0E3X1L2
A	661	SER	ALA	conflict	UNP A0A0E3X1L2
A	663	ASP	VAL	conflict	UNP A0A0E3X1L2
A	664	LYS	GLN	conflict	UNP A0A0E3X1L2
A	665	ILE	SER	conflict	UNP A0A0E3X1L2
A	718	GLN	GLU	conflict	UNP A0A0E3X1L2
A	719	VAL	ALA	conflict	UNP A0A0E3X1L2
A	722	ASN	ASP	conflict	UNP A0A0E3X1L2
A	795	SER	LEU	conflict	UNP A0A0E3X1L2
A	872	HIS	TYR	conflict	UNP A0A0E3X1L2
A	885	ALA	GLY	conflict	UNP A0A0E3X1L2

- Molecule 2 is a protein called Transferrin Binding Protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	600	Total	C	N	O	S	0	0
			4720	2939	817	958	6		

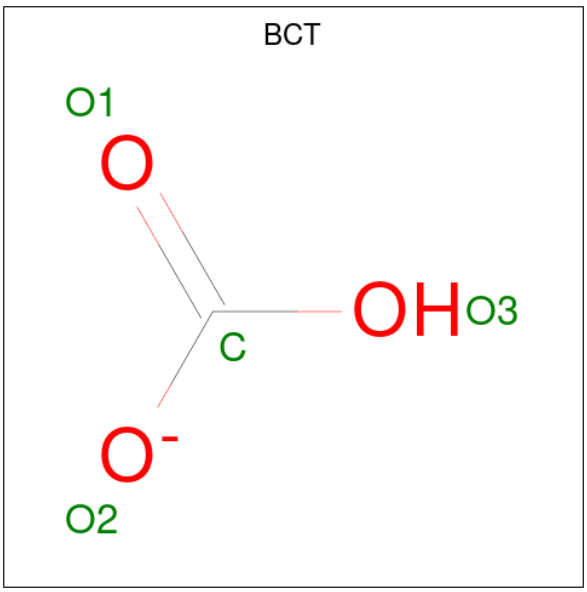
- Molecule 3 is a protein called Transferrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	675	Total	C	N	O	S	1	0
			5176	3256	896	977	47		
3	G	675	Total	C	N	O	S	0	0
			5192	3263	896	986	47		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	448	VAL	ILE	conflict	UNP P02787
G	448	VAL	ILE	conflict	UNP P02787

- Molecule 4 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	F	1	Total	C	O		0
			4	1	3		
4	G	1	Total	C	O		0
			4	1	3		
4	G	1	Total	C	O		0
			4	1	3		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

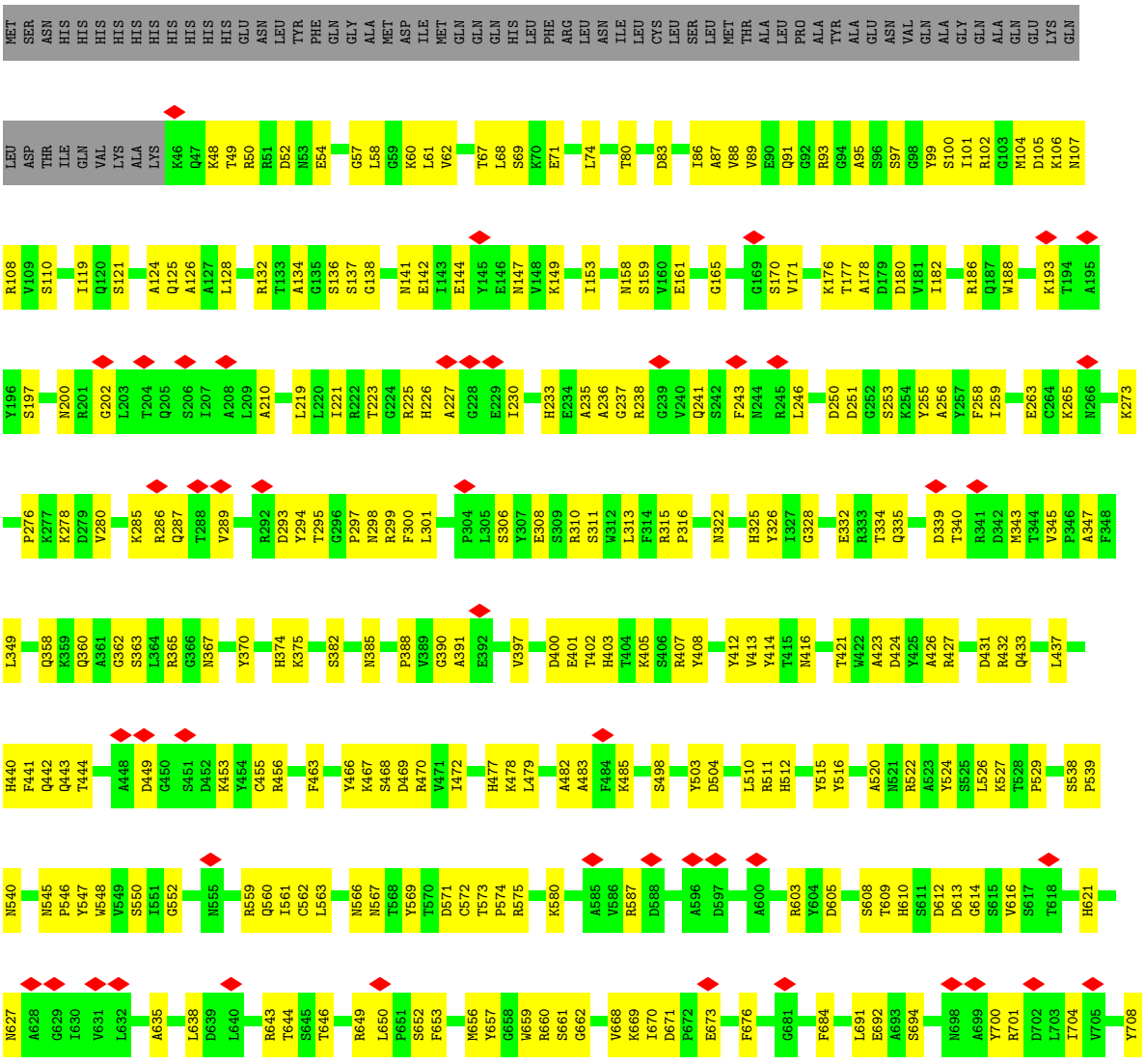
Mol	Chain	Residues	Atoms	AltConf
5	F	1	Total Fe 1 1	0
5	G	2	Total Fe 2 2	0

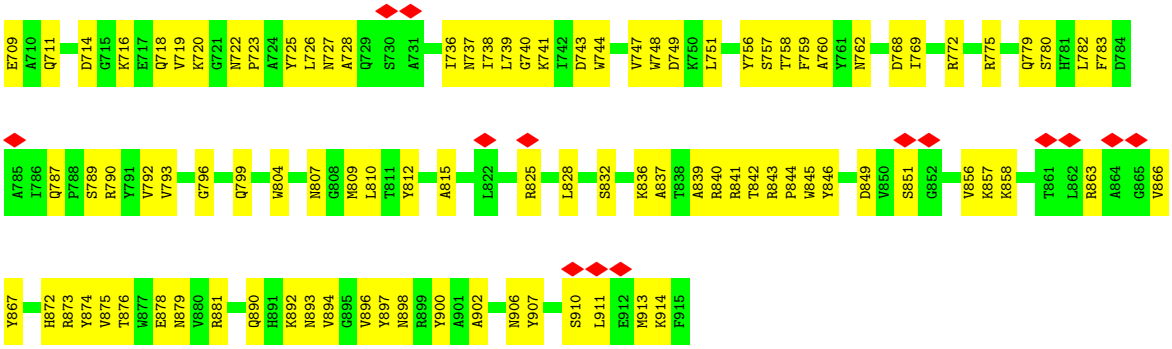
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transferrin Binding Protein A

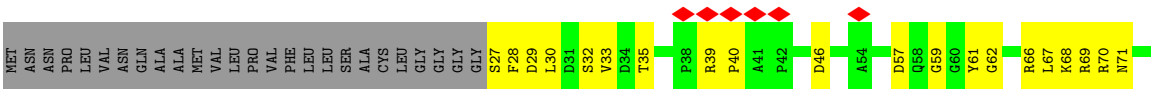
Chain A:

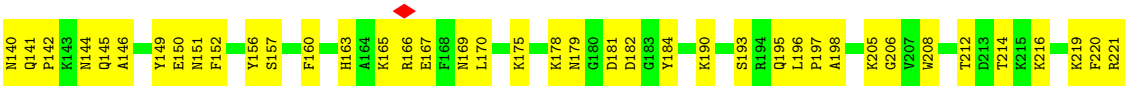


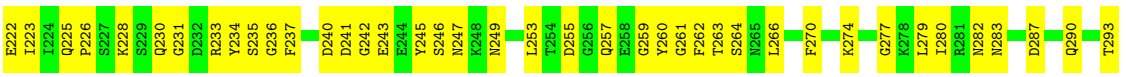


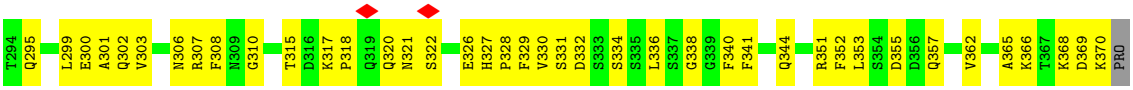
• Molecule 2: Transferrin Binding Protein B

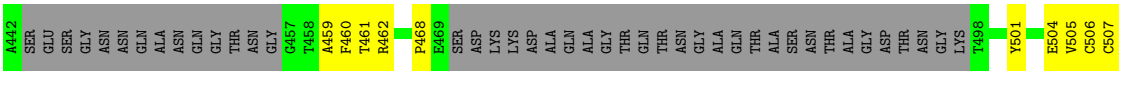
Chain B:

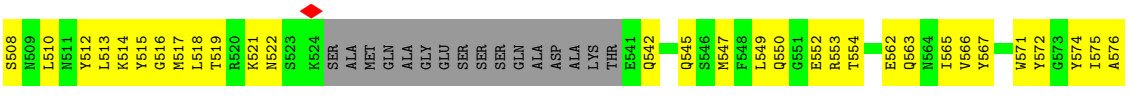


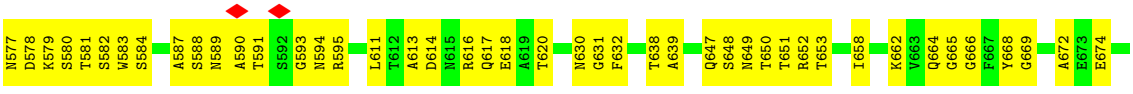


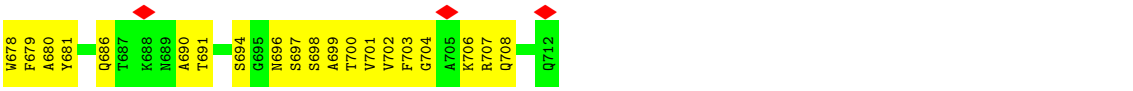






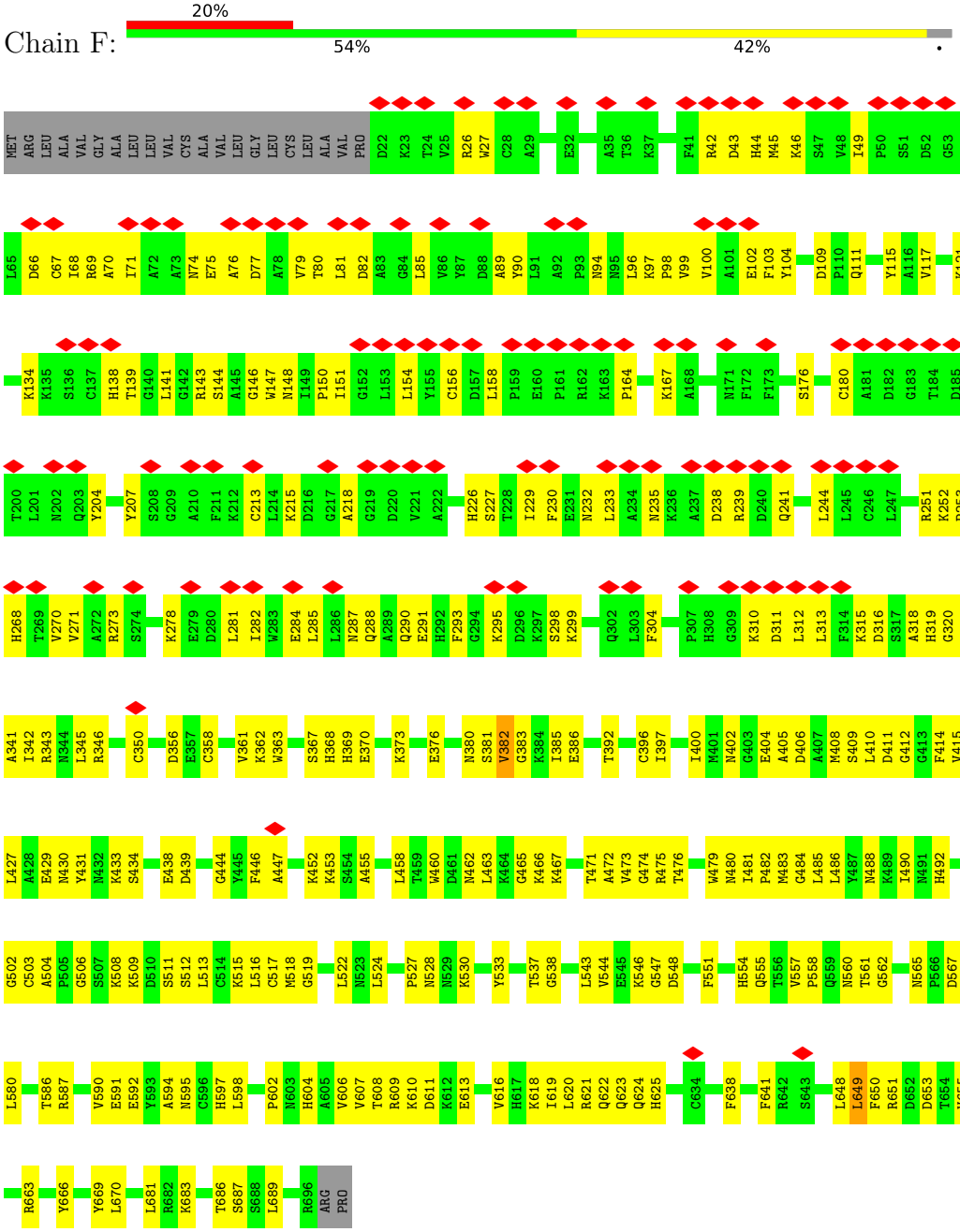






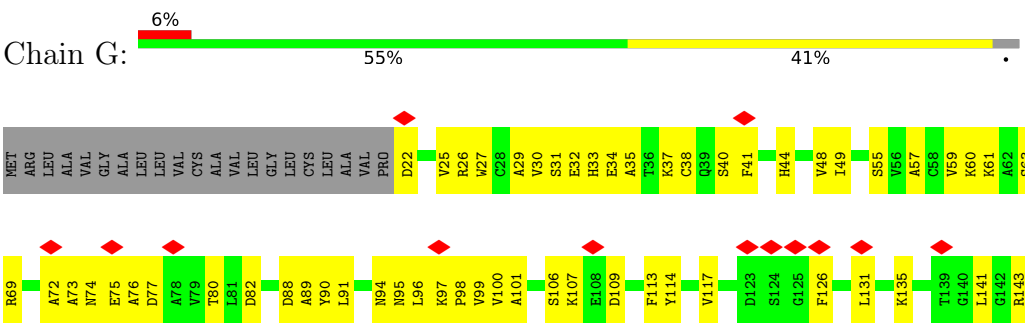
• Molecule 3: Transferrin

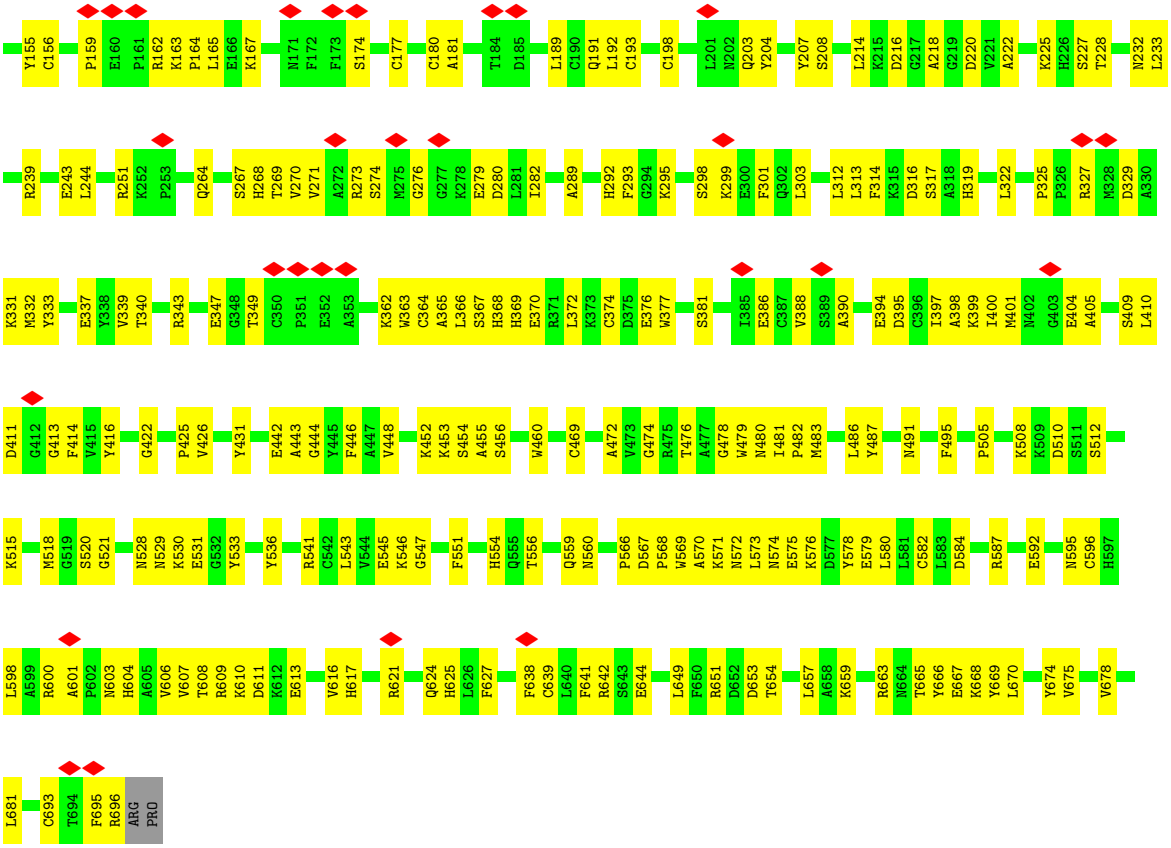
Chain F:



• Molecule 3: Transferrin

Chain G:




Y155 C156 P159 E160 P161 R162 K163 P164 L165 E166 K167 N171 F172 F173 S174 C177 C180 A181 T184 D185 L189 C190 Q191 L192 C193 C198 L201 N202 Q203 Y204 Y207 S208 L214 K215 D216 G217 A218 G219 D220 V221 A222 K225 H226 S227 T228 N232 L233
R239 E243 L244 R251 K252 P253 Q264 S267 H268 T269 V270 V271 A272 R273 S274 M275 G276 G277 K278 E279 D280 L281 I282 A289 H292 F293 G294 K295 S298 K299 E300 F301 Q302 L303 L312 L313 F314 K315 D316 S317 A318 H319 L322 P325 P326 R327 M328 D329 A330
K331 M332 Y333 E337 Y338 V339 T340 R343 E347 G348 T349 C350 P351 E352 A353 K362 W363 C364 A365 L366 S367 H368 H369 E370 R371 L372 K373 C374 D375 E376 W377 S381 I385 E386 C387 V388 S389 A390 E394 D395 C396 I397 A398 K399 I400 M401 N402 G403 E404 A405 S409 L410
D411 G412 G413 F414 V415 Y416 G422 P425 V426 Y431 E442 A443 G444 Y445 F446 A447 V448 K452 K453 S454 A455 S456 W460 C469 A472 V473 G474 R475 T476 A477 G478 W479 N480 I481 P482 M483 L486 Y487 M491 F495 P505 K508 K509 D510 S511 S512
K515 M518 G519 S520 G521 N528 N529 K530 E531 G532 Y533 Y536 R541 C542 L543 V544 E545 K546 G547 F551 H554 Q555 T556 Q559 N560 P566 D567 P568 W569 A570 K571 N572 L573 N574 E575 K576 D577 Y578 E579 L580 L581 C582 L583 D584 R587 E592 N595 C596 H597
L598 A599 R600 A601 P602 N603 H604 A605 V606 V607 T608 R609 K610 D611 K612 E613 V616 H617 R621 Q624 H625 L626 F627 F638 C639 L640 F641 R642 S643 E644 L649 F650 R651 D652 D653 T654 L657 A658 K659 R663 N664 T665 Y666 E667 K668 Y669 L670 Y674 V675 V678
L681 C693 T694 F695 R696 ARG PRO

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47147	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 ($e^-/Å^2$)	53.52	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.435	Depositor
Minimum map value	-0.160	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0888	Depositor
Map size (Å)	323.4, 323.4, 323.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.078, 1.078, 1.078	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/7020	0.37	0/9478
2	B	0.19	0/4818	0.38	0/6493
3	F	0.17	0/5293	0.42	1/7161 (0.0%)
3	G	0.15	0/5309	0.35	0/7179
All	All	0.17	0/22440	0.38	1/30311 (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
2	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	358	CYS	CB-CA-C	-5.16	110.64	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	96	GLU	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	6869	0	6669	284	0
2	B	4720	0	4504	291	0
3	F	5176	0	4942	252	0
3	G	5192	0	4970	223	0
4	F	4	0	1	2	0
4	G	8	0	2	5	0
5	F	1	0	0	0	0
5	G	2	0	0	0	0
All	All	21972	0	21088	991	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 23.

All (991) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:576:ALA:O	2:B:697:SER:HA	1.64	0.96
2:B:169:ASN:O	2:B:175:LYS:HA	1.66	0.95
3:G:556:THR:O	3:G:560:ASN:HB2	1.69	0.91
1:A:149:LYS:HG2	1:A:176:LYS:HA	1.56	0.88
2:B:566:VAL:HG23	2:B:708:GLN:HB2	1.58	0.85
1:A:691:LEU:HD23	1:A:740:GLY:HA3	1.58	0.85
2:B:501:TYR:HB3	2:B:518:LEU:HD11	1.60	0.82
1:A:237:GLY:HA2	1:A:898:ASN:HB3	1.63	0.81
3:F:99:VAL:HG23	3:F:100:VAL:HG23	1.62	0.80
2:B:163:HIS:ND1	2:B:181:ASP:OD1	2.16	0.79
2:B:571:TRP:HB3	2:B:703:PHE:HB3	1.65	0.78
1:A:250:ASP:HA	1:A:280:VAL:HG12	1.65	0.78
1:A:511:ARG:NH2	1:A:512:HIS:O	2.17	0.77
2:B:68:LYS:NZ	2:B:69:ARG:O	2.18	0.77
2:B:90:ALA:O	2:B:103:ARG:NH2	2.18	0.76
3:F:144:SER:HA	3:F:148:ASN:HB2	1.67	0.76
3:G:370:GLU:HB3	3:G:649:LEU:HD11	1.68	0.75
3:G:177:CYS:HB2	3:G:192:LEU:HB2	1.67	0.75
2:B:310:GLY:O	2:B:336:LEU:HB3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:LYS:HG2	3:F:508:LYS:HD3	1.68	0.74
3:F:594:ALA:O	3:F:597:HIS:ND1	2.19	0.74
3:G:99:VAL:HG23	3:G:100:VAL:HG23	1.68	0.74
2:B:228:LYS:NZ	2:B:241:ASP:OD1	2.19	0.74
2:B:412:LEU:HD12	2:B:545:GLN:HB2	1.68	0.74
3:G:98:PRO:HA	3:G:271:VAL:HA	1.69	0.74
1:A:841:ARG:O	1:A:843:ARG:NH1	2.21	0.73
1:A:400:ASP:HB2	1:A:440:HIS:HB3	1.70	0.73
3:G:327:ARG:O	3:G:327:ARG:NH1	2.21	0.73
1:A:455:CYS:O	1:A:456:ARG:NH1	2.20	0.72
2:B:225:GLN:O	2:B:230:GLN:NE2	2.18	0.72
2:B:553:ARG:NH1	2:B:630:ASN:OD1	2.22	0.72
1:A:560:GLN:NE2	1:A:562:CYS:SG	2.63	0.72
3:G:528:ASN:HD21	3:G:530:LYS:HE2	1.53	0.72
2:B:193:SER:O	2:B:306:ASN:ND2	2.22	0.71
3:G:365:ALA:HB1	3:G:370:GLU:HB2	1.72	0.71
2:B:150:GLU:N	2:B:369:ASP:OD2	2.23	0.71
3:F:238:ASP:OD1	3:F:241:GLN:NE2	2.23	0.71
3:G:40:SER:O	3:G:44:HIS:ND1	2.24	0.71
1:A:711:GLN:NE2	1:A:719:VAL:O	2.23	0.71
3:G:400:ILE:O	3:G:609:ARG:NH1	2.23	0.71
1:A:709:GLU:HB3	1:A:720:LYS:HB3	1.72	0.70
2:B:221:ARG:HD3	3:G:567:ASP:HA	1.73	0.70
3:F:328:MET:HE1	3:F:689:LEU:HD13	1.73	0.70
3:F:100:VAL:HB	3:F:270:VAL:HB	1.74	0.70
2:B:127:PRO:HG2	2:B:131:GLN:HG2	1.73	0.70
1:A:125:GLN:NE2	1:A:660:ARG:O	2.25	0.69
1:A:809:MET:HB2	1:A:849:ASP:HB2	1.72	0.69
3:F:176:SER:HA	3:F:192:LEU:HD22	1.74	0.69
2:B:410:LEU:HD23	2:B:700:THR:HG23	1.74	0.69
1:A:48:LYS:HZ2	1:A:52:ASP:HB2	1.56	0.69
1:A:522:ARG:HH11	1:A:552:GLY:H	1.38	0.69
1:A:241:GLN:HE22	1:A:298:ASN:HB2	1.58	0.69
1:A:48:LYS:NZ	1:A:52:ASP:HB2	2.08	0.69
3:F:130:GLN:O	3:F:134:LYS:NZ	2.26	0.69
3:F:139:THR:HG23	3:F:143:ARG:HD3	1.75	0.69
1:A:61:LEU:HB2	1:A:153:ILE:HB	1.75	0.68
1:A:843:ARG:NE	2:B:29:ASP:O	2.26	0.68
3:G:90:TYR:O	3:G:95:ASN:ND2	2.21	0.68
1:A:360:GLN:NE2	3:F:653:ASP:OD2	2.26	0.68
3:G:399:LYS:O	3:G:405:ALA:N	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:PHE:N	1:A:520:ALA:O	2.21	0.68
2:B:616:ARG:HH11	2:B:617:GLN:H	1.42	0.68
1:A:856:VAL:HG12	1:A:857:LYS:HG3	1.75	0.68
2:B:208:TRP:NE1	2:B:263:THR:O	2.23	0.68
1:A:828:LEU:HD11	3:F:382:VAL:HA	1.75	0.67
3:F:117:VAL:HA	3:F:262:LEU:HD23	1.76	0.67
3:G:144:SER:HA	3:G:148:ASN:HB2	1.77	0.67
3:F:433:LYS:HA	3:F:655:VAL:HG11	1.77	0.67
3:G:663:ARG:HH21	3:G:669:TYR:HA	1.60	0.67
3:F:409:SER:OG	3:F:651:ARG:NH2	2.26	0.67
2:B:648:SER:OG	3:F:475:ARG:NH1	2.27	0.67
3:G:32:GLU:OE1	3:G:33:HIS:ND1	2.27	0.67
3:F:97:LYS:HD2	3:F:98:PRO:HD2	1.76	0.67
3:G:442:GLU:OE1	3:G:603:ASN:ND2	2.26	0.67
1:A:516:TYR:HA	1:A:561:ILE:HG13	1.77	0.67
3:F:102:GLU:HG3	3:F:315:LYS:HZ1	1.59	0.67
3:G:487:TYR:O	3:G:491:ASN:N	2.26	0.67
1:A:74:LEU:HG	1:A:197:SER:HB2	1.77	0.67
1:A:653:PHE:HA	1:A:656:MET:HE2	1.77	0.66
1:A:67:THR:O	1:A:71:GLU:HB2	1.95	0.66
2:B:39:ARG:NH2	2:B:40:PRO:O	2.28	0.66
2:B:366:LYS:NZ	2:B:369:ASP:OD1	2.28	0.66
3:F:164:PRO:HG2	3:F:167:LYS:HB3	1.77	0.66
3:G:422:GLY:O	3:G:610:LYS:NZ	2.29	0.66
3:F:504:ALA:N	3:F:517:CYS:SG	2.68	0.66
1:A:223:THR:HB	1:A:311:SER:HB3	1.78	0.66
3:F:327:ARG:O	3:F:327:ARG:NH1	2.25	0.66
3:G:151:ILE:O	3:G:155:TYR:N	2.29	0.66
3:G:295:LYS:NZ	3:G:316:ASP:O	2.28	0.66
2:B:631:GLY:HA2	2:B:666:GLY:HA2	1.78	0.66
3:F:362:LYS:H	3:F:406:ASP:HB2	1.61	0.65
3:F:356:ASP:OD1	3:F:618:LYS:NZ	2.30	0.65
3:F:481:ILE:HG13	3:F:482:PRO:HD3	1.77	0.65
3:F:402:ASN:ND2	3:F:404:GLU:OE2	2.29	0.65
3:F:543:LEU:HA	3:F:547:GLY:HA3	1.79	0.65
3:G:233:LEU:O	3:G:239:ARG:NH1	2.29	0.65
1:A:89:VAL:HG21	1:A:105:ASP:HB2	1.79	0.64
2:B:571:TRP:O	2:B:594:ASN:ND2	2.28	0.64
3:G:444:GLY:HA3	3:G:601:ALA:O	1.98	0.64
3:F:126:PHE:HB2	3:F:130:GLN:HB3	1.80	0.64
1:A:879:ASN:HB3	1:A:900:TYR:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:LYS:O	2:B:708:GLN:NE2	2.31	0.64
3:F:580:LEU:HD23	3:F:590:VAL:HA	1.80	0.64
1:A:91:GLN:HE21	1:A:95:ALA:H	1.43	0.64
2:B:152:PHE:HB2	2:B:156:TYR:CZ	2.33	0.64
2:B:595:ARG:NH2	2:B:616:ARG:O	2.30	0.64
3:G:76:ALA:O	3:G:273:ARG:NH2	2.31	0.63
2:B:554:THR:O	2:B:630:ASN:ND2	2.23	0.63
2:B:686:GLN:N	2:B:686:GLN:OE1	2.32	0.63
3:G:405:ALA:O	3:G:609:ARG:NH1	2.29	0.63
2:B:104:GLN:N	2:B:104:GLN:OE1	2.29	0.63
3:G:106:SER:OG	3:G:109:ASP:OD1	2.15	0.63
1:A:193:LYS:HA	1:A:911:LEU:O	1.99	0.63
1:A:97:SER:OG	1:A:106:LYS:NZ	2.27	0.63
2:B:95:ASP:OD1	2:B:96:GLU:N	2.32	0.63
3:G:48:VAL:HG23	3:G:49:ILE:HG12	1.80	0.63
3:G:452:LYS:O	3:G:587:ARG:NH2	2.32	0.63
1:A:363:SER:HB3	1:A:367:ASN:HD21	1.64	0.62
3:G:143:ARG:NH2	3:G:207:TYR:OH	2.32	0.62
1:A:50:ARG:NH2	1:A:57:GLY:O	2.29	0.62
1:A:226:HIS:ND1	1:A:308:GLU:OE2	2.28	0.62
1:A:233:HIS:CE1	1:A:873:ARG:HE	2.16	0.62
2:B:412:LEU:HD11	3:F:522:LEU:HB2	1.81	0.62
3:F:423:LEU:HD12	3:F:607:VAL:HG12	1.80	0.62
2:B:410:LEU:HD21	2:B:680:ALA:HB2	1.81	0.62
1:A:365:ARG:HB3	1:A:524:TYR:HB3	1.82	0.62
3:F:483:MET:HG3	3:F:681:LEU:HD21	1.81	0.62
1:A:49:THR:OG1	1:A:52:ASP:OD1	2.16	0.62
2:B:588:SER:HB3	2:B:593:GLY:HA3	1.79	0.62
3:F:362:LYS:HG2	3:F:386:GLU:HB2	1.80	0.62
3:F:427:LEU:HD13	3:F:620:LEU:HD22	1.82	0.62
3:G:156:CYS:O	3:G:162:ARG:NH2	2.33	0.62
1:A:68:LEU:HA	1:A:71:GLU:HB3	1.82	0.62
3:F:369:HIS:HB3	3:F:648:LEU:HD21	1.81	0.62
1:A:661:SER:OG	3:F:621:ARG:NH2	2.31	0.62
3:F:331:LYS:HE2	3:F:402:ASN:HD21	1.64	0.62
3:G:444:GLY:C	3:G:600:ARG:HE	2.07	0.62
1:A:158:ASN:ND2	1:A:170:SER:OG	2.26	0.62
1:A:405:LYS:HE3	1:A:433:GLN:HE22	1.65	0.62
1:A:635:ALA:HB3	1:A:638:LEU:HB2	1.80	0.62
2:B:212:THR:OG1	2:B:236:GLY:N	2.33	0.62
1:A:840:ARG:NH1	1:A:897:TYR:OH	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:CYS:HB2	2:B:510:LEU:HD23	1.82	0.61
3:G:416:TYR:HE1	3:G:675:VAL:HG13	1.64	0.61
1:A:176:LYS:O	1:A:315:ARG:NH1	2.33	0.61
1:A:684:PHE:HB2	1:A:691:LEU:HB2	1.82	0.61
1:A:873:ARG:HD2	2:B:27:SER:HA	1.81	0.61
2:B:591:THR:OG1	2:B:595:ARG:NH1	2.34	0.61
2:B:167:GLU:OE2	2:B:169:ASN:ND2	2.33	0.61
1:A:692:GLU:HB3	1:A:739:LEU:HG	1.81	0.61
2:B:426:ALA:N	2:B:552:GLU:OE2	2.31	0.61
3:G:126:PHE:O	3:G:251:ARG:NH2	2.33	0.61
3:G:425:PRO:HA	3:G:607:VAL:HA	1.82	0.61
2:B:61:TYR:HE2	2:B:433:GLY:HA2	1.65	0.61
2:B:575:ILE:HG22	2:B:583:TRP:HE3	1.66	0.61
1:A:295:THR:HG21	1:A:347:ALA:HB2	1.83	0.61
1:A:616:VAL:HG22	1:A:657:TYR:HA	1.83	0.61
1:A:843:ARG:HH21	2:B:30:LEU:HA	1.66	0.61
3:G:74:ASN:OD1	3:G:273:ARG:NH1	2.33	0.61
2:B:579:LYS:HG2	3:F:508:LYS:HB3	1.82	0.61
3:F:71:ILE:HG13	3:F:96:LEU:HD21	1.83	0.61
2:B:575:ILE:HA	2:B:698:SER:O	2.01	0.61
2:B:674:GLU:OE2	2:B:706:LYS:NZ	2.32	0.61
1:A:69:SER:HB3	1:A:193:LYS:HZ3	1.65	0.60
1:A:661:SER:O	3:F:621:ARG:NE	2.29	0.60
3:G:101:ALA:HB3	3:G:322:LEU:HD11	1.83	0.60
1:A:815:ALA:HB2	1:A:844:PRO:HD3	1.83	0.60
3:G:592:GLU:O	3:G:596:CYS:N	2.33	0.60
3:F:147:TRP:HA	3:F:151:ILE:HD13	1.83	0.60
3:F:397:ILE:HD11	3:F:410:LEU:HD11	1.83	0.60
1:A:876:THR:OG1	1:A:879:ASN:OD1	2.16	0.60
2:B:69:ARG:HD3	2:B:178:LYS:HB3	1.84	0.60
3:G:89:ALA:O	3:G:96:LEU:N	2.32	0.60
1:A:325:HIS:HA	1:A:412:TYR:HE1	1.67	0.60
3:F:370:GLU:OE1	3:F:649:LEU:N	2.27	0.60
1:A:289:VAL:HB	1:A:293:ASP:HB2	1.82	0.60
3:G:174:SER:O	3:G:191:GLN:NE2	2.35	0.60
3:G:479:TRP:O	3:G:483:MET:HG3	2.01	0.60
1:A:722:ASN:OD1	1:A:723:PRO:HD2	2.02	0.60
2:B:208:TRP:HD1	2:B:264:SER:HB3	1.65	0.60
3:F:502:GLY:HA2	3:F:516:LEU:HD12	1.82	0.60
1:A:294:TYR:O	1:A:299:ARG:NH1	2.34	0.60
3:G:97:LYS:HZ3	3:G:274:SER:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:LYS:HG3	1:A:718:GLN:HE22	1.67	0.60
2:B:243:GLU:OE2	2:B:246:SER:N	2.35	0.60
3:F:285:LEU:O	3:F:288:GLN:NE2	2.34	0.60
3:G:571:LYS:NZ	3:G:572:ASN:OD1	2.35	0.59
2:B:589:ASN:OD1	2:B:590:ALA:N	2.34	0.59
3:F:80:THR:HB	3:F:270:VAL:HG22	1.83	0.59
3:F:89:ALA:HB1	3:F:96:LEU:HB2	1.84	0.59
3:F:474:GLY:H	3:F:479:TRP:CD1	2.19	0.59
2:B:67:LEU:HG	2:B:235:SER:HB3	1.84	0.59
2:B:562:GLU:OE1	2:B:707:ARG:NH2	2.34	0.59
2:B:649:ASN:HD21	2:B:652:ARG:HB2	1.68	0.59
1:A:748:TRP:HB3	1:A:751:LEU:HG	1.85	0.59
1:A:812:TYR:CD1	1:A:846:TYR:HB3	2.38	0.59
2:B:649:ASN:HA	3:F:474:GLY:HA3	1.83	0.59
3:F:381:SER:OG	3:F:623:GLN:NE2	2.27	0.59
3:G:531:GLU:HG3	3:G:533:TYR:H	1.68	0.59
1:A:539:PRO:HB2	1:A:547:TYR:HD1	1.67	0.59
2:B:243:GLU:OE2	2:B:245:TYR:N	2.36	0.59
3:F:128:MET:HA	3:F:131:LEU:HD23	1.84	0.59
3:G:453:LYS:NZ	3:G:578:TYR:O	2.33	0.59
3:G:536:TYR:OH	3:G:651:ARG:NH1	2.35	0.59
1:A:841:ARG:H	2:B:33:VAL:HG12	1.67	0.59
3:F:343:ARG:O	3:F:346:ARG:HG2	2.02	0.59
2:B:142:PRO:HD3	3:G:520:SER:HB3	1.84	0.58
2:B:320:GLN:NE2	2:B:321:ASN:OD1	2.36	0.58
3:G:163:LYS:NZ	3:G:347:GLU:O	2.28	0.58
3:G:448:VAL:HB	3:G:580:LEU:HD22	1.85	0.58
1:A:332:GLU:OE2	1:A:407:ARG:HB3	2.04	0.58
2:B:151:ASN:N	2:B:369:ASP:OD2	2.34	0.58
2:B:247:ASN:ND2	2:B:259:GLY:O	2.34	0.58
2:B:613:ALA:N	2:B:620:THR:OG1	2.31	0.58
2:B:152:PHE:O	2:B:156:TYR:OH	2.16	0.58
3:G:146:GLY:N	4:G:701:BCT:O3	2.30	0.58
2:B:690:ALA:O	2:B:696:ASN:ND2	2.36	0.58
3:F:396:CYS:HB3	3:F:408:MET:HE2	1.86	0.58
1:A:571:ASP:OD1	1:A:573:THR:OG1	2.15	0.58
3:G:31:SER:OG	3:G:32:GLU:N	2.31	0.58
2:B:266:LEU:HD23	2:B:277:GLY:HA3	1.85	0.58
1:A:125:GLN:HE22	1:A:660:ARG:H	1.52	0.57
2:B:437:PRO:O	2:B:462:ARG:NH2	2.34	0.57
1:A:760:ALA:HB3	1:A:792:VAL:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:VAL:HA	2:B:308:PHE:HB3	1.84	0.57
2:B:282:ASN:HA	2:B:293:THR:HG22	1.85	0.57
2:B:547:MET:HE1	2:B:702:VAL:HG13	1.87	0.57
2:B:571:TRP:CD1	2:B:611:LEU:HD22	2.40	0.57
3:F:66:ASP:OD1	3:F:69:ARG:NH2	2.34	0.57
3:F:473:VAL:HG13	3:F:479:TRP:CE2	2.38	0.57
1:A:159:SER:OG	1:A:646:THR:O	2.21	0.57
3:G:401:MET:SD	3:G:401:MET:N	2.75	0.57
1:A:443:GLN:HB3	1:A:467:LYS:HG2	1.86	0.57
3:G:474:GLY:H	3:G:479:TRP:CD1	2.22	0.57
1:A:559:ARG:NH1	1:A:560:GLN:O	2.36	0.57
2:B:578:ASP:HA	2:B:696:ASN:HB2	1.87	0.57
1:A:812:TYR:HD1	1:A:846:TYR:HB3	1.68	0.57
3:G:452:LYS:NZ	3:G:543:LEU:O	2.34	0.57
3:G:472:ALA:HA	3:G:505:PRO:HD2	1.85	0.57
3:G:279:GLU:HA	3:G:282:ILE:HG12	1.86	0.57
3:G:666:TYR:O	3:G:670:LEU:N	2.35	0.57
2:B:591:THR:O	2:B:595:ARG:NH1	2.38	0.57
2:B:89:GLU:OE1	2:B:103:ARG:NH2	2.38	0.56
1:A:762:ASN:O	1:A:789:SER:OG	2.21	0.56
2:B:103:ARG:HH21	2:B:104:GLN:HE22	1.52	0.56
3:G:570:ALA:HA	3:G:573:LEU:HD23	1.87	0.56
1:A:841:ARG:NH1	1:A:842:THR:O	2.38	0.56
2:B:516:GLY:HA2	2:B:572:TYR:HD2	1.70	0.56
3:G:82:ASP:HA	3:G:268:HIS:CG	2.40	0.56
3:G:411:ASP:OD1	3:G:604:HIS:NE2	2.38	0.56
3:G:592:GLU:HG2	3:G:596:CYS:H	1.69	0.56
2:B:234:TYR:HE2	2:B:237:PHE:HE1	1.52	0.56
3:G:608:THR:HG21	3:G:616:VAL:HG11	1.87	0.56
1:A:744:TRP:NE1	1:A:757:SER:OG	2.38	0.56
2:B:170:LEU:HA	2:B:175:LYS:HD2	1.86	0.56
2:B:119:ILE:HD13	2:B:129:ASN:H	1.70	0.56
3:G:362:LYS:HZ1	3:G:388:VAL:HB	1.71	0.56
1:A:397:VAL:HG13	1:A:441:PHE:HE1	1.71	0.56
1:A:538:SER:HB2	3:F:587:ARG:HB2	1.86	0.56
1:A:787:GLN:OE1	1:A:790:ARG:NH2	2.39	0.56
2:B:107:VAL:O	2:B:110:LYS:HG2	2.05	0.56
3:G:453:LYS:HE3	3:G:576:LYS:HD3	1.88	0.56
2:B:277:GLY:O	2:B:299:LEU:N	2.29	0.56
3:G:145:ALA:HA	3:G:149:ILE:HD12	1.87	0.56
1:A:728:ALA:O	1:A:772:ARG:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:35:ALA:HA	3:G:60:LYS:HZ2	1.71	0.56
2:B:196:LEU:HB3	2:B:270:PHE:CE1	2.42	0.55
3:F:103:PHE:CE2	3:F:320:GLY:HA3	2.42	0.55
3:F:508:LYS:O	3:F:511:SER:OG	2.22	0.55
1:A:124:ALA:N	1:A:136:SER:OG	2.39	0.55
2:B:95:ASP:H	2:B:102:LYS:HZ3	1.54	0.55
2:B:166:ARG:HB2	2:B:179:ASN:HD22	1.70	0.55
3:F:109:ASP:O	3:F:111:GLN:NE2	2.39	0.55
3:F:290:GLN:NE2	3:F:291:GLU:OE2	2.39	0.55
3:G:476:THR:HA	3:G:480:ASN:HB2	1.87	0.55
3:G:666:TYR:HD2	3:G:670:LEU:HD12	1.69	0.55
3:F:150:PRO:HG2	3:F:151:ILE:HD12	1.88	0.55
2:B:84:ASP:OD2	2:B:86:SER:OG	2.15	0.55
2:B:422:ASN:OD1	2:B:423:PHE:N	2.38	0.55
1:A:416:ASN:HB3	1:A:424:ASP:HA	1.88	0.55
3:F:82:ASP:OD1	3:F:268:HIS:NE2	2.39	0.55
3:F:518:MET:HB2	3:F:533:TYR:HE2	1.72	0.55
3:G:26:ARG:NH2	3:G:273:ARG:HH22	2.05	0.55
3:G:34:GLU:OE1	3:G:34:GLU:N	2.39	0.55
1:A:609:THR:O	1:A:610:HIS:ND1	2.37	0.55
1:A:711:GLN:HG3	1:A:718:GLN:HB2	1.88	0.55
2:B:46:ASP:HA	2:B:708:GLN:HA	1.89	0.55
2:B:257:GLN:HA	2:B:293:THR:HG23	1.89	0.55
3:F:207:TYR:OH	4:F:701:BCT:O1	2.24	0.55
3:F:229:ILE:HD12	3:F:232:ASN:HD21	1.72	0.55
3:G:225:LYS:HG3	3:G:227:SER:H	1.70	0.55
2:B:208:TRP:CE2	2:B:279:LEU:HB3	2.42	0.55
3:F:97:LYS:NZ	3:F:328:MET:O	2.33	0.55
3:G:204:TYR:OH	3:G:216:ASP:OD2	2.19	0.55
3:G:364:CYS:SG	3:G:365:ALA:N	2.80	0.55
3:G:556:THR:O	3:G:560:ASN:CB	2.50	0.55
3:G:639:CYS:HB2	3:G:642:ARG:HD2	1.89	0.55
1:A:890:GLN:O	1:A:892:LYS:NZ	2.32	0.55
3:F:76:ALA:O	3:F:273:ARG:NH1	2.39	0.55
1:A:668:VAL:HG23	1:A:670:ILE:HD11	1.89	0.54
3:F:561:THR:HA	3:F:565:ASN:HB2	1.88	0.54
1:A:221:ILE:HD13	1:A:313:LEU:HD23	1.89	0.54
1:A:563:LEU:HB2	1:A:566:ASN:HD22	1.72	0.54
1:A:840:ARG:HD3	2:B:33:VAL:HB	1.88	0.54
1:A:840:ARG:HA	2:B:33:VAL:HB	1.89	0.54
2:B:69:ARG:HH21	2:B:182:ASP:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:42:ARG:HB3	3:F:56:VAL:HG22	1.89	0.54
3:G:368:HIS:CE1	3:G:372:LEU:HD11	2.42	0.54
1:A:297:PRO:HB2	1:A:893:ASN:O	2.06	0.54
3:F:648:LEU:O	3:F:650:PHE:N	2.40	0.54
3:G:141:LEU:HA	3:G:147:TRP:CG	2.43	0.54
2:B:122:SER:HB2	2:B:125:LEU:HG	1.87	0.54
3:F:641:PHE:HE1	3:F:650:PHE:HD2	1.56	0.54
2:B:69:ARG:NH1	2:B:179:ASN:O	2.41	0.54
3:F:98:PRO:HA	3:F:271:VAL:HG22	1.90	0.54
3:F:207:TYR:HH	4:F:701:BCT:C	2.19	0.54
2:B:223:ILE:HD11	2:B:262:PHE:CZ	2.43	0.54
3:F:312:LEU:HG	3:F:313:LEU:HG	1.90	0.54
3:G:135:LYS:HB3	3:G:192:LEU:HD11	1.89	0.54
3:G:575:GLU:HG2	3:G:576:LYS:HE3	1.88	0.54
3:G:27:TRP:HE1	3:G:313:LEU:HD13	1.71	0.54
1:A:258:PHE:HA	1:A:546:PRO:HB2	1.89	0.53
3:F:342:ILE:HA	3:F:345:LEU:HD12	1.90	0.53
3:F:518:MET:HE2	3:F:533:TYR:CE2	2.43	0.53
2:B:237:PHE:CE1	2:B:240:ASP:HB2	2.43	0.53
1:A:200:ASN:HB3	1:A:230:ILE:HG12	1.90	0.53
1:A:567:ASN:HB2	1:A:662:GLY:C	2.34	0.53
3:F:104:TYR:HA	3:F:319:HIS:HB2	1.90	0.53
1:A:539:PRO:HA	1:A:545:ASN:HD21	1.73	0.53
3:G:267:SER:O	3:G:333:TYR:OH	2.27	0.53
2:B:334:SER:N	2:B:355:ASP:OD1	2.39	0.53
1:A:253:SER:HB3	3:F:576:LYS:HE3	1.90	0.53
2:B:571:TRP:CB	2:B:703:PHE:HB3	2.37	0.53
3:F:74:ASN:OD1	3:F:273:ARG:NE	2.42	0.53
3:G:94:ASN:OD1	3:G:95:ASN:N	2.40	0.53
3:F:282:ILE:HA	3:F:285:LEU:HD12	1.89	0.53
2:B:93:LEU:HD12	2:B:94:PRO:HD2	1.90	0.53
2:B:197:PRO:HD2	2:B:270:PHE:CE1	2.44	0.53
1:A:235:ALA:HA	1:A:238:ARG:HD2	1.90	0.53
1:A:692:GLU:O	1:A:738:ILE:HD12	2.09	0.53
1:A:726:LEU:HB3	1:A:775:ARG:CZ	2.39	0.53
2:B:249:ASN:OD1	3:G:520:SER:OG	2.27	0.53
3:F:501:GLU:OE2	3:F:516:LEU:HG	2.09	0.53
3:G:298:SER:N	3:G:299:LYS:HA	2.24	0.53
2:B:579:LYS:O	3:F:509:LYS:HB2	2.08	0.53
2:B:69:ARG:HH11	2:B:178:LYS:HB3	1.73	0.52
1:A:416:ASN:ND2	1:A:421:THR:OG1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:SER:OG	1:A:653:PHE:N	2.40	0.52
2:B:27:SER:OG	2:B:28:PHE:N	2.40	0.52
2:B:567:TYR:OH	2:B:672:ALA:O	2.28	0.52
3:F:55:SER:OG	3:F:56:VAL:N	2.42	0.52
2:B:221:ARG:N	2:B:326:GLU:OE2	2.43	0.52
3:F:485:LEU:O	3:F:488:ASN:ND2	2.36	0.52
1:A:256:ALA:HB2	3:F:576:LYS:NZ	2.25	0.52
1:A:510:LEU:HD23	1:A:575:ARG:HD2	1.91	0.52
1:A:727:ASN:OD1	1:A:775:ARG:NH2	2.22	0.52
1:A:866:VAL:HG13	1:A:907:TYR:CE1	2.45	0.52
2:B:198:ALA:N	2:B:400:LYS:O	2.42	0.52
1:A:669:LYS:NZ	1:A:671:ASP:OD1	2.33	0.52
1:A:840:ARG:HD2	1:A:897:TYR:CZ	2.44	0.52
2:B:257:GLN:NE2	2:B:283:ASN:O	2.42	0.52
3:F:361:VAL:HG23	3:F:385:ILE:HG22	1.92	0.52
3:F:592:GLU:HB3	3:F:595:ASN:HB2	1.91	0.52
2:B:195:GLN:OE1	2:B:403:THR:OG1	2.20	0.52
2:B:233:ARG:NE	3:G:376:GLU:OE2	2.41	0.52
3:G:193:CYS:HB3	3:G:204:TYR:HB2	1.90	0.52
1:A:431:ASP:N	1:A:431:ASP:OD1	2.41	0.52
2:B:59:GLY:HA2	2:B:307:ARG:NH1	2.25	0.52
2:B:327:HIS:CE1	2:B:329:PHE:HB2	2.45	0.52
2:B:62:GLY:O	2:B:91:THR:N	2.31	0.52
1:A:110:SER:HB3	1:A:165:GLY:C	2.35	0.52
1:A:121:SER:OG	1:A:138:GLY:O	2.15	0.52
2:B:27:SER:HB3	2:B:30:LEU:HB3	1.92	0.52
3:F:400:ILE:HA	3:F:405:ALA:HB3	1.92	0.52
3:G:469:CYS:SG	3:G:547:GLY:HA3	2.49	0.52
1:A:708:TYR:HD2	3:F:382:VAL:HG11	1.75	0.51
2:B:617:GLN:OE1	3:F:368:HIS:N	2.43	0.51
3:G:193:CYS:HA	3:G:203:GLN:HE22	1.74	0.51
1:A:107:ASN:HD21	1:A:649:ARG:HH21	1.59	0.51
1:A:149:LYS:HE3	1:A:180:ASP:HB2	1.92	0.51
1:A:407:ARG:HD3	1:A:433:GLN:NE2	2.26	0.51
2:B:616:ARG:NH1	2:B:617:GLN:H	2.07	0.51
3:F:233:LEU:HD11	3:F:239:ARG:HG3	1.91	0.51
3:G:164:PRO:O	3:G:167:LYS:HG2	2.10	0.51
2:B:430:VAL:HG13	2:B:435:MET:HE1	1.93	0.51
3:F:397:ILE:O	3:F:400:ILE:HG22	2.10	0.51
1:A:367:ASN:N	3:F:591:GLU:OE2	2.43	0.51
1:A:427:ARG:H	1:A:483:ALA:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:458:LEU:HD22	3:F:462:ASN:HD22	1.74	0.51
3:G:410:LEU:HD23	3:G:414:PHE:HB2	1.93	0.51
1:A:297:PRO:O	1:A:894:VAL:HA	2.11	0.51
2:B:78:GLU:OE2	2:B:80:GLU:N	2.44	0.51
3:F:561:THR:HG23	3:F:562:GLY:H	1.76	0.51
3:G:61:LYS:HD2	3:G:66:ASP:HB3	1.93	0.51
1:A:836:LYS:HD2	2:B:35:THR:OG1	2.11	0.51
2:B:280:ILE:HG22	2:B:295:GLN:HA	1.92	0.51
2:B:287:ASP:HB2	2:B:290:GLN:HG2	1.92	0.51
1:A:186:ARG:HG3	1:A:188:TRP:H	1.76	0.51
1:A:741:LYS:HE3	1:A:756:TYR:CD1	2.45	0.51
1:A:756:TYR:CZ	1:A:796:GLY:HA3	2.45	0.51
1:A:385:ASN:H	3:F:434:SER:CB	2.23	0.50
1:A:737:ASN:OD1	1:A:738:ILE:N	2.44	0.50
2:B:100:LEU:HD22	2:B:105:LYS:HG3	1.92	0.50
2:B:208:TRP:CZ2	2:B:262:PHE:HB3	2.46	0.50
3:G:663:ARG:HG2	3:G:668:LYS:HD3	1.92	0.50
1:A:256:ALA:HB2	3:F:576:LYS:HZ2	1.76	0.50
2:B:562:GLU:HB3	2:B:565:ILE:HD11	1.92	0.50
3:F:490:ILE:HG13	3:F:492:HIS:HD2	1.76	0.50
3:G:362:LYS:NZ	3:G:363:TRP:O	2.40	0.50
1:A:161:GLU:N	1:A:161:GLU:OE1	2.44	0.50
1:A:704:ILE:HG13	1:A:725:TYR:HB3	1.93	0.50
2:B:571:TRP:CD2	2:B:611:LEU:HD13	2.46	0.50
2:B:691:THR:H	2:B:694:SER:HB3	1.75	0.50
3:F:472:ALA:O	3:F:479:TRP:HB2	2.11	0.50
3:G:100:VAL:O	3:G:269:THR:OG1	2.12	0.50
1:A:839:ALA:C	1:A:840:ARG:HE	2.19	0.50
2:B:415:LYS:NZ	2:B:681:TYR:H	2.09	0.50
2:B:415:LYS:NZ	2:B:699:ALA:O	2.45	0.50
3:G:377:TRP:O	3:G:381:SER:N	2.34	0.50
3:G:559:GLN:HE22	3:G:653:ASP:HA	1.76	0.50
3:G:665:THR:HG22	3:G:668:LYS:HG2	1.93	0.50
1:A:779:GLN:NE2	1:A:780:SER:O	2.32	0.50
2:B:70:ARG:NH1	2:B:71:ASN:O	2.45	0.50
2:B:422:ASN:ND2	2:B:550:GLN:OE1	2.45	0.50
2:B:553:ARG:HB3	2:B:630:ASN:ND2	2.27	0.50
3:F:304:PHE:HB3	3:F:316:ASP:HA	1.94	0.50
3:F:460:TRP:CD2	3:F:463:LEU:HD21	2.46	0.50
1:A:132:ARG:HH12	1:A:345:VAL:HG23	1.75	0.50
2:B:578:ASP:HB3	2:B:696:ASN:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:455:ALA:O	3:F:587:ARG:NH2	2.45	0.50
3:F:481:ILE:HG13	3:F:482:PRO:CD	2.42	0.50
2:B:245:TYR:OH	3:G:568:PRO:HD2	2.12	0.50
3:F:408:MET:HE1	3:F:410:LEU:HD11	1.94	0.50
3:F:430:ASN:HD21	3:F:658:ALA:HB2	1.77	0.50
3:F:227:SER:HA	3:F:230:PHE:CD2	2.46	0.50
3:F:410:LEU:HD13	3:F:414:PHE:HB3	1.93	0.50
1:A:91:GLN:NE2	1:A:93:ARG:H	2.10	0.49
1:A:522:ARG:NH1	1:A:552:GLY:H	2.08	0.49
1:A:124:ALA:HB2	1:A:136:SER:H	1.76	0.49
1:A:300:PHE:CE1	1:A:896:VAL:HG21	2.48	0.49
2:B:430:VAL:HG22	2:B:435:MET:HE1	1.94	0.49
2:B:578:ASP:OD1	2:B:578:ASP:N	2.45	0.49
3:G:41:PHE:CE1	3:G:303:LEU:HD11	2.47	0.49
3:G:143:ARG:NH2	4:G:701:BCT:O2	2.42	0.49
3:G:613:GLU:HA	3:G:616:VAL:HG12	1.93	0.49
1:A:306:SER:HB3	1:A:339:ASP:HB2	1.93	0.49
1:A:649:ARG:N	1:A:673:GLU:OE1	2.44	0.49
2:B:101:PRO:HB2	2:B:104:GLN:OE1	2.11	0.49
3:G:483:MET:HA	3:G:486:LEU:HB2	1.95	0.49
1:A:566:ASN:OD1	1:A:571:ASP:HB2	2.12	0.49
3:G:89:ALA:HB1	3:G:96:LEU:HB2	1.95	0.49
1:A:89:VAL:HG13	1:A:881:ARG:NH1	2.28	0.49
1:A:256:ALA:O	1:A:278:LYS:HA	2.12	0.49
2:B:197:PRO:HD2	2:B:270:PHE:HE1	1.77	0.49
1:A:58:LEU:HB2	1:A:643:ARG:CZ	2.43	0.49
3:F:343:ARG:HA	3:F:346:ARG:NE	2.28	0.49
3:F:519:GLY:HA3	3:F:524:LEU:HA	1.95	0.49
3:F:616:VAL:HA	3:F:619:ILE:HG22	1.94	0.49
3:G:347:GLU:HG3	3:G:349:THR:HG23	1.94	0.49
1:A:374:HIS:O	1:A:374:HIS:ND1	2.45	0.49
1:A:421:THR:OG1	1:A:423:ALA:O	2.29	0.49
3:F:287:ASN:O	3:F:290:GLN:HG3	2.12	0.49
3:F:579:GLU:OE1	3:F:579:GLU:N	2.46	0.49
3:F:611:ASP:OD1	3:F:611:ASP:N	2.43	0.49
1:A:144:GLU:OE2	1:A:225:ARG:NH2	2.45	0.49
1:A:382:SER:HA	1:A:388:PRO:HA	1.94	0.49
3:F:537:THR:HA	3:F:560:ASN:HD21	1.77	0.49
1:A:251:ASP:CG	3:F:576:LYS:HZ1	2.20	0.49
2:B:212:THR:H	2:B:235:SER:HG	1.59	0.49
2:B:575:ILE:HD11	2:B:658:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:479:TRP:CZ2	3:G:483:MET:HE3	2.48	0.49
3:G:621:ARG:O	3:G:625:HIS:ND1	2.42	0.49
1:A:527:LYS:HB2	1:A:550:SER:HB2	1.94	0.48
2:B:351:ARG:HB2	2:B:362:VAL:HG12	1.94	0.48
2:B:516:GLY:HA2	2:B:572:TYR:CD2	2.48	0.48
2:B:571:TRP:CE2	2:B:611:LEU:HB3	2.48	0.48
2:B:674:GLU:HG2	2:B:706:LYS:HD3	1.95	0.48
3:F:452:LYS:NZ	3:F:544:VAL:O	2.41	0.48
3:G:460:TRP:HZ2	3:G:598:LEU:HD11	1.78	0.48
1:A:759:PHE:HD1	1:A:793:VAL:HG22	1.78	0.48
2:B:101:PRO:HG2	2:B:104:GLN:HB2	1.95	0.48
2:B:327:HIS:ND1	2:B:329:PHE:HB2	2.28	0.48
3:F:397:ILE:HA	3:F:400:ILE:HG22	1.95	0.48
3:F:411:ASP:O	3:F:415:VAL:HG23	2.13	0.48
3:F:471:THR:OG1	3:F:472:ALA:N	2.46	0.48
1:A:511:ARG:NH1	1:A:512:HIS:H	2.11	0.48
2:B:221:ARG:HD3	3:G:568:PRO:HD3	1.94	0.48
2:B:344:GLN:HG2	2:B:401:LEU:HD11	1.96	0.48
3:G:365:ALA:HB2	3:G:374:CYS:SG	2.52	0.48
2:B:593:GLY:HA2	2:B:614:ASP:OD2	2.12	0.48
1:A:326:TYR:HB3	1:A:413:VAL:HB	1.94	0.48
1:A:414:TYR:HB3	1:A:426:ALA:HB3	1.95	0.48
1:A:432:ARG:HA	1:A:477:HIS:O	2.14	0.48
2:B:353:LEU:HD11	2:B:357:GLN:HA	1.96	0.48
2:B:517:MET:HA	2:B:547:MET:HA	1.96	0.48
3:G:483:MET:SD	3:G:681:LEU:HD13	2.54	0.48
3:G:611:ASP:OD1	3:G:611:ASP:N	2.43	0.48
2:B:145:GLN:HB2	2:B:150:GLU:HG2	1.94	0.48
3:F:154:LEU:O	3:F:158:LEU:N	2.46	0.48
3:G:135:LYS:O	3:G:220:ASP:N	2.47	0.48
1:A:529:PRO:HG3	1:A:548:TRP:HB2	1.96	0.48
1:A:716:LYS:HG3	1:A:718:GLN:NE2	2.28	0.48
1:A:782:LEU:HD13	1:A:837:ALA:HB2	1.95	0.48
2:B:301:ALA:HA	2:B:310:GLY:HA3	1.96	0.48
3:F:426:VAL:HG23	3:F:660:LEU:HD23	1.96	0.48
3:G:80:THR:OG1	3:G:270:VAL:HG22	2.14	0.48
3:G:604:HIS:CE1	3:G:651:ARG:HD2	2.49	0.48
1:A:603:ARG:HE	1:A:605:ASP:CG	2.22	0.48
1:A:744:TRP:O	1:A:751:LEU:HD12	2.14	0.48
2:B:650:THR:OG1	3:F:474:GLY:HA2	2.14	0.48
3:G:143:ARG:HB3	4:G:701:BCT:C	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HB	1:A:313:LEU:HB3	1.96	0.48
3:F:80:THR:HA	3:F:270:VAL:HA	1.95	0.48
2:B:70:ARG:NH1	2:B:78:GLU:O	2.47	0.48
3:F:192:LEU:HD23	3:F:218:ALA:HB1	1.95	0.48
3:F:427:LEU:HD23	3:F:659:LYS:HA	1.95	0.48
3:G:545:GLU:OE1	3:G:546:LYS:HG3	2.14	0.48
3:F:474:GLY:H	3:F:479:TRP:CG	2.32	0.47
3:F:586:THR:C	3:F:587:ARG:HD2	2.39	0.47
3:F:141:LEU:HD12	3:F:147:TRP:CZ3	2.49	0.47
3:F:304:PHE:CE1	3:F:318:ALA:HB3	2.49	0.47
3:G:474:GLY:HA2	3:G:480:ASN:HD21	1.80	0.47
2:B:521:LYS:NZ	2:B:542:GLN:HG2	2.29	0.47
3:F:68:ILE:HA	3:F:71:ILE:HG12	1.95	0.47
3:G:627:PHE:HB3	3:G:638:PHE:CE2	2.50	0.47
1:A:738:ILE:HG23	1:A:759:PHE:HE2	1.80	0.47
1:A:874:TYR:CZ	1:A:902:ALA:HB1	2.49	0.47
1:A:878:GLU:HA	1:A:881:ARG:HB3	1.96	0.47
2:B:166:ARG:HB2	2:B:179:ASN:ND2	2.28	0.47
2:B:330:VAL:HG23	2:B:331:SER:H	1.79	0.47
3:F:373:LYS:O	3:F:376:GLU:HG3	2.14	0.47
3:F:412:GLY:HA2	3:F:415:VAL:HB	1.96	0.47
3:F:512:SER:HA	3:F:515:LYS:HD3	1.96	0.47
1:A:621:HIS:ND1	1:A:650:LEU:HD22	2.30	0.47
1:A:708:TYR:HE1	1:A:723:PRO:HA	1.79	0.47
2:B:97:PRO:HB2	2:B:156:TYR:CD1	2.49	0.47
3:G:386:GLU:N	3:G:386:GLU:OE1	2.48	0.47
3:G:479:TRP:CE2	3:G:483:MET:HG2	2.50	0.47
1:A:466:TYR:CZ	1:A:468:SER:HB2	2.50	0.47
1:A:540:ASN:HA	3:F:453:LYS:NZ	2.29	0.47
1:A:846:TYR:O	1:A:872:HIS:ND1	2.42	0.47
2:B:223:ILE:HD11	2:B:262:PHE:HZ	1.79	0.47
2:B:587:ALA:HA	2:B:594:ASN:HB2	1.96	0.47
3:F:465:GLY:HA2	3:F:499:PHE:HA	1.97	0.47
3:F:503:CYS:HB2	3:F:516:LEU:HB2	1.97	0.47
3:G:25:VAL:O	3:G:57:ALA:N	2.30	0.47
3:G:117:VAL:HB	3:G:244:LEU:HD22	1.95	0.47
3:G:289:ALA:O	3:G:293:PHE:N	2.39	0.47
3:G:317:SER:O	3:G:319:HIS:ND1	2.46	0.47
3:G:331:LYS:HA	3:G:331:LYS:HD2	1.61	0.47
2:B:124:TYR:OH	2:B:157:SER:O	2.31	0.47
2:B:206:GLY:HA3	2:B:365:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:GLU:H	2:B:326:GLU:CD	2.22	0.47
3:F:102:GLU:HG3	3:F:315:LYS:NZ	2.27	0.47
1:A:498:SER:HB2	1:A:587:ARG:HG2	1.97	0.47
3:G:399:LYS:HB3	3:G:404:GLU:HB3	1.96	0.47
1:A:408:TYR:CE1	1:A:432:ARG:HB2	2.50	0.46
1:A:472:ILE:O	1:A:510:LEU:HD12	2.15	0.46
3:G:100:VAL:HB	3:G:270:VAL:HB	1.97	0.46
3:G:143:ARG:HE	4:G:701:BCT:C	2.28	0.46
1:A:93:ARG:HD2	1:A:340:THR:OG1	2.15	0.46
1:A:427:ARG:HH22	1:A:482:ALA:N	2.13	0.46
1:A:708:TYR:HE1	1:A:723:PRO:CA	2.29	0.46
2:B:300:GLU:O	2:B:300:GLU:HG2	2.14	0.46
2:B:515:TYR:HB3	2:B:549:LEU:HD13	1.96	0.46
3:F:115:TYR:HA	3:F:263:ALA:O	2.16	0.46
3:G:413:GLY:N	3:G:476:THR:OG1	2.48	0.46
1:A:202:GLY:HA2	1:A:227:ALA:HA	1.97	0.46
1:A:259:ILE:HG21	1:A:273:LYS:HA	1.98	0.46
1:A:401:GLU:HG2	1:A:403:HIS:CE1	2.50	0.46
3:F:453:LYS:HG2	3:F:579:GLU:OE1	2.16	0.46
3:F:554:HIS:CD2	3:F:555:GLN:HE21	2.34	0.46
3:G:394:GLU:HA	3:G:397:ILE:HD12	1.97	0.46
1:A:390:GLY:N	1:A:463:PHE:HB3	2.30	0.46
2:B:149:TYR:CD1	2:B:205:LYS:HB2	2.50	0.46
1:A:310:ARG:HB2	1:A:335:GLN:HE22	1.79	0.46
2:B:459:ALA:O	2:B:508:SER:HB3	2.15	0.46
3:F:81:LEU:HD21	3:F:85:LEU:HD13	1.96	0.46
3:F:311:ASP:OD1	3:F:315:LYS:HA	2.16	0.46
1:A:83:ASP:OD1	1:A:83:ASP:N	2.46	0.46
1:A:285:LYS:NZ	1:A:286:ARG:O	2.38	0.46
1:A:310:ARG:HB2	1:A:335:GLN:NE2	2.30	0.46
1:A:621:HIS:CE1	1:A:650:LEU:HD22	2.50	0.46
2:B:61:TYR:CZ	2:B:93:LEU:HD13	2.51	0.46
2:B:461:THR:OG1	2:B:504:GLU:OE2	2.27	0.46
2:B:577:ASN:OD1	2:B:581:THR:N	2.49	0.46
3:G:592:GLU:HG2	3:G:595:ASN:HB3	1.98	0.46
3:G:693:CYS:O	3:G:696:ARG:NH1	2.39	0.46
2:B:208:TRP:CD1	2:B:279:LEU:HD22	2.51	0.46
2:B:221:ARG:CZ	3:G:566:PRO:HG2	2.46	0.46
2:B:225:GLN:N	2:B:242:GLY:O	2.44	0.46
2:B:519:THR:OG1	2:B:545:GLN:HG2	2.16	0.46
3:F:44:HIS:HB3	3:F:293:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:77:ASP:HB3	3:F:282:ILE:HD11	1.98	0.46
3:F:465:GLY:O	3:F:466:LYS:HG3	2.15	0.46
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.78	0.46
1:A:485:LYS:HD3	1:A:498:SER:HA	1.97	0.46
1:A:879:ASN:HB3	1:A:900:TYR:CD1	2.50	0.46
2:B:505:VAL:HA	2:B:515:TYR:O	2.15	0.46
2:B:571:TRP:CD1	2:B:594:ASN:HB3	2.50	0.46
3:G:273:ARG:HG3	3:G:274:SER:O	2.16	0.46
1:A:741:LYS:HD3	1:A:758:THR:HB	1.97	0.46
1:A:846:TYR:H	1:A:872:HIS:CE1	2.34	0.46
2:B:113:THR:OG1	2:B:116:ASP:O	2.29	0.46
2:B:574:TYR:CE2	3:F:522:LEU:HD21	2.51	0.46
3:F:97:LYS:C	3:F:271:VAL:HG13	2.40	0.46
3:F:244:LEU:O	3:F:252:LYS:N	2.40	0.46
3:F:381:SER:O	3:F:382:VAL:HG12	2.16	0.46
3:F:446:PHE:H	3:F:554:HIS:CE1	2.34	0.46
3:G:113:PHE:CD2	3:G:264:GLN:HB3	2.51	0.46
1:A:137:SER:OG	1:A:401:GLU:OE2	2.26	0.45
2:B:27:SER:HB3	2:B:30:LEU:HD22	1.96	0.45
2:B:83:LEU:N	2:B:357:GLN:O	2.33	0.45
2:B:632:PHE:CZ	2:B:665:GLY:HA3	2.51	0.45
2:B:681:TYR:HB3	2:B:699:ALA:HB3	1.97	0.45
3:F:156:CYS:HB3	3:F:350:CYS:HB3	1.46	0.45
3:G:44:HIS:HB3	3:G:293:PHE:CE1	2.51	0.45
1:A:87:ALA:HB3	1:A:100:SER:HB2	1.98	0.45
2:B:66:ARG:NH2	2:B:184:TYR:OH	2.48	0.45
2:B:112:GLU:OE2	2:B:165:LYS:HE2	2.15	0.45
2:B:220:PHE:HD1	2:B:326:GLU:O	1.99	0.45
2:B:353:LEU:HD21	2:B:357:GLN:HG3	1.98	0.45
3:F:253:PRO:HG2	3:F:256:GLU:OE2	2.16	0.45
3:F:281:LEU:HA	3:F:284:GLU:CD	2.41	0.45
3:F:439:ASP:OD1	3:F:439:ASP:N	2.49	0.45
1:A:142:GLU:H	1:A:142:GLU:CD	2.22	0.45
1:A:233:HIS:CE1	1:A:235:ALA:HB3	2.52	0.45
1:A:479:LEU:HD13	1:A:504:ASP:HB2	1.98	0.45
2:B:94:PRO:HG2	2:B:190:LYS:HB3	1.99	0.45
2:B:140:ASN:C	3:G:521:GLY:H	2.23	0.45
2:B:616:ARG:NH1	2:B:618:GLU:H	2.13	0.45
3:F:115:TYR:H	3:F:226:HIS:HE1	1.64	0.45
3:G:568:PRO:O	3:G:571:LYS:HG2	2.17	0.45
1:A:839:ALA:HB1	1:A:840:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:LYS:HE3	2:B:221:ARG:NH2	2.32	0.45
2:B:234:TYR:OH	2:B:240:ASP:OD2	2.22	0.45
2:B:274:LYS:HD2	2:B:302:GLN:NE2	2.32	0.45
2:B:547:MET:HE3	2:B:700:THR:HG22	1.99	0.45
2:B:576:ALA:HB3	2:B:698:SER:OG	2.16	0.45
3:F:94:ASN:HB3	3:F:96:LEU:HD23	1.97	0.45
3:F:453:LYS:HE2	3:F:578:TYR:O	2.17	0.45
3:F:517:CYS:O	3:F:524:LEU:HG	2.16	0.45
3:G:26:ARG:N	3:G:77:ASP:OD2	2.40	0.45
3:G:192:LEU:HD22	3:G:218:ALA:HB1	1.97	0.45
1:A:233:HIS:HD1	1:A:236:ALA:H	1.65	0.45
2:B:412:LEU:HD21	3:F:522:LEU:HD13	1.97	0.45
3:F:43:ASP:HA	3:F:46:LYS:HG2	1.98	0.45
3:F:496:ASP:N	3:F:496:ASP:OD1	2.47	0.45
3:G:162:ARG:O	3:G:165:LEU:HD22	2.17	0.45
1:A:126:ALA:C	3:F:625:HIS:HE2	2.25	0.45
1:A:178:ALA:HA	1:A:219:LEU:HD22	1.99	0.45
1:A:511:ARG:HH11	1:A:574:PRO:HA	1.81	0.45
1:A:676:PHE:HB3	1:A:701:ARG:NH2	2.32	0.45
2:B:100:LEU:HD11	2:B:160:PHE:CD1	2.52	0.45
1:A:627:ASN:HB2	1:A:644:THR:O	2.17	0.45
1:A:799:GLN:HB2	1:A:804:TRP:CD2	2.52	0.45
2:B:226:PRO:HA	2:B:230:GLN:OE1	2.17	0.45
2:B:591:THR:HA	2:B:595:ARG:HD2	1.99	0.45
3:F:331:LYS:HE2	3:F:402:ASN:ND2	2.30	0.45
3:G:141:LEU:HA	3:G:147:TRP:CD1	2.52	0.45
1:A:472:ILE:CG1	1:A:511:ARG:HB2	2.47	0.45
1:A:479:LEU:HD12	1:A:503:TYR:O	2.17	0.45
2:B:91:THR:HA	2:B:104:GLN:HE22	1.81	0.45
2:B:231:GLY:N	2:B:234:TYR:O	2.30	0.45
3:G:214:LEU:HB2	3:G:222:ALA:HB2	1.98	0.45
3:G:481:ILE:N	3:G:482:PRO:HD2	2.32	0.45
1:A:360:GLN:HE22	3:F:431:TYR:HD1	1.65	0.44
1:A:540:ASN:OD1	1:A:545:ASN:ND2	2.50	0.44
2:B:368:LYS:HB3	2:B:370:LYS:HE3	1.99	0.44
2:B:408:VAL:HG21	2:B:678:TRP:CD2	2.52	0.44
3:F:298:SER:HB2	3:F:299:LYS:C	2.42	0.44
3:G:61:LYS:HA	3:G:61:LYS:HD3	1.78	0.44
1:A:407:ARG:HG3	1:A:432:ARG:O	2.17	0.44
1:A:714:ASP:HB2	1:A:716:LYS:NZ	2.32	0.44
1:A:828:LEU:HD21	3:F:383:GLY:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:PHE:O	3:F:319:HIS:HB2	2.18	0.44
1:A:80:THR:HG21	1:A:88:VAL:HG23	1.99	0.44
1:A:349:LEU:HD12	1:A:391:ALA:HA	1.99	0.44
1:A:768:ASP:N	1:A:768:ASP:OD1	2.49	0.44
1:A:769:ILE:HD11	1:A:783:PHE:HE1	1.82	0.44
1:A:793:VAL:HB	1:A:810:LEU:HD21	1.99	0.44
3:F:620:LEU:HD21	3:F:657:LEU:HD13	1.98	0.44
3:G:431:TYR:HA	3:G:654:THR:HA	1.99	0.44
1:A:182:ILE:HA	1:A:210:ALA:HB1	1.99	0.44
2:B:71:ASN:HB2	2:B:178:LYS:NZ	2.32	0.44
2:B:255:ASP:OD1	2:B:255:ASP:N	2.46	0.44
3:F:126:PHE:O	3:F:251:ARG:NH2	2.50	0.44
3:F:339:VAL:HA	3:F:342:ILE:HG12	1.99	0.44
3:F:363:TRP:CZ2	3:F:650:PHE:HE1	2.35	0.44
3:G:25:VAL:N	3:G:55:SER:O	2.49	0.44
3:G:159:PRO:O	3:G:162:ARG:HG3	2.17	0.44
3:G:327:ARG:HH21	3:G:398:ALA:HB1	1.82	0.44
3:G:329:ASP:OD1	3:G:332:MET:HE1	2.17	0.44
3:G:390:ALA:HB1	3:G:395:ASP:HB3	1.98	0.44
1:A:310:ARG:HB2	1:A:335:GLN:OE1	2.18	0.44
2:B:91:THR:HA	2:B:104:GLN:NE2	2.31	0.44
2:B:220:PHE:CZ	2:B:328:PRO:HB3	2.53	0.44
2:B:240:ASP:OD1	2:B:242:GLY:N	2.44	0.44
2:B:658:ILE:HG23	2:B:681:TYR:CD1	2.53	0.44
3:F:327:ARG:HA	3:F:327:ARG:HD2	1.69	0.44
2:B:504:GLU:O	2:B:516:GLY:HA3	2.16	0.44
2:B:662:LYS:O	2:B:679:PHE:HB2	2.17	0.44
3:F:561:THR:HG23	3:F:562:GLY:N	2.32	0.44
3:G:107:LYS:NZ	3:G:319:HIS:O	2.51	0.44
3:G:325:PRO:HD3	3:G:695:PHE:CD2	2.53	0.44
1:A:147:ASN:O	1:A:176:LYS:N	2.43	0.44
1:A:440:HIS:HB2	1:A:470:ARG:HE	1.82	0.44
1:A:539:PRO:HA	1:A:545:ASN:ND2	2.32	0.44
1:A:756:TYR:OH	1:A:807:ASN:ND2	2.36	0.44
2:B:310:GLY:C	2:B:336:LEU:HB3	2.42	0.44
2:B:336:LEU:HA	2:B:352:PHE:HB3	2.00	0.44
3:F:64:TYR:CE2	3:F:85:LEU:HD11	2.53	0.44
3:G:369:HIS:CD2	3:G:529:ASN:HB2	2.52	0.44
3:G:455:ALA:HA	3:G:456:SER:HA	1.70	0.44
1:A:86:ILE:HG23	1:A:101:ILE:HD11	2.00	0.44
1:A:100:SER:C	1:A:101:ILE:HD12	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LYS:O	1:A:375:LYS:NZ	2.50	0.44
2:B:583:TRP:CD1	3:F:528:ASN:HD22	2.36	0.44
3:F:411:ASP:OD1	3:F:412:GLY:N	2.49	0.44
3:F:424:VAL:HB	3:F:610:LYS:NZ	2.33	0.44
3:F:458:LEU:HD22	3:F:462:ASN:ND2	2.32	0.44
3:F:608:THR:HG22	3:F:609:ARG:N	2.33	0.44
3:F:608:THR:HG21	3:F:613:GLU:HA	1.99	0.44
3:G:69:ARG:HA	3:G:72:ALA:HB3	1.99	0.44
3:G:109:ASP:OD1	3:G:109:ASP:N	2.49	0.44
1:A:99:TYR:HD2	1:A:171:VAL:HG21	1.82	0.44
1:A:613:ASP:OD1	1:A:614:GLY:N	2.51	0.44
2:B:434:ILE:HG12	2:B:468:PRO:HB3	1.99	0.44
3:F:444:GLY:HA3	3:F:602:PRO:HA	2.00	0.44
3:G:180:CYS:HA	3:G:198:CYS:HB2	2.00	0.44
1:A:316:PRO:O	1:A:328:GLY:HA2	2.18	0.43
1:A:442:GLN:NE2	1:A:453:LYS:O	2.45	0.43
1:A:843:ARG:HH21	1:A:875:VAL:HG21	1.83	0.43
3:F:70:ALA:HB1	3:F:75:GLU:HB3	2.00	0.43
3:G:339:VAL:O	3:G:343:ARG:HG2	2.17	0.43
3:G:409:SER:HA	3:G:606:VAL:HA	2.00	0.43
1:A:449:ASP:OD1	1:A:449:ASP:N	2.51	0.43
1:A:743:ASP:O	1:A:747:VAL:HG23	2.17	0.43
3:G:508:LYS:HB3	3:G:510:ASP:OD1	2.18	0.43
3:G:582:CYS:HB2	3:G:584:ASP:OD1	2.18	0.43
1:A:659:TRP:CD1	1:A:723:PRO:HB2	2.54	0.43
2:B:565:ILE:H	2:B:565:ILE:HD12	1.83	0.43
2:B:577:ASN:OD1	2:B:580:SER:N	2.51	0.43
3:F:429:GLU:HA	3:F:657:LEU:HD23	2.00	0.43
3:G:29:ALA:N	3:G:59:VAL:O	2.51	0.43
3:G:193:CYS:HA	3:G:203:GLN:NE2	2.33	0.43
2:B:105:LYS:HA	2:B:108:ILE:HG12	2.01	0.43
2:B:116:ASP:OD2	2:B:118:ASN:HB2	2.18	0.43
3:F:278:LYS:NZ	3:F:281:LEU:HD22	2.34	0.43
3:F:467:LYS:O	3:F:548:ASP:HB2	2.19	0.43
3:G:624:GLN:NE2	3:G:657:LEU:HB2	2.34	0.43
1:A:444:THR:HG22	1:A:466:TYR:CD1	2.53	0.43
3:F:473:VAL:HA	3:F:479:TRP:CD2	2.54	0.43
1:A:255:TYR:HB3	1:A:540:ASN:O	2.19	0.43
1:A:325:HIS:HA	1:A:412:TYR:CE1	2.50	0.43
1:A:334:THR:OG1	1:A:405:LYS:HB3	2.18	0.43
1:A:358:GLN:O	1:A:362:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:HIS:HB3	1:A:572:CYS:HA	2.00	0.43
1:A:580:LYS:HG2	1:A:608:SER:HG	1.83	0.43
2:B:122:SER:H	2:B:125:LEU:HD12	1.83	0.43
2:B:220:PHE:CG	2:B:328:PRO:HD3	2.53	0.43
2:B:317:LYS:NZ	2:B:318:PRO:HD2	2.33	0.43
3:F:82:ASP:HA	3:F:268:HIS:CG	2.53	0.43
3:G:454:SER:OG	3:G:455:ALA:N	2.52	0.43
2:B:208:TRP:CD1	2:B:264:SER:HB3	2.50	0.43
2:B:512:TYR:CD2	2:B:669:GLY:HA2	2.54	0.43
2:B:658:ILE:HG23	2:B:681:TYR:CG	2.53	0.43
3:F:321:PHE:C	3:F:322:LEU:HD12	2.44	0.43
3:G:280:ASP:OD1	3:G:280:ASP:N	2.49	0.43
1:A:233:HIS:HE1	1:A:235:ALA:HB3	1.84	0.43
1:A:612:ASP:OD1	1:A:612:ASP:N	2.52	0.43
1:A:807:ASN:HB2	1:A:851:SER:OG	2.19	0.43
1:A:843:ARG:HG2	2:B:29:ASP:HB3	2.00	0.43
1:A:913:MET:HE3	1:A:914:LYS:N	2.34	0.43
3:F:380:ASN:ND2	3:F:638:PHE:HB3	2.33	0.43
3:F:516:LEU:HD22	3:F:546:LYS:HE2	2.01	0.43
3:G:400:ILE:HD13	3:G:405:ALA:HB3	2.01	0.43
3:G:663:ARG:HA	3:G:668:LYS:HD2	2.00	0.43
2:B:650:THR:O	3:F:687:SER:OG	2.27	0.43
3:F:27:TRP:CZ3	3:F:79:VAL:HG23	2.54	0.43
3:F:484:GLY:HA2	3:F:681:LEU:HB2	2.00	0.43
3:G:426:VAL:HG21	3:G:616:VAL:HG13	2.01	0.43
1:A:182:ILE:HG12	1:A:210:ALA:HB1	2.01	0.43
1:A:866:VAL:HG13	1:A:907:TYR:HE1	1.83	0.43
2:B:46:ASP:HB2	2:B:707:ARG:O	2.19	0.43
2:B:131:GLN:HB3	2:B:135:THR:OG1	2.19	0.43
3:F:204:TYR:CD2	3:F:213:CYS:HB2	2.54	0.43
3:G:27:TRP:O	3:G:59:VAL:N	2.47	0.43
2:B:321:ASN:OD1	2:B:322:SER:N	2.52	0.42
2:B:575:ILE:HD12	2:B:698:SER:O	2.18	0.42
3:F:26:ARG:HH21	3:F:76:ALA:HB2	1.83	0.42
3:F:282:ILE:HA	3:F:285:LEU:HB2	2.01	0.42
3:F:506:GLY:HA2	3:F:527:PRO:HD3	2.01	0.42
1:A:299:ARG:HG2	1:A:301:LEU:H	1.83	0.42
2:B:178:LYS:HD3	2:B:178:LYS:HA	1.84	0.42
2:B:460:PHE:CG	2:B:589:ASN:HB3	2.54	0.42
3:F:619:ILE:HA	3:F:622:GLN:OE1	2.18	0.42
3:G:181:ALA:HB1	3:G:189:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:446:PHE:O	3:G:554:HIS:HB3	2.19	0.42
3:G:512:SER:HB2	3:G:515:LYS:HD2	2.00	0.42
1:A:142:GLU:OE1	1:A:142:GLU:N	2.42	0.42
2:B:27:SER:N	2:B:30:LEU:HD22	2.34	0.42
2:B:163:HIS:ND1	3:G:368:HIS:CG	2.88	0.42
2:B:279:LEU:HD21	2:B:299:LEU:HD11	1.99	0.42
2:B:513:LEU:C	2:B:514:LYS:HZ2	2.25	0.42
2:B:522:ASN:H	2:B:542:GLN:HG3	1.83	0.42
3:F:138:HIS:HB3	3:F:147:TRP:HE1	1.84	0.42
3:G:30:VAL:O	3:G:34:GLU:HB2	2.19	0.42
3:G:63:SER:N	3:G:66:ASP:OD2	2.52	0.42
3:G:367:SER:OG	3:G:368:HIS:N	2.52	0.42
1:A:158:ASN:OD1	1:A:161:GLU:HB2	2.19	0.42
2:B:226:PRO:O	3:G:644:GLU:HG3	2.19	0.42
3:F:124:SER:HG	3:F:251:ARG:HH12	1.61	0.42
3:F:341:ALA:O	3:F:345:LEU:HG	2.20	0.42
3:F:557:VAL:HB	3:F:558:PRO:HD3	2.01	0.42
3:G:453:LYS:HG2	3:G:579:GLU:HG3	2.01	0.42
3:G:674:TYR:O	3:G:678:VAL:HG12	2.20	0.42
1:A:54:GLU:OE1	1:A:57:GLY:N	2.46	0.42
1:A:402:THR:O	1:A:437:LEU:HA	2.20	0.42
2:B:149:TYR:CG	2:B:205:LYS:HB2	2.54	0.42
2:B:163:HIS:HA	2:B:181:ASP:OD1	2.18	0.42
2:B:411:LYS:HD3	2:B:414:ASP:OD2	2.20	0.42
3:F:666:TYR:O	3:F:670:LEU:HD13	2.19	0.42
1:A:694:SER:O	1:A:736:ILE:HG13	2.19	0.42
3:F:61:LYS:HD2	3:F:67:CYS:SG	2.60	0.42
3:F:281:LEU:HA	3:F:284:GLU:OE2	2.20	0.42
3:F:453:LYS:HE2	3:F:579:GLU:HB3	2.01	0.42
3:F:476:THR:HA	3:F:480:ASN:HD22	1.84	0.42
3:G:479:TRP:HD1	3:G:480:ASN:ND2	2.18	0.42
3:G:483:MET:HE2	3:G:495:PHE:HZ	1.85	0.42
1:A:134:ALA:HB2	1:A:469:ASP:HB3	2.02	0.42
1:A:863:ARG:HB2	1:A:910:SER:HB2	2.02	0.42
2:B:99:GLU:OE1	2:B:99:GLU:N	2.53	0.42
3:F:516:LEU:HB3	3:F:546:LYS:NZ	2.34	0.42
3:G:243:GLU:OE2	3:G:251:ARG:NH1	2.51	0.42
3:G:362:LYS:HD2	3:G:363:TRP:H	1.85	0.42
1:A:322:ASN:HD21	1:A:325:HIS:CD2	2.38	0.42
2:B:415:LYS:HZ3	2:B:699:ALA:H	1.68	0.42
2:B:680:ALA:HA	2:B:699:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:397:ILE:HD11	3:F:410:LEU:CD1	2.49	0.42
3:F:537:THR:HA	3:F:560:ASN:ND2	2.34	0.42
3:G:88:ASP:HA	3:G:91:LEU:HD12	2.01	0.42
3:G:208:SER:HA	3:G:232:ASN:HD21	1.84	0.42
3:G:292:HIS:O	3:G:298:SER:HA	2.20	0.42
1:A:89:VAL:HG13	1:A:881:ARG:HH12	1.83	0.42
1:A:102:ARG:O	1:A:700:TYR:OH	2.33	0.42
1:A:692:GLU:OE2	1:A:694:SER:HB3	2.19	0.42
2:B:221:ARG:NH2	3:G:566:PRO:HG2	2.34	0.42
2:B:691:THR:N	2:B:694:SER:HB3	2.35	0.42
3:F:45:MET:O	3:F:49:ILE:HB	2.20	0.42
3:F:265:VAL:HG12	3:F:266:PRO:O	2.19	0.42
3:G:163:LYS:HD3	3:G:163:LYS:HA	1.74	0.42
1:A:653:PHE:HD1	1:A:656:MET:HE2	1.85	0.42
1:A:867:TYR:HB2	1:A:906:ASN:OD1	2.19	0.42
2:B:223:ILE:HD12	2:B:223:ILE:HA	1.88	0.42
2:B:295:GLN:HG2	2:B:315:THR:HG21	2.02	0.42
3:F:411:ASP:HB2	3:F:604:HIS:ND1	2.35	0.42
3:F:565:ASN:ND2	3:F:567:ASP:HB2	2.35	0.42
1:A:134:ALA:HB3	1:A:569:TYR:OH	2.20	0.41
1:A:299:ARG:HD2	1:A:343:MET:HB2	2.02	0.41
1:A:440:HIS:HB2	1:A:470:ARG:NE	2.35	0.41
1:A:510:LEU:HB3	1:A:575:ARG:HB2	2.02	0.41
1:A:512:HIS:O	1:A:572:CYS:HB2	2.20	0.41
1:A:515:TYR:CD2	1:A:561:ILE:HB	2.55	0.41
2:B:515:TYR:CE1	2:B:704:GLY:HA3	2.54	0.41
2:B:583:TRP:HD1	3:F:528:ASN:HD22	1.68	0.41
2:B:583:TRP:CG	2:B:584:SER:N	2.87	0.41
3:F:621:ARG:O	3:F:624:GLN:HG2	2.20	0.41
1:A:128:LEU:HG	3:F:625:HIS:ND1	2.35	0.41
1:A:243:PHE:CZ	1:A:287:GLN:HB3	2.55	0.41
1:A:273:LYS:O	1:A:276:PRO:HD3	2.20	0.41
2:B:144:ASN:OD1	2:B:261:GLY:HA3	2.20	0.41
2:B:196:LEU:O	2:B:402:THR:N	2.46	0.41
2:B:651:THR:OG1	2:B:652:ARG:HD2	2.20	0.41
3:F:235:ASN:OD1	3:F:235:ASN:N	2.54	0.41
3:F:340:THR:O	3:F:343:ARG:HG2	2.20	0.41
3:F:501:GLU:HG2	3:F:512:SER:HB2	2.02	0.41
3:F:533:TYR:HA	3:F:538:GLY:HA3	2.02	0.41
3:G:65:LEU:HA	3:G:68:ILE:HD12	2.02	0.41
3:G:312:LEU:C	3:G:314:PHE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:HB3	1:A:108:ARG:HD3	2.02	0.41
2:B:57:ASP:OD2	2:B:307:ARG:NH1	2.53	0.41
2:B:462:ARG:HB3	2:B:505:VAL:HG13	2.03	0.41
2:B:647:GLN:HA	3:F:392:THR:HG23	2.02	0.41
2:B:650:THR:OG1	3:F:480:ASN:OD1	2.31	0.41
2:B:652:ARG:HG3	3:F:686:THR:HG22	2.02	0.41
2:B:664:GLN:HB2	2:B:678:TRP:CZ2	2.55	0.41
3:F:346:ARG:HB3	3:F:346:ARG:NH1	2.35	0.41
3:G:274:SER:C	3:G:276:GLY:H	2.27	0.41
2:B:416:LYS:O	2:B:418:GLN:NE2	2.54	0.41
3:G:641:PHE:CE2	3:G:654:THR:HG23	2.56	0.41
1:A:526:LEU:HD22	3:F:592:GLU:CD	2.45	0.41
1:A:727:ASN:O	1:A:772:ARG:HD3	2.19	0.41
1:A:841:ARG:HH12	1:A:843:ARG:HA	1.85	0.41
2:B:513:LEU:HD13	2:B:668:TYR:CE2	2.56	0.41
2:B:578:ASP:CA	2:B:696:ASN:H	2.33	0.41
3:F:43:ASP:HA	3:F:46:LYS:HZ2	1.86	0.41
3:F:471:THR:OG1	3:F:475:ARG:HG3	2.21	0.41
3:G:114:TYR:CD2	3:G:225:LYS:HB2	2.55	0.41
3:G:541:ARG:HG3	3:G:569:TRP:CE3	2.55	0.41
3:G:574:ASN:OD1	3:G:575:GLU:N	2.47	0.41
1:A:119:ILE:CG2	1:A:141:ASN:H	2.34	0.41
2:B:405:LEU:HD13	2:B:422:ASN:HB3	2.03	0.41
3:F:90:TYR:CE2	3:F:330:ALA:HB3	2.55	0.41
3:F:104:TYR:CE1	3:F:318:ALA:HA	2.55	0.41
3:F:683:LYS:HD3	3:F:683:LYS:HA	1.83	0.41
2:B:212:THR:N	2:B:235:SER:HG	2.17	0.41
2:B:584:SER:O	3:F:530:LYS:NZ	2.40	0.41
3:F:367:SER:HB2	3:F:370:GLU:HG2	2.02	0.41
3:F:485:LEU:HD22	3:F:486:LEU:HD22	2.02	0.41
3:G:146:GLY:H	4:G:701:BCT:HO3	1.61	0.41
3:G:368:HIS:O	3:G:372:LEU:HG	2.20	0.41
3:G:400:ILE:HA	3:G:405:ALA:O	2.21	0.41
3:G:518:MET:HG3	3:G:531:GLU:OE2	2.21	0.41
1:A:125:GLN:HE22	1:A:660:ARG:N	2.15	0.41
1:A:149:LYS:HE2	1:A:177:THR:H	1.86	0.41
1:A:540:ASN:H	1:A:545:ASN:ND2	2.19	0.41
2:B:39:ARG:NH1	2:B:40:PRO:HD2	2.35	0.41
2:B:221:ARG:CD	3:G:568:PRO:HD3	2.51	0.41
2:B:331:SER:OG	2:B:332:ASP:N	2.54	0.41
2:B:340:PHE:C	2:B:341:PHE:HD1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LEU:HG	3:F:522:LEU:HD22	2.03	0.41
2:B:522:ASN:O	2:B:542:GLN:NE2	2.40	0.41
3:F:115:TYR:O	3:F:226:HIS:ND1	2.54	0.41
3:G:27:TRP:HD1	3:G:38:CYS:SG	2.44	0.41
3:G:193:CYS:HB3	3:G:204:TYR:CD2	2.56	0.41
1:A:263:GLU:HA	1:A:265:LYS:HZ2	1.85	0.41
1:A:432:ARG:HG2	1:A:478:LYS:HG2	2.03	0.41
1:A:749:ASP:N	1:A:749:ASP:OD1	2.54	0.41
1:A:867:TYR:HD2	1:A:906:ASN:OD1	2.04	0.41
2:B:75:GLN:OE1	2:B:75:GLN:N	2.54	0.41
2:B:208:TRP:CE2	2:B:262:PHE:HB3	2.56	0.41
2:B:653:THR:HG23	3:F:687:SER:HA	2.03	0.41
3:F:146:GLY:C	3:F:147:TRP:HD1	2.29	0.41
3:F:180:CYS:N	3:F:198:CYS:HB2	2.35	0.41
3:F:396:CYS:CB	3:F:408:MET:HE2	2.51	0.41
3:F:408:MET:SD	3:F:410:LEU:HG	2.61	0.41
3:F:409:SER:HA	3:F:606:VAL:HA	2.02	0.41
3:G:37:LYS:HG3	3:G:301:PHE:HZ	1.86	0.41
3:G:73:ALA:HB3	3:G:75:GLU:OE1	2.21	0.41
3:G:343:ARG:NH1	3:G:343:ARG:HA	2.36	0.41
3:G:567:ASP:HB2	3:G:569:TRP:CD1	2.55	0.41
3:G:567:ASP:OD1	3:G:570:ALA:HB3	2.20	0.41
1:A:370:TYR:CZ	1:A:375:LYS:HD3	2.56	0.41
3:F:121:LYS:NZ	3:F:215:LYS:HA	2.36	0.41
3:F:438:GLU:HG3	3:F:659:LYS:HG2	2.03	0.41
3:F:482:PRO:HB3	3:F:551:PHE:CE1	2.55	0.41
3:F:663:ARG:HE	3:F:669:TYR:HD1	1.69	0.41
3:G:29:ALA:HB3	3:G:60:LYS:HD3	2.02	0.41
3:G:244:LEU:O	3:G:251:ARG:HA	2.21	0.41
1:A:60:LYS:NZ	1:A:62:VAL:HG22	2.36	0.40
1:A:708:TYR:CD2	3:F:382:VAL:HG11	2.54	0.40
1:A:857:LYS:O	1:A:858:LYS:HG2	2.21	0.40
2:B:679:PHE:CE1	2:B:701:VAL:HB	2.57	0.40
3:G:77:ASP:HA	3:G:273:ARG:HH21	1.86	0.40
3:G:443:ALA:HB3	3:G:600:ARG:CZ	2.51	0.40
3:G:478:GLY:HA2	3:G:551:PHE:O	2.21	0.40
1:A:841:ARG:HG2	2:B:32:SER:O	2.21	0.40
1:A:845:TRP:HB2	1:A:872:HIS:HE1	1.86	0.40
2:B:77:LYS:NZ	2:B:216:LYS:HD2	2.37	0.40
2:B:80:GLU:HA	2:B:214:THR:O	2.22	0.40
2:B:146:ALA:HB3	2:B:149:TYR:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:LEU:O	2:B:620:THR:N	2.54	0.40
2:B:638:THR:OG1	2:B:639:ALA:N	2.53	0.40
3:F:592:GLU:O	3:F:595:ASN:HB2	2.21	0.40
3:G:337:GLU:O	3:G:340:THR:OG1	2.30	0.40
1:A:86:ILE:HG12	1:A:101:ILE:HG12	2.04	0.40
2:B:308:PHE:CE2	2:B:338:GLY:HA3	2.56	0.40
2:B:562:GLU:HG2	2:B:563:GLN:H	1.87	0.40
2:B:575:ILE:O	2:B:582:SER:HB2	2.21	0.40
3:F:613:GLU:H	3:F:613:GLU:CD	2.28	0.40
3:G:22:ASP:OD1	3:G:22:ASP:N	2.54	0.40
3:G:131:LEU:HD23	3:G:131:LEU:HA	1.97	0.40
3:G:366:LEU:HD21	3:G:528:ASN:HA	2.02	0.40
3:G:411:ASP:HA	3:G:604:HIS:CG	2.57	0.40
3:G:617:HIS:CE1	3:G:659:LYS:HE2	2.56	0.40
1:A:132:ARG:HH22	1:A:345:VAL:HA	1.85	0.40
2:B:135:THR:HA	2:B:141:GLN:HE22	1.86	0.40
2:B:208:TRP:CH2	2:B:262:PHE:HB3	2.56	0.40
2:B:253:LEU:HD21	2:B:260:TYR:CE1	2.56	0.40
2:B:506:CYS:HA	2:B:507:CYS:HA	1.78	0.40
3:F:310:LYS:HD2	3:F:310:LYS:HA	1.84	0.40
3:F:447:ALA:HB3	3:F:598:LEU:HB2	2.03	0.40
3:F:502:GLY:HA3	3:F:513:LEU:HD13	2.02	0.40
3:G:425:PRO:HA	3:G:607:VAL:HG12	2.02	0.40
3:G:667:GLU:OE1	3:G:675:VAL:HG21	2.21	0.40
1:A:825:ARG:O	1:A:832:SER:HA	2.21	0.40
2:B:344:GLN:HB3	2:B:401:LEU:HD21	2.04	0.40
3:F:295:LYS:NZ	3:F:318:ALA:O	2.52	0.40
3:G:97:LYS:NZ	3:G:274:SER:HA	2.36	0.40
3:G:225:LYS:HG2	3:G:228:THR:OG1	2.22	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	868/939 (92%)	832 (96%)	36 (4%)	0	100	100
2	B	590/712 (83%)	546 (92%)	44 (8%)	0	100	100
3	F	672/698 (96%)	584 (87%)	86 (13%)	2 (0%)	36	71
3	G	671/698 (96%)	614 (92%)	57 (8%)	0	100	100
All	All	2801/3047 (92%)	2576 (92%)	223 (8%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	382	VAL
3	F	649	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	708/768 (92%)	708 (100%)	0	100	100
2	B	507/580 (87%)	507 (100%)	0	100	100
3	F	547/585 (94%)	547 (100%)	0	100	100
3	G	554/585 (95%)	554 (100%)	0	100	100
All	All	2316/2518 (92%)	2316 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	125	GLN
1	A	241	GLN
1	A	275	ASN
1	A	360	GLN
1	A	495	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	545	ASN
1	A	831	ASN
1	A	889	ASN
2	B	141	GLN
2	B	257	GLN
2	B	601	ASN
3	F	138	HIS
3	F	555	GLN
3	F	595	ASN
3	G	39	GLN
3	G	287	ASN
3	G	369	HIS
3	G	380	ASN
3	G	480	ASN
3	G	491	ASN
3	G	565	ASN
3	G	623	GLN
3	G	637	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
4	BCT	G	701	-	3,3,3	0.78	0	2,3,3	3.25	2 (100%)
4	BCT	G	702	5	3,3,3	0.79	0	2,3,3	3.27	2 (100%)
4	BCT	F	701	5	3,3,3	0.78	0	2,3,3	3.30	2 (100%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	702	BCT	O2-C-O1	4.05	130.03	119.68
4	F	701	BCT	O2-C-O1	4.04	130.02	119.68
4	G	701	BCT	O2-C-O1	3.98	129.87	119.68
4	F	701	BCT	O3-C-O1	-2.33	113.73	119.68
4	G	701	BCT	O3-C-O1	-2.29	113.83	119.68
4	G	702	BCT	O3-C-O1	-2.25	113.92	119.68

There are no chirality outliers.

There are no torsion outliers.

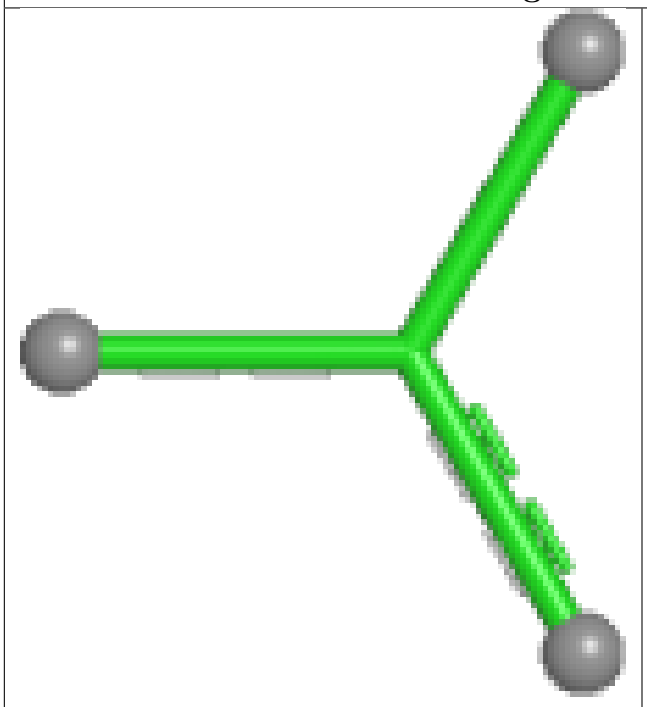
There are no ring outliers.

2 monomers are involved in 7 short contacts:

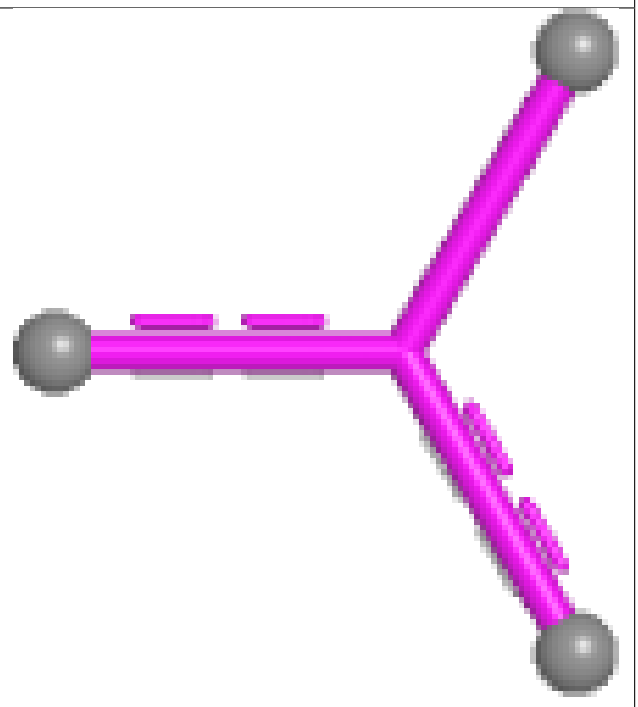
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	701	BCT	5	0
4	F	701	BCT	2	0

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.

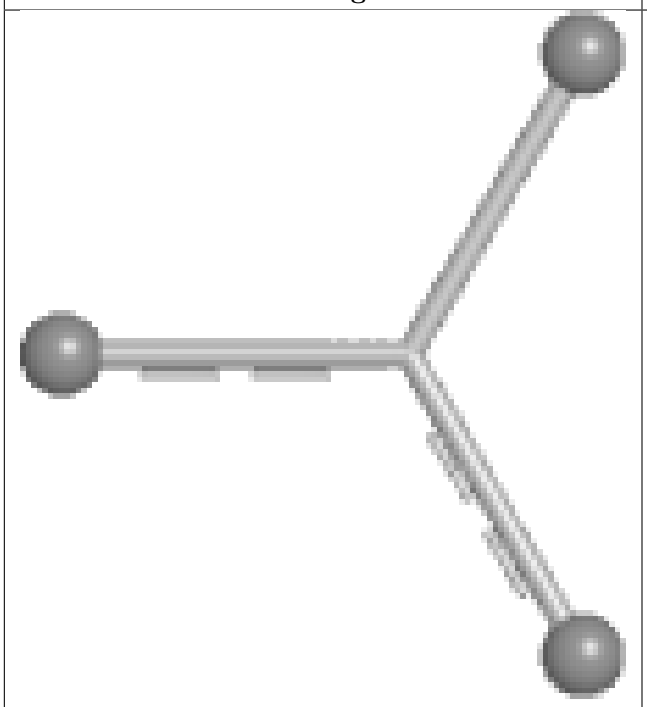
Ligand BCT G 701



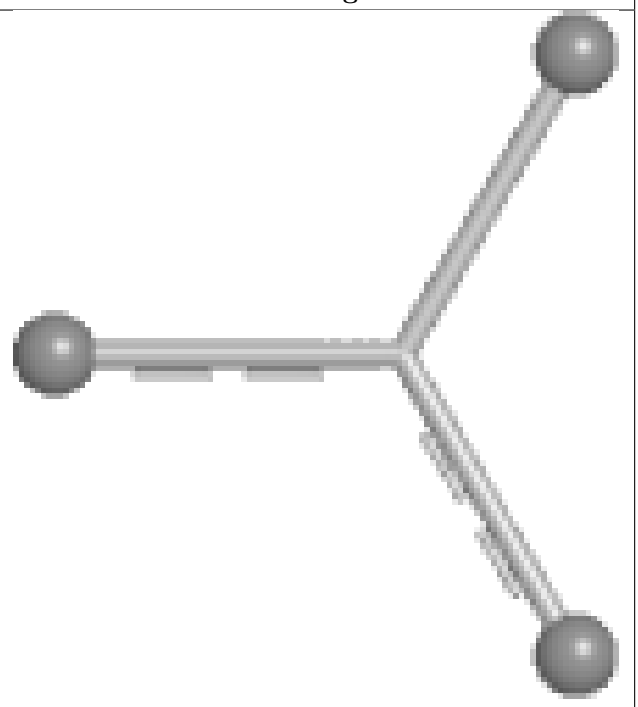
Bond lengths



Bond angles

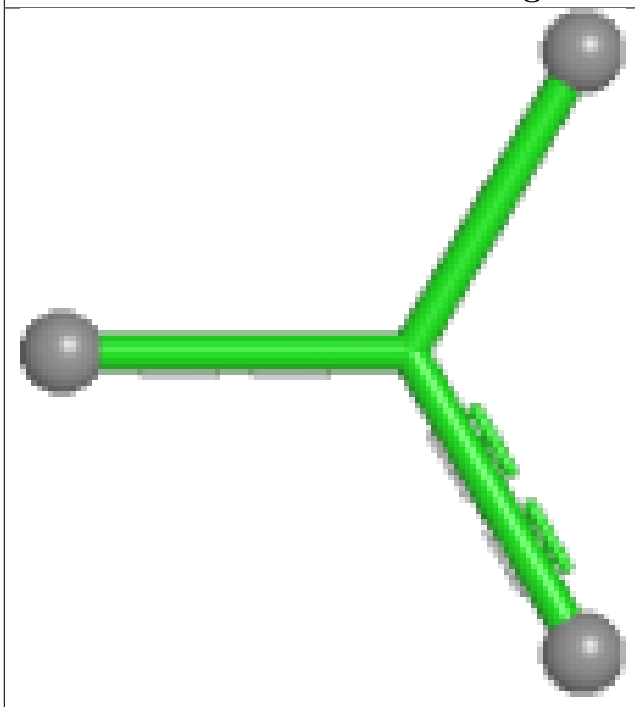


Torsions

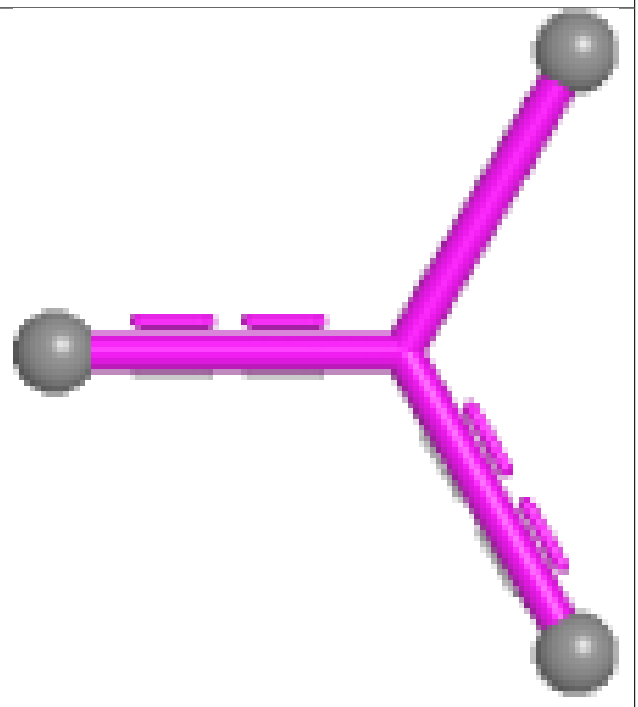


Rings

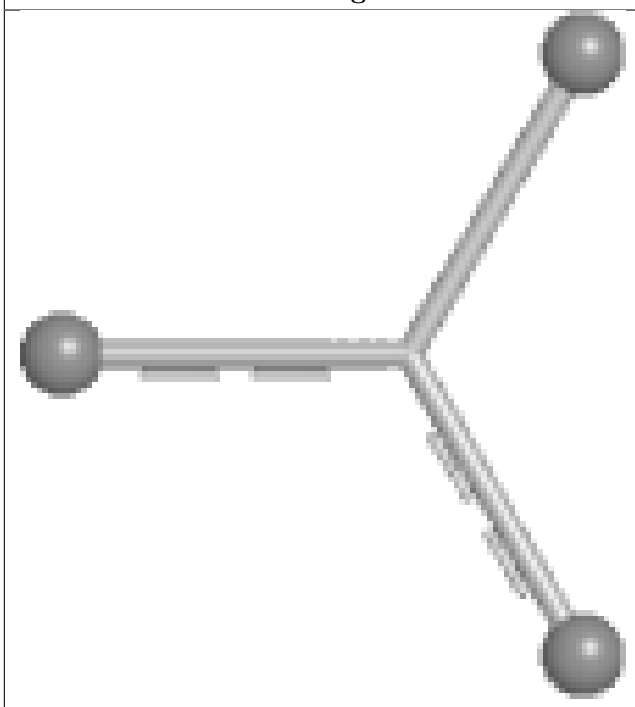
Ligand BCT G 702



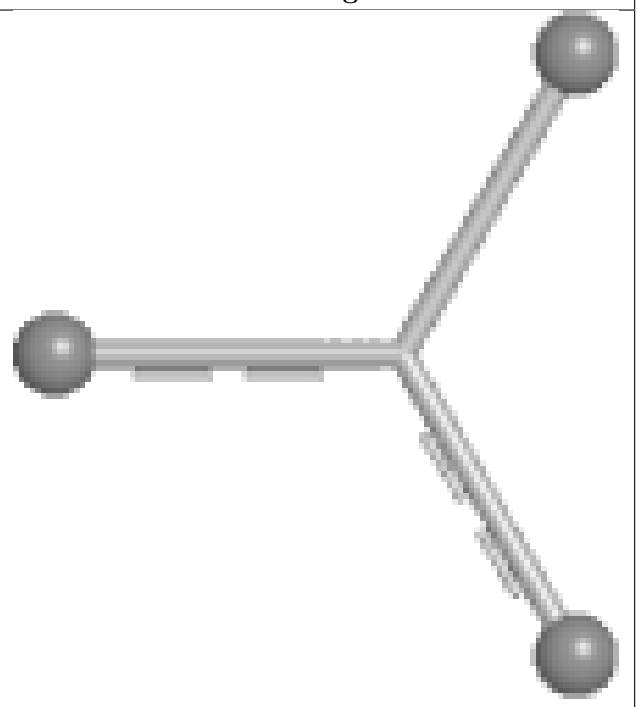
Bond lengths



Bond angles

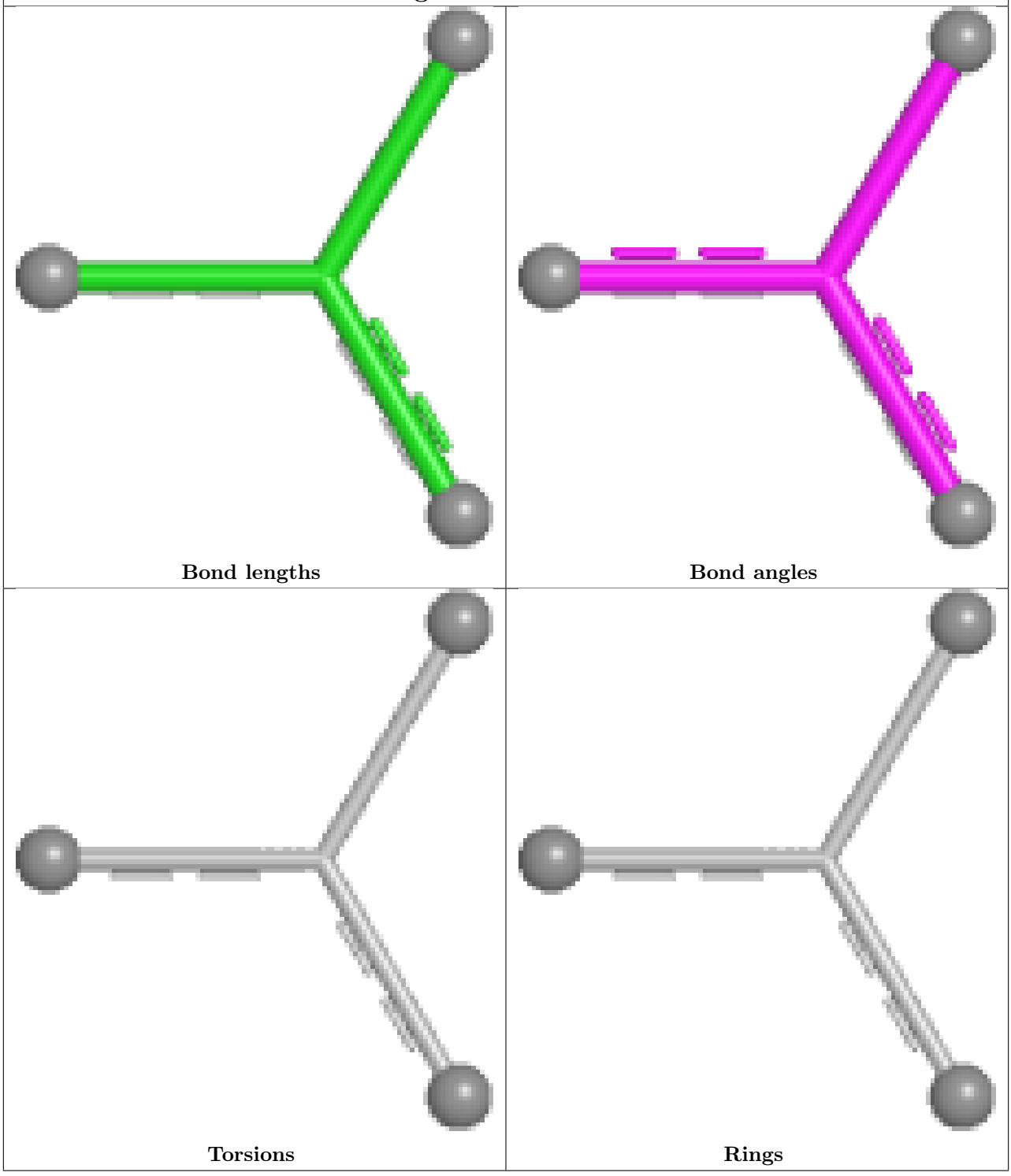


Torsions



Rings

Ligand BCT F 701



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
3	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	206:GLY	C	207:TYR	N	3.18

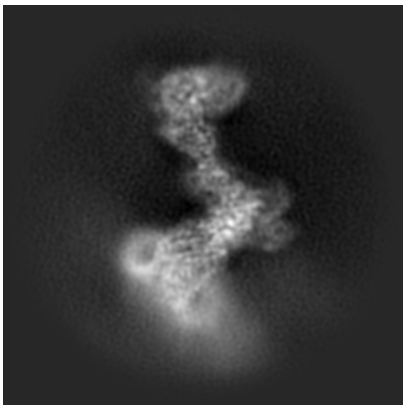
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45682. These allow visual inspection of the internal detail of the map and identification of artifacts.

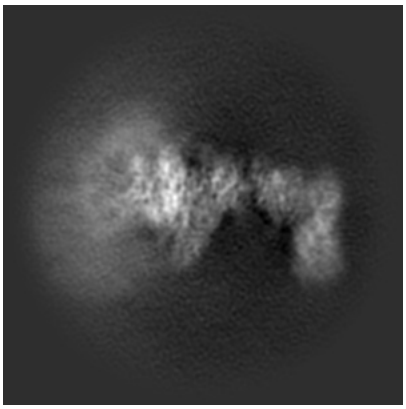
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

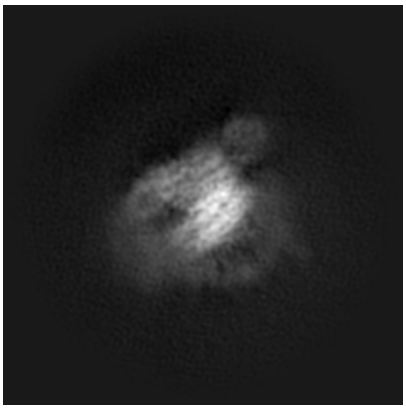
6.1.1 Primary map



X

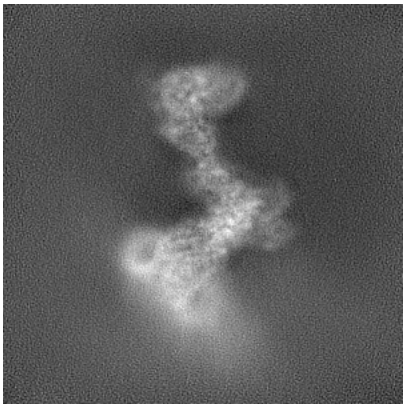


Y

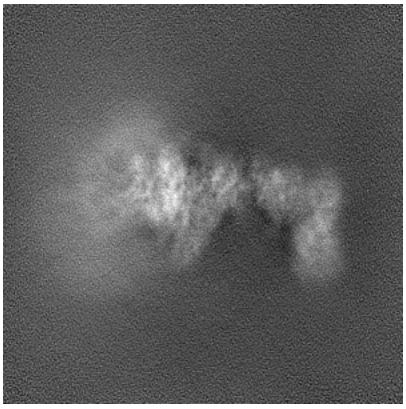


Z

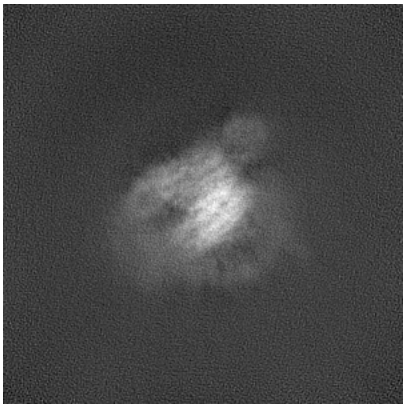
6.1.2 Raw map



X



Y

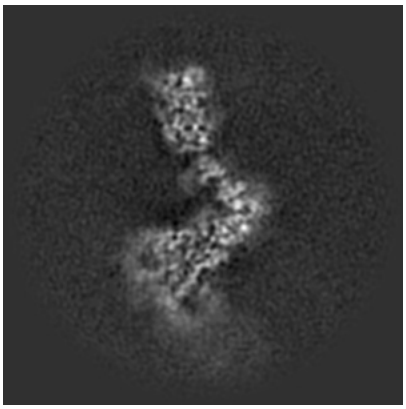


Z

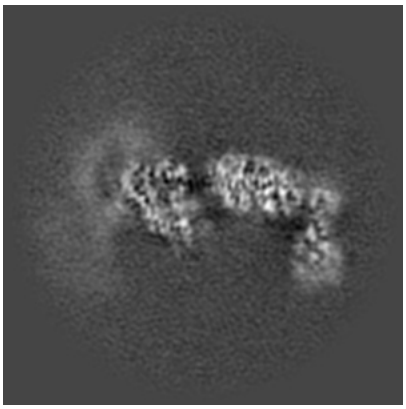
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

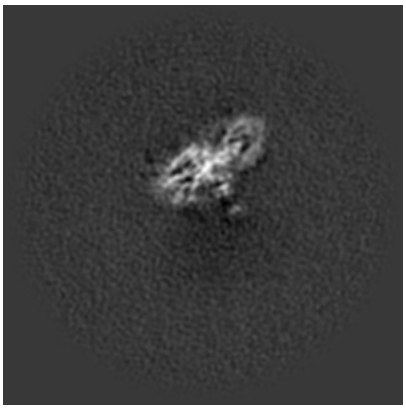
6.2.1 Primary map



X Index: 150

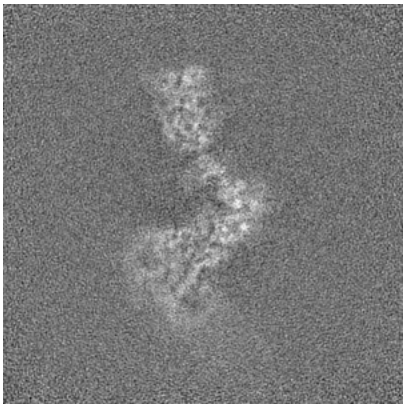


Y Index: 150

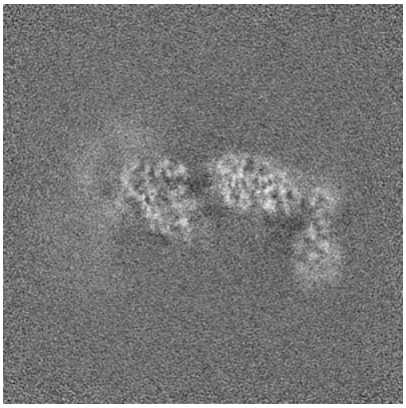


Z Index: 150

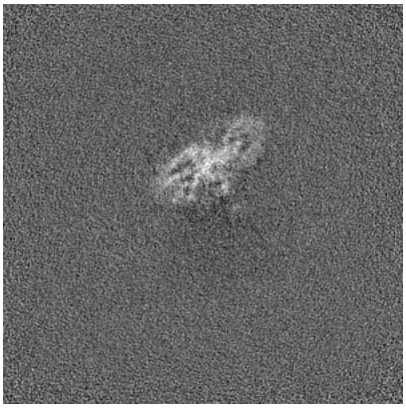
6.2.2 Raw map



X Index: 150



Y Index: 150

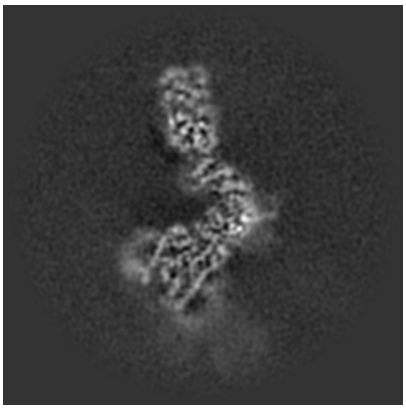


Z Index: 150

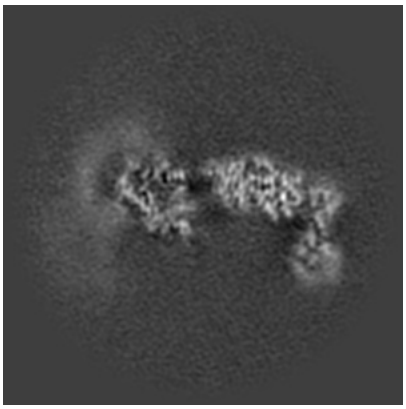
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

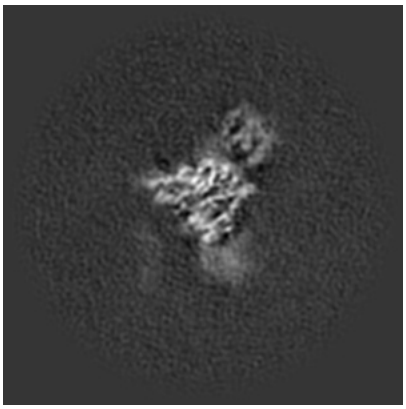
6.3.1 Primary map



X Index: 157

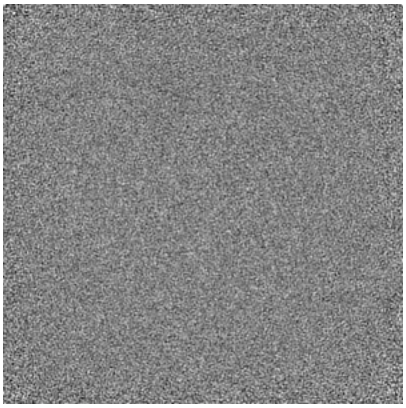


Y Index: 148

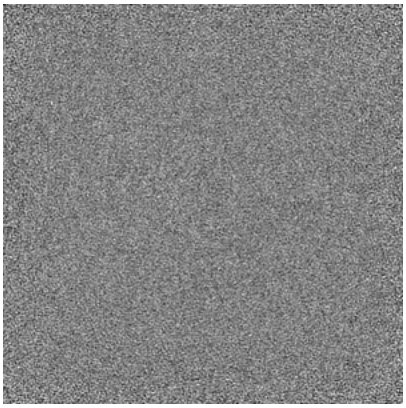


Z Index: 129

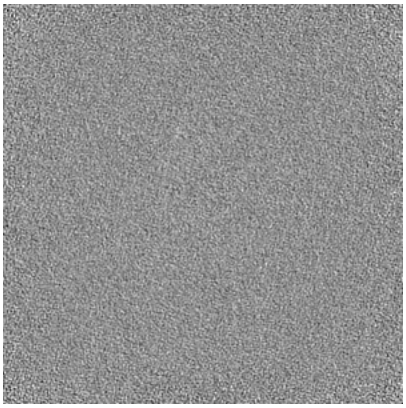
6.3.2 Raw map



X Index: 0



Y Index: 0

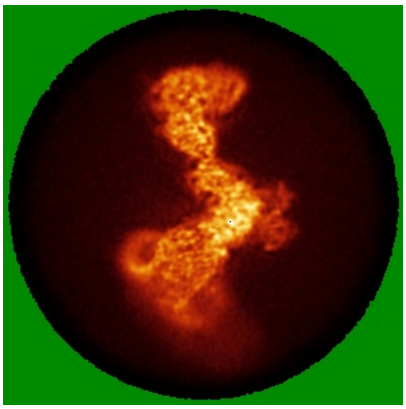


Z Index: 0

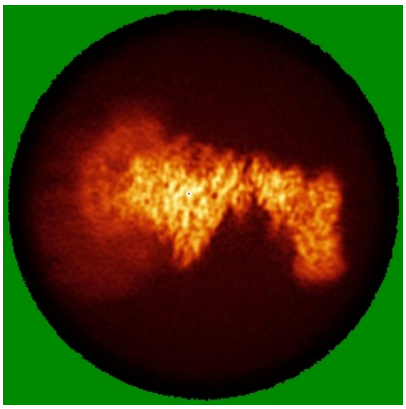
The images above show the largest variance slices of the map in three orthogonal directions.

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

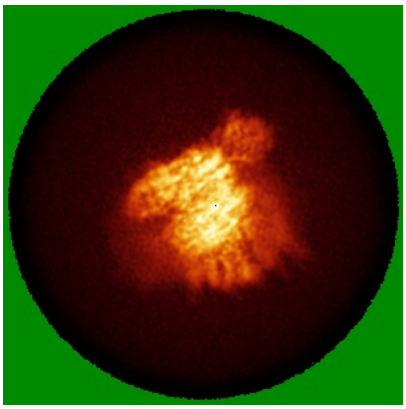
6.4.1 Primary map



X

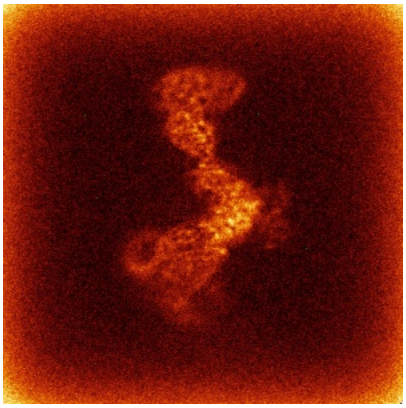


Y

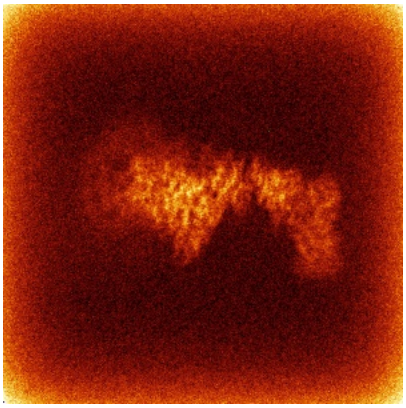


Z

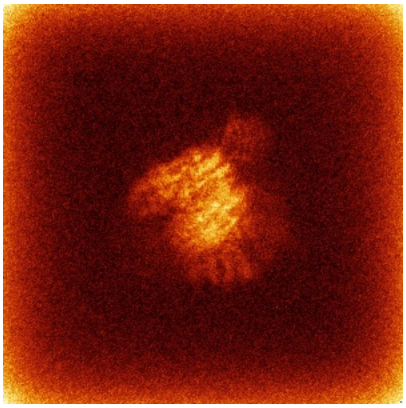
6.4.2 Raw map



X



Y



Z

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

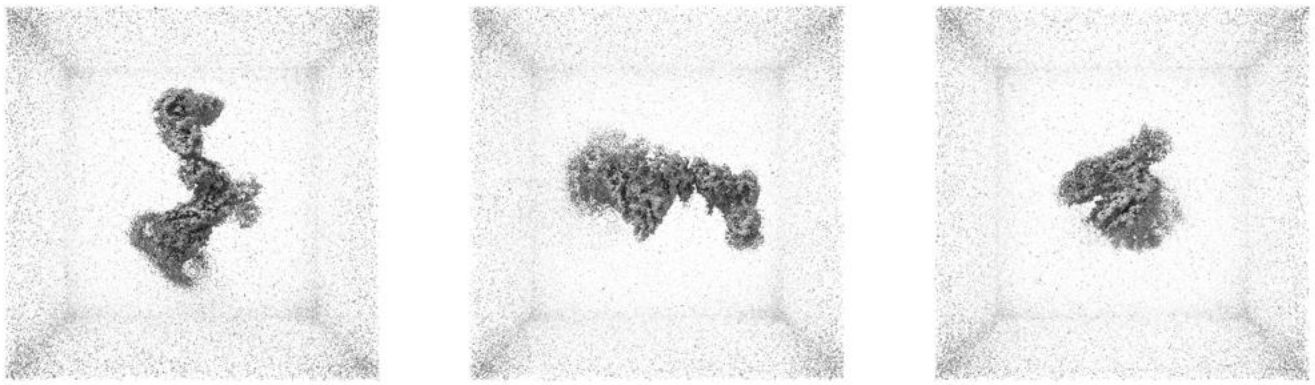
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0888. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

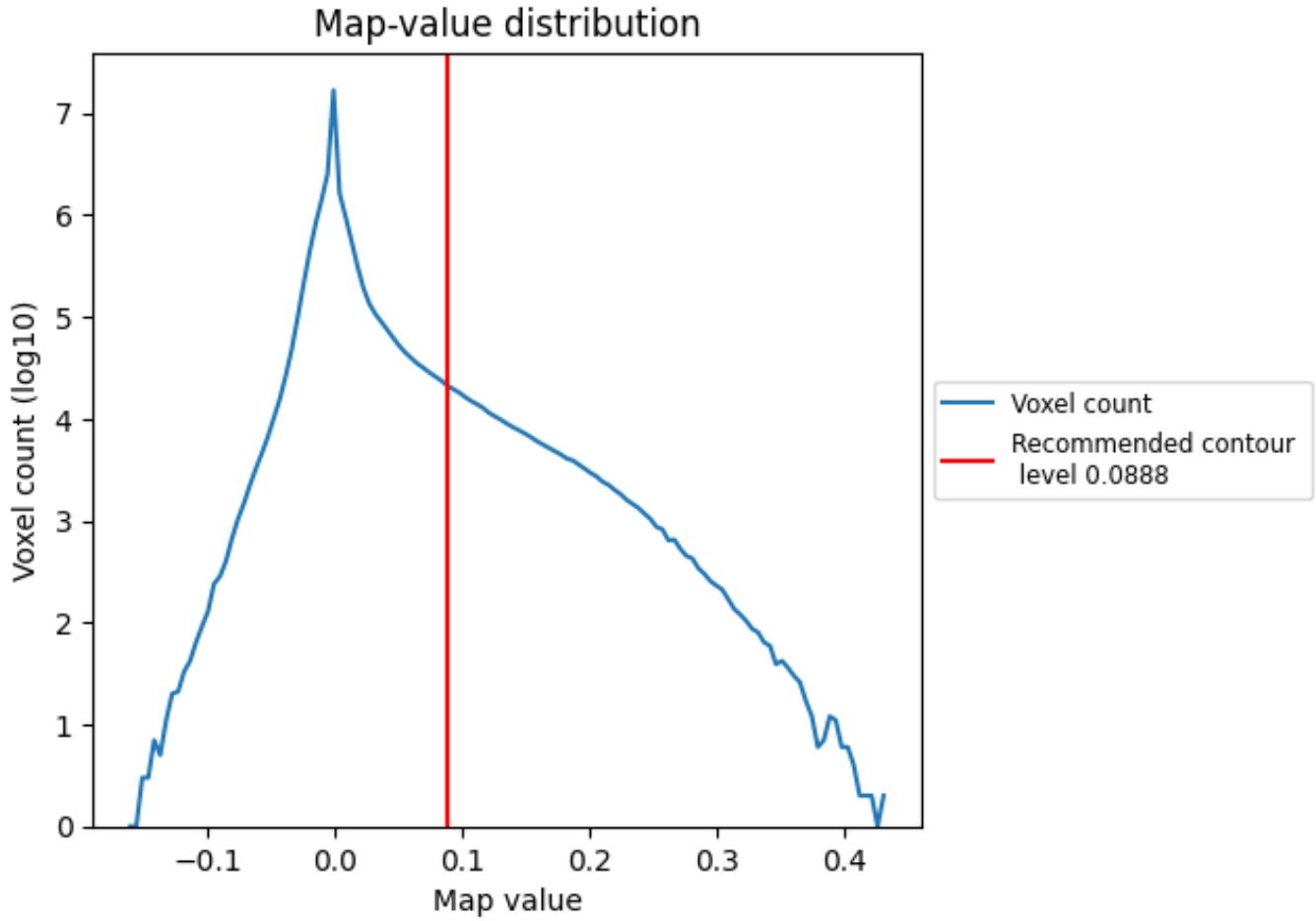
6.6 Mask visualisation (i)

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

7 Map analysis

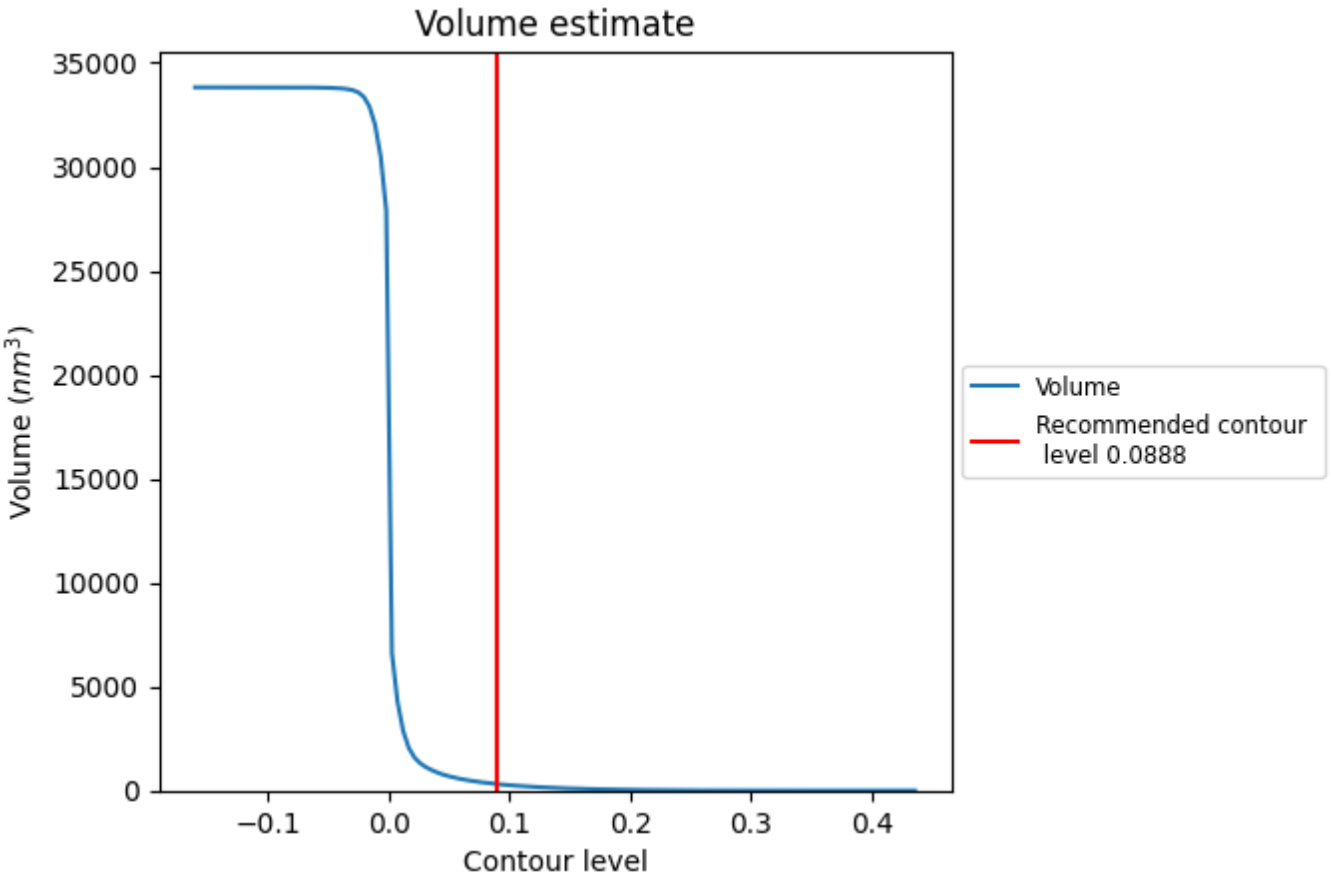
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

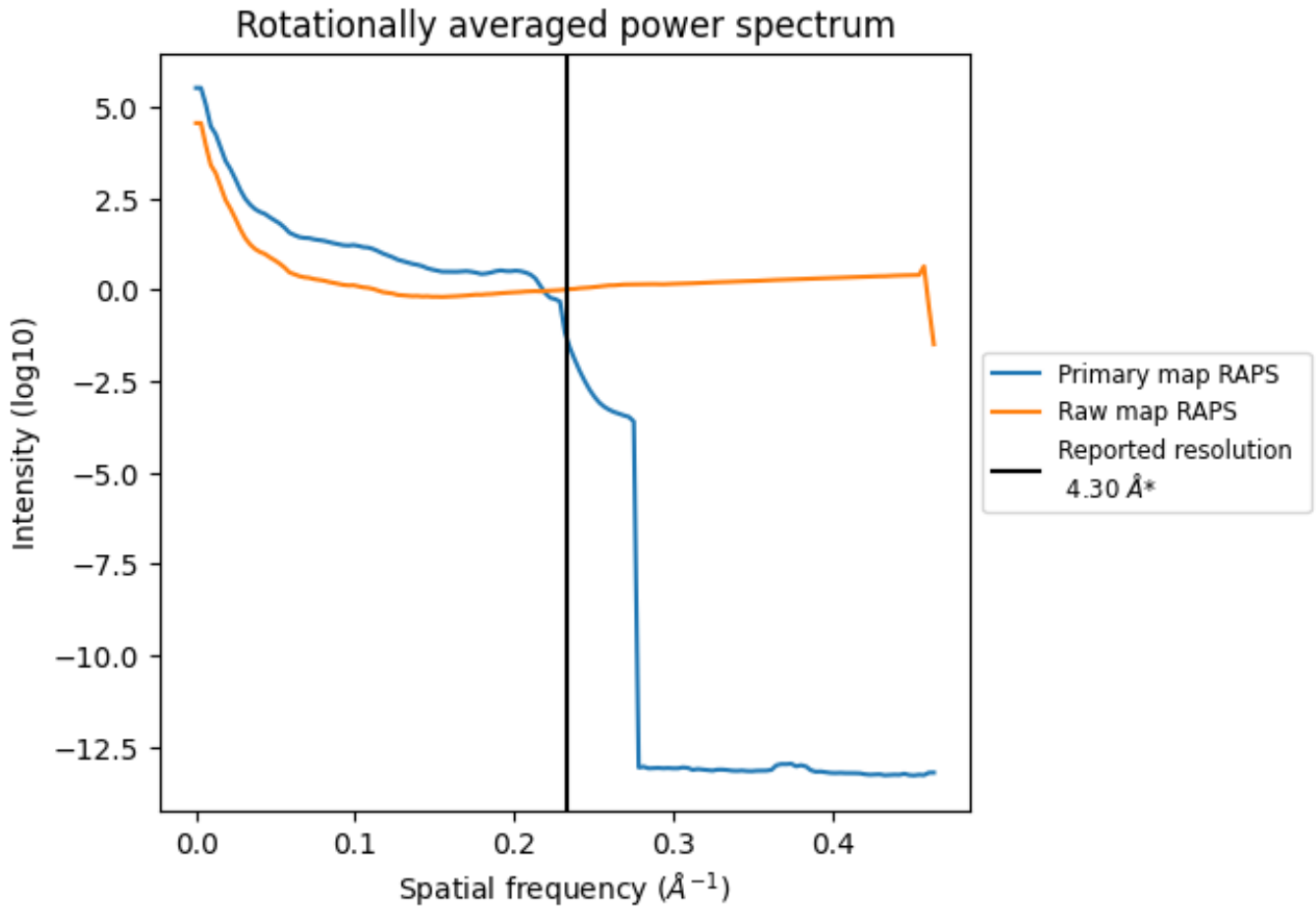
7.2 Volume estimate



The volume at the recommended contour level is 318 nm^3; this corresponds to an approximate mass of 287 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)

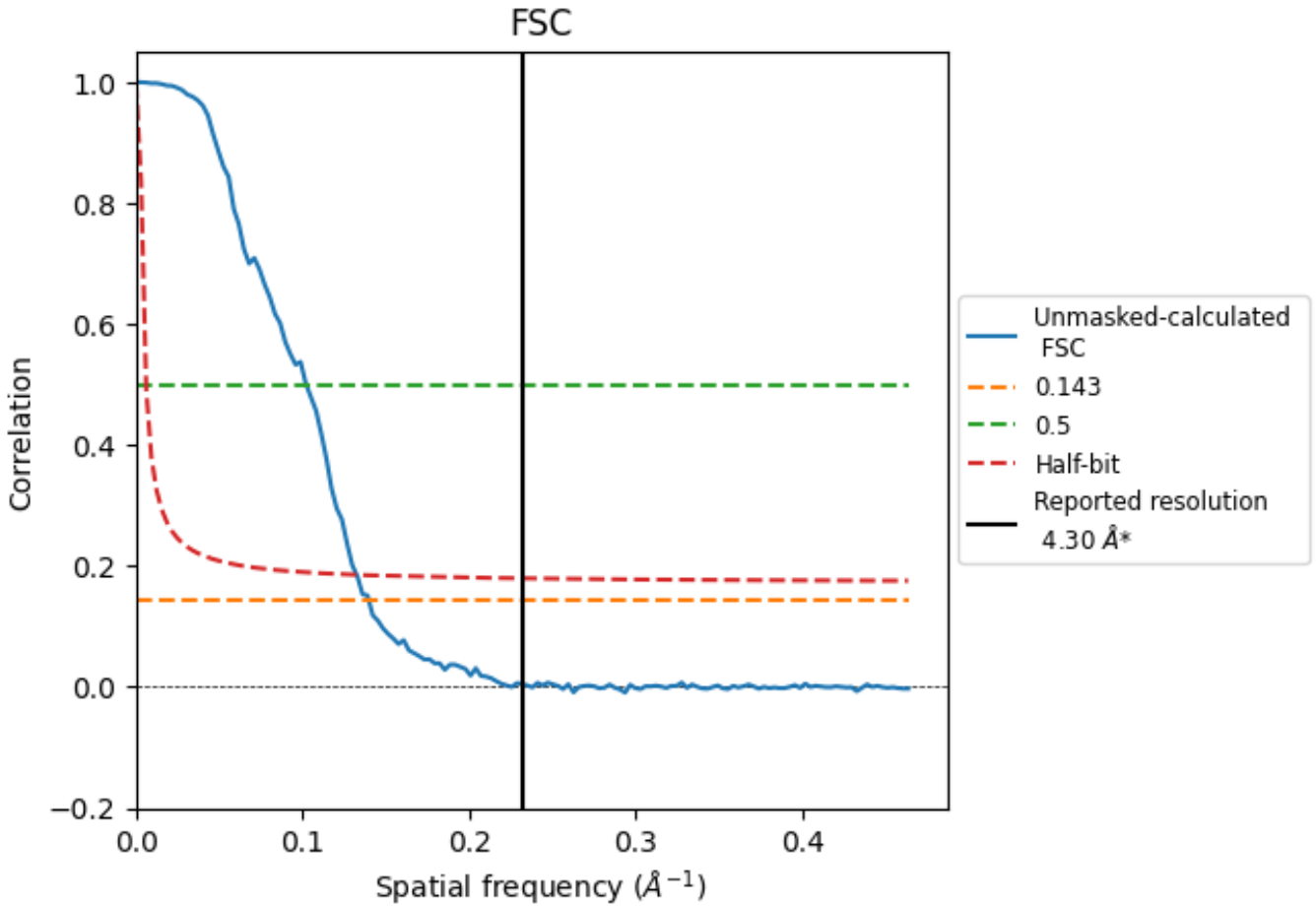


*Reported resolution corresponds to spatial frequency of 0.233 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

8.2 Resolution estimates (i)

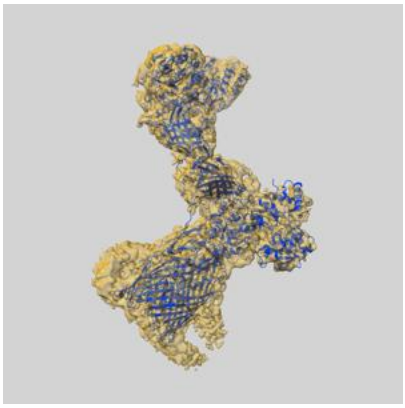
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.15	9.78	7.55

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.15 differs from the reported value 4.3 by more than 10 %

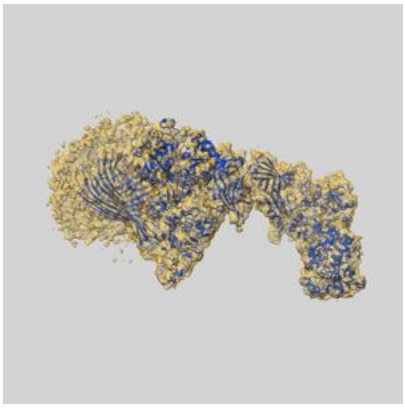
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45682 and PDB model 9CLM. Per-residue inclusion information can be found in section 3 on page 8.

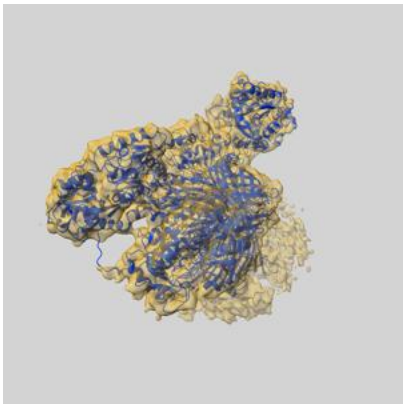
9.1 Map-model overlay



X



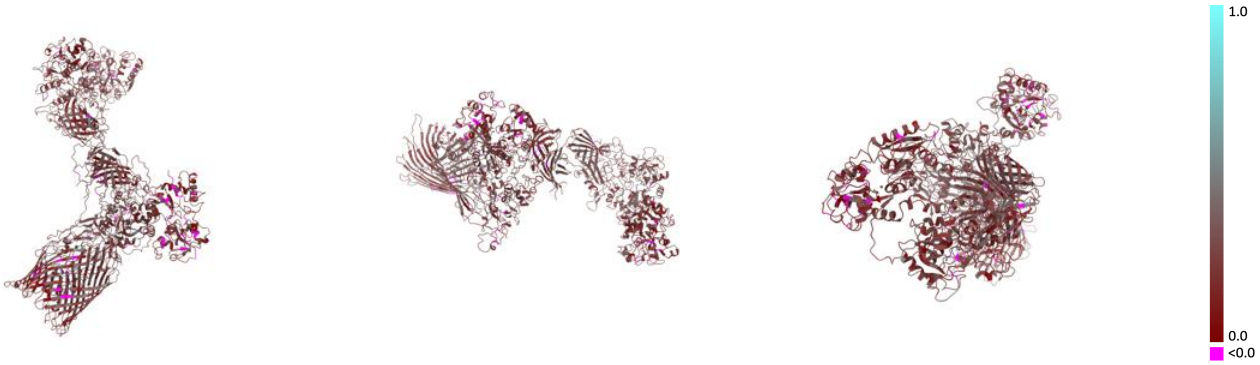
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0888 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.

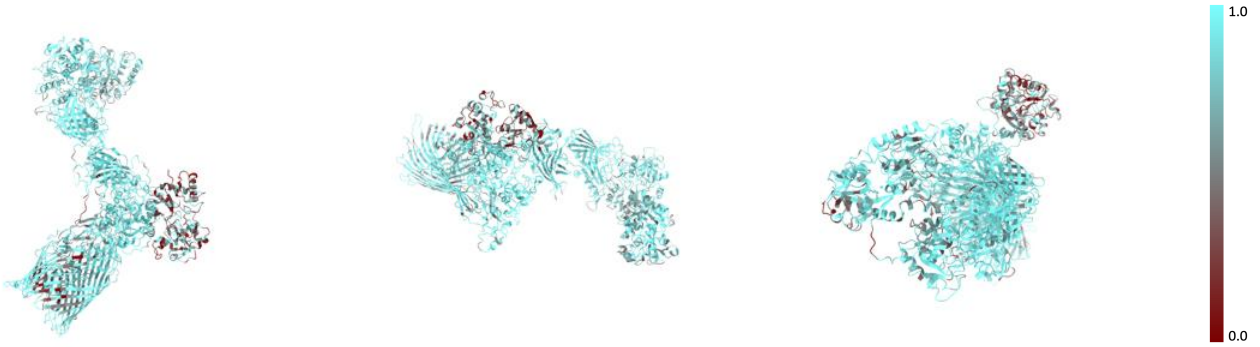
9.2 Q-score mapped to coordinate model (i)



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.

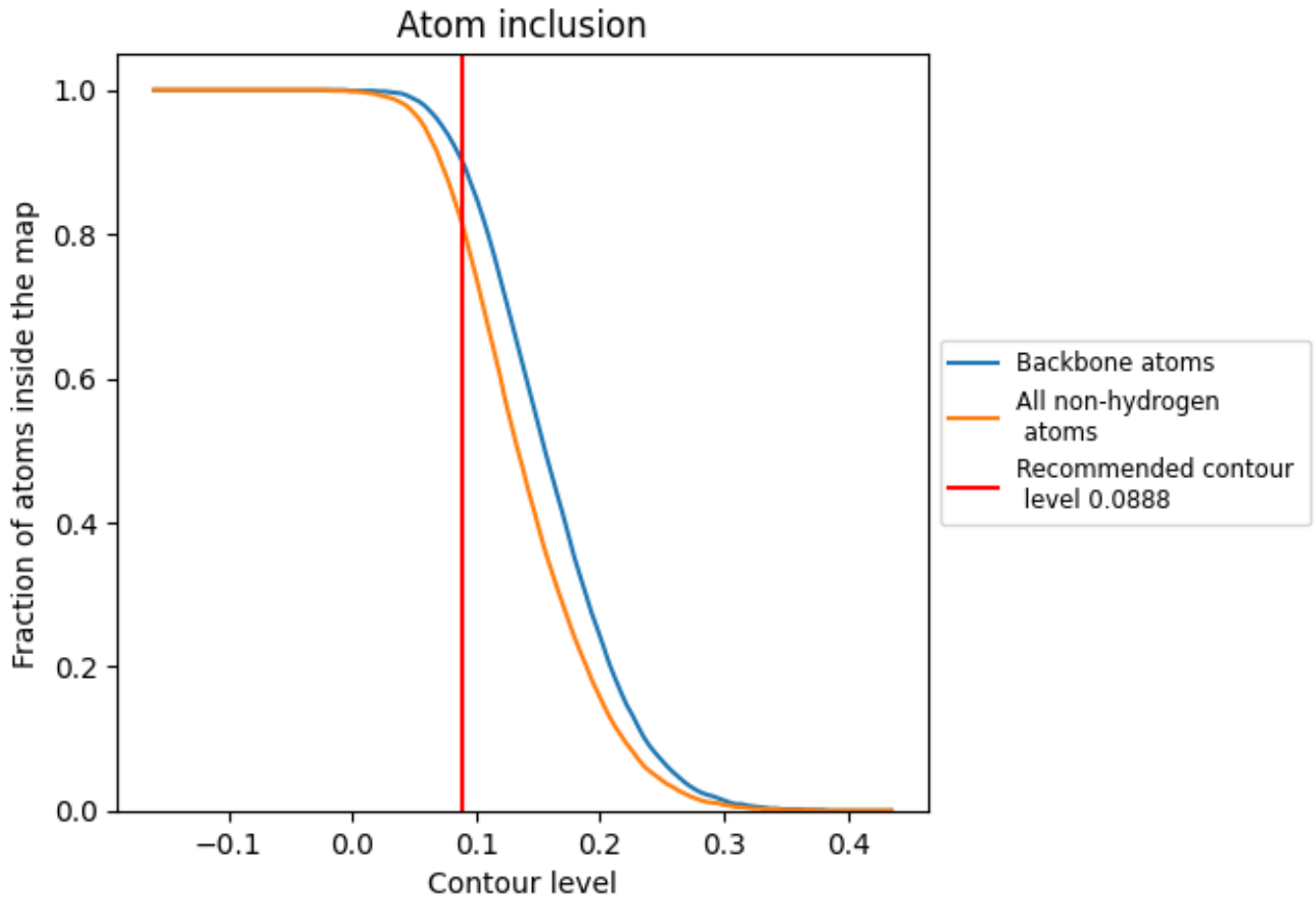
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0888).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.0888) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.2650
A	0.8290	0.2730
B	0.8850	0.2980
F	0.7400	0.2550
G	0.8010	0.2350