Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 10:12 PM EDT

PDB ID	:	9CE0 / pdb_00009ce0
EMDB ID	:	EMD-45489
Title	:	DosP Apo Bent form
Authors	:	Kumar, P.; Kober, D.L.
Deposited on	:	2024-06-25
Resolution	:	3.97 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

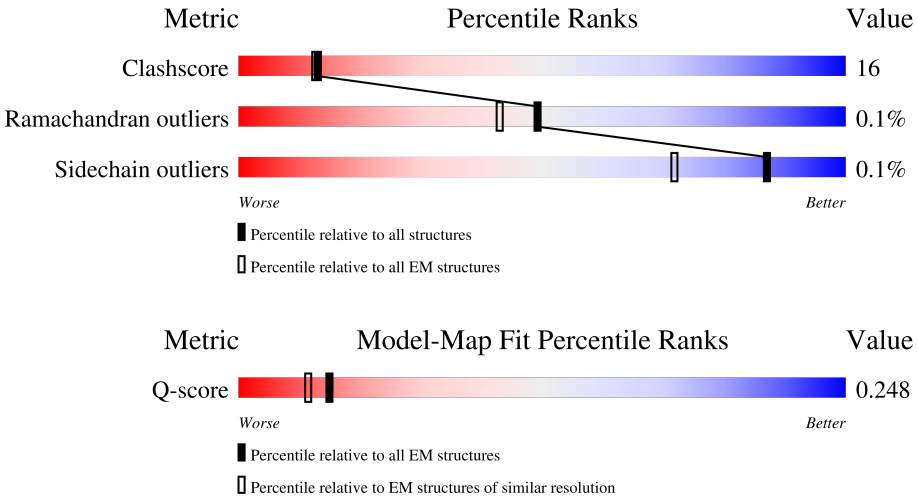
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

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 3.97 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	7578 (3.47 - 4.47)

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	7% 67% 31% .
1	B	806	6% 65% 32% .

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
3	OXY	A	902	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12551 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.

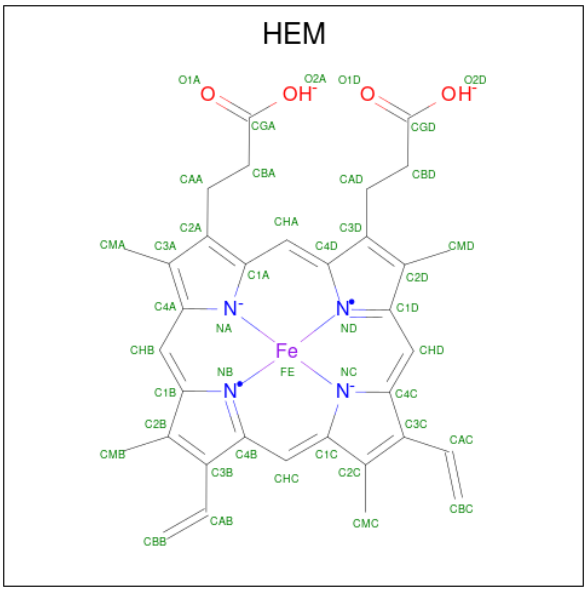
- Molecule 1 is a protein called Oxygen sensor protein DosP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	787	Total	C	N	O	S	0	0
			6257	3961	1095	1168	33		
1	B	781	Total	C	N	O	S	0	0
			6204	3928	1085	1158	33		

There are 20 discrepancies between the modelled and reference sequences:

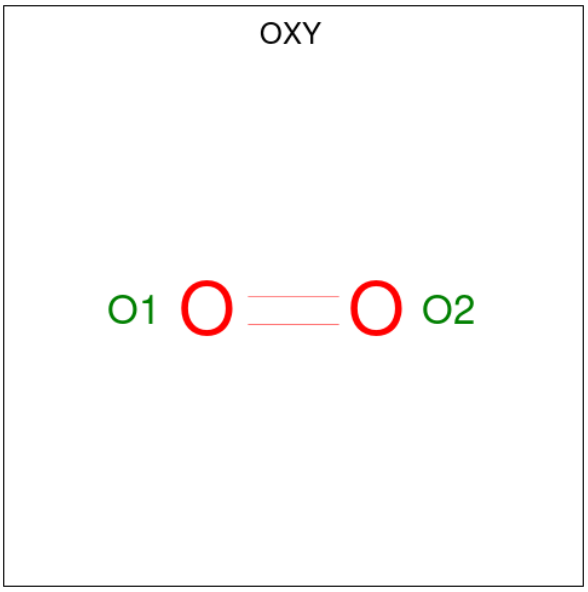
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P76129
A	2	ARG	-	expression tag	UNP P76129
A	3	GLN	-	expression tag	UNP P76129
A	4	ASP	-	expression tag	UNP P76129
A	5	ALA	-	expression tag	UNP P76129
A	6	GLU	-	expression tag	UNP P76129
A	7	VAL	-	expression tag	UNP P76129
A	8	ILE	-	expression tag	UNP P76129
A	16	SER	ASN	conflict	UNP P76129
A	195	THR	ILE	conflict	UNP P76129
B	1	MET	-	expression tag	UNP P76129
B	2	ARG	-	expression tag	UNP P76129
B	3	GLN	-	expression tag	UNP P76129
B	4	ASP	-	expression tag	UNP P76129
B	5	ALA	-	expression tag	UNP P76129
B	6	GLU	-	expression tag	UNP P76129
B	7	VAL	-	expression tag	UNP P76129
B	8	ILE	-	expression tag	UNP P76129
B	16	SER	ASN	conflict	UNP P76129
B	195	THR	ILE	conflict	UNP P76129

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	O	0
			2	2	

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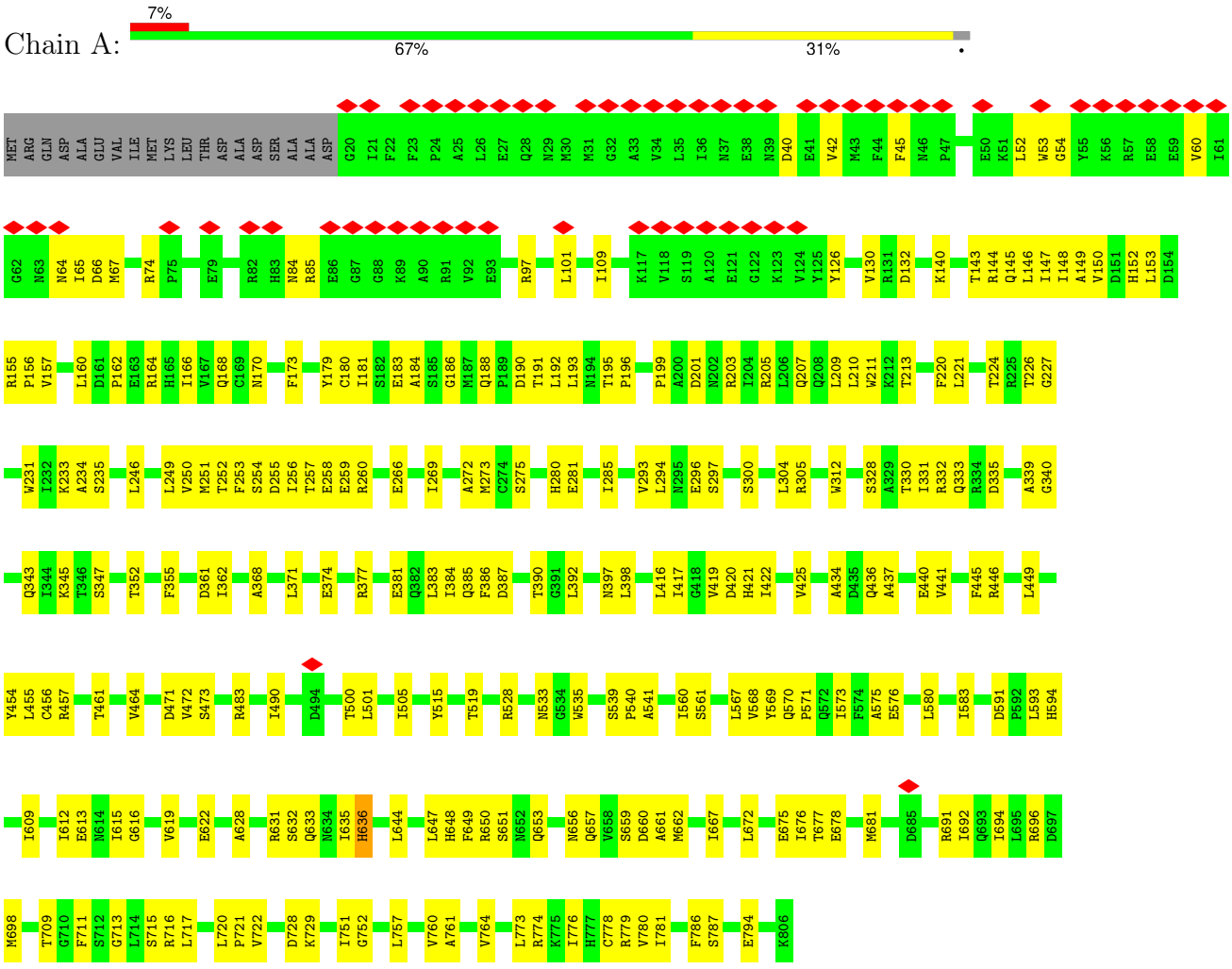
Mol	Chain	Residues	Atoms	AltConf
3	B	1	Total O 2 2	0

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: Oxygen sensor protein DosP

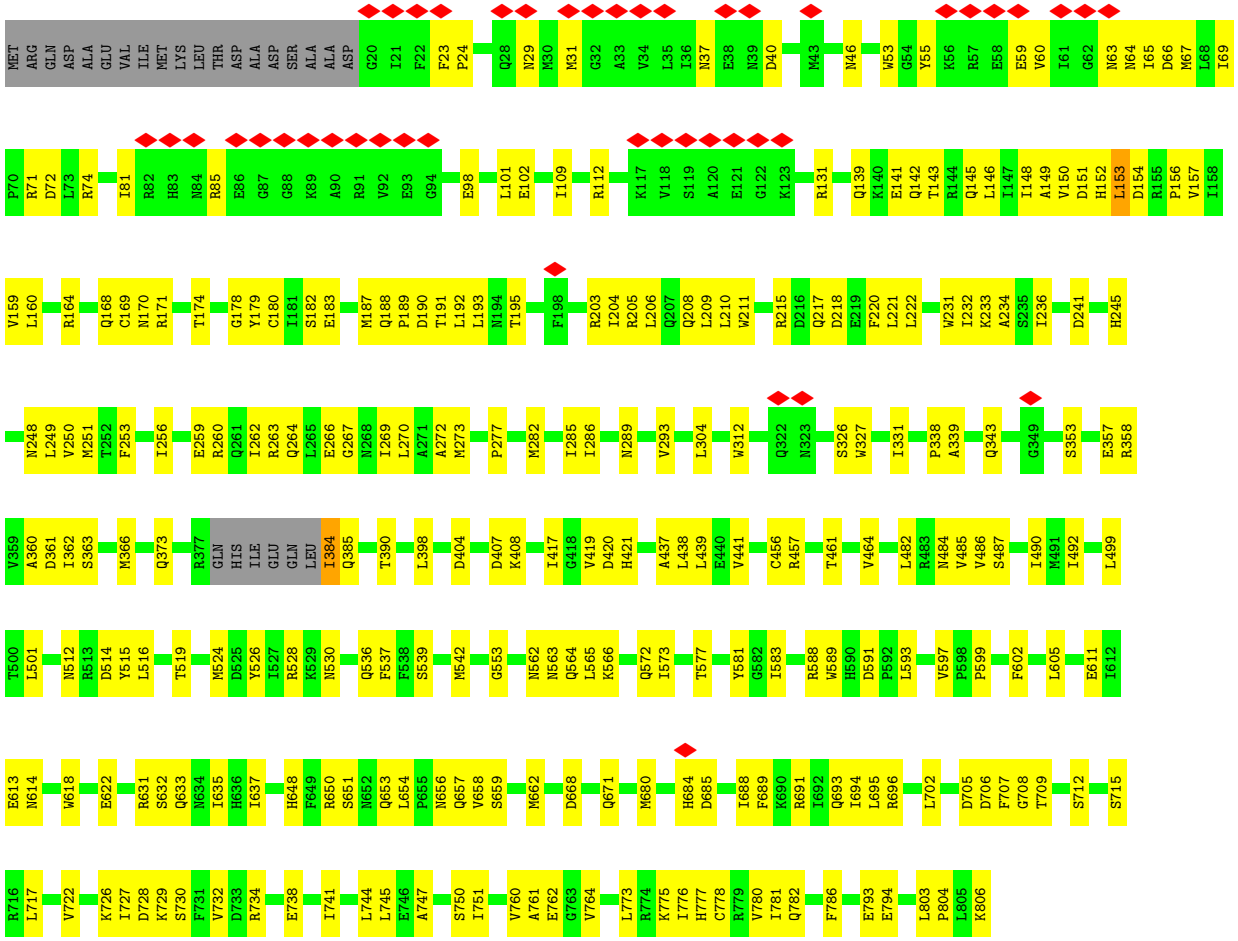
Chain A:



• Molecule 1: Oxygen sensor protein DosP

Chain B:




MET ARG GLN ASP ALA GLU VAL ILE MET LYS LEU THR ASP ALA ASP SER ALA ALA ASP G20 I21 F22 F23 P24 Q28 N29 M30 M31 G32 A33 V34 L35 I36 N37 E38 N39 D40 M43 N46 W53 G54 Y55 K56 R57 E58 E59 V60 I61 G62 N63 N64 I65 D66 M67 L68 I69
P70 R71 D72 L73 R74 I81 R82 H83 N84 R85 E86 G87 G88 K89 A90 R91 V92 E93 G94 E98 L101 E102 I109 R112 K117 V118 S119 A120 E121 G122 K123 R131 Q139 K140 E141 Q142 T143 R144 Q145 L146 I147 I148 A149 V150 D151 H152 L153 D154 R155 P156 V157 I158
V159 L160 R164 Q168 C169 N170 R171 T174 G178 Y179 C180 I181 S182 E183 M187 Q188 P189 D190 T191 L192 L193 N194 T195 F198 R203 I204 R205 L206 Q207 Q208 L209 L210 W211 R215 D216 Q217 D218 E219 F220 L221 L222 W231 I232 K233 A234 S235 I236 D241 H245
N248 L249 V250 M251 T252 F253 I256 E259 R260 Q261 I262 R263 Q264 L265 E266 G267 N268 I269 L270 A271 A272 M273 P277 M282 I285 I286 N289 V293 L304 W312 Q322 N323 S326 W327 I331 P338 A339 Q343 G349 S353 E357 R358
V359 A360 D361 I362 S363 M366 Q373 R377 GLN HIS ILE GLU GLN LEU I384 Q385 T390 L398 D404 D407 K408 I417 G418 V419 D420 H421 A437 L438 L439 E440 V441 C456 R457 T461 V464 L482 R483 N484 V485 V486 S487 I490 M491 I492 L499
T500 L501 N512 R513 D514 Y515 L516 T519 M524 D525 Y526 I527 R528 K529 N530 Q536 F537 F538 S539 M542 G553 N562 N563 Q564 L565 K566 Q572 I573 T577 Y581 G582 I583 R588 W589 H590 D591 P592 L593 V597 P598 P599 F602 L605 E611 I612
E613 N614 W618 E622 R631 S632 Q633 N634 I635 H636 I637 H648 F649 R650 S651 N652 Q653 L654 P655 N656 Q657 V658 S659 M662 D668 Q671 M680 H684 D685 I688 F689 K690 R691 I692 Q693 I694 L695 R696 L702 D705 D706 F707 G708 T709 S712 S715
R716 L717 V722 K726 I727 D728 K729 S730 F731 V732 D733 R734 E738 I741 L744 L745 E746 A747 S750 I751 V760 A761 E762 G763 V764 L773 R774 K775 I776 H777 C778 R779 V780 I781 Q782 F786 E793 E794 L803 P804 L805 K806

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154173	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.985	Depositor
Minimum map value	-0.226	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.123	Depositor
Map size (Å)	413.30002, 413.30002, 413.30002	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6144532, 1.6144532, 1.6144532	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	0/6385	0.41	0/8650
1	B	0.22	0/6330	0.42	0/8574
All	All	0.22	0/12715	0.41	0/17224

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	6257	0	6236	213	0
1	B	6204	0	6184	213	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	2	0	0	2	0
3	B	2	0	0	0	0
All	All	12551	0	12480	410	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 16.

All (410) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:O	1:A:143:THR:OG1	1.93	0.87
1:B:326:SER:OG	1:B:343:GLN:NE2	2.10	0.85
1:B:164:ARG:NE	1:B:210:LEU:O	2.09	0.84
1:B:536:GLN:OE1	1:B:537:PHE:N	2.10	0.84
1:A:422:ILE:HG21	1:A:461:THR:HG21	1.56	0.84
1:A:272:ALA:O	1:A:275:SER:OG	1.96	0.83
1:A:728:ASP:OD1	1:A:729:LYS:N	2.13	0.81
1:B:190:ASP:OD1	1:B:191:THR:N	2.13	0.81
1:A:84:ASN:O	1:A:126:TYR:OH	1.98	0.80
1:B:236:ILE:HD11	1:B:249:LEU:HD23	1.63	0.79
1:B:514:ASP:OD1	1:B:515:TYR:N	2.14	0.79
1:B:160:LEU:HD21	1:B:189:PRO:HG2	1.65	0.78
1:B:71:ARG:NH2	1:B:102:GLU:OE2	2.17	0.78
1:A:764:VAL:HG21	1:A:781:ILE:HG23	1.64	0.78
1:B:632:SER:OG	1:B:633:GLN:OE1	2.00	0.78
1:A:273:MET:HE1	1:B:270:LEU:HD13	1.65	0.77
1:A:613:GLU:OE1	1:A:653:GLN:NE2	2.18	0.75
1:A:201:ASP:OD2	1:A:205:ARG:NE	2.20	0.75
1:B:441:VAL:HG22	1:B:490:ILE:HD13	1.68	0.75
1:B:572:GLN:OE1	1:B:782:GLN:NE2	2.20	0.75
1:B:708:GLY:O	1:B:709:THR:OG1	2.05	0.75
1:B:760:VAL:HG22	1:B:780:VAL:CG2	2.17	0.74
1:A:343:GLN:O	1:A:343:GLN:NE2	2.20	0.74
1:A:419:VAL:O	1:A:528:ARG:NH1	2.21	0.74
1:A:195:THR:OG1	1:A:203:ARG:NH2	2.21	0.73
1:A:255:ASP:OD1	1:A:256:ILE:N	2.21	0.73
1:B:613:GLU:OE2	1:B:613:GLU:N	2.20	0.73
1:B:611:GLU:OE2	1:B:614:ASN:ND2	2.22	0.73
1:A:188:GLN:OE1	1:A:210:LEU:HD21	1.89	0.72
1:A:255:ASP:OD1	1:A:257:THR:N	2.22	0.72
1:B:728:ASP:OD1	1:B:729:LYS:N	2.22	0.72
1:B:180:CYS:SG	1:B:182:SER:OG	2.48	0.72
1:A:233:LYS:HB2	1:A:256:ILE:HD11	1.71	0.72
1:B:730:SER:O	1:B:734:ARG:NH1	2.23	0.72
1:B:151:ASP:O	1:B:171:ARG:NH2	2.23	0.72
1:A:97:ARG:NH1	3:A:902:OXY:O1	2.24	0.71
1:B:67:MET:O	1:B:74:ARG:NH1	2.24	0.70
1:B:153:LEU:HD23	1:B:154:ASP:H	1.57	0.70
1:B:209:LEU:HD12	1:B:220:PHE:CZ	2.26	0.70
1:B:727:ILE:HG21	1:B:745:LEU:HD11	1.73	0.70
1:B:591:ASP:OD2	1:B:593:LEU:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:ILE:HD13	1:B:745:LEU:CD1	2.21	0.69
1:B:262:ILE:HG23	1:B:362:ILE:HG12	1.74	0.69
1:A:471:ASP:OD1	1:A:472:VAL:N	2.26	0.68
1:A:720:LEU:HD12	1:A:720:LEU:O	1.93	0.68
1:B:512:ASN:ND2	1:B:514:ASP:OD1	2.27	0.68
1:A:297:SER:OG	1:A:345:LYS:O	2.08	0.67
1:A:234:ALA:HB1	1:A:251:MET:CE	2.24	0.67
1:A:573:ILE:HD11	1:A:786:PHE:CD2	2.30	0.67
2:B:901:HEM:HBC2	2:B:901:HEM:HHD	1.77	0.67
1:A:387:ASP:OD2	1:A:390:THR:OG1	2.09	0.67
1:A:143:THR:CG2	1:B:143:THR:HG22	2.25	0.66
1:A:252:THR:HG21	1:B:152:HIS:CD2	2.31	0.66
1:A:715:SER:HB3	1:B:744:LEU:HD12	1.77	0.66
1:A:381:GLU:O	1:A:384:ILE:HG22	1.96	0.65
1:A:651:SER:O	1:A:691:ARG:NE	2.28	0.65
1:A:333:GLN:NE2	1:A:335:ASP:O	2.30	0.65
1:B:139:GLN:O	1:B:143:THR:HG23	1.97	0.65
1:A:233:LYS:N	1:A:256:ILE:HD11	2.12	0.64
1:B:188:GLN:OE1	1:B:190:ASP:N	2.28	0.64
1:B:583:ILE:HD13	1:B:637:ILE:HD11	1.79	0.64
1:A:573:ILE:HD11	1:A:786:PHE:CG	2.34	0.63
1:B:182:SER:OG	1:B:183:GLU:OE2	2.16	0.63
1:B:66:ASP:O	1:B:74:ARG:NE	2.31	0.63
1:B:512:ASN:OD1	1:B:514:ASP:N	2.28	0.63
1:A:422:ILE:CG2	1:A:461:THR:HG21	2.29	0.63
1:A:233:LYS:CB	1:A:256:ILE:HD11	2.29	0.63
1:B:456:CYS:SG	1:B:457:ARG:N	2.71	0.63
1:B:573:ILE:HD11	1:B:786:PHE:CE2	2.35	0.62
1:A:794:GLU:OE2	1:A:794:GLU:N	2.32	0.62
1:B:727:ILE:HD13	1:B:745:LEU:HD13	1.81	0.62
1:B:648:HIS:O	1:B:650:ARG:NH2	2.33	0.62
1:A:779:ARG:O	1:A:780:VAL:HG13	2.00	0.62
1:B:248:ASN:C	1:B:249:LEU:HD12	2.24	0.62
1:A:162:PRO:O	1:A:164:ARG:NH2	2.32	0.62
1:A:300:SER:O	1:A:343:GLN:NE2	2.30	0.62
1:B:209:LEU:HD11	1:B:218:ASP:HB2	1.82	0.62
1:B:407:ASP:OD1	1:B:408:LYS:N	2.33	0.62
1:B:712:SER:O	1:B:715:SER:OG	2.17	0.62
1:A:660:ASP:OD1	1:A:661:ALA:N	2.33	0.61
1:B:656:ASN:OD1	1:B:657:GLN:N	2.33	0.61
1:A:711:PHE:N	1:B:706:ASP:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ALA:HB1	1:A:251:MET:HE3	1.82	0.61
1:A:456:CYS:SG	1:A:457:ARG:N	2.74	0.61
1:A:751:ILE:HG23	1:B:751:ILE:CD1	2.31	0.61
1:B:437:ALA:O	1:B:441:VAL:HG23	2.01	0.61
1:B:734:ARG:NH2	1:B:738:GLU:OE2	2.34	0.60
1:B:760:VAL:HG22	1:B:780:VAL:HG21	1.82	0.60
1:A:694:ILE:HG22	1:A:698:MET:HE1	1.82	0.60
1:A:571:PRO:HA	1:A:583:ILE:HG22	1.84	0.60
1:B:526:TYR:O	1:B:530:ASN:ND2	2.35	0.60
1:B:98:GLU:OE2	1:B:112:ARG:NH2	2.33	0.60
1:A:166:ILE:O	1:A:186:GLY:N	2.34	0.59
1:A:280:HIS:ND1	1:A:312:TRP:O	2.34	0.59
1:B:282:MET:HA	1:B:285:ILE:HD12	1.83	0.59
1:A:143:THR:HG21	1:B:143:THR:HG22	1.84	0.59
1:A:146:LEU:HD13	1:B:146:LEU:HB3	1.83	0.59
1:A:515:TYR:CZ	1:A:519:THR:HG21	2.38	0.59
1:A:328:SER:O	1:B:215:ARG:NH1	2.34	0.59
1:B:193:LEU:HD22	1:B:222:LEU:CD2	2.31	0.59
1:B:153:LEU:HD23	1:B:154:ASP:N	2.17	0.59
1:A:199:PRO:O	1:A:203:ARG:NH1	2.35	0.59
1:A:613:GLU:OE1	1:A:657:GLN:NE2	2.36	0.59
1:B:160:LEU:HD21	1:B:189:PRO:CG	2.33	0.59
1:B:234:ALA:HB2	1:B:253:PHE:HE1	1.67	0.59
1:A:52:LEU:O	1:A:54:GLY:N	2.35	0.59
1:B:581:TYR:CD2	1:B:780:VAL:HG11	2.38	0.59
1:B:668:ASP:N	1:B:671:GLN:OE1	2.30	0.59
1:A:266:GLU:OE2	1:A:362:ILE:HG23	2.03	0.59
1:B:515:TYR:CZ	1:B:519:THR:HG21	2.38	0.58
1:A:207:GLN:OE1	1:A:210:LEU:HD23	2.03	0.58
1:A:420:ASP:OD2	1:A:500:THR:OG1	2.18	0.58
1:A:709:THR:O	1:B:709:THR:N	2.31	0.58
1:B:589:TRP:CE3	1:B:597:VAL:HG11	2.39	0.58
1:A:149:ALA:O	1:A:152:HIS:C	2.47	0.58
1:A:146:LEU:HD11	1:B:146:LEU:HD13	1.86	0.57
1:A:148:ILE:HG23	1:B:250:VAL:HG21	1.87	0.57
1:B:680:MET:O	1:B:688:ILE:HD12	2.04	0.57
1:A:221:LEU:HD22	1:A:231:TRP:CD1	2.40	0.57
1:B:539:SER:HB3	1:B:542:MET:HE2	1.87	0.57
1:A:190:ASP:OD2	1:A:207:GLN:NE2	2.37	0.57
1:A:256:ILE:N	1:A:256:ILE:HD12	2.19	0.57
1:B:637:ILE:HG23	1:B:637:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:760:VAL:HA	1:A:780:VAL:HG23	1.87	0.56
1:B:651:SER:O	1:B:691:ARG:NE	2.39	0.56
1:A:421:HIS:O	1:A:425:VAL:HG23	2.05	0.56
1:B:486:VAL:HG11	1:B:501:LEU:HD23	1.87	0.56
1:A:196:PRO:O	1:A:203:ARG:NH2	2.37	0.56
1:A:352:THR:HG23	1:A:355:PHE:H	1.70	0.56
1:A:97:ARG:NE	2:A:901:HEM:O1A	2.38	0.56
1:A:540:PRO:HA	1:A:541:ALA:C	2.31	0.56
1:A:776:ILE:O	1:A:776:ILE:HG22	2.05	0.56
1:B:221:LEU:O	1:B:222:LEU:HD12	2.07	0.55
1:A:644:LEU:HD12	1:A:649:PHE:CG	2.41	0.55
1:B:361:ASP:OD1	1:B:362:ILE:N	2.40	0.55
1:B:597:VAL:HG13	1:B:597:VAL:O	2.05	0.55
2:B:901:HEM:HMB1	2:B:901:HEM:HBB2	1.88	0.55
1:A:235:SER:OG	1:A:252:THR:O	2.15	0.54
1:A:64:ASN:ND2	1:A:66:ASP:OD2	2.40	0.54
1:A:694:ILE:CG2	1:A:698:MET:HE1	2.38	0.54
1:B:512:ASN:O	1:B:516:LEU:HD23	2.07	0.54
1:A:387:ASP:OD2	1:A:390:THR:N	2.38	0.54
1:A:422:ILE:HG21	1:A:461:THR:CG2	2.31	0.54
1:B:717:LEU:HD12	1:B:722:VAL:HG11	1.90	0.54
1:B:577:THR:OG1	1:B:806:LYS:NZ	2.40	0.54
1:A:180:CYS:SG	1:A:181:ILE:N	2.81	0.54
1:B:59:GLU:O	1:B:63:ASN:ND2	2.41	0.53
1:B:331:ILE:O	1:B:339:ALA:N	2.36	0.53
1:A:66:ASP:O	1:A:74:ARG:NE	2.41	0.53
1:A:146:LEU:HD12	1:A:147:ILE:N	2.22	0.53
1:B:441:VAL:HG22	1:B:490:ILE:CD1	2.36	0.53
1:B:241:ASP:OD1	1:B:245:HIS:N	2.35	0.53
1:A:224:THR:OG1	1:A:227:GLY:N	2.42	0.53
2:A:901:HEM:HBB2	2:A:901:HEM:HMB1	1.91	0.53
1:B:266:GLU:O	1:B:267:GLY:C	2.50	0.53
1:B:764:VAL:HG21	1:B:781:ILE:HG23	1.91	0.52
1:B:187:MET:HE1	1:B:192:LEU:HA	1.91	0.52
1:B:747:ALA:O	1:B:750:SER:OG	2.24	0.52
1:A:437:ALA:O	1:A:441:VAL:HG23	2.10	0.52
1:A:656:ASN:OD1	1:A:657:GLN:N	2.41	0.52
1:A:190:ASP:O	1:A:193:LEU:C	2.52	0.52
1:A:576:GLU:OE2	1:A:576:GLU:N	2.38	0.52
1:A:149:ALA:HA	1:B:250:VAL:HG11	1.91	0.52
1:A:417:ILE:HG22	1:A:501:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASP:OD1	1:B:217:GLN:NE2	2.43	0.52
1:B:142:GLN:O	1:B:143:THR:C	2.53	0.52
1:A:293:VAL:HG23	1:A:294:LEU:H	1.74	0.51
1:A:609:ILE:O	1:A:609:ILE:HG22	2.09	0.51
1:A:659:SER:OG	1:A:698:MET:HE3	2.10	0.51
1:A:505:ILE:HD12	1:A:535:TRP:CZ3	2.45	0.51
1:B:101:LEU:N	1:B:109:ILE:O	2.43	0.51
1:B:204:ILE:O	1:B:208:GLN:OE1	2.27	0.51
1:B:437:ALA:HA	1:B:492:ILE:HD11	1.91	0.51
1:B:482:LEU:O	1:B:485:VAL:HG12	2.11	0.51
1:B:565:LEU:HD22	1:B:588:ARG:O	2.11	0.51
1:A:648:HIS:O	1:A:650:ARG:NE	2.40	0.51
1:B:174:THR:O	1:B:178:GLY:N	2.40	0.51
1:B:289:ASN:O	1:B:293:VAL:HG23	2.11	0.51
1:B:484:ASN:O	1:B:487:SER:OG	2.28	0.51
1:A:384:ILE:O	1:A:384:ILE:HG23	2.11	0.50
1:A:591:ASP:OD1	1:A:593:LEU:N	2.39	0.50
1:A:471:ASP:OD1	1:A:473:SER:N	2.39	0.50
1:A:385:GLN:O	1:A:386:PHE:CG	2.64	0.50
1:A:296:GLU:OE2	1:A:347:SER:OG	2.27	0.50
1:A:397:ASN:OD1	1:A:454:TYR:OH	2.27	0.50
1:A:751:ILE:HG23	1:B:751:ILE:HD11	1.91	0.50
1:B:685:ASP:OD1	1:B:685:ASP:C	2.55	0.50
1:A:184:ALA:HA	1:A:192:LEU:HD13	1.94	0.50
1:A:720:LEU:O	1:A:721:PRO:C	2.55	0.50
1:B:31:MET:SD	1:B:131:ARG:NH2	2.85	0.50
1:B:633:GLN:OE1	1:B:633:GLN:N	2.45	0.50
1:B:708:GLY:C	1:B:709:THR:HG1	2.16	0.50
2:A:901:HEM:CHD	2:A:901:HEM:HBC2	2.42	0.50
1:B:269:ILE:HG21	1:B:366:MET:SD	2.51	0.50
2:B:901:HEM:HBC2	2:B:901:HEM:CHD	2.41	0.49
1:A:145:GLN:HB3	1:B:159:VAL:HG21	1.94	0.49
1:A:220:PHE:C	1:A:221:LEU:HD23	2.37	0.49
1:A:416:LEU:CD1	1:A:464:VAL:HG22	2.42	0.49
1:B:286:ILE:O	1:B:289:ASN:OD1	2.29	0.49
1:A:160:LEU:HD23	1:A:166:ILE:HA	1.94	0.49
1:A:179:TYR:CE2	1:A:193:LEU:HD23	2.47	0.49
1:A:540:PRO:HA	1:A:541:ALA:HB3	1.93	0.49
1:B:206:LEU:O	1:B:210:LEU:HD23	2.13	0.49
1:A:761:ALA:HB2	1:A:778:CYS:SG	2.53	0.49
1:A:97:ARG:NH1	3:A:902:OXY:O2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:SER:OG	1:A:633:GLN:NE2	2.43	0.49
1:B:29:ASN:O	1:B:46:ASN:ND2	2.45	0.49
1:A:644:LEU:HD12	1:A:649:PHE:CD2	2.49	0.48
1:A:64:ASN:OD1	1:A:65:ILE:N	2.45	0.48
1:A:483:ARG:NH1	1:A:533:ASN:O	2.41	0.48
1:B:187:MET:SD	1:B:191:THR:OG1	2.69	0.48
1:B:263:ARG:O	1:B:264:GLN:C	2.55	0.48
2:B:901:HEM:HBB2	2:B:901:HEM:CMB	2.44	0.48
1:A:711:PHE:CE1	1:B:705:ASP:O	2.66	0.48
1:B:23:PHE:HB3	1:B:24:PRO:HD3	1.95	0.48
1:B:193:LEU:HD22	1:B:222:LEU:HD21	1.94	0.48
1:B:654:LEU:O	1:B:658:VAL:HG22	2.13	0.48
1:A:156:PRO:HD2	1:A:254:SER:HA	1.96	0.48
1:B:726:LYS:NZ	1:B:760:VAL:HG11	2.29	0.48
2:B:901:HEM:HBD2	2:B:901:HEM:HHA	1.96	0.48
1:B:691:ARG:O	1:B:694:ILE:HG22	2.14	0.48
1:B:384:ILE:O	1:B:385:GLN:HB2	2.14	0.48
1:A:667:ILE:HG21	1:A:672:LEU:HD23	1.95	0.48
1:A:226:THR:HG22	1:A:226:THR:O	2.13	0.47
1:B:195:THR:OG1	1:B:203:ARG:NE	2.47	0.47
1:B:353:SER:OG	1:B:357:GLU:OE2	2.32	0.47
1:A:157:VAL:HG21	1:B:149:ALA:HB1	1.97	0.47
1:A:339:ALA:HB1	1:A:371:LEU:HD22	1.95	0.47
1:A:449:LEU:HD11	1:A:455:LEU:HD22	1.96	0.47
2:A:901:HEM:HBB2	2:A:901:HEM:CMB	2.45	0.47
1:B:205:ARG:HA	1:B:208:GLN:OE1	2.15	0.47
1:A:209:LEU:HD23	1:A:251:MET:HE1	1.95	0.47
1:A:568:VAL:HG12	1:A:569:TYR:N	2.29	0.47
1:A:67:MET:O	1:A:74:ARG:NH1	2.45	0.47
1:A:305:ARG:NH1	1:A:374:GLU:OE2	2.47	0.47
1:B:358:ARG:O	1:B:361:ASP:OD1	2.32	0.47
1:B:362:ILE:HG23	1:B:363:SER:N	2.30	0.47
1:B:461:THR:O	1:B:461:THR:HG22	2.15	0.47
1:B:564:GLN:O	1:B:566:LYS:NZ	2.48	0.47
1:B:262:ILE:HG23	1:B:362:ILE:CG1	2.44	0.46
1:A:570:GLN:NE2	1:A:787:SER:O	2.40	0.46
1:B:273:MET:O	1:B:373:GLN:NE2	2.45	0.46
1:A:612:ILE:HD11	1:A:647:LEU:O	2.16	0.46
1:B:689:PHE:O	1:B:693:GLN:OE1	2.34	0.46
1:A:681:MET:HG3	1:A:716:ARG:HE	1.81	0.46
1:A:153:LEU:HD11	1:B:153:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PHE:HZ	1:A:193:LEU:HD21	1.81	0.46
1:B:174:THR:HA	1:B:179:TYR:O	2.16	0.46
1:B:231:TRP:CD1	1:B:260:ARG:HD3	2.50	0.46
1:A:143:THR:HG22	1:B:143:THR:HG22	1.97	0.46
1:A:255:ASP:OD2	1:A:259:GLU:N	2.48	0.46
1:B:741:ILE:O	1:B:745:LEU:HD23	2.16	0.46
1:A:616:GLY:O	1:A:619:VAL:HG12	2.16	0.46
1:B:417:ILE:HG23	1:B:501:LEU:CD1	2.45	0.46
1:B:524:MET:SD	1:B:528:ARG:NH1	2.89	0.46
1:A:293:VAL:HG23	1:A:294:LEU:N	2.30	0.46
1:A:593:LEU:C	1:A:593:LEU:HD23	2.41	0.46
1:A:716:ARG:HH22	1:A:720:LEU:HD11	1.80	0.46
1:B:775:LYS:O	1:B:777:HIS:ND1	2.49	0.46
1:A:392:LEU:HD23	1:A:446:ARG:NH1	2.31	0.46
2:A:901:HEM:HBD2	2:A:901:HEM:HHA	1.96	0.46
1:B:60:VAL:HG22	1:B:67:MET:HE2	1.97	0.46
1:B:72:ASP:N	1:B:72:ASP:OD1	2.49	0.46
1:A:612:ILE:HA	1:A:615:ILE:HG22	1.97	0.46
1:B:40:ASP:OD1	1:B:81:ILE:HG21	2.15	0.46
1:B:599:PRO:HA	1:B:602:PHE:CE2	2.51	0.46
1:A:60:VAL:HG12	1:A:60:VAL:O	2.15	0.45
1:A:335:ASP:N	1:A:335:ASP:OD1	2.49	0.45
1:A:575:ALA:HB1	1:A:774:ARG:HD2	1.97	0.45
1:B:64:ASN:OD1	1:B:65:ILE:N	2.50	0.45
1:A:257:THR:HG23	1:A:258:GLU:N	2.31	0.45
1:A:713:GLY:O	1:A:717:LEU:HD23	2.17	0.45
1:B:193:LEU:HD22	1:B:222:LEU:HD23	1.97	0.45
1:B:420:ASP:OD1	1:B:421:HIS:N	2.42	0.45
1:B:696:ARG:HD2	1:B:702:LEU:HD23	1.99	0.45
1:B:168:GLN:NE2	1:B:169:CYS:O	2.50	0.45
1:B:360:ALA:O	1:B:363:SER:OG	2.34	0.45
1:B:209:LEU:HD12	1:B:220:PHE:HZ	1.78	0.45
1:A:155:ARG:O	1:A:157:VAL:HG13	2.17	0.45
1:A:539:SER:O	1:A:541:ALA:HB3	2.17	0.45
1:B:142:GLN:O	1:B:145:GLN:HG3	2.17	0.45
1:B:761:ALA:HB2	1:B:778:CYS:SG	2.57	0.45
1:A:779:ARG:O	1:A:780:VAL:CG1	2.66	0.45
1:B:156:PRO:O	1:B:157:VAL:HG13	2.17	0.45
1:B:684:HIS:O	1:B:685:ASP:OD1	2.34	0.45
1:B:773:LEU:HA	1:B:776:ILE:HG12	1.99	0.45
1:A:195:THR:HG1	1:A:203:ARG:NH2	2.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:HG22	1:A:260:ARG:NH2	2.32	0.44
1:B:304:LEU:HD12	1:B:338:PRO:O	2.16	0.44
1:B:419:VAL:CG1	1:B:499:LEU:HD23	2.47	0.44
1:B:637:ILE:O	1:B:637:ILE:CG2	2.65	0.44
1:A:42:VAL:HG11	1:A:45:PHE:CZ	2.52	0.44
1:A:696:ARG:NH1	1:A:721:PRO:O	2.50	0.44
1:B:209:LEU:HD11	1:B:218:ASP:CB	2.47	0.44
1:A:752:GLY:HA2	1:A:757:LEU:HB2	2.00	0.44
1:A:398:LEU:HD21	1:A:464:VAL:HG11	1.99	0.44
1:A:173:PHE:CZ	1:A:193:LEU:HD21	2.52	0.44
1:B:272:ALA:O	1:B:277:PRO:HD3	2.18	0.44
1:A:246:LEU:HD23	1:A:249:LEU:HD11	1.98	0.44
1:B:273:MET:HA	1:B:282:MET:HE1	2.00	0.44
1:A:635:ILE:O	1:A:636:HIS:C	2.60	0.44
1:A:760:VAL:HG22	1:A:780:VAL:HG21	1.99	0.44
1:B:251:MET:HE1	1:B:253:PHE:CE2	2.53	0.44
1:B:256:ILE:HG22	1:B:259:GLU:OE1	2.18	0.44
1:A:168:GLN:HG3	1:B:145:GLN:HG2	2.00	0.43
1:B:732:VAL:HG21	1:B:762:GLU:O	2.18	0.43
1:A:144:ARG:O	1:A:147:ILE:HG22	2.18	0.43
1:A:567:LEU:HD22	1:A:622:GLU:HB3	1.99	0.43
1:A:150:VAL:O	1:A:153:LEU:HB3	2.17	0.43
1:A:593:LEU:HD22	1:A:594:HIS:CE1	2.52	0.43
1:A:675:GLU:O	1:A:676:ILE:HD13	2.19	0.43
1:A:722:VAL:HG23	1:A:757:LEU:HD21	2.00	0.43
1:A:144:ARG:HA	1:A:147:ILE:HG22	2.00	0.43
1:A:304:LEU:HD23	1:A:340:GLY:HA2	1.99	0.43
1:B:366:MET:SD	1:B:366:MET:C	3.02	0.43
1:B:419:VAL:HG12	1:B:499:LEU:HD23	2.01	0.43
1:A:145:GLN:O	1:A:148:ILE:HG22	2.18	0.43
1:A:250:VAL:CG1	1:B:148:ILE:HG22	2.49	0.43
1:A:266:GLU:HA	1:A:269:ILE:HG22	2.01	0.43
1:B:150:VAL:O	1:B:153:LEU:O	2.37	0.43
1:B:565:LEU:CD2	1:B:589:TRP:HB2	2.49	0.43
1:B:618:TRP:CZ2	1:B:622:GLU:HG3	2.53	0.43
1:A:164:ARG:HG3	1:A:211:TRP:CD2	2.54	0.43
1:A:383:LEU:HD11	1:B:439:LEU:HD13	2.00	0.43
1:B:419:VAL:O	1:B:461:THR:HG21	2.17	0.43
1:A:255:ASP:OD2	1:A:258:GLU:N	2.51	0.43
1:B:773:LEU:HD23	1:B:776:ILE:HD11	2.01	0.43
1:A:440:GLU:OE1	1:A:440:GLU:N	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:GLU:C	1:B:141:GLU:CD	2.87	0.43
1:A:101:LEU:N	1:A:109:ILE:O	2.41	0.42
1:A:612:ILE:O	1:A:615:ILE:HG22	2.19	0.42
1:B:659:SER:HA	1:B:662:MET:HG2	2.00	0.42
1:A:331:ILE:HG23	1:A:368:ALA:N	2.34	0.42
1:A:420:ASP:OD1	1:A:528:ARG:NE	2.52	0.42
1:A:422:ILE:HD11	1:A:434:ALA:HB1	2.00	0.42
1:B:260:ARG:O	1:B:264:GLN:HG2	2.18	0.42
1:B:398:LEU:HD11	1:B:464:VAL:HG11	2.02	0.42
1:A:157:VAL:HA	1:A:252:THR:HG22	2.00	0.42
1:A:676:ILE:HG21	1:A:681:MET:HE2	2.00	0.42
1:A:132:ASP:OD1	1:A:132:ASP:N	2.51	0.42
1:A:330:THR:HG21	1:A:332:ARG:CZ	2.49	0.42
1:B:55:TYR:HB3	1:B:60:VAL:HG23	2.02	0.42
1:A:188:GLN:HB3	1:A:191:THR:HG23	2.01	0.42
1:A:662:MET:HA	1:A:667:ILE:HD13	2.02	0.42
1:A:778:CYS:O	1:A:779:ARG:HB3	2.19	0.42
1:B:390:THR:HA	1:B:439:LEU:HD21	2.02	0.42
1:A:694:ILE:HG22	1:A:698:MET:CE	2.49	0.42
1:A:715:SER:CB	1:B:744:LEU:HD12	2.48	0.42
1:B:562:ASN:OD1	1:B:562:ASN:C	2.62	0.42
1:B:803:LEU:HB3	1:B:804:PRO:HD3	2.01	0.42
1:A:471:ASP:OD1	1:A:471:ASP:C	2.63	0.42
1:B:312:TRP:CD1	1:B:312:TRP:C	2.97	0.42
1:A:195:THR:HG1	1:A:203:ARG:HH21	1.68	0.42
1:A:252:THR:OG1	1:B:152:HIS:NE2	2.51	0.42
1:A:436:GLN:O	1:A:440:GLU:OE1	2.38	0.42
1:B:208:GLN:O	1:B:211:TRP:N	2.40	0.42
1:B:744:LEU:C	1:B:744:LEU:HD23	2.45	0.42
2:B:901:HEM:HHA	2:B:901:HEM:HBA2	2.01	0.42
1:A:383:LEU:HD11	1:B:439:LEU:CD1	2.50	0.42
1:A:628:ALA:HA	1:A:631:ARG:HG2	2.02	0.42
1:A:183:GLU:O	1:A:192:LEU:HD13	2.20	0.41
1:A:312:TRP:CD1	1:A:312:TRP:C	2.98	0.41
1:B:157:VAL:HG22	1:B:170:ASN:ND2	2.35	0.41
1:A:213:THR:HG22	1:A:246:LEU:HD21	2.02	0.41
1:A:580:LEU:HD23	1:A:580:LEU:C	2.45	0.41
1:A:773:LEU:HD23	1:A:781:ILE:CD1	2.50	0.41
1:B:553:GLY:HA2	1:B:605:LEU:HD21	2.02	0.41
1:B:793:GLU:O	1:B:794:GLU:HG2	2.20	0.41
1:A:220:PHE:CE1	1:A:234:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ALA:HB1	1:A:285:ILE:HD13	2.03	0.41
1:A:681:MET:SD	1:A:692:ILE:HD13	2.60	0.41
1:B:180:CYS:N	1:B:183:GLU:OE1	2.53	0.41
1:B:602:PHE:CD1	1:B:602:PHE:C	2.98	0.41
1:A:437:ALA:HB1	1:A:490:ILE:HD13	2.02	0.41
1:A:560:ILE:HG13	1:A:561:SER:N	2.36	0.41
1:B:327:TRP:O	1:B:343:GLN:NE2	2.53	0.41
1:B:658:VAL:HG23	1:B:659:SER:N	2.36	0.41
1:A:445:PHE:O	1:A:449:LEU:HD13	2.20	0.41
1:A:760:VAL:HA	1:A:780:VAL:CG2	2.50	0.41
1:B:65:ILE:O	1:B:69:ILE:HG12	2.21	0.41
1:B:233:LYS:HB2	1:B:256:ILE:HG21	2.02	0.41
1:B:259:GLU:O	1:B:263:ARG:HG2	2.21	0.41
1:B:631:ARG:HG3	1:B:635:ILE:HG22	2.03	0.41
1:A:190:ASP:OD1	1:A:191:THR:N	2.53	0.41
1:A:417:ILE:CG2	1:A:501:LEU:HD22	2.50	0.41
1:B:142:GLN:O	1:B:145:GLN:N	2.53	0.41
1:B:707:PHE:CD2	1:B:707:PHE:O	2.74	0.41
1:A:40:ASP:OD1	1:A:85:ARG:NH1	2.44	0.41
1:B:581:TYR:CG	1:B:780:VAL:HG11	2.55	0.41
1:B:651:SER:HA	1:B:688:ILE:HG22	2.02	0.41
1:B:37:ASN:O	1:B:85:ARG:NH1	2.53	0.41
1:B:234:ALA:HB2	1:B:253:PHE:CE1	2.52	0.41
1:A:150:VAL:HG12	1:A:170:ASN:HB2	2.03	0.41
1:A:677:THR:O	1:A:678:GLU:HB3	2.21	0.41
1:B:653:GLN:O	1:B:657:GLN:HG2	2.21	0.41
1:B:658:VAL:HG21	1:B:695:LEU:HD13	2.02	0.41
1:B:53:TRP:CE2	1:B:101:LEU:HD11	2.55	0.41
1:B:64:ASN:ND2	1:B:66:ASP:OD2	2.53	0.41
1:B:404:ASP:O	1:B:407:ASP:OD1	2.39	0.41
1:B:438:LEU:HD13	1:B:457:ARG:NH1	2.36	0.40
1:B:562:ASN:O	1:B:563:ASN:OD1	2.39	0.40
1:A:233:LYS:O	1:A:253:PHE:HB3	2.22	0.40
1:A:281:GLU:OE2	1:A:285:ILE:HD12	2.21	0.40
1:A:332:ARG:O	1:A:368:ALA:HB1	2.22	0.40
1:A:52:LEU:HD13	1:A:130:VAL:HB	2.04	0.40
1:A:374:GLU:O	1:A:377:ARG:HG2	2.21	0.40
1:B:514:ASP:OD1	1:B:514:ASP:C	2.63	0.40
1:B:729:LYS:O	1:B:730:SER:C	2.64	0.40
1:B:208:GLN:HG2	1:B:209:LEU:N	2.37	0.40
1:B:222:LEU:HD13	1:B:232:ILE:HD11	2.02	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	785/806 (97%)	730 (93%)	53 (7%)	2 (0%)	36 70
1	B	777/806 (96%)	732 (94%)	45 (6%)	0	100 100
All	All	1562/1612 (97%)	1462 (94%)	98 (6%)	2 (0%)	49 80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	TRP
1	A	636	HIS

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	683/698 (98%)	683 (100%)	0	100 100
1	B	677/698 (97%)	675 (100%)	2 (0%)	86 85
All	All	1360/1396 (97%)	1358 (100%)	2 (0%)	87 89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	153	LEU

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Mol	Chain	Res	Type
1	B	384	ILE

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

Mol	Chain	Res	Type
1	A	39	ASN
1	A	268	ASN
1	A	289	ASN
1	A	343	GLN
1	A	462	GLN
1	A	562	ASN
1	A	563	ASN
1	A	648	HIS
1	A	663	HIS
1	A	670	HIS
1	A	684	HIS
1	B	139	GLN
1	B	194	ASN
1	B	247	GLN
1	B	343	GLN
1	B	653	GLN
1	B	693	GLN

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

4 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	HEM	B	901	3,1	50,50,50	1.41	9 (18%)	67,82,82	1.11	4 (5%)
2	HEM	A	901	3	50,50,50	1.49	10 (20%)	67,82,82	1.14	5 (7%)
3	OXY	A	902	2	1,1,1	0.17	0	-		
3	OXY	B	902	2	1,1,1	0.17	0	-		

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	HEM	B	901	3,1	-	2/14/54/54	-
2	HEM	A	901	3	-	6/14/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	FE-NC	4.11	2.08	1.95
2	A	901	HEM	FE-NA	3.72	2.07	1.95
2	A	901	HEM	FE-ND	3.35	2.05	1.94
2	B	901	HEM	FE-NB	3.21	2.04	1.94
2	A	901	HEM	FE-NB	3.17	2.04	1.94
2	B	901	HEM	FE-NA	3.14	2.05	1.95
2	B	901	HEM	FE-NC	3.12	2.05	1.95
2	B	901	HEM	FE-ND	3.08	2.04	1.94
2	B	901	HEM	CAB-C3B	2.96	1.55	1.47
2	B	901	HEM	CAC-C3C	2.95	1.55	1.47
2	A	901	HEM	CAC-C3C	2.93	1.55	1.47
2	A	901	HEM	CAB-C3B	2.90	1.55	1.47
2	B	901	HEM	CMB-C2B	2.09	1.55	1.50
2	B	901	HEM	CMD-C2D	2.07	1.55	1.50
2	A	901	HEM	CMB-C2B	2.04	1.55	1.50
2	A	901	HEM	CMA-C3A	2.04	1.54	1.50
2	A	901	HEM	CMC-C2C	2.03	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	CMD-C2D	2.03	1.54	1.50
2	B	901	HEM	CMC-C2C	2.01	1.54	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	HEM	C4D-ND-C1D	2.53	108.20	105.21
2	B	901	HEM	C4D-ND-C1D	2.49	108.15	105.21
2	B	901	HEM	C1B-NB-C4B	2.36	108.00	105.21
2	A	901	HEM	C1B-NB-C4B	2.34	107.98	105.21
2	A	901	HEM	C3D-C4D-ND	-2.23	107.73	110.17
2	B	901	HEM	C3B-C2B-C1B	2.15	108.02	106.41
2	A	901	HEM	C3B-C2B-C1B	2.09	107.98	106.41
2	A	901	HEM	C2A-C1A-NA	-2.05	107.88	110.15
2	B	901	HEM	C3D-C4D-ND	-2.03	107.95	110.17

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	HEM	C2A-CAA-CBA-CGA
2	A	901	HEM	C4D-C3D-CAD-CBD
2	A	901	HEM	C2D-C3D-CAD-CBD
2	B	901	HEM	C4C-C3C-CAC-CBC
2	A	901	HEM	C4C-C3C-CAC-CBC
2	A	901	HEM	CAA-CBA-CGA-O1A
2	A	901	HEM	CAA-CBA-CGA-O2A
2	B	901	HEM	C4D-C3D-CAD-CBD

There are no ring outliers.

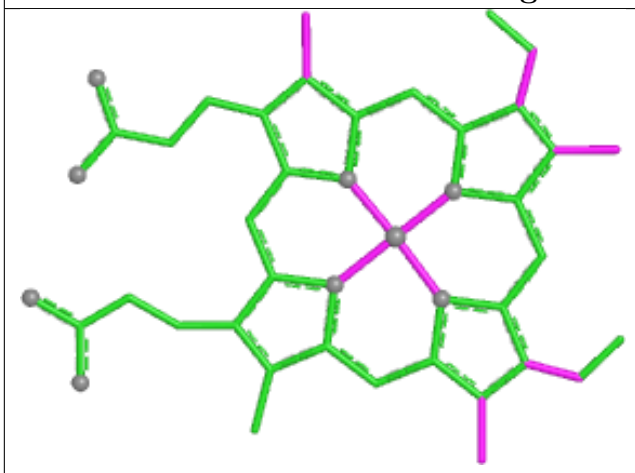
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	HEM	6	0
2	A	901	HEM	5	0
3	A	902	OXY	2	0

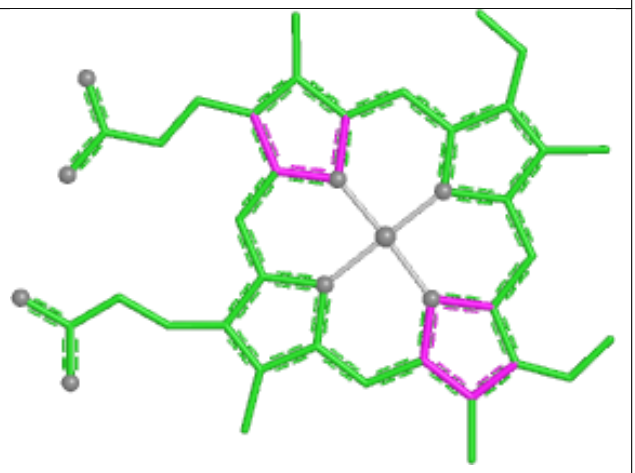
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

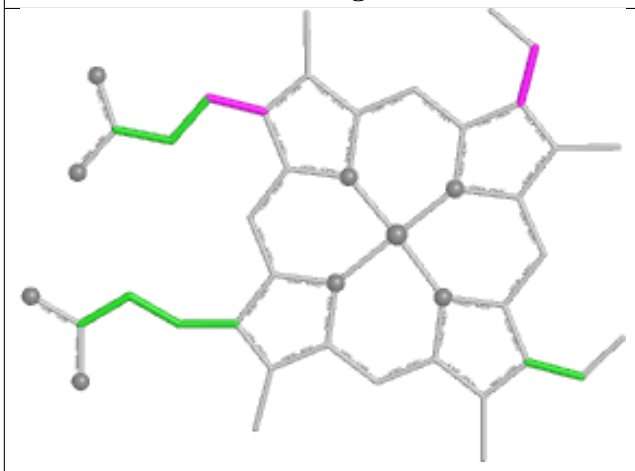
Ligand HEM B 901



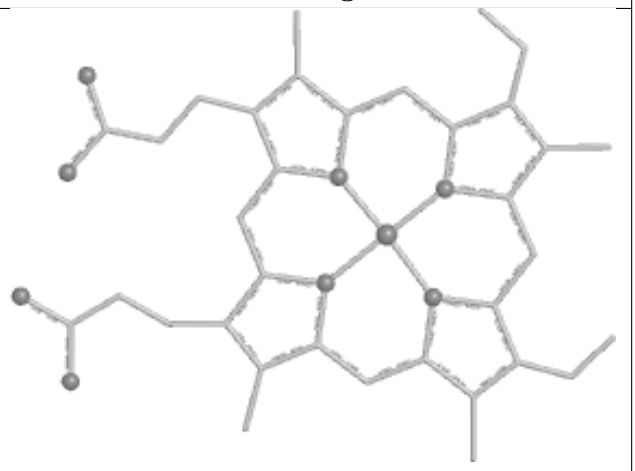
Bond lengths



Bond angles

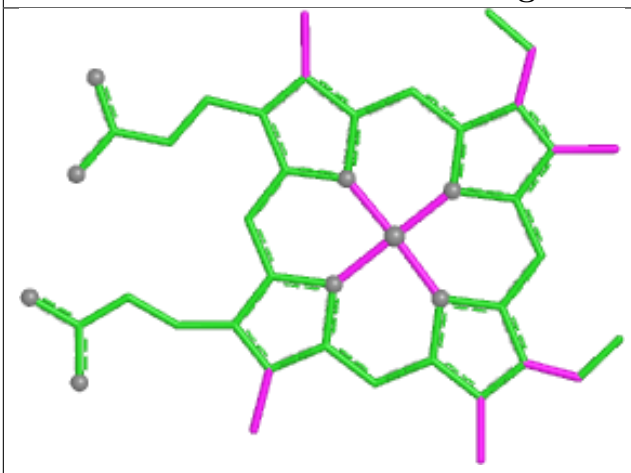


Torsions

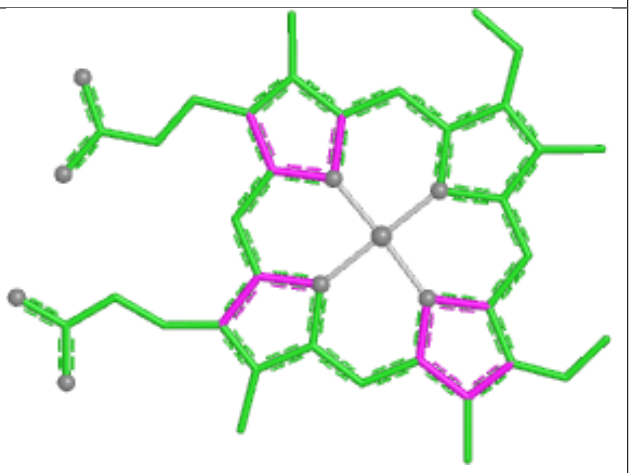


Rings

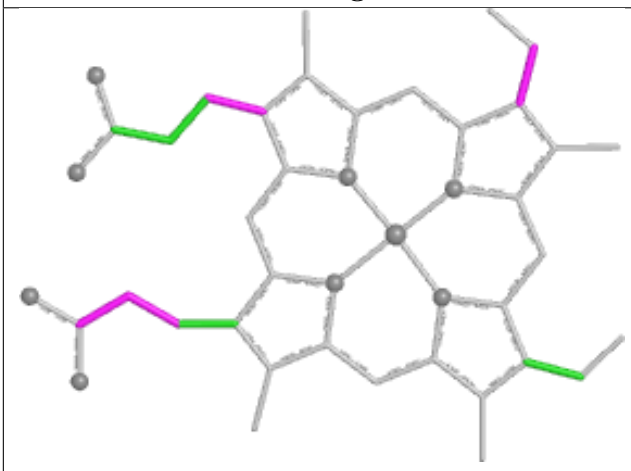
Ligand HEM A 901



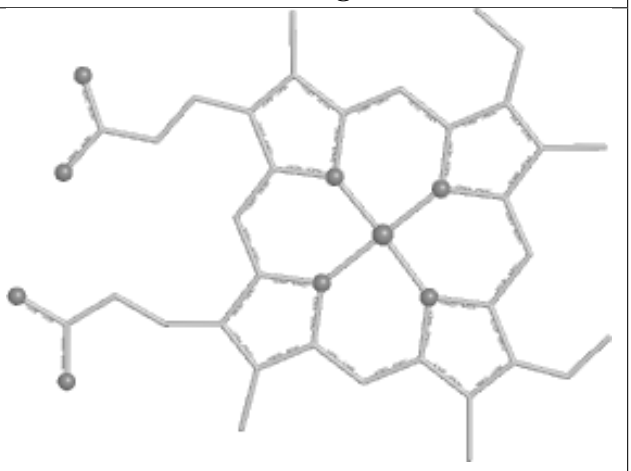
Bond lengths



Bond angles

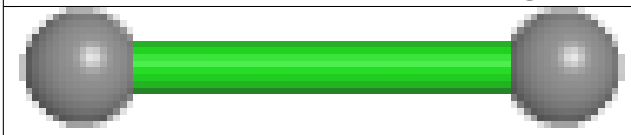


Torsions



Rings

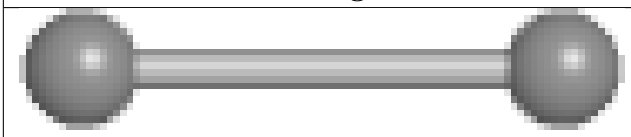
Ligand OXY A 902



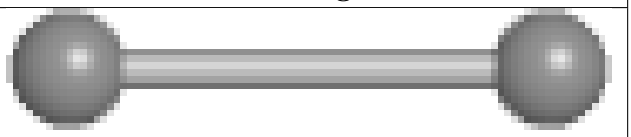
Bond lengths



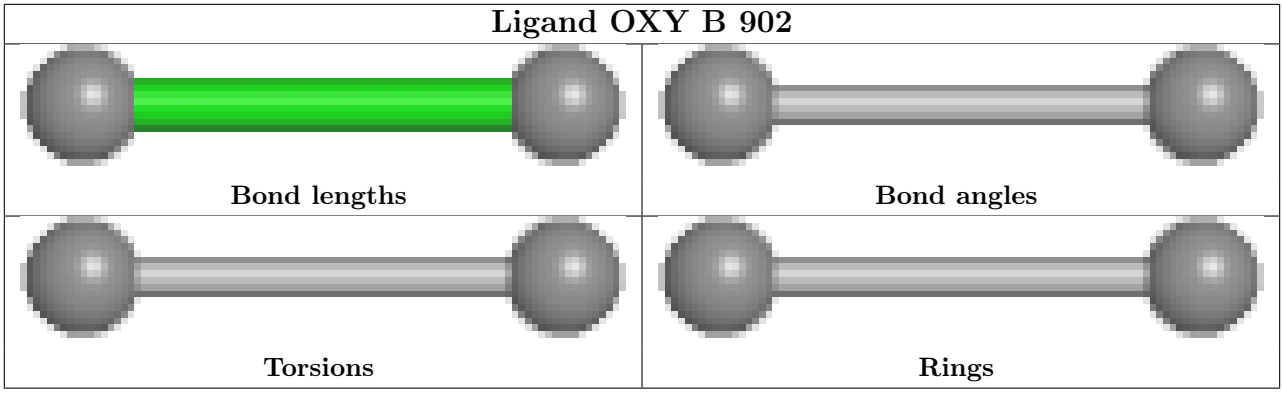
Bond angles



Torsions



Rings



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.

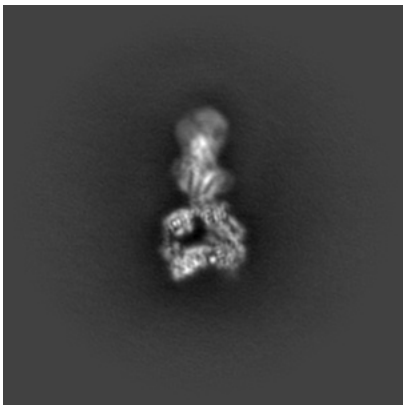
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45489. These allow visual inspection of the internal detail of the map and identification of artifacts.

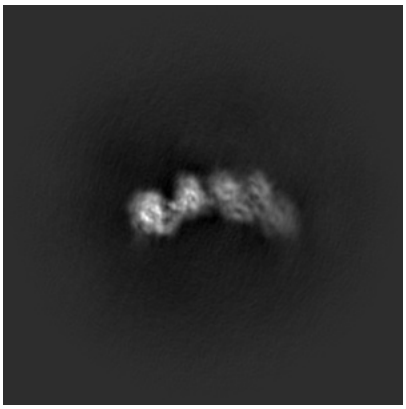
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

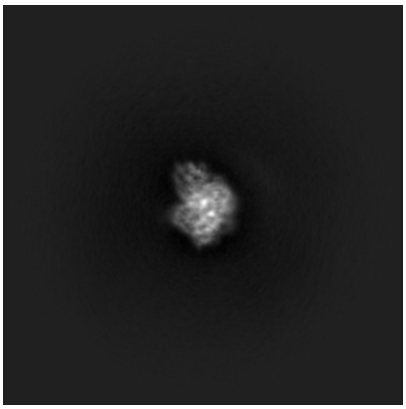
6.1.1 Primary map



X

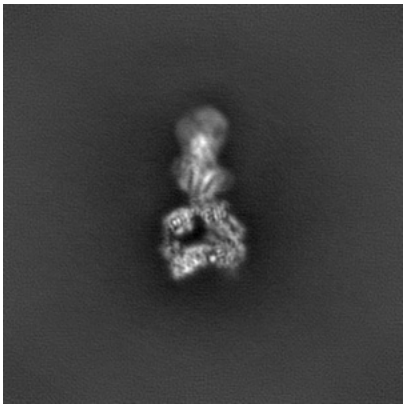


Y

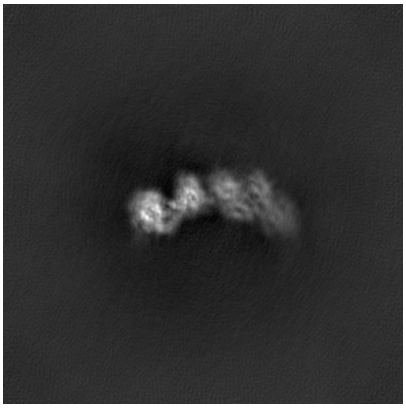


Z

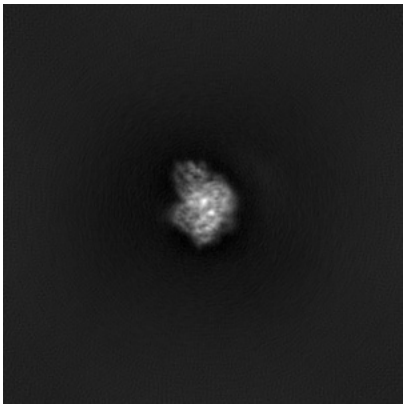
6.1.2 Raw map



X



Y

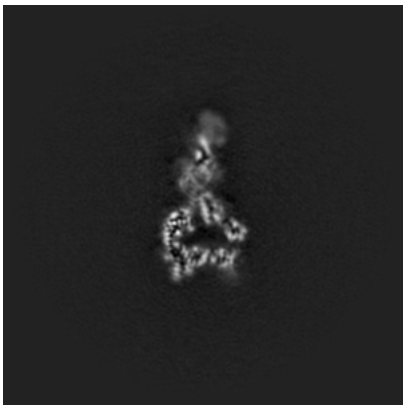


Z

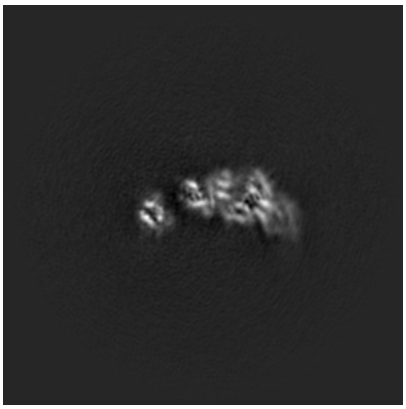
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

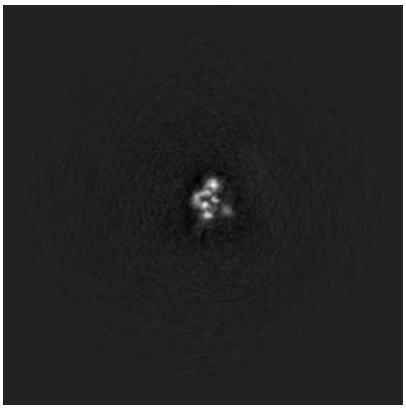
6.2.1 Primary map



X Index: 128

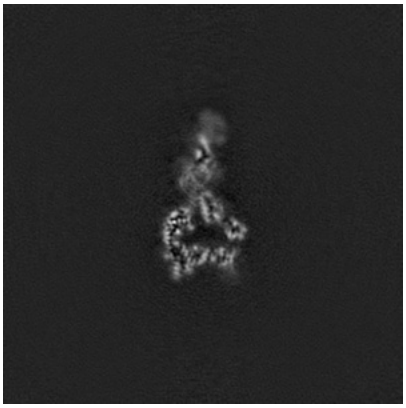


Y Index: 128

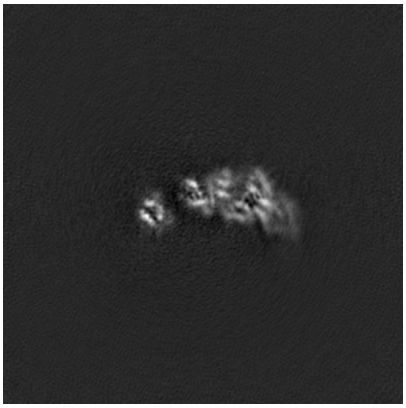


Z Index: 128

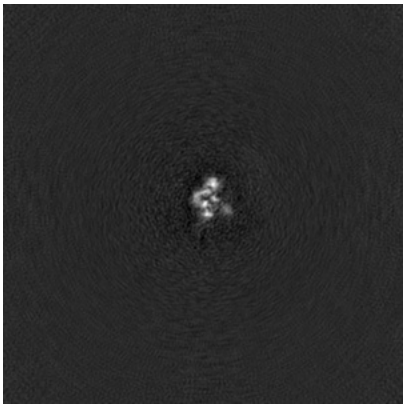
6.2.2 Raw map



X Index: 128



Y Index: 128

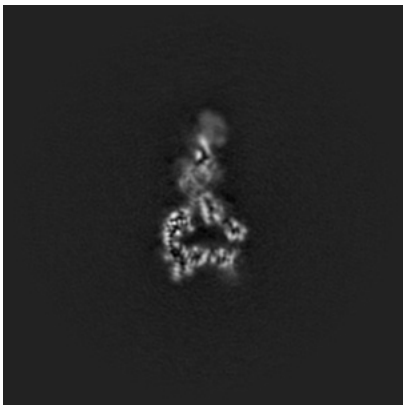


Z Index: 128

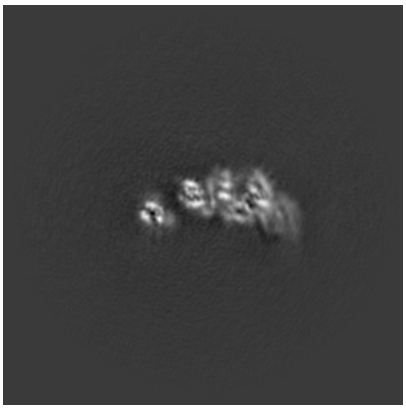
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

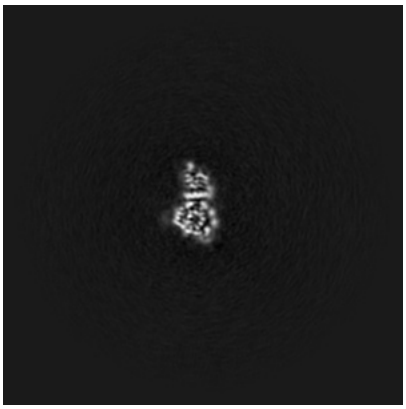
6.3.1 Primary map



X Index: 128

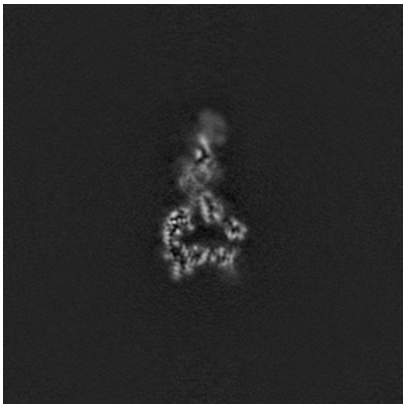


Y Index: 129

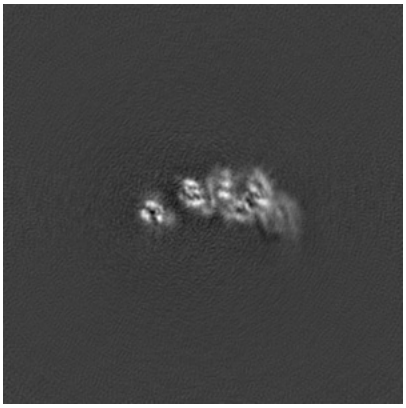


Z Index: 92

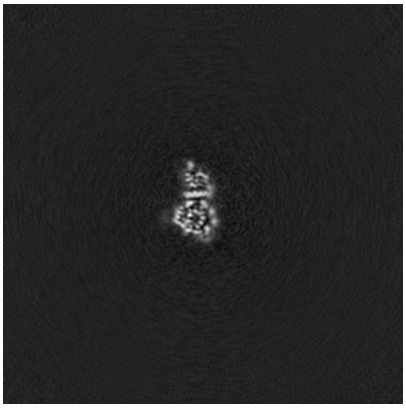
6.3.2 Raw map



X Index: 128



Y Index: 129



Z Index: 92

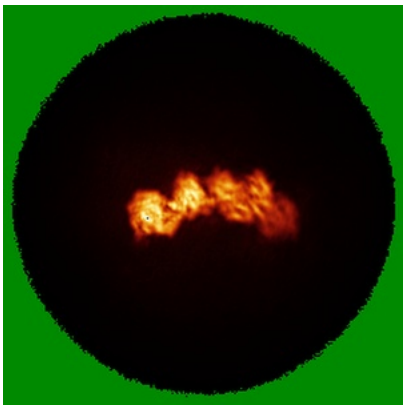
The images above show the largest variance slices of the map in three orthogonal directions.

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

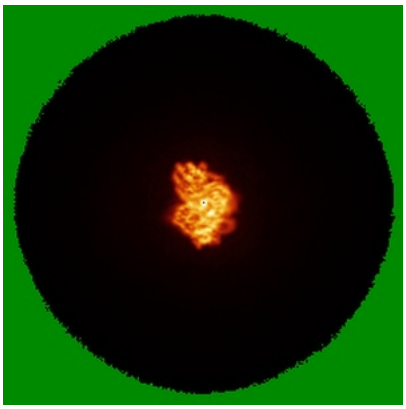
6.4.1 Primary map



X

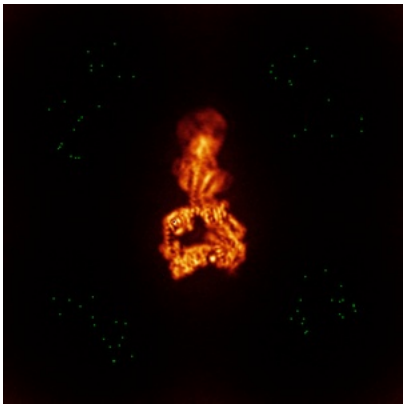


Y

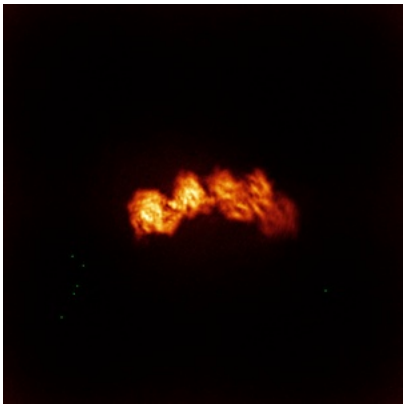


Z

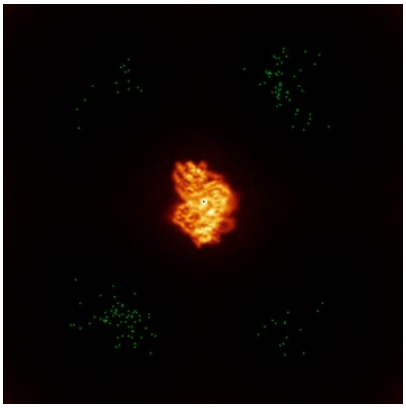
6.4.2 Raw map



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 0.123. 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.

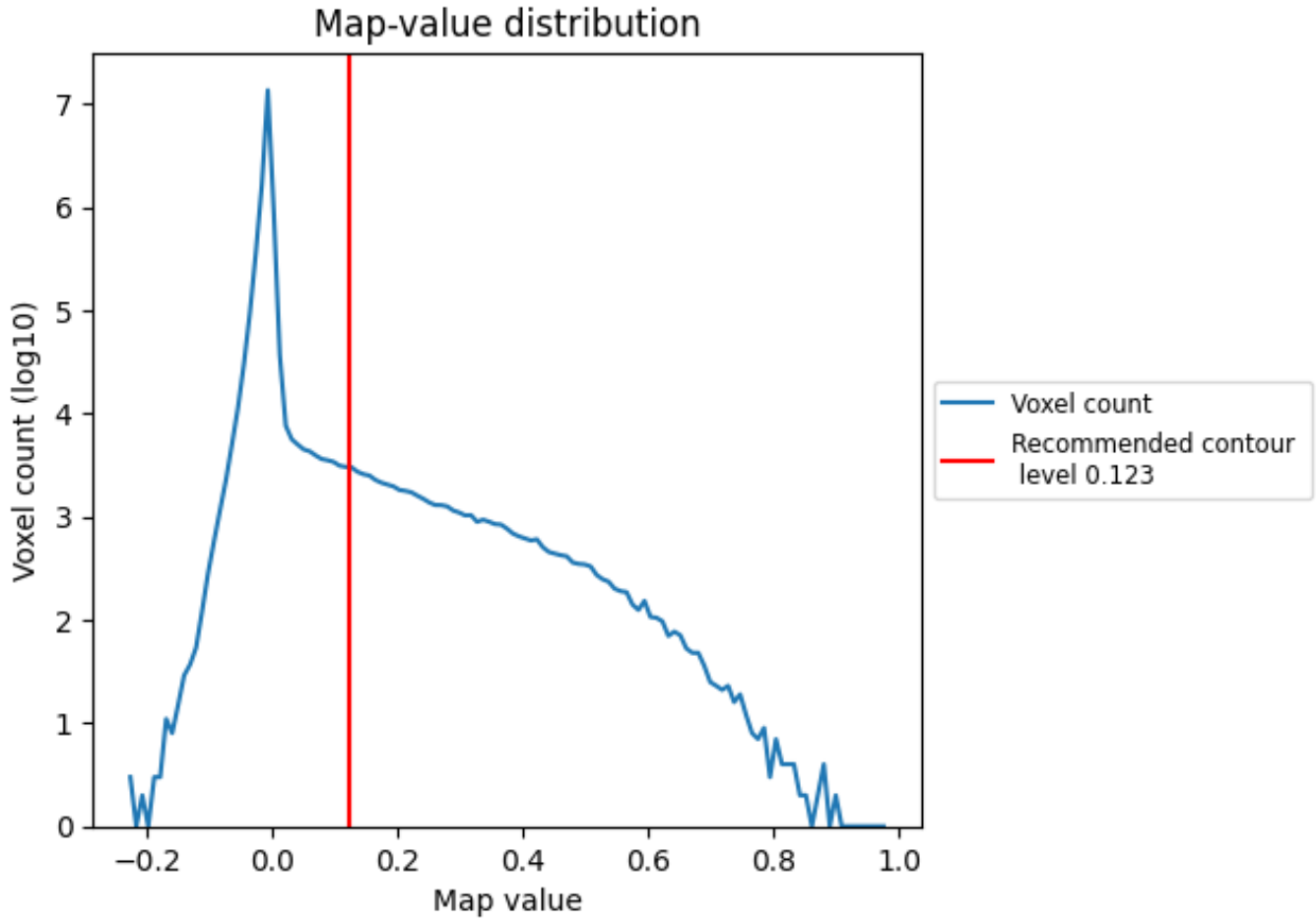
6.6 Mask visualisation (i)

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

7 Map analysis

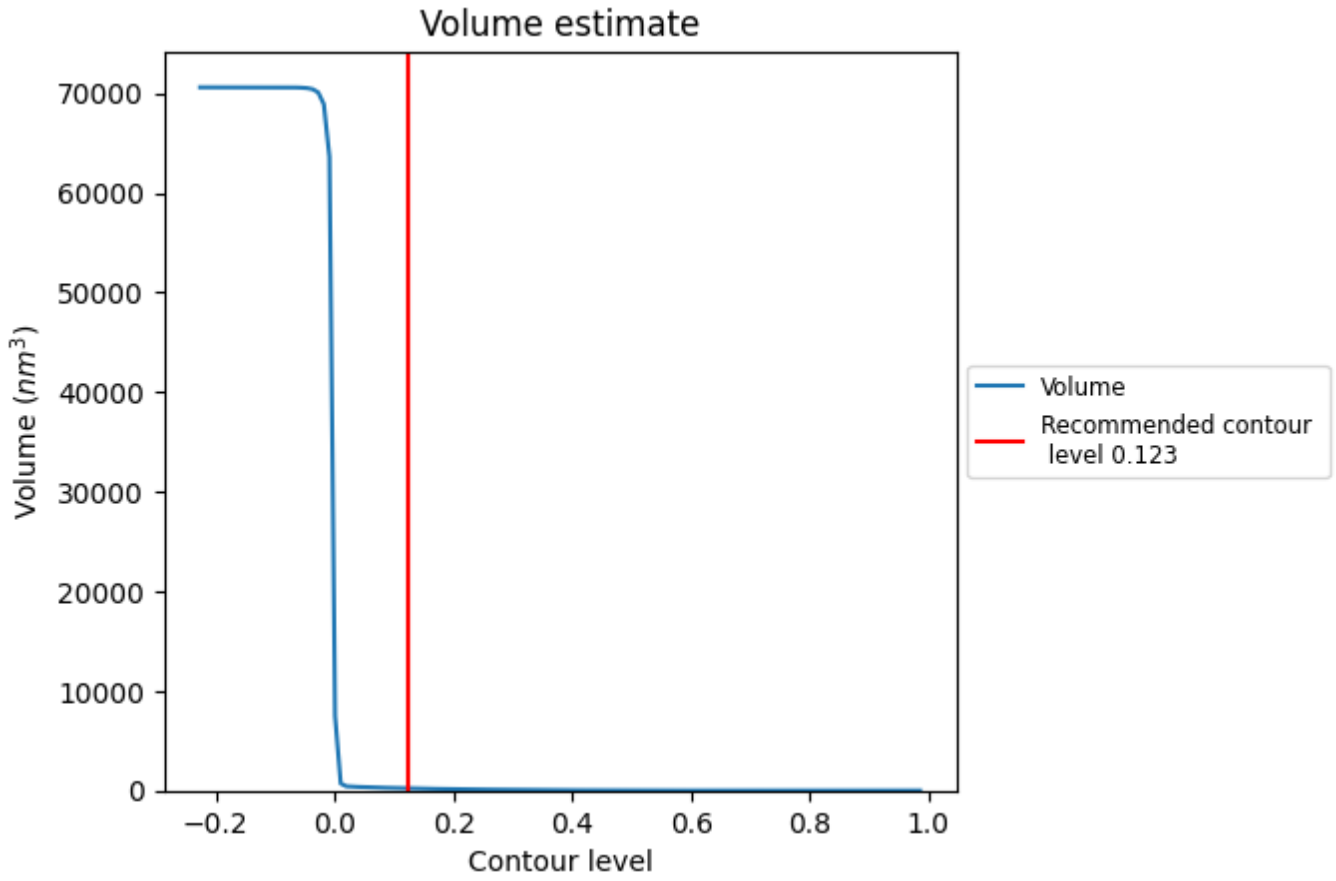
This section contains the results of statistical analysis of the map.

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.

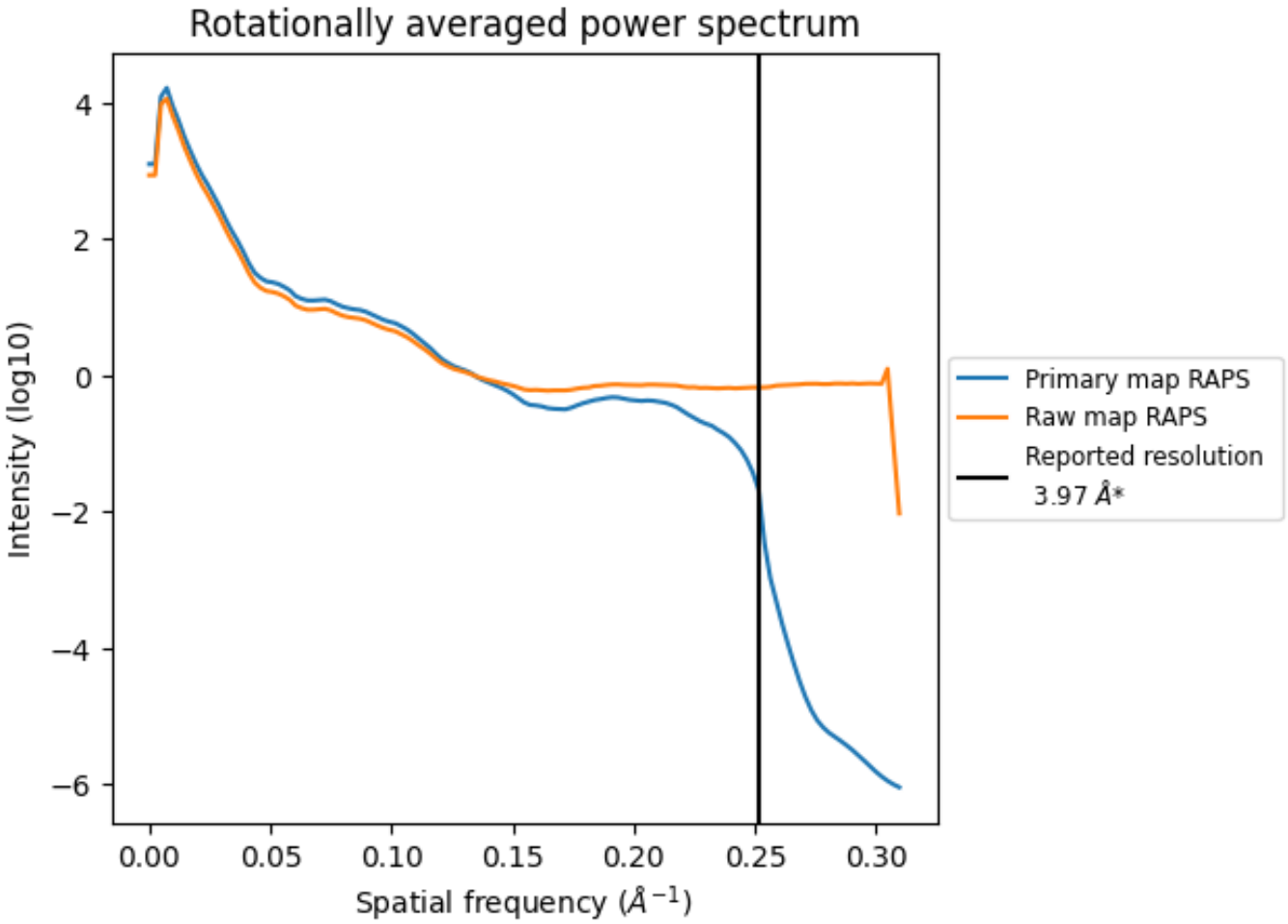
7.2 Volume estimate



The volume at the recommended contour level is 223 nm^3; this corresponds to an approximate mass of 202 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)

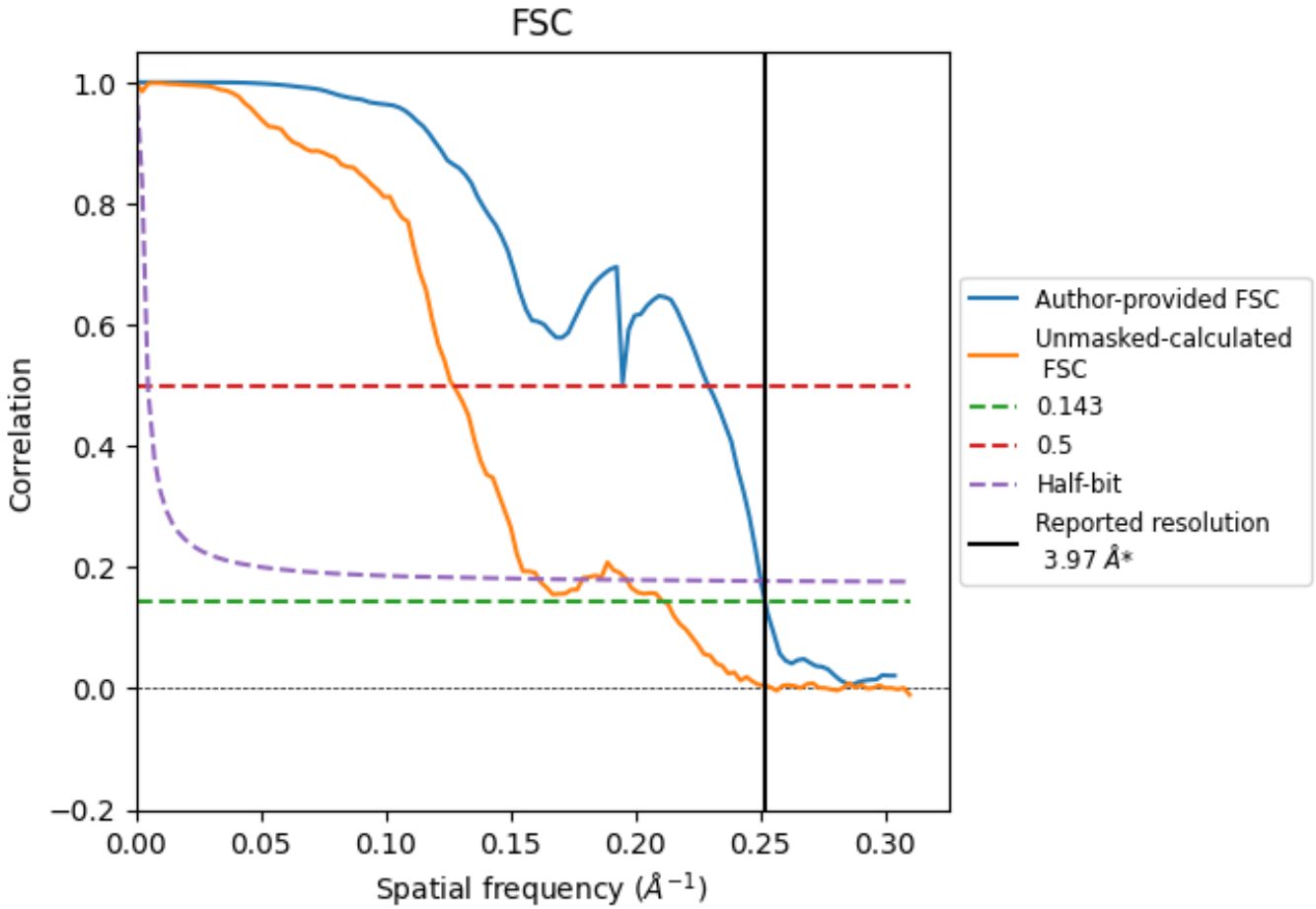


*Reported resolution corresponds to spatial frequency of 0.252 Å^{-1}

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 0.252 Å^{-1}

8.2 Resolution estimates (i)

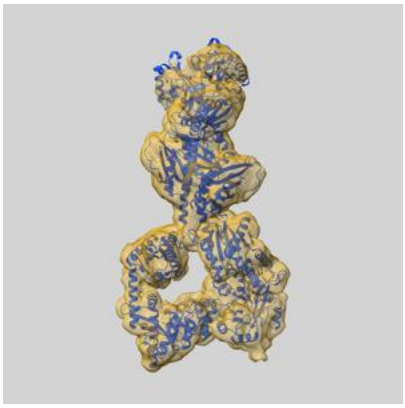
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.97	-	-
Author-provided FSC curve	3.97	4.36	4.00
Unmasked-calculated*	4.73	7.87	6.20

*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 4.73 differs from the reported value 3.97 by more than 10 %

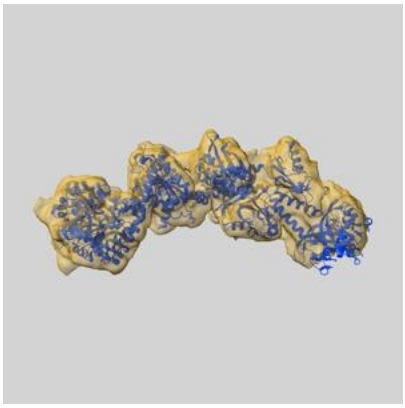
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45489 and PDB model 9CE0. Per-residue inclusion information can be found in section 3 on page 7.

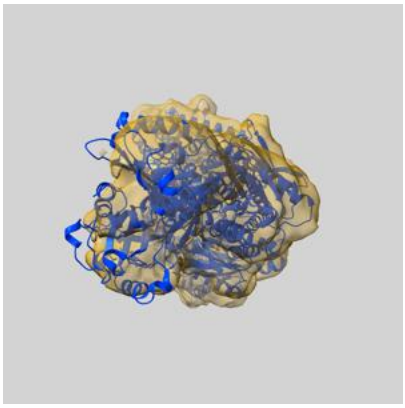
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.123 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.

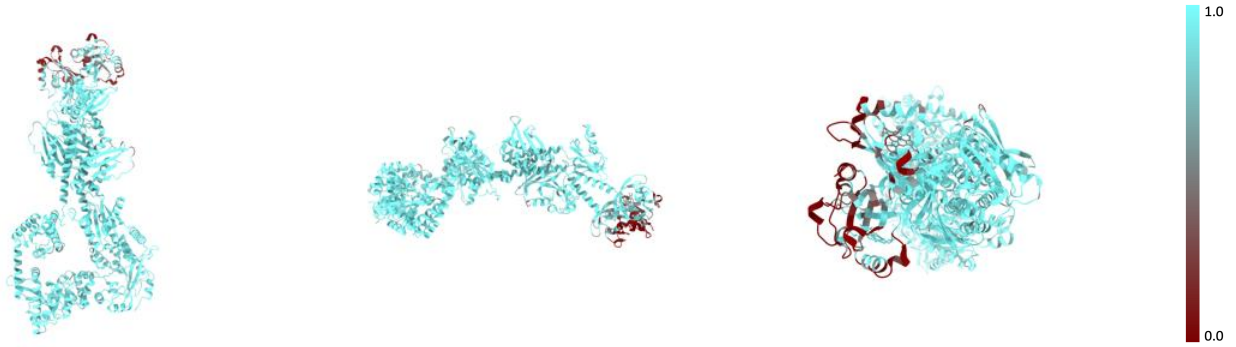
9.2 Q-score mapped to coordinate model (i)



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.

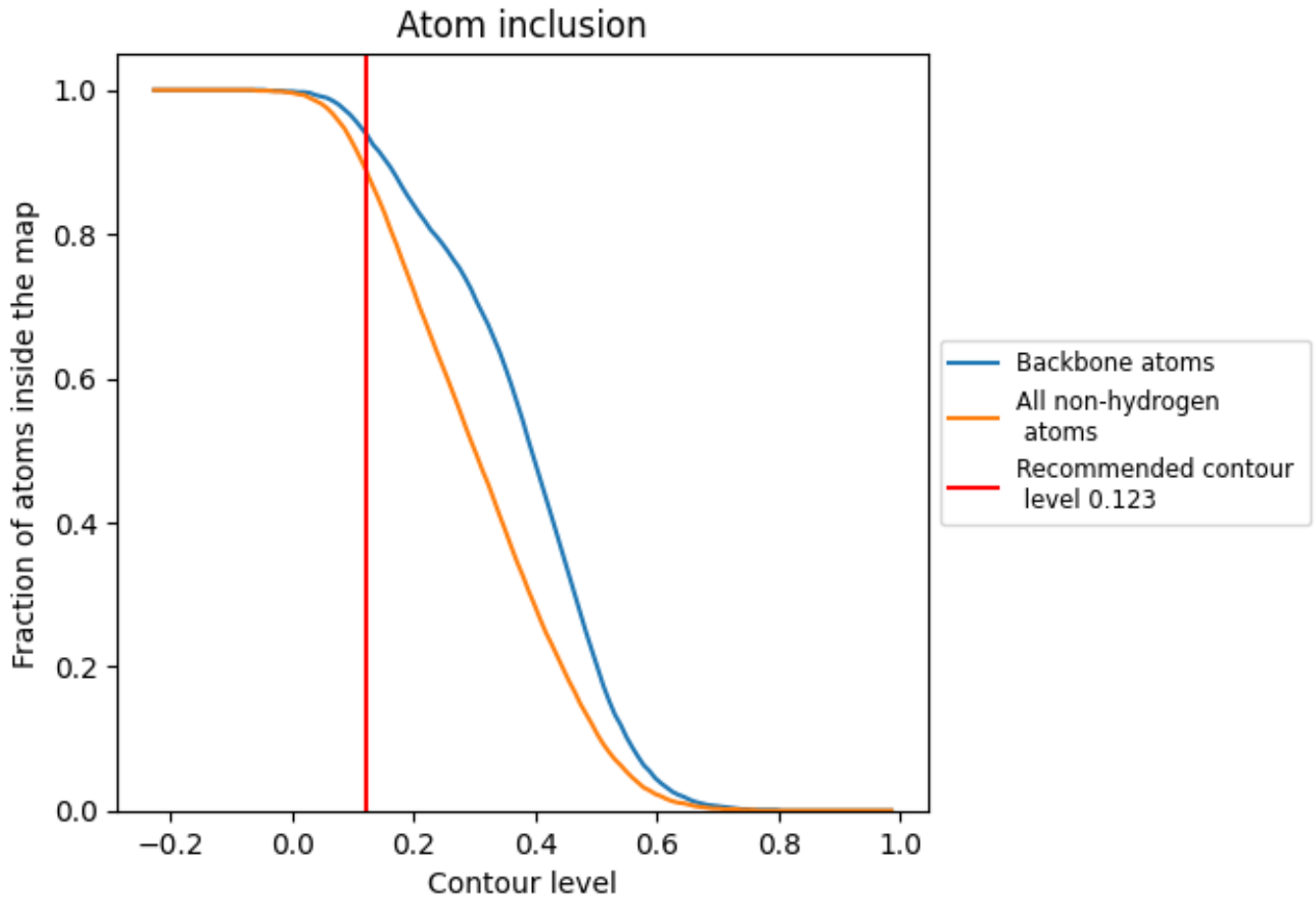
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.123).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% 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 (0.123) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8870	0.2480
A	0.8770	0.2490
B	0.8980	0.2470