Full wwPDB EM Validation Report (i)

Mar 19, 2024 – 07:58 PM JST

PDB ID	:	6JQN
EMDB ID	:	EMD-9875
Title	:	Structure of PaaZ, a bifunctional enzyme in complex with NADP+ and OCoA
Authors	:	Gakher, L.; Vinothkumar, K.R.; Katagihallimath, N.; Sowdhamini, R.; Sathyanarayanan, N.; Cannone, G.
Deposited on	:	2019-03-31
Resolution	:	3.10 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

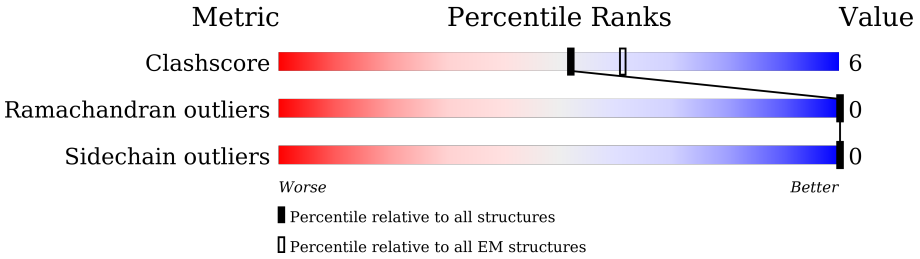
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	688	84% 15%
1	B	688	84% 15%
1	C	688	83% 15%
1	D	688	84% 15%
1	E	688	83% 16%
1	F	688	84% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31278 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 Bifunctional protein PaaZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	678	5108	3224	904	955	25	0	0
1	B	678	5108	3224	904	955	25	0	0
1	C	678	5108	3224	904	955	25	0	0
1	D	678	5108	3224	904	955	25	0	0
1	E	678	5108	3224	904	955	25	0	0
1	F	678	5108	3224	904	955	25	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP P77455
A	-5	GLY	-	expression tag	UNP P77455
A	-4	HIS	-	expression tag	UNP P77455
A	-3	HIS	-	expression tag	UNP P77455
A	-2	HIS	-	expression tag	UNP P77455
A	-1	HIS	-	expression tag	UNP P77455
A	0	HIS	-	expression tag	UNP P77455
A	1	HIS	-	expression tag	UNP P77455
B	-6	MET	-	initiating methionine	UNP P77455
B	-5	GLY	-	expression tag	UNP P77455
B	-4	HIS	-	expression tag	UNP P77455
B	-3	HIS	-	expression tag	UNP P77455
B	-2	HIS	-	expression tag	UNP P77455
B	-1	HIS	-	expression tag	UNP P77455
B	0	HIS	-	expression tag	UNP P77455
B	1	HIS	-	expression tag	UNP P77455
C	-6	MET	-	initiating methionine	UNP P77455
C	-5	GLY	-	expression tag	UNP P77455

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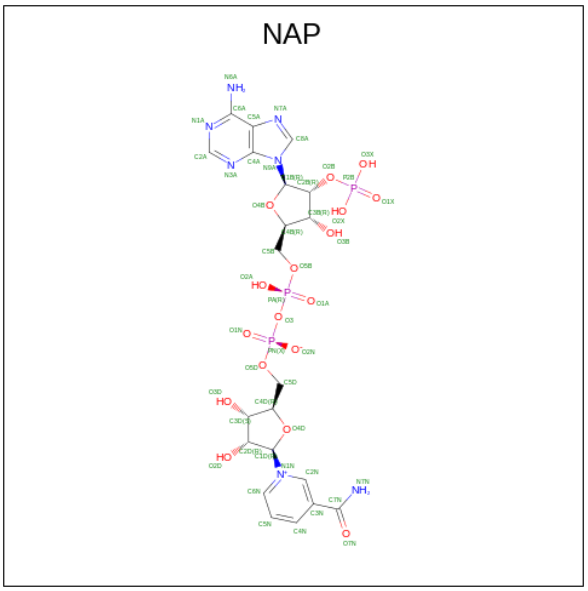
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P77455
C	-3	HIS	-	expression tag	UNP P77455
C	-2	HIS	-	expression tag	UNP P77455
C	-1	HIS	-	expression tag	UNP P77455
C	0	HIS	-	expression tag	UNP P77455
C	1	HIS	-	expression tag	UNP P77455
D	-6	MET	-	initiating methionine	UNP P77455
D	-5	GLY	-	expression tag	UNP P77455
D	-4	HIS	-	expression tag	UNP P77455
D	-3	HIS	-	expression tag	UNP P77455
D	-2	HIS	-	expression tag	UNP P77455
D	-1	HIS	-	expression tag	UNP P77455
D	0	HIS	-	expression tag	UNP P77455
D	1	HIS	-	expression tag	UNP P77455
E	-6	MET	-	initiating methionine	UNP P77455
E	-5	GLY	-	expression tag	UNP P77455
E	-4	HIS	-	expression tag	UNP P77455
E	-3	HIS	-	expression tag	UNP P77455
E	-2	HIS	-	expression tag	UNP P77455
E	-1	HIS	-	expression tag	UNP P77455
E	0	HIS	-	expression tag	UNP P77455
E	1	HIS	-	expression tag	UNP P77455
F	-6	MET	-	initiating methionine	UNP P77455
F	-5	GLY	-	expression tag	UNP P77455
F	-4	HIS	-	expression tag	UNP P77455
F	-3	HIS	-	expression tag	UNP P77455
F	-2	HIS	-	expression tag	UNP P77455
F	-1	HIS	-	expression tag	UNP P77455
F	0	HIS	-	expression tag	UNP P77455
F	1	HIS	-	expression tag	UNP P77455

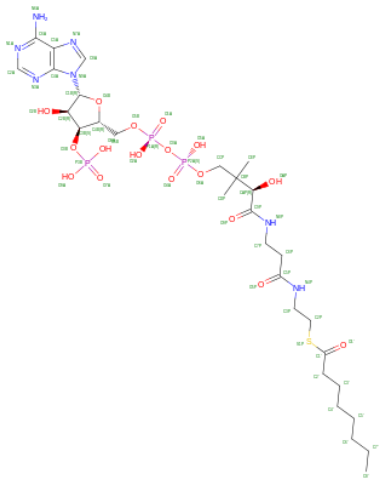
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	48	21	7	17	3	0
2	B	1	48	21	7	17	3	0
2	C	1	48	21	7	17	3	0
2	D	1	48	21	7	17	3	0
2	E	1	48	21	7	17	3	0
2	F	1	48	21	7	17	3	0

- Molecule 3 is OCTANOYL-COENZYME A (three-letter code: CO8) (formula: $C_{29}H_{50}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).

CO8



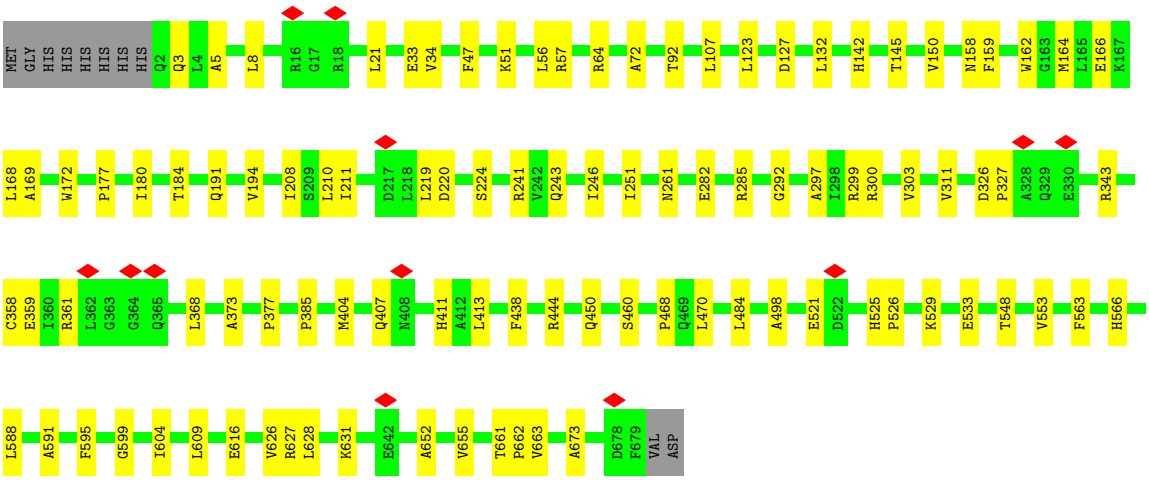
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	A	1	57	29	7	17	3	1	0
3	B	1	57	29	7	17	3	1	0
3	C	1	57	29	7	17	3	1	0
3	D	1	57	29	7	17	3	1	0
3	E	1	57	29	7	17	3	1	0
3	F	1	57	29	7	17	3	1	0

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.

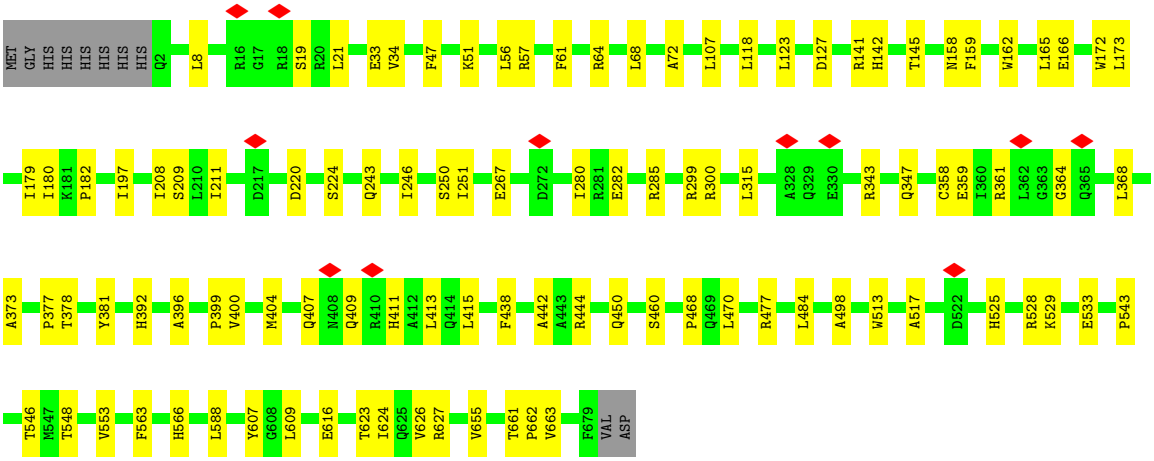
• Molecule 1: Bifunctional protein PaaZ

Chain A: 84% 15%



• Molecule 1: Bifunctional protein PaaZ

Chain B: 84% 15%



• Molecule 1: Bifunctional protein PaaZ

Chain C: 83% 15%

MET GLY HIS HIS HIS HIS HIS HIS Q2 L8 R16 G17 R18 S19 R20 L21 E33 V34 F47 K51 L56 R57 R64 A72 L107 G114 L118 L123 D127 S133 F138 H142 T145 V150 N158 F159 P160 C161 W162 G163 M164

L165 E166 K167 L168 A169 W172 L173 P177 A178 I179 I180 T184 I197 I208 S209 L210 I211 D217 D220 S224 R241 V242 Q243 I246 I251 N261 E267 D272 E282 R285 C295 R299 R300 V303 V311 A328 Q329 E330

R343 Q347 C358 E359 I360 R361 L362 G363 G364 Q365 L368 A373 P377 T378 A396 P399 V400 M404 Q407 N408 Q409 R410 H411 A412 L413 Q414 L415 F438 R444 Q450 S460 P468 Q469 L470 L484 V490 A498 K511 V519 R523

K529 E533 T548 V553 F563 H566 A591 I604 E616 I624 Q625 V626 R627 K631 S640 E643 A652 V655 V663 A673 F679 VAL ASP

• Molecule 1: Bifunctional protein PaaZ

Chain D: 84% 15%

MET GLY HIS HIS HIS HIS HIS HIS Q2 L8 G15 R16 G17 R18 L21 E33 F47 K51 L56 R57 R64 T92 Y110 L123 D127 L132 H142 T145 N158 F159 W162 G163 M164 L165 E166 K167 L168 A169 P170 T171 W172 L173

I180 V194 I197 I208 S209 L210 I211 D217 L218 L219 D220 Q243 I246 S250 I251 L260 E282 R285 K290 A291 G292 R299 R300 V303 V311 P327 A328 Q329 E330 R343 Q347 C358 E359 I360 R361 L362 G363 G364 Q365 L368

A373 P377 P385 H392 M404 Q407 N408 H411 A412 L413 Q414 L415 G421 R436 Q437 F438 R444 T445 Q450 S460 L470 R477 L484 V490 A498 E521 H525 P526 K529 E533 R544 T548 V553 F563 H566

L588 A591 F595 G599 L609 L612 E616 Q625 V626 R627 L628 K631 R639 E642 A652 V663 F679 VAL ASP

• Molecule 1: Bifunctional protein PaaZ

Chain E: 83% 16%

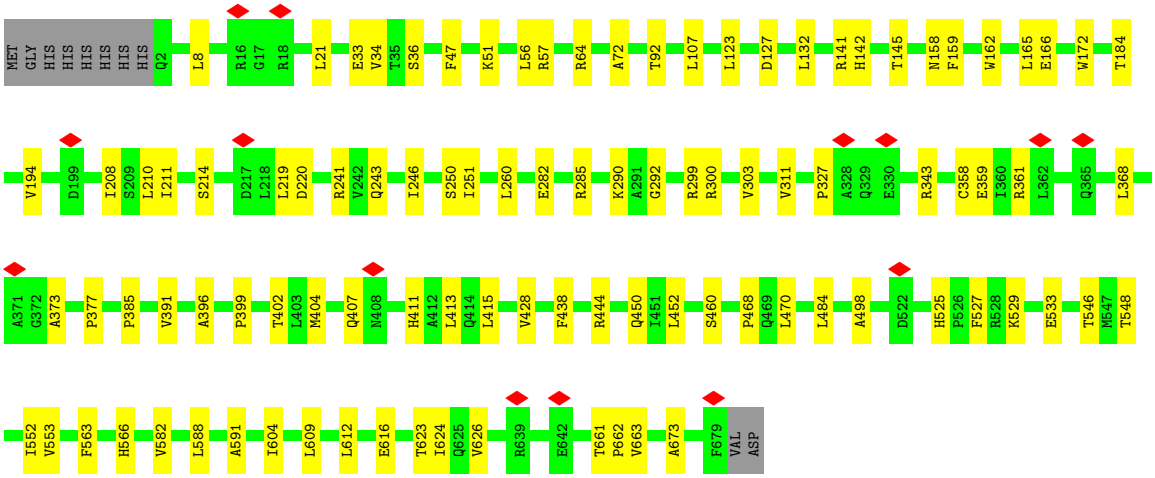
MET GLY HIS HIS HIS HIS HIS HIS Q2 L8 R16 G17 R18 S19 R20 L21 A30 E33 F47 K51 L56 R57 R64 L68 A72 L107 G114 L118 L123 D127 H142 T145 V150 N158 F159 W162 L165 E166

W172 L173 P177 A178 I179 I180 K181 P182 I197 I208 S209 L210 I211 D217 D220 S224 R241 V242 Q243 I246 S250 I251 V264 E267 D272 E282 R285 G292 R299 R300 V303 V311 A328 Q329 E330 R343 C358 E359 I360

R361 L362 Q365 A366 D367 L368 A373 P377 T378 H392 A396 P399 V400 Q407 N408 Q409 R410 H411 A412 L413 Q414 L415 T426 F438 R444 Q450 S460 P468 Q469 L470 R477 L484 V490 A498 E521 D522 H525 P526 F527 R528 K529

• Molecule 1: Bifunctional protein PaaZ

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	101503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; CTF was corrected on each particle during refinement and reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	132075	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.797	Depositor
Minimum map value	-0.350	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	436.71997, 436.71997, 436.71997	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, CO8

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	0.33	0/5211	0.56	0/7073
1	B	0.33	0/5211	0.56	0/7073
1	C	0.33	0/5211	0.55	0/7073
1	D	0.33	0/5211	0.55	0/7073
1	E	0.33	0/5211	0.56	0/7073
1	F	0.33	0/5211	0.55	0/7073
All	All	0.33	0/31266	0.55	0/42438

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 (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	5108	0	5122	60	0
1	B	5108	0	5122	65	0
1	C	5108	0	5122	66	0
1	D	5108	0	5122	59	0
1	E	5108	0	5122	71	0
1	F	5108	0	5122	63	0
2	A	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	25	2	0
2	C	48	0	25	2	0
2	D	48	0	25	0	0
2	E	48	0	25	2	0
2	F	48	0	25	2	0
3	A	57	0	46	1	0
3	B	57	0	46	0	0
3	C	57	0	46	1	0
3	D	57	0	46	2	0
3	E	57	0	46	0	0
3	F	57	0	46	1	0
All	All	31278	0	31158	357	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 6.

All (357) 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:F:361:ARG:HH12	1:F:377:PRO:HB2	1.58	0.69
1:E:158:ASN:HD22	2:E:801:NAP:H6N	1.58	0.68
1:C:616:GLU:HB2	1:C:663:VAL:HG12	1.75	0.68
1:B:158:ASN:HD22	2:B:801:NAP:H6N	1.59	0.66
1:D:361:ARG:HH12	1:D:377:PRO:HB2	1.59	0.66
1:A:166:GLU:HB2	1:A:484:LEU:HD21	1.78	0.65
1:A:361:ARG:HH12	1:A:377:PRO:HB2	1.62	0.64
1:B:616:GLU:HB2	1:B:663:VAL:HG12	1.79	0.64
1:C:158:ASN:HD22	2:C:801:NAP:H6N	1.62	0.63
1:C:166:GLU:HB2	1:C:484:LEU:HD21	1.80	0.63
1:C:361:ARG:HH12	1:C:377:PRO:HB2	1.64	0.62
1:B:361:ARG:HH12	1:B:377:PRO:HB2	1.64	0.62
1:E:361:ARG:HH12	1:E:377:PRO:HB2	1.64	0.61
1:D:166:GLU:HB2	1:D:484:LEU:HD21	1.83	0.61
1:F:563:PHE:HB3	1:F:566:HIS:HD2	1.66	0.61
1:E:631:LYS:HD2	1:E:652:ALA:HB2	1.83	0.60
1:E:616:GLU:HB2	1:E:663:VAL:HG12	1.83	0.60
1:A:159:PHE:HB3	1:A:162:TRP:HB3	1.84	0.60
1:A:127:ASP:OD2	1:A:142:HIS:ND1	2.33	0.60
1:B:220:ASP:OD1	1:B:243:GLN:NE2	2.35	0.59
1:B:166:GLU:HB2	1:B:484:LEU:HD21	1.84	0.59
1:C:220:ASP:OD1	1:C:243:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:ASP:OD1	1:D:243:GLN:NE2	2.36	0.59
1:D:56:LEU:O	1:D:64:ARG:NH1	2.35	0.59
1:C:563:PHE:HB3	1:C:566:HIS:HD2	1.67	0.59
1:D:616:GLU:HB2	1:D:663:VAL:HG12	1.84	0.59
1:E:220:ASP:OD1	1:E:243:GLN:NE2	2.36	0.58
1:F:159:PHE:HB3	1:F:162:TRP:HB3	1.85	0.58
1:B:413:LEU:HD11	1:B:438:PHE:HA	1.85	0.58
1:F:220:ASP:OD1	1:F:243:GLN:NE2	2.37	0.58
1:D:127:ASP:OD2	1:D:142:HIS:ND1	2.36	0.58
1:A:220:ASP:OD1	1:A:243:GLN:NE2	2.36	0.57
1:D:631:LYS:HD2	1:D:652:ALA:HB2	1.85	0.57
1:C:150:VAL:HG12	1:C:177:PRO:HG2	1.86	0.57
1:C:626:VAL:HG22	1:C:655:VAL:HG22	1.86	0.57
1:E:563:PHE:HB3	1:E:566:HIS:HD2	1.68	0.57
1:C:127:ASP:OD2	1:C:142:HIS:ND1	2.38	0.57
1:A:92:THR:HA	1:A:327:PRO:HB3	1.87	0.57
1:C:631:LYS:HD2	1:C:652:ALA:HB2	1.86	0.57
1:C:343:ARG:HH11	1:C:373:ALA:HA	1.70	0.57
1:F:158:ASN:HD22	2:F:801:NAP:H6N	1.70	0.56
1:A:413:LEU:HD11	1:A:438:PHE:HA	1.87	0.56
1:B:159:PHE:HB3	1:B:162:TRP:HB3	1.88	0.56
1:A:450:GLN:NE2	1:A:460:SER:OG	2.39	0.56
1:D:343:ARG:HE	1:D:368:LEU:HD23	1.70	0.56
1:F:166:GLU:HB2	1:F:484:LEU:HD21	1.86	0.56
1:C:343:ARG:HE	1:C:368:LEU:HD23	1.70	0.56
1:F:127:ASP:OD2	1:F:142:HIS:ND1	2.37	0.56
1:F:343:ARG:HE	1:F:368:LEU:HD23	1.70	0.56
1:F:56:LEU:O	1:F:64:ARG:NH1	2.37	0.56
1:E:56:LEU:O	1:E:64:ARG:NH1	2.39	0.56
1:A:21:LEU:HA	1:A:33:GLU:HA	1.87	0.56
1:A:563:PHE:HB3	1:A:566:HIS:HD2	1.71	0.56
1:E:123:LEU:HG	1:E:145:THR:HG22	1.88	0.56
1:B:358:CYS:SG	1:B:359:GLU:N	2.79	0.55
1:D:407:GLN:H	1:D:411:HIS:HB3	1.72	0.55
1:A:343:ARG:HE	1:A:368:LEU:HD23	1.69	0.55
1:A:358:CYS:SG	1:A:359:GLU:N	2.79	0.55
1:A:56:LEU:O	1:A:64:ARG:NH1	2.39	0.55
1:A:616:GLU:HB2	1:A:663:VAL:HG12	1.88	0.55
1:B:127:ASP:OD2	1:B:142:HIS:ND1	2.38	0.55
1:D:563:PHE:HB3	1:D:566:HIS:HD2	1.71	0.55
1:F:92:THR:HA	1:F:327:PRO:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:413:LEU:HD11	1:F:438:PHE:HA	1.88	0.55
1:B:56:LEU:O	1:B:64:ARG:NH1	2.39	0.55
1:D:343:ARG:HH11	1:D:373:ALA:HA	1.71	0.55
1:B:224:SER:HA	1:B:251:ILE:HG22	1.88	0.55
1:C:224:SER:HA	1:C:251:ILE:HG22	1.87	0.55
1:F:450:GLN:NE2	1:F:460:SER:OG	2.40	0.55
1:E:413:LEU:HD11	1:E:438:PHE:HA	1.89	0.54
1:E:159:PHE:HB3	1:E:162:TRP:HB3	1.88	0.54
1:C:56:LEU:O	1:C:64:ARG:NH1	2.41	0.54
1:A:588:LEU:HD11	1:A:609:LEU:HD11	1.89	0.54
1:A:626:VAL:HG22	1:A:655:VAL:HG22	1.90	0.54
1:A:343:ARG:HH11	1:A:373:ALA:HA	1.73	0.54
1:C:519:VAL:HG21	1:C:627:ARG:HH21	1.71	0.54
1:D:385:PRO:HB3	1:D:404:MET:HB2	1.89	0.54
1:A:261:ASN:ND2	1:A:297:ALA:O	2.39	0.54
1:C:358:CYS:SG	1:C:359:GLU:N	2.80	0.54
1:C:413:LEU:HD11	1:C:438:PHE:HA	1.89	0.54
1:D:260:LEU:HB3	1:D:300:ARG:HE	1.73	0.53
1:B:127:ASP:O	1:B:141:ARG:NH2	2.41	0.53
1:D:413:LEU:HD11	1:D:438:PHE:HA	1.88	0.53
1:A:246:ILE:HG12	1:A:251:ILE:HD11	1.90	0.53
1:C:246:ILE:HG12	1:C:251:ILE:HD11	1.90	0.53
1:D:168:LEU:HD13	1:D:180:ILE:HD11	1.89	0.53
1:C:159:PHE:HB3	1:C:162:TRP:HB3	1.90	0.53
1:D:358:CYS:SG	1:D:359:GLU:N	2.80	0.53
1:E:626:VAL:HG22	1:E:655:VAL:HG22	1.91	0.53
1:F:616:GLU:HB2	1:F:663:VAL:HG12	1.90	0.53
1:F:385:PRO:HB3	1:F:404:MET:HB2	1.90	0.53
1:A:292:GLY:O	1:A:299:ARG:NH2	2.39	0.53
1:B:407:GLN:H	1:B:411:HIS:HB3	1.73	0.53
1:D:159:PHE:HB3	1:D:162:TRP:HB3	1.91	0.53
1:E:166:GLU:HB2	1:E:484:LEU:HD21	1.91	0.53
1:B:282:GLU:OE1	1:B:285:ARG:NH2	2.42	0.53
1:D:21:LEU:HA	1:D:33:GLU:HA	1.90	0.53
1:E:343:ARG:HE	1:E:368:LEU:HD23	1.74	0.53
1:B:563:PHE:HB3	1:B:566:HIS:HD2	1.75	0.52
1:D:246:ILE:HG12	1:D:251:ILE:HD11	1.91	0.52
1:A:591:ALA:HA	1:A:626:VAL:HG21	1.92	0.52
1:C:123:LEU:HG	1:C:145:THR:HG22	1.90	0.52
1:E:609:LEU:HB3	1:F:612:LEU:HB3	1.91	0.52
1:F:107:LEU:HD21	1:F:165:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ARG:HH11	1:B:373:ALA:HA	1.74	0.52
1:A:72:ALA:HB2	1:A:107:LEU:HB3	1.92	0.52
1:D:347:GLN:NE2	1:D:364:GLY:O	2.43	0.52
1:F:21:LEU:HA	1:F:33:GLU:HA	1.91	0.52
1:A:631:LYS:HD2	1:A:652:ALA:HB2	1.92	0.51
1:E:246:ILE:HG12	1:E:251:ILE:HD11	1.91	0.51
1:B:343:ARG:HE	1:B:368:LEU:HD23	1.75	0.51
1:E:172:TRP:HZ2	1:E:208:ILE:HB	1.76	0.51
1:E:343:ARG:HH11	1:E:373:ALA:HA	1.75	0.51
1:A:57:ARG:HH11	1:B:444:ARG:HH22	1.59	0.51
1:C:347:GLN:NE2	1:C:364:GLY:O	2.44	0.51
1:B:246:ILE:HG12	1:B:251:ILE:HD11	1.93	0.51
1:D:158:ASN:O	1:D:290:LYS:NZ	2.44	0.51
1:F:343:ARG:HH11	1:F:373:ALA:HA	1.76	0.51
1:F:529:LYS:HB3	1:F:533:GLU:HG3	1.93	0.51
1:B:529:LYS:HB3	1:B:533:GLU:HG3	1.93	0.51
1:C:450:GLN:NE2	1:C:460:SER:OG	2.44	0.51
1:F:123:LEU:HG	1:F:145:THR:HG22	1.92	0.50
1:B:300:ARG:NH1	1:B:415:LEU:O	2.43	0.50
1:E:21:LEU:HA	1:E:33:GLU:HA	1.92	0.50
1:E:300:ARG:NH1	1:E:415:LEU:O	2.44	0.50
1:E:407:GLN:H	1:E:411:HIS:HB3	1.75	0.50
1:E:595:PHE:HB2	1:E:628:LEU:HD22	1.94	0.50
1:F:407:GLN:H	1:F:411:HIS:HB3	1.77	0.50
1:C:107:LEU:HD22	1:C:169:ALA:HB2	1.93	0.50
1:D:282:GLU:OE1	1:D:285:ARG:NH2	2.44	0.50
1:F:246:ILE:HG12	1:F:251:ILE:HD11	1.93	0.50
1:C:168:LEU:HD13	1:C:180:ILE:HD11	1.93	0.50
1:A:407:GLN:H	1:A:411:HIS:HB3	1.77	0.50
1:C:468:PRO:HA	1:C:484:LEU:HD22	1.94	0.50
1:F:358:CYS:SG	1:F:359:GLU:N	2.80	0.50
1:C:8:LEU:HD21	1:C:211:ILE:HG23	1.93	0.50
1:D:123:LEU:HG	1:D:145:THR:HG22	1.93	0.50
1:D:529:LYS:HB3	1:D:533:GLU:HG3	1.94	0.50
1:B:123:LEU:HG	1:B:145:THR:HG22	1.93	0.50
1:F:282:GLU:OE1	1:F:285:ARG:NH2	2.45	0.50
1:E:282:GLU:OE1	1:E:285:ARG:NH2	2.45	0.49
1:E:358:CYS:SG	1:E:359:GLU:N	2.79	0.49
1:B:280:ILE:HG23	1:B:315:LEU:HD23	1.93	0.49
1:B:450:GLN:NE2	1:B:460:SER:OG	2.44	0.49
1:F:591:ALA:HA	1:F:626:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:LEU:HA	1:B:33:GLU:HA	1.94	0.49
1:E:361:ARG:NH1	1:E:377:PRO:O	2.45	0.49
1:C:303:VAL:HG11	1:C:311:VAL:HG11	1.94	0.49
1:A:123:LEU:HG	1:A:145:THR:HG22	1.94	0.49
1:B:172:TRP:HZ2	1:B:208:ILE:HB	1.77	0.49
1:C:604:ILE:HD11	1:C:673:ALA:HB2	1.94	0.49
1:A:158:ASN:HD22	2:A:801:NAP:H6N	1.76	0.49
1:F:588:LEU:HD11	1:F:609:LEU:HD11	1.94	0.49
1:E:525:HIS:CD2	1:E:597:ASP:HB2	2.48	0.49
1:C:72:ALA:HB2	1:C:107:LEU:HB3	1.94	0.49
1:D:450:GLN:NE2	1:D:460:SER:OG	2.46	0.49
1:D:92:THR:HA	1:D:327:PRO:HB3	1.94	0.48
1:D:172:TRP:HZ2	1:D:208:ILE:HB	1.77	0.48
1:D:591:ALA:HA	1:D:626:VAL:HG21	1.95	0.48
1:F:428:VAL:HG22	1:F:452:LEU:HB3	1.96	0.48
1:C:21:LEU:HA	1:C:33:GLU:HA	1.94	0.48
1:C:282:GLU:OE1	1:C:285:ARG:NH2	2.47	0.48
1:B:107:LEU:HD21	1:B:165:LEU:HD12	1.96	0.48
1:C:407:GLN:H	1:C:411:HIS:HB3	1.77	0.48
1:E:8:LEU:HD21	1:E:211:ILE:HG23	1.96	0.48
1:F:72:ALA:HB2	1:F:107:LEU:HB3	1.95	0.48
1:A:529:LYS:HB3	1:A:533:GLU:HG3	1.96	0.48
1:B:8:LEU:HD21	1:B:211:ILE:HG23	1.96	0.47
1:E:303:VAL:HG11	1:E:311:VAL:HG11	1.95	0.47
1:E:378:THR:HB	1:E:400:VAL:HG22	1.96	0.47
1:D:292:GLY:O	1:D:299:ARG:NH2	2.46	0.47
1:A:3:GLN:NE2	1:A:33:GLU:OE2	2.48	0.47
1:E:468:PRO:HA	1:E:484:LEU:HD22	1.96	0.47
1:D:8:LEU:HD21	1:D:211:ILE:HG23	1.97	0.47
1:A:385:PRO:HB3	1:A:404:MET:HB2	1.96	0.47
3:A:802:CO8:O9A	1:B:607:TYR:OH	2.30	0.47
1:C:548:THR:HG21	1:E:553:VAL:HG21	1.96	0.47
1:D:15:GLY:O	1:D:16:ARG:NE	2.47	0.47
1:F:303:VAL:HG11	1:F:311:VAL:HG11	1.95	0.47
1:A:224:SER:HA	1:A:251:ILE:HG22	1.98	0.46
1:E:150:VAL:HG12	1:E:177:PRO:HG2	1.97	0.46
1:E:224:SER:HA	1:E:251:ILE:HG22	1.98	0.46
1:F:260:LEU:HB3	1:F:300:ARG:HE	1.81	0.46
1:E:114:GLY:HA2	1:E:118:LEU:HD13	1.96	0.46
1:C:300:ARG:NH1	1:C:415:LEU:O	2.44	0.46
1:B:377:PRO:HA	1:B:399:PRO:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:HD2	1:D:444:ARG:HH22	1.80	0.46
1:C:361:ARG:NH1	1:C:377:PRO:O	2.49	0.46
1:E:292:GLY:O	1:E:299:ARG:NH2	2.45	0.46
1:C:470:LEU:HD22	1:D:498:ALA:HB1	1.98	0.46
1:D:525:HIS:HD2	1:D:526:PRO:HD2	1.80	0.46
1:E:127:ASP:OD2	1:E:142:HIS:ND1	2.31	0.46
1:E:158:ASN:HD21	2:E:801:NAP:H52N	1.80	0.46
1:A:282:GLU:OE1	1:A:285:ARG:NH2	2.49	0.46
1:E:47:PHE:O	1:E:51:LYS:HB3	2.16	0.46
1:A:468:PRO:HA	1:A:484:LEU:HD22	1.98	0.45
1:C:173:LEU:HD23	1:C:490:VAL:HG11	1.98	0.45
1:E:72:ALA:HB2	1:E:107:LEU:HB3	1.98	0.45
1:A:300:ARG:HD2	1:A:404:MET:HE1	1.97	0.45
1:B:19:SER:OG	1:B:34:VAL:O	2.34	0.45
1:C:591:ALA:HA	1:C:626:VAL:HG21	1.98	0.45
1:F:8:LEU:HD21	1:F:211:ILE:HG23	1.97	0.45
1:A:8:LEU:HD21	1:A:211:ILE:HG23	1.98	0.45
1:C:172:TRP:HZ2	1:C:208:ILE:HB	1.82	0.45
1:C:299:ARG:NH1	1:C:396:ALA:O	2.50	0.45
1:A:164:MET:HG2	1:A:180:ILE:HG12	1.99	0.45
1:B:543:PRO:HB3	1:D:599:GLY:HA2	1.99	0.45
3:D:802:CO8:H10	3:D:802:CO8:H72	1.69	0.45
1:E:470:LEU:HD22	1:F:498:ALA:HB1	1.97	0.45
1:A:599:GLY:HA2	1:E:543:PRO:HB3	1.98	0.45
1:C:164:MET:HG3	1:C:180:ILE:HG12	1.99	0.45
1:C:498:ALA:HB1	1:D:470:LEU:HD22	1.99	0.45
1:E:529:LYS:HB3	1:E:533:GLU:HG3	1.99	0.45
1:C:133:SER:HB3	1:C:138:PHE:HB3	1.97	0.45
1:E:444:ARG:HH22	1:F:57:ARG:HD2	1.81	0.45
1:E:591:ALA:HA	1:E:626:VAL:HG21	1.98	0.45
1:A:470:LEU:HD22	1:B:498:ALA:HB1	1.98	0.45
1:A:525:HIS:HD2	1:A:526:PRO:HD2	1.82	0.45
1:E:299:ARG:NH1	1:E:396:ALA:O	2.50	0.45
1:C:114:GLY:HA2	1:C:118:LEU:HD13	1.99	0.45
1:B:72:ALA:HB2	1:B:107:LEU:HB3	1.97	0.45
1:E:521:GLU:OE2	1:E:627:ARG:NH2	2.50	0.45
1:F:604:ILE:HD11	1:F:673:ALA:HB2	1.98	0.45
1:A:444:ARG:HH22	1:B:57:ARG:HD2	1.83	0.44
1:A:34:VAL:HG21	1:A:184:THR:HB	2.00	0.44
1:A:47:PHE:O	1:A:51:LYS:HB3	2.17	0.44
1:A:168:LEU:HD13	1:A:180:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLU:OE2	1:A:627:ARG:NH2	2.50	0.44
1:D:392:HIS:O	1:D:477:ARG:NH1	2.38	0.44
1:E:57:ARG:HD2	1:F:444:ARG:HH22	1.82	0.44
1:A:219:LEU:HD22	1:A:246:ILE:HD11	1.99	0.44
1:D:421:GLY:HA2	1:D:445:THR:HB	1.99	0.44
1:F:127:ASP:O	1:F:141:ARG:NH2	2.50	0.44
1:B:299:ARG:NH1	1:B:396:ALA:O	2.51	0.44
1:C:300:ARG:HD2	1:C:404:MET:HE1	1.99	0.44
1:C:444:ARG:HH22	1:D:57:ARG:HD2	1.83	0.44
1:D:194:VAL:HG21	1:D:210:LEU:HD13	1.99	0.44
1:A:172:TRP:HZ2	1:A:208:ILE:HB	1.82	0.44
1:D:164:MET:HG3	1:D:180:ILE:HG12	1.99	0.44
1:F:299:ARG:NH1	1:F:396:ALA:O	2.50	0.44
1:D:173:LEU:HD23	1:D:490:VAL:HG11	2.00	0.44
1:E:68:LEU:HD11	1:E:173:LEU:HB2	1.99	0.44
1:E:173:LEU:HD23	1:E:490:VAL:HG11	1.99	0.44
1:E:498:ALA:HB1	1:F:470:LEU:HD22	1.99	0.44
1:F:194:VAL:HG21	1:F:210:LEU:HD13	1.99	0.44
1:F:377:PRO:HA	1:F:399:PRO:HB2	1.99	0.44
1:A:107:LEU:HD22	1:A:169:ALA:HB2	1.99	0.44
1:B:378:THR:HB	1:B:400:VAL:HG22	2.00	0.44
1:C:34:VAL:HG21	1:C:184:THR:HB	1.99	0.44
1:A:548:THR:HG21	1:F:553:VAL:HG21	1.99	0.43
1:B:553:VAL:HG21	1:E:548:THR:HG21	2.00	0.43
1:E:470:LEU:HD11	1:F:132:LEU:HD11	1.99	0.43
1:B:525:HIS:HB3	1:B:528:ARG:HG3	2.00	0.43
1:C:470:LEU:HD11	1:D:132:LEU:HD11	2.00	0.43
1:D:588:LEU:HD11	1:D:609:LEU:HD11	1.99	0.43
1:E:241:ARG:HH12	1:F:250:SER:HA	1.83	0.43
1:D:303:VAL:HG11	1:D:311:VAL:HG11	2.00	0.43
1:F:36:SER:OG	1:F:214:SER:O	2.31	0.43
1:A:661:THR:HA	1:A:662:PRO:HD3	1.87	0.43
1:B:158:ASN:HD21	2:B:801:NAP:H52N	1.83	0.43
1:C:47:PHE:O	1:C:51:LYS:HB3	2.18	0.43
1:C:161:CYS:O	1:C:165:LEU:HB2	2.19	0.43
1:C:172:TRP:HH2	1:C:197:ILE:HG21	1.83	0.43
1:D:172:TRP:HH2	1:D:197:ILE:HG21	1.83	0.43
1:F:300:ARG:HD2	1:F:404:MET:HE1	2.01	0.43
1:D:219:LEU:HD22	1:D:246:ILE:HD11	2.00	0.43
1:E:179:ILE:HG12	1:E:209:SER:HB2	1.99	0.43
1:F:219:LEU:HD22	1:F:246:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD11	1:B:470:LEU:HD11	2.01	0.43
1:D:521:GLU:OE2	1:D:627:ARG:NH2	2.51	0.43
1:E:377:PRO:HA	1:E:399:PRO:HB2	2.01	0.43
1:E:392:HIS:O	1:E:477:ARG:NH1	2.42	0.43
1:E:525:HIS:CD2	1:E:527:PHE:H	2.37	0.43
1:E:604:ILE:HD11	1:E:673:ALA:HB2	2.01	0.42
1:F:34:VAL:HG21	1:F:184:THR:HB	2.01	0.42
1:F:525:HIS:CD2	1:F:527:PHE:H	2.37	0.42
1:B:172:TRP:HH2	1:B:197:ILE:HG21	1.84	0.42
1:B:180:ILE:HG22	1:B:182:PRO:HD3	2.01	0.42
1:E:640:SER:HB2	1:E:643:GLU:HG2	2.01	0.42
1:F:172:TRP:HZ2	1:F:208:ILE:HB	1.82	0.42
1:B:548:THR:HG21	1:C:553:VAL:HG21	2.01	0.42
1:B:626:VAL:HG22	1:B:655:VAL:HG22	2.01	0.42
1:C:640:SER:HB2	1:C:643:GLU:HG2	2.01	0.42
1:E:21:LEU:HD13	1:E:30:ALA:HB2	2.01	0.42
1:F:47:PHE:O	1:F:51:LYS:HB3	2.19	0.42
1:A:498:ALA:HB1	1:B:470:LEU:HD22	2.01	0.42
1:B:358:CYS:HB3	1:B:381:TYR:HB3	2.02	0.42
1:C:377:PRO:HA	1:C:399:PRO:HB2	2.01	0.42
1:E:267:GLU:HG2	1:E:409:GLN:HG2	2.01	0.42
1:F:552:ILE:HG12	1:F:582:VAL:HA	2.02	0.42
1:C:261:ASN:ND2	1:C:295:CYS:O	2.52	0.42
1:E:450:GLN:NE2	1:E:460:SER:OG	2.52	0.42
1:F:391:VAL:HG13	1:F:402:THR:HG21	2.01	0.42
1:C:241:ARG:HH12	1:D:250:SER:HA	1.84	0.42
1:C:267:GLU:HG2	1:C:409:GLN:HG2	2.01	0.42
1:E:172:TRP:HH2	1:E:197:ILE:HG21	1.84	0.42
1:B:588:LEU:HD11	1:B:609:LEU:HD11	2.00	0.42
3:C:802:CO8:O6A	3:C:802:CO8:OAP	2.29	0.42
1:A:5:ALA:HB3	1:A:191:GLN:HE22	1.84	0.42
1:C:624:ILE:HG23	1:C:655:VAL:HG13	2.02	0.42
1:D:300:ARG:NH1	1:D:415:LEU:O	2.49	0.42
1:A:303:VAL:HG11	1:A:311:VAL:HG11	2.01	0.42
1:B:47:PHE:O	1:B:51:LYS:HB3	2.20	0.42
1:F:292:GLY:O	1:F:299:ARG:NH2	2.46	0.42
1:B:468:PRO:HA	1:B:484:LEU:HD22	2.00	0.41
1:C:511:LYS:HE3	1:D:436:ARG:HE	1.85	0.41
1:D:553:VAL:HG21	1:F:548:THR:HG21	2.02	0.41
1:F:546:THR:HA	1:F:623:THR:HA	2.02	0.41
1:C:179:ILE:HG12	1:C:209:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:PHE:O	1:D:51:LYS:HB3	2.20	0.41
1:D:595:PHE:HB2	1:D:628:LEU:HD22	2.01	0.41
1:E:19:SER:OG	1:E:33:GLU:OE1	2.38	0.41
1:B:68:LEU:HD11	1:B:173:LEU:HB2	2.02	0.41
1:B:624:ILE:HG23	1:B:655:VAL:HG13	2.03	0.41
1:E:250:SER:HA	1:F:241:ARG:HH12	1.86	0.41
1:A:241:ARG:HH12	1:B:250:SER:HA	1.85	0.41
1:B:19:SER:OG	1:B:33:GLU:OE1	2.37	0.41
1:B:392:HIS:O	1:B:477:ARG:NH1	2.41	0.41
1:B:438:PHE:O	1:B:442:ALA:HB3	2.20	0.41
1:B:661:THR:HA	1:B:662:PRO:HD3	1.89	0.41
1:E:107:LEU:HD21	1:E:165:LEU:HD22	2.02	0.41
1:B:546:THR:HA	1:B:623:THR:HA	2.02	0.41
1:B:627:ARG:HD2	1:B:627:ARG:HA	1.95	0.41
1:E:548:THR:HG23	1:E:551:ASP:H	1.86	0.41
1:B:61:PHE:HB3	1:B:118:LEU:HD23	2.03	0.41
1:B:347:GLN:NE2	1:B:364:GLY:O	2.54	0.41
1:D:544:ARG:HG2	1:D:625:GLN:HB2	2.03	0.41
1:F:468:PRO:HA	1:F:484:LEU:HD22	2.03	0.41
1:A:595:PHE:HB2	1:A:628:LEU:HD22	2.03	0.41
1:C:378:THR:HB	1:C:400:VAL:HG22	2.03	0.41
1:E:180:ILE:HG22	1:E:182:PRO:HD3	2.03	0.41
1:B:267:GLU:HG2	1:B:409:GLN:HG2	2.02	0.41
1:C:19:SER:OG	1:C:33:GLU:OE1	2.38	0.41
3:D:802:CO8:O6A	3:D:802:CO8:OAP	2.32	0.41
1:E:546:THR:HA	1:E:623:THR:HA	2.03	0.41
1:F:300:ARG:NH1	1:F:415:LEU:O	2.49	0.41
1:F:624:ILE:HD13	1:F:624:ILE:HA	1.95	0.41
1:A:194:VAL:HG21	1:A:210:LEU:HD13	2.02	0.41
1:A:326:ASP:HA	1:A:327:PRO:HD3	1.98	0.41
1:B:300:ARG:HD2	1:B:404:MET:HE1	2.02	0.41
1:B:513:TRP:CD1	1:B:517:ALA:HB3	2.56	0.41
1:D:609:LEU:HD21	1:D:612:LEU:HB2	2.03	0.41
1:C:158:ASN:HD21	2:C:801:NAP:H52N	1.86	0.40
1:E:264:VAL:N	1:E:426:THR:O	2.51	0.40
1:F:661:THR:HA	1:F:662:PRO:HD3	1.88	0.40
1:B:179:ILE:HG12	1:B:209:SER:HB2	2.03	0.40
1:D:110:TYR:CZ	1:D:170:PRO:HG3	2.56	0.40
1:F:158:ASN:HD21	2:F:801:NAP:H52N	1.87	0.40
3:F:802:CO8:HN4	3:F:802:CO8:H71	1.75	0.40
1:A:150:VAL:HG12	1:A:177:PRO:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:VAL:HG21	1:D:548:THR:HG21	2.04	0.40
1:A:604:ILE:HD11	1:A:673:ALA:HB2	2.04	0.40
1:E:612:LEU:HD23	1:F:609:LEU:HB3	2.03	0.40
1:F:158:ASN:O	1:F:290:LYS:NZ	2.48	0.40
1:C:57:ARG:HD2	1:D:444:ARG:NH2	2.37	0.40
1:C:529:LYS:HB3	1:C:533:GLU:HG3	2.03	0.40
1:E:525:HIS:HA	1:E:526:PRO:HD3	1.95	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	676/688 (98%)	638 (94%)	38 (6%)	0	100	100
1	B	676/688 (98%)	633 (94%)	43 (6%)	0	100	100
1	C	676/688 (98%)	637 (94%)	39 (6%)	0	100	100
1	D	676/688 (98%)	633 (94%)	43 (6%)	0	100	100
1	E	676/688 (98%)	638 (94%)	38 (6%)	0	100	100
1	F	676/688 (98%)	634 (94%)	42 (6%)	0	100	100
All	All	4056/4128 (98%)	3813 (94%)	243 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	529/538 (98%)	529 (100%)	0	100	100
1	B	529/538 (98%)	529 (100%)	0	100	100
1	C	529/538 (98%)	529 (100%)	0	100	100
1	D	529/538 (98%)	529 (100%)	0	100	100
1	E	529/538 (98%)	529 (100%)	0	100	100
1	F	529/538 (98%)	529 (100%)	0	100	100
All	All	3174/3228 (98%)	3174 (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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	392	HIS
1	A	450	GLN
1	B	158	ASN
1	B	450	GLN
1	C	158	ASN
1	C	450	GLN
1	D	450	GLN
1	E	158	ASN
1	E	450	GLN
1	E	525	HIS
1	F	158	ASN
1	F	191	GLN
1	F	392	HIS
1	F	450	GLN
1	F	525	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAP	F	801	-	45,52,52	1.18	3 (6%)	56,80,80	1.24	5 (8%)
3	CO8	C	802	-	51,59,59	0.92	2 (3%)	62,85,85	1.38	8 (12%)
3	CO8	B	802	-	51,59,59	0.92	2 (3%)	62,85,85	1.26	6 (9%)
3	CO8	E	802	-	51,59,59	0.92	2 (3%)	62,85,85	1.23	5 (8%)
2	NAP	C	801	-	45,52,52	1.17	3 (6%)	56,80,80	1.26	6 (10%)
2	NAP	E	801	-	45,52,52	1.16	3 (6%)	56,80,80	1.24	6 (10%)
2	NAP	B	801	-	45,52,52	1.16	3 (6%)	56,80,80	1.23	6 (10%)
3	CO8	A	802	-	51,59,59	0.95	2 (3%)	62,85,85	1.24	6 (9%)
3	CO8	F	802	-	51,59,59	0.94	2 (3%)	62,85,85	1.25	6 (9%)
2	NAP	A	801	-	45,52,52	1.17	3 (6%)	56,80,80	1.23	6 (10%)
3	CO8	D	802	-	51,59,59	0.92	2 (3%)	62,85,85	1.28	6 (9%)
2	NAP	D	801	-	45,52,52	1.16	3 (6%)	56,80,80	1.23	5 (8%)

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	NAP	F	801	-	-	4/31/67/67	0/5/5/5
3	CO8	C	802	-	-	11/54/74/74	0/3/3/3
3	CO8	B	802	-	-	18/54/74/74	0/3/3/3
3	CO8	E	802	-	-	12/54/74/74	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	801	-	-	11/31/67/67	0/5/5/5
2	NAP	E	801	-	-	4/31/67/67	0/5/5/5
2	NAP	B	801	-	-	7/31/67/67	0/5/5/5
3	CO8	A	802	-	-	15/54/74/74	0/3/3/3
3	CO8	F	802	-	-	16/54/74/74	0/3/3/3
2	NAP	A	801	-	-	10/31/67/67	0/5/5/5
3	CO8	D	802	-	-	14/54/74/74	0/3/3/3
2	NAP	D	801	-	-	4/31/67/67	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	NAP	C6N-N1N	4.63	1.46	1.35
2	F	801	NAP	C6N-N1N	4.62	1.46	1.35
2	C	801	NAP	C6N-N1N	4.62	1.46	1.35
2	B	801	NAP	C6N-N1N	4.60	1.46	1.35
2	A	801	NAP	C6N-N1N	4.53	1.46	1.35
2	D	801	NAP	C6N-N1N	4.48	1.46	1.35
3	A	802	CO8	C1'-S1P	-3.97	1.66	1.76
3	D	802	CO8	C1'-S1P	-3.91	1.66	1.76
3	F	802	CO8	C1'-S1P	-3.86	1.66	1.76
3	E	802	CO8	C1'-S1P	-3.83	1.66	1.76
3	C	802	CO8	C1'-S1P	-3.81	1.66	1.76
3	B	802	CO8	C1'-S1P	-3.80	1.66	1.76
2	F	801	NAP	C6N-C5N	3.36	1.46	1.38
2	E	801	NAP	C6N-C5N	3.29	1.45	1.38
2	C	801	NAP	C6N-C5N	3.27	1.45	1.38
2	B	801	NAP	C6N-C5N	3.26	1.45	1.38
2	A	801	NAP	C6N-C5N	3.25	1.45	1.38
2	D	801	NAP	C6N-C5N	3.22	1.45	1.38
3	F	802	CO8	C5A-C4A	2.50	1.47	1.40
3	A	802	CO8	C5A-C4A	2.49	1.47	1.40
3	B	802	CO8	C5A-C4A	2.44	1.47	1.40
3	E	802	CO8	C5A-C4A	2.36	1.47	1.40
2	A	801	NAP	C5A-C4A	2.36	1.47	1.40
2	E	801	NAP	C5A-C4A	2.36	1.47	1.40
3	D	802	CO8	C5A-C4A	2.35	1.47	1.40
2	F	801	NAP	C5A-C4A	2.34	1.47	1.40
3	C	802	CO8	C5A-C4A	2.34	1.47	1.40
2	D	801	NAP	C5A-C4A	2.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	NAP	C5A-C4A	2.31	1.47	1.40
2	B	801	NAP	C5A-C4A	2.30	1.47	1.40

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	802	CO8	C2'-C1'-S1P	6.00	120.44	113.46
3	D	802	CO8	C2'-C1'-S1P	5.28	119.60	113.46
3	F	802	CO8	C2'-C1'-S1P	5.12	119.42	113.46
3	B	802	CO8	C2'-C1'-S1P	5.09	119.39	113.46
3	E	802	CO8	C2'-C1'-S1P	5.00	119.28	113.46
3	A	802	CO8	C2'-C1'-S1P	4.89	119.15	113.46
2	B	801	NAP	C5N-C6N-N1N	-4.04	114.61	120.40
2	F	801	NAP	C5N-C6N-N1N	-4.03	114.63	120.40
2	C	801	NAP	C5N-C6N-N1N	-4.01	114.65	120.40
2	F	801	NAP	PN-O3-PA	-4.01	119.06	132.83
2	E	801	NAP	C5N-C6N-N1N	-4.01	114.65	120.40
2	A	801	NAP	C5N-C6N-N1N	-3.97	114.71	120.40
2	C	801	NAP	PN-O3-PA	-3.90	119.44	132.83
2	D	801	NAP	C5N-C6N-N1N	-3.86	114.86	120.40
2	B	801	NAP	PN-O3-PA	-3.85	119.60	132.83
2	A	801	NAP	PN-O3-PA	-3.74	119.99	132.83
2	D	801	NAP	PN-O3-PA	-3.73	120.04	132.83
2	E	801	NAP	PN-O3-PA	-3.71	120.09	132.83
3	B	802	CO8	P2A-O3A-P1A	-3.56	120.59	132.83
3	D	802	CO8	P2A-O3A-P1A	-3.51	120.77	132.83
3	C	802	CO8	O1'-C1'-C2'	-3.47	119.89	123.99
2	C	801	NAP	N3A-C2A-N1A	-3.40	123.36	128.68
2	F	801	NAP	N3A-C2A-N1A	-3.34	123.46	128.68
2	A	801	NAP	N3A-C2A-N1A	-3.31	123.51	128.68
2	D	801	NAP	N3A-C2A-N1A	-3.30	123.52	128.68
2	B	801	NAP	N3A-C2A-N1A	-3.30	123.52	128.68
2	E	801	NAP	N3A-C2A-N1A	-3.30	123.53	128.68
3	D	802	CO8	N3A-C2A-N1A	-3.23	123.62	128.68
3	C	802	CO8	N3A-C2A-N1A	-3.23	123.62	128.68
3	E	802	CO8	N3A-C2A-N1A	-3.22	123.65	128.68
3	A	802	CO8	N3A-C2A-N1A	-3.18	123.71	128.68
3	F	802	CO8	N3A-C2A-N1A	-3.17	123.72	128.68
3	B	802	CO8	N3A-C2A-N1A	-3.16	123.75	128.68
3	D	802	CO8	O1'-C1'-C2'	-3.04	120.40	123.99
3	A	802	CO8	O1'-C1'-C2'	-3.02	120.42	123.99
3	F	802	CO8	O1'-C1'-C2'	-2.99	120.46	123.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	CO8	O1'-C1'-C2'	-2.97	120.48	123.99
3	A	802	CO8	O4B-C1B-C2B	-2.97	102.59	106.93
3	E	802	CO8	O1'-C1'-C2'	-2.84	120.64	123.99
2	D	801	NAP	C4A-C5A-N7A	-2.81	106.47	109.40
3	D	802	CO8	C4A-C5A-N7A	-2.80	106.48	109.40
2	C	801	NAP	C4A-C5A-N7A	-2.71	106.57	109.40
3	F	802	CO8	P2A-O3A-P1A	-2.71	123.52	132.83
2	D	801	NAP	C2N-C3N-C4N	2.67	121.28	118.26
3	B	802	CO8	O4B-C1B-C2B	-2.62	103.10	106.93
2	A	801	NAP	C4A-C5A-N7A	-2.60	106.69	109.40
2	F	801	NAP	C4A-C5A-N7A	-2.59	106.70	109.40
3	C	802	CO8	C4A-C5A-N7A	-2.58	106.71	109.40
2	F	801	NAP	C2N-C3N-C4N	2.54	121.14	118.26
3	C	802	CO8	P2A-O3A-P1A	-2.54	124.11	132.83
2	E	801	NAP	C4A-C5A-N7A	-2.52	106.78	109.40
2	B	801	NAP	C4A-C5A-N7A	-2.48	106.81	109.40
3	C	802	CO8	C7P-C6P-C5P	-2.45	108.28	112.36
3	E	802	CO8	C4A-C5A-N7A	-2.42	106.88	109.40
3	E	802	CO8	P2A-O3A-P1A	-2.40	124.58	132.83
2	E	801	NAP	C2N-C3N-C4N	2.40	120.97	118.26
2	C	801	NAP	C2N-C3N-C4N	2.40	120.97	118.26
2	A	801	NAP	C2N-C3N-C4N	2.39	120.97	118.26
3	C	802	CO8	C3B-C2B-C1B	2.37	105.14	99.89
3	F	802	CO8	C4A-C5A-N7A	-2.35	106.95	109.40
3	B	802	CO8	C4A-C5A-N7A	-2.35	106.95	109.40
3	A	802	CO8	C4A-C5A-N7A	-2.31	106.99	109.40
2	B	801	NAP	C2N-C3N-C4N	2.30	120.87	118.26
3	C	802	CO8	O1'-C1'-S1P	-2.27	119.67	122.61
2	A	801	NAP	O4D-C1D-C2D	-2.15	103.79	106.93
2	C	801	NAP	C3D-C2D-C1D	2.07	104.09	100.98
3	F	802	CO8	O4B-C1B-C2B	-2.05	103.92	106.93
2	E	801	NAP	C3D-C2D-C1D	2.05	104.06	100.98
3	A	802	CO8	C7P-C6P-C5P	-2.04	108.95	112.36
3	D	802	CO8	O1'-C1'-S1P	-2.02	120.00	122.61
2	B	801	NAP	C3D-C2D-C1D	2.00	103.99	100.98

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C5B-O5B-PA-O3
2	B	801	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	801	NAP	C5B-O5B-PA-O3
2	C	801	NAP	C5B-O5B-PA-O1A
2	C	801	NAP	C5B-O5B-PA-O2A
2	C	801	NAP	C5B-O5B-PA-O3
2	D	801	NAP	C5B-O5B-PA-O1A
3	A	802	CO8	CAP-C9P-N8P-C7P
3	A	802	CO8	O9P-C9P-N8P-C7P
3	B	802	CO8	CAP-CBP-CCP-O6A
3	B	802	CO8	OAP-CAP-CBP-CCP
3	B	802	CO8	C9P-CAP-CBP-CCP
3	B	802	CO8	OAP-CAP-CBP-CDP
3	B	802	CO8	O9P-C9P-CAP-OAP
3	B	802	CO8	CAP-C9P-N8P-C7P
3	B	802	CO8	O9P-C9P-N8P-C7P
3	C	802	CO8	P1A-O3A-P2A-O6A
3	C	802	CO8	CAP-C9P-N8P-C7P
3	C	802	CO8	O9P-C9P-N8P-C7P
3	C	802	CO8	C5P-C6P-C7P-N8P
3	D	802	CO8	C3B-O3B-P3B-O8A
3	D	802	CO8	C5B-O5B-P1A-O3A
3	D	802	CO8	CAP-C9P-N8P-C7P
3	D	802	CO8	C5P-C6P-C7P-N8P
3	D	802	CO8	C1'-C2'-C3'-C4'
3	E	802	CO8	CAP-C9P-N8P-C7P
3	E	802	CO8	C5P-C6P-C7P-N8P
3	F	802	CO8	C3B-C4B-C5B-O5B
3	F	802	CO8	O4B-C4B-C5B-O5B
3	F	802	CO8	C9P-CAP-CBP-CCP
3	F	802	CO8	C5P-C6P-C7P-N8P
3	E	802	CO8	O9P-C9P-N8P-C7P
3	D	802	CO8	O9P-C9P-N8P-C7P
2	A	801	NAP	O4B-C4B-C5B-O5B
2	A	801	NAP	C3B-C4B-C5B-O5B
3	B	802	CO8	C3'-C4'-C5'-C6'
3	B	802	CO8	C4'-C5'-C6'-C7'
3	A	802	CO8	S1P-C2P-C3P-N4P
3	A	802	CO8	C3B-C4B-C5B-O5B
3	B	802	CO8	CDP-CBP-CCP-O6A
3	B	802	CO8	CEP-CBP-CCP-O6A
2	C	801	NAP	PN-O3-PA-O1A
2	F	801	NAP	O4B-C4B-C5B-O5B
2	D	801	NAP	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
3	A	802	CO8	N8P-C9P-CAP-CBP
3	C	802	CO8	N8P-C9P-CAP-CBP
3	E	802	CO8	C4'-C5'-C6'-C7'
3	A	802	CO8	O4B-C4B-C5B-O5B
3	D	802	CO8	O4B-C4B-C5B-O5B
3	F	802	CO8	C4'-C5'-C6'-C7'
2	F	801	NAP	C4D-C5D-O5D-PN
3	C	802	CO8	C4'-C5'-C6'-C7'
3	E	802	CO8	P1A-O3A-P2A-O6A
3	A	802	CO8	C1'-C2'-C3'-C4'
3	B	802	CO8	C5'-C6'-C7'-C8'
2	B	801	NAP	C2B-O2B-P2B-O1X
2	F	801	NAP	C2B-O2B-P2B-O1X
2	A	801	NAP	C4D-C5D-O5D-PN
3	C	802	CO8	C4B-C5B-O5B-P1A
3	B	802	CO8	C9P-CAP-CBP-CDP
3	B	802	CO8	C9P-CAP-CBP-CEP
3	F	802	CO8	C9P-CAP-CBP-CEP
2	C	801	NAP	C5D-O5D-PN-O3
3	F	802	CO8	CCP-O6A-P2A-O3A
2	B	801	NAP	C4D-C5D-O5D-PN
2	C	801	NAP	C4D-C5D-O5D-PN
2	E	801	NAP	C4D-C5D-O5D-PN
2	A	801	NAP	C5B-O5B-PA-O1A
2	A	801	NAP	C5B-O5B-PA-O2A
2	B	801	NAP	C5D-O5D-PN-O1N
2	C	801	NAP	C5D-O5D-PN-O1N
2	C	801	NAP	C5D-O5D-PN-O2N
3	D	802	CO8	C5B-O5B-P1A-O2A
3	F	802	CO8	CCP-O6A-P2A-O4A
3	F	802	CO8	CCP-O6A-P2A-O5A
3	E	802	CO8	C2'-C3'-C4'-C5'
2	F	801	NAP	C3B-C4B-C5B-O5B
3	F	802	CO8	OAP-CAP-CBP-CCP
3	A	802	CO8	O9P-C9P-CAP-OAP
3	C	802	CO8	O9P-C9P-CAP-OAP
3	D	802	CO8	O9P-C9P-CAP-OAP
3	E	802	CO8	O9P-C9P-CAP-OAP
3	F	802	CO8	O9P-C9P-CAP-OAP
3	D	802	CO8	C3'-C4'-C5'-C6'
3	F	802	CO8	OAP-CAP-CBP-CDP
3	B	802	CO8	C5P-C6P-C7P-N8P

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	B	802	CO8	S1P-C2P-C3P-N4P
3	D	802	CO8	S1P-C2P-C3P-N4P
3	F	802	CO8	CDP-CBP-CCP-O6A
3	E	802	CO8	N8P-C9P-CAP-CBP
3	C	802	CO8	C3P-C2P-S1P-C1'
3	E	802	CO8	C3P-C2P-S1P-C1'
2	A	801	NAP	PN-O3-PA-O1A
3	A	802	CO8	C4B-C5B-O5B-P1A
3	A	802	CO8	P1A-O3A-P2A-O4A
2	C	801	NAP	O4B-C4B-C5B-O5B
3	D	802	CO8	C3B-C4B-C5B-O5B
3	D	802	CO8	O1'-C1'-S1P-C2P
2	C	801	NAP	C2B-O2B-P2B-O1X
3	A	802	CO8	N8P-C9P-CAP-OAP
3	B	802	CO8	N8P-C9P-CAP-OAP
3	C	802	CO8	N8P-C9P-CAP-OAP
3	E	802	CO8	C3B-O3B-P3B-O7A
3	E	802	CO8	N8P-C9P-CAP-OAP
3	A	802	CO8	CDP-CBP-CCP-O6A
3	A	802	CO8	C3'-C4'-C5'-C6'
3	F	802	CO8	C9P-CAP-CBP-CDP
3	F	802	CO8	O5P-C5P-C6P-C7P
2	A	801	NAP	C2B-O2B-P2B-O2X
2	B	801	NAP	C5D-O5D-PN-O3
2	C	801	NAP	C2B-O2B-P2B-O2X
2	D	801	NAP	C2B-O2B-P2B-O2X
2	E	801	NAP	C2B-O2B-P2B-O2X
3	F	802	CO8	N4P-C5P-C6P-C7P
2	A	801	NAP	PN-O3-PA-O2A
2	A	801	NAP	C5D-O5D-PN-O1N
2	B	801	NAP	C5B-O5B-PA-O2A
2	D	801	NAP	C5D-O5D-PN-O1N
2	E	801	NAP	C5B-O5B-PA-O1A
2	E	801	NAP	C5D-O5D-PN-O1N
3	A	802	CO8	C5B-O5B-P1A-O1A
3	B	802	CO8	CCP-O6A-P2A-O4A
3	D	802	CO8	CDP-CBP-CCP-O6A
3	A	802	CO8	O9P-C9P-CAP-CBP
3	C	802	CO8	O9P-C9P-CAP-CBP
3	E	802	CO8	O9P-C9P-CAP-CBP

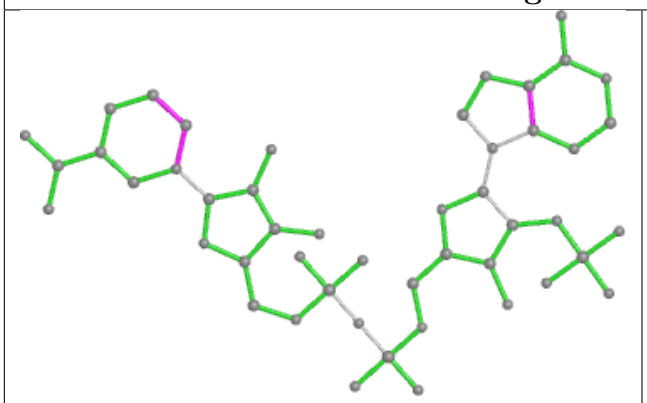
There are no ring outliers.

9 monomers are involved in 14 short contacts:

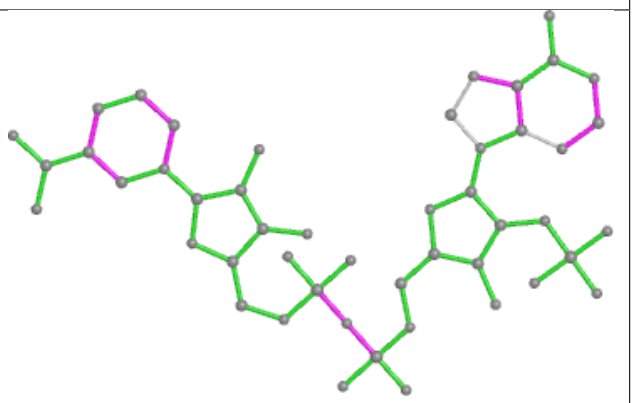
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	801	NAP	2	0
3	C	802	CO8	1	0
2	C	801	NAP	2	0
2	E	801	NAP	2	0
2	B	801	NAP	2	0
3	A	802	CO8	1	0
3	F	802	CO8	1	0
2	A	801	NAP	1	0
3	D	802	CO8	2	0

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.

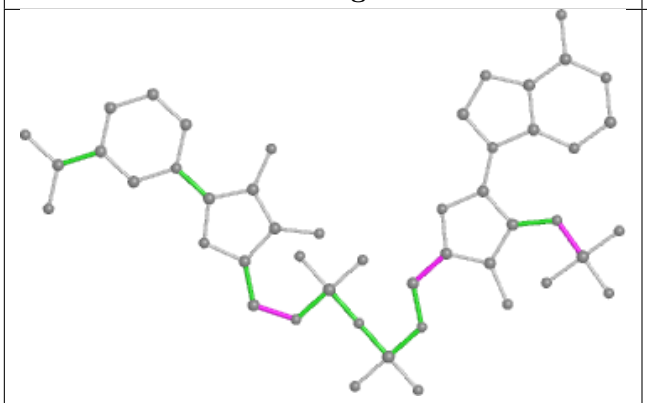
Ligand NAP F 801



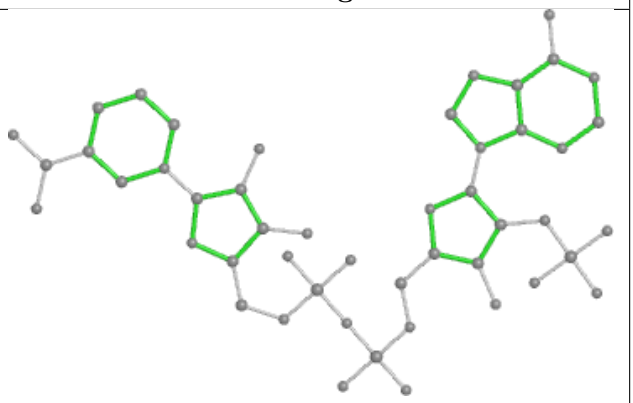
Bond lengths



Bond angles

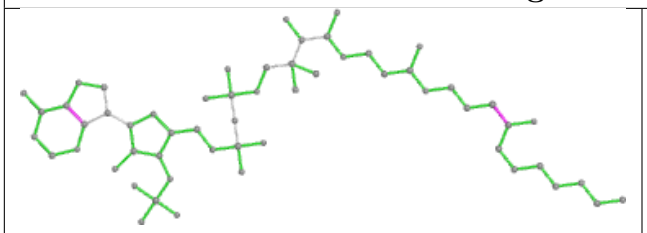


Torsions



Rings

Ligand CO8 C 802



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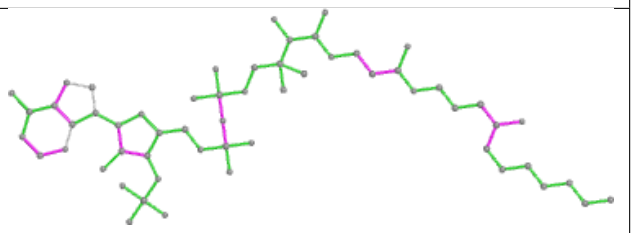
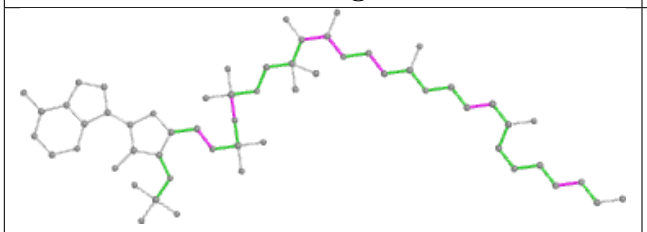


Bond angles



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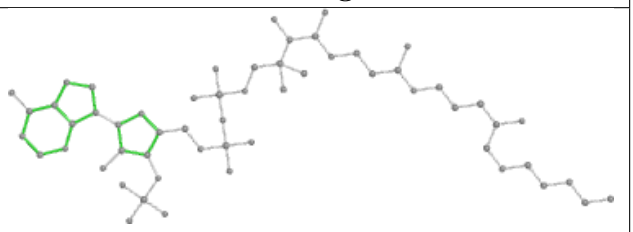
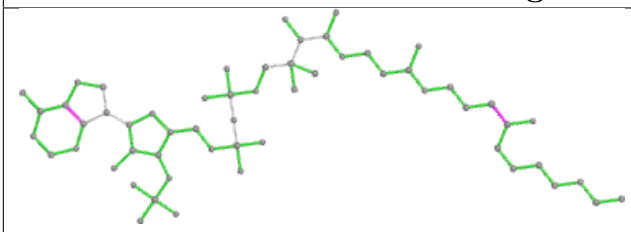
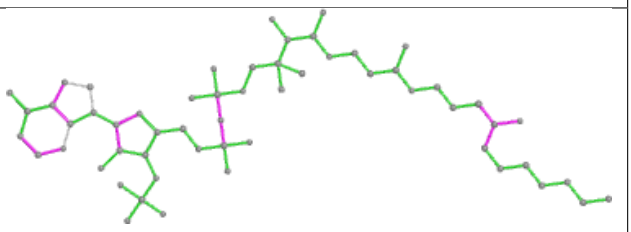
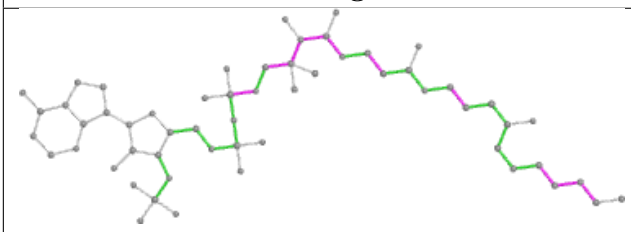
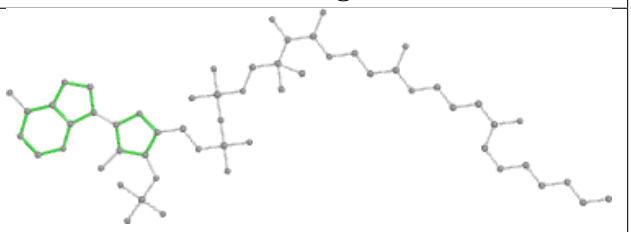


Rings

Ligand CO8 B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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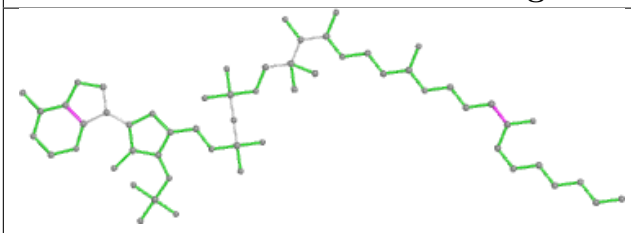
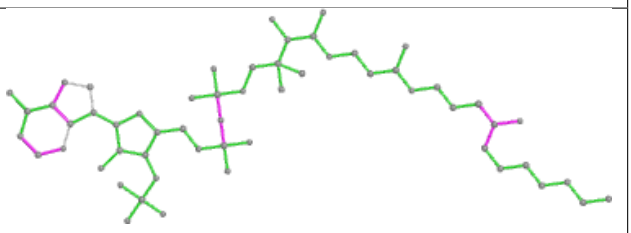
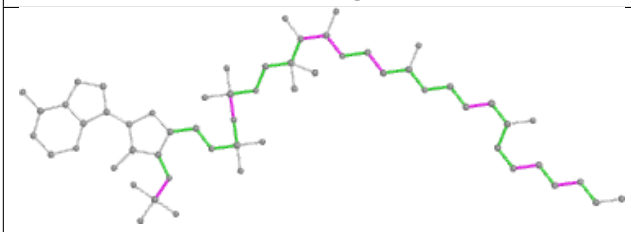
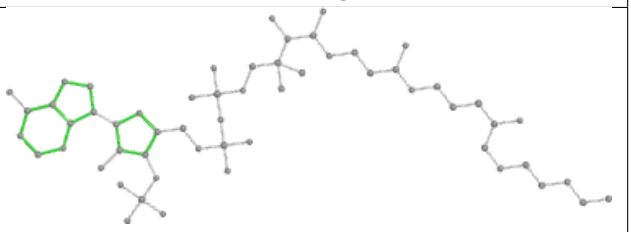
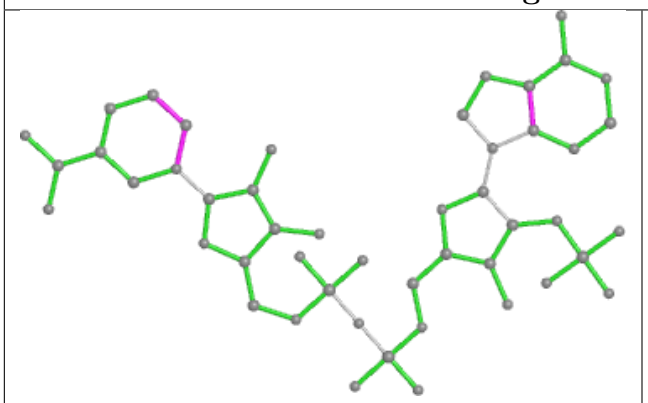
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAP C 801



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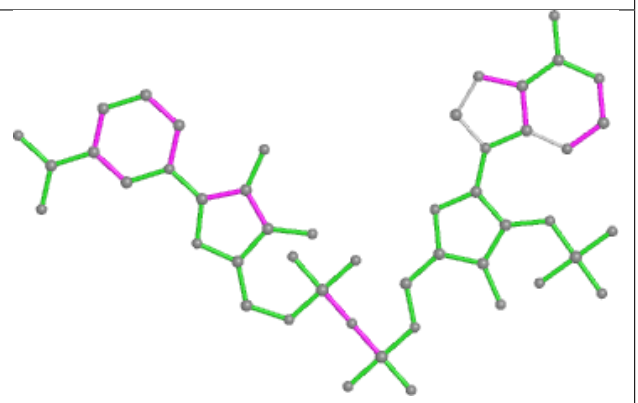

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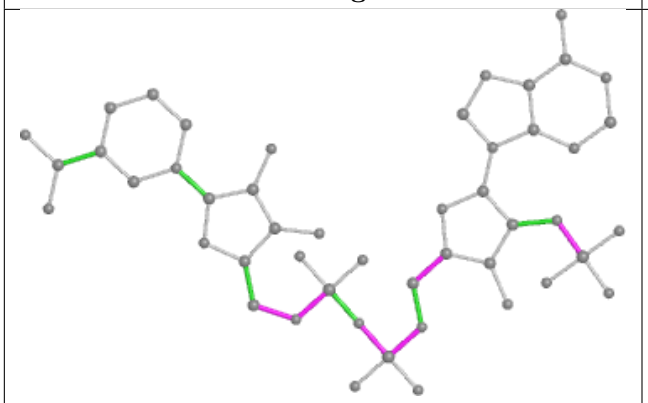

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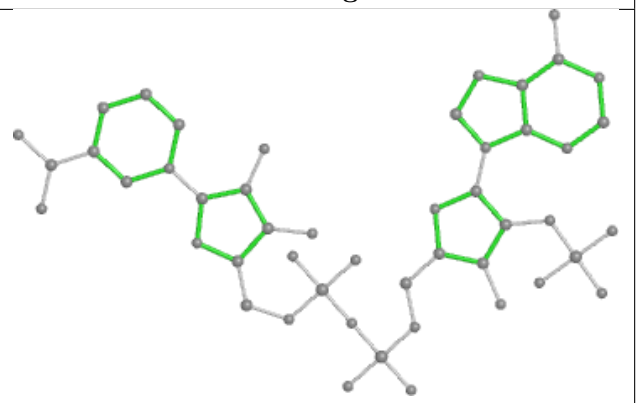

Rings

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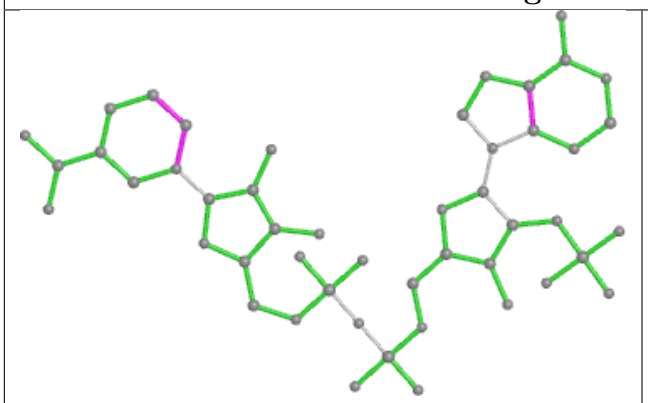

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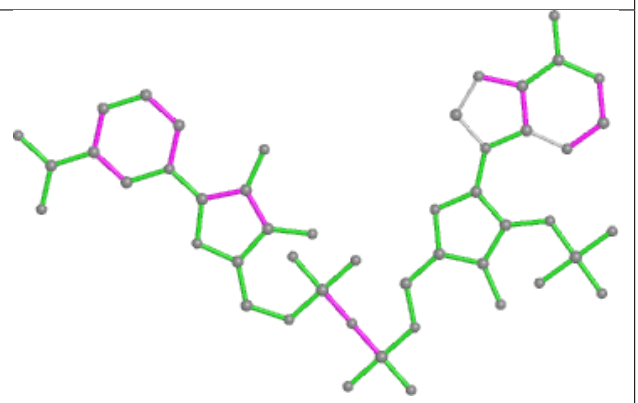
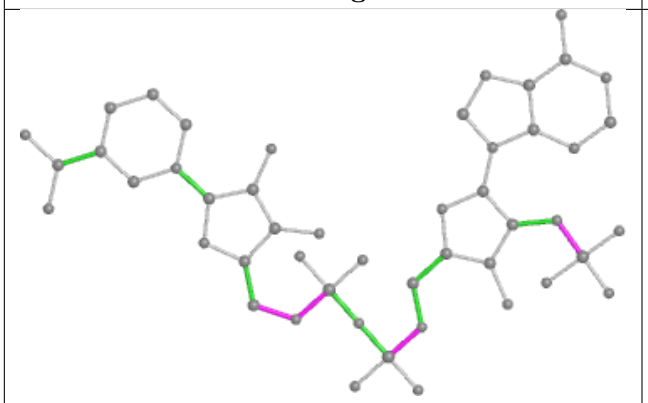


Bond angles



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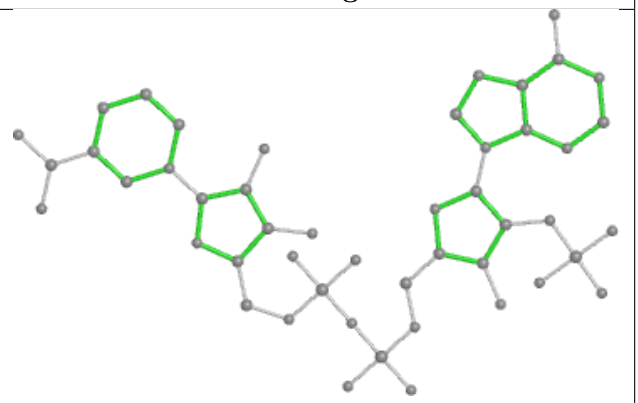

Rings

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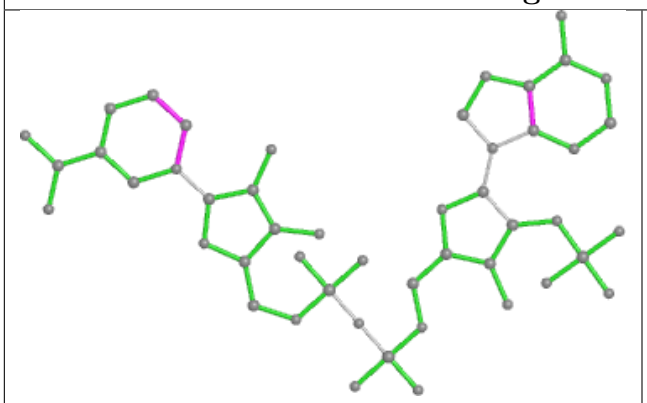

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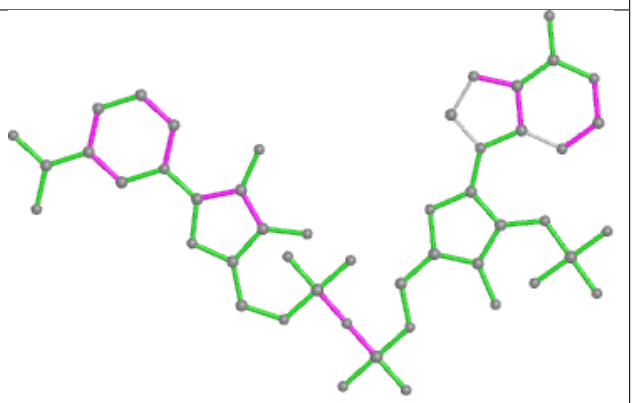

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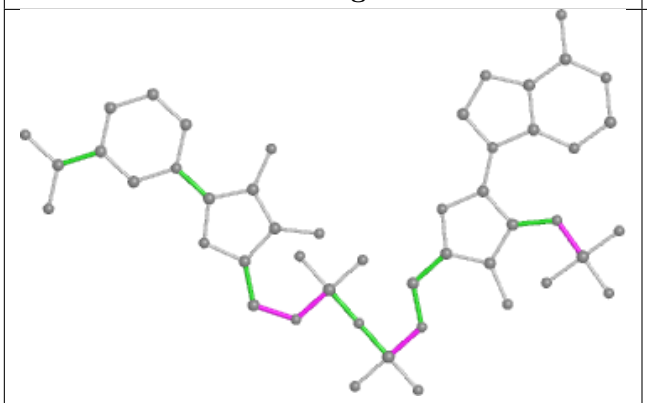

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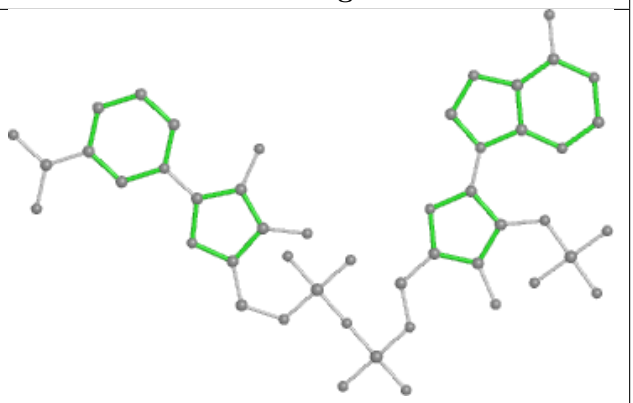
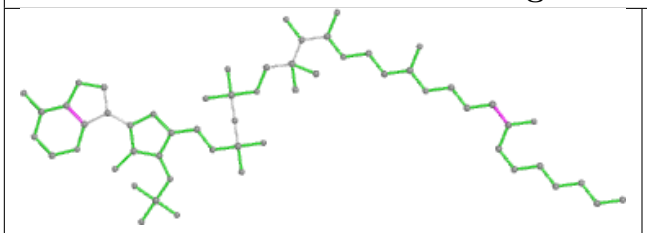


Rings

Ligand CO8 A 802



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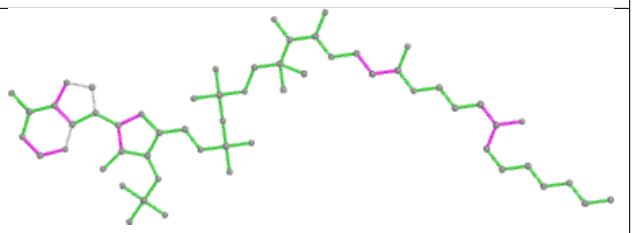
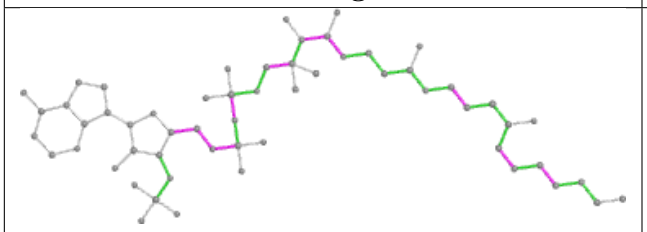


Bond angles



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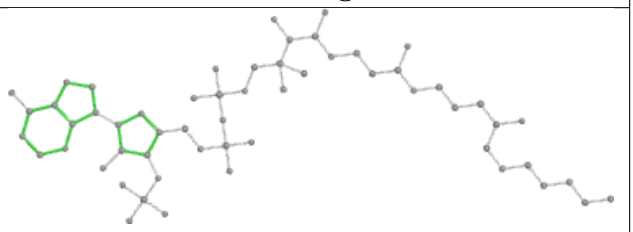
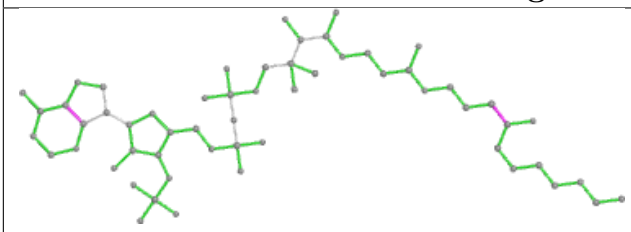
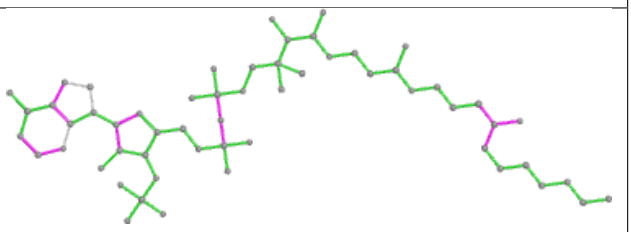
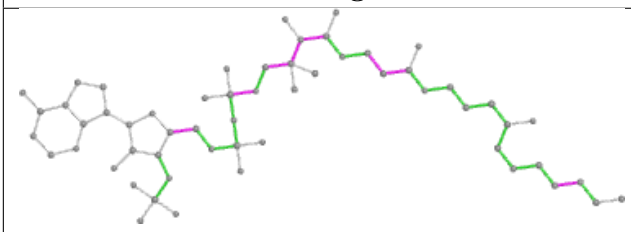
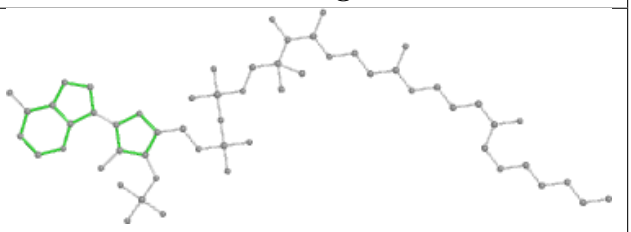
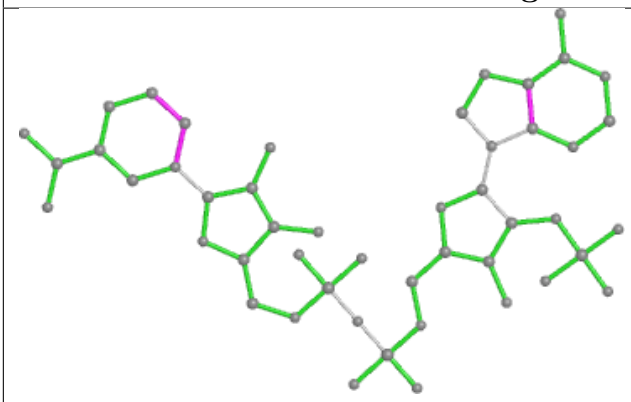
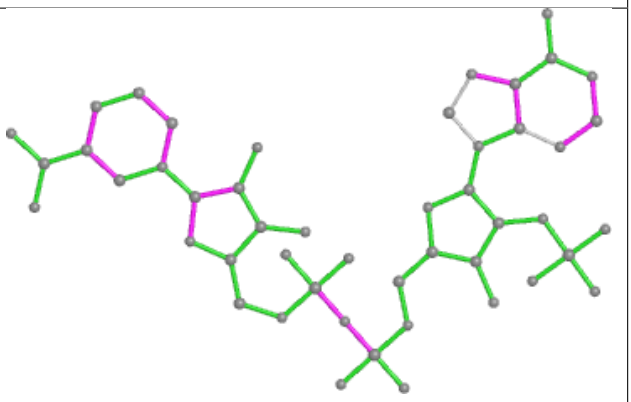
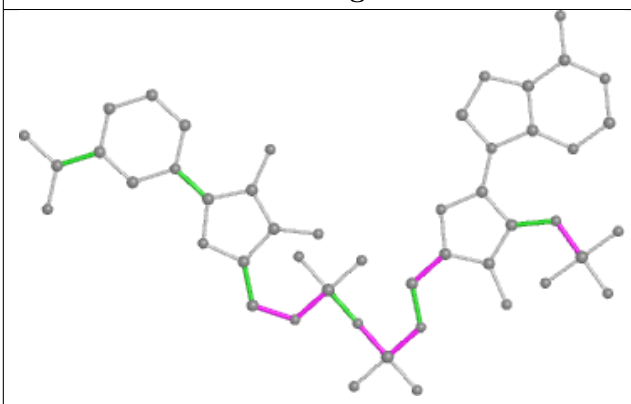
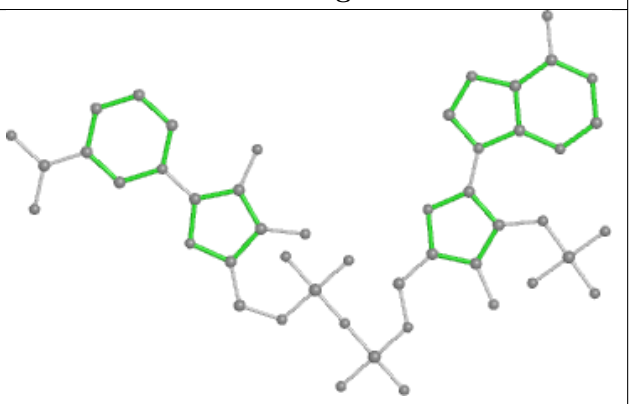
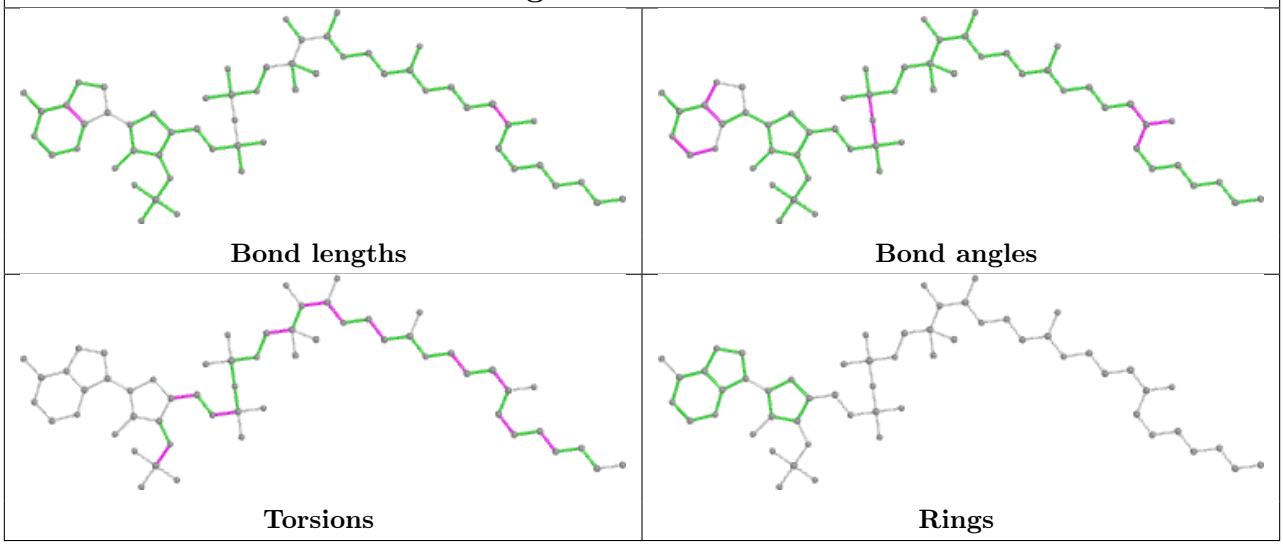


Rings

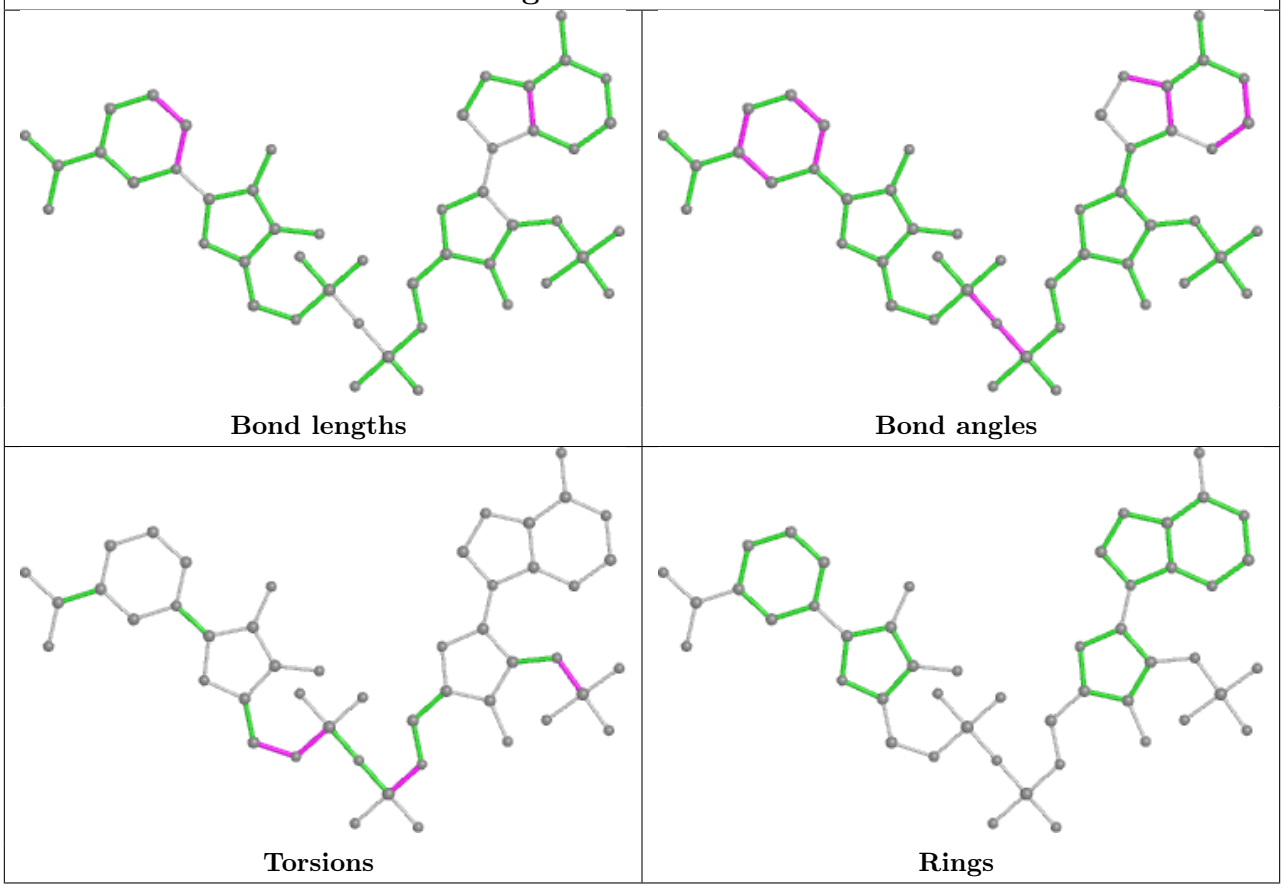
Ligand CO8 F 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand NAP A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CO8 D 802



Ligand NAP D 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

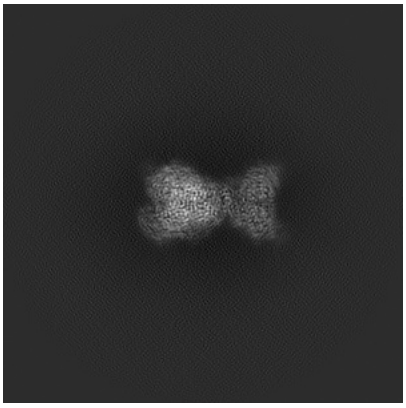
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-9875. These allow visual inspection of the internal detail of the map and identification of artifacts.

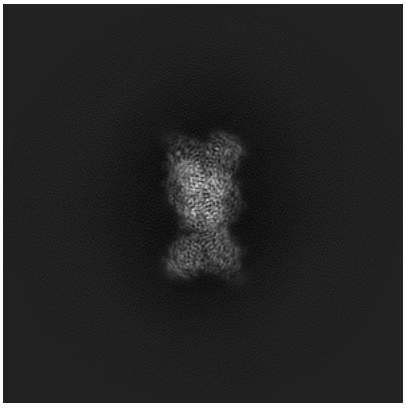
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

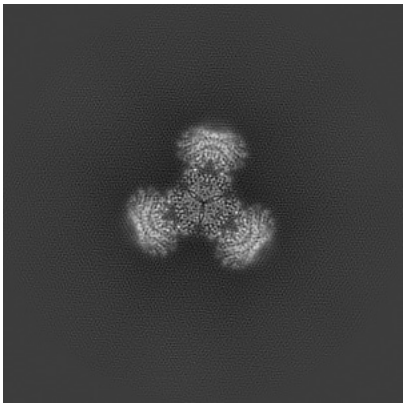
6.1.1 Primary map



X



Y

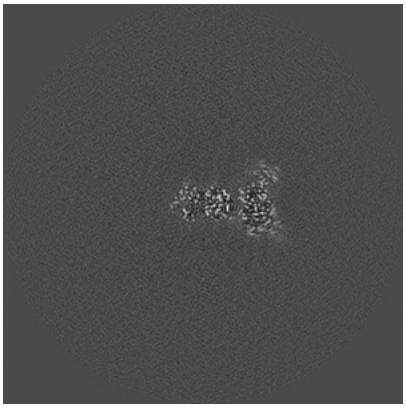


Z

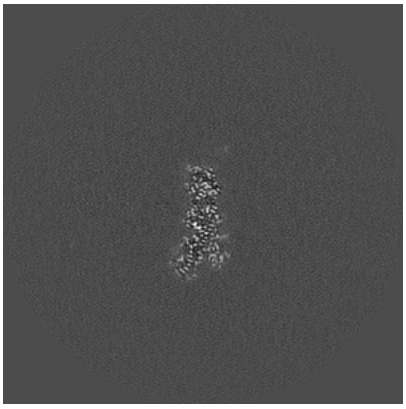
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

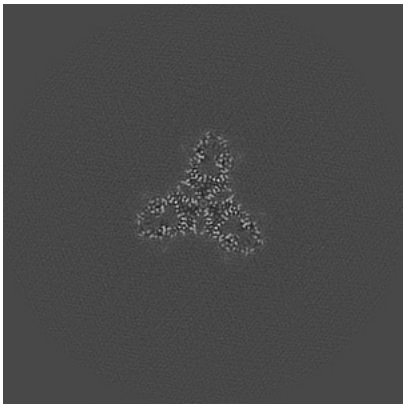
6.2.1 Primary map



X Index: 206



Y Index: 206

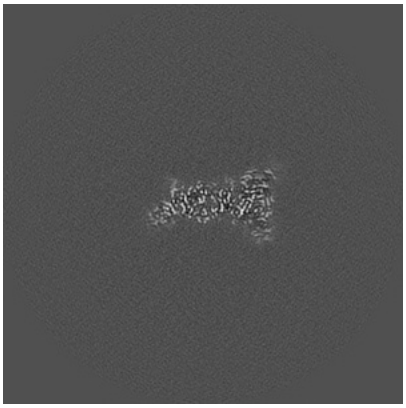


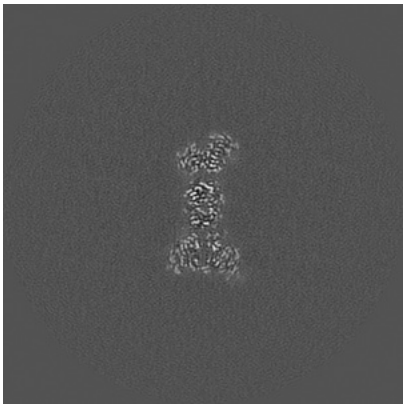
Z Index: 206

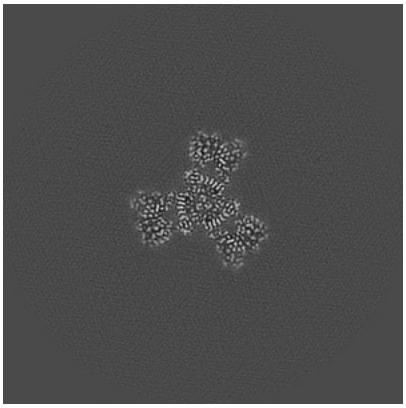
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 223

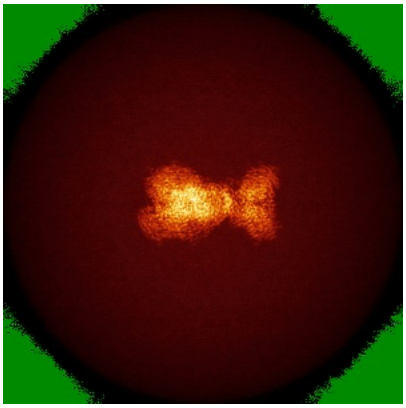

Y Index: 187

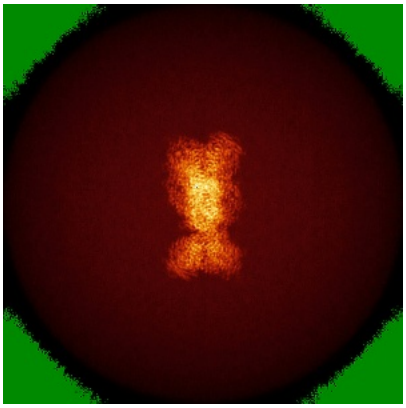

Z Index: 198

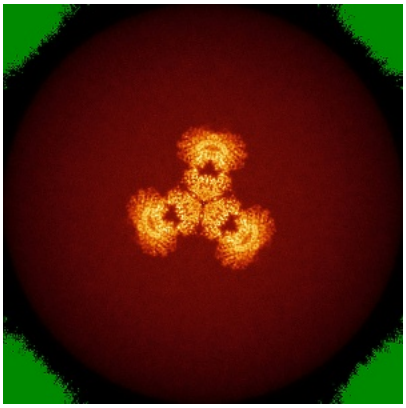
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

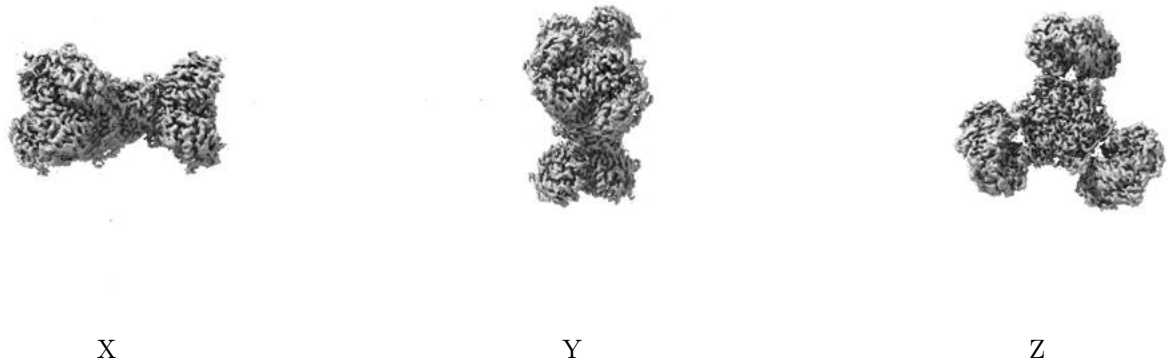

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

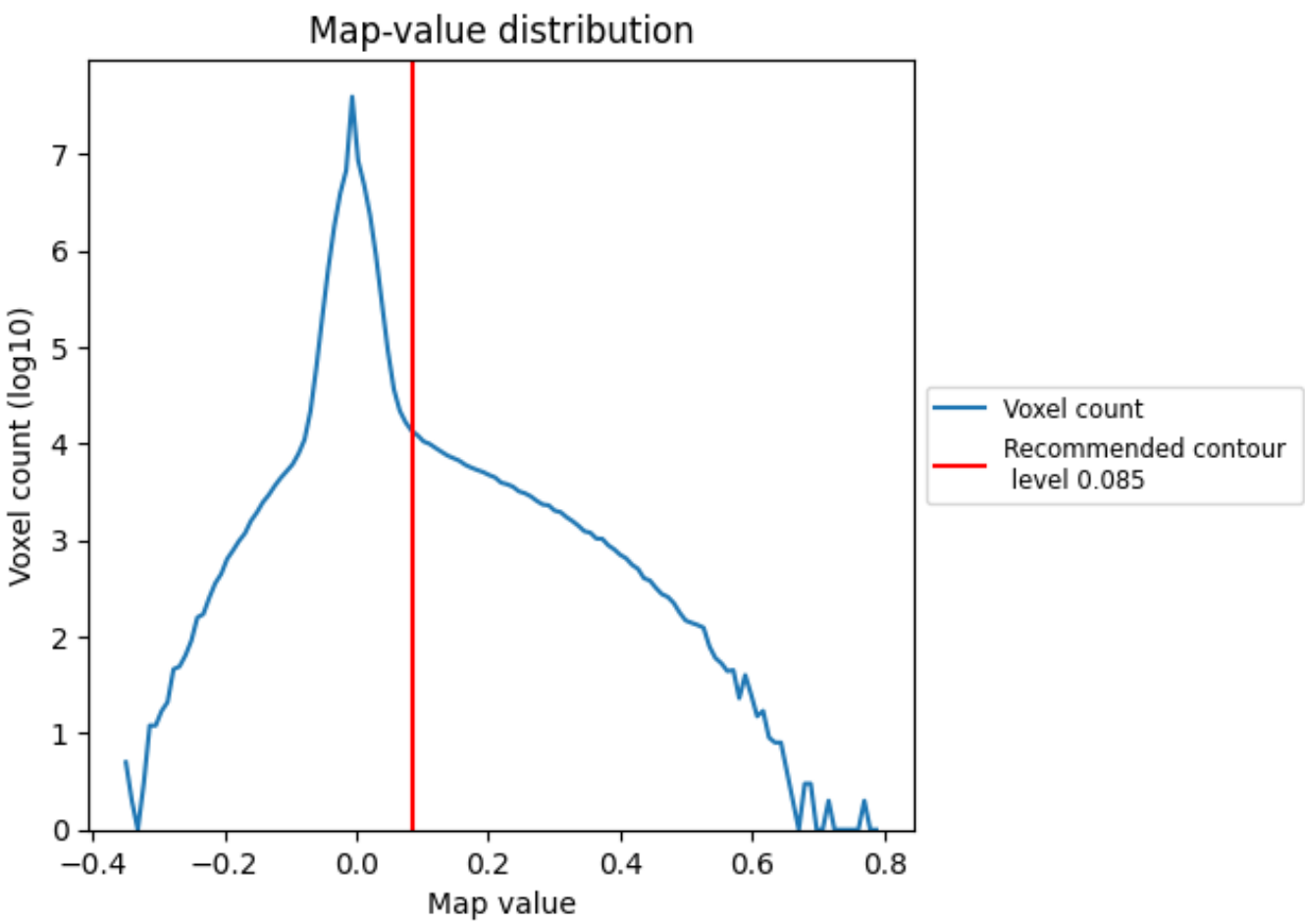
6.6 Mask visualisation (i)

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

7 Map analysis (i)

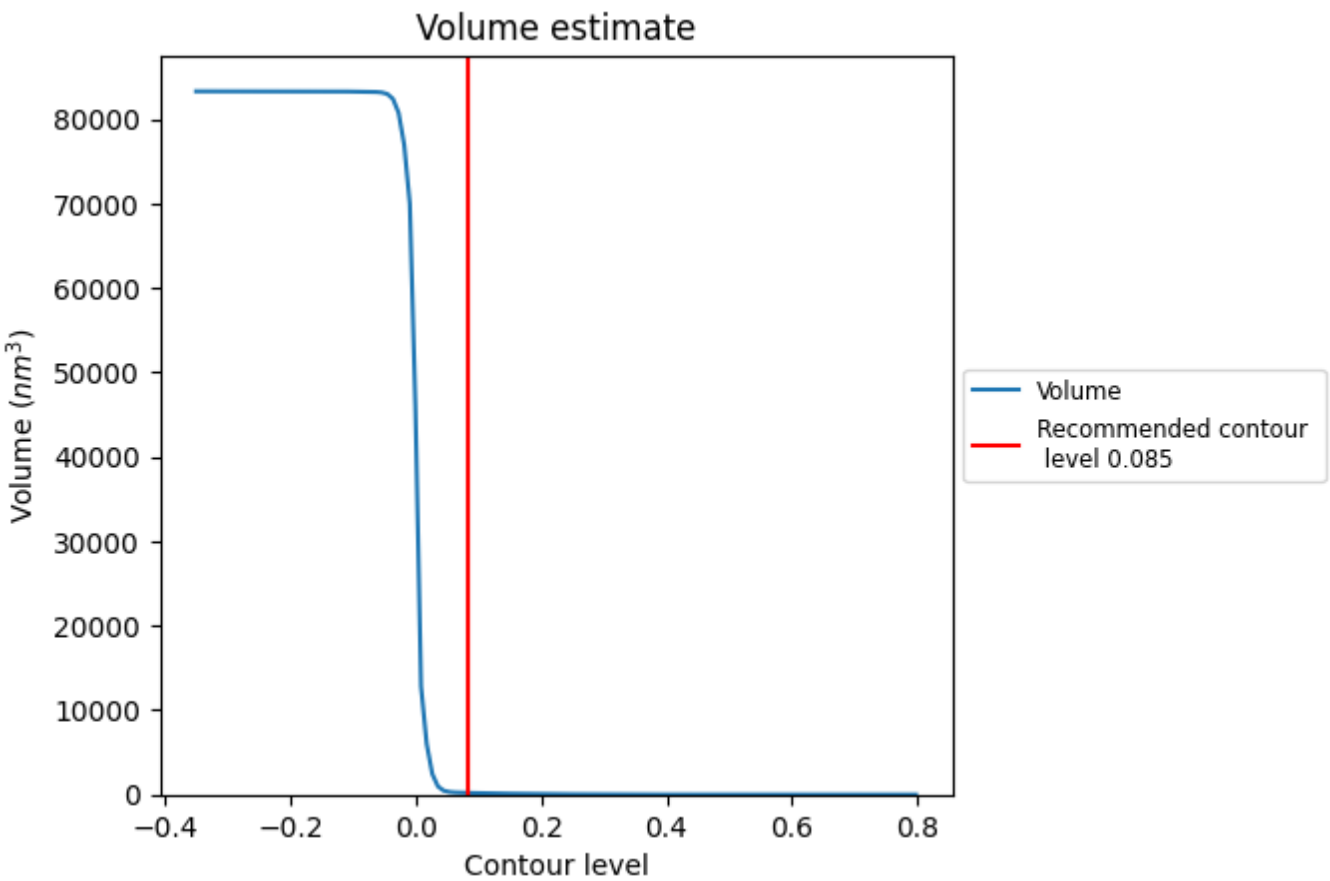
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

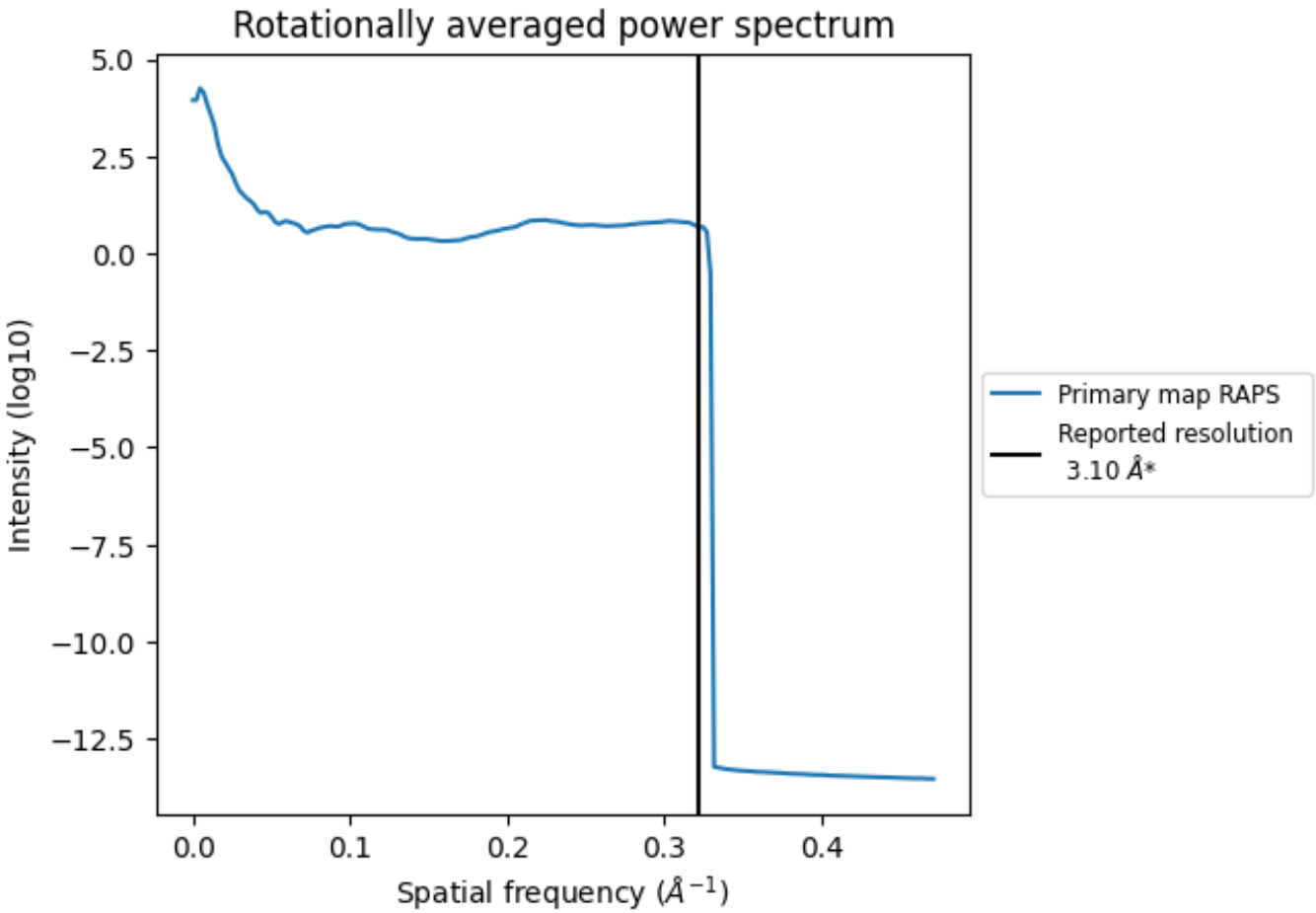
7.2 Volume estimate (i)



The volume at the recommended contour level is 193 nm^3; this corresponds to an approximate mass of 174 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)

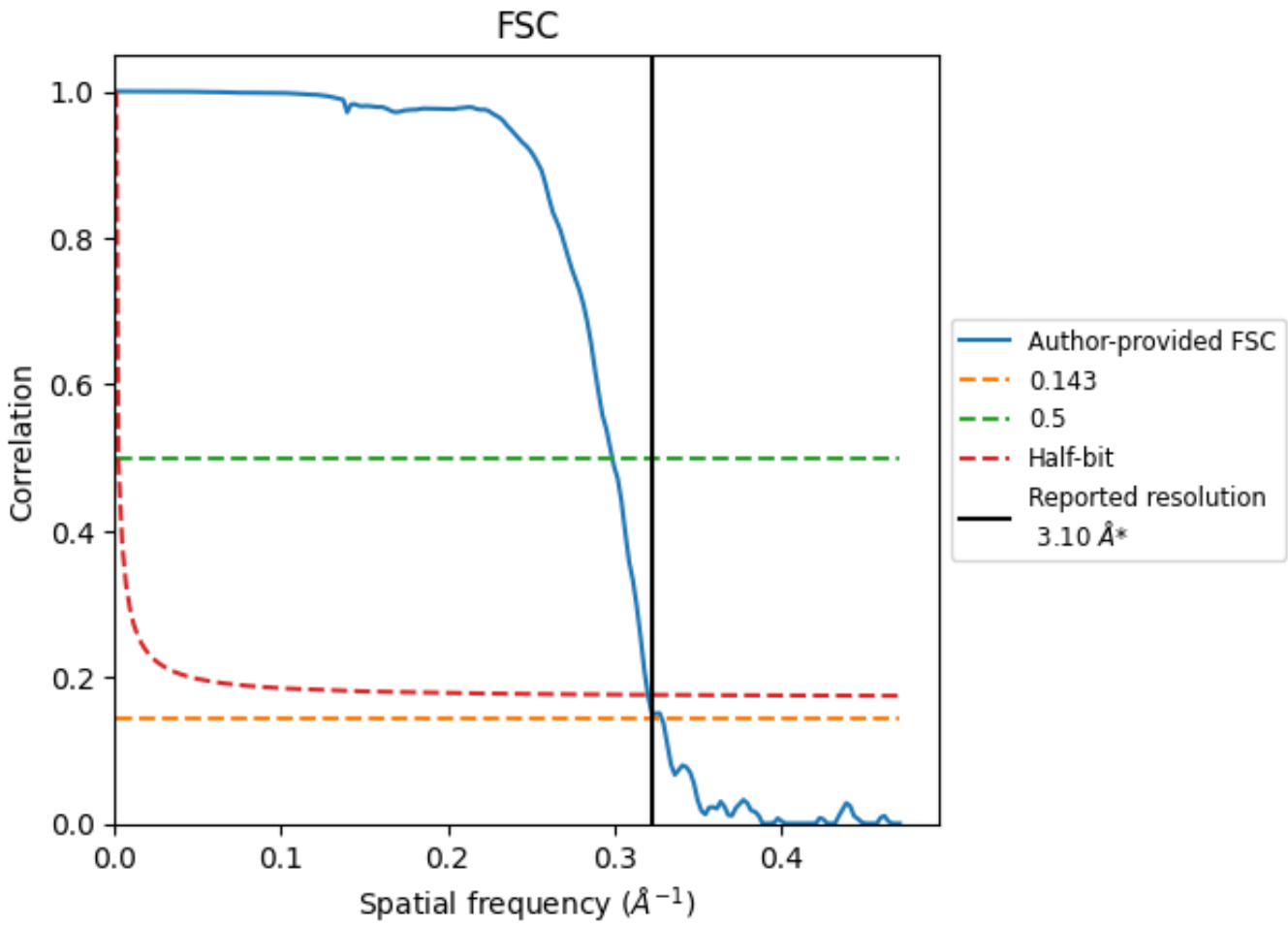


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

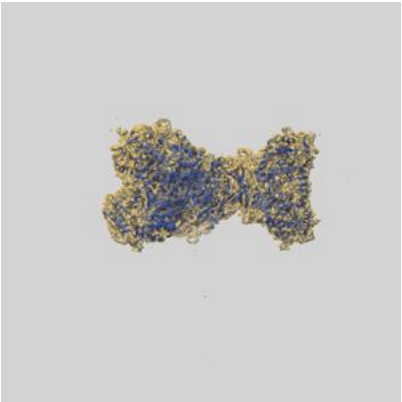
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.35	3.12
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

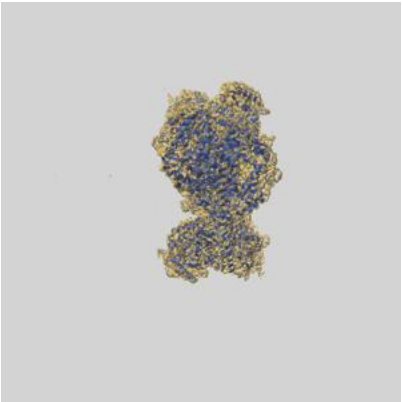
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-9875 and PDB model 6JQN. Per-residue inclusion information can be found in section 3 on page 7.

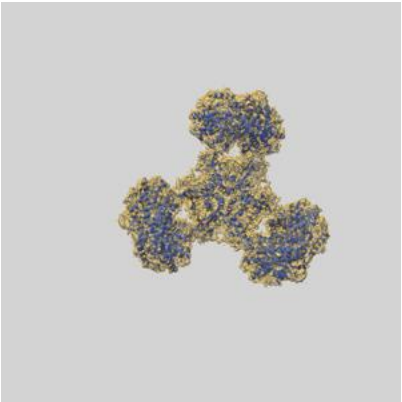
9.1 Map-model overlay (i)



X



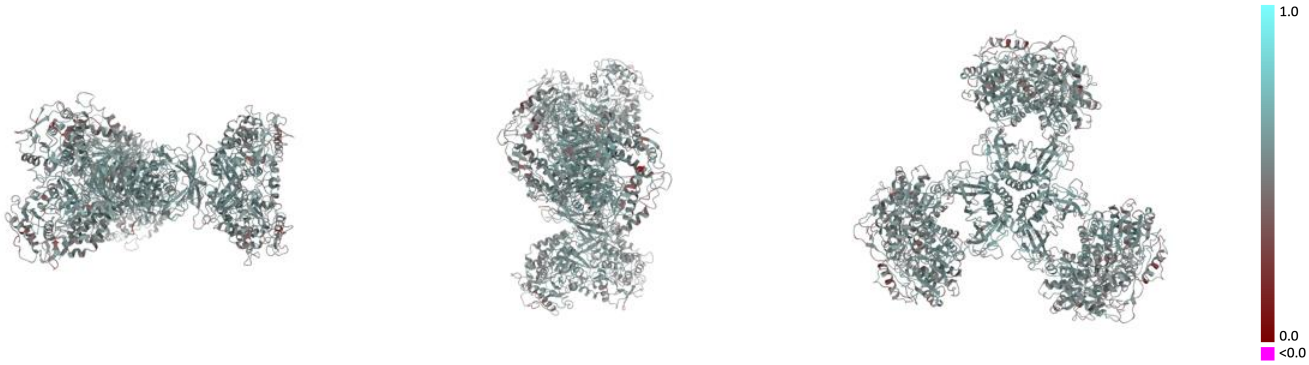
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085 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.

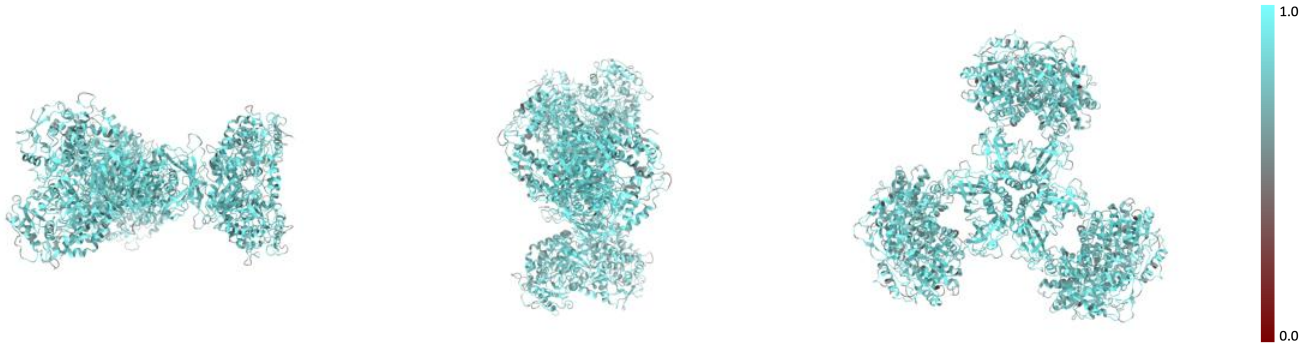
9.2 Q-score mapped to coordinate model (i)



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.

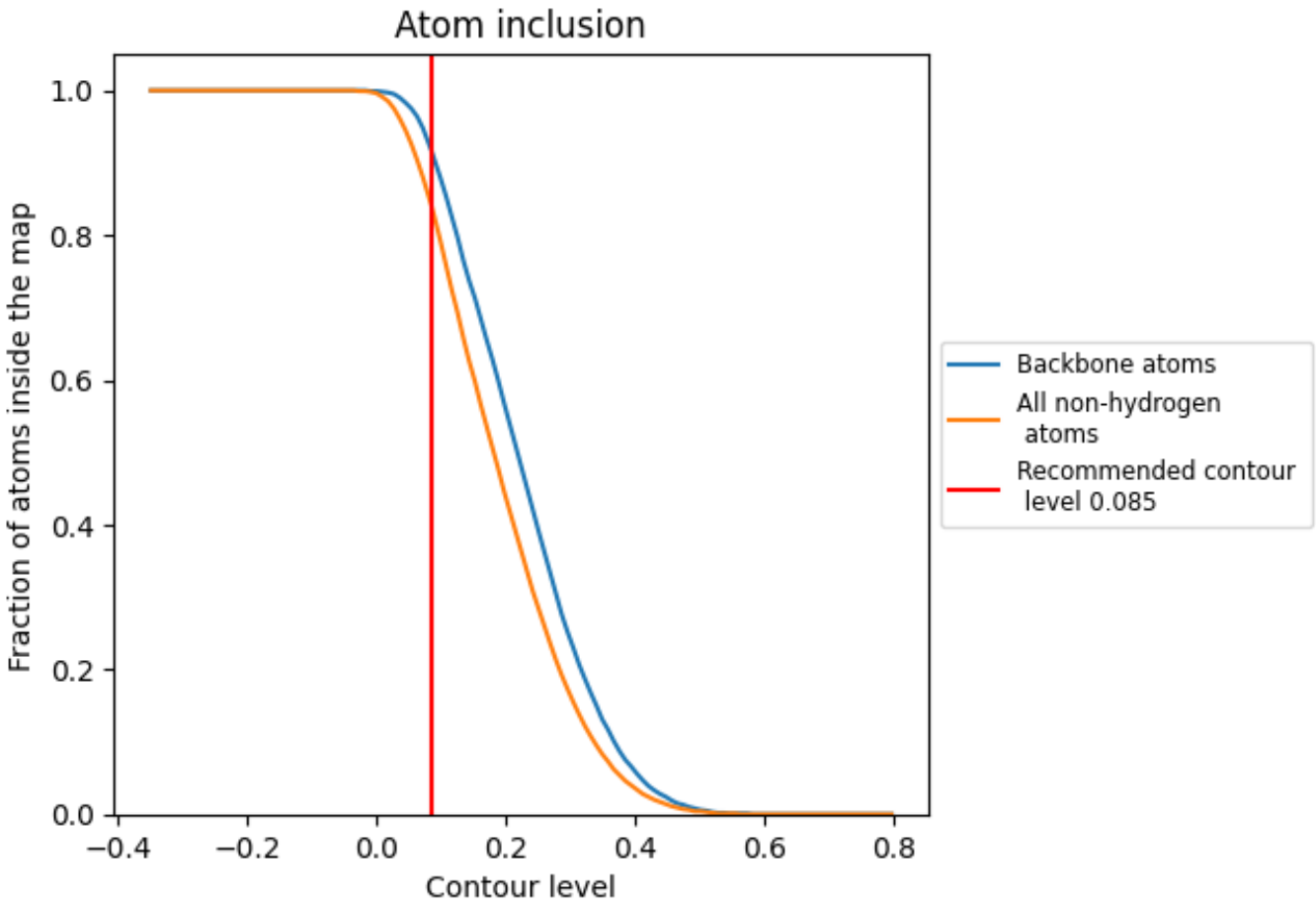
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.085).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.5340
A	0.8400	0.5330
B	0.8380	0.5340
C	0.8390	0.5330
D	0.8410	0.5330
E	0.8410	0.5330
F	0.8390	0.5350