Full wwPDB EM Validation Report (i)

Dec 10, 2022 – 07:25 pm GMT

PDB ID	:	6QS6
EMDB ID	:	EMD-4624
Title	:	ClpB (DWB and K476C mutant) bound to casein in presence of ATPgammaS - state KC-1
Authors	:	Deville, C.; Saibil, H.R.
Deposited on	:	2019-02-20
Resolution	:	3.90 Å(reported)
Based on initial model	:	1CIU

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:

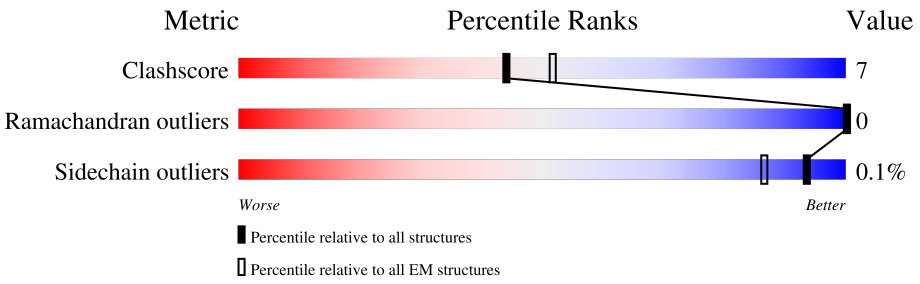
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.90 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	858	29% 56% 11% 33%
1	B	858	20% 55% 13% 32%
1	C	858	23% 58% 16% 27%
1	D	858	29% 58% 15% 27%
1	E	858	38% 55% 12% 33%
1	F	858	45% 56% 11% 33%
2	S	24	38% 100%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28557 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 Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	577	4538	2850	825	847	16	0	0
1	B	582	4562	2864	830	852	16	0	0
1	C	630	4976	3120	900	938	18	0	0
1	D	625	4952	3106	895	933	18	0	0
1	E	577	4538	2850	825	847	16	0	0
1	F	577	4538	2850	825	847	16	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	GLU	engineered mutation	UNP P63284
A	476	CYS	LYS	engineered mutation	UNP P63284
A	678	ALA	GLU	engineered mutation	UNP P63284
A	858	HIS	-	expression tag	UNP P63284
B	279	ALA	GLU	engineered mutation	UNP P63284
B	476	CYS	LYS	engineered mutation	UNP P63284
B	678	ALA	GLU	engineered mutation	UNP P63284
B	858	HIS	-	expression tag	UNP P63284
C	279	ALA	GLU	engineered mutation	UNP P63284
C	476	CYS	LYS	engineered mutation	UNP P63284
C	678	ALA	GLU	engineered mutation	UNP P63284
C	858	HIS	-	expression tag	UNP P63284
D	279	ALA	GLU	engineered mutation	UNP P63284
D	476	CYS	LYS	engineered mutation	UNP P63284
D	678	ALA	GLU	engineered mutation	UNP P63284
D	858	HIS	-	expression tag	UNP P63284
E	279	ALA	GLU	engineered mutation	UNP P63284
E	476	CYS	LYS	engineered mutation	UNP P63284

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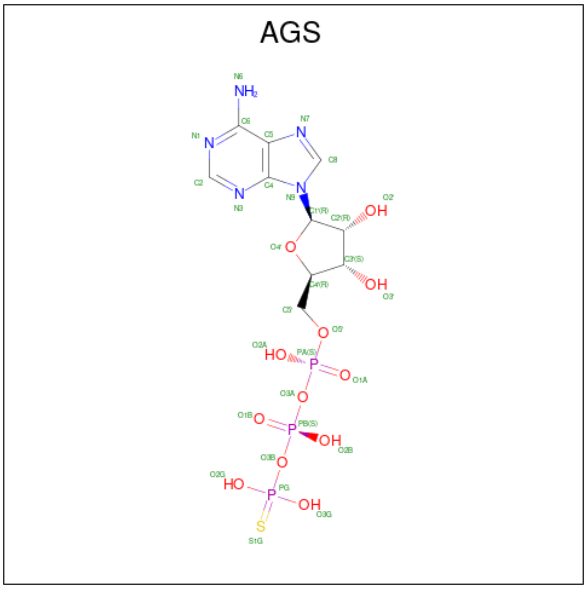
Chain	Residue	Modelled	Actual	Comment	Reference
E	678	ALA	GLU	engineered mutation	UNP P63284
E	858	HIS	-	expression tag	UNP P63284
F	279	ALA	GLU	engineered mutation	UNP P63284
F	476	CYS	LYS	engineered mutation	UNP P63284
F	678	ALA	GLU	engineered mutation	UNP P63284
F	858	HIS	-	expression tag	UNP P63284

- Molecule 2 is a protein called casein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	S	24	120	72	24	24	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	A	1	31	10	5	12	3	1	0
3	B	1	62	20	10	24	6	2	0
3	B	1	62	20	10	24	6	2	0
3	C	1	62	20	10	24	6	2	0
3	C	1	62	20	10	24	6	2	0

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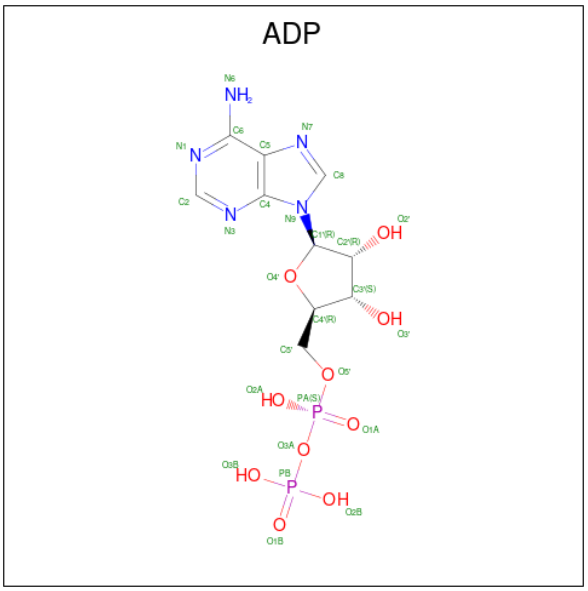
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	D	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
3	D	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
3	E	1	62	20	10	24	6	2	0
			Total	C	N	O	P	S	
3	E	1	62	20	10	24	6	2	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



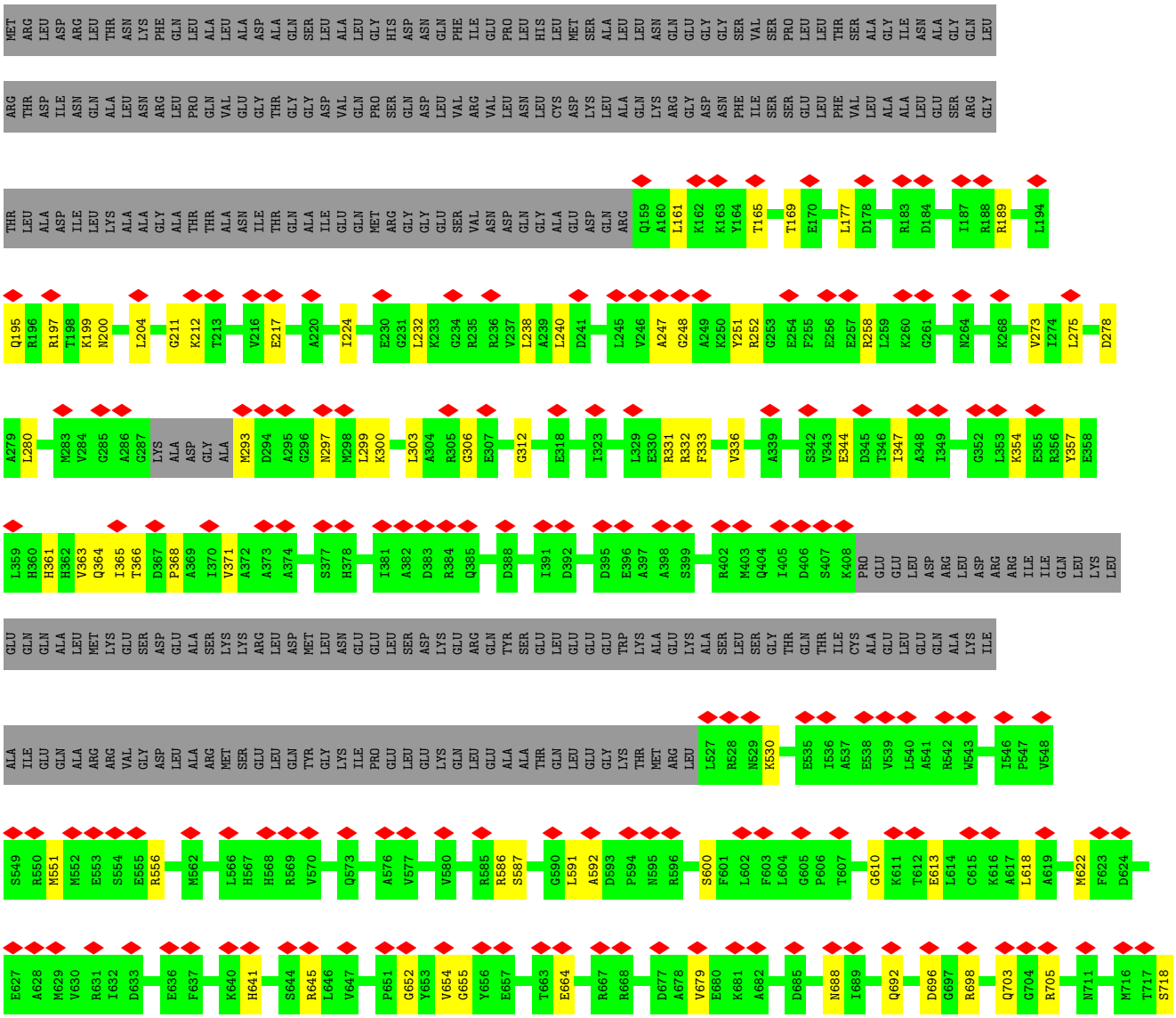
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	F	1	27	10	5	10	2	0

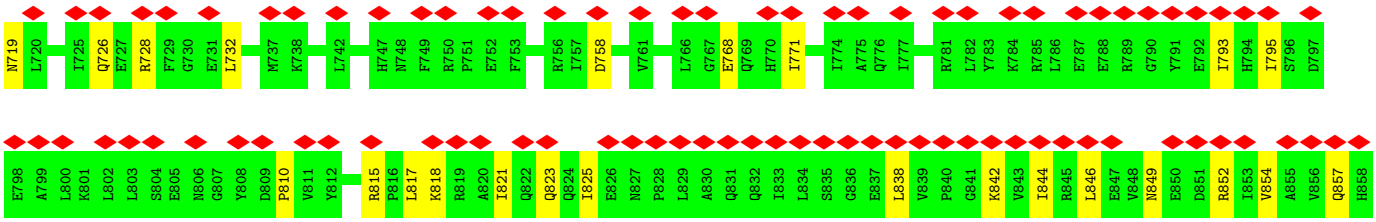
3 Residue-property plots (i)

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: Chaperone protein ClpB

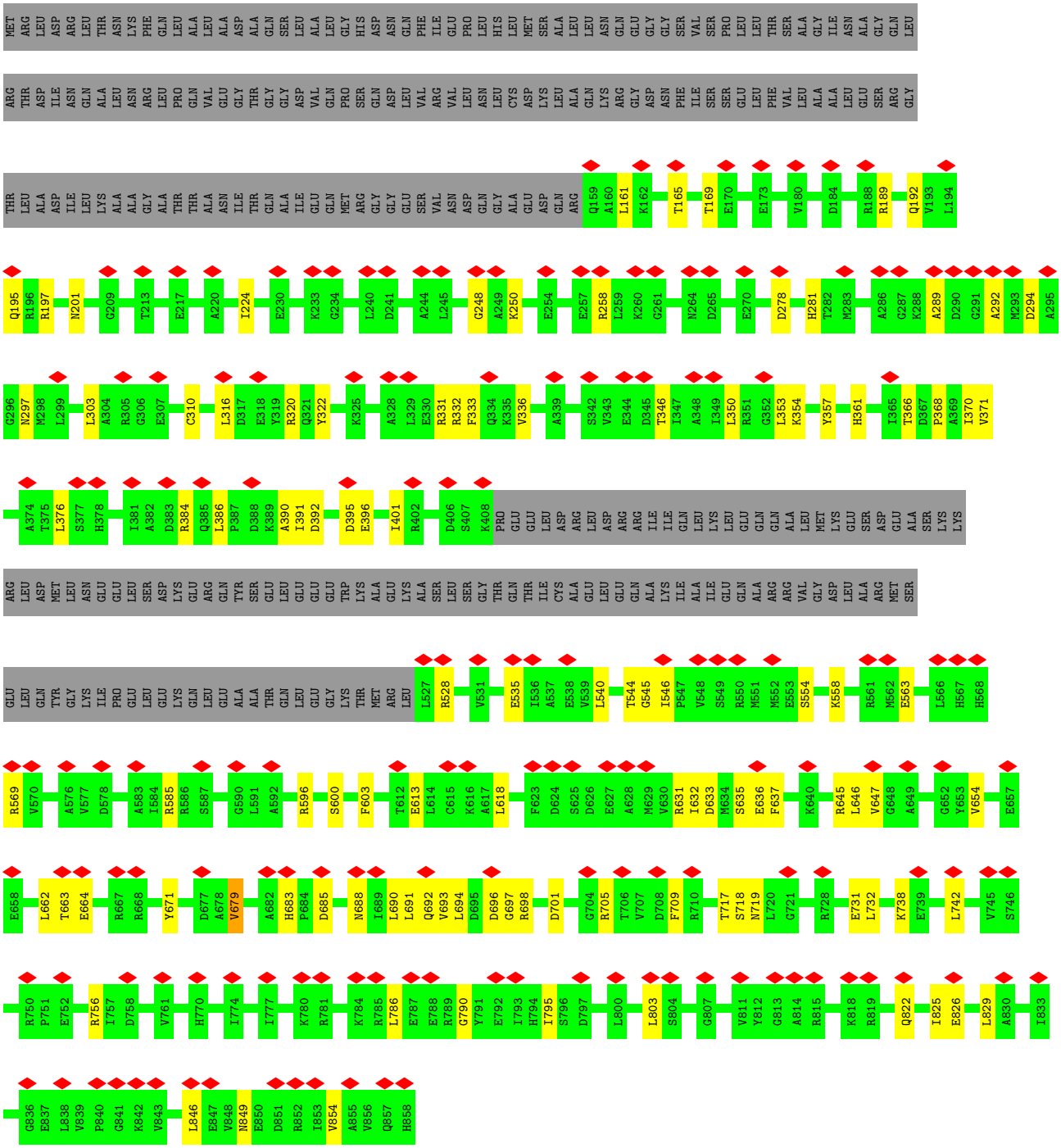
Chain A: 29% 56% 11% 33%





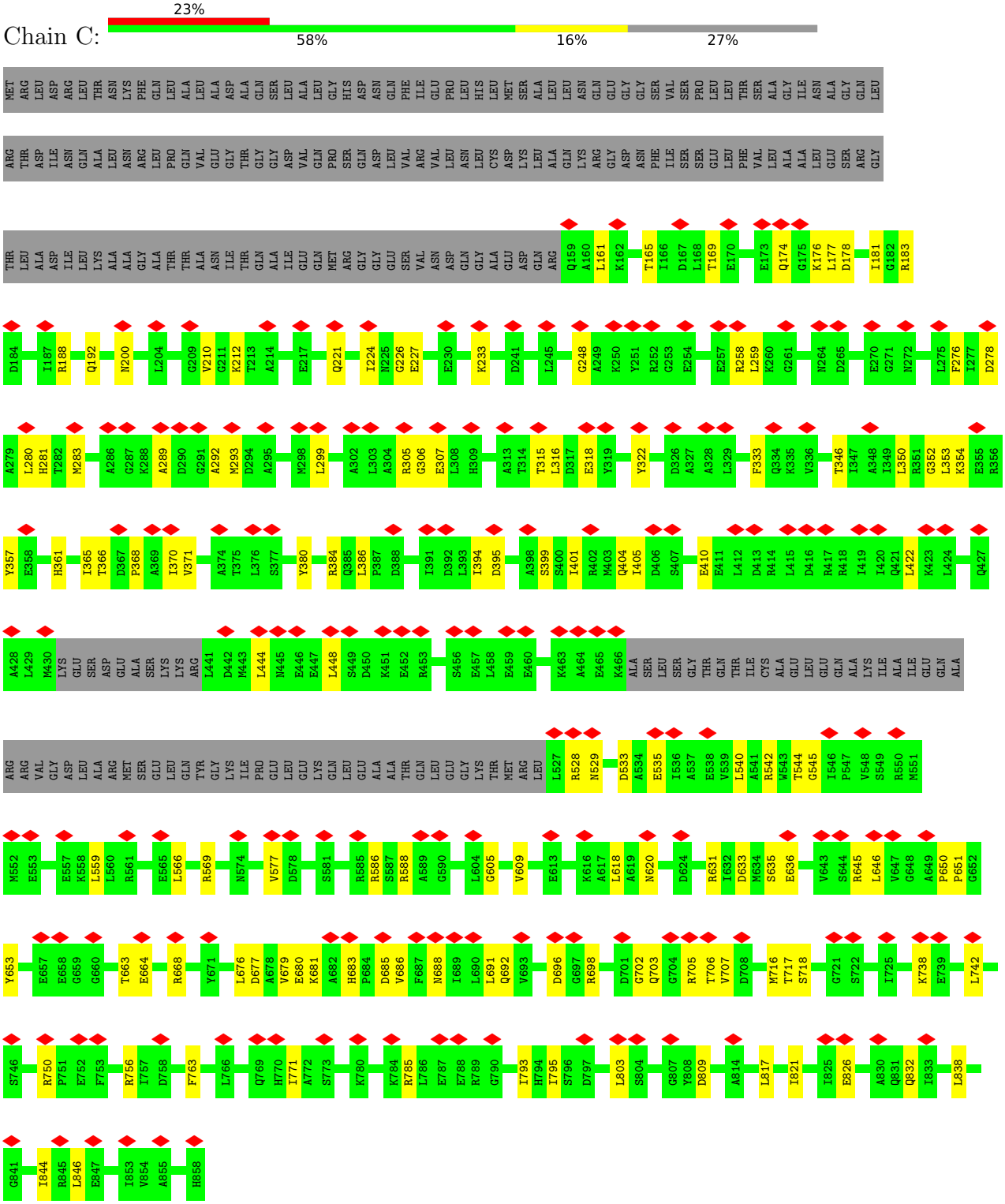
- Molecule 1: Chaperone protein ClpB

Chain B:



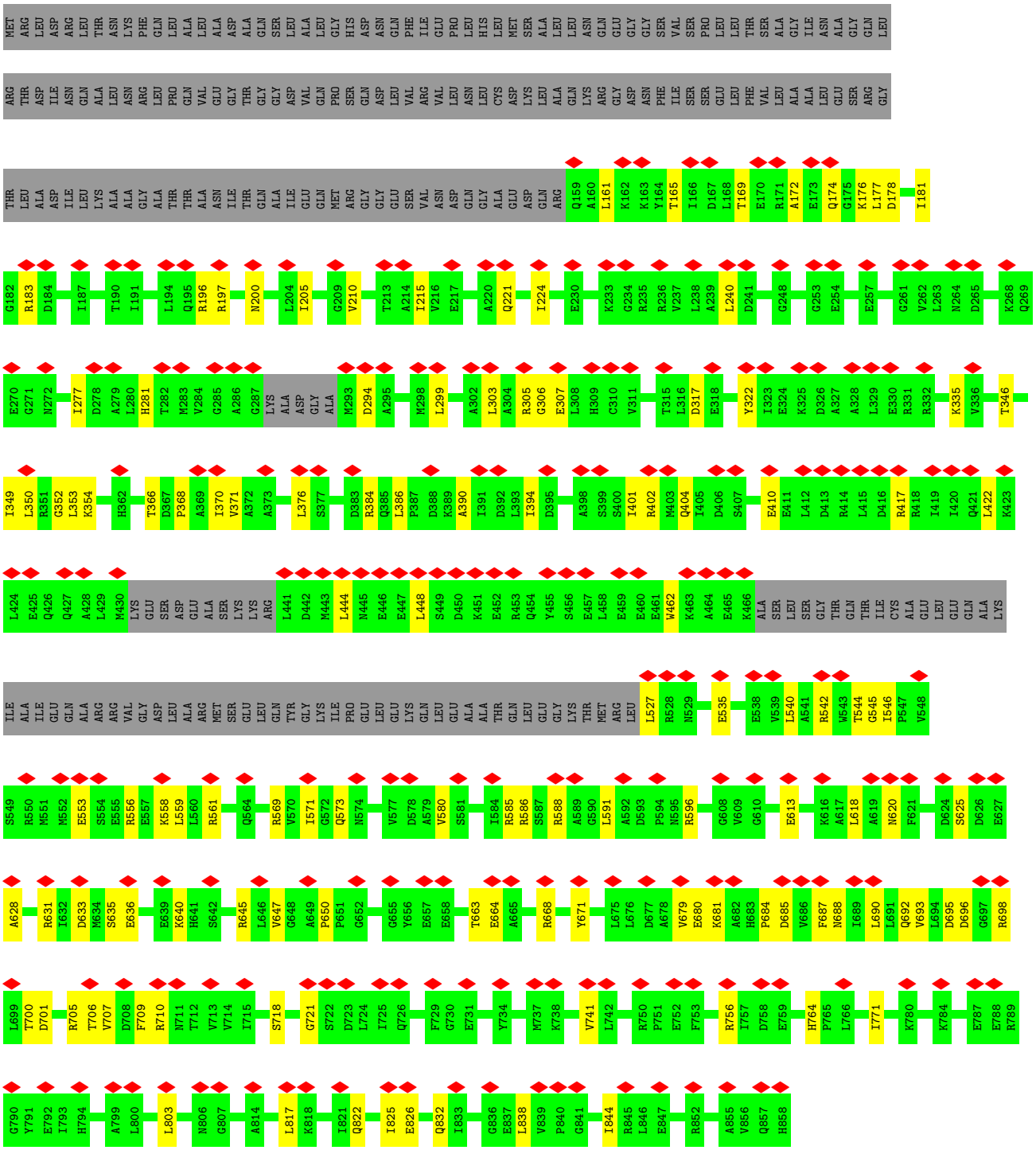
- Molecule 1: Chaperone protein ClpB

Chain C:



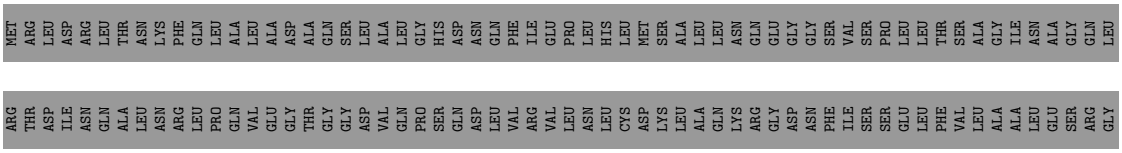
- Molecule 1: Chaperone protein ClpB

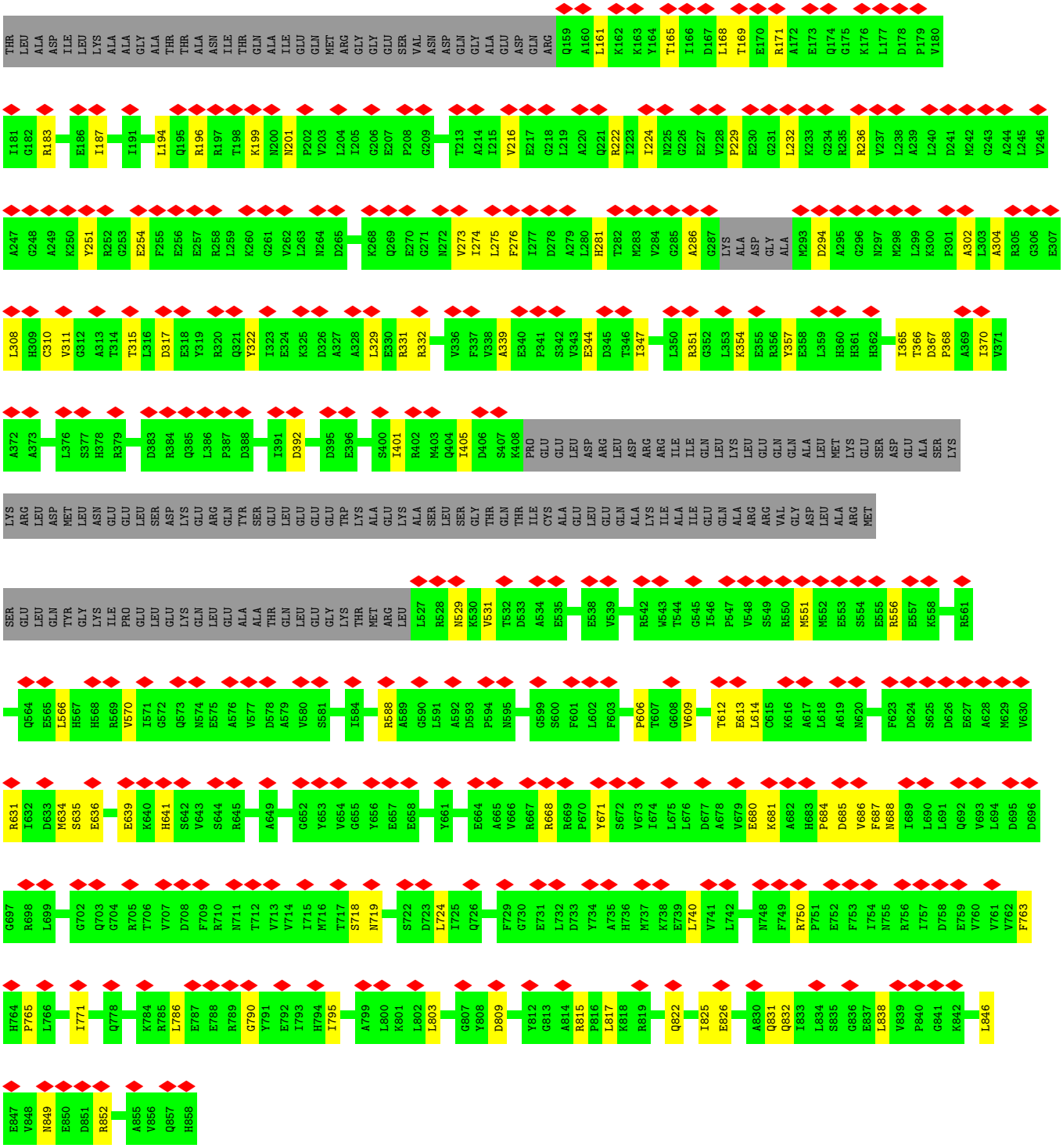
Chain D:



- Molecule 1: Chaperone protein ClpB

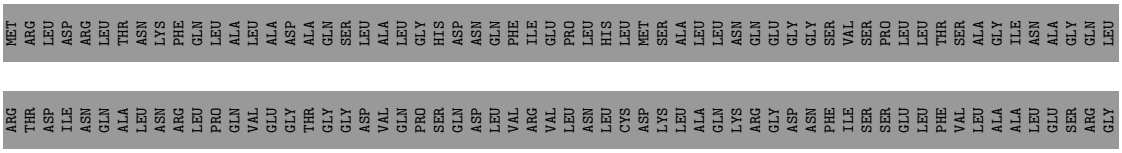
Chain E:





- Molecule 1: Chaperone protein ClpB

Chain F:



THR LEU ALA ASP ILE LEU LYS ALA ALA GLY ALA THR THR ALA ASN ILE THR GLN ALA ILE GLU GLN MET ARG GLY GLY GLU SER VAL ASN ASP GLN GLY ALA GLU ASP GLN ARG Q159 A160 L161 K162 K163 Y164 T165 I166 D167 L168 T169 E170 R171 A172 E173 Q174 G175 K176 L177 D178 P179 V180

R183 E186 I187 T190 R197 T198 K199 N200 G206 E207 P208 G209 T213 A214 E217 A220 Q221 R222 I223 I224 N225 G226 E227 V228 P229 E230 K233 G234 R235 R236 V237 L238 A239 L240 D241 M242 G243 A244 L245 V246 A247 G248 A249 K250 Y251 R252 G253 E254 F255 E256 E257

R258 L259 K260 G261 N264 D265 L266 A267 K268 Q269 E270 L275 F276 I277 D278 A279 L280 H281 T282 M283 V284 G285 A286 G287 LYS ALA ASP GLY ALA M293 D294 N297 M298 L299 K300 P301 A302 L303 A304 R305 G306 E307 L308 H309 C310 V311 G312 A313 E318 Y319 Y322 I323 E324 K325 D326

L329 E330 R331 R332 V336 F337 V338 A339 E340 P341 S342 V343 E344 D345 T346 I347 A348 I349 L350 L353 K354 E355 R356 Y357 E358 L359 H360 H361 H362 V363 Q364 I365 T366 D367 P368 A369 I370 V371 A372 A373 A374 T375 L376 S377 H378 R379 Y380 I381 A382 D383 R384 Q385 D388 K389 A390 I391

D392 D395 E396 S399 S400 I401 R402 M403 Q404 I405 D406 S407 K408 PRO GLU GLU LEU ASP ARG LEU ASP ARG ARG ILE ILE GLN LEU LYS LEU GLU GLN GLN ALA LEU MET LYS GLU SER ASP GLU ALA SER LYS LYS ARG LEU ASP MET LEU ASN GLU GLU LEU SER ASP LYS GLU ARG

GLN TYR SER GLU LEU GLU GLU GLU TRP LYS ALA GLU LYS ALA SER LEU SER GLY THR GLN THR ILE CYS ALA GLU LEU GLU ASP ALA LYS ILE ALA ILE GLU GLN GLN ALA ARG ARG VAL GLY ASP LEU ALA ARG MET SER GLU LEU GLN TYR GLY LYS ILE PRO GLU LEU GLU LYS GLN LEU

GLU ALA ALA THR GLN LEU GLU GLY LYS THR MET ARG LEU L527 R528 N529 K530 V531 A534 E535 E538 V539 L540 A541 R542 W543 T544 G545 I546 R550 M551 M552 E553 S554 E555 R556 E557 K558 L559 L560 R561 M562 E563 Q564 E565 L566 H567 H568 R569 V570 I571 G572 Q573 N574 E575 A576 V577

V580 S581 N582 A583 I584 R585 R586 S587 R588 A589 G590 L591 A592 D593 P594 N595 R596 P597 I598 G599 S600 F601 L602 F603 L604 G605 P606 T607 G608 V609 G610 K611 T612 E613 K616 A619 M620 F621 M622 F623 D624 S625 D626 E627 A628 M629 V630 R631 I632 D633 M634 S635 E636 F637 M638 E639 K640

H641 S642 V643 S644 R645 G648 A649 P650 P651 G652 Y653 V654 G655 Y656 E657 E658 G659 G660 Y661 L662 T663 E664 A665 V666 R667 R668 R669 S672 V673 I674 L675 L676 D677 A678 V679 E680 K681 A682 H683 P684 D685 V686 F687 N688 I689 L690 L691 Q692 V693 L694 D695 D696 G697 R698 L699 T700 D701 G702

Q703 G704 R705 T706 V707 D708 F709 R710 N711 T712 V713 V714 I715 M716 T717 S718 N719 L720 G721 S722 D723 L724 I725 Q726 E727 R728 F729 G730 E731 L732 D733 Y734 A735 H736 M737 K738 E739 L740 V741 L742 G743 V744 V745 S746 H747 N748 F749 R750 P751 E752 F753 I754 N755 R756 I757 D758 E759 V760 V761 V762

F763 H764 P765 L766 G767 E768 Q769 H770 I771 Q778 R781 L782 R785 L786 E787 E788 R789 G790 Y791 E792 I793 H794 I795 A799 L800 K801 L802 L803 N806 G807 Y808 D809 P810 V811 Y812 G813 A814 R815 R819 A820 I821 Q822 I825 E826 N827 P828 L829 A830 L834 S835 G836 E837

L838 V839 P840 G841 K842 V843 I844 R845 L846 E847 V848 N849 E850 D851 R852 I853 V854 A855 V856 Q857 H858

- Molecule 2: casein

Chain S: 38% 100%

X1 X2 X3 X10 X11 X12 X13 X14 X15 X22 X23 X24

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77469	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: AGS, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.43	0/4605	0.57	0/6213
1	B	0.56	0/4630	0.66	2/6249 (0.0%)
1	C	0.61	0/5047	0.69	2/6805 (0.0%)
1	D	0.53	1/5022 (0.0%)	0.67	2/6769 (0.0%)
1	E	0.38	0/4605	0.57	1/6213 (0.0%)
1	F	0.29	0/4605	0.51	0/6213
All	All	0.48	1/28514 (0.0%)	0.62	7/38462 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	580	VAL	CB-CG1	-5.12	1.42	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	618	LEU	CB-CG-CD1	-6.42	100.09	111.00
1	B	618	LEU	CB-CG-CD2	-5.51	101.62	111.00
1	B	353	LEU	CA-CB-CG	-5.45	102.77	115.30
1	C	646	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	618	LEU	CB-CG-CD2	-5.12	102.29	111.00
1	D	353	LEU	CA-CB-CG	-5.11	103.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	329	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	293	MET	Peptide
1	C	685	ASP	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4538	0	4603	67	0
1	B	4562	0	4624	78	0
1	C	4976	0	5031	89	0
1	D	4952	0	5014	88	0
1	E	4538	0	4604	62	0
1	F	4538	0	4604	58	0
2	S	120	0	29	0	0
3	A	31	0	11	3	0
3	B	62	0	23	4	0
3	C	62	0	24	7	0
3	D	62	0	24	6	0
3	E	62	0	23	6	0
4	A	27	0	10	0	0
4	F	27	0	10	0	0
All	All	28557	0	28634	393	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 7.

All (393) 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:B:692:GLN:HE22	1:C:636:GLU:HG3	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLY:H	1:B:258:ARG:HH12	1.35	0.73
1:D:573:GLN:HE22	1:D:764:HIS:H	1.39	0.71
1:C:692:GLN:HE22	1:D:636:GLU:HG3	1.55	0.70
1:B:366:THR:HG22	1:B:368:PRO:HD2	1.73	0.68
1:A:366:THR:HG22	1:A:368:PRO:HD2	1.76	0.68
1:C:366:THR:HG22	1:C:368:PRO:HD2	1.74	0.68
1:C:688:ASN:HB3	1:D:635:SER:HB2	1.75	0.68
1:A:688:ASN:HB3	1:B:635:SER:HB2	1.76	0.68
1:D:688:ASN:HB3	1:E:635:SER:HB2	1.76	0.67
1:D:366:THR:HG22	1:D:368:PRO:HD2	1.77	0.66
1:A:357:TYR:HE1	1:F:197:ARG:HE	1.42	0.65
1:A:692:GLN:NE2	1:B:635:SER:OG	2.28	0.65
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.77	0.64
1:C:227:GLU:HB3	1:D:417:ARG:HH22	1.62	0.64
1:B:698:ARG:NH1	1:C:633:ASP:OD2	2.31	0.64
1:B:331:ARG:NH1	3:C:1001:AGS:S1G	2.71	0.63
1:A:692:GLN:HE22	1:B:636:GLU:HG3	1.64	0.63
1:B:756:ARG:NH2	3:C:1002:AGS:S1G	2.70	0.62
1:C:679:VAL:HG12	1:C:718:SER:HB2	1.82	0.62
1:A:645:ARG:HA	1:F:651:PRO:HD2	1.81	0.62
1:B:546:ILE:HG13	1:B:671:TYR:HB2	1.81	0.61
1:F:310:CYS:SG	1:F:311:VAL:N	2.73	0.61
1:F:821:ILE:HG23	1:F:825:ILE:HD12	1.82	0.61
1:C:692:GLN:NE2	1:D:635:SER:OG	2.33	0.61
1:C:354:LYS:HB2	1:C:370:ILE:HD11	1.83	0.60
1:B:361:HIS:NE2	1:B:395:ASP:OD1	2.30	0.60
3:D:902:AGS:O2B	3:D:902:AGS:O2A	2.19	0.60
1:B:376:LEU:HB3	1:B:540:LEU:HD22	1.83	0.60
1:A:331:ARG:NH1	3:B:1001:AGS:S1G	2.75	0.59
1:B:822:GLN:O	1:B:826:GLU:HB2	2.02	0.59
1:E:566:LEU:O	1:E:570:VAL:N	2.35	0.59
1:D:174:GLN:OE1	1:D:176:LYS:NZ	2.36	0.58
1:A:821:ILE:HG23	1:A:825:ILE:HD12	1.85	0.58
1:C:544:THR:OG1	1:C:545:GLY:N	2.36	0.58
1:D:692:GLN:NE2	1:E:635:SER:OG	2.36	0.58
1:F:628:ALA:HB1	1:F:672:SER:HA	1.85	0.58
1:B:192:GLN:HE22	1:C:542:ARG:HH22	1.51	0.58
1:F:183:ARG:NH2	1:F:339:ALA:O	2.36	0.58
1:A:169:THR:HB	1:A:224:ILE:HD11	1.86	0.58
1:C:785:ARG:NH2	1:C:826:GLU:OE2	2.37	0.57
1:A:664:GLU:OE2	1:A:705:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:582:ASN:OD1	1:F:585:ARG:NH2	2.38	0.57
1:B:600:SER:HB2	1:B:694:LEU:HD22	1.86	0.57
1:B:281:HIS:HB2	1:B:322:TYR:HD2	1.70	0.57
1:B:569:ARG:NH2	1:B:613:GLU:OE1	2.36	0.57
1:D:197:ARG:HE	1:E:357:TYR:HE1	1.51	0.57
1:B:696:ASP:OD2	1:C:631:ARG:NH1	2.34	0.57
1:D:640:LYS:NZ	1:E:639:GLU:OE2	2.38	0.57
1:C:404:GLN:NE2	1:C:410:GLU:OE1	2.38	0.56
1:D:346:THR:HG21	1:D:386:LEU:HD22	1.86	0.56
1:A:586:ARG:HH12	1:B:822:GLN:HE21	1.53	0.56
1:C:174:GLN:OE1	1:C:176:LYS:NZ	2.38	0.56
1:D:664:GLU:OE2	1:D:705:ARG:NH2	2.39	0.56
1:A:679:VAL:HG12	1:A:718:SER:HB2	1.89	0.55
1:F:172:ALA:HB2	1:F:177:LEU:HD12	1.88	0.55
1:B:690:LEU:HA	1:B:693:VAL:HB	1.87	0.55
1:C:248:GLY:H	1:C:258:ARG:HH12	1.53	0.55
1:A:703:GLN:OE1	1:A:705:ARG:NH1	2.35	0.55
3:B:1001:AGS:O1B	3:B:1001:AGS:O2G	2.24	0.55
3:C:1002:AGS:O1B	3:C:1002:AGS:O2G	2.23	0.55
1:B:350:LEU:HD11	1:B:390:ALA:HB1	1.88	0.55
3:B:1002:AGS:O2G	3:B:1002:AGS:O1B	2.23	0.55
3:C:1002:AGS:O2B	3:C:1002:AGS:O2A	2.24	0.55
1:E:634:MET:HE1	1:E:686:VAL:HG11	1.87	0.55
1:A:211:GLY:HA3	3:A:1001:AGS:H8	1.89	0.55
1:D:350:LEU:HD11	1:D:390:ALA:HB1	1.89	0.55
1:D:692:GLN:HE22	1:E:636:GLU:HG3	1.72	0.55
1:C:528:ARG:NH2	1:C:535:GLU:OE2	2.39	0.55
1:D:680:GLU:OE2	1:D:681:LYS:NZ	2.40	0.55
1:D:696:ASP:OD2	1:E:631:ARG:NH2	2.38	0.55
1:F:571:ILE:O	1:F:770:HIS:NE2	2.39	0.55
1:B:169:THR:HB	1:B:224:ILE:HD11	1.88	0.55
1:F:563:GLU:OE2	1:F:585:ARG:NH1	2.39	0.55
1:A:726:GLN:NE2	1:A:810:PRO:O	2.41	0.54
1:D:663:THR:HB	1:D:707:VAL:HG21	1.88	0.54
1:A:199:LYS:NZ	1:B:392:ASP:OD2	2.40	0.54
1:B:303:LEU:HB3	1:B:332:ARG:HG2	1.88	0.54
3:E:1002:AGS:O2A	3:E:1002:AGS:O1B	2.24	0.54
1:C:680:GLU:OE2	1:C:681:LYS:NZ	2.41	0.54
1:D:553:GLU:OE1	1:D:556:ARG:NH2	2.41	0.54
1:D:832:GLN:HB3	1:D:838:LEU:HD13	1.89	0.54
1:A:654:VAL:H	1:F:652:GLY:HA2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ASP:OD1	1:E:668:ARG:NH2	2.37	0.54
1:F:350:LEU:HD11	1:F:390:ALA:HB1	1.90	0.54
1:A:344:GLU:HA	1:A:347:ILE:HD12	1.90	0.53
3:A:1001:AGS:O2G	3:A:1001:AGS:O1B	2.26	0.53
1:C:677:ASP:OD1	1:C:717:THR:OG1	2.24	0.53
1:D:698:ARG:HH21	1:D:706:THR:HG22	1.72	0.53
1:C:756:ARG:NH2	3:D:902:AGS:O2G	2.42	0.53
1:C:192:GLN:HE22	1:D:542:ARG:HH22	1.56	0.53
3:C:1001:AGS:O2G	3:C:1001:AGS:O1B	2.24	0.53
1:D:698:ARG:NH2	1:D:700:THR:OG1	2.42	0.53
1:A:195:GLN:HE21	1:A:232:LEU:HG	1.74	0.53
1:D:544:THR:OG1	1:D:545:GLY:N	2.42	0.53
1:E:685:ASP:N	1:E:685:ASP:OD1	2.40	0.53
1:B:646:LEU:HD12	1:B:647:VAL:HG13	1.90	0.53
1:C:683:HIS:HB3	1:C:686:VAL:HG23	1.91	0.53
1:B:354:LYS:HB2	1:B:370:ILE:HD11	1.91	0.53
3:E:1001:AGS:O1A	3:E:1001:AGS:O2G	2.26	0.53
1:C:333:PHE:O	1:D:384:ARG:NH2	2.39	0.53
1:C:676:LEU:HB2	1:C:716:MET:HG2	1.91	0.53
1:D:569:ARG:HH11	1:D:620:ASN:HD22	1.57	0.53
1:B:688:ASN:HB3	1:C:635:SER:HB2	1.90	0.52
1:A:551:MET:HB3	1:A:556:ARG:HB2	1.91	0.52
1:D:169:THR:HB	1:D:224:ILE:HD11	1.91	0.52
1:E:405:ILE:HD11	1:E:529:ASN:HA	1.92	0.52
1:A:793:ILE:HG12	1:A:844:ILE:HB	1.90	0.52
1:B:197:ARG:NH2	1:C:178:ASP:OD1	2.42	0.52
1:B:554:SER:O	1:B:558:LYS:HB2	2.10	0.52
1:C:559:LEU:HD11	1:C:588:ARG:HG3	1.91	0.52
1:E:684:PRO:HA	1:E:687:PHE:HD2	1.74	0.52
1:B:632:ILE:HD11	1:B:662:LEU:HD13	1.92	0.52
1:B:738:LYS:O	1:B:742:LEU:HB2	2.10	0.52
1:F:180:VAL:HG21	1:F:214:ALA:HB1	1.90	0.52
1:C:832:GLN:HB3	1:C:838:LEU:HD13	1.90	0.52
1:D:294:ASP:OD1	1:D:294:ASP:N	2.41	0.52
3:D:901:AGS:O2G	3:D:901:AGS:O1B	2.26	0.52
1:A:252:ARG:HD3	1:B:289:ALA:HB2	1.90	0.52
1:D:172:ALA:HB2	1:D:177:LEU:HD12	1.92	0.52
1:D:181:ILE:HD11	1:D:352:GLY:HA3	1.92	0.52
1:B:528:ARG:NH2	1:B:535:GLU:OE2	2.43	0.51
1:B:731:GLU:HG2	1:B:732:LEU:HD12	1.92	0.51
1:D:368:PRO:HA	1:D:371:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:688:ASN:OD1	1:E:750:ARG:NH1	2.43	0.51
1:F:606:PRO:HB3	1:F:726:GLN:HE21	1.76	0.51
1:C:771:ILE:HG23	1:C:817:LEU:HD22	1.91	0.51
1:D:613:GLU:HG3	3:D:902:AGS:H2'	1.92	0.51
1:E:832:GLN:HB3	1:E:838:LEU:HD13	1.91	0.51
1:C:361:HIS:NE2	1:C:395:ASP:OD1	2.37	0.51
1:D:693:VAL:HG13	1:D:709:PHE:HD2	1.75	0.51
1:E:613:GLU:HG3	3:E:1002:AGS:H2'	1.91	0.51
1:B:664:GLU:OE2	1:B:705:ARG:NH2	2.43	0.51
1:C:169:THR:HB	1:C:224:ILE:HD11	1.92	0.51
1:D:695:ASP:HB2	1:D:756:ARG:HD2	1.93	0.51
1:C:161:LEU:O	1:C:165:THR:OG1	2.26	0.51
1:D:183:ARG:NH2	1:D:210:VAL:O	2.43	0.51
1:B:294:ASP:N	1:B:294:ASP:OD1	2.34	0.50
1:C:212:LYS:NZ	3:C:1001:AGS:O3B	2.42	0.50
1:F:842:LYS:HD2	1:F:857:GLN:HE21	1.76	0.50
1:C:281:HIS:HB2	1:C:322:TYR:HD2	1.76	0.50
1:D:559:LEU:HD11	1:D:588:ARG:HG3	1.93	0.50
1:A:768:GLU:HA	1:A:771:ILE:HD12	1.93	0.50
1:D:591:LEU:HD23	1:E:826:GLU:HG2	1.93	0.50
1:E:194:LEU:HD21	1:E:274:ILE:HD13	1.91	0.50
1:B:692:GLN:NE2	1:C:635:SER:OG	2.36	0.50
1:C:401:ILE:HD11	1:C:535:GLU:HG3	1.94	0.50
1:D:281:HIS:HB2	1:D:322:TYR:HD2	1.77	0.50
1:D:663:THR:HG21	1:D:701:ASP:HB3	1.93	0.50
1:C:795:ILE:HG13	1:C:846:LEU:HB2	1.93	0.50
1:A:333:PHE:O	1:B:384:ARG:NH2	2.42	0.50
1:F:603:PHE:HB2	1:F:717:THR:HG22	1.94	0.50
1:B:316:LEU:HD21	1:C:668:ARG:HD2	1.94	0.49
1:B:346:THR:HG21	1:B:386:LEU:HD22	1.95	0.49
1:B:688:ASN:HA	1:B:691:LEU:HG	1.95	0.49
1:A:293:MET:N	1:A:297:ASN:OD1	2.46	0.49
1:B:683:HIS:ND1	1:B:685:ASP:OD1	2.44	0.49
1:C:305:ARG:NH1	1:C:307:GLU:OE2	2.46	0.49
1:E:588:ARG:NH2	1:E:671:TYR:OH	2.34	0.49
1:F:366:THR:HG22	1:F:368:PRO:HD2	1.94	0.49
1:A:200:ASN:ND2	1:A:306:GLY:O	2.46	0.49
1:A:251:TYR:HD2	1:B:250:LYS:HD2	1.78	0.49
1:C:183:ARG:NH2	1:C:210:VAL:O	2.45	0.49
1:C:422:LEU:HB2	1:C:448:LEU:HD13	1.95	0.49
1:C:703:GLN:OE1	1:C:705:ARG:NH1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:ARG:O	1:F:176:LYS:N	2.41	0.49
1:C:636:GLU:OE1	1:C:645:ARG:NH2	2.46	0.49
1:E:606:PRO:HG3	1:E:765:PRO:HG3	1.95	0.49
1:F:293:MET:HA	1:F:298:MET:HG3	1.95	0.49
1:F:679:VAL:HG11	1:F:716:MET:HB3	1.94	0.49
1:E:236:ARG:HB2	1:E:273:VAL:HA	1.95	0.49
1:A:248:GLY:H	1:A:258:ARG:HH22	1.61	0.49
1:A:332:ARG:NH2	3:B:1001:AGS:S1G	2.72	0.49
1:C:259:LEU:HD11	1:C:299:LEU:HD11	1.95	0.49
1:F:786:LEU:HD13	1:F:793:ILE:HD12	1.94	0.48
1:C:793:ILE:HG12	1:C:844:ILE:HB	1.95	0.48
1:D:354:LYS:HB2	1:D:370:ILE:HD11	1.94	0.48
1:F:404:GLN:HA	1:F:407:SER:HB3	1.94	0.48
1:C:533:ASP:OD1	1:C:533:ASP:N	2.45	0.48
1:D:181:ILE:HD12	1:D:349:ILE:HA	1.94	0.48
1:C:698:ARG:HH21	1:C:706:THR:HG21	1.78	0.48
1:E:251:TYR:HB2	1:E:254:GLU:HG2	1.96	0.48
1:E:849:ASN:HD22	1:E:852:ARG:HB2	1.79	0.48
1:F:698:ARG:HH21	1:F:706:THR:HG22	1.78	0.48
1:B:161:LEU:O	1:B:165:THR:OG1	2.31	0.48
1:A:618:LEU:O	1:A:622:MET:HB2	2.14	0.48
1:B:679:VAL:HG12	1:B:718:SER:HB2	1.95	0.48
1:F:380:TYR:OH	1:F:552:MET:SD	2.59	0.47
1:A:641:HIS:HD2	1:F:650:PRO:HG3	1.79	0.47
1:B:663:THR:HG21	1:B:701:ASP:HB3	1.96	0.47
1:A:698:ARG:NH1	1:B:633:ASP:OD2	2.46	0.47
1:B:718:SER:OG	1:B:719:ASN:N	2.48	0.47
1:D:404:GLN:NE2	1:D:410:GLU:OE1	2.34	0.47
1:D:558:LYS:HA	1:D:561:ARG:HE	1.79	0.47
1:B:333:PHE:O	1:C:384:ARG:NH2	2.47	0.47
1:C:688:ASN:HA	1:C:691:LEU:HG	1.95	0.47
1:E:201:ASN:OD1	1:E:310:CYS:N	2.47	0.47
1:F:728:ARG:HB3	1:F:732:LEU:HD12	1.97	0.47
1:A:718:SER:OG	1:A:719:ASN:N	2.48	0.47
1:B:697:GLY:O	1:B:709:PHE:N	2.36	0.47
1:D:803:LEU:HD11	1:D:825:ILE:HD11	1.97	0.47
1:E:304:ALA:HA	1:E:332:ARG:HH11	1.79	0.47
1:E:809:ASP:N	1:E:809:ASP:OD1	2.47	0.47
1:A:238:LEU:HD13	1:A:273:VAL:HG13	1.96	0.47
1:E:795:ILE:HA	1:E:846:LEU:HB2	1.97	0.47
1:F:684:PRO:HA	1:F:687:PHE:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HB2	1:A:275:LEU:HD11	1.97	0.46
1:A:815:ARG:HA	1:A:818:LYS:HD3	1.97	0.46
1:C:380:TYR:HB2	1:C:540:LEU:HD21	1.97	0.46
1:E:281:HIS:HB2	1:E:322:TYR:HD2	1.79	0.46
1:F:161:LEU:O	1:F:165:THR:OG1	2.31	0.46
1:D:196:ARG:NH2	1:E:392:ASP:OD1	2.49	0.46
1:E:344:GLU:HA	1:E:347:ILE:HD12	1.96	0.46
1:C:354:LYS:HG3	1:C:365:ILE:HB	1.98	0.46
1:F:354:LYS:HG3	1:F:365:ILE:HB	1.96	0.46
1:C:226:GLY:O	1:C:233:LYS:NZ	2.48	0.46
1:F:680:GLU:HA	1:F:687:PHE:HZ	1.80	0.46
1:B:189:ARG:HH11	1:B:336:VAL:HG22	1.81	0.46
1:B:297:ASN:HD21	1:C:281:HIS:HE1	1.64	0.46
1:C:664:GLU:O	1:C:668:ARG:HG2	2.16	0.46
1:E:315:THR:HG22	1:E:317:ASP:H	1.80	0.46
1:F:642:SER:HA	1:F:645:ARG:HE	1.81	0.46
1:B:201:ASN:OD1	1:B:310:CYS:N	2.49	0.46
1:C:289:ALA:H	1:C:292:ALA:HB2	1.81	0.46
1:C:405:ILE:HD11	1:C:529:ASN:HA	1.98	0.46
1:D:200:ASN:ND2	1:D:306:GLY:O	2.49	0.46
1:E:815:ARG:NH1	3:E:1002:AGS:S1G	2.89	0.46
1:B:693:VAL:HG13	1:B:709:PHE:HD2	1.81	0.45
1:A:591:LEU:HD21	1:B:829:LEU:HD23	1.97	0.45
1:B:544:THR:OG1	1:B:545:GLY:N	2.48	0.45
1:C:422:LEU:HD22	1:C:444:LEU:HD11	1.97	0.45
1:C:738:LYS:O	1:C:742:LEU:HB2	2.16	0.45
1:D:401:ILE:HD11	1:D:535:GLU:HG3	1.99	0.45
1:E:771:ILE:HG23	1:E:817:LEU:HD22	1.98	0.45
1:F:169:THR:HB	1:F:224:ILE:HD11	1.98	0.45
1:D:161:LEU:O	1:D:165:THR:OG1	2.34	0.45
1:D:422:LEU:HD22	1:D:444:LEU:HD11	1.97	0.45
1:A:280:LEU:HD22	1:A:312:GLY:HA3	1.99	0.45
1:A:299:LEU:HB3	1:A:303:LEU:HD13	1.98	0.45
1:A:849:ASN:HB2	1:A:852:ARG:H	1.81	0.45
1:D:771:ILE:HG23	1:D:817:LEU:HD22	1.97	0.45
1:E:229:PRO:HD2	1:E:232:LEU:HD12	1.99	0.45
1:B:320:ARG:HH12	1:C:668:ARG:HH21	1.65	0.45
1:C:609:VAL:HG23	1:C:763:PHE:HD2	1.81	0.45
1:D:650:PRO:HG3	1:E:641:HIS:HD2	1.82	0.45
1:D:721:GLY:HA3	1:D:741:VAL:HG23	1.99	0.45
1:D:838:LEU:HD23	1:D:844:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:724:LEU:HD21	1:E:740:LEU:HG	1.99	0.45
1:A:204:LEU:HD23	1:A:336:VAL:HB	1.98	0.45
1:A:696:ASP:OD2	1:B:631:ARG:NH1	2.36	0.45
1:B:637:PHE:HE1	1:B:645:ARG:HD2	1.81	0.45
3:C:1001:AGS:O2B	3:C:1001:AGS:O2A	2.34	0.45
1:F:245:LEU:HB3	1:F:255:PHE:HE1	1.81	0.45
1:A:728:ARG:HB3	1:A:732:LEU:HD12	1.99	0.45
1:D:183:ARG:HD2	1:D:215:ILE:HD11	1.99	0.45
1:E:718:SER:OG	1:E:719:ASN:N	2.50	0.45
1:F:793:ILE:HG12	1:F:844:ILE:HB	1.99	0.45
1:D:647:VAL:HG13	1:D:701:ASP:HA	1.99	0.44
1:E:354:LYS:HD3	1:E:370:ILE:HD11	1.98	0.44
1:F:344:GLU:HA	1:F:347:ILE:HD12	1.99	0.44
1:A:587:SER:HA	1:A:592:ALA:HB2	1.99	0.44
1:E:401:ILE:HG13	1:E:531:VAL:HG22	1.99	0.44
1:F:207:GLU:HG2	1:F:385:GLN:HE22	1.83	0.44
1:A:842:LYS:HD2	1:A:857:GLN:HE21	1.83	0.44
1:C:809:ASP:OD1	1:C:809:ASP:N	2.50	0.44
1:E:286:ALA:N	1:E:294:ASP:OD2	2.46	0.44
1:F:368:PRO:HA	1:F:371:VAL:HG12	1.98	0.44
1:F:786:LEU:HB3	1:F:791:TYR:HB2	1.99	0.44
1:A:212:LYS:NZ	3:A:1001:AGS:O3B	2.48	0.44
1:C:276:PHE:CZ	1:C:278:ASP:HB3	2.53	0.44
1:D:299:LEU:HB3	1:D:303:LEU:HD13	2.00	0.44
1:A:247:ALA:HB2	1:F:293:MET:HB3	1.99	0.44
1:B:849:ASN:HD21	1:B:854:VAL:HB	1.83	0.44
1:C:569:ARG:HH11	1:C:620:ASN:HD22	1.66	0.44
1:E:351:ARG:NE	1:E:367:ASP:OD1	2.51	0.44
1:D:422:LEU:HB2	1:D:448:LEU:HD13	1.99	0.44
1:D:625:SER:HB3	1:D:628:ALA:HB2	2.00	0.44
1:D:679:VAL:HG12	1:D:718:SER:HB2	1.99	0.44
1:D:822:GLN:O	1:D:826:GLU:HB2	2.18	0.44
1:E:302:ALA:HB1	1:E:308:LEU:HB2	1.99	0.44
1:A:600:SER:HG	1:A:758:ASP:H	1.62	0.44
1:D:585:ARG:NE	1:E:831:GLN:OE1	2.51	0.44
1:F:663:THR:HB	1:F:707:VAL:HG11	2.00	0.44
1:A:610:GLY:HA2	1:A:613:GLU:HB2	2.00	0.43
1:C:350:LEU:HD22	1:C:394:ILE:HG13	2.00	0.43
1:C:803:LEU:HD13	1:C:821:ILE:HG12	2.00	0.43
1:D:402:ARG:HA	1:D:402:ARG:HD2	1.84	0.43
1:D:650:PRO:HG3	1:E:641:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:690:LEU:HA	1:D:693:VAL:HB	2.00	0.43
1:A:771:ILE:HG23	1:A:817:LEU:HD22	2.00	0.43
1:E:169:THR:HB	1:E:224:ILE:HD11	2.01	0.43
1:F:222:ARG:O	1:F:227:GLU:N	2.49	0.43
1:C:605:GLY:HA3	1:C:763:PHE:HB2	1.99	0.43
1:C:698:ARG:NH1	1:D:633:ASP:OD2	2.51	0.43
1:A:849:ASN:HD21	1:A:854:VAL:HB	1.84	0.43
1:B:603:PHE:HB2	1:B:717:THR:HA	1.99	0.43
1:D:178:ASP:O	1:D:221:GLN:NE2	2.51	0.43
1:E:803:LEU:HD11	1:E:825:ILE:HD11	2.00	0.43
1:C:651:PRO:HD2	1:D:645:ARG:HA	1.99	0.43
1:E:199:LYS:HE2	1:E:331:ARG:HA	1.99	0.43
1:F:178:ASP:OD1	1:F:356:ARG:NH1	2.51	0.43
1:A:189:ARG:NH2	1:B:396:GLU:OE2	2.52	0.43
1:B:278:ASP:OD1	1:B:278:ASP:N	2.52	0.43
1:A:823:GLN:NE2	1:F:755:ASN:OD1	2.46	0.43
1:C:586:ARG:CZ	1:D:822:GLN:HE21	2.32	0.43
1:D:376:LEU:HB3	1:D:540:LEU:HD22	2.01	0.43
1:B:636:GLU:OE1	1:B:645:ARG:NH1	2.52	0.43
1:C:346:THR:HG21	1:C:386:LEU:HD22	2.01	0.43
3:D:902:AGS:O2G	3:D:902:AGS:O1B	2.37	0.43
1:E:609:VAL:HG23	1:E:763:PHE:HD2	1.84	0.43
1:A:354:LYS:HG3	1:A:365:ILE:HB	2.00	0.43
1:A:364:GLN:HB2	1:A:530:LYS:HG2	2.00	0.43
1:E:187:ILE:HG21	1:E:222:ARG:HD2	2.00	0.43
1:F:695:ASP:HB2	1:F:756:ARG:HH12	1.84	0.43
1:A:197:ARG:HD3	1:B:357:TYR:CE1	2.54	0.43
3:D:901:AGS:O2A	3:D:901:AGS:O2B	2.37	0.43
1:A:645:ARG:HB2	1:F:650:PRO:HB3	2.01	0.42
1:E:168:LEU:HD23	1:E:171:ARG:HD3	2.00	0.42
1:F:637:PHE:HA	1:F:642:SER:HB3	2.00	0.42
1:A:795:ILE:HA	1:A:846:LEU:HB2	2.01	0.42
1:D:684:PRO:HA	1:D:687:PHE:HD2	1.83	0.42
1:E:612:THR:N	3:E:1002:AGS:O2A	2.51	0.42
1:F:683:HIS:ND1	1:F:685:ASP:OD1	2.52	0.42
1:F:795:ILE:HA	1:F:846:LEU:HB2	2.01	0.42
1:A:652:GLY:HA2	1:B:654:VAL:H	1.84	0.42
1:B:289:ALA:HB3	1:B:292:ALA:HB3	2.00	0.42
1:C:280:LEU:HD11	1:C:283:MET:HE1	2.01	0.42
1:C:315:THR:HB	1:C:318:GLU:HB2	2.02	0.42
1:E:196:ARG:NH2	1:E:199:LYS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ILE:HD12	1:D:335:LYS:HG2	2.01	0.42
1:D:462:TRP:HD1	1:D:527:LEU:HD21	1.85	0.42
1:D:596:ARG:NH2	1:D:756:ARG:O	2.52	0.42
1:E:786:LEU:O	1:E:790:GLY:N	2.53	0.42
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.91	0.42
1:C:702:GLY:HA2	1:D:645:ARG:HE	1.84	0.42
1:B:786:LEU:O	1:B:790:GLY:N	2.52	0.42
1:C:368:PRO:HA	1:C:371:VAL:HG12	2.01	0.42
1:C:750:ARG:HH11	1:D:681:LYS:HE3	1.85	0.42
1:E:354:LYS:HG3	1:E:365:ILE:HB	2.02	0.42
1:B:368:PRO:HA	1:B:371:VAL:HG12	2.02	0.42
1:C:177:LEU:HB2	1:C:221:GLN:HE21	1.84	0.42
1:C:566:LEU:HD12	1:C:577:VAL:HG13	2.01	0.42
1:D:417:ARG:HA	1:D:417:ARG:HD3	1.85	0.42
1:E:275:LEU:O	1:E:311:VAL:N	2.52	0.42
1:E:680:GLU:OE2	1:E:681:LYS:NZ	2.53	0.42
3:E:1002:AGS:O2G	3:E:1002:AGS:O1A	2.38	0.42
1:F:768:GLU:HA	1:F:771:ILE:HD12	2.01	0.42
1:B:401:ILE:HD13	1:B:401:ILE:HA	1.85	0.42
1:A:838:LEU:HD23	1:A:844:ILE:HD13	2.00	0.41
1:C:188:ARG:HD3	1:D:410:GLU:HG2	2.01	0.41
1:F:178:ASP:HA	1:F:179:PRO:HD3	1.94	0.41
1:B:192:GLN:NE2	1:C:542:ARG:HH22	2.17	0.41
1:C:663:THR:HB	1:C:707:VAL:HG21	2.01	0.41
1:F:323:ILE:HG23	1:F:329:LEU:HG	2.02	0.41
1:B:197:ARG:HD3	1:C:357:TYR:CE1	2.56	0.41
1:B:596:ARG:NH2	1:B:756:ARG:O	2.53	0.41
1:D:350:LEU:HD22	1:D:394:ILE:HG13	2.02	0.41
1:D:586:ARG:CZ	1:E:822:GLN:HE21	2.33	0.41
1:E:551:MET:HB3	1:E:556:ARG:HD3	2.02	0.41
1:F:304:ALA:HA	1:F:332:ARG:HE	1.86	0.41
1:F:380:TYR:HD2	1:F:540:LEU:HD21	1.85	0.41
1:A:278:ASP:OD1	1:A:278:ASP:N	2.52	0.41
1:A:655:GLY:H	1:F:652:GLY:N	2.18	0.41
1:D:693:VAL:HG13	1:D:709:PHE:CD2	2.54	0.41
1:C:394:ILE:HD13	1:C:394:ILE:HA	1.89	0.41
1:D:305:ARG:NH1	1:D:307:GLU:OE2	2.45	0.41
1:E:183:ARG:NH2	1:E:339:ALA:O	2.49	0.41
1:F:559:LEU:HD13	1:F:585:ARG:HG2	2.03	0.41
1:B:795:ILE:HG13	1:B:846:LEU:HB2	2.03	0.41
1:C:200:ASN:ND2	1:C:306:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:ILE:HD12	1:D:571:ILE:HA	2.00	0.41
1:D:685:ASP:OD1	1:D:685:ASP:N	2.54	0.41
1:E:161:LEU:O	1:E:165:THR:OG1	2.39	0.41
1:F:242:MET:O	1:F:246:VAL:HB	2.21	0.41
1:A:300:LYS:HG2	1:A:332:ARG:NH1	2.35	0.41
1:A:361:HIS:HB2	1:A:363:VAL:HG22	2.02	0.41
1:B:563:GLU:OE2	1:B:585:ARG:NH1	2.54	0.41
1:E:614:LEU:HD12	1:E:614:LEU:HA	1.93	0.41
1:D:546:ILE:HG13	1:D:671:TYR:HB2	2.03	0.40
1:A:177:LEU:HD13	1:A:217:GLU:HB3	2.03	0.40
1:B:357:TYR:HE2	1:B:391:ILE:HG23	1.86	0.40
1:C:696:ASP:OD2	1:D:631:ARG:NH1	2.42	0.40
1:A:347:ILE:HD11	1:A:371:VAL:HG23	2.03	0.40
1:E:216:VAL:HG21	1:E:276:PHE:CE1	2.56	0.40
1:F:625:SER:OG	1:F:626:ASP:N	2.54	0.40
1:A:161:LEU:O	1:A:165:THR:OG1	2.30	0.40
1:D:240:LEU:HD23	1:D:277:ILE:HG12	2.03	0.40
1:B:195:GLN:O	1:C:399:SER:OG	2.32	0.40
1:B:803:LEU:HD11	1:B:825:ILE:HD11	2.03	0.40
1:C:181:ILE:HD11	1:C:352:GLY:HA3	2.04	0.40
1:C:316:LEU:HD21	1:D:668:ARG:HG2	2.03	0.40
1:C:650:PRO:HG2	1:C:653:TYR:CD2	2.56	0.40
1:F:244:ALA:O	1:F:258:ARG:NH1	2.54	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	571/858 (67%)	526 (92%)	45 (8%)	0	100	100
1	B	578/858 (67%)	527 (91%)	51 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	624/858 (73%)	572 (92%)	52 (8%)	0	100	100
1	D	617/858 (72%)	576 (93%)	41 (7%)	0	100	100
1	E	571/858 (67%)	517 (90%)	54 (10%)	0	100	100
1	F	571/858 (67%)	526 (92%)	45 (8%)	0	100	100
All	All	3532/5148 (69%)	3244 (92%)	288 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	481/714 (67%)	481 (100%)	0	100	100
1	B	481/714 (67%)	480 (100%)	1 (0%)	93	96
1	C	527/714 (74%)	527 (100%)	0	100	100
1	D	527/714 (74%)	526 (100%)	1 (0%)	93	96
1	E	481/714 (67%)	481 (100%)	0	100	100
1	F	481/714 (67%)	480 (100%)	1 (0%)	93	96
All	All	2978/4284 (70%)	2975 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	679	VAL
1	D	710	ARG
1	F	331	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN

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Mol	Chain	Res	Type
1	A	641	HIS
1	A	692	GLN
1	A	849	ASN
1	A	858	HIS
1	B	281	HIS
1	B	297	ASN
1	B	567	HIS
1	B	574	ASN
1	B	692	GLN
1	B	822	GLN
1	B	849	ASN
1	C	620	ASN
1	C	641	HIS
1	C	692	GLN
1	C	806	ASN
1	C	858	HIS
1	D	620	ASN
1	D	692	GLN
1	E	309	HIS
1	E	822	GLN
1	E	849	ASN
1	E	858	HIS
1	F	281	HIS
1	F	726	GLN
1	F	849	ASN
1	F	857	GLN

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)

11 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	$\#\|Z\| > 2$
3	AGS	E	1001	-	26,33,33	0.72	0	26,52,52	1.06	2 (7%)
3	AGS	C	1001	-	26,33,33	0.76	1 (3%)	26,52,52	1.48	2 (7%)
3	AGS	D	901	-	26,33,33	0.82	1 (3%)	26,52,52	1.31	2 (7%)
4	ADP	A	1002	-	24,29,29	1.05	2 (8%)	29,45,45	1.90	6 (20%)
3	AGS	E	1002	-	26,33,33	0.68	0	26,52,52	1.40	5 (19%)
3	AGS	B	1002	-	26,33,33	0.76	0	26,52,52	1.41	2 (7%)
3	AGS	B	1001	-	26,33,33	0.82	1 (3%)	26,52,52	1.18	2 (7%)
3	AGS	D	902	-	26,33,33	0.84	0	26,52,52	1.31	2 (7%)
4	ADP	F	1001	-	24,29,29	0.97	1 (4%)	29,45,45	1.60	5 (17%)
3	AGS	C	1002	-	26,33,33	0.80	0	26,52,52	1.53	4 (15%)
3	AGS	A	1001	-	26,33,33	0.80	0	26,52,52	1.41	2 (7%)

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
3	AGS	E	1001	-	-	7/17/38/38	0/3/3/3
3	AGS	C	1001	-	-	0/17/38/38	0/3/3/3
3	AGS	D	901	-	-	2/17/38/38	0/3/3/3
4	ADP	A	1002	-	-	3/12/32/32	0/3/3/3
3	AGS	E	1002	-	-	4/17/38/38	0/3/3/3
3	AGS	B	1002	-	-	6/17/38/38	0/3/3/3
3	AGS	B	1001	-	-	3/17/38/38	0/3/3/3
3	AGS	D	902	-	-	1/17/38/38	0/3/3/3
4	ADP	F	1001	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	C	1002	-	-	5/17/38/38	0/3/3/3
3	AGS	A	1001	-	-	2/17/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	ADP	C5-C4	2.59	1.47	1.40
4	F	1001	ADP	C5-C4	2.49	1.47	1.40
4	A	1002	ADP	C2-N3	2.38	1.35	1.32
3	D	901	AGS	C8-N7	-2.06	1.31	1.34
3	B	1001	AGS	C8-N7	-2.01	1.31	1.34
3	C	1001	AGS	C8-N7	-2.01	1.31	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1001	AGS	PA-O3A-PB	-6.02	112.18	132.83
3	A	1001	AGS	PA-O3A-PB	-5.89	112.62	132.83
4	A	1002	ADP	C3'-C2'-C1'	5.86	109.80	100.98
3	C	1002	AGS	PA-O3A-PB	-5.41	114.26	132.83
3	D	901	AGS	PA-O3A-PB	-5.41	114.27	132.83
3	B	1002	AGS	PA-O3A-PB	-5.28	114.72	132.83
3	D	902	AGS	PA-O3A-PB	-4.86	116.16	132.83
4	A	1002	ADP	C1'-N9-C4	4.57	134.67	126.64
3	B	1001	AGS	PA-O3A-PB	-4.42	117.66	132.83
4	F	1001	ADP	PA-O3A-PB	-4.18	118.47	132.83
3	E	1002	AGS	PA-O3A-PB	-4.09	118.80	132.83
3	E	1001	AGS	PA-O3A-PB	-3.61	120.43	132.83
4	F	1001	ADP	N3-C2-N1	-3.39	123.38	128.68
4	A	1002	ADP	N3-C2-N1	-3.21	123.66	128.68
4	F	1001	ADP	C3'-C2'-C1'	2.96	105.43	100.98
3	E	1002	AGS	C1'-N9-C4	2.84	131.62	126.64
4	A	1002	ADP	PA-O3A-PB	-2.80	123.22	132.83
3	C	1002	AGS	C3'-C2'-C1'	2.77	105.15	100.98
4	F	1001	ADP	C4-C5-N7	-2.72	106.56	109.40
3	E	1002	AGS	C5-C6-N6	2.62	124.34	120.35
3	B	1002	AGS	C5-C6-N6	2.59	124.29	120.35
4	A	1002	ADP	O4'-C1'-C2'	-2.56	103.18	106.93
3	D	901	AGS	C5-C6-N6	2.28	123.81	120.35
3	E	1001	AGS	C5-C6-N6	2.23	123.73	120.35
3	B	1001	AGS	C5-C6-N6	2.22	123.72	120.35
3	A	1001	AGS	C5-C6-N6	2.17	123.65	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1002	AGS	O2G-PG-O3B	2.17	111.87	104.64
3	C	1001	AGS	C5-C6-N6	2.15	123.61	120.35
4	A	1002	ADP	C4-C5-N7	-2.13	107.17	109.40
3	E	1002	AGS	C3'-C2'-C1'	2.13	104.18	100.98
3	C	1002	AGS	C5-C6-N6	2.12	123.57	120.35
3	D	902	AGS	C5-C6-N6	2.11	123.55	120.35
3	C	1002	AGS	C1'-N9-C4	2.09	130.31	126.64
4	F	1001	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	AGS	O4'-C4'-C5'-O5'
3	B	1001	AGS	PB-O3B-PG-O2G
3	B	1002	AGS	PB-O3B-PG-O2G
3	B	1002	AGS	PB-O3B-PG-O3G
3	B	1002	AGS	C5'-O5'-PA-O1A
3	B	1002	AGS	C5'-O5'-PA-O3A
3	C	1002	AGS	C5'-O5'-PA-O1A
3	C	1002	AGS	O4'-C4'-C5'-O5'
3	C	1002	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	PB-O3B-PG-O2G
3	E	1001	AGS	PB-O3B-PG-O3G
3	E	1001	AGS	C5'-O5'-PA-O1A
3	E	1001	AGS	C5'-O5'-PA-O2A
3	E	1001	AGS	C5'-O5'-PA-O3A
3	E	1002	AGS	C5'-O5'-PA-O1A
3	A	1001	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	O4'-C4'-C5'-O5'
4	A	1002	ADP	O4'-C4'-C5'-O5'
3	D	901	AGS	O4'-C4'-C5'-O5'
3	D	901	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	C3'-C4'-C5'-O5'
4	A	1002	ADP	PA-O3A-PB-O1B
4	A	1002	ADP	PA-O3A-PB-O3B
3	C	1002	AGS	C5'-O5'-PA-O3A
4	F	1001	ADP	C3'-C4'-C5'-O5'
3	B	1001	AGS	PA-O3A-PB-O1B
3	B	1002	AGS	C5'-O5'-PA-O2A
3	C	1002	AGS	C5'-O5'-PA-O2A
3	B	1001	AGS	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	902	AGS	PB-O3B-PG-O2G
3	E	1002	AGS	PG-O3B-PB-O1B
3	E	1002	AGS	PG-O3B-PB-O2B
3	B	1002	AGS	PB-O3A-PA-O2A
4	F	1001	ADP	PB-O3A-PA-O1A
3	E	1002	AGS	PG-O3B-PB-O3A

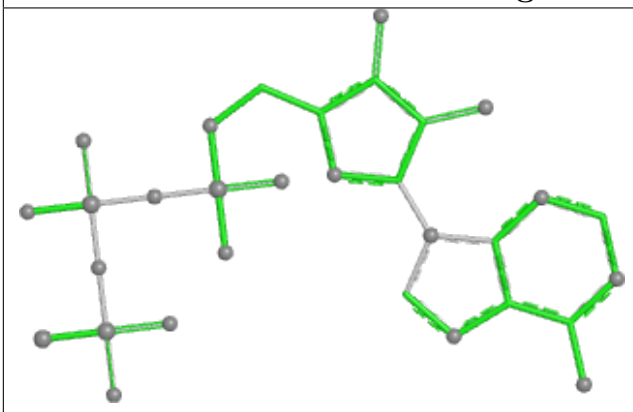
There are no ring outliers.

9 monomers are involved in 26 short contacts:

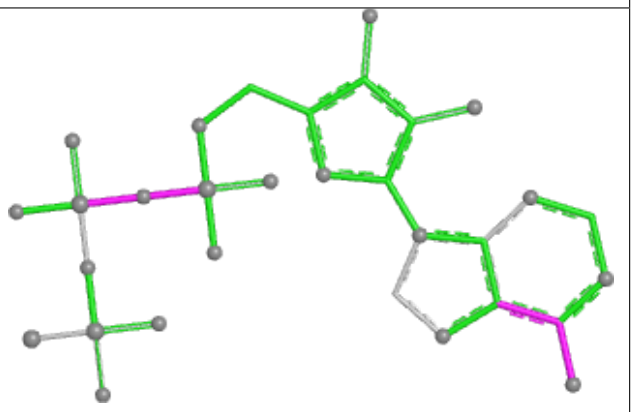
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1001	AGS	1	0
3	C	1001	AGS	4	0
3	D	901	AGS	2	0
3	E	1002	AGS	5	0
3	B	1002	AGS	1	0
3	B	1001	AGS	3	0
3	D	902	AGS	4	0
3	C	1002	AGS	3	0
3	A	1001	AGS	3	0

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.

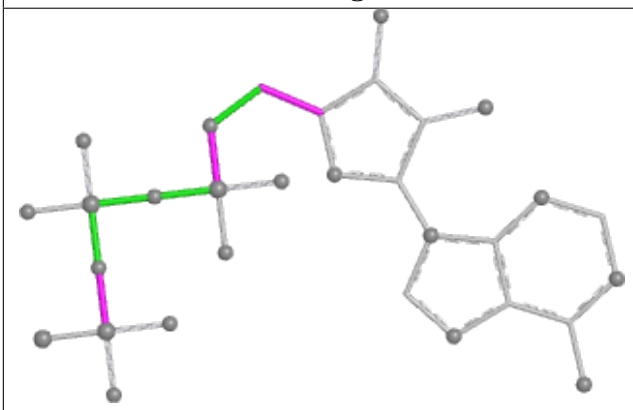
Ligand AGS E 1001



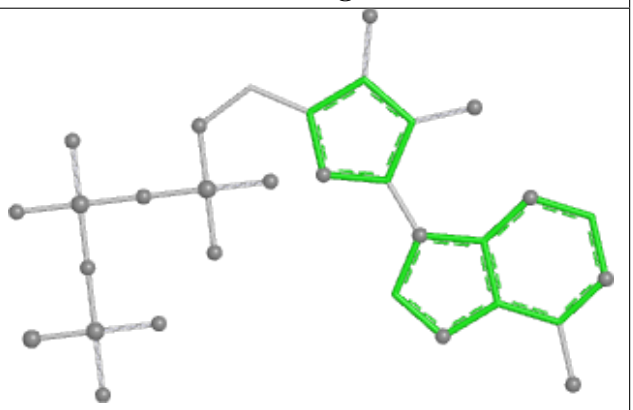
Bond lengths



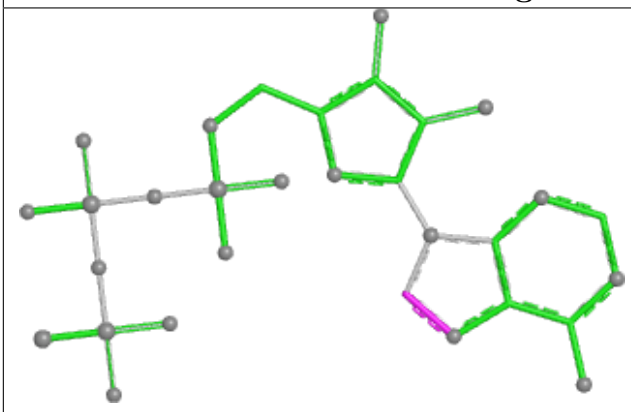
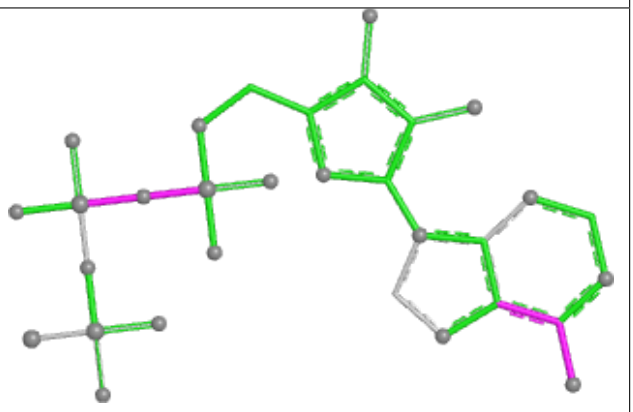
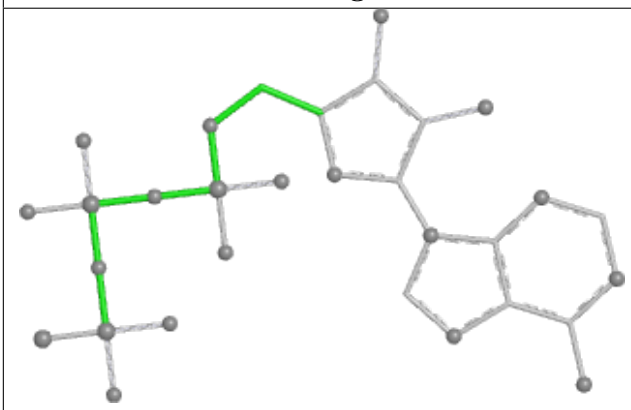
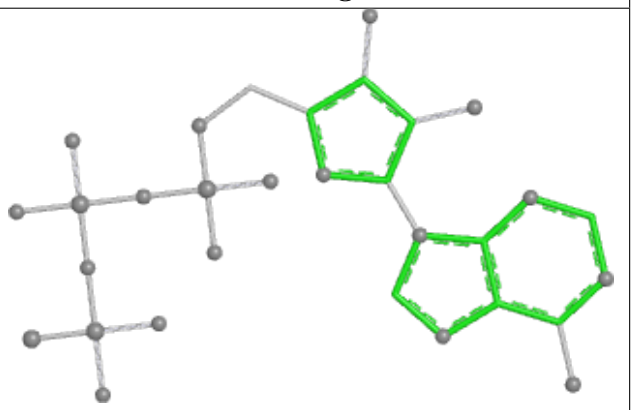
Bond angles



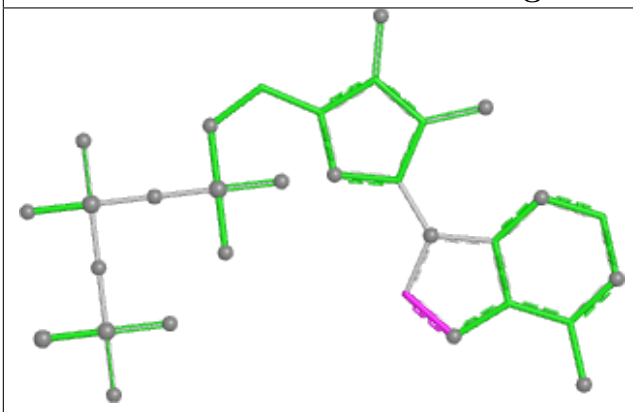
Torsions



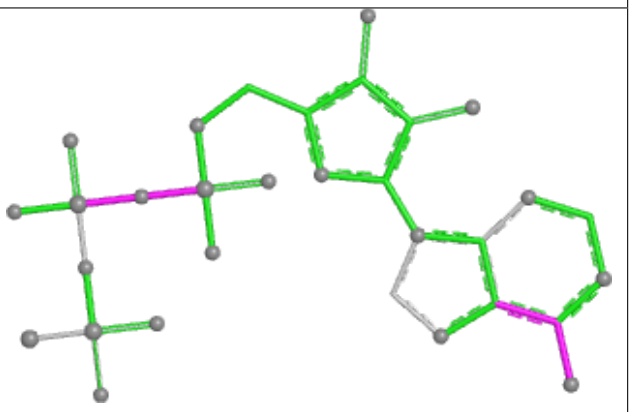
Rings

Ligand AGS C 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

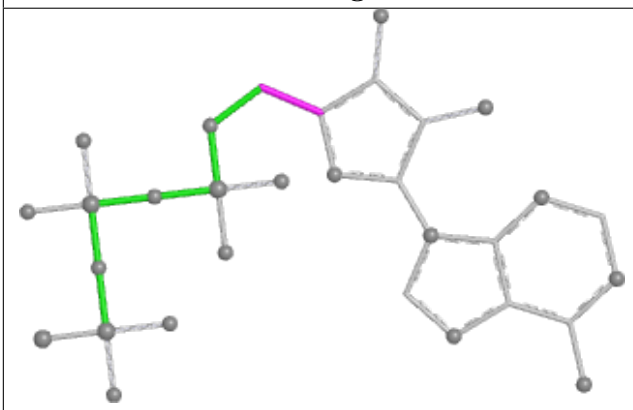
Ligand AGS D 901



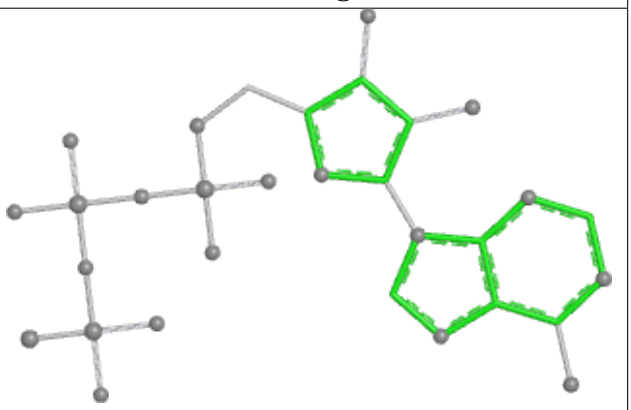
Bond lengths



Bond angles

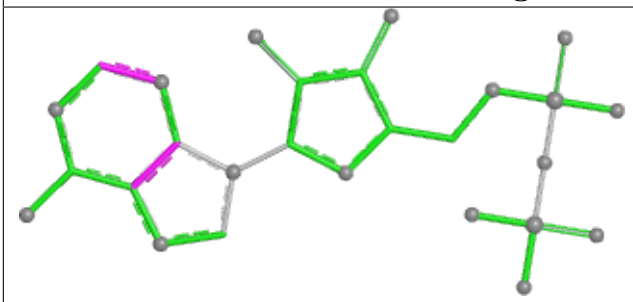


Torsions

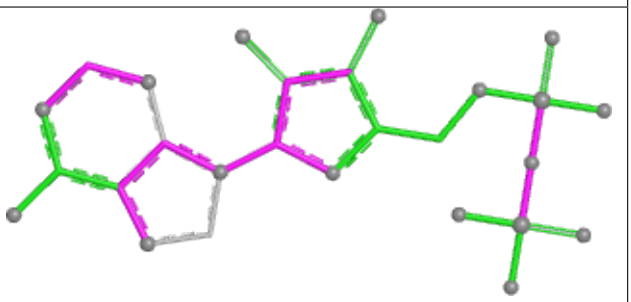


Rings

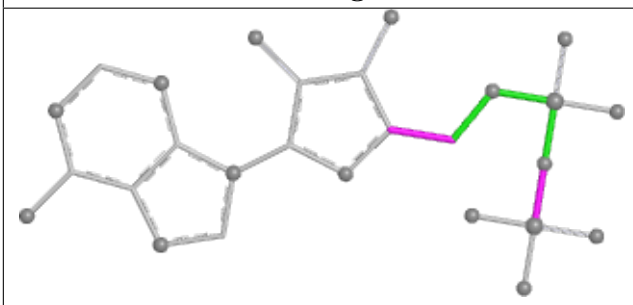
Ligand ADP A 1002



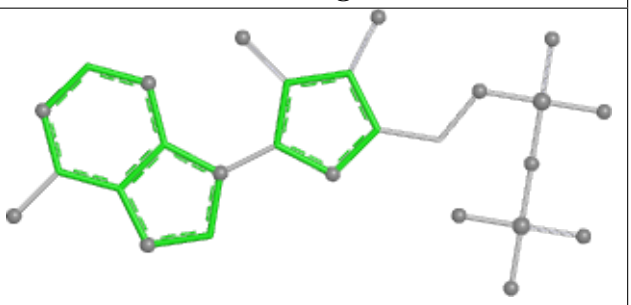
Bond lengths



Bond angles

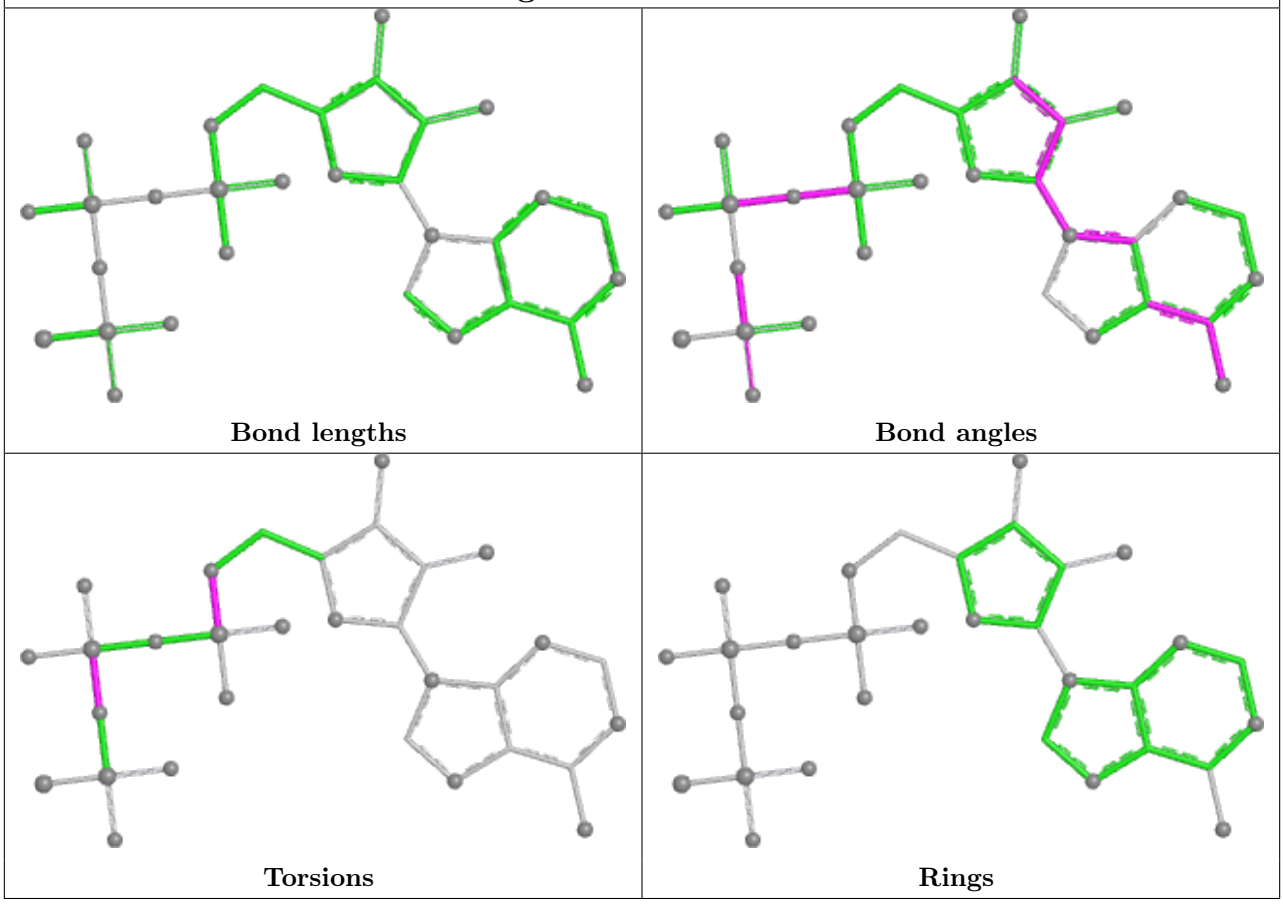


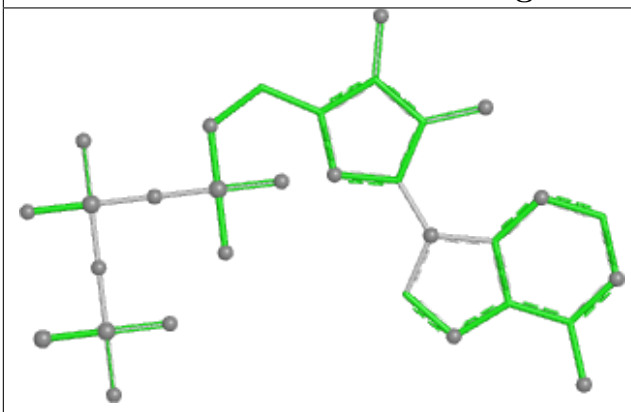
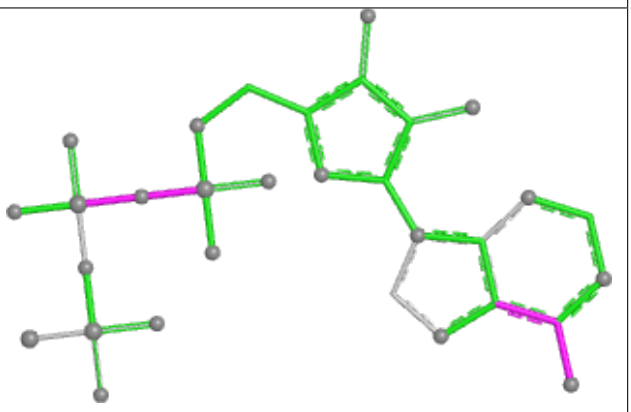
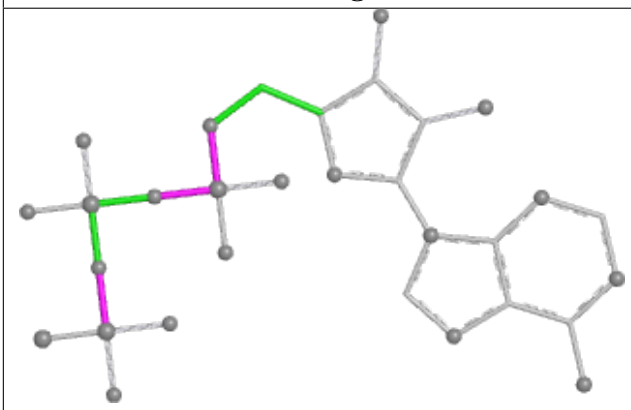
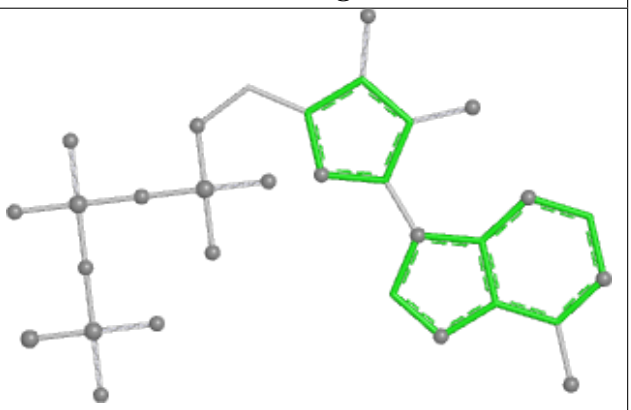
Torsions

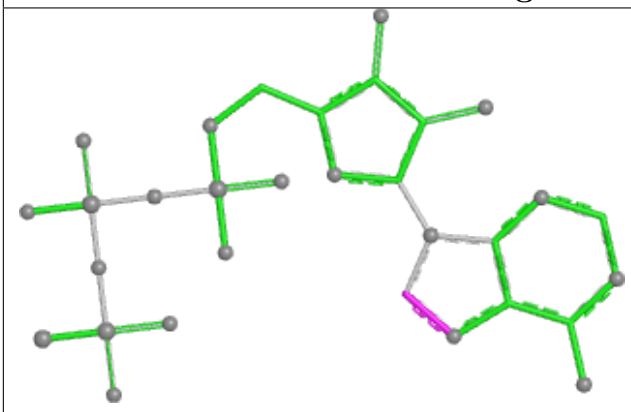
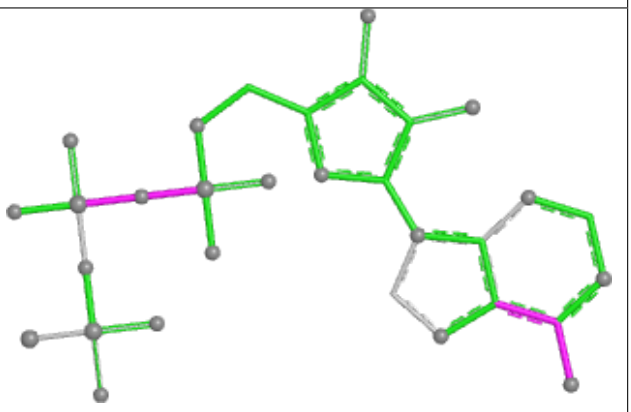
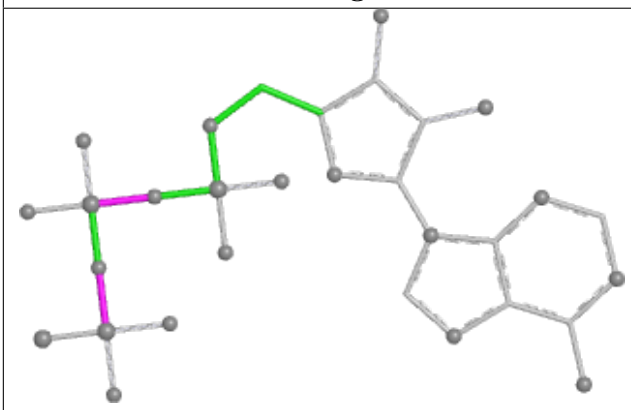
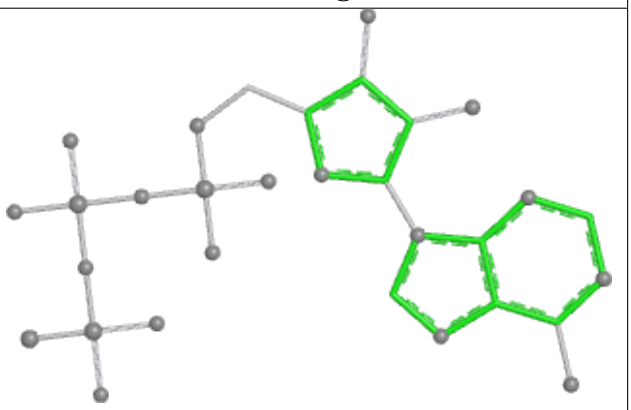


Rings

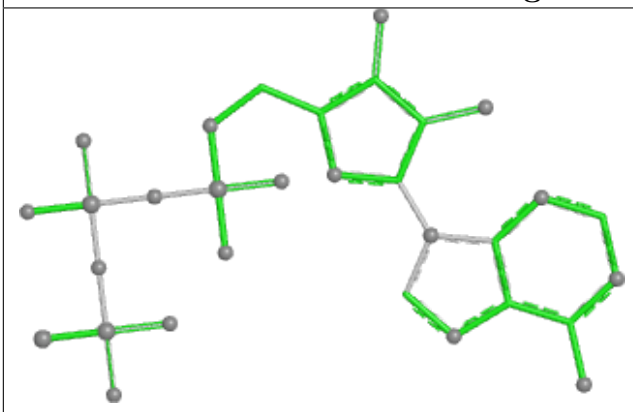
Ligand AGS E 1002



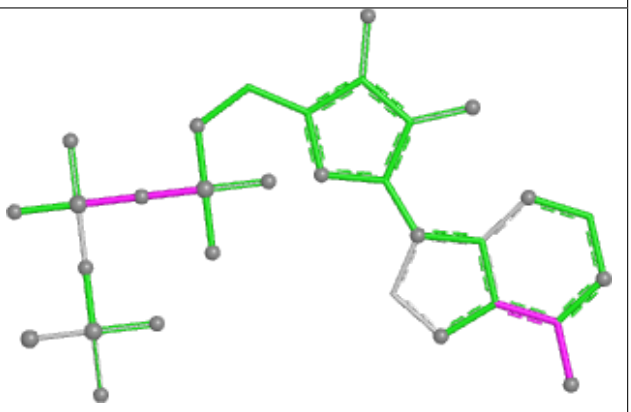
Ligand AGS B 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AGS B 1001	
 Bond lengths	 Bond angles
 Torsions	 Rings

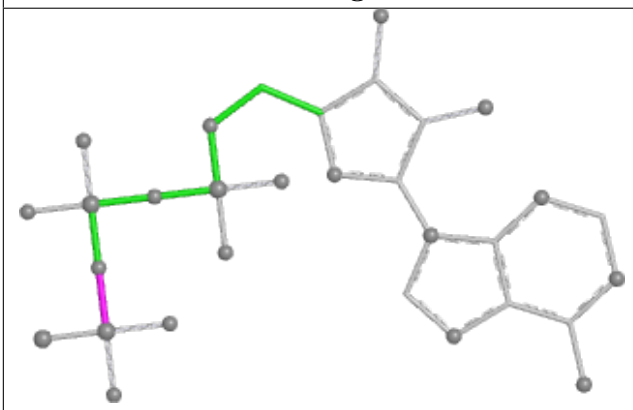
Ligand AGS D 902



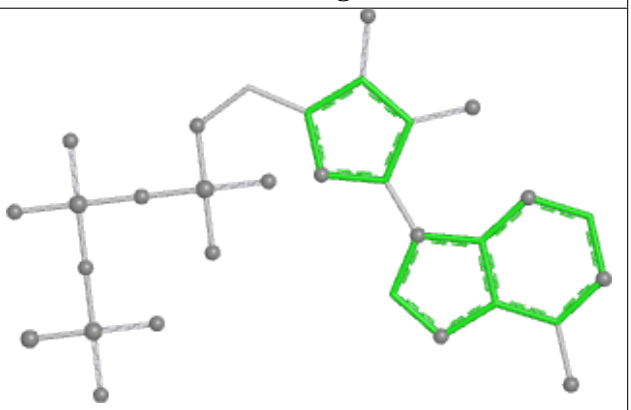
Bond lengths



Bond angles

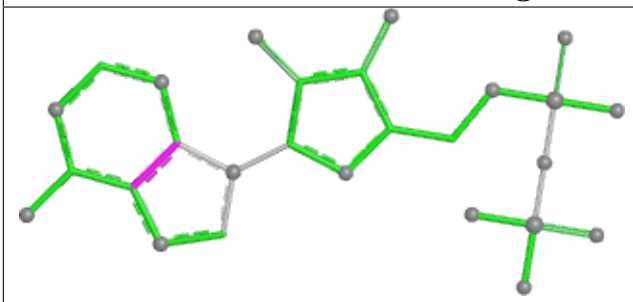


Torsions

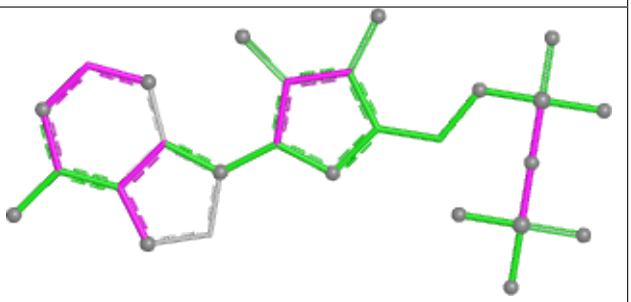


Rings

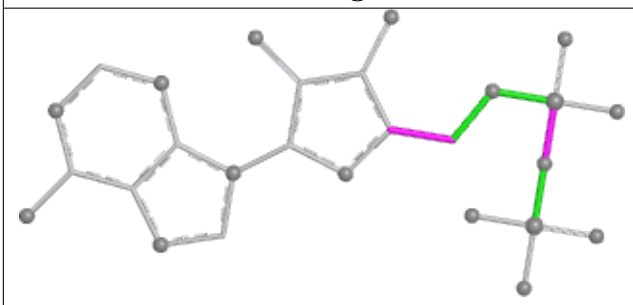
Ligand ADP F 1001



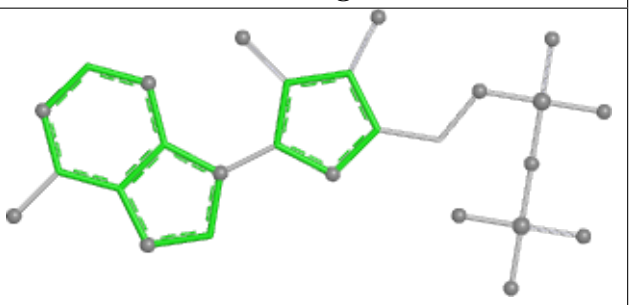
Bond lengths



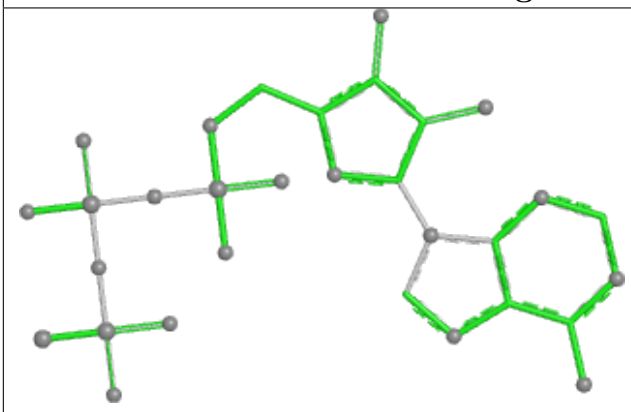
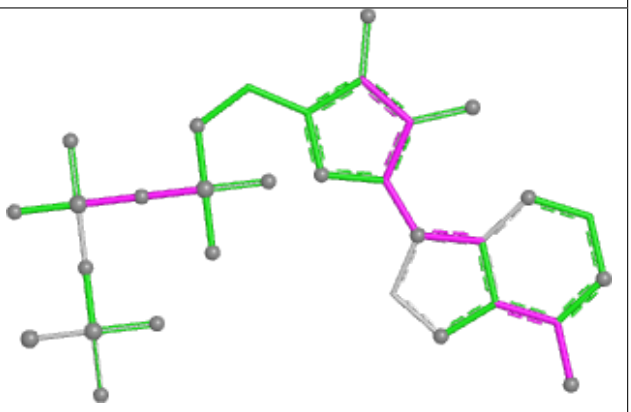
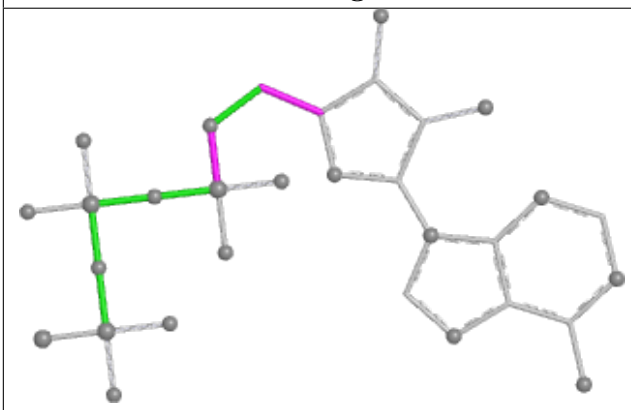
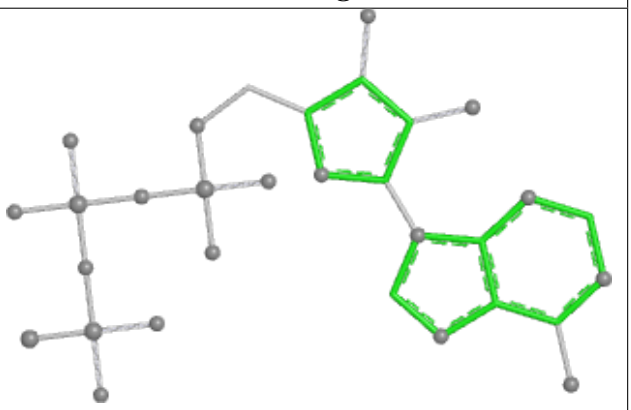
Bond angles

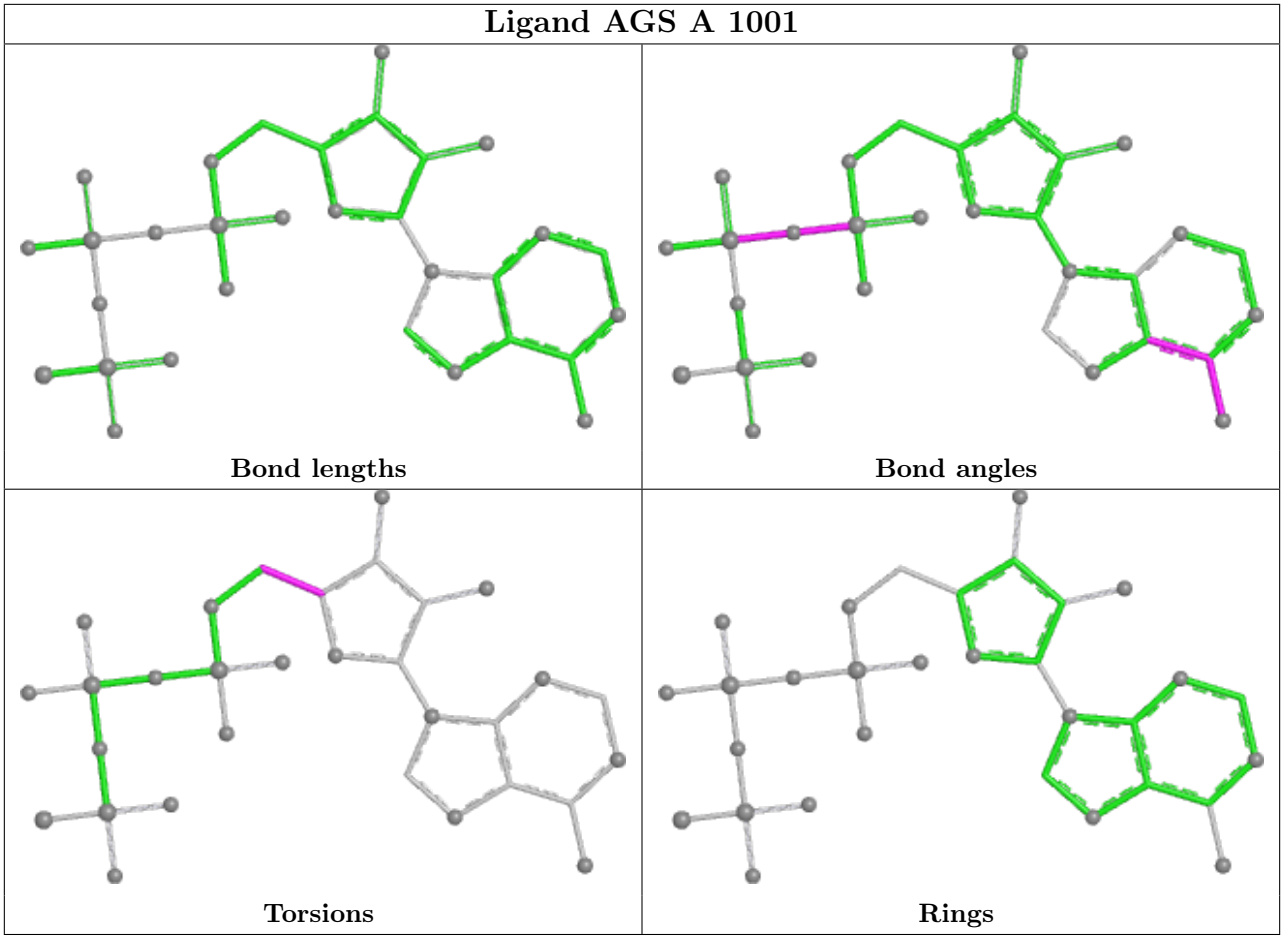


Torsions



Rings

Ligand AGS C 1002	
 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.

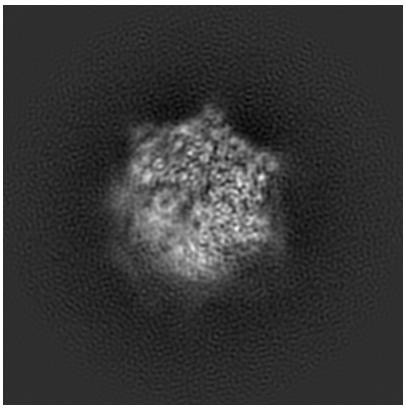
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4624. These allow visual inspection of the internal detail of the map and identification of artifacts.

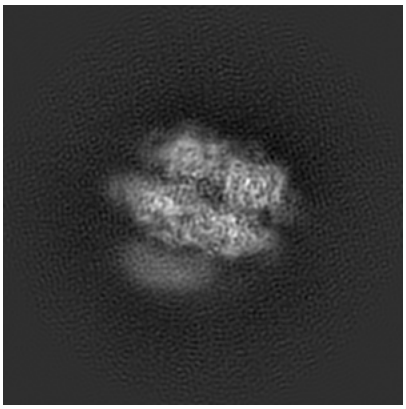
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

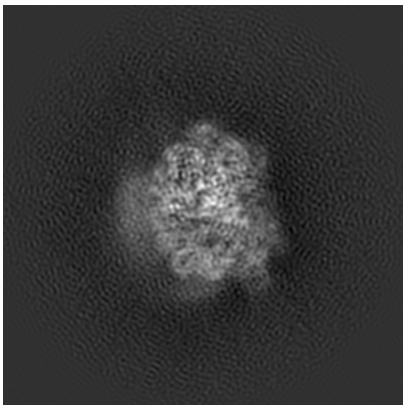
6.1.1 Primary map



X

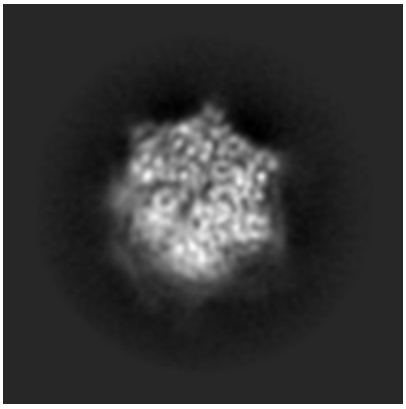


Y

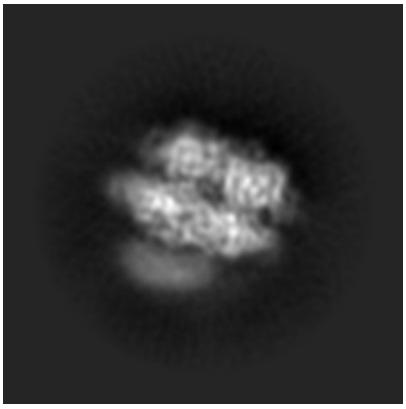


Z

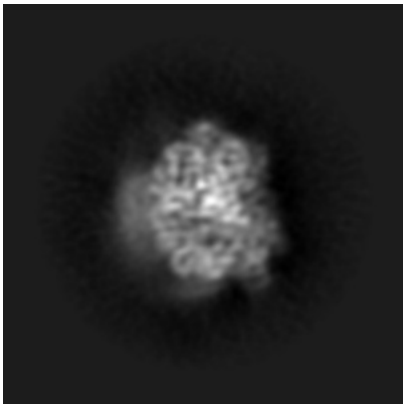
6.1.2 Raw map



X



Y

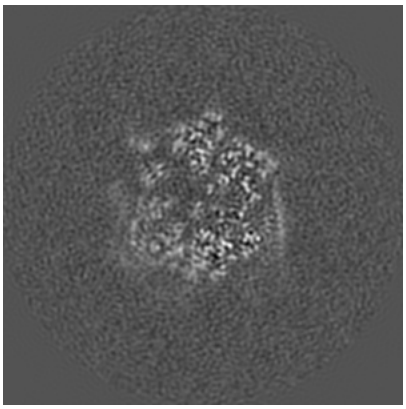


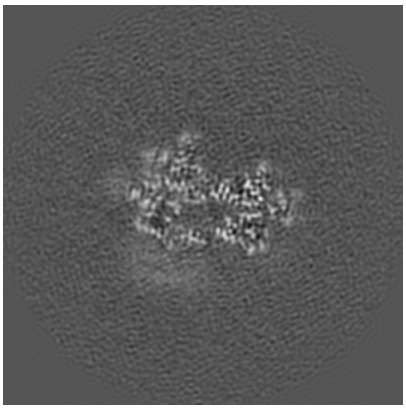
Z

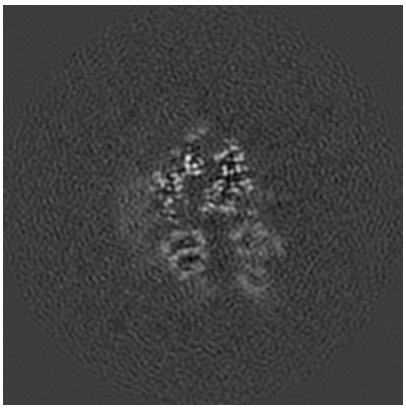
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

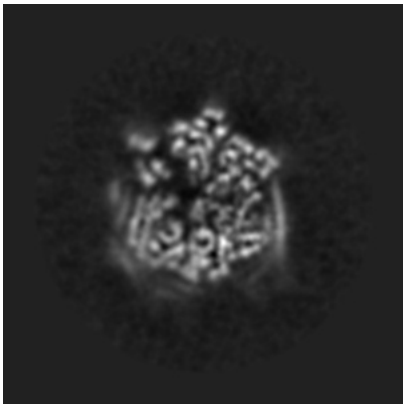
6.2.1 Primary map

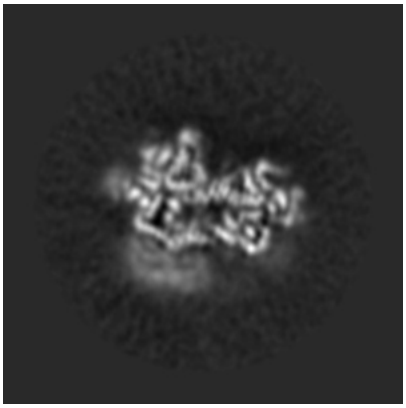

X Index: 144

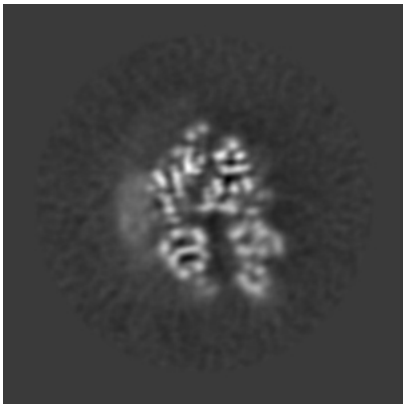

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

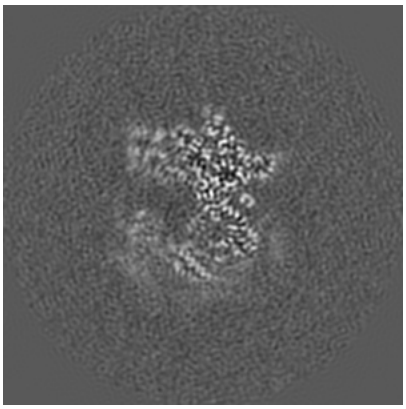

Y Index: 144

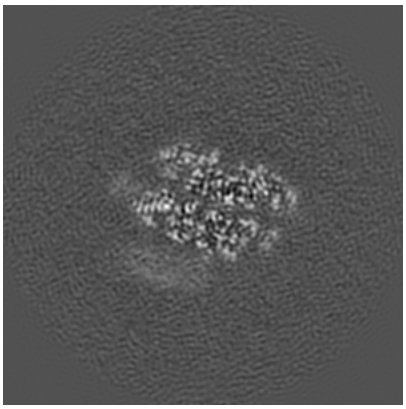

Z Index: 144

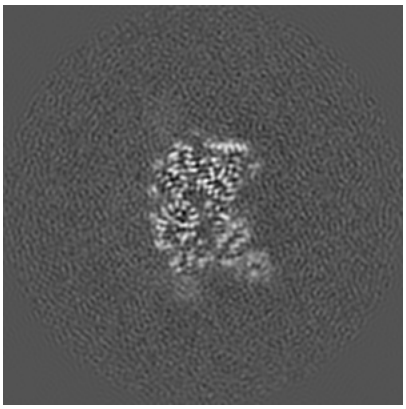
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

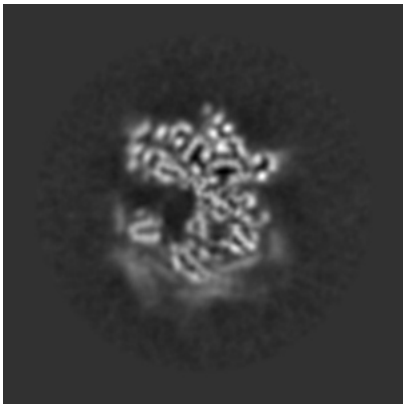
6.3.1 Primary map

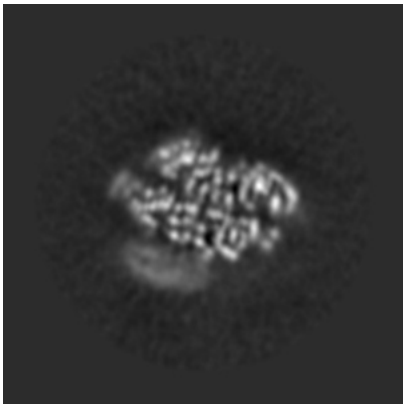

X Index: 153

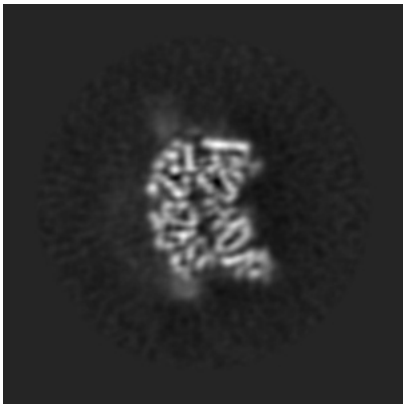

Y Index: 157


Z Index: 163

6.3.2 Raw map


X Index: 155


Y Index: 156


Z Index: 164

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

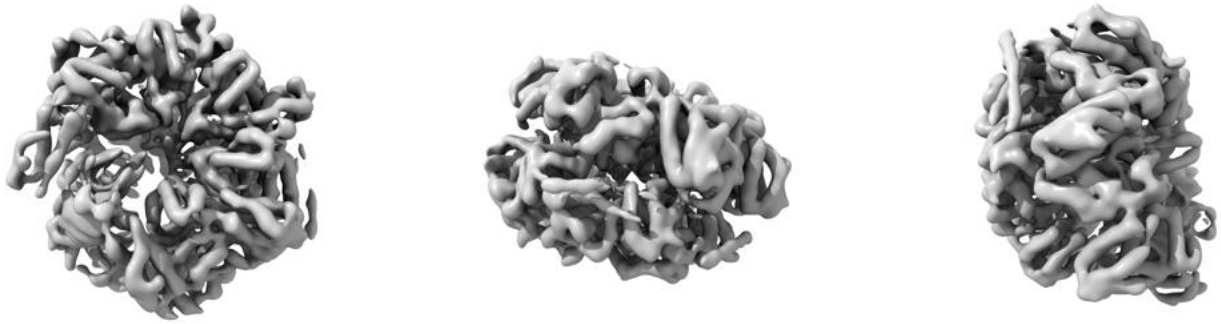
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

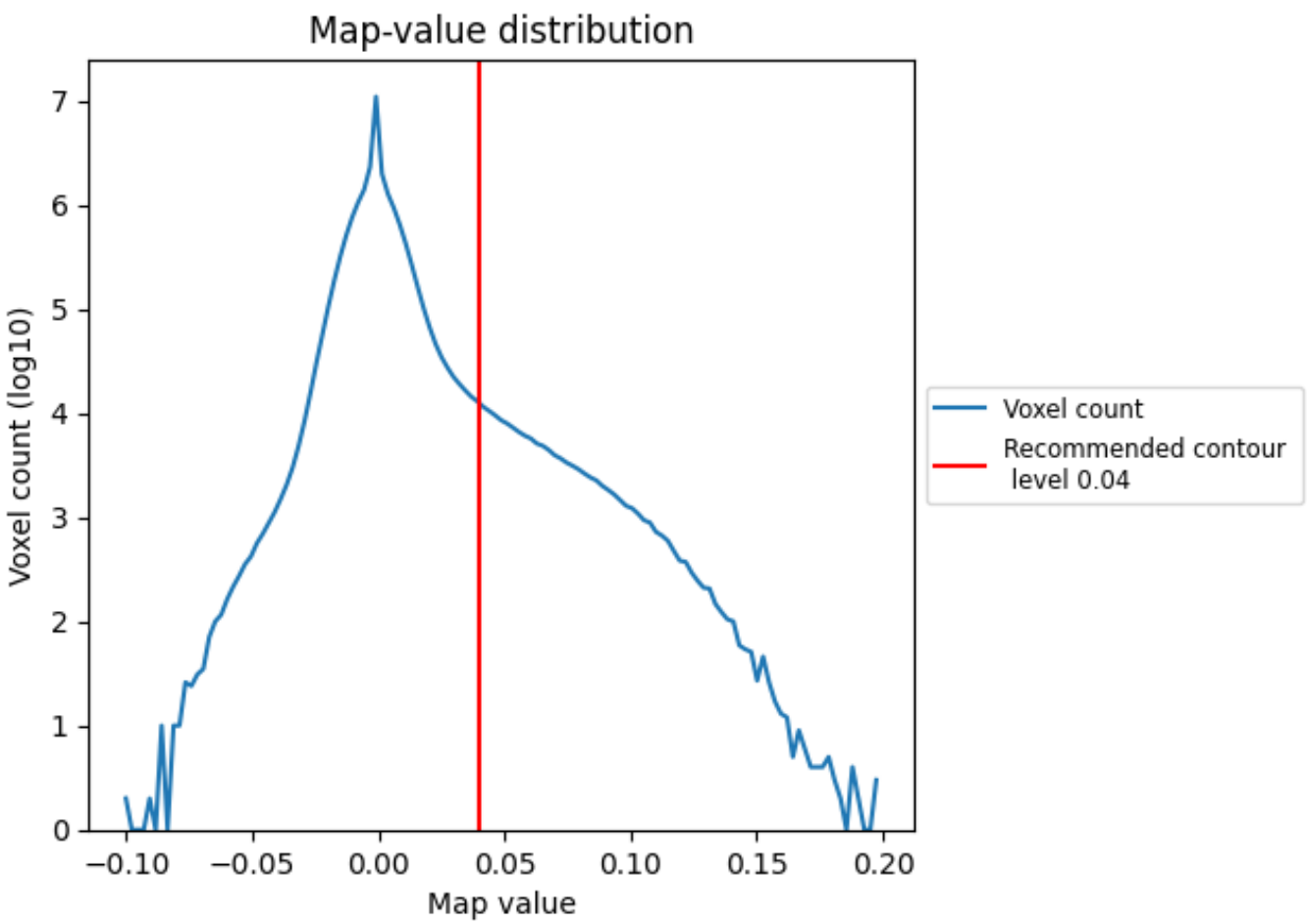
6.5 Mask visualisation (i)

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

7 Map analysis (i)

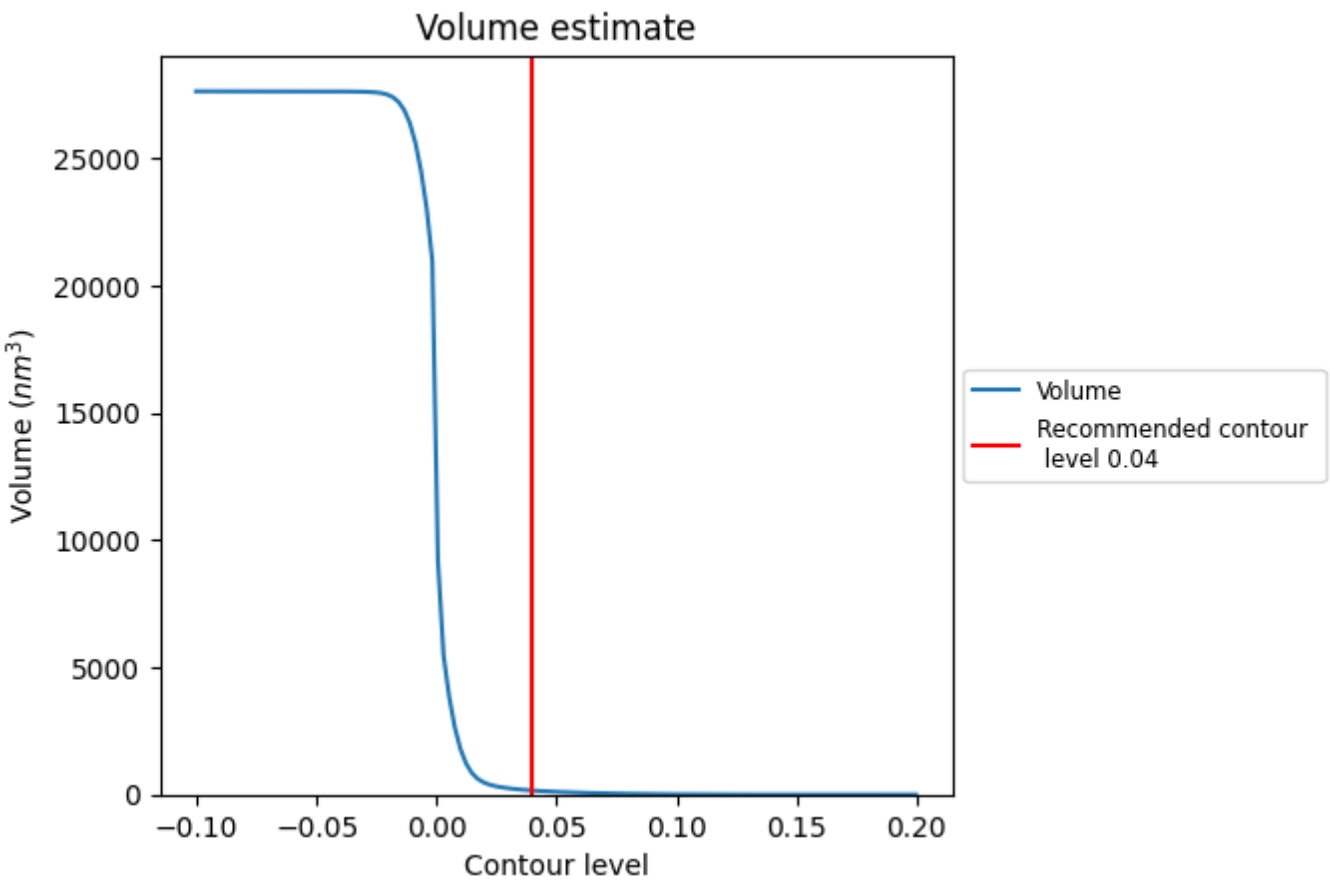
This section contains the results of statistical analysis of the map.

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.

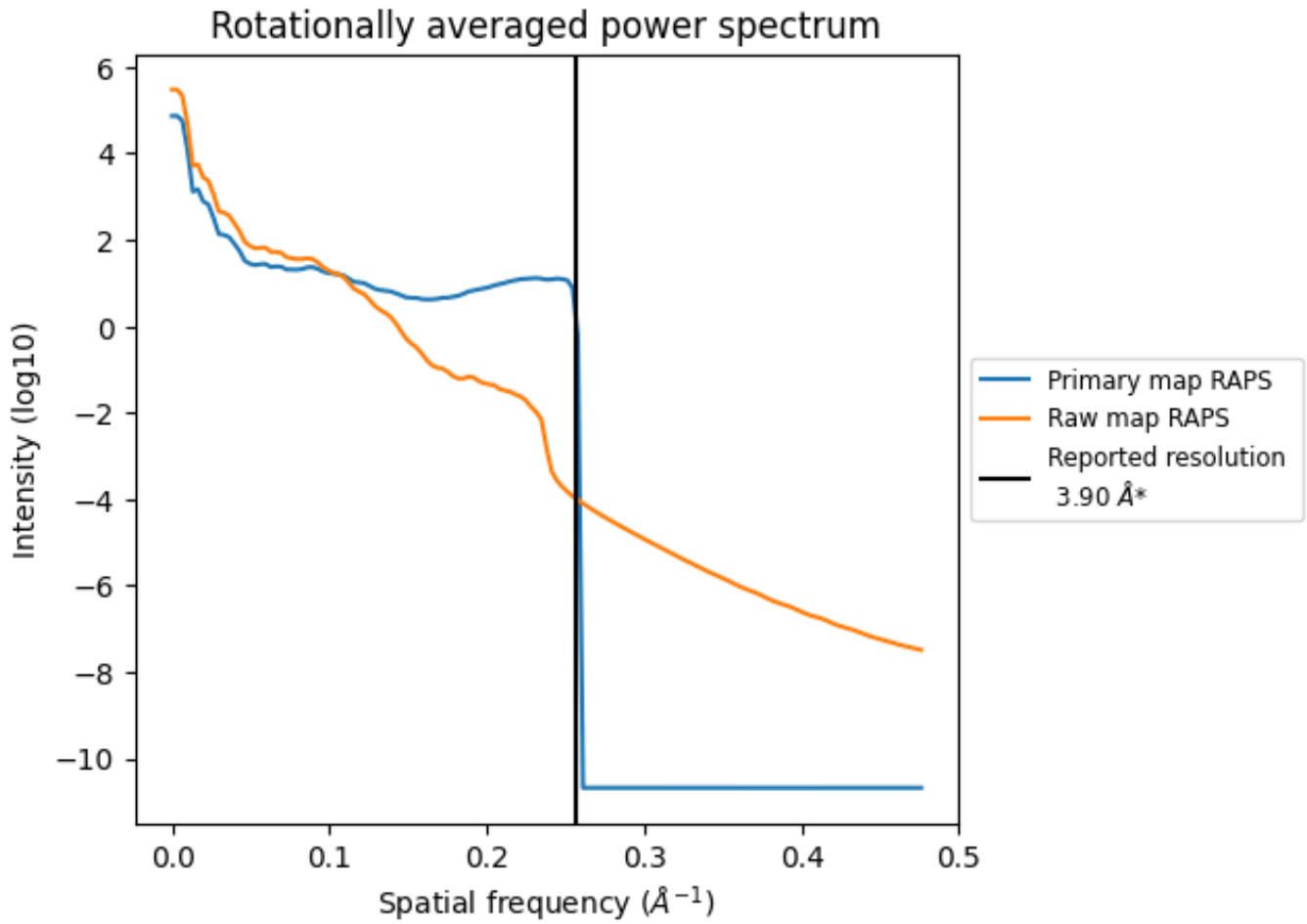
7.2 Volume estimate (i)



The volume at the recommended contour level is 160 nm^3; this corresponds to an approximate mass of 144 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)

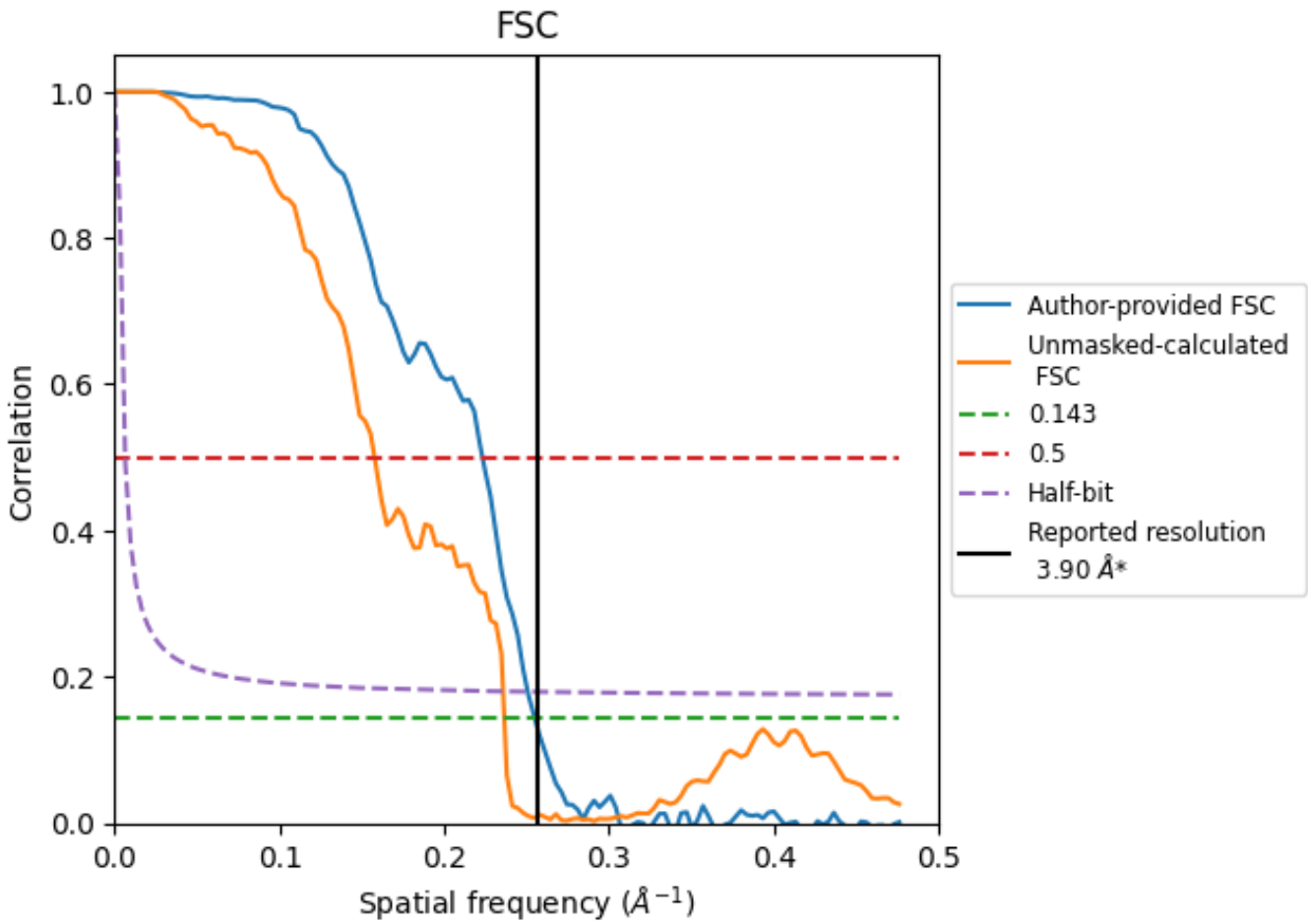


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

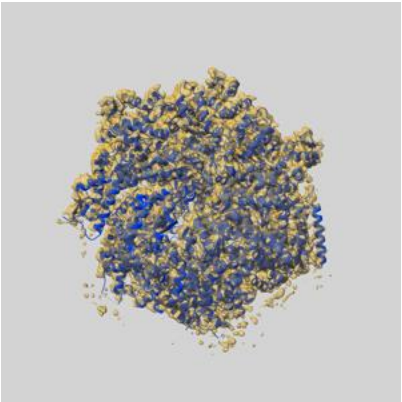
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.92	4.48	3.99
Unmasked-calculated*	4.23	6.34	4.24

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

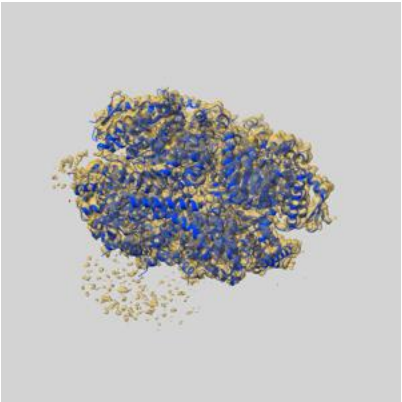
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4624 and PDB model 6QS6. Per-residue inclusion information can be found in section 3 on page 6.

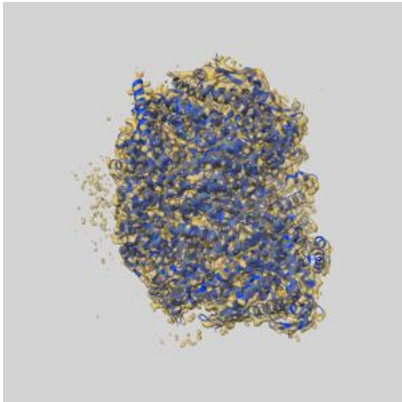
9.1 Map-model overlay (i)



X



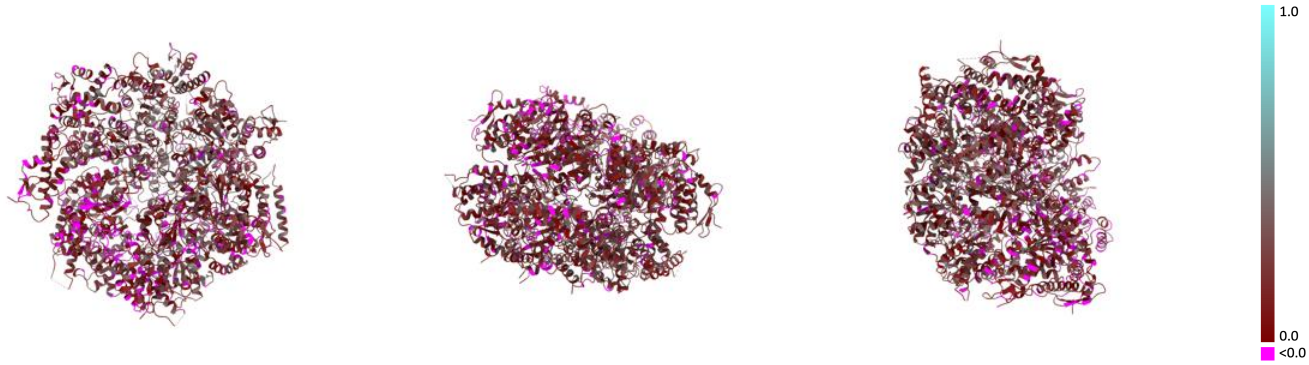
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

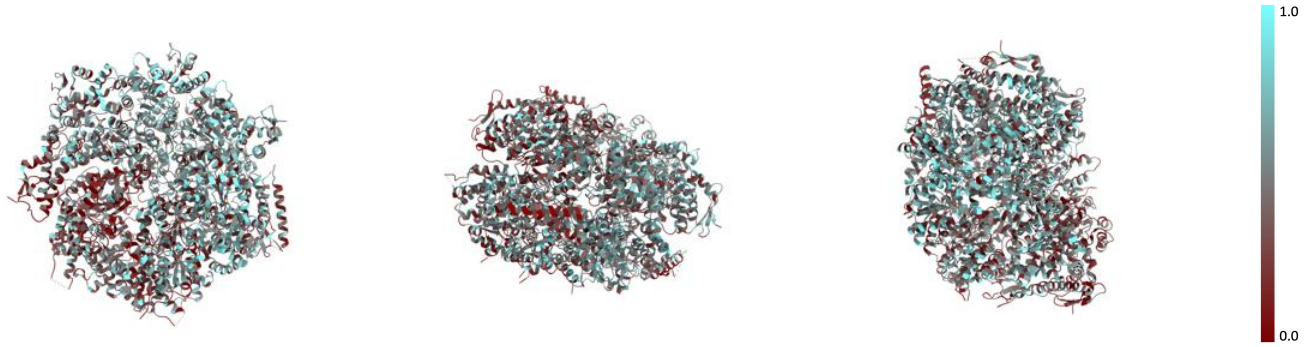
9.2 Q-score mapped to coordinate model (i)



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.

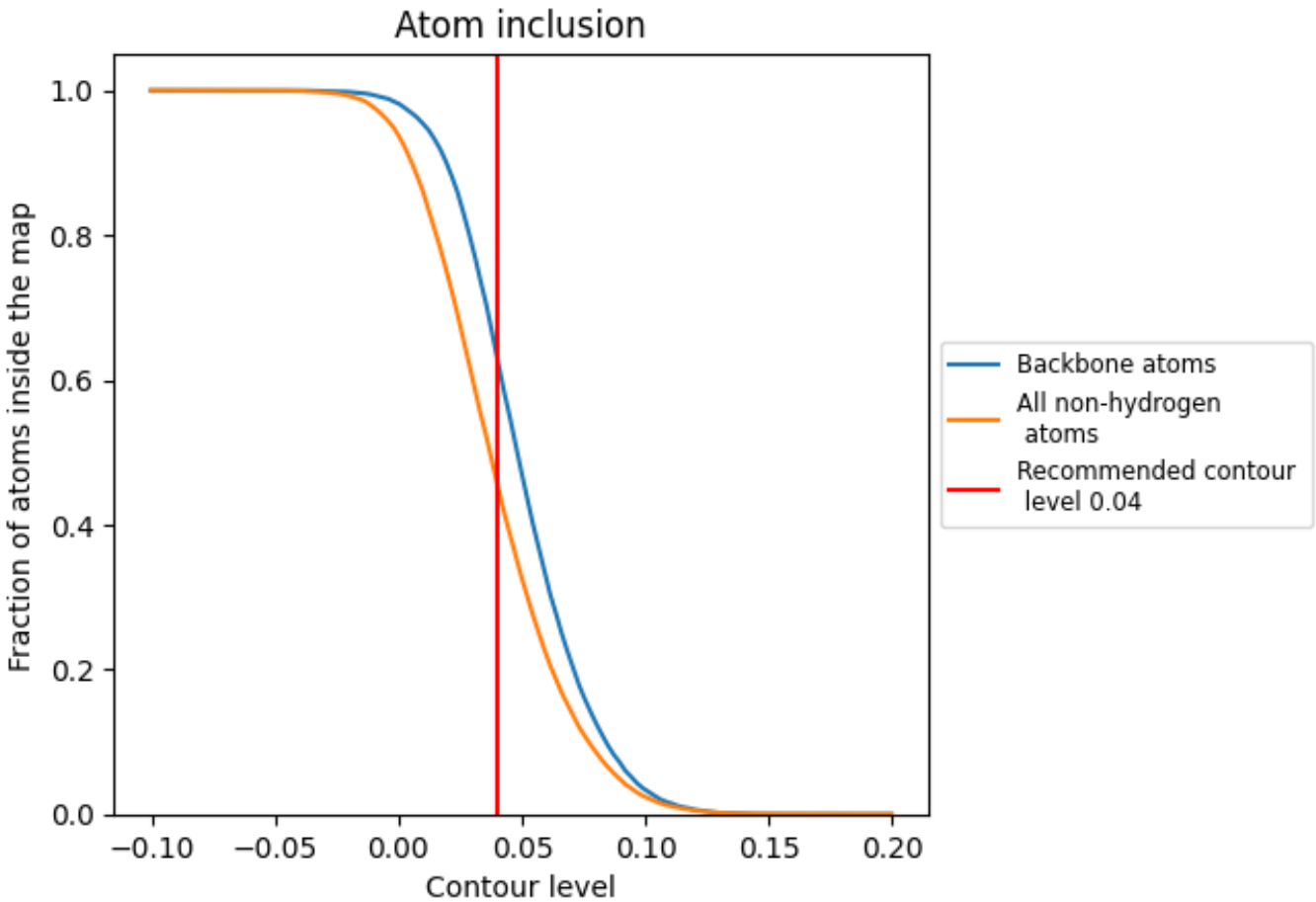
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 46% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4569	0.1750
A	0.4523	0.1790
B	0.5432	0.2060
C	0.5279	0.1950
D	0.4916	0.1880
E	0.3893	0.1440
F	0.3216	0.1320
S	0.6167	0.3050