Full wwPDB EM Validation Report (i)

Feb 24, 2024 – 01:49 PM EST

PDB ID	:	7LFX
EMDB ID	:	EMD-23308
Title	:	Cryo-EM structure of human cGMP-bound open CNGA1 channel in Na+/Ca2+
Authors	:	Xue, J.; Han, Y.; Jiang, Y.
Deposited on	:	2021-01-19
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:

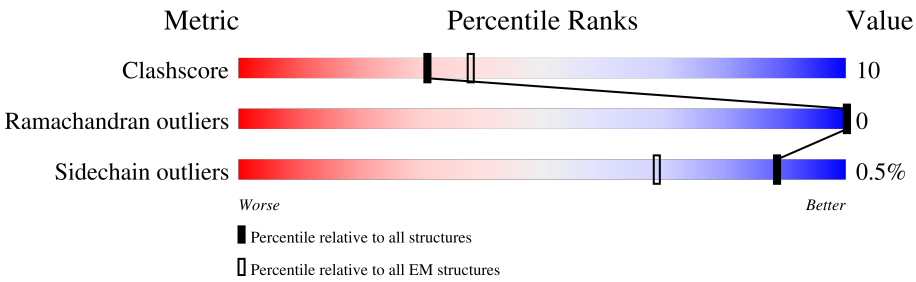
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	560	17% 59% 21% 20%
1	B	560	17% 58% 22% 20%
1	C	560	17% 58% 22% 20%
1	D	560	17% 59% 21% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14846 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 cGMP-gated cation channel alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	450	3688	2411	594	664	19	0	0
1	B	450	3688	2411	594	664	19	0	0
1	C	450	3688	2411	594	664	19	0	0
1	D	450	3688	2411	594	664	19	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	initiating methionine	UNP P29973
A	132	ASP	-	expression tag	UNP P29973
A	133	TYR	-	expression tag	UNP P29973
A	134	LYS	-	expression tag	UNP P29973
A	135	ASP	-	expression tag	UNP P29973
A	136	ASP	-	expression tag	UNP P29973
A	137	ASP	-	expression tag	UNP P29973
A	138	ASP	-	expression tag	UNP P29973
A	139	LYS	-	expression tag	UNP P29973
A	140	GLY	-	expression tag	UNP P29973
A	141	GLY	-	expression tag	UNP P29973
A	142	SER	-	expression tag	UNP P29973
A	143	ALA	-	expression tag	UNP P29973
B	131	MET	-	initiating methionine	UNP P29973
B	132	ASP	-	expression tag	UNP P29973
B	133	TYR	-	expression tag	UNP P29973
B	134	LYS	-	expression tag	UNP P29973
B	135	ASP	-	expression tag	UNP P29973
B	136	ASP	-	expression tag	UNP P29973
B	137	ASP	-	expression tag	UNP P29973
B	138	ASP	-	expression tag	UNP P29973
B	139	LYS	-	expression tag	UNP P29973

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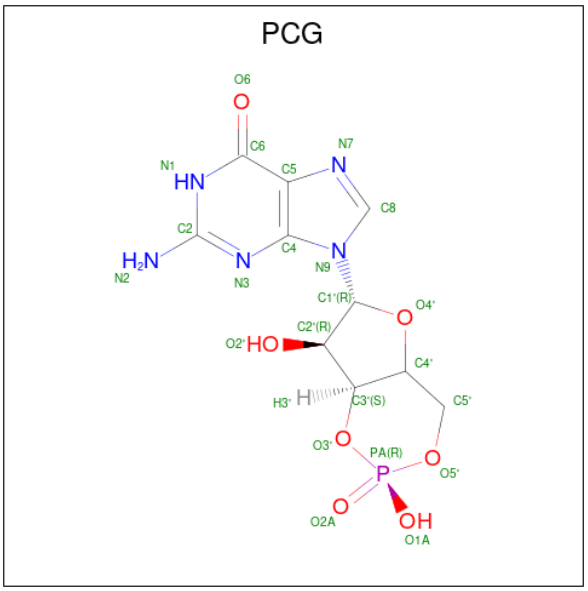
Chain	Residue	Modelled	Actual	Comment	Reference
B	140	GLY	-	expression tag	UNP P29973
B	141	GLY	-	expression tag	UNP P29973
B	142	SER	-	expression tag	UNP P29973
B	143	ALA	-	expression tag	UNP P29973
C	131	MET	-	initiating methionine	UNP P29973
C	132	ASP	-	expression tag	UNP P29973
C	133	TYR	-	expression tag	UNP P29973
C	134	LYS	-	expression tag	UNP P29973
C	135	ASP	-	expression tag	UNP P29973
C	136	ASP	-	expression tag	UNP P29973
C	137	ASP	-	expression tag	UNP P29973
C	138	ASP	-	expression tag	UNP P29973
C	139	LYS	-	expression tag	UNP P29973
C	140	GLY	-	expression tag	UNP P29973
C	141	GLY	-	expression tag	UNP P29973
C	142	SER	-	expression tag	UNP P29973
C	143	ALA	-	expression tag	UNP P29973
D	131	MET	-	initiating methionine	UNP P29973
D	132	ASP	-	expression tag	UNP P29973
D	133	TYR	-	expression tag	UNP P29973
D	134	LYS	-	expression tag	UNP P29973
D	135	ASP	-	expression tag	UNP P29973
D	136	ASP	-	expression tag	UNP P29973
D	137	ASP	-	expression tag	UNP P29973
D	138	ASP	-	expression tag	UNP P29973
D	139	LYS	-	expression tag	UNP P29973
D	140	GLY	-	expression tag	UNP P29973
D	141	GLY	-	expression tag	UNP P29973
D	142	SER	-	expression tag	UNP P29973
D	143	ALA	-	expression tag	UNP P29973

- Molecule 2 is CYCLIC GUANOSINE MONOPHOSPHATE (three-letter code: PCG) (formula: $C_{10}H_{12}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	B	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	C	1	Total	C	N	O	P	0
			23	10	5	7	1	
2	D	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

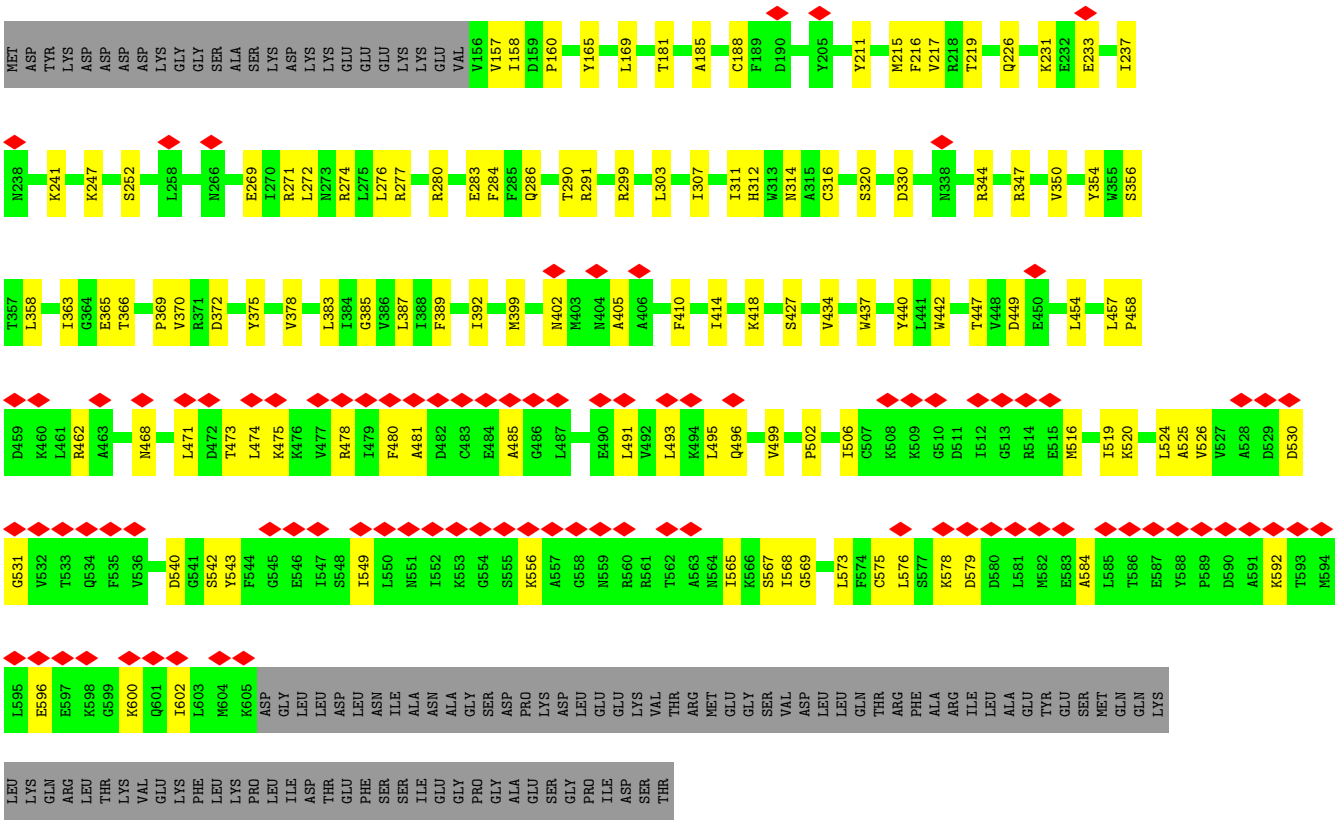
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Ca	0
			2	2	

3 Residue-property plots (i)

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

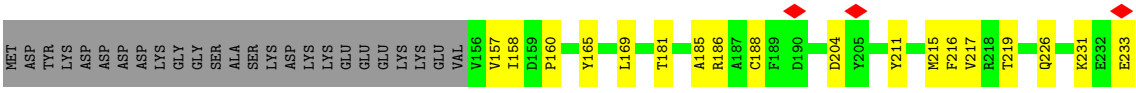
- Molecule 1: cGMP-gated cation channel alpha-1

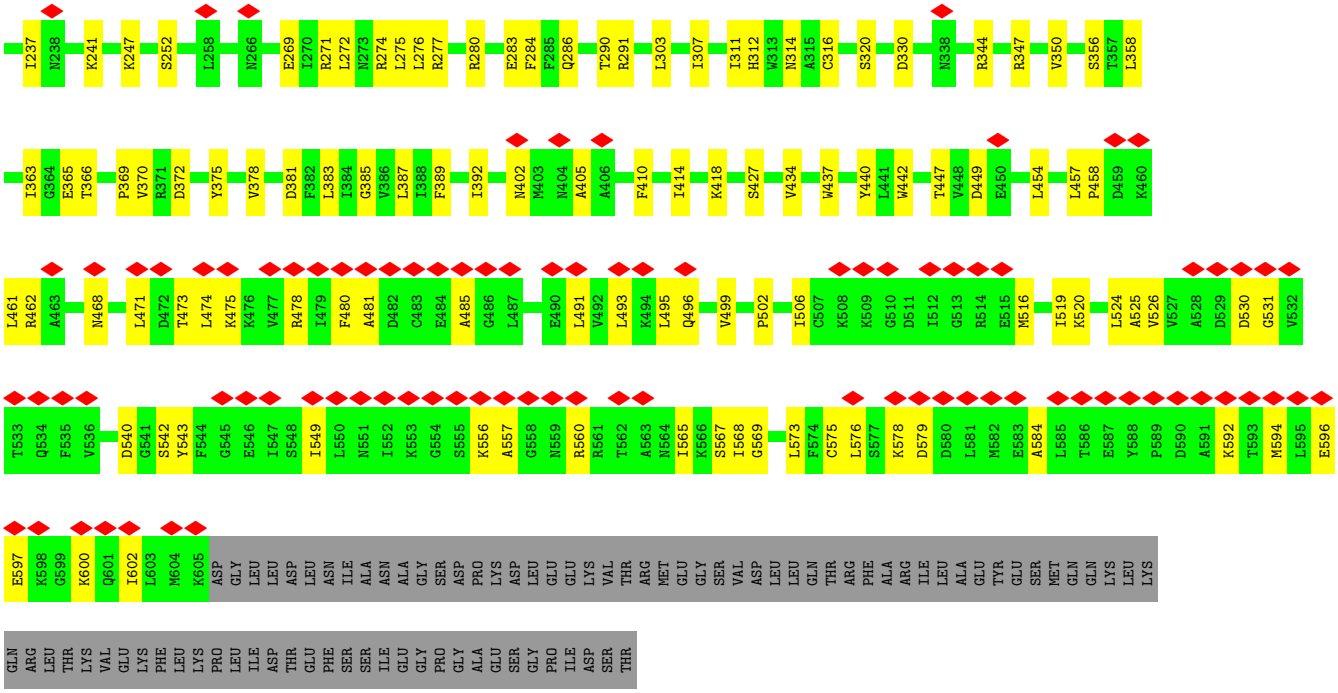
Chain A:



- Molecule 1: cGMP-gated cation channel alpha-1

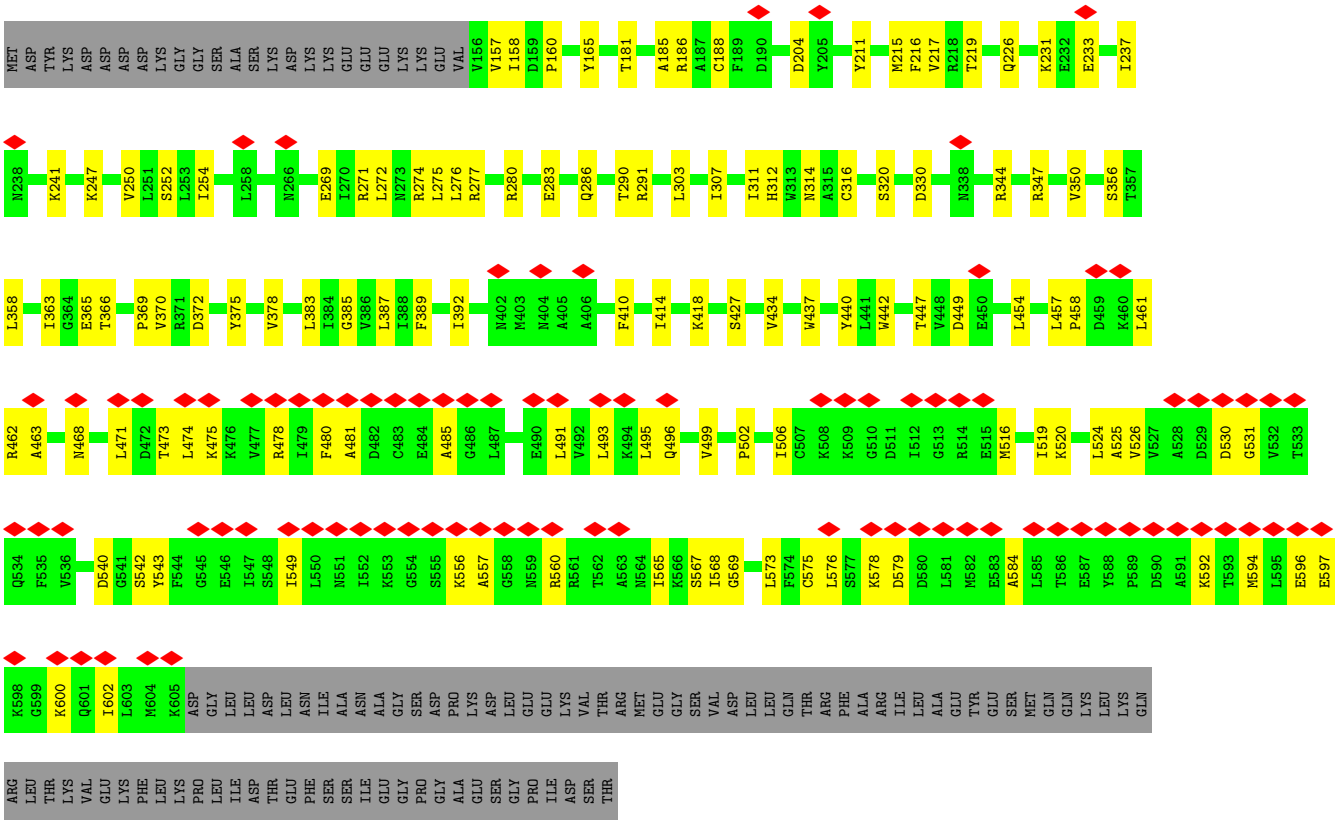
Chain B:





- Molecule 1: cGMP-gated cation channel alpha-1

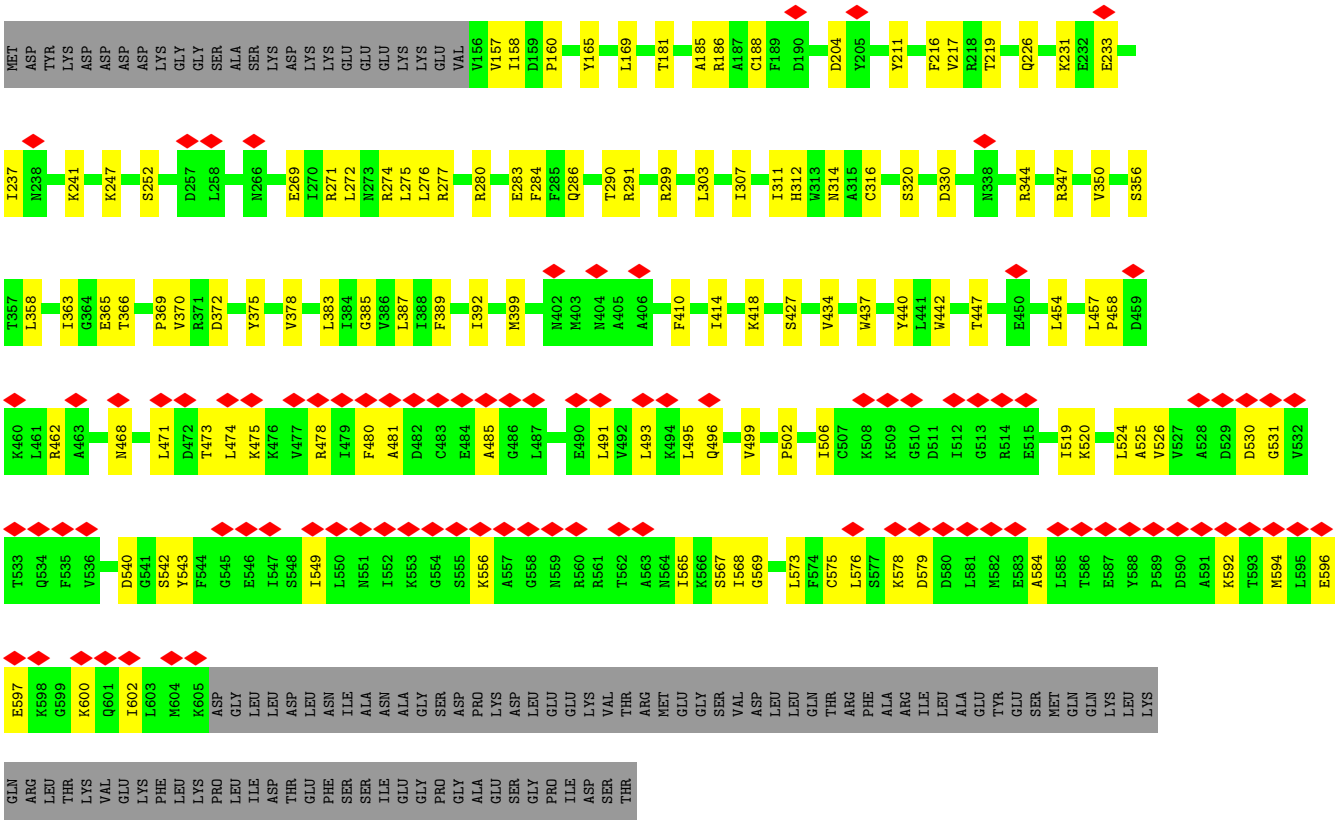
Chain C:



- Molecule 1: cGMP-gated cation channel alpha-1

Chain D:

17%
59%
21%
20%


MET ASP TYR LYS ASP ASP ASP ASP LYS GLY GLY SER ALA SER LYS ASP LYS LYS LYS GLU GLU GLU LYS LYS GLU VAL V156 V157 I158 D159 P160 Y165 L169 T181 A185 R186 A187 C188 F189 D190 D204 Y205 Y211 F216 V217 R218 T219 Q226 K231 E232 E233
I237 N238 K241 K247 S252 D257 L258 N266 E269 I270 R271 L272 N273 R274 L275 L276 R277 R280 E283 F284 F285 Q286 T290 R291 R299 L303 I307 I311 H312 W313 N314 A315 C316 S320 D330 N338 R344 R347 V350 S356
T357 L358 I363 G364 E365 T366 P369 V370 R371 D372 Y375 V378 L383 I384 G385 V386 L387 I388 F389 I392 M399 N402 M403 N404 A405 A406 F410 I414 K418 S427 V434 W437 Y440 L441 W442 T447 E450 L454 L457 P458 D459
K460 L461 R462 A463 N468 L471 D472 T473 L474 K475 K476 V477 R478 I479 F480 A481 D482 C483 E484 A485 G486 L487 E490 L491 V492 L493 K494 L495 Q496 V499 P502 I506 C507 K508 K509 G510 D511 I512 G513 R514 E515 I519 K520 L524 A525 V526 V527 A528 D529 D530 G531 V532
T533 Q534 F535 V536 D540 G541 S542 Y543 F544 G545 E546 I547 S548 I549 L550 N551 I552 K553 G554 S555 K556 A557 G558 N559 R560 R561 T562 A563 N564 I565 K566 S567 I568 G569 L573 F574 C575 L576 S577 K578 D579 D580 L581 M582 E583 A584 L585 T586 E587 Y588 P589 D590 A591 K592 T593 M594 L595 E596
E597 K598 G599 K600 Q601 I602 L603 M604 K605 ASP GLY LEU LEU ASP LEU ASN ILE ALA ASN ALA GLY SER ASP PRO LYS ASP LEU GLU GLU LYS VAL THR ARG MET GLU GLY SER VAL ASP LEU LEU GLN THR ARG PHE ALA ARG ILE LEU ALA GLU TYR GLU SER MET GLN GLN LYS LEU LYS
GLN ARG LEU THR LYS VAL GLU LYS PHE LEU LYS PRO LEU ILE ASP THR GLU PHE SER SER ILE GLU GLY PRO GLY ALA GLU SER GLY PRO ILE ASP SER THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76571	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.107	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	231.84, 231.84, 231.84	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.805, 0.805, 0.805	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: PCG, CA

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	0.28	0/3773	0.41	0/5111
1	B	0.28	0/3773	0.41	0/5111
1	C	0.28	0/3773	0.41	0/5111
1	D	0.28	0/3773	0.41	0/5111
All	All	0.28	0/15092	0.41	0/20444

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	3688	0	3737	82	0
1	B	3688	0	3737	86	0
1	C	3688	0	3737	84	0
1	D	3688	0	3737	80	0
2	A	23	0	11	1	0
2	B	23	0	11	1	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	A	2	0	0	0	0
All	All	14846	0	14992	288	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 10.

All (288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ALA:HA	1:A:485:ALA:HA	1.83	0.60
1:C:385:GLY:O	1:C:389:PHE:HB2	2.02	0.60
1:D:481:ALA:HA	1:D:485:ALA:HA	1.84	0.60
1:C:481:ALA:HA	1:C:485:ALA:HA	1.84	0.59
1:B:481:ALA:HA	1:B:485:ALA:HA	1.83	0.59
1:D:385:GLY:O	1:D:389:PHE:HB2	2.02	0.59
1:A:347:ARG:NH2	1:B:370:VAL:O	2.36	0.59
1:B:385:GLY:O	1:B:389:PHE:HB2	2.02	0.59
1:C:347:ARG:NH2	1:D:370:VAL:O	2.36	0.58
1:B:347:ARG:NH2	1:C:370:VAL:O	2.36	0.58
1:A:385:GLY:O	1:A:389:PHE:HB2	2.02	0.58
1:A:370:VAL:O	1:D:347:ARG:NH2	2.36	0.58
1:A:540:ASP:OD2	1:B:226:GLN:NE2	2.38	0.57
1:A:226:GLN:NE2	1:D:540:ASP:OD2	2.38	0.57
1:B:252:SER:HB3	1:B:276:LEU:HB2	1.87	0.57
1:D:252:SER:HB3	1:D:276:LEU:HB2	1.87	0.57
1:C:252:SER:HB3	1:C:276:LEU:HB2	1.87	0.56
1:D:491:LEU:HD21	1:D:584:ALA:HB3	1.87	0.56
1:B:540:ASP:OD2	1:C:226:GLN:NE2	2.37	0.56
1:C:540:ASP:OD2	1:D:226:GLN:NE2	2.38	0.56
1:C:491:LEU:HD21	1:C:584:ALA:HB3	1.87	0.56
1:B:440:TYR:HE2	1:B:499:VAL:HG11	1.71	0.56
1:C:440:TYR:HE2	1:C:499:VAL:HG11	1.71	0.56
1:A:491:LEU:HD21	1:A:584:ALA:HB3	1.87	0.56
1:A:252:SER:HB3	1:A:276:LEU:HB2	1.87	0.55
1:A:440:TYR:HE2	1:A:499:VAL:HG11	1.71	0.55
1:A:468:ASN:HD21	1:D:427:SER:H	1.55	0.55
1:D:440:TYR:HE2	1:D:499:VAL:HG11	1.71	0.55
1:B:491:LEU:HD21	1:B:584:ALA:HB3	1.87	0.55
1:C:427:SER:H	1:D:468:ASN:HD21	1.55	0.55
1:B:181:THR:O	1:B:312:HIS:NE2	2.40	0.55
1:A:303:LEU:HD22	1:A:392:ILE:HG23	1.89	0.54
1:B:307:ILE:HD13	1:C:387:LEU:HD21	1.90	0.54
1:A:307:ILE:HD13	1:B:387:LEU:HD21	1.90	0.54
1:D:303:LEU:HD22	1:D:392:ILE:HG23	1.89	0.54
1:C:181:THR:O	1:C:312:HIS:NE2	2.40	0.54
1:B:427:SER:H	1:C:468:ASN:HD21	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:THR:O	1:D:312:HIS:NE2	2.40	0.54
1:B:303:LEU:HD22	1:B:392:ILE:HG23	1.89	0.53
1:A:387:LEU:HD21	1:D:307:ILE:HD13	1.90	0.53
1:C:307:ILE:HD13	1:D:387:LEU:HD21	1.90	0.53
1:A:181:THR:O	1:A:312:HIS:NE2	2.40	0.53
1:B:495:LEU:HD23	1:B:576:LEU:HD13	1.91	0.53
1:C:495:LEU:HD23	1:C:576:LEU:HD13	1.91	0.53
1:D:519:ILE:HD12	1:D:542:SER:HB2	1.91	0.53
1:A:427:SER:H	1:B:468:ASN:HD21	1.55	0.53
1:C:519:ILE:HD12	1:C:542:SER:HB2	1.91	0.53
1:B:283:GLU:O	1:B:286:GLN:HG3	2.10	0.52
1:C:303:LEU:HD22	1:C:392:ILE:HG23	1.89	0.52
1:D:188:CYS:SG	1:D:320:SER:OG	2.68	0.52
1:B:188:CYS:SG	1:B:320:SER:OG	2.68	0.52
1:B:519:ILE:HD12	1:B:542:SER:HB2	1.91	0.52
1:C:283:GLU:O	1:C:286:GLN:HG3	2.10	0.52
1:D:283:GLU:O	1:D:286:GLN:HG3	2.10	0.52
1:A:519:ILE:HD12	1:A:542:SER:HB2	1.91	0.52
1:C:188:CYS:SG	1:C:320:SER:OG	2.68	0.52
1:A:462:ARG:HD2	1:A:493:LEU:HD22	1.92	0.52
1:D:462:ARG:HD2	1:D:493:LEU:HD22	1.92	0.52
1:A:188:CYS:SG	1:A:320:SER:OG	2.68	0.52
1:B:462:ARG:HD2	1:B:493:LEU:HD22	1.92	0.52
1:D:165:TYR:OH	1:D:280:ARG:NH2	2.42	0.51
1:A:495:LEU:HD23	1:A:576:LEU:HD13	1.91	0.51
1:C:462:ARG:HD2	1:C:493:LEU:HD22	1.92	0.51
1:D:495:LEU:HD23	1:D:576:LEU:HD13	1.91	0.51
1:B:216:PHE:O	1:B:219:THR:OG1	2.23	0.51
1:B:165:TYR:OH	1:B:280:ARG:NH2	2.42	0.51
1:A:283:GLU:O	1:A:286:GLN:HG3	2.10	0.51
1:D:480:PHE:HZ	1:D:491:LEU:HD13	1.76	0.51
1:A:241:LYS:O	1:A:247:LYS:NZ	2.44	0.51
1:D:442:TRP:HE3	1:D:447:THR:HG21	1.76	0.51
1:A:442:TRP:HE3	1:A:447:THR:HG21	1.76	0.50
1:B:480:PHE:HZ	1:B:491:LEU:HD13	1.76	0.50
1:D:216:PHE:O	1:D:219:THR:OG1	2.23	0.50
1:B:185:ALA:HB2	1:B:312:HIS:CE1	2.47	0.50
1:A:369:PRO:HG3	1:A:378:VAL:HG21	1.94	0.50
1:A:414:ILE:HG22	1:A:418:LYS:HE2	1.94	0.50
1:B:442:TRP:HE3	1:B:447:THR:HG21	1.76	0.50
1:C:185:ALA:HB2	1:C:312:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:PHE:HZ	1:A:491:LEU:HD13	1.76	0.50
1:B:157:VAL:HG11	1:B:231:LYS:HA	1.94	0.50
1:C:480:PHE:HZ	1:C:491:LEU:HD13	1.76	0.50
1:A:474:LEU:HD22	1:A:480:PHE:HD2	1.77	0.49
1:A:478:ARG:HG3	1:A:543:TYR:HE1	1.77	0.49
1:C:165:TYR:OH	1:C:280:ARG:NH2	2.42	0.49
1:C:474:LEU:HD22	1:C:480:PHE:HD2	1.77	0.49
1:D:369:PRO:HG3	1:D:378:VAL:HG21	1.94	0.49
1:B:414:ILE:HG22	1:B:418:LYS:HE2	1.94	0.49
1:A:165:TYR:OH	1:A:280:ARG:NH2	2.42	0.49
1:A:185:ALA:HB2	1:A:312:HIS:CE1	2.47	0.49
1:C:188:CYS:SG	1:C:316:CYS:HB3	2.52	0.49
1:D:185:ALA:HB2	1:D:312:HIS:CE1	2.47	0.49
1:D:188:CYS:SG	1:D:316:CYS:HB3	2.52	0.49
1:D:478:ARG:HG3	1:D:543:TYR:HE1	1.78	0.49
1:A:468:ASN:ND2	1:D:427:SER:H	2.11	0.49
1:B:188:CYS:SG	1:B:316:CYS:HB3	2.52	0.49
1:B:474:LEU:HD22	1:B:480:PHE:HD2	1.77	0.49
1:B:478:ARG:HG3	1:B:543:TYR:HE1	1.77	0.49
1:C:157:VAL:HG11	1:C:231:LYS:HA	1.94	0.49
1:C:369:PRO:HG3	1:C:378:VAL:HG21	1.94	0.49
1:C:414:ILE:HG22	1:C:418:LYS:HE2	1.94	0.49
1:D:241:LYS:O	1:D:247:LYS:NZ	2.44	0.49
1:D:414:ILE:HG22	1:D:418:LYS:HE2	1.94	0.49
1:A:157:VAL:HG11	1:A:231:LYS:HA	1.94	0.49
1:A:427:SER:H	1:B:468:ASN:ND2	2.11	0.49
1:A:458:PRO:HG3	1:D:437:TRP:CE2	2.48	0.49
1:C:478:ARG:HG3	1:C:543:TYR:HE1	1.77	0.49
1:C:442:TRP:HE3	1:C:447:THR:HG21	1.76	0.49
1:C:427:SER:H	1:D:468:ASN:ND2	2.10	0.48
1:C:437:TRP:CE2	1:D:458:PRO:HG3	2.48	0.48
1:A:188:CYS:SG	1:A:316:CYS:HB3	2.52	0.48
1:D:474:LEU:HD22	1:D:480:PHE:HD2	1.77	0.48
1:A:383:LEU:HD21	1:D:311:ILE:CD1	2.43	0.48
1:B:369:PRO:HG3	1:B:378:VAL:HG21	1.94	0.48
1:B:427:SER:H	1:C:468:ASN:ND2	2.11	0.48
1:C:241:LYS:O	1:C:247:LYS:NZ	2.44	0.48
1:A:437:TRP:CE2	1:B:458:PRO:HG3	2.48	0.48
1:B:241:LYS:O	1:B:247:LYS:NZ	2.44	0.48
1:C:480:PHE:CZ	1:C:491:LEU:HD13	2.49	0.48
1:B:480:PHE:CZ	1:B:491:LEU:HD13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:VAL:HG11	1:D:231:LYS:HA	1.94	0.47
1:B:311:ILE:CD1	1:C:383:LEU:HD21	2.44	0.47
1:B:437:TRP:CE2	1:C:458:PRO:HG3	2.48	0.47
1:D:307:ILE:HG13	1:D:392:ILE:HG21	1.97	0.47
1:A:290:THR:HG23	1:D:414:ILE:HD13	1.96	0.47
1:A:307:ILE:HG13	1:A:392:ILE:HG21	1.97	0.47
1:B:414:ILE:HD13	1:C:290:THR:HG23	1.96	0.47
1:C:311:ILE:CD1	1:D:383:LEU:HD21	2.44	0.47
1:A:372:ASP:CG	1:D:344:ARG:HH12	2.17	0.47
1:B:449:ASP:OD1	1:B:449:ASP:N	2.45	0.47
1:D:480:PHE:CZ	1:D:491:LEU:HD13	2.49	0.47
1:A:311:ILE:CD1	1:B:383:LEU:HD21	2.44	0.47
1:A:480:PHE:CZ	1:A:491:LEU:HD13	2.49	0.46
1:A:506:ILE:HD11	1:A:567:SER:HB2	1.98	0.46
1:C:307:ILE:HG13	1:C:392:ILE:HG21	1.97	0.46
1:D:473:THR:HG21	1:D:520:LYS:HA	1.97	0.46
1:B:307:ILE:HG13	1:B:392:ILE:HG21	1.96	0.46
1:C:271:ARG:O	1:C:274:ARG:HB2	2.16	0.46
1:D:233:GLU:O	1:D:237:ILE:HG12	2.16	0.46
1:B:344:ARG:HH12	1:C:372:ASP:CG	2.18	0.46
1:C:506:ILE:HD11	1:C:567:SER:HB2	1.97	0.46
1:C:473:THR:HG21	1:C:520:LYS:HA	1.97	0.46
1:C:211:TYR:O	1:C:277:ARG:NH1	2.49	0.46
1:C:414:ILE:HD13	1:D:290:THR:HG23	1.96	0.46
1:A:233:GLU:O	1:A:237:ILE:HG12	2.16	0.46
1:A:271:ARG:O	1:A:274:ARG:HB2	2.16	0.46
1:B:530:ASP:OD1	1:B:531:GLY:N	2.48	0.46
1:D:358:LEU:HD12	1:D:366:THR:HG23	1.98	0.46
1:D:506:ILE:HD11	1:D:567:SER:HB2	1.97	0.46
1:A:344:ARG:HH12	1:B:372:ASP:CG	2.18	0.46
1:A:530:ASP:OD1	1:A:531:GLY:N	2.48	0.46
1:C:233:GLU:O	1:C:237:ILE:HG12	2.16	0.46
1:C:344:ARG:HH12	1:D:372:ASP:CG	2.17	0.46
1:C:530:ASP:OD1	1:C:531:GLY:N	2.49	0.46
1:D:530:ASP:OD1	1:D:531:GLY:N	2.48	0.46
1:A:211:TYR:O	1:A:277:ARG:NH1	2.49	0.46
1:A:414:ILE:HD13	1:B:290:THR:HG23	1.96	0.46
1:B:233:GLU:O	1:B:237:ILE:HG12	2.16	0.46
1:B:502:PRO:HG3	1:B:569:GLY:HA2	1.98	0.46
1:A:358:LEU:HD12	1:A:366:THR:HG23	1.98	0.45
1:B:271:ARG:O	1:B:274:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:PRO:HG3	1:D:569:GLY:HA2	1.98	0.45
1:A:457:LEU:HD21	1:D:434:VAL:HG13	1.99	0.45
1:A:434:VAL:HG13	1:B:457:LEU:HD21	1.99	0.45
1:A:473:THR:HG21	1:A:520:LYS:HA	1.97	0.45
1:C:434:VAL:HG13	1:D:457:LEU:HD21	1.98	0.45
1:B:473:THR:HG21	1:B:520:LYS:HA	1.97	0.45
1:B:506:ILE:HD11	1:B:567:SER:HB2	1.98	0.45
1:D:269:GLU:O	1:D:272:LEU:HB2	2.17	0.45
1:C:502:PRO:HG3	1:C:569:GLY:HA2	1.99	0.45
1:D:211:TYR:O	1:D:277:ARG:NH1	2.49	0.45
1:D:271:ARG:O	1:D:274:ARG:HB2	2.16	0.45
1:B:211:TYR:O	1:B:277:ARG:NH1	2.49	0.45
1:C:358:LEU:HD12	1:C:366:THR:HG23	1.98	0.45
1:B:160:PRO:HA	1:B:165:TYR:CG	2.52	0.45
1:B:596:GLU:HG3	1:B:600:LYS:HZ1	1.81	0.45
1:A:596:GLU:HG3	1:A:600:LYS:HZ1	1.82	0.45
1:A:502:PRO:HG3	1:A:569:GLY:HA2	1.99	0.45
1:D:186:ARG:NH1	1:D:204:ASP:OD2	2.38	0.45
1:A:160:PRO:HA	1:A:165:TYR:CG	2.52	0.45
1:A:269:GLU:O	1:A:272:LEU:HB2	2.17	0.45
1:B:434:VAL:HG13	1:C:457:LEU:HD21	1.99	0.45
1:C:160:PRO:HA	1:C:165:TYR:CG	2.52	0.45
1:D:160:PRO:HA	1:D:165:TYR:CG	2.52	0.45
1:D:524:LEU:HD11	1:D:573:LEU:HD21	1.99	0.45
1:B:358:LEU:HD12	1:B:366:THR:HG23	1.98	0.44
1:A:524:LEU:HD11	1:A:573:LEU:HD21	1.99	0.44
1:A:410:PHE:CE2	1:A:442:TRP:HB2	2.53	0.44
1:B:314:ASN:ND2	1:B:381:ASP:OD2	2.44	0.44
1:B:269:GLU:O	1:B:272:LEU:HB2	2.17	0.44
1:C:516:MET:N	1:C:576:LEU:O	2.41	0.44
1:C:269:GLU:O	1:C:272:LEU:HB2	2.17	0.44
1:C:496:GLN:HB2	1:C:575:CYS:SG	2.58	0.44
1:A:516:MET:N	1:A:576:LEU:O	2.41	0.44
1:B:410:PHE:CE2	1:B:442:TRP:HB2	2.53	0.44
1:B:496:GLN:HB2	1:B:575:CYS:SG	2.58	0.44
1:B:549:ILE:HD12	1:B:578:LYS:HB3	2.00	0.44
1:C:350:VAL:HG12	1:D:375:TYR:HB3	2.00	0.44
1:C:410:PHE:CE2	1:C:442:TRP:HB2	2.53	0.44
1:C:524:LEU:HD11	1:C:573:LEU:HD21	1.99	0.44
1:C:549:ILE:HD12	1:C:578:LYS:HB3	2.00	0.44
1:D:549:ILE:HD12	1:D:578:LYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:PHE:O	1:A:219:THR:OG1	2.23	0.44
1:A:496:GLN:HB2	1:A:575:CYS:SG	2.58	0.44
1:A:549:ILE:HD12	1:A:578:LYS:HB3	2.00	0.44
1:D:496:GLN:HB2	1:D:575:CYS:SG	2.58	0.44
1:A:375:TYR:HB3	1:D:350:VAL:HG12	2.00	0.43
1:A:350:VAL:HG12	1:B:375:TYR:HB3	2.00	0.43
1:D:410:PHE:CE2	1:D:442:TRP:HB2	2.53	0.43
1:B:602:ILE:HD11	2:B:701:PCG:C6	2.49	0.43
1:C:186:ARG:NH1	1:C:204:ASP:OD2	2.38	0.43
1:B:350:VAL:HG12	1:C:375:TYR:HB3	2.00	0.43
1:C:596:GLU:HG3	1:C:600:LYS:HZ1	1.84	0.43
1:D:303:LEU:HD23	1:D:303:LEU:HA	1.89	0.43
1:B:524:LEU:HD11	1:B:573:LEU:HD21	2.00	0.43
1:D:454:LEU:HB3	1:D:462:ARG:HG3	2.01	0.43
1:B:525:ALA:HB2	1:B:568:ILE:HD11	2.01	0.43
1:D:596:GLU:HG3	1:D:600:LYS:HZ1	1.84	0.43
1:A:578:LYS:HG3	1:A:579:ASP:N	2.34	0.43
1:B:516:MET:N	1:B:576:LEU:O	2.41	0.43
1:D:602:ILE:HD11	2:D:701:PCG:C6	2.49	0.43
1:C:525:ALA:HB2	1:C:568:ILE:HD11	2.01	0.43
1:D:363:ILE:HG22	1:D:365:GLU:HG2	2.01	0.43
1:D:578:LYS:HG3	1:D:579:ASP:N	2.34	0.43
1:B:186:ARG:NH1	1:B:204:ASP:OD2	2.38	0.42
1:B:578:LYS:HG3	1:B:579:ASP:N	2.34	0.42
1:C:454:LEU:HB3	1:C:462:ARG:HG3	2.01	0.42
1:C:578:LYS:HG3	1:C:579:ASP:N	2.34	0.42
1:A:602:ILE:HD11	2:A:701:PCG:C6	2.49	0.42
1:A:363:ILE:HG22	1:A:365:GLU:HG2	2.01	0.42
1:C:216:PHE:O	1:C:219:THR:OG1	2.23	0.42
1:A:525:ALA:HB2	1:A:568:ILE:HD11	2.01	0.42
1:D:158:ILE:HD12	1:D:217:VAL:HG13	2.02	0.42
1:D:330:ASP:HB2	1:D:370:VAL:HG21	2.02	0.42
1:B:158:ILE:HD12	1:B:217:VAL:HG13	2.02	0.42
1:B:314:ASN:HB3	1:B:356:SER:OG	2.20	0.42
1:C:526:VAL:HG22	1:C:565:ILE:HD12	2.02	0.42
1:A:158:ILE:HD12	1:A:217:VAL:HG13	2.02	0.42
1:A:454:LEU:HB3	1:A:462:ARG:HG3	2.01	0.42
1:C:158:ILE:HD12	1:C:217:VAL:HG13	2.02	0.42
1:C:330:ASP:HB2	1:C:370:VAL:HG21	2.02	0.42
1:C:602:ILE:HD11	2:C:701:PCG:C6	2.49	0.42
1:A:471:LEU:HD11	1:A:475:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ILE:HG22	1:B:365:GLU:HG2	2.01	0.42
1:B:526:VAL:HG22	1:B:565:ILE:HD12	2.02	0.41
1:D:525:ALA:HB2	1:D:568:ILE:HD11	2.01	0.41
1:B:454:LEU:HB3	1:B:462:ARG:HG3	2.01	0.41
1:C:314:ASN:HB3	1:C:356:SER:OG	2.20	0.41
1:D:314:ASN:HB3	1:D:356:SER:OG	2.20	0.41
1:C:363:ILE:HG22	1:C:365:GLU:HG2	2.01	0.41
1:A:314:ASN:HB3	1:A:356:SER:OG	2.20	0.41
1:B:594:MET:O	1:B:597:GLU:HB3	2.20	0.41
1:D:471:LEU:HD11	1:D:475:LYS:HE2	2.02	0.41
1:C:449:ASP:OD1	1:C:449:ASP:N	2.45	0.41
1:D:272:LEU:O	1:D:275:LEU:HG	2.21	0.41
1:B:169:LEU:HB3	1:B:284:PHE:HB2	2.03	0.41
1:B:471:LEU:HD11	1:B:475:LYS:HE2	2.02	0.41
1:C:594:MET:O	1:C:597:GLU:HB3	2.21	0.41
1:A:330:ASP:HB2	1:A:370:VAL:HG21	2.02	0.41
1:B:330:ASP:HB2	1:B:370:VAL:HG21	2.02	0.41
1:D:169:LEU:HB3	1:D:284:PHE:HB2	2.03	0.41
1:A:410:PHE:CE2	1:A:414:ILE:HD11	2.56	0.41
1:A:449:ASP:OD1	1:A:449:ASP:N	2.45	0.41
1:A:402:ASN:HA	1:A:405:ALA:HB2	2.03	0.41
1:B:402:ASN:HA	1:B:405:ALA:HB2	2.03	0.41
1:B:410:PHE:CE2	1:B:414:ILE:HD11	2.56	0.41
1:B:592:LYS:HG2	1:B:596:GLU:OE1	2.21	0.41
1:C:272:LEU:O	1:C:275:LEU:HG	2.21	0.41
1:C:471:LEU:HD11	1:C:475:LYS:HE2	2.02	0.41
1:C:557:ALA:HB1	1:C:560:ARG:HB2	2.03	0.41
1:A:215:MET:HG3	1:A:277:ARG:HH12	1.86	0.40
1:A:354:TYR:CZ	1:A:358:LEU:HD11	2.57	0.40
1:C:215:MET:HG3	1:C:277:ARG:HH12	1.86	0.40
1:C:463:ALA:HB2	1:C:493:LEU:HD11	2.04	0.40
1:C:592:LYS:HG2	1:C:596:GLU:OE1	2.21	0.40
1:D:526:VAL:HG22	1:D:565:ILE:HD12	2.02	0.40
1:B:272:LEU:O	1:B:275:LEU:HG	2.21	0.40
1:B:458:PRO:HD2	1:B:461:LEU:HB3	2.03	0.40
1:A:169:LEU:HB3	1:A:284:PHE:HB2	2.03	0.40
1:A:526:VAL:HG22	1:A:565:ILE:HD12	2.02	0.40
1:A:592:LYS:HG2	1:A:596:GLU:OE1	2.21	0.40
1:B:215:MET:HG3	1:B:277:ARG:HH12	1.86	0.40
1:B:557:ALA:HB1	1:B:560:ARG:HB2	2.03	0.40
1:D:594:MET:O	1:D:597:GLU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:HB3	1:A:399:MET:SD	2.62	0.40
1:C:250:VAL:O	1:C:254:ILE:HG13	2.22	0.40
1:C:458:PRO:HD2	1:C:461:LEU:HB3	2.03	0.40
1:D:299:ARG:HB3	1:D:399:MET:SD	2.62	0.40
1:D:592:LYS:HG2	1:D:596:GLU:OE1	2.21	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	448/560 (80%)	437 (98%)	11 (2%)	0	100	100
1	B	448/560 (80%)	438 (98%)	10 (2%)	0	100	100
1	C	448/560 (80%)	438 (98%)	10 (2%)	0	100	100
1	D	448/560 (80%)	438 (98%)	10 (2%)	0	100	100
All	All	1792/2240 (80%)	1751 (98%)	41 (2%)	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	405/502 (81%)	403 (100%)	2 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	405/502 (81%)	403 (100%)	2 (0%)	88	94
1	C	405/502 (81%)	403 (100%)	2 (0%)	88	94
1	D	405/502 (81%)	403 (100%)	2 (0%)	88	94
All	All	1620/2008 (81%)	1612 (100%)	8 (0%)	89	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	291	ARG
1	A	556	LYS
1	B	291	ARG
1	B	556	LYS
1	C	291	ARG
1	C	556	LYS
1	D	291	ARG
1	D	556	LYS

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

Mol	Chain	Res	Type
1	A	302	ASN
1	A	402	ASN
1	A	404	ASN
1	A	411	GLN
1	A	468	ASN
1	A	534	GLN
1	B	302	ASN
1	B	338	ASN
1	B	402	ASN
1	B	404	ASN
1	B	411	GLN
1	B	468	ASN
1	B	534	GLN
1	C	338	ASN
1	C	402	ASN
1	C	404	ASN
1	C	411	GLN
1	C	468	ASN
1	C	534	GLN
1	D	402	ASN

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Mol	Chain	Res	Type
1	D	404	ASN
1	D	411	GLN
1	D	468	ASN
1	D	534	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PCG	C	701	-	22,26,26	2.15	5 (22%)	25,41,41	1.91	7 (28%)
2	PCG	A	701	-	22,26,26	2.15	5 (22%)	25,41,41	1.90	7 (28%)
2	PCG	D	701	-	22,26,26	2.16	5 (22%)	25,41,41	1.91	8 (32%)
2	PCG	B	701	-	22,26,26	2.15	5 (22%)	25,41,41	1.90	7 (28%)

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	PCG	C	701	-	-	0/0/31/31	0/4/4/4
2	PCG	A	701	-	-	0/0/31/31	0/4/4/4
2	PCG	D	701	-	-	0/0/31/31	0/4/4/4
2	PCG	B	701	-	-	0/0/31/31	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	PCG	PA-O5'	5.45	1.63	1.57
2	A	701	PCG	PA-O5'	5.43	1.63	1.57
2	B	701	PCG	PA-O5'	5.41	1.63	1.57
2	C	701	PCG	PA-O5'	5.41	1.63	1.57
2	B	701	PCG	O4'-C1'	5.10	1.48	1.41
2	D	701	PCG	O4'-C1'	5.10	1.48	1.41
2	A	701	PCG	O4'-C1'	5.09	1.48	1.41
2	C	701	PCG	O4'-C1'	5.07	1.48	1.41
2	D	701	PCG	C5-C6	-3.88	1.39	1.47
2	C	701	PCG	C5-C6	-3.84	1.39	1.47
2	A	701	PCG	C5-C6	-3.81	1.39	1.47
2	B	701	PCG	C5-C6	-3.81	1.39	1.47
2	B	701	PCG	PA-O3'	3.68	1.63	1.57
2	C	701	PCG	PA-O3'	3.67	1.63	1.57
2	D	701	PCG	PA-O3'	3.67	1.63	1.57
2	A	701	PCG	PA-O3'	3.61	1.63	1.57
2	B	701	PCG	C6-N1	2.09	1.41	1.37
2	A	701	PCG	C6-N1	2.05	1.40	1.37
2	C	701	PCG	C6-N1	2.04	1.40	1.37
2	D	701	PCG	C6-N1	2.04	1.40	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	PCG	O3'-C3'-C4'	-4.57	107.26	110.71
2	D	701	PCG	O3'-C3'-C4'	-4.53	107.29	110.71
2	B	701	PCG	O3'-C3'-C4'	-4.51	107.31	110.71
2	A	701	PCG	O3'-C3'-C4'	-4.49	107.32	110.71
2	B	701	PCG	O1A-PA-O2A	3.13	118.54	108.73
2	C	701	PCG	O1A-PA-O2A	3.13	118.52	108.73
2	D	701	PCG	O1A-PA-O2A	3.11	118.49	108.73
2	A	701	PCG	O1A-PA-O2A	3.11	118.46	108.73
2	D	701	PCG	C5-C6-N1	3.02	119.28	113.95
2	A	701	PCG	C5-C6-N1	2.98	119.22	113.95
2	C	701	PCG	C5-C6-N1	2.97	119.20	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	PCG	C5-C6-N1	2.97	119.19	113.95
2	B	701	PCG	O5'-PA-O3'	-2.87	101.72	105.68
2	D	701	PCG	O5'-PA-O3'	-2.86	101.73	105.68
2	C	701	PCG	C2-N1-C6	-2.85	119.84	125.10
2	D	701	PCG	C2-N1-C6	-2.85	119.84	125.10
2	B	701	PCG	C2-N1-C6	-2.85	119.85	125.10
2	C	701	PCG	O5'-PA-O3'	-2.85	101.75	105.68
2	A	701	PCG	O5'-PA-O3'	-2.84	101.77	105.68
2	A	701	PCG	C2-N1-C6	-2.83	119.88	125.10
2	D	701	PCG	C8-N7-C5	2.74	108.20	102.99
2	C	701	PCG	C8-N7-C5	2.70	108.14	102.99
2	A	701	PCG	C8-N7-C5	2.69	108.11	102.99
2	B	701	PCG	C8-N7-C5	2.66	108.06	102.99
2	A	701	PCG	N1-C2-N3	-2.12	119.36	123.32
2	C	701	PCG	N1-C2-N3	-2.10	119.40	123.32
2	D	701	PCG	N1-C2-N3	-2.10	119.40	123.32
2	B	701	PCG	N1-C2-N3	-2.08	119.43	123.32
2	D	701	PCG	O6-C6-C5	-2.01	120.44	124.37

There are no chirality outliers.

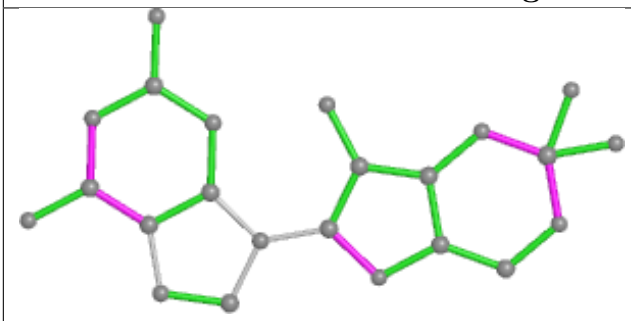
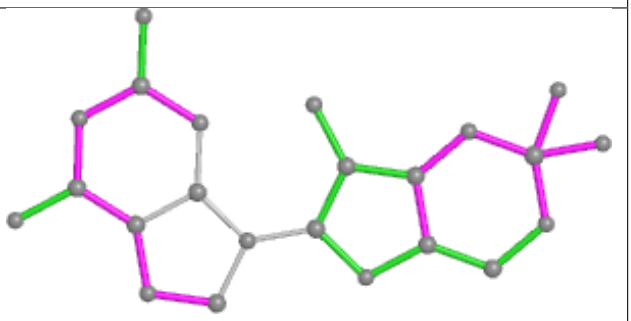
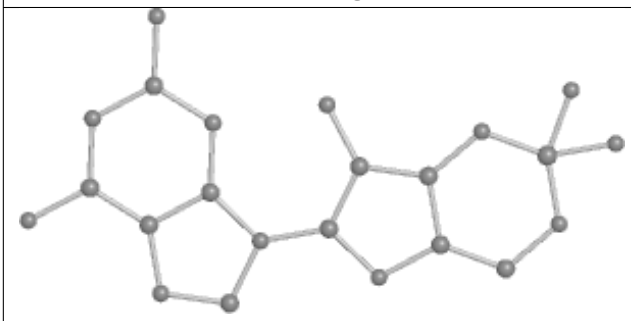
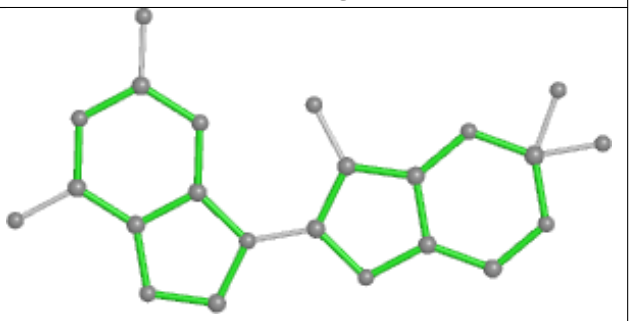
There are no torsion outliers.

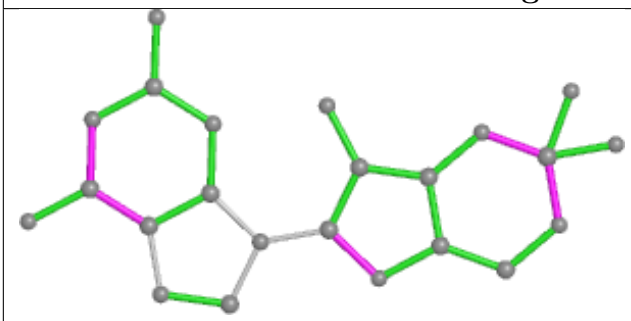
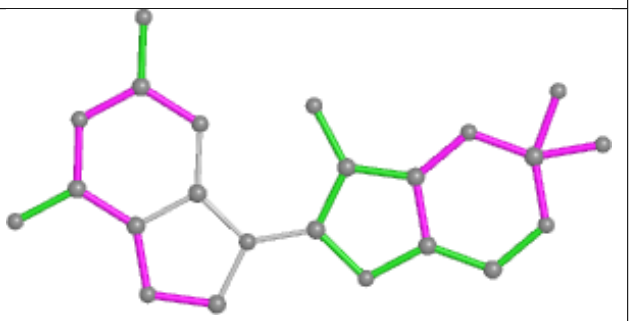
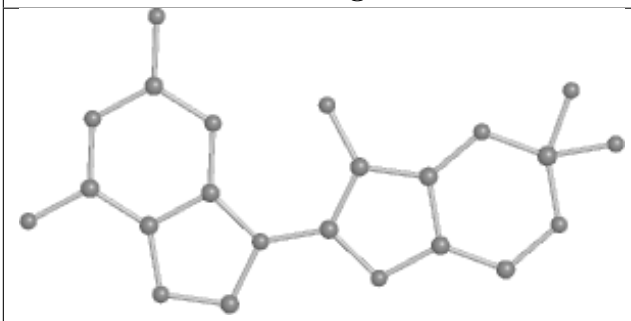
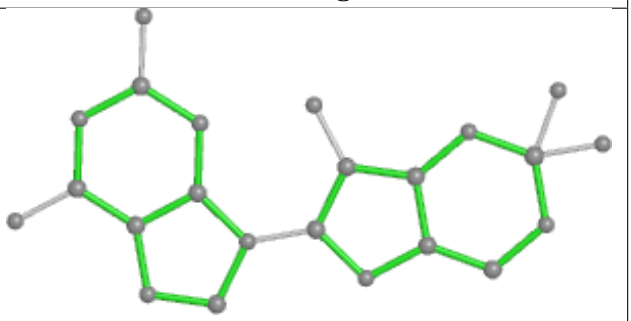
There are no ring outliers.

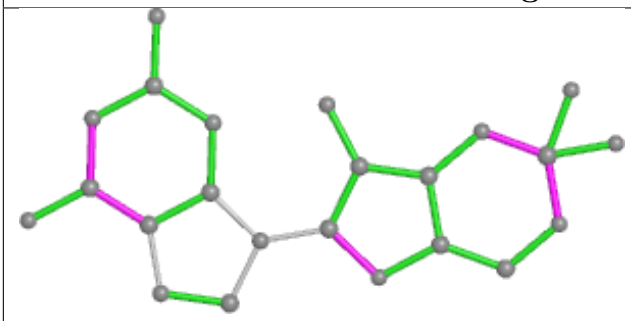
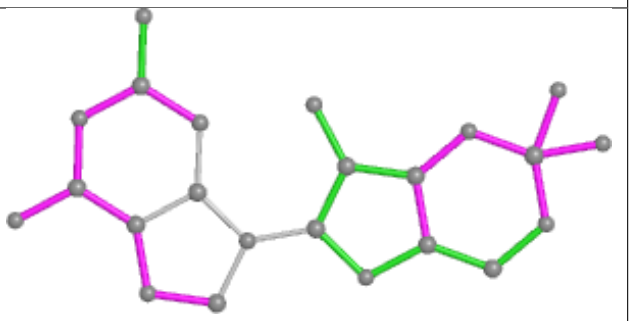
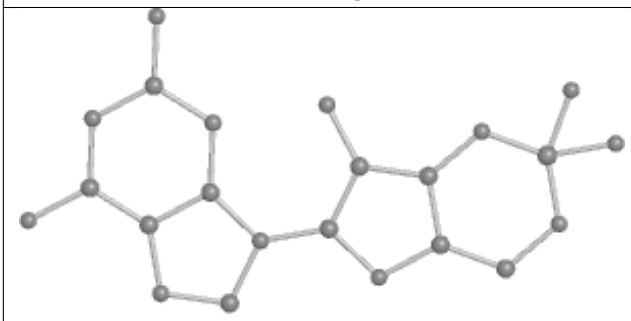
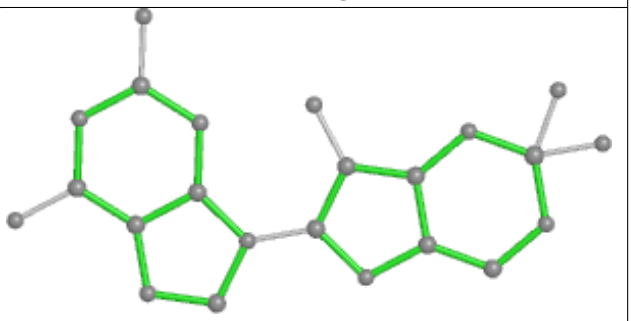
4 monomers are involved in 4 short contacts:

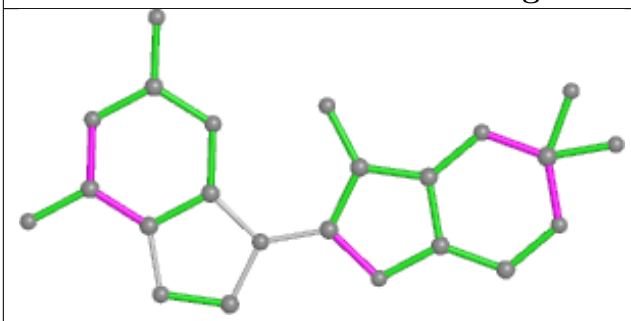
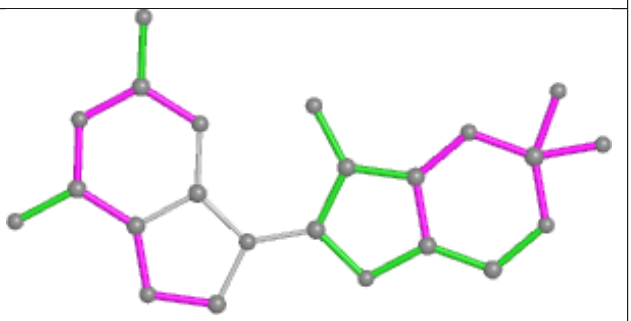
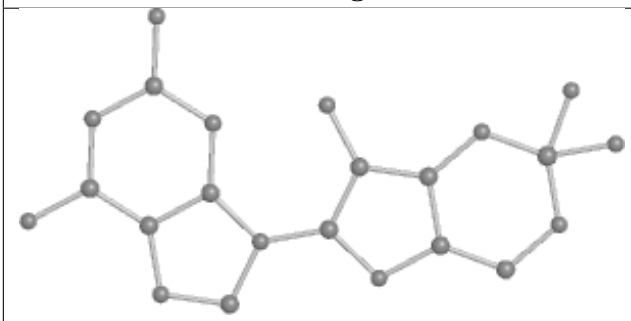
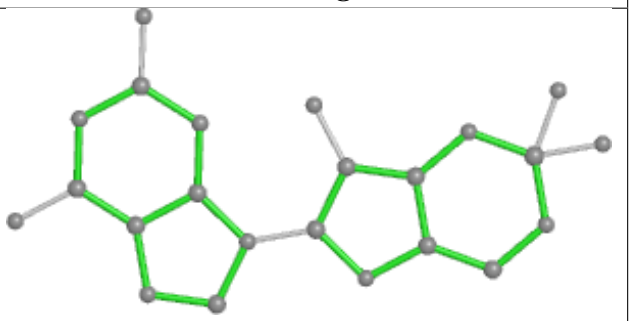
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	PCG	1	0
2	A	701	PCG	1	0
2	D	701	PCG	1	0
2	B	701	PCG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PCG C 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCG A 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCG D 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PCG B 701	
 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.

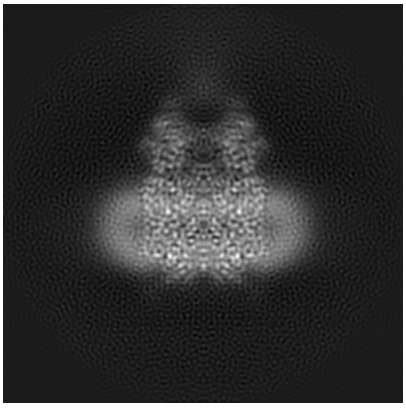
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23308. These allow visual inspection of the internal detail of the map and identification of artifacts.

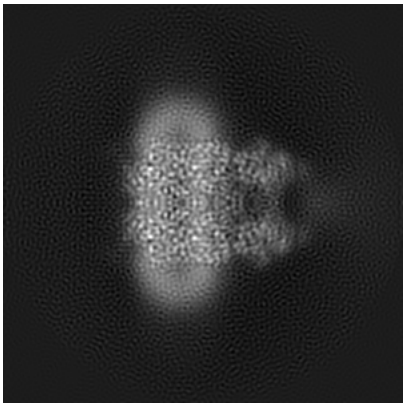
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

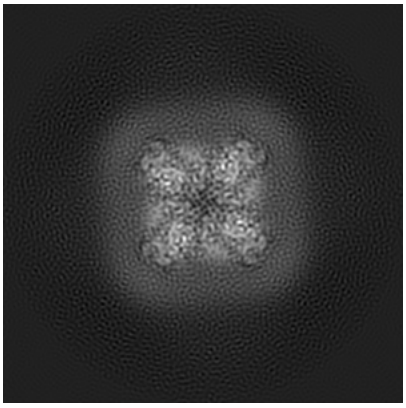
6.1.1 Primary map



X



Y

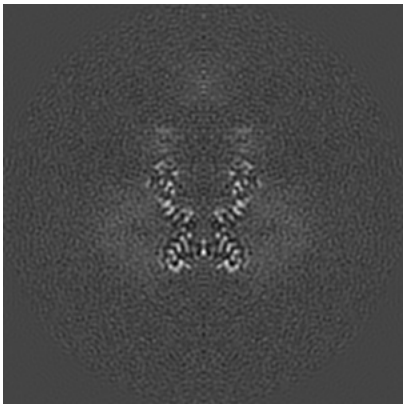


Z

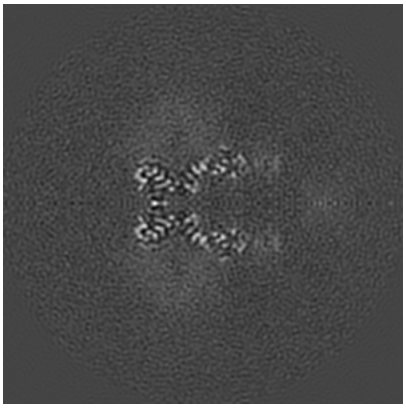
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

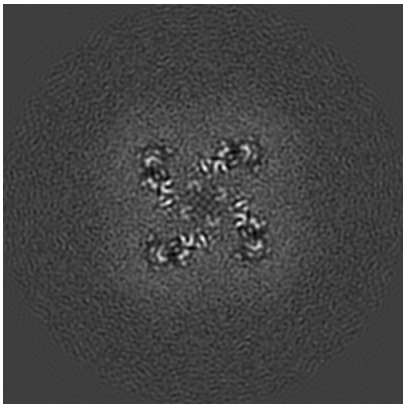
6.2.1 Primary map



X Index: 144



Y Index: 144

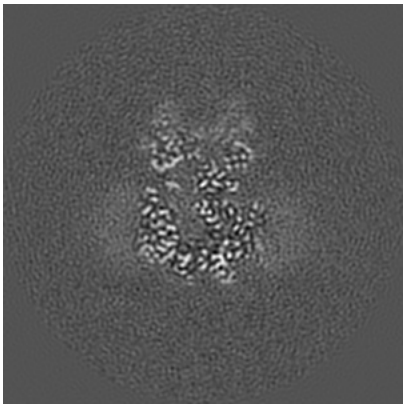


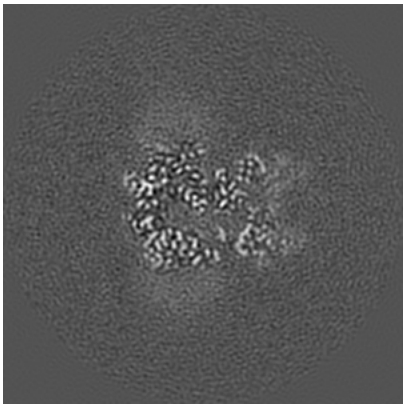
Z Index: 144

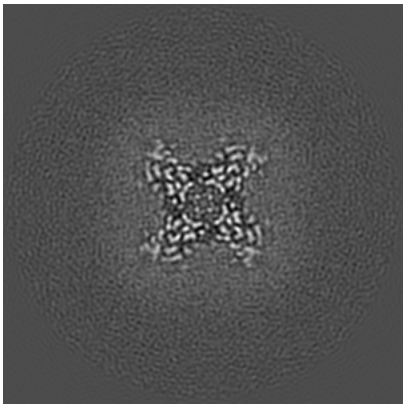
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 120

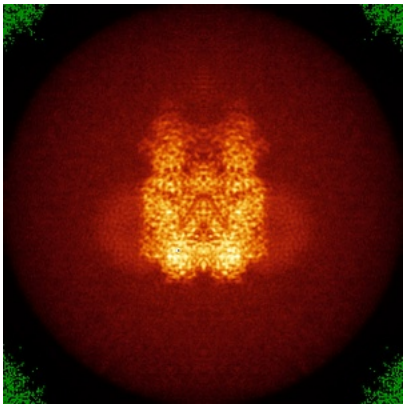

Y Index: 168

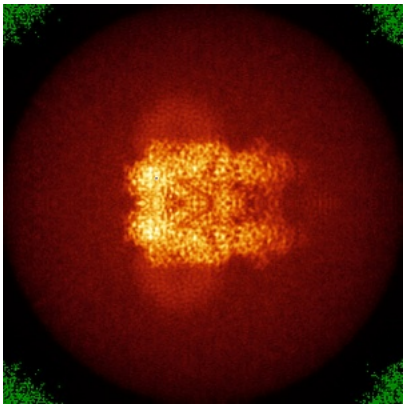

Z Index: 106

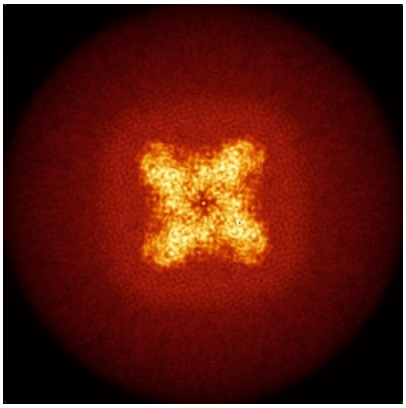
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

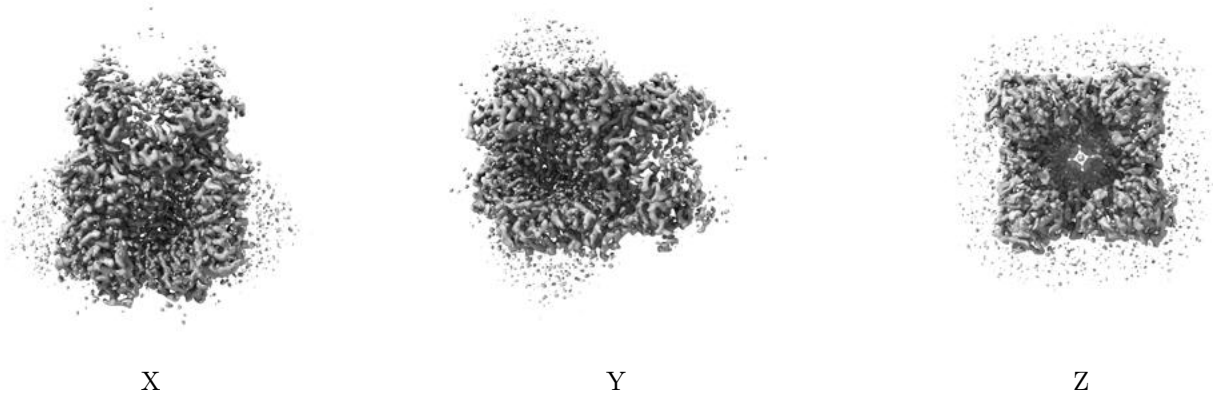

Y


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 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

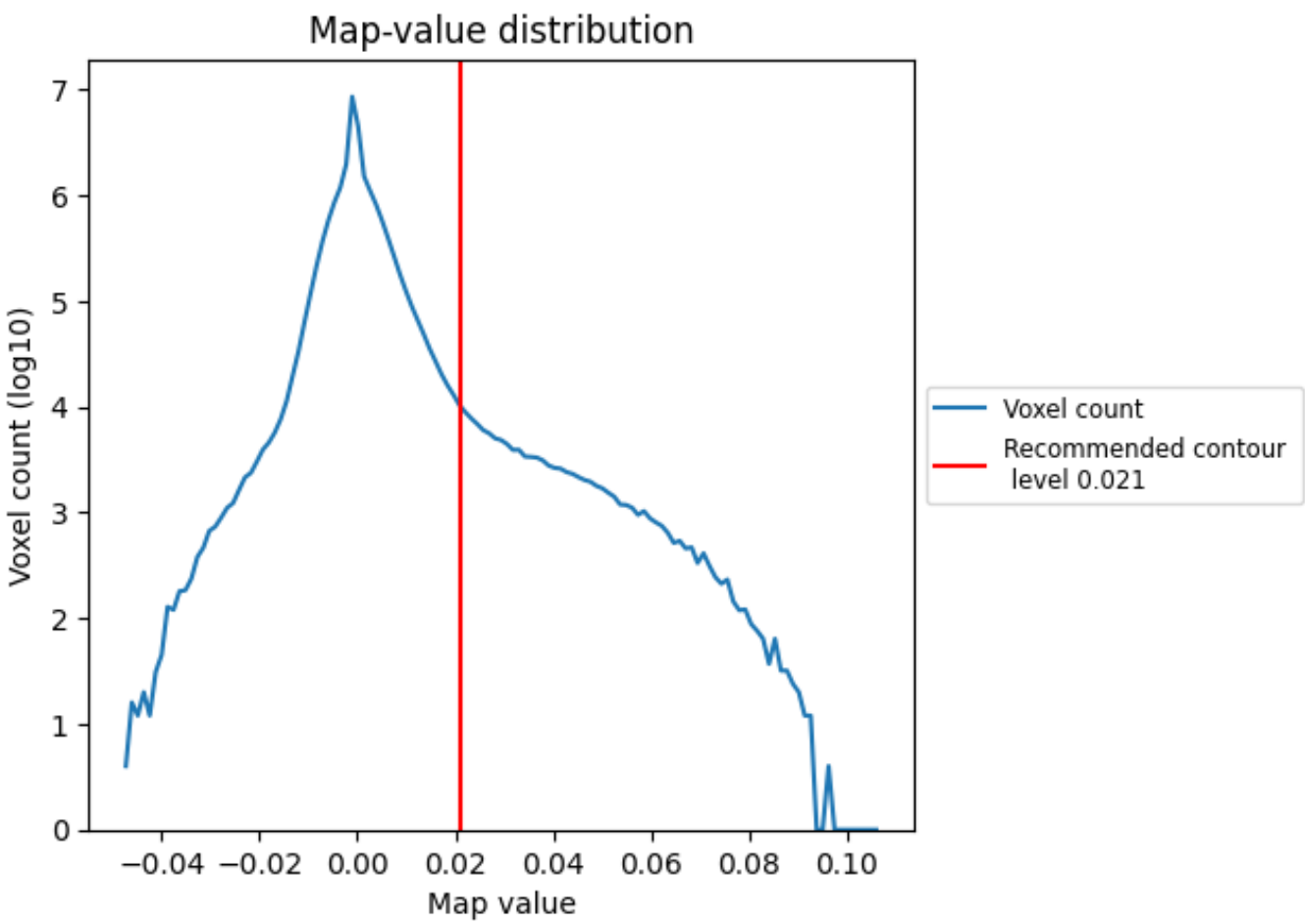
6.6 Mask visualisation (i)

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

7 Map analysis (i)

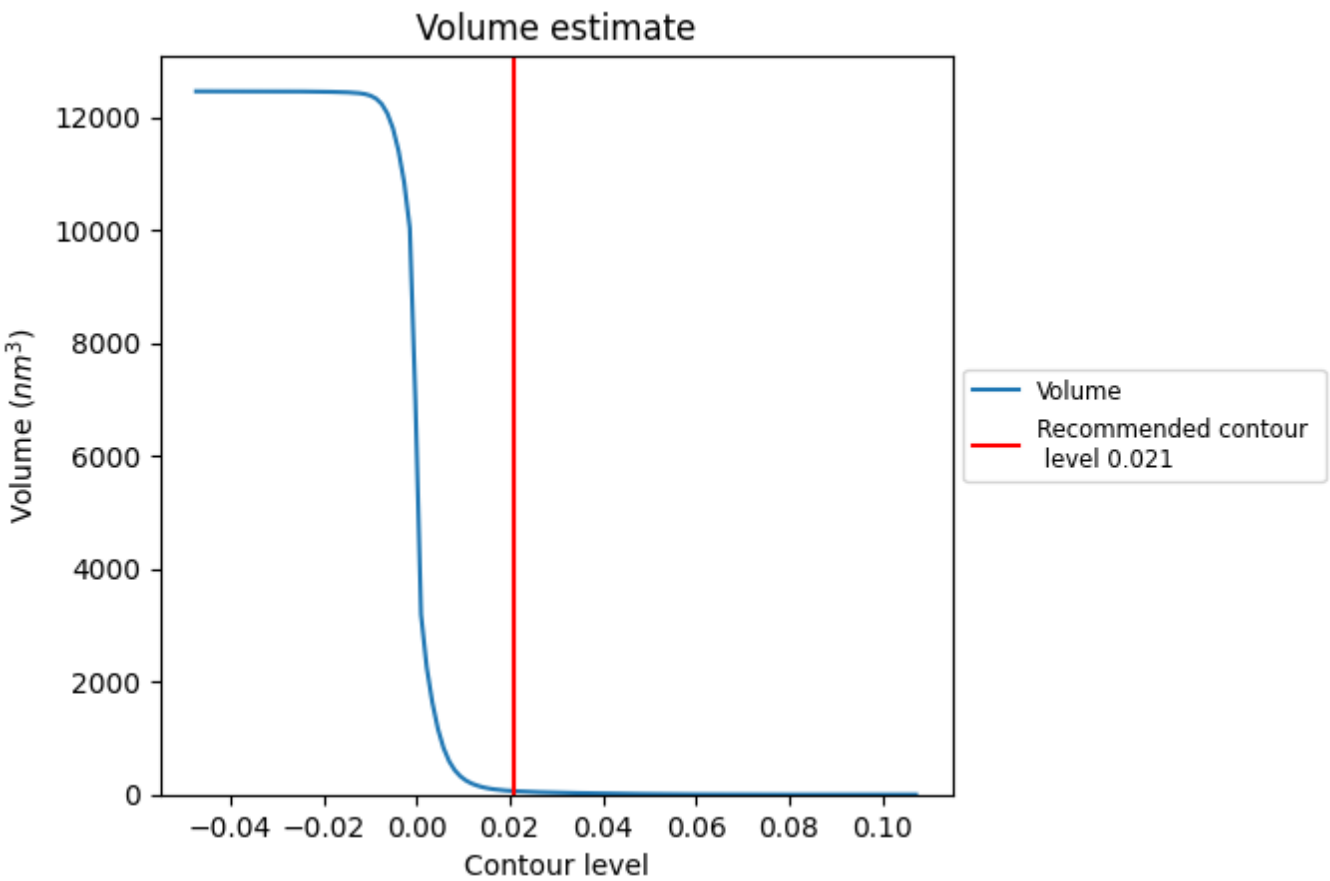
This section contains the results of statistical analysis of the map.

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.

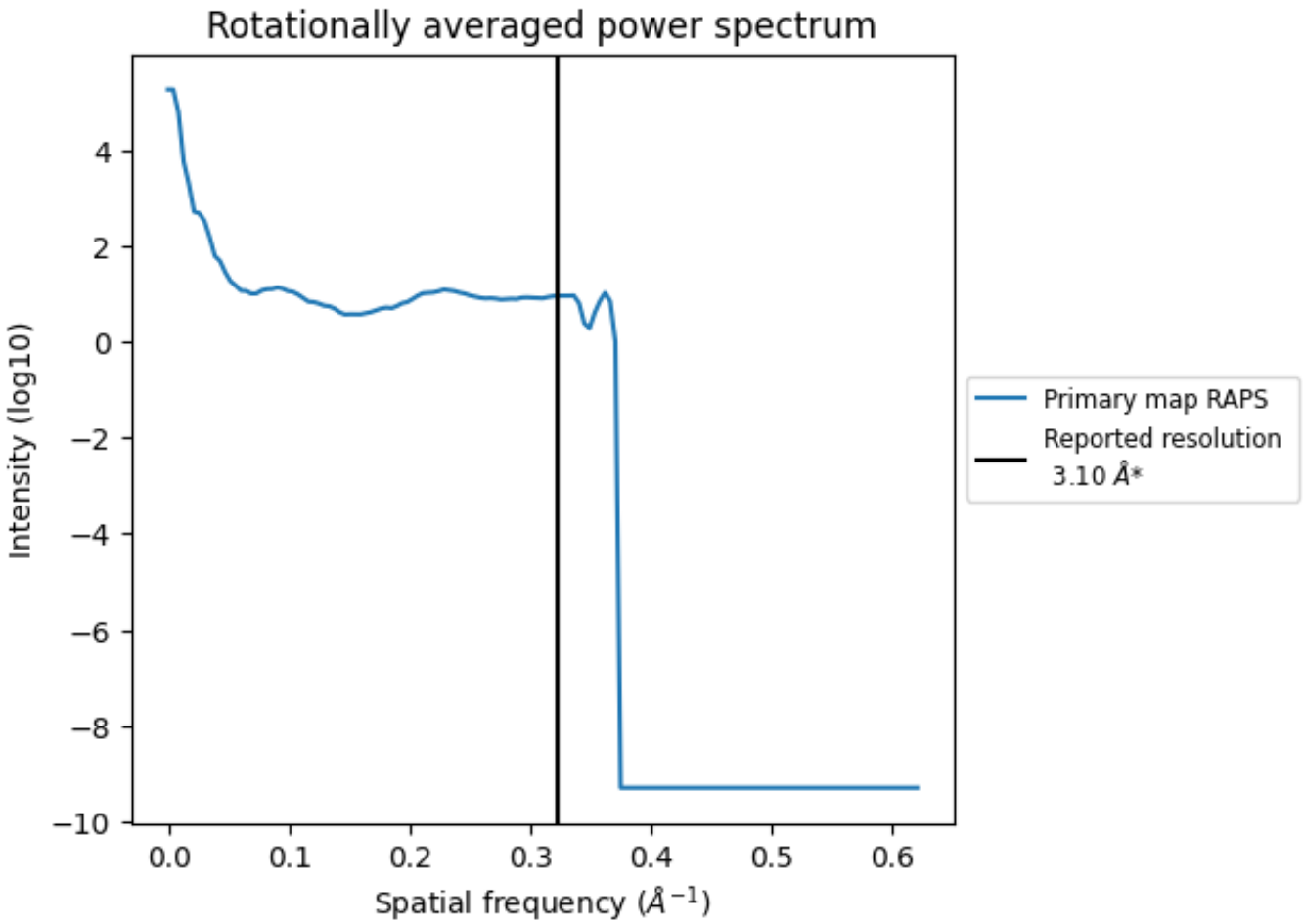
7.2 Volume estimate (i)



The volume at the recommended contour level is 62 nm^3; this corresponds to an approximate mass of 56 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)

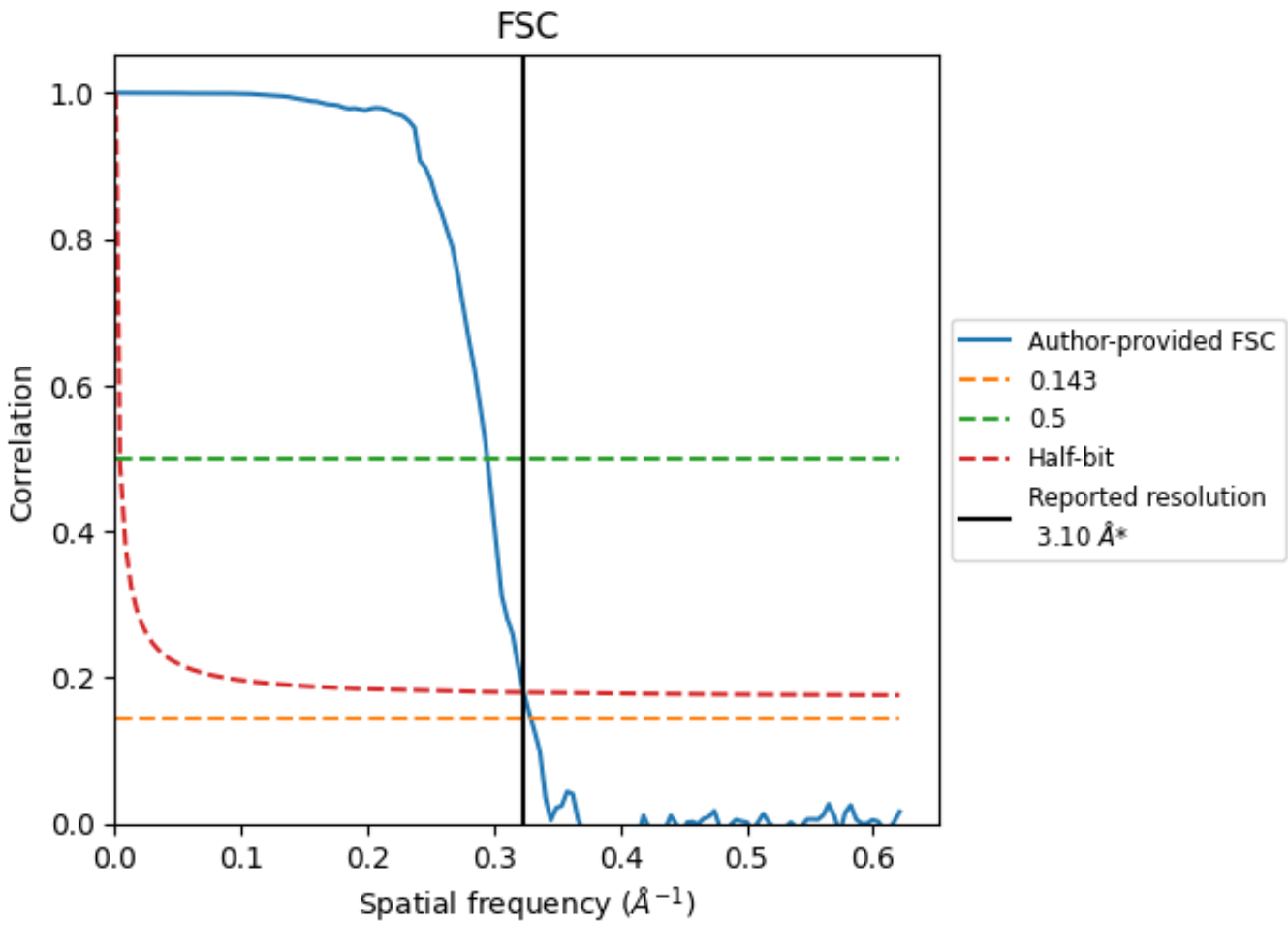


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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)

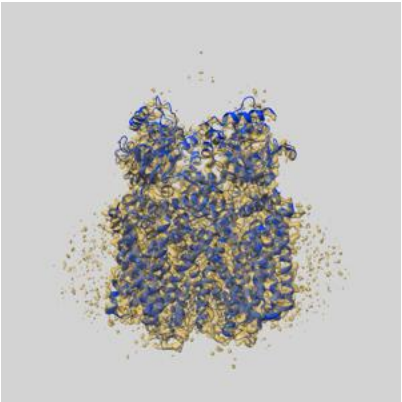
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.04	3.39	3.09
Unmasked-calculated*	-	-	-

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

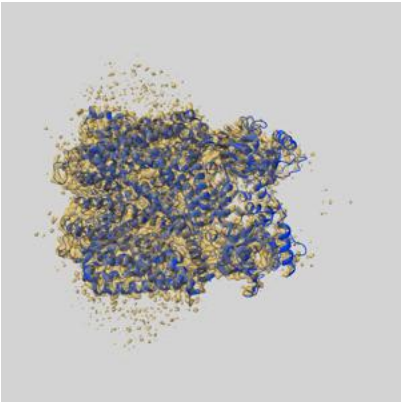
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23308 and PDB model 7LFX. Per-residue inclusion information can be found in section 3 on page 6.

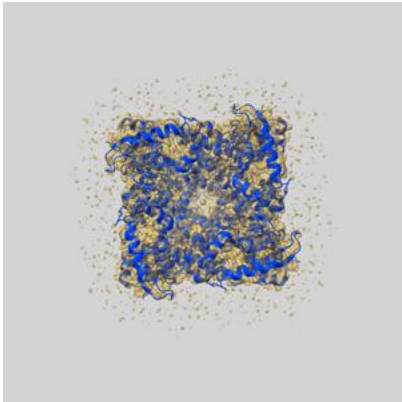
9.1 Map-model overlay (i)



X



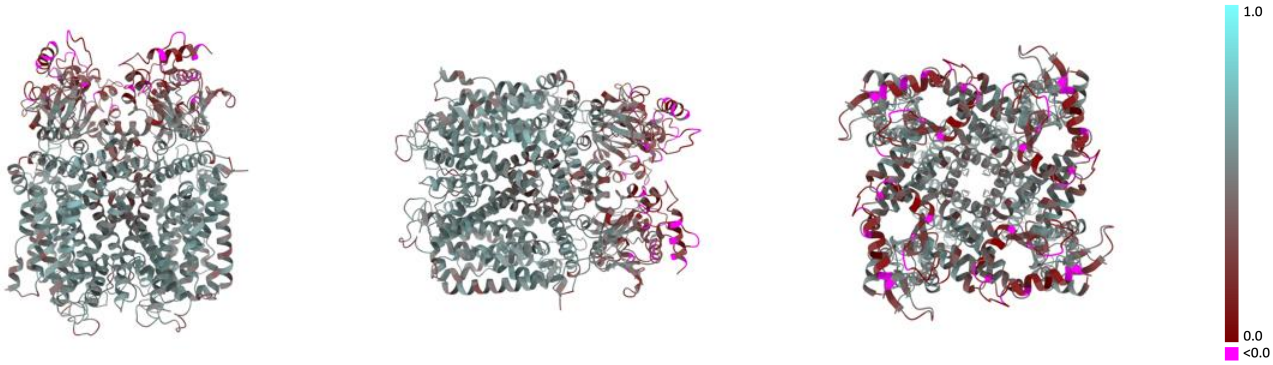
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.021 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.

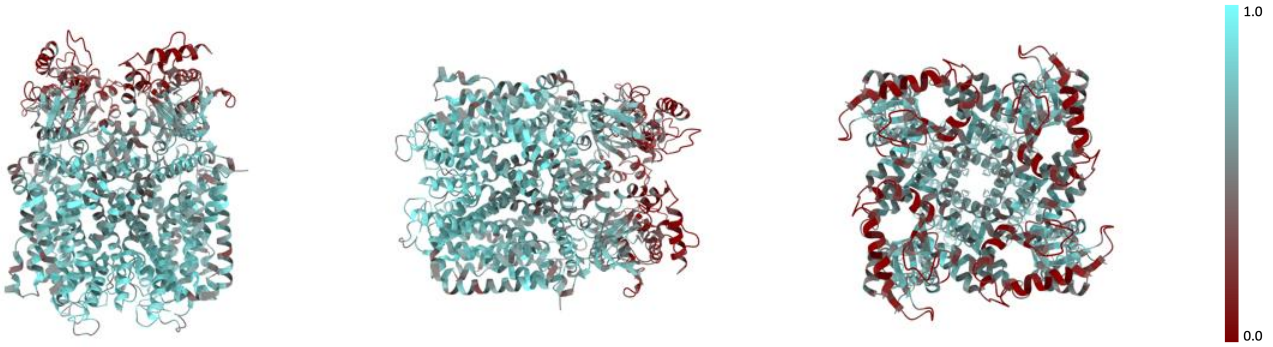
9.2 Q-score mapped to coordinate model (i)



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.

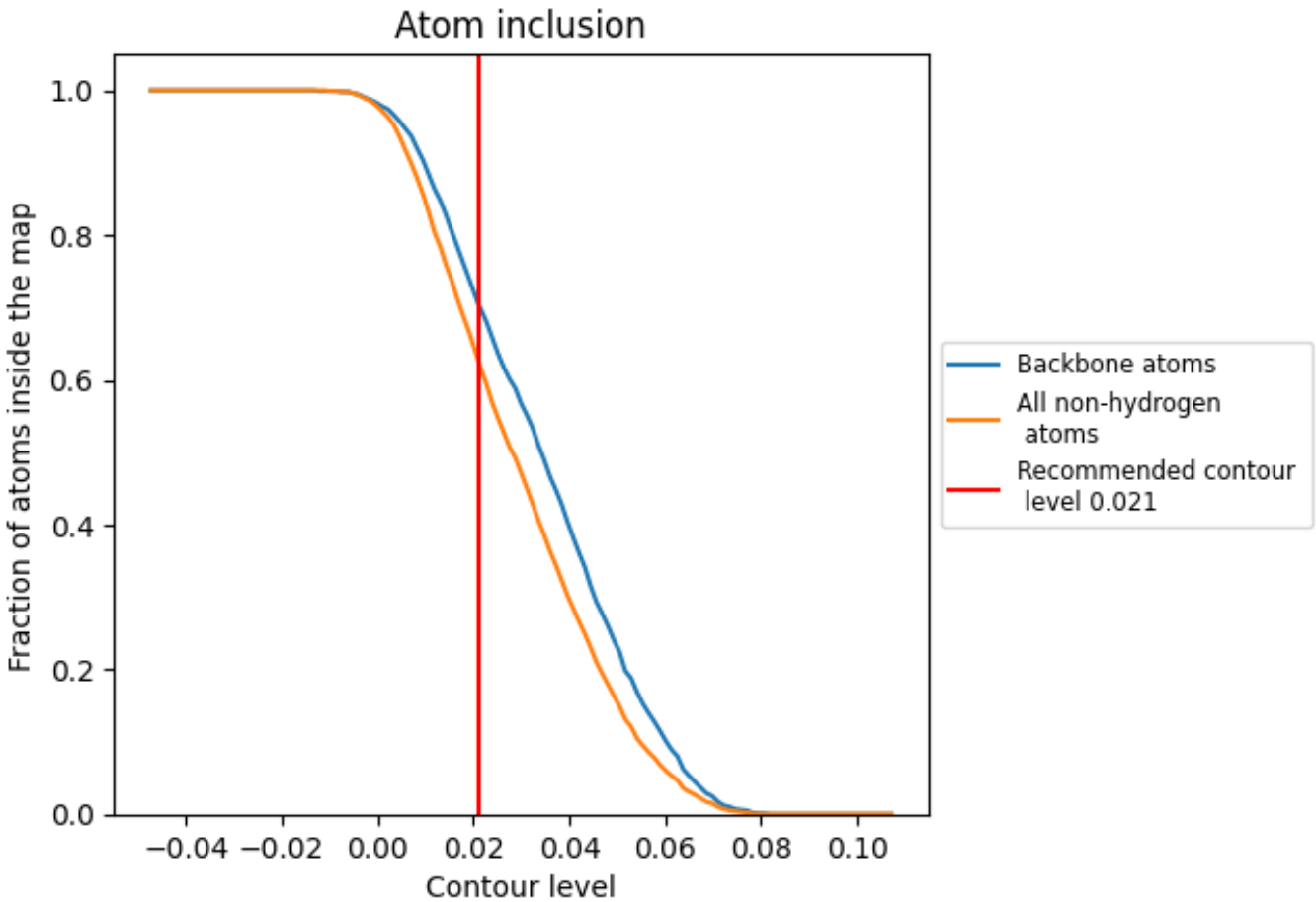
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.021).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 63% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6270	0.4580
A	0.6270	0.4580
B	0.6270	0.4580
C	0.6270	0.4580
D	0.6260	0.4580