Full wwPDB EM Validation Report (i)

Mar 11, 2024 – 03:32 AM EDT

PDB ID	:	6P4K
EMDB ID	:	EMD-20251
Title	:	mouse norovirus complexed with TCA
Authors	:	Smith, T.J.
Deposited on	:	2019-05-27
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:

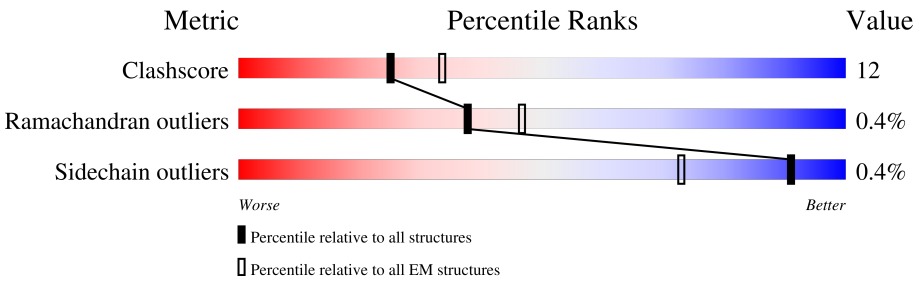
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	516	81% 73% 26%
1	B	516	80% 76% 23% •
1	C	516	78% 80% 17% •

2 Entry composition (i)

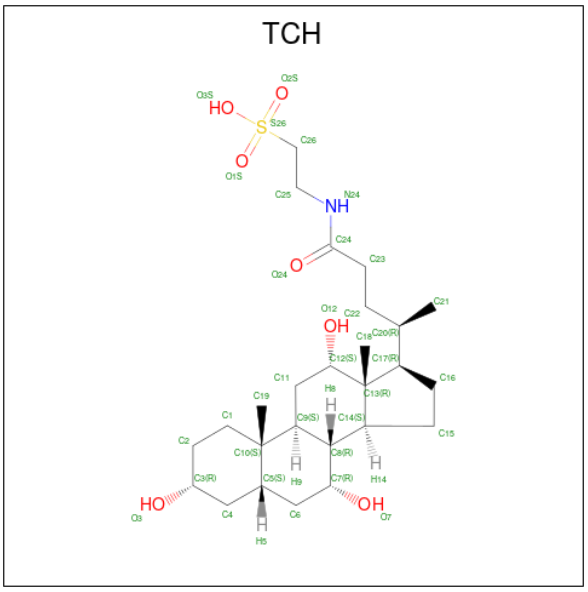
There are 2 unique types of molecules in this entry. The entry contains 11963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	514	3948	2544	650	738	16	0	0
1	B	513	3941	2539	649	737	16	0	0
1	C	502	3864	2493	636	719	16	0	0

- Molecule 2 is TAUROCHOLIC ACID (three-letter code: TCH) (formula: $C_{26}H_{45}NO_7S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	A	1	35	26	1	7	1	0
2	A	1	35	26	1	7	1	0
2	B	1	35	26	1	7	1	0
2	B	1	35	26	1	7	1	0

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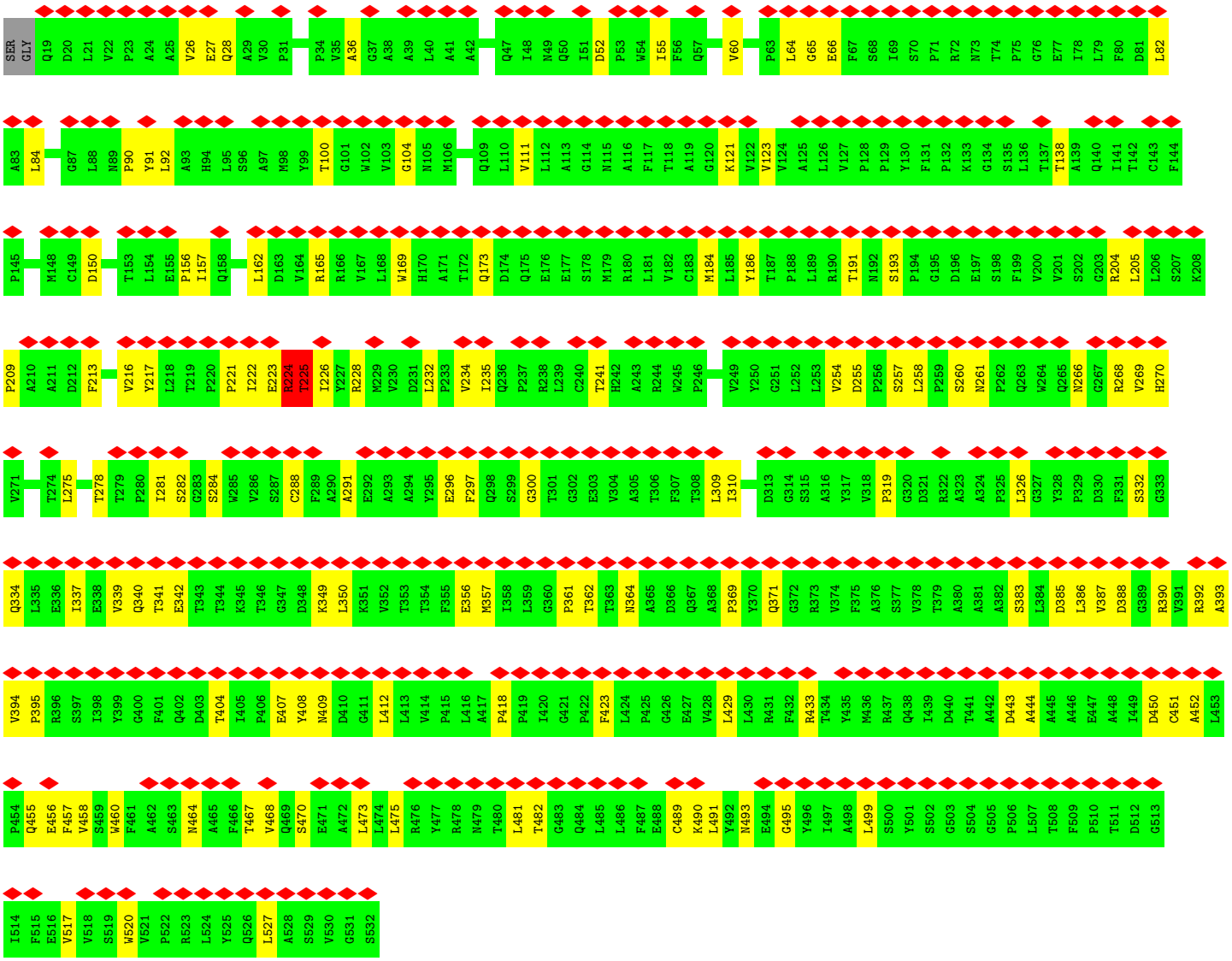
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	C	1	35	26	1	7	1	0
			Total	C	N	O	S	
2	C	1	35	26	1	7	1	0

3 Residue-property plots (i)

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

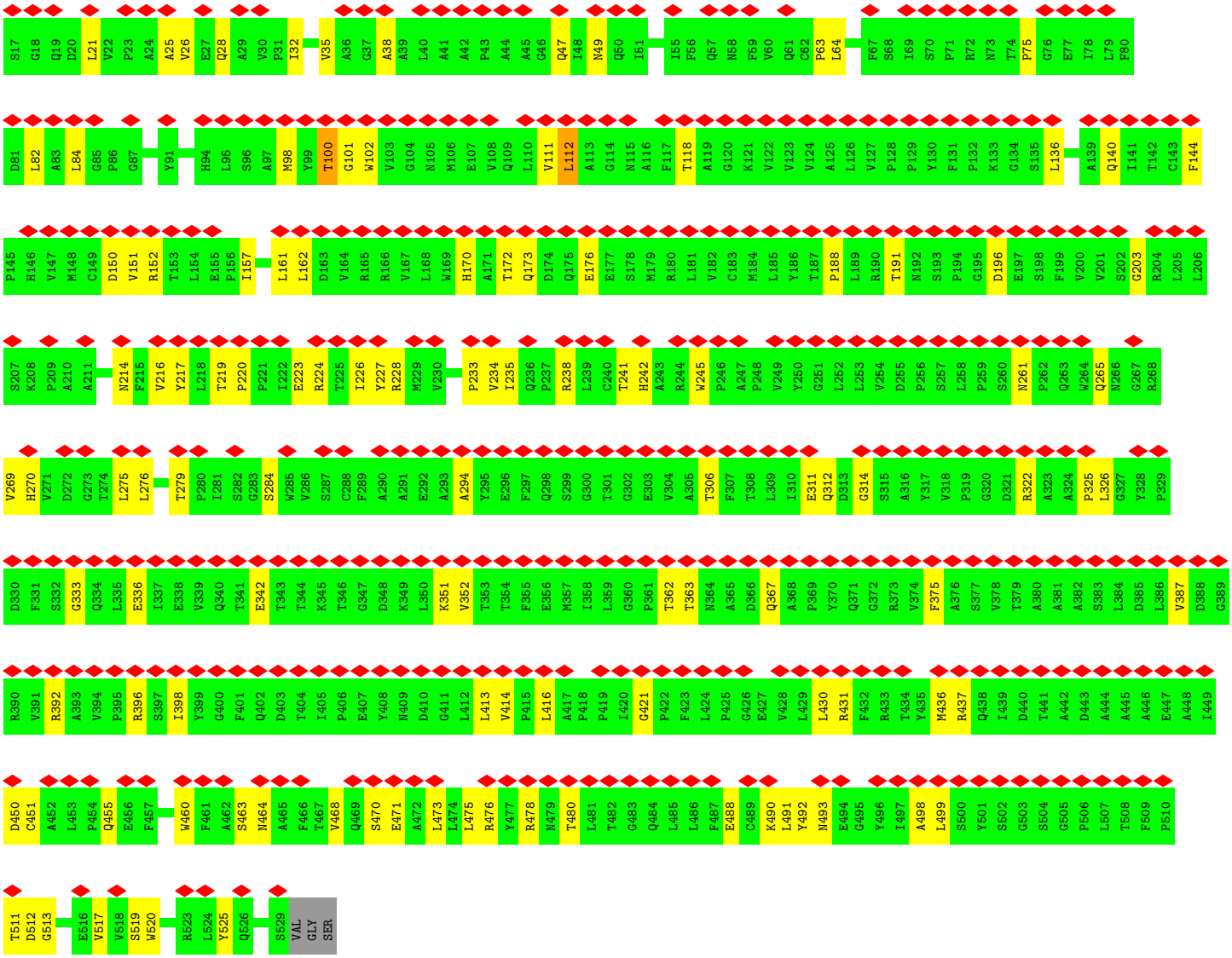
- Molecule 1: Capsid protein

Chain A: 81% 73% 26%



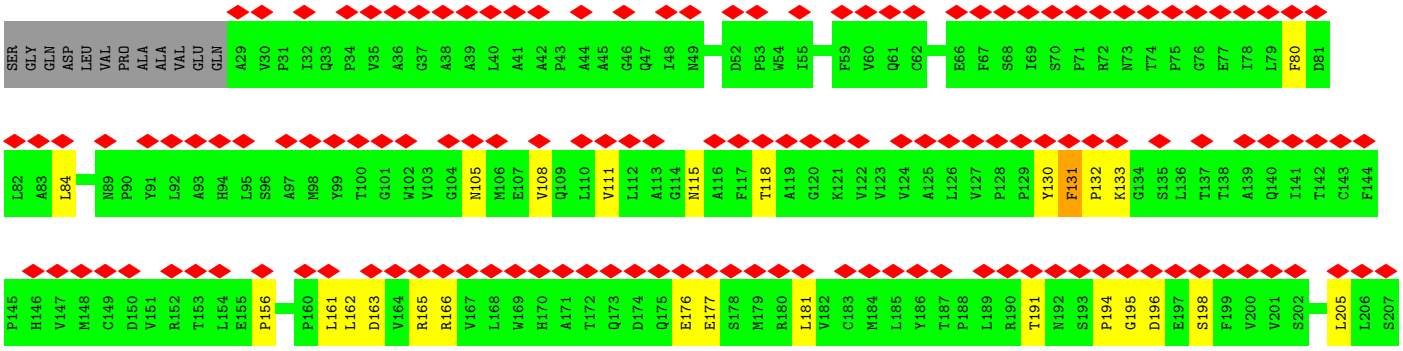
- Molecule 1: Capsid protein

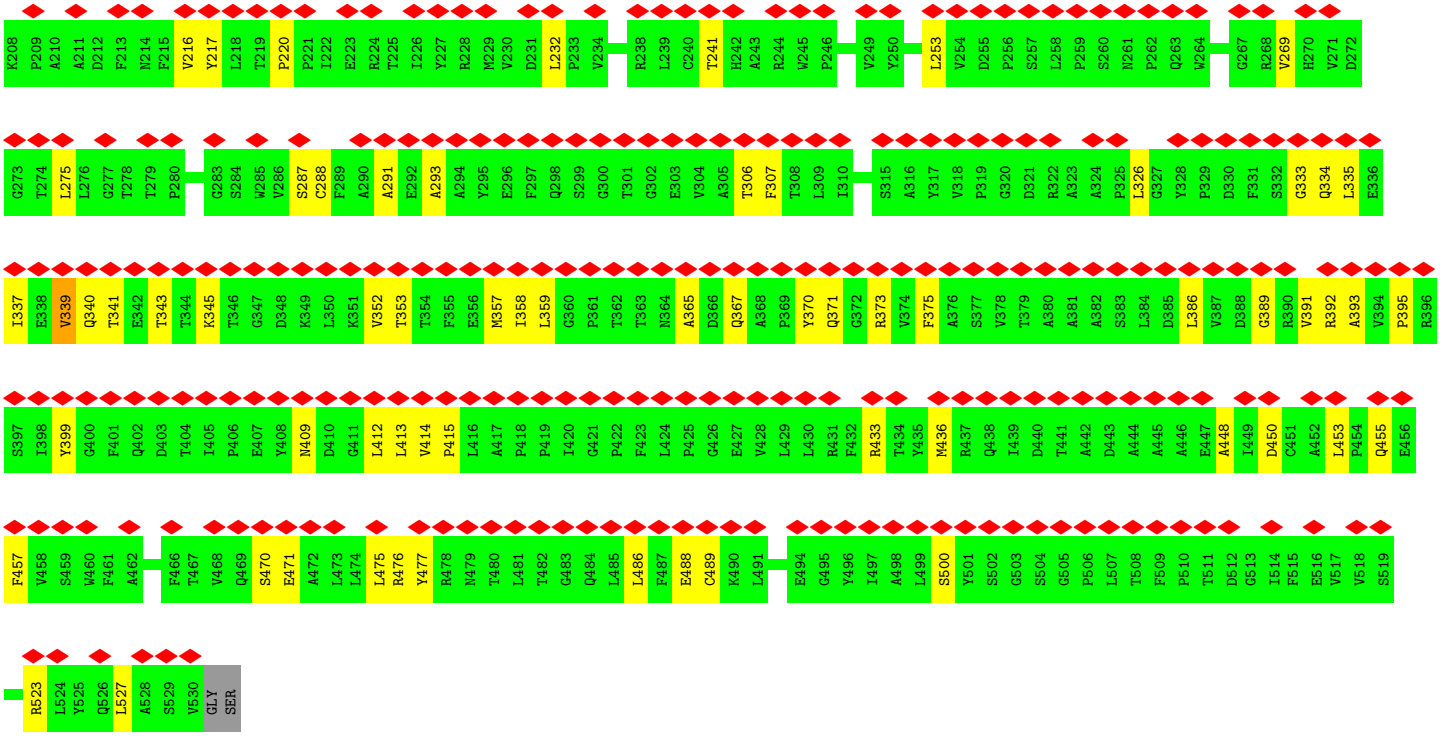
Chain B:



- Molecule 1: Capsid protein

Chain C:




K208 P209 A210 A211 D212 F213 N214 F215 V216 Y217 L218 T219 P220 P221 I222 E223 R224 T225 I226 Y227 R228 M229 V230 D231 L232 P233 V234 R238 L239 C240 T241 H242 A243 R244 W245 P246 V249 Y250 L253 V254 D255 P256 S257 L258 P259 S260 N261 P262 Q263 W264 G267 R268 V269 H270 V271 D272
G273 T274 L275 L276 G277 T278 T279 P280 G283 S284 W285 V286 S287 C288 F289 A290 A291 E292 A293 A294 Y295 E296 F297 Q298 S299 G300 T301 G302 E303 V304 A305 T306 F307 T308 L309 I310 S315 A316 Y317 V318 P319 G320 D321 R322 A323 A324 P325 L326 G327 Y328 P329 D330 F331 S332 G333 Q334 L335 E336
I337 E338 V339 Q340 T341 E342 T343 T344 K345 T346 G347 D348 K349 L350 K351 V352 T353 T354 F355 E356 M357 I358 L359 G360 P361 T362 T363 N364 A365 D366 Q367 A368 P369 Y370 Q371 G372 R373 V374 F375 A376 S377 V378 T379 A380 A381 A382 S383 L384 D385 L386 V387 D388 G389 R390 V391 R392 A393 V394 P395 R396
S397 I398 Y399 G400 F401 Q402 D403 T404 I405 P406 E407 Y408 N409 D410 G411 L412 L413 V414 P415 L416 A417 P418 P419 I420 G421 P422 F423 L424 P425 G426 E427 V428 L429 L430 R431 F432 R433 T434 Y435 M436 R437 Q438 I439 D440 T441 A442 D443 A444 A445 A446 E447 A448 I449 D450 C451 A452 L453 P454 Q455 E456
F457 V458 S459 W460 F461 A462 F466 T467 V468 Q469 S470 E471 A472 L473 L474 L475 R476 Y477 R478 N479 T480 L481 T482 G483 Q484 L485 L486 F487 E488 C489 K490 L491 E494 G495 Y496 I497 A498 L499 S500 Y501 S502 G503 S504 G505 P506 L507 T508 F509 P510 T511 D512 G513 I514 F515 E516 V517 V518 S519
R523 L524 Y525 Q526 L527 A528 S529 V530 GLY SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25000	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	19.155	Depositor
Minimum map value	-13.334	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.647	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	624.456, 624.456, 624.456	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1564, 1.1564, 1.1564	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: TCH

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	0.59	0/4056	0.59	0/5561
1	B	0.58	0/4050	0.58	0/5554
1	C	0.58	0/3972	0.57	0/5447
All	All	0.59	0/12078	0.58	0/16562

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	A	0	5
1	C	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	GLN	Peptide
1	A	221	PRO	Peptide
1	A	224	ARG	Peptide
1	A	225	THR	Peptide
1	A	458	VAL	Peptide
1	C	131	PHE	Peptide
1	C	339	VAL	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	3948	0	3893	86	0
1	B	3941	0	3883	78	0
1	C	3864	0	3812	60	0
2	A	70	0	76	21	0
2	B	70	0	76	24	0
2	C	70	0	78	20	0
All	All	11963	0	11818	276	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 12.

All (276) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:602:TCH:C17	2:A:602:TCH:C16	1.76	1.63
2:B:601:TCH:C7	2:B:601:TCH:C6	1.75	1.63
2:A:602:TCH:C7	2:A:602:TCH:C6	1.76	1.62
2:B:602:TCH:C16	2:B:602:TCH:C17	1.76	1.61
2:B:601:TCH:C17	2:B:601:TCH:C16	1.76	1.60
2:C:601:TCH:C7	2:C:601:TCH:C6	1.75	1.59
2:A:601:TCH:C7	2:A:601:TCH:C6	1.75	1.59
2:B:602:TCH:C7	2:B:602:TCH:C6	1.75	1.58
2:C:602:TCH:C7	2:C:602:TCH:C6	1.75	1.57
2:A:601:TCH:C16	2:A:601:TCH:C17	1.76	1.55
2:C:602:TCH:C16	2:C:602:TCH:C17	1.76	1.53
2:C:601:TCH:C16	2:C:601:TCH:C17	1.76	1.45
2:B:602:TCH:H37	2:B:602:TCH:H16A	1.32	1.09
2:C:601:TCH:H37	2:C:601:TCH:H16A	1.36	1.05
2:B:602:TCH:C6	2:B:602:TCH:C8	2.40	0.97
2:C:602:TCH:C6	2:C:602:TCH:C8	2.40	0.94
2:C:601:TCH:C16	2:C:601:TCH:H37	1.98	0.93
2:A:601:TCH:H37	2:A:601:TCH:H16A	1.51	0.93
2:A:601:TCH:C6	2:A:601:TCH:C8	2.41	0.90
2:B:602:TCH:C16	2:B:602:TCH:H37	2.02	0.88
2:C:602:TCH:H16A	2:C:602:TCH:H37	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:602:TCH:C16	2:A:602:TCH:C20	2.52	0.86
2:B:601:TCH:C6	2:B:601:TCH:C8	2.42	0.86
2:A:602:TCH:H16A	2:A:602:TCH:H37	1.58	0.85
2:B:601:TCH:C16	2:B:601:TCH:C20	2.53	0.85
2:C:602:TCH:C16	2:C:602:TCH:C20	2.54	0.85
1:B:32:ILE:HD13	1:B:162:LEU:HD12	1.61	0.83
1:C:337:ILE:HB	1:C:393:ALA:HB1	1.61	0.82
2:B:602:TCH:C16	2:B:602:TCH:C20	2.57	0.81
1:A:409:ASN:HD22	1:A:412:LEU:HB2	1.46	0.80
2:C:601:TCH:C6	2:C:601:TCH:C8	2.41	0.79
2:A:602:TCH:C6	2:A:602:TCH:C8	2.42	0.79
2:C:601:TCH:C16	2:C:601:TCH:C20	2.57	0.78
2:C:601:TCH:C16	2:C:601:TCH:C22	2.62	0.78
2:B:602:TCH:H16A	2:B:602:TCH:C22	2.14	0.77
1:B:101:GLY:H	1:B:172:THR:HG23	1.48	0.77
2:C:602:TCH:C16	2:C:602:TCH:H37	2.16	0.76
2:B:601:TCH:C16	2:B:601:TCH:C22	2.64	0.75
2:A:601:TCH:C16	2:A:601:TCH:H37	2.16	0.75
1:B:314:GLY:HA2	2:B:601:TCH:H1	1.67	0.75
2:B:602:TCH:C16	2:B:602:TCH:C22	2.65	0.75
1:A:319:PRO:HG2	1:C:413:LEU:HB2	1.69	0.75
2:A:601:TCH:C16	2:A:601:TCH:C20	2.60	0.74
1:C:334:GLN:HB2	1:C:399:TYR:HB3	1.69	0.74
2:B:601:TCH:C22	2:B:601:TCH:H16A	2.18	0.73
1:B:49:ASN:ND2	1:B:216:VAL:O	2.20	0.73
2:B:601:TCH:H16A	2:B:601:TCH:H37	1.68	0.73
1:C:241:THR:HG23	1:C:455:GLN:HB3	1.71	0.73
1:A:224:ARG:O	1:A:225:THR:OG1	2.06	0.73
1:B:473:LEU:HD12	1:B:491:LEU:HD23	1.68	0.73
2:A:602:TCH:C16	2:A:602:TCH:C22	2.67	0.72
1:A:36:ALA:O	1:A:165:ARG:NH2	2.24	0.71
1:B:336:GLU:OE2	1:B:396:ARG:NH2	2.23	0.71
1:B:480:THR:HG23	1:B:513:GLY:HA2	1.72	0.71
1:A:111:VAL:HG12	1:A:156:PRO:HB3	1.73	0.70
1:C:339:VAL:HG11	1:C:353:THR:H	1.55	0.70
2:C:601:TCH:H16A	2:C:601:TCH:C22	2.16	0.69
1:A:473:LEU:HD12	1:A:491:LEU:HD23	1.73	0.69
2:C:602:TCH:C16	2:C:602:TCH:C22	2.72	0.67
1:B:170:HIS:HB3	1:B:176:GLU:HG3	1.74	0.67
2:A:602:TCH:H16A	2:A:602:TCH:C22	2.23	0.67
1:C:108:VAL:HG21	1:C:181:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:602:TCH:H16A	2:C:602:TCH:C22	2.25	0.67
1:C:470:SER:OG	1:C:471:GLU:N	2.28	0.66
1:B:75:PRO:HG3	1:B:188:PRO:HD3	1.77	0.66
1:C:358:ILE:O	1:C:367:GLN:NE2	2.29	0.66
1:B:47:GLN:HE21	1:B:49:ASN:HD21	1.42	0.65
1:B:100:THR:O	1:B:100:THR:OG1	2.04	0.65
2:A:601:TCH:C16	2:A:601:TCH:C22	2.74	0.65
1:B:98:MET:O	1:B:219:THR:N	2.27	0.64
1:B:112:LEU:HD13	1:B:151:VAL:HA	1.78	0.64
1:C:453:LEU:HD22	1:C:457:PHE:HD2	1.60	0.64
1:A:470:SER:O	1:A:493:ASN:ND2	2.29	0.64
1:C:293:ALA:HB3	1:C:389:GLY:H	1.63	0.64
1:B:270:HIS:HD2	1:B:276:LEU:HD11	1.63	0.64
1:B:26:VAL:O	1:B:28:GLN:NE2	2.31	0.64
1:A:222:ILE:HG13	1:A:223:GLU:N	2.13	0.63
1:A:121:LYS:HE2	1:A:150:ASP:HB3	1.79	0.63
1:A:268:ARG:NH1	1:A:418:PRO:O	2.31	0.63
1:B:32:ILE:CD1	1:B:162:LEU:HD12	2.27	0.63
1:A:443:ASP:OD1	1:A:444:ALA:N	2.32	0.62
1:C:333:GLY:H	1:C:359:LEU:HB2	1.65	0.62
1:B:312:GLN:NE2	1:B:326:LEU:O	2.30	0.61
1:B:224:ARG:NH2	1:B:463:SER:O	2.32	0.61
1:B:351:LYS:NZ	1:B:352:VAL:O	2.26	0.61
1:A:216:VAL:HG12	1:A:217:TYR:HB2	1.82	0.61
1:A:228:ARG:HH22	1:A:464:ASN:HB2	1.65	0.61
1:C:118:THR:HA	1:C:191:THR:HG22	1.83	0.61
1:A:52:ASP:HB3	1:A:55:ILE:HG13	1.82	0.60
1:A:222:ILE:HG13	1:A:223:GLU:HG3	1.83	0.60
1:A:490:LYS:HG3	1:A:527:LEU:HD21	1.82	0.60
1:C:370:TYR:HE1	1:C:415:PRO:HD2	1.66	0.60
1:B:476:ARG:HH11	1:B:488:GLU:HB3	1.67	0.60
1:C:253:LEU:HD21	1:C:433:ARG:HD2	1.83	0.59
1:A:341:THR:HB	1:A:386:LEU:HD22	1.83	0.59
1:B:241:THR:HG23	1:B:455:GLN:HB3	1.85	0.59
1:B:284:SER:O	1:B:392:ARG:NH2	2.36	0.59
1:B:64:LEU:HG	1:B:520:TRP:HB2	1.84	0.59
1:C:288:CYS:SG	1:C:392:ARG:NH2	2.76	0.59
1:A:291:ALA:HB2	1:A:309:LEU:HD23	1.85	0.58
1:B:367:GLN:NE2	1:B:375:PHE:O	2.36	0.58
1:A:296:GLU:OE1	1:A:296:GLU:N	2.33	0.58
1:B:470:SER:OG	1:B:471:GLU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:HIS:CD2	1:B:276:LEU:HD11	2.39	0.57
1:C:84:LEU:HB2	1:C:161:LEU:HG	1.87	0.57
1:A:282:SER:HG	1:A:284:SER:HG	1.50	0.57
1:B:101:GLY:HA2	1:B:170:HIS:O	2.06	0.56
1:A:310:ILE:HD11	2:A:601:TCH:H1	1.88	0.56
1:B:333:GLY:HA3	1:B:398:ILE:HD11	1.88	0.56
1:A:255:ASP:HB3	1:A:258:LEU:HD12	1.88	0.55
1:C:105:ASN:HD22	1:C:162:LEU:HA	1.71	0.55
1:C:291:ALA:HB1	1:C:307:PHE:HB3	1.88	0.55
1:C:371:GLN:HE22	1:C:409:ASN:HD21	1.53	0.55
2:C:602:TCH:C7	2:C:602:TCH:C5	2.66	0.55
1:C:339:VAL:HG21	1:C:352:VAL:HA	1.88	0.55
1:A:92:LEU:HD11	1:A:209:PRO:HG3	1.89	0.54
1:B:392:ARG:NH1	2:B:601:TCH:O3S	2.34	0.54
1:B:275:LEU:HB3	1:B:279:THR:HG23	1.90	0.54
1:A:275:LEU:HD11	1:A:281:ILE:HD11	1.90	0.54
1:A:241:THR:HB	1:A:455:GLN:HB2	1.89	0.53
1:A:26:VAL:HG23	1:A:27:GLU:H	1.72	0.53
1:C:198:SER:O	1:C:198:SER:OG	2.26	0.53
1:A:423:PHE:HZ	1:A:429:LEU:HD12	1.74	0.52
1:B:460:TRP:O	1:B:464:ASN:ND2	2.37	0.52
2:B:601:TCH:C7	2:B:601:TCH:C5	2.65	0.52
1:A:64:LEU:O	1:A:64:LEU:HD23	2.10	0.52
1:A:266:ASN:OD1	1:A:278:THR:OG1	2.27	0.52
1:B:431:ARG:HB3	1:B:450:ASP:HB3	1.92	0.52
1:A:467:THR:HG22	1:A:468:VAL:H	1.74	0.52
1:C:216:VAL:HG12	1:C:217:TYR:HB2	1.90	0.52
1:B:490:LYS:NZ	1:B:525:TYR:O	2.42	0.52
1:C:500:SER:HB3	1:C:527:LEU:HB2	1.91	0.52
1:C:340:GLN:HB3	1:C:391:VAL:HG12	1.92	0.51
1:B:21:LEU:HD23	1:B:152:ARG:O	2.10	0.51
1:A:82:LEU:HD11	1:A:205:LEU:HD13	1.93	0.51
1:B:102:TRP:HD1	1:B:172:THR:HG22	1.75	0.51
1:C:433:ARG:HG2	1:C:448:ALA:HB1	1.93	0.51
1:A:340:GLN:HE21	1:A:350:LEU:HD22	1.75	0.51
1:C:340:GLN:HG2	2:C:601:TCH:H21	1.93	0.50
1:B:322:ARG:HH12	1:B:325:PRO:HA	1.76	0.50
2:C:601:TCH:C7	2:C:601:TCH:C5	2.66	0.50
1:B:233:PRO:HB2	1:B:235:ILE:HG12	1.93	0.50
1:A:100:THR:HG22	1:A:217:TYR:HB3	1.94	0.50
1:B:242:HIS:CE1	1:B:451:CYS:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:OG1	1:A:193:SER:O	2.19	0.50
1:C:196:ASP:OD1	1:C:196:ASP:N	2.42	0.50
1:A:392:ARG:HD3	2:A:601:TCH:H26	1.93	0.50
1:A:475:LEU:HB2	1:A:489:CYS:SG	2.52	0.50
1:B:437:ARG:HG3	2:B:602:TCH:N24	2.26	0.49
1:C:475:LEU:HB2	1:C:489:CYS:SG	2.53	0.49
1:A:371:GLN:OE1	1:C:412:LEU:HB3	2.13	0.48
1:C:111:VAL:HG12	1:C:156:PRO:HB3	1.93	0.48
1:A:361:PRO:HA	1:A:407:GLU:HG2	1.95	0.48
1:C:365:ALA:HB1	1:C:367:GLN:HG2	1.95	0.48
1:A:284:SER:O	1:A:392:ARG:NH2	2.45	0.48
1:A:339:VAL:HG23	1:A:341:THR:HG23	1.95	0.48
2:B:601:TCH:H21	2:B:601:TCH:H23	1.65	0.48
1:A:234:VAL:O	1:A:235:ILE:HD13	2.13	0.48
1:B:430:LEU:HD13	1:B:499:LEU:HD21	1.96	0.48
1:A:451:CYS:SG	1:A:452:ALA:N	2.87	0.48
1:B:261:ASN:HD22	1:B:421:GLY:HA3	1.78	0.48
1:B:492:TYR:HE2	1:B:498:ALA:HB3	1.79	0.48
1:B:223:GLU:CD	1:B:223:GLU:H	2.17	0.47
1:A:369:PRO:HG2	1:A:408:TYR:HA	1.96	0.47
1:C:130:TYR:O	1:C:131:PHE:HB3	2.14	0.47
1:C:343:THR:HG22	1:C:345:LYS:H	1.80	0.47
1:B:35:VAL:HG23	1:B:162:LEU:HD13	1.97	0.47
1:C:433:ARG:HG3	1:C:450:ASP:HB3	1.97	0.47
1:A:157:ILE:O	1:A:157:ILE:HG13	2.13	0.47
1:C:339:VAL:HG13	1:C:353:THR:O	2.15	0.47
1:A:455:GLN:O	1:A:456:GLU:HB2	2.15	0.46
1:B:478:ARG:O	1:B:513:GLY:HA3	2.16	0.46
1:C:306:THR:HG1	1:C:375:PHE:HE1	1.62	0.46
1:A:481:LEU:O	1:A:482:THR:OG1	2.31	0.46
1:C:477:TYR:CE2	1:C:486:LEU:HD12	2.51	0.46
1:C:293:ALA:HB2	1:C:391:VAL:HG13	1.98	0.45
1:A:260:SER:OG	1:A:261:ASN:OD1	2.31	0.45
1:B:265:GLN:NE2	1:B:416:LEU:HD22	2.32	0.45
1:A:383:SER:O	1:A:383:SER:OG	2.34	0.45
1:C:133:LYS:HD3	1:C:133:LYS:HA	1.74	0.45
1:A:169:TRP:O	1:C:166:ARG:HD2	2.17	0.45
1:B:269:VAL:HG22	1:B:270:HIS:O	2.17	0.45
1:B:342:GLU:HB3	1:B:387:VAL:HB	1.99	0.45
1:A:254:VAL:HG11	1:A:499:LEU:HD23	1.97	0.45
1:B:84:LEU:HD13	1:B:161:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:PHE:O	1:C:373:ARG:HA	2.17	0.45
1:A:288:CYS:HB2	1:A:393:ALA:O	2.17	0.45
1:A:60:VAL:HG23	1:A:90:PRO:HD2	1.99	0.44
1:A:184:MET:HE3	1:A:184:MET:HB3	1.80	0.44
1:B:475:LEU:HD23	1:B:517:VAL:HA	1.98	0.44
1:B:219:THR:OG1	1:B:220:PRO:HD2	2.17	0.44
1:B:234:VAL:O	1:B:234:VAL:HG23	2.18	0.44
1:A:225:THR:HG22	1:A:226:ILE:N	2.32	0.44
1:A:332:SER:OG	1:A:404:THR:O	2.33	0.44
1:B:150:ASP:OD2	1:B:151:VAL:N	2.50	0.44
1:A:288:CYS:HB3	1:A:395:PRO:HD3	1.99	0.44
1:B:468:VAL:HB	1:B:493:ASN:ND2	2.32	0.44
1:B:111:VAL:O	1:B:203:GLY:HA2	2.17	0.44
1:C:335:LEU:O	1:C:357:MET:N	2.42	0.44
1:A:269:VAL:O	1:A:495:GLY:HA3	2.18	0.44
1:A:342:GLU:O	1:A:387:VAL:HG23	2.18	0.44
1:A:390:ARG:HB3	2:A:601:TCH:H11A	1.99	0.44
1:C:163:ASP:OD2	1:C:165:ARG:HD3	2.18	0.44
1:C:453:LEU:HD22	1:C:457:PHE:CD2	2.48	0.44
1:A:223:GLU:OE2	1:A:224:ARG:N	2.51	0.43
1:A:150:ASP:OD1	1:A:150:ASP:N	2.49	0.43
1:B:63:PRO:O	1:B:519:SER:HB2	2.18	0.43
1:B:118:THR:HG22	1:B:191:THR:HG22	2.00	0.43
1:A:334:GLN:NE2	1:A:356:GLU:HG2	2.33	0.43
1:A:334:GLN:HG2	1:A:357:MET:O	2.18	0.43
2:A:602:TCH:H11A	2:A:602:TCH:H1A	1.79	0.43
1:C:115:ASN:OD1	1:C:118:THR:HG23	2.19	0.43
1:A:65:GLY:O	1:A:66:GLU:HG2	2.17	0.43
2:C:601:TCH:H18B	2:C:601:TCH:H20	1.78	0.43
1:A:455:GLN:C	1:A:457:PHE:H	2.22	0.43
1:B:216:VAL:HG12	1:B:217:TYR:HB2	2.00	0.43
1:A:60:VAL:HG11	1:A:91:TYR:HE2	1.83	0.43
1:B:227:TYR:O	1:B:228:ARG:HB3	2.19	0.42
2:B:602:TCH:C7	2:B:602:TCH:C5	2.66	0.42
1:C:477:TYR:CD2	1:C:486:LEU:HD12	2.54	0.42
1:A:297:PHE:HD1	1:A:300:GLY:HA3	1.84	0.42
1:B:238:ARG:NH1	1:B:512:ASP:OD1	2.51	0.42
1:B:476:ARG:NH1	1:B:488:GLU:OE1	2.52	0.42
1:C:476:ARG:HG3	1:C:488:GLU:HG2	2.00	0.42
2:B:602:TCH:H18B	2:B:602:TCH:H20	1.63	0.42
1:C:326:LEU:HD23	1:C:326:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:HA3	1:A:213:PHE:HA	2.02	0.42
1:A:392:ARG:HH11	2:A:601:TCH:H26	1.84	0.42
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.75	0.42
1:A:111:VAL:HG22	1:A:204:ARG:HB2	2.01	0.42
1:C:471:GLU:CD	1:C:523:ARG:HG3	2.40	0.42
1:B:38:ALA:HB2	1:B:214:ASN:HB2	2.01	0.42
1:A:84:LEU:HD22	1:A:162:LEU:O	2.20	0.42
2:A:601:TCH:H11	2:A:601:TCH:H19B	1.80	0.42
1:B:413:LEU:HD23	1:B:414:VAL:N	2.35	0.42
1:A:433:ARG:NH2	1:A:450:ASP:OD1	2.36	0.41
1:A:337:ILE:HA	1:A:394:VAL:O	2.19	0.41
1:B:362:THR:O	1:B:363:THR:OG1	2.36	0.41
1:A:361:PRO:O	1:A:362:THR:OG1	2.33	0.41
1:A:385:ASP:OD2	1:A:385:ASP:N	2.38	0.41
1:C:176:GLU:HG2	1:C:177:GLU:H	1.85	0.41
1:C:436:MET:H	1:C:436:MET:HG2	1.66	0.41
1:C:500:SER:O	1:C:500:SER:OG	2.37	0.41
1:B:101:GLY:N	1:B:172:THR:HG23	2.26	0.41
1:B:245:TRP:HE1	2:B:602:TCH:HO3S	1.66	0.41
1:B:306:THR:HG22	1:B:375:PHE:CD1	2.56	0.41
1:C:269:VAL:HG23	1:C:275:LEU:HD23	2.02	0.41
1:A:232:LEU:HD13	1:A:517:VAL:HG23	2.02	0.41
1:A:326:LEU:HD23	1:A:326:LEU:HA	1.90	0.41
1:A:123:VAL:HG12	1:A:186:TYR:HB2	2.02	0.41
2:A:602:TCH:H21	2:A:602:TCH:H23	1.80	0.41
1:B:25:ALA:HB3	1:B:157:ILE:HG12	2.02	0.41
1:C:339:VAL:HG11	1:C:353:THR:N	2.28	0.41
1:A:387:VAL:HG12	1:A:388:ASP:H	1.86	0.41
1:B:173:GLN:HA	1:B:226:ILE:HD13	2.02	0.41
1:B:238:ARG:HD3	1:B:511:THR:HG23	2.03	0.41
1:B:478:ARG:O	1:B:513:GLY:CA	2.68	0.41
2:B:601:TCH:H18B	2:B:601:TCH:H20	1.73	0.41
1:A:28:GLN:HA	1:A:28:GLN:OE1	2.21	0.41
1:A:470:SER:HB3	1:A:520:TRP:HB3	2.03	0.41
1:B:136:LEU:HA	1:B:140:GLN:HE21	1.86	0.41
1:A:342:GLU:OE1	1:A:349:LYS:HD2	2.21	0.40
1:B:136:LEU:HD12	1:B:140:GLN:HE21	1.85	0.40
1:A:362:THR:O	1:A:364:ASN:ND2	2.54	0.40
1:C:341:THR:HB	1:C:386:LEU:HD22	2.02	0.40
1:A:255:ASP:OD1	1:A:257:SER:OG	2.36	0.40
1:A:269:VAL:HG22	1:A:270:HIS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:TRP:CD1	1:A:460:TRP:O	2.74	0.40
1:B:82:LEU:O	1:B:82:LEU:HD12	2.21	0.40
1:B:144:PHE:CE1	1:C:220:PRO:HD2	2.57	0.40
1:C:80:PHE:CZ	1:C:205:LEU:HD13	2.56	0.40
1:C:287:SER:O	1:C:395:PRO:HD3	2.21	0.40
1:C:339:VAL:CG1	1:C:353:THR:H	2.28	0.40
1:B:294:ALA:HB3	1:B:306:THR:OG1	2.22	0.40
1:B:311:GLU:OE1	1:B:322:ARG:NH2	2.54	0.40
1:B:436:MET:HE2	1:B:436:MET:HB3	1.97	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	510/516 (99%)	453 (89%)	55 (11%)	2 (0%)	34	69
1	B	511/516 (99%)	445 (87%)	65 (13%)	1 (0%)	47	79
1	C	500/516 (97%)	440 (88%)	57 (11%)	3 (1%)	25	59
All	All	1521/1548 (98%)	1338 (88%)	177 (12%)	6 (0%)	38	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	225	THR
1	A	224	ARG
1	C	194	PRO
1	B	196	ASP
1	C	132	PRO
1	C	195	GLY

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	426/427 (100%)	424 (100%)	2 (0%)	88 94
1	B	425/427 (100%)	423 (100%)	2 (0%)	88 94
1	C	417/427 (98%)	416 (100%)	1 (0%)	93 97
All	All	1268/1281 (99%)	1263 (100%)	5 (0%)	91 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	THR
1	A	224	ARG
1	B	100	THR
1	B	112	LEU
1	C	414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	57	GLN
1	A	170	HIS
1	A	270	HIS
1	A	340	GLN
1	A	364	ASN
1	A	367	GLN
1	A	402	GLN
1	A	409	ASN
1	B	28	GLN
1	B	33	GLN
1	B	47	GLN
1	B	73	ASN
1	B	105	ASN
1	B	140	GLN
1	B	266	ASN

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Mol	Chain	Res	Type
1	B	270	HIS
1	B	455	GLN
1	C	105	ASN
1	C	173	GLN
1	C	409	ASN
1	C	464	ASN
1	C	469	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)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TCH	B	602	-	38,38,38	8.79	30 (78%)	59,60,60	2.38	25 (42%)
2	TCH	A	602	-	38,38,38	8.79	30 (78%)	59,60,60	2.50	22 (37%)
2	TCH	C	601	-	38,38,38	8.80	30 (78%)	59,60,60	2.48	23 (38%)
2	TCH	B	601	-	38,38,38	8.78	30 (78%)	59,60,60	2.61	22 (37%)
2	TCH	A	601	-	38,38,38	8.76	30 (78%)	59,60,60	2.69	30 (50%)
2	TCH	C	602	-	38,38,38	8.79	30 (78%)	59,60,60	2.36	23 (38%)

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	TCH	B	602	-	-	9/16/81/81	0/4/4/4
2	TCH	A	602	-	-	6/16/81/81	0/4/4/4
2	TCH	C	601	-	-	11/16/81/81	0/4/4/4
2	TCH	B	601	-	-	9/16/81/81	0/4/4/4
2	TCH	A	601	-	-	10/16/81/81	0/4/4/4
2	TCH	C	602	-	-	11/16/81/81	0/4/4/4

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TCH	C8-C14	-25.31	1.04	1.53
2	A	602	TCH	C8-C14	-25.25	1.04	1.53
2	C	601	TCH	C8-C14	-25.22	1.04	1.53
2	B	602	TCH	C8-C14	-25.13	1.04	1.53
2	C	602	TCH	C8-C14	-24.97	1.05	1.53
2	A	601	TCH	C8-C7	-24.89	1.11	1.53
2	A	601	TCH	C8-C14	-24.80	1.05	1.53
2	B	602	TCH	C8-C7	-24.79	1.11	1.53
2	C	602	TCH	C8-C7	-24.77	1.11	1.53
2	C	601	TCH	C8-C7	-24.72	1.11	1.53
2	B	601	TCH	C8-C7	-24.54	1.11	1.53
2	A	602	TCH	C8-C7	-24.52	1.11	1.53
2	A	601	TCH	C11-C12	-15.51	1.27	1.53
2	C	601	TCH	C11-C12	-15.45	1.27	1.53
2	B	602	TCH	C11-C12	-15.26	1.27	1.53
2	A	602	TCH	C11-C12	-15.25	1.27	1.53
2	C	602	TCH	C11-C12	-15.17	1.27	1.53
2	B	601	TCH	C11-C12	-15.14	1.27	1.53
2	C	601	TCH	C10-C5	-14.82	1.31	1.55
2	A	602	TCH	C10-C5	-14.79	1.31	1.55
2	B	601	TCH	C10-C5	-14.69	1.31	1.55
2	C	602	TCH	C10-C5	-14.57	1.31	1.55
2	B	602	TCH	C10-C5	-14.52	1.31	1.55
2	A	601	TCH	C10-C5	-14.32	1.32	1.55
2	C	601	TCH	C20-C17	-13.90	1.30	1.54
2	B	601	TCH	C20-C17	-13.88	1.30	1.54
2	A	602	TCH	C20-C17	-13.84	1.30	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	TCH	C20-C17	-13.62	1.30	1.54
2	C	602	TCH	C20-C17	-13.54	1.30	1.54
2	A	602	TCH	C6-C7	13.44	1.76	1.52
2	B	601	TCH	C6-C7	13.34	1.75	1.52
2	C	602	TCH	C6-C7	13.34	1.75	1.52
2	C	601	TCH	C6-C7	13.33	1.75	1.52
2	A	601	TCH	C20-C17	-13.26	1.31	1.54
2	B	602	TCH	C6-C7	13.18	1.75	1.52
2	A	601	TCH	C6-C7	13.18	1.75	1.52
2	C	601	TCH	O12-C12	11.54	1.62	1.43
2	C	602	TCH	O12-C12	11.51	1.62	1.43
2	B	602	TCH	O12-C12	11.50	1.62	1.43
2	A	601	TCH	O12-C12	11.49	1.62	1.43
2	A	602	TCH	O12-C12	11.46	1.62	1.43
2	B	601	TCH	O12-C12	11.14	1.62	1.43
2	A	601	TCH	C13-C12	-11.11	1.37	1.54
2	C	602	TCH	C13-C12	-11.06	1.37	1.54
2	C	601	TCH	C13-C12	-11.03	1.37	1.54
2	B	602	TCH	C13-C12	-10.90	1.37	1.54
2	A	602	TCH	C16-C17	10.87	1.76	1.54
2	B	601	TCH	C16-C17	10.77	1.76	1.54
2	B	602	TCH	C16-C17	10.75	1.76	1.54
2	C	601	TCH	C16-C17	10.69	1.76	1.54
2	A	601	TCH	C16-C17	10.58	1.76	1.54
2	B	601	TCH	C13-C12	-10.58	1.38	1.54
2	C	602	TCH	C16-C17	10.54	1.76	1.54
2	A	602	TCH	C13-C12	-10.53	1.38	1.54
2	A	601	TCH	C4-C5	9.45	1.69	1.53
2	B	601	TCH	C4-C5	9.11	1.68	1.53
2	C	602	TCH	C4-C5	9.06	1.68	1.53
2	A	602	TCH	C4-C5	8.94	1.68	1.53
2	C	601	TCH	C4-C5	8.91	1.68	1.53
2	B	602	TCH	C4-C5	8.88	1.68	1.53
2	C	602	TCH	C13-C17	8.69	1.70	1.55
2	A	602	TCH	C13-C17	8.39	1.69	1.55
2	B	602	TCH	C13-C17	8.29	1.69	1.55
2	B	601	TCH	C13-C17	8.23	1.69	1.55
2	A	601	TCH	C13-C17	8.02	1.69	1.55
2	C	601	TCH	C13-C17	7.87	1.69	1.55
2	B	602	TCH	C6-C5	-7.00	1.42	1.53
2	C	602	TCH	C6-C5	-6.95	1.42	1.53
2	C	601	TCH	C6-C5	-6.94	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TCH	C6-C5	-6.94	1.42	1.53
2	C	602	TCH	C24-N24	6.93	1.49	1.33
2	A	602	TCH	C6-C5	-6.82	1.42	1.53
2	B	602	TCH	C24-N24	6.82	1.48	1.33
2	A	602	TCH	C24-N24	6.79	1.48	1.33
2	A	601	TCH	C24-N24	6.79	1.48	1.33
2	B	601	TCH	C24-N24	6.73	1.48	1.33
2	A	601	TCH	C15-C14	6.71	1.68	1.54
2	C	601	TCH	C24-N24	6.70	1.48	1.33
2	B	602	TCH	C15-C14	6.51	1.67	1.54
2	B	601	TCH	C15-C14	6.44	1.67	1.54
2	A	601	TCH	C6-C5	-6.40	1.43	1.53
2	A	602	TCH	C15-C14	6.36	1.67	1.54
2	C	601	TCH	C15-C14	6.33	1.67	1.54
2	B	602	TCH	C1-C10	6.25	1.65	1.54
2	B	601	TCH	O7-C7	6.23	1.56	1.43
2	C	602	TCH	C15-C14	6.22	1.67	1.54
2	A	602	TCH	O7-C7	6.19	1.56	1.43
2	C	601	TCH	O7-C7	6.18	1.56	1.43
2	C	602	TCH	O7-C7	6.17	1.56	1.43
2	B	602	TCH	O7-C7	6.13	1.56	1.43
2	A	601	TCH	O7-C7	6.10	1.56	1.43
2	A	601	TCH	C1-C10	6.02	1.64	1.54
2	C	602	TCH	C1-C10	5.89	1.64	1.54
2	A	602	TCH	C1-C10	5.79	1.64	1.54
2	B	601	TCH	C1-C10	5.71	1.64	1.54
2	C	601	TCH	C1-C10	5.63	1.64	1.54
2	B	602	TCH	C13-C14	5.16	1.64	1.55
2	A	601	TCH	C13-C14	5.10	1.64	1.55
2	A	602	TCH	C13-C14	5.09	1.64	1.55
2	C	602	TCH	C13-C14	4.99	1.64	1.55
2	B	601	TCH	C13-C14	4.99	1.64	1.55
2	C	601	TCH	C13-C14	4.84	1.63	1.55
2	A	602	TCH	C2-C3	-4.77	1.40	1.51
2	C	602	TCH	C2-C3	-4.71	1.40	1.51
2	B	601	TCH	C2-C3	-4.68	1.40	1.51
2	B	602	TCH	C2-C3	-4.67	1.40	1.51
2	C	601	TCH	C2-C3	-4.63	1.40	1.51
2	A	601	TCH	C2-C3	-4.32	1.41	1.51
2	A	602	TCH	C26-S26	4.27	1.83	1.77
2	B	601	TCH	C26-S26	4.26	1.83	1.77
2	C	602	TCH	C26-S26	4.25	1.83	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	602	TCH	C22-C20	4.03	1.64	1.54
2	C	601	TCH	C26-S26	3.97	1.83	1.77
2	A	602	TCH	C22-C20	3.93	1.64	1.54
2	A	601	TCH	C26-S26	3.92	1.83	1.77
2	A	601	TCH	C22-C20	3.91	1.64	1.54
2	B	601	TCH	C22-C20	3.91	1.64	1.54
2	B	602	TCH	C22-C20	3.84	1.64	1.54
2	C	601	TCH	C22-C20	3.79	1.64	1.54
2	B	602	TCH	C26-S26	3.62	1.82	1.77
2	A	602	TCH	C21-C20	3.62	1.61	1.53
2	B	601	TCH	C21-C20	3.62	1.61	1.53
2	A	601	TCH	C16-C15	3.49	1.63	1.54
2	B	602	TCH	C21-C20	3.49	1.61	1.53
2	A	601	TCH	C21-C20	3.48	1.61	1.53
2	C	602	TCH	C21-C20	3.45	1.61	1.53
2	C	601	TCH	C21-C20	3.41	1.61	1.53
2	C	601	TCH	C16-C15	3.34	1.63	1.54
2	C	602	TCH	C16-C15	3.26	1.62	1.54
2	B	602	TCH	C16-C15	3.23	1.62	1.54
2	B	601	TCH	C16-C15	3.23	1.62	1.54
2	A	602	TCH	C16-C15	3.15	1.62	1.54
2	C	602	TCH	C23-C24	3.07	1.57	1.51
2	A	601	TCH	C23-C24	2.83	1.56	1.51
2	A	601	TCH	C10-C9	2.79	1.61	1.56
2	B	601	TCH	C10-C9	2.74	1.61	1.56
2	B	601	TCH	C23-C24	2.65	1.56	1.51
2	C	602	TCH	C10-C9	2.64	1.61	1.56
2	A	602	TCH	C23-C24	2.64	1.56	1.51
2	C	601	TCH	C23-C24	2.63	1.56	1.51
2	B	602	TCH	C23-C24	2.60	1.56	1.51
2	B	602	TCH	C10-C9	2.58	1.60	1.56
2	C	601	TCH	C11-C9	-2.54	1.49	1.53
2	C	602	TCH	C1-C2	2.52	1.58	1.53
2	A	602	TCH	C10-C9	2.46	1.60	1.56
2	B	602	TCH	C1-C2	2.45	1.58	1.53
2	A	601	TCH	C1-C2	2.44	1.58	1.53
2	A	601	TCH	C11-C9	-2.40	1.49	1.53
2	B	602	TCH	O2S-S26	2.38	1.52	1.45
2	A	601	TCH	O24-C24	-2.37	1.18	1.23
2	C	601	TCH	O2S-S26	2.34	1.51	1.45
2	A	602	TCH	C1-C2	2.30	1.58	1.53
2	C	602	TCH	C11-C9	-2.30	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	TCH	C1-C2	2.28	1.58	1.53
2	A	602	TCH	C11-C9	-2.27	1.50	1.53
2	B	602	TCH	O24-C24	-2.26	1.18	1.23
2	A	602	TCH	O24-C24	-2.26	1.18	1.23
2	B	601	TCH	O24-C24	-2.26	1.18	1.23
2	B	601	TCH	C1-C2	2.26	1.58	1.53
2	C	601	TCH	O24-C24	-2.24	1.18	1.23
2	A	602	TCH	C19-C10	2.24	1.58	1.54
2	C	602	TCH	O2S-S26	2.24	1.51	1.45
2	A	601	TCH	O1S-S26	2.23	1.51	1.45
2	B	602	TCH	C11-C9	-2.23	1.50	1.53
2	B	602	TCH	O1S-S26	2.23	1.51	1.45
2	C	601	TCH	O1S-S26	2.21	1.51	1.45
2	B	602	TCH	C19-C10	2.21	1.58	1.54
2	B	601	TCH	C11-C9	-2.20	1.50	1.53
2	B	601	TCH	O1S-S26	2.18	1.51	1.45
2	A	602	TCH	O1S-S26	2.18	1.51	1.45
2	B	601	TCH	O2S-S26	2.17	1.51	1.45
2	B	601	TCH	C19-C10	2.17	1.58	1.54
2	C	602	TCH	O24-C24	-2.16	1.18	1.23
2	A	601	TCH	O2S-S26	2.15	1.51	1.45
2	A	601	TCH	C19-C10	2.15	1.58	1.54
2	C	601	TCH	C10-C9	2.14	1.60	1.56
2	A	602	TCH	O2S-S26	2.13	1.51	1.45
2	C	602	TCH	O1S-S26	2.11	1.51	1.45
2	C	601	TCH	C19-C10	2.11	1.58	1.54
2	C	602	TCH	C19-C10	2.09	1.58	1.54

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	TCH	C14-C13-C12	8.18	115.02	107.40
2	A	602	TCH	C14-C13-C12	7.14	114.05	107.40
2	A	601	TCH	C13-C17-C20	-7.04	111.09	119.50
2	B	602	TCH	C13-C17-C20	-7.00	111.13	119.50
2	C	601	TCH	C14-C13-C12	6.81	113.75	107.40
2	C	601	TCH	C13-C17-C20	-6.78	111.40	119.50
2	B	601	TCH	C13-C17-C20	-6.09	112.22	119.50
2	C	602	TCH	O2S-S26-C26	5.66	113.73	106.92
2	C	602	TCH	C13-C17-C20	-5.65	112.75	119.50
2	B	602	TCH	C14-C13-C12	5.60	112.62	107.40
2	A	602	TCH	C13-C17-C20	-5.26	113.22	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	TCH	C11-C9-C10	-5.24	108.33	113.73
2	A	602	TCH	C11-C9-C10	-5.22	108.34	113.73
2	A	601	TCH	C11-C9-C10	-5.21	108.35	113.73
2	C	601	TCH	C11-C9-C10	-5.11	108.46	113.73
2	A	601	TCH	C14-C13-C12	5.08	112.14	107.40
2	B	602	TCH	C11-C9-C10	-4.93	108.65	113.73
2	A	601	TCH	C18-C13-C17	-4.91	103.53	111.21
2	B	601	TCH	C17-C13-C12	4.86	122.10	117.67
2	C	602	TCH	C11-C9-C10	-4.71	108.87	113.73
2	A	601	TCH	O1S-S26-C26	4.71	112.58	106.92
2	C	601	TCH	C17-C13-C12	4.68	121.94	117.67
2	A	602	TCH	C17-C13-C12	4.62	121.89	117.67
2	A	601	TCH	C9-C10-C5	4.60	115.04	108.58
2	C	602	TCH	C17-C13-C14	4.51	104.64	100.09
2	B	601	TCH	C18-C13-C17	-4.36	104.39	111.21
2	C	602	TCH	C17-C13-C12	4.33	121.62	117.67
2	A	602	TCH	C1-C10-C9	-4.30	104.59	111.35
2	A	602	TCH	C1-C10-C5	4.29	114.11	107.77
2	B	602	TCH	C18-C13-C17	-4.24	104.57	111.21
2	A	602	TCH	O1S-S26-C26	4.19	111.96	106.92
2	B	602	TCH	O1S-S26-C26	4.16	111.93	106.92
2	C	602	TCH	O2S-S26-O1S	-4.12	99.68	113.95
2	C	601	TCH	C18-C13-C17	-4.12	104.77	111.21
2	B	602	TCH	C17-C13-C12	4.11	121.42	117.67
2	A	602	TCH	C18-C13-C17	-4.05	104.88	111.21
2	A	602	TCH	C23-C22-C20	-4.03	107.16	114.52
2	B	602	TCH	C1-C10-C5	4.01	113.70	107.77
2	C	602	TCH	C18-C13-C17	-3.99	104.97	111.21
2	A	601	TCH	C4-C3-C2	3.90	115.21	110.55
2	A	601	TCH	C17-C13-C14	3.87	104.00	100.09
2	A	601	TCH	C14-C8-C9	3.85	114.99	109.71
2	B	601	TCH	O1S-S26-C26	3.85	111.55	106.92
2	B	601	TCH	O2S-S26-C26	3.84	111.54	106.92
2	A	601	TCH	C23-C24-N24	3.83	122.86	116.42
2	A	601	TCH	O2S-S26-O1S	-3.81	100.75	113.95
2	B	601	TCH	O2S-S26-O1S	-3.81	100.76	113.95
2	A	601	TCH	C17-C13-C12	3.79	121.13	117.67
2	C	601	TCH	O1S-S26-C26	3.78	111.47	106.92
2	A	602	TCH	O2S-S26-O1S	-3.73	101.05	113.95
2	B	601	TCH	C23-C22-C20	-3.72	107.73	114.52
2	B	601	TCH	C18-C13-C12	-3.71	105.29	109.07
2	A	601	TCH	O2S-S26-C26	3.67	111.34	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	TCH	C6-C5-C4	-3.67	106.97	111.19
2	B	601	TCH	C9-C10-C5	3.63	113.68	108.58
2	A	601	TCH	C6-C5-C10	3.58	116.46	112.66
2	C	602	TCH	C15-C14-C8	3.56	123.31	118.33
2	C	601	TCH	C14-C8-C9	3.55	114.58	109.71
2	C	601	TCH	O2S-S26-O1S	-3.54	101.69	113.95
2	B	601	TCH	C15-C14-C8	3.53	123.27	118.33
2	C	601	TCH	C9-C11-C12	-3.51	109.67	114.30
2	C	601	TCH	O2S-S26-C26	3.46	111.08	106.92
2	B	602	TCH	C23-C22-C20	-3.45	108.21	114.52
2	C	602	TCH	C9-C10-C5	3.44	113.42	108.58
2	B	601	TCH	C11-C12-C13	3.41	114.74	111.24
2	A	602	TCH	O2S-S26-C26	3.40	111.01	106.92
2	C	601	TCH	C1-C10-C5	3.39	112.79	107.77
2	A	601	TCH	C15-C14-C8	3.38	123.06	118.33
2	A	602	TCH	C15-C14-C8	3.37	123.04	118.33
2	B	602	TCH	O2S-S26-O1S	-3.35	102.35	113.95
2	A	602	TCH	C9-C10-C5	3.34	113.27	108.58
2	A	602	TCH	C18-C13-C14	-3.34	105.99	111.21
2	B	601	TCH	C18-C13-C14	-3.29	106.06	111.21
2	C	602	TCH	C6-C5-C4	-3.28	107.41	111.19
2	C	601	TCH	C23-C22-C20	-3.26	108.57	114.52
2	C	602	TCH	C1-C10-C5	3.25	112.57	107.77
2	B	601	TCH	C6-C5-C4	-3.24	107.47	111.19
2	B	601	TCH	C1-C10-C5	3.22	112.54	107.77
2	C	602	TCH	O12-C12-C13	-3.22	105.58	111.03
2	B	601	TCH	C1-C10-C9	-3.22	106.29	111.35
2	B	602	TCH	C15-C14-C8	3.21	122.83	118.33
2	B	602	TCH	C17-C13-C14	3.20	103.32	100.09
2	C	601	TCH	C22-C23-C24	-3.19	105.91	113.04
2	C	602	TCH	C14-C13-C12	3.17	110.35	107.40
2	A	602	TCH	C22-C23-C24	-3.15	106.01	113.04
2	A	601	TCH	C23-C22-C20	-3.12	108.82	114.52
2	C	602	TCH	C14-C8-C9	3.11	113.98	109.71
2	A	601	TCH	C22-C23-C24	-3.11	106.10	113.04
2	B	602	TCH	C9-C10-C5	3.08	112.91	108.58
2	C	602	TCH	C23-C22-C20	-3.07	108.91	114.52
2	A	602	TCH	C18-C13-C12	-3.03	105.98	109.07
2	C	602	TCH	O1S-S26-C26	3.01	110.54	106.92
2	C	601	TCH	C15-C14-C8	2.95	122.46	118.33
2	B	602	TCH	C14-C8-C9	2.94	113.75	109.71
2	A	602	TCH	O3S-S26-C26	2.93	110.50	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	TCH	C22-C23-C24	-2.90	106.57	113.04
2	C	601	TCH	C21-C20-C17	-2.85	108.55	112.92
2	A	601	TCH	C21-C20-C17	-2.79	108.66	112.92
2	C	601	TCH	C23-C24-N24	2.76	121.06	116.42
2	B	602	TCH	C6-C5-C4	-2.76	108.02	111.19
2	B	601	TCH	C22-C23-C24	-2.74	106.91	113.04
2	C	601	TCH	C1-C10-C9	-2.72	107.07	111.35
2	B	601	TCH	O3S-S26-C26	2.70	110.13	105.77
2	B	602	TCH	C1-C10-C9	-2.69	107.12	111.35
2	A	601	TCH	C1-C2-C3	2.69	113.92	110.47
2	A	601	TCH	C1-C10-C5	2.68	111.73	107.77
2	A	602	TCH	C17-C13-C14	2.68	102.79	100.09
2	B	602	TCH	C18-C13-C12	-2.66	106.36	109.07
2	C	602	TCH	C23-C24-N24	2.63	120.85	116.42
2	A	601	TCH	O12-C12-C13	-2.62	106.60	111.03
2	B	602	TCH	C23-C24-N24	2.58	120.76	116.42
2	A	602	TCH	C6-C5-C4	-2.54	108.26	111.19
2	A	601	TCH	C9-C11-C12	-2.54	110.95	114.30
2	C	602	TCH	C18-C13-C14	-2.54	107.24	111.21
2	C	602	TCH	O3S-S26-C26	2.54	109.87	105.77
2	C	602	TCH	C9-C11-C12	-2.53	110.96	114.30
2	A	602	TCH	C23-C24-N24	2.52	120.67	116.42
2	C	601	TCH	O12-C12-C13	-2.51	106.79	111.03
2	B	601	TCH	C17-C13-C14	2.49	102.60	100.09
2	A	601	TCH	C18-C13-C14	-2.49	107.32	111.21
2	A	601	TCH	C19-C10-C9	-2.39	107.88	111.18
2	C	601	TCH	C18-C13-C14	-2.39	107.47	111.21
2	B	602	TCH	O12-C12-C13	-2.37	107.02	111.03
2	B	602	TCH	O2S-S26-C26	2.36	109.76	106.92
2	C	601	TCH	C9-C10-C5	2.36	111.89	108.58
2	B	602	TCH	C21-C20-C17	-2.34	109.34	112.92
2	C	602	TCH	C1-C10-C9	-2.30	107.73	111.35
2	C	602	TCH	C21-C20-C17	-2.29	109.42	112.92
2	C	601	TCH	O3S-S26-C26	2.28	109.46	105.77
2	A	601	TCH	C5-C4-C3	2.26	116.08	112.76
2	B	602	TCH	C18-C13-C14	-2.25	107.69	111.21
2	C	602	TCH	C19-C10-C9	-2.23	108.11	111.18
2	A	601	TCH	O24-C24-N24	-2.23	118.81	123.01
2	A	602	TCH	C11-C12-C13	2.19	113.50	111.24
2	A	601	TCH	C4-C5-C10	2.15	114.94	112.66
2	B	602	TCH	O3S-S26-C26	2.14	109.22	105.77
2	B	601	TCH	O12-C12-C13	-2.13	107.43	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	TCH	C1-C10-C9	-2.12	108.02	111.35
2	B	601	TCH	C23-C24-N24	2.10	119.96	116.42
2	B	602	TCH	C9-C11-C12	-2.09	111.54	114.30
2	B	602	TCH	C19-C10-C9	-2.08	108.31	111.18
2	C	601	TCH	C18-C13-C12	-2.06	106.97	109.07
2	A	602	TCH	C14-C8-C9	2.02	112.48	109.71
2	A	601	TCH	C9-C8-C7	-2.02	109.46	111.88
2	A	601	TCH	O24-C24-C23	-2.02	118.33	122.02

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TCH	C13-C17-C20-C21
2	A	601	TCH	N24-C25-C26-S26
2	A	602	TCH	N24-C25-C26-S26
2	B	601	TCH	N24-C25-C26-S26
2	B	602	TCH	C13-C17-C20-C21
2	B	602	TCH	N24-C25-C26-S26
2	C	601	TCH	C13-C17-C20-C21
2	C	601	TCH	C25-C26-S26-O1S
2	C	601	TCH	C25-C26-S26-O2S
2	C	601	TCH	C25-C26-S26-O3S
2	C	602	TCH	N24-C25-C26-S26
2	C	601	TCH	C16-C17-C20-C21
2	C	601	TCH	C13-C17-C20-C22
2	A	601	TCH	C16-C17-C20-C21
2	B	602	TCH	C16-C17-C20-C21
2	A	601	TCH	C13-C17-C20-C22
2	B	602	TCH	C13-C17-C20-C22
2	A	601	TCH	C23-C24-N24-C25
2	A	602	TCH	C23-C24-N24-C25
2	B	601	TCH	C23-C24-N24-C25
2	B	602	TCH	C23-C24-N24-C25
2	C	601	TCH	C23-C24-N24-C25
2	C	602	TCH	C23-C24-N24-C25
2	A	601	TCH	C16-C17-C20-C22
2	B	602	TCH	C16-C17-C20-C22
2	C	601	TCH	C16-C17-C20-C22
2	C	602	TCH	C13-C17-C20-C21
2	B	602	TCH	C17-C20-C22-C23
2	C	601	TCH	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
2	B	602	TCH	C21-C20-C22-C23
2	C	601	TCH	C21-C20-C22-C23
2	C	602	TCH	C21-C20-C22-C23
2	A	601	TCH	O24-C24-N24-C25
2	A	602	TCH	O24-C24-N24-C25
2	B	601	TCH	O24-C24-N24-C25
2	B	602	TCH	O24-C24-N24-C25
2	C	601	TCH	O24-C24-N24-C25
2	C	602	TCH	O24-C24-N24-C25
2	C	602	TCH	C17-C20-C22-C23
2	B	601	TCH	C13-C17-C20-C21
2	A	601	TCH	C20-C22-C23-C24
2	B	601	TCH	C20-C22-C23-C24
2	B	601	TCH	C13-C17-C20-C22
2	C	602	TCH	C13-C17-C20-C22
2	C	602	TCH	C20-C22-C23-C24
2	A	601	TCH	C21-C20-C22-C23
2	C	602	TCH	C16-C17-C20-C21
2	A	602	TCH	C13-C17-C20-C21
2	B	601	TCH	C16-C17-C20-C21
2	A	601	TCH	C17-C20-C22-C23
2	C	602	TCH	C16-C17-C20-C22
2	A	602	TCH	C13-C17-C20-C22
2	B	601	TCH	C16-C17-C20-C22
2	A	602	TCH	C16-C17-C20-C21
2	B	601	TCH	C21-C20-C22-C23
2	C	602	TCH	C26-C25-N24-C24

There are no ring outliers.

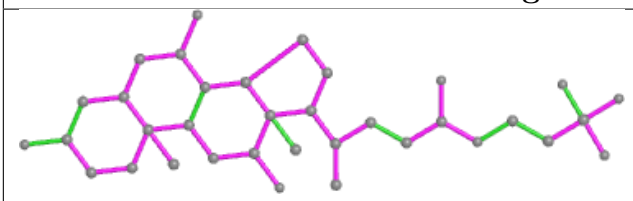
6 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	TCH	12	0
2	A	602	TCH	9	0
2	C	601	TCH	11	0
2	B	601	TCH	12	0
2	A	601	TCH	12	0
2	C	602	TCH	9	0

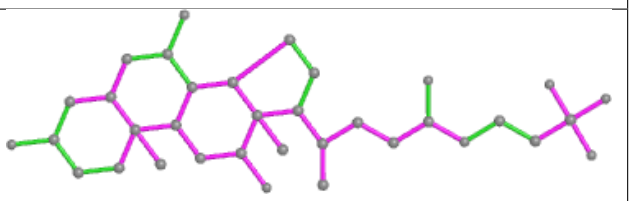
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

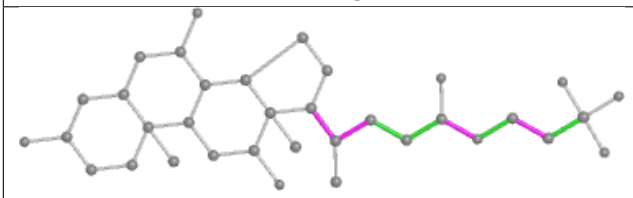
Ligand TCH B 602



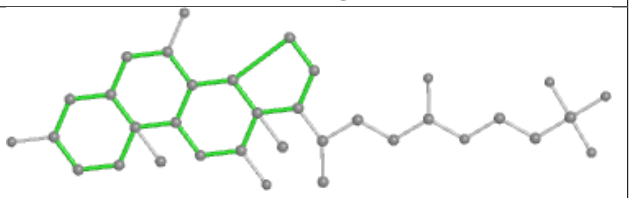
Bond lengths



Bond angles

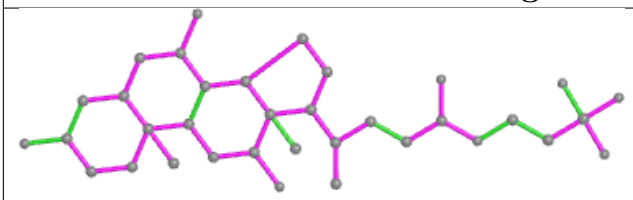


Torsions

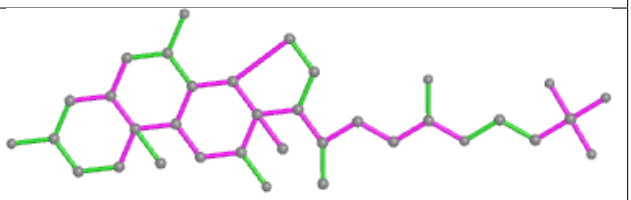


Rings

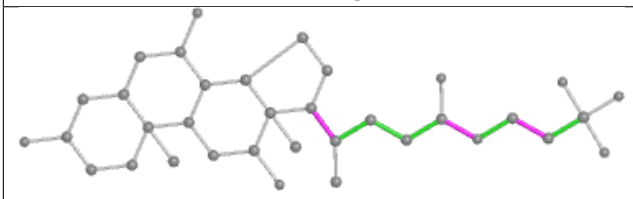
Ligand TCH A 602



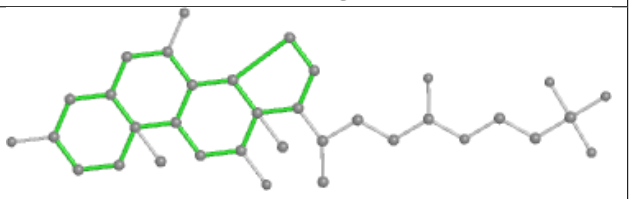
Bond lengths



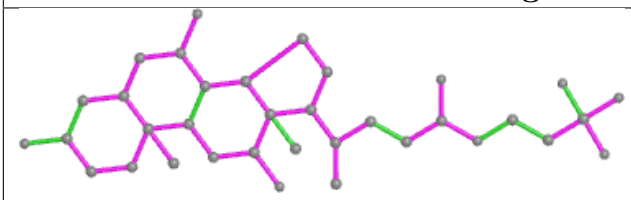
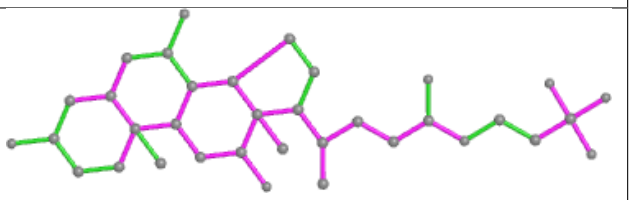
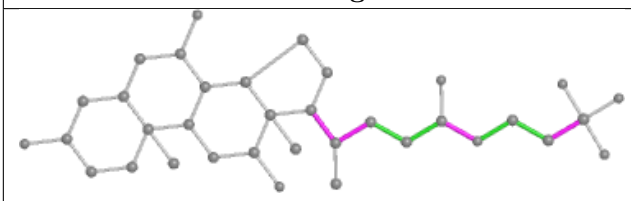
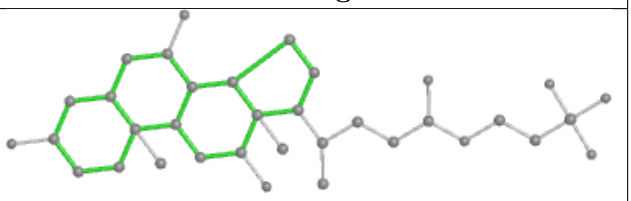
Bond angles

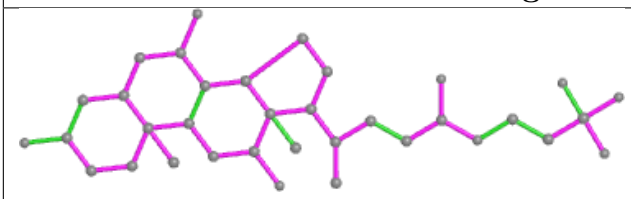
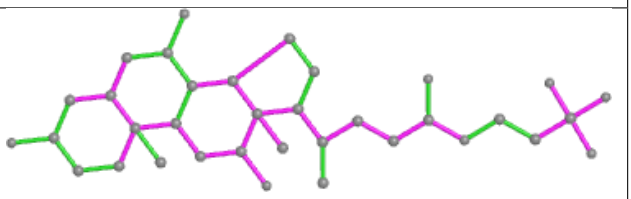
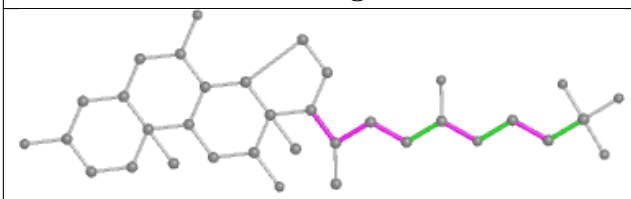
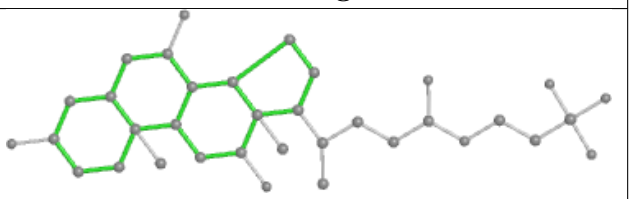


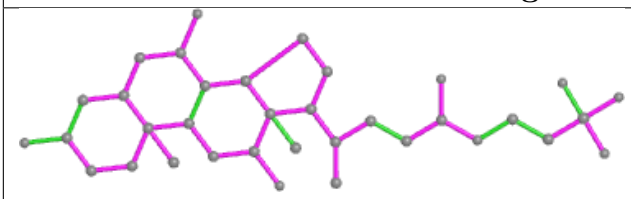
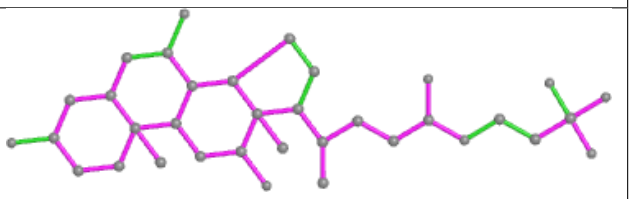
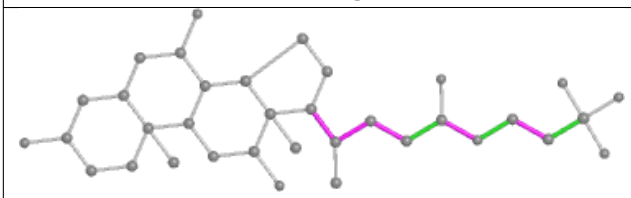
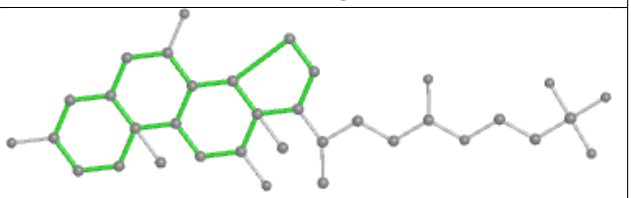
Torsions

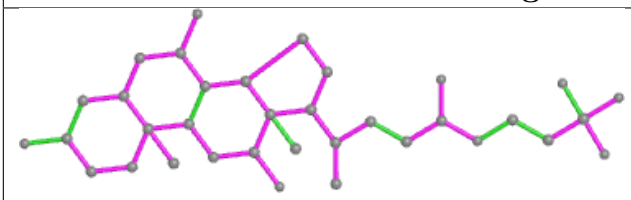
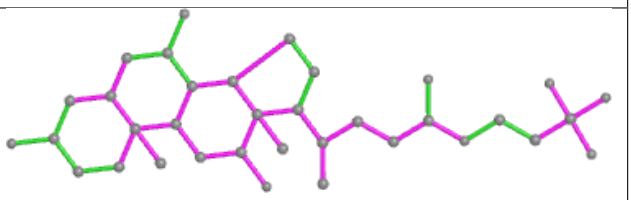
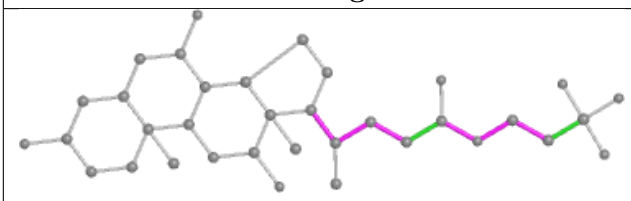
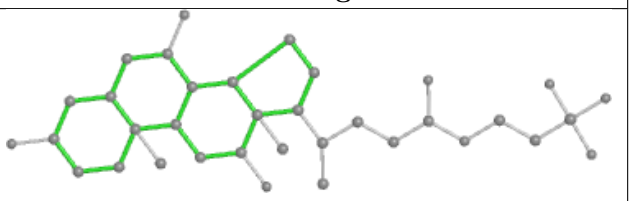


Rings

Ligand TCH C 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TCH B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TCH A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TCH C 602	
 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	296:GLU	C	297:PHE	N	5.74

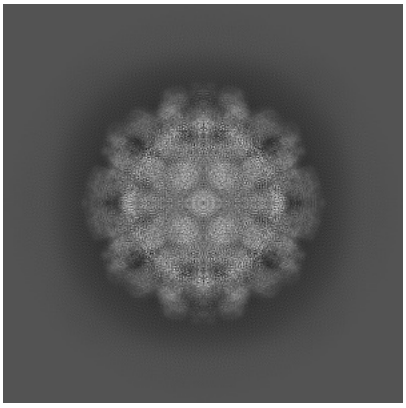
6 Map visualisation (i)

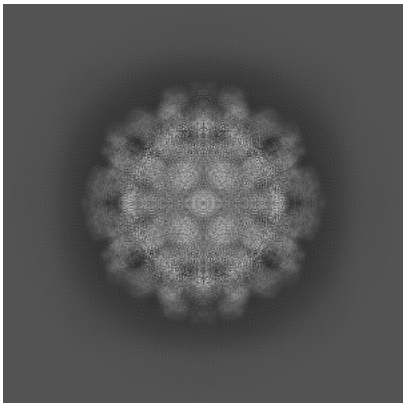
This section contains visualisations of the EMDB entry EMD-20251. These allow visual inspection of the internal detail of the map and identification of artifacts.

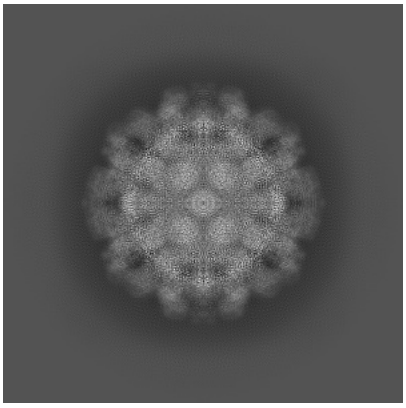
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

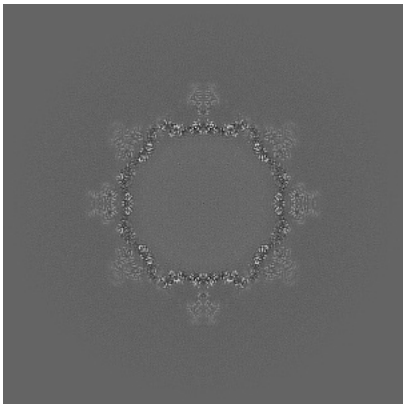

Y

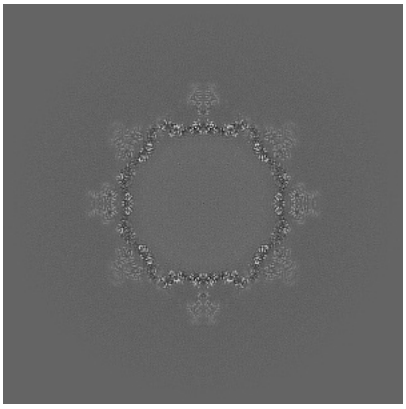

Z

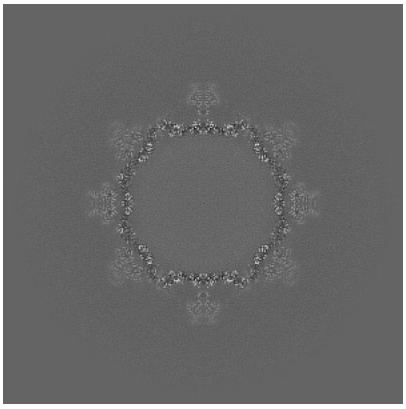
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 270

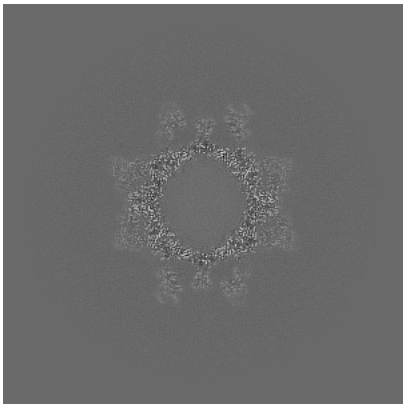

Y Index: 270

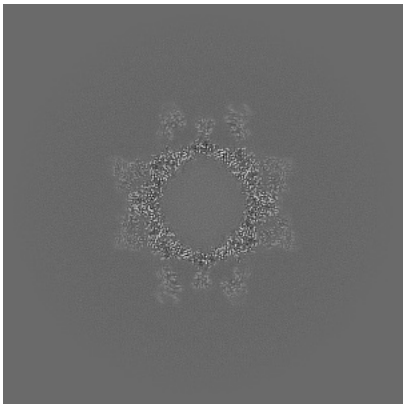

Z Index: 270

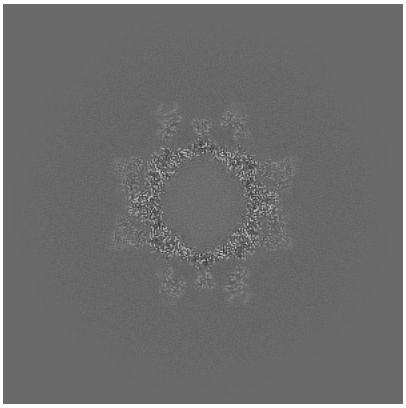
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 345

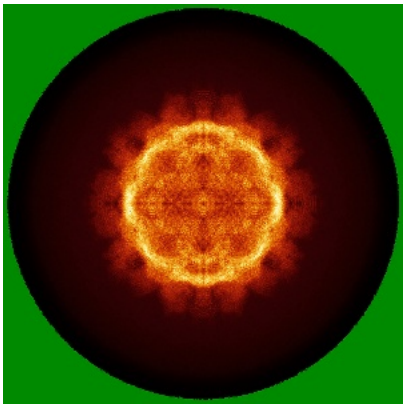

Y Index: 345

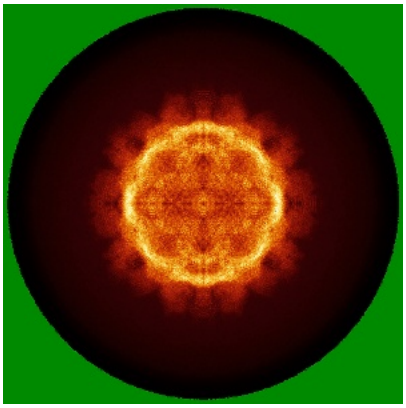

Z Index: 195

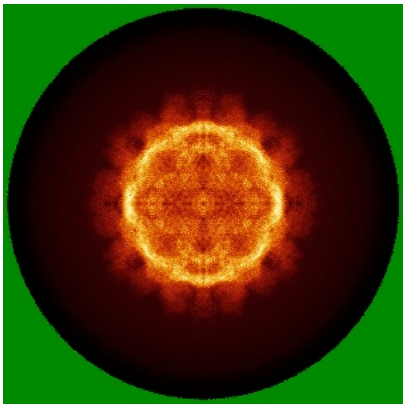
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

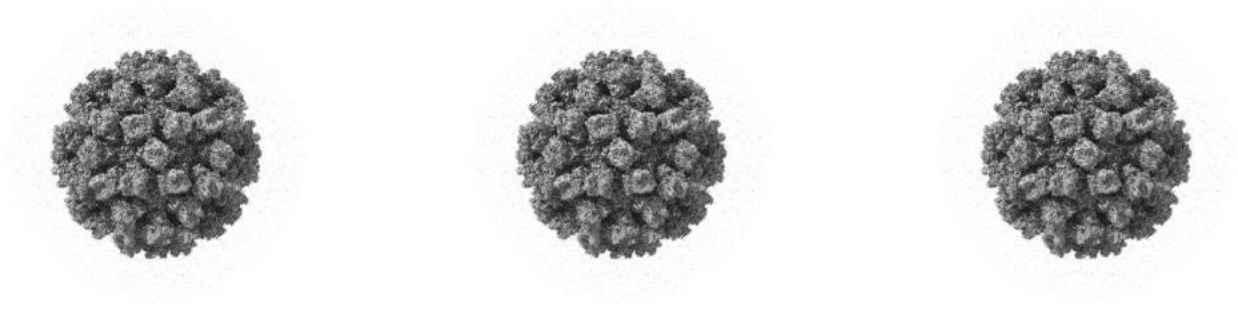

Y


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

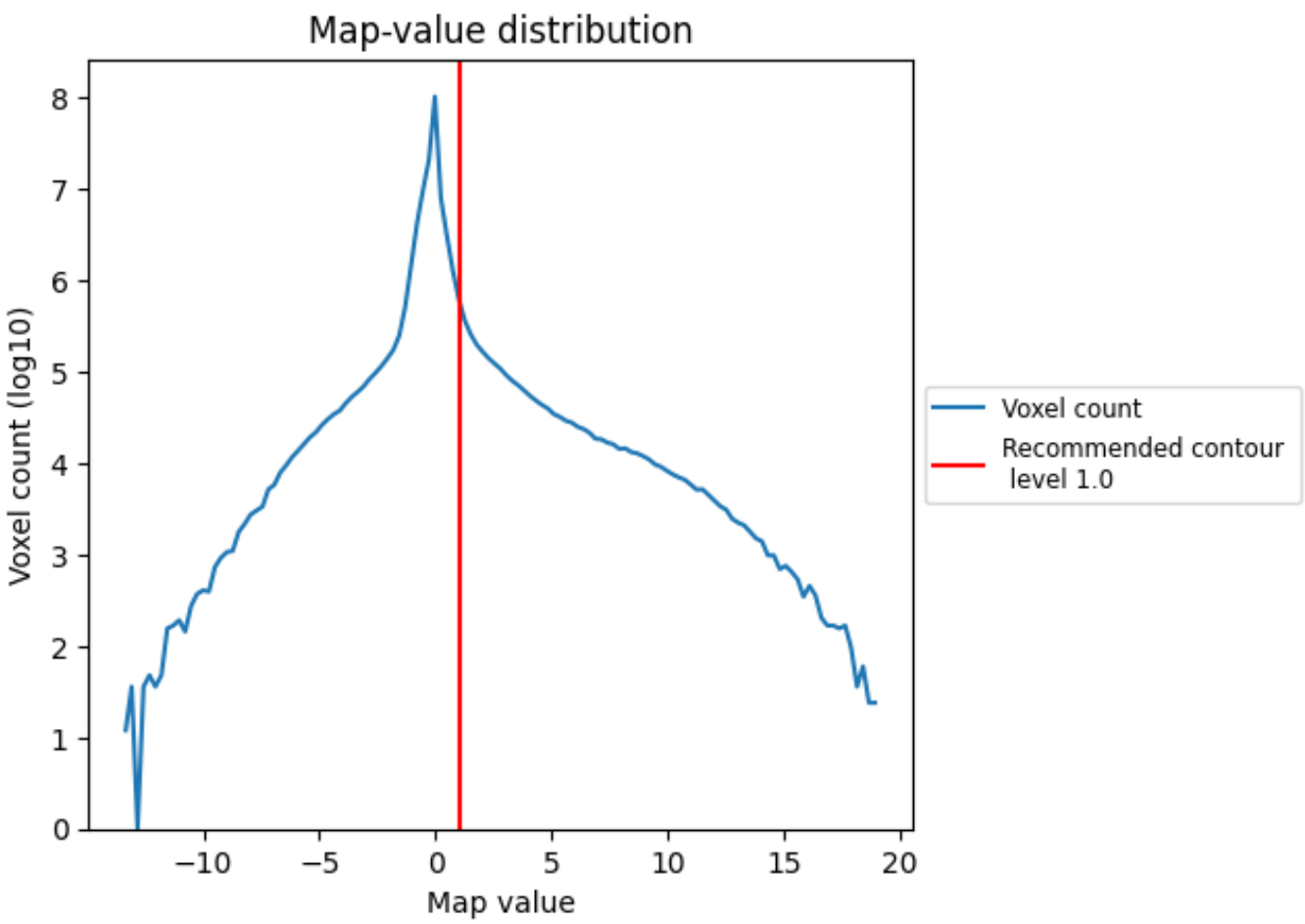
6.6 Mask visualisation (i)

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

7 Map analysis (i)

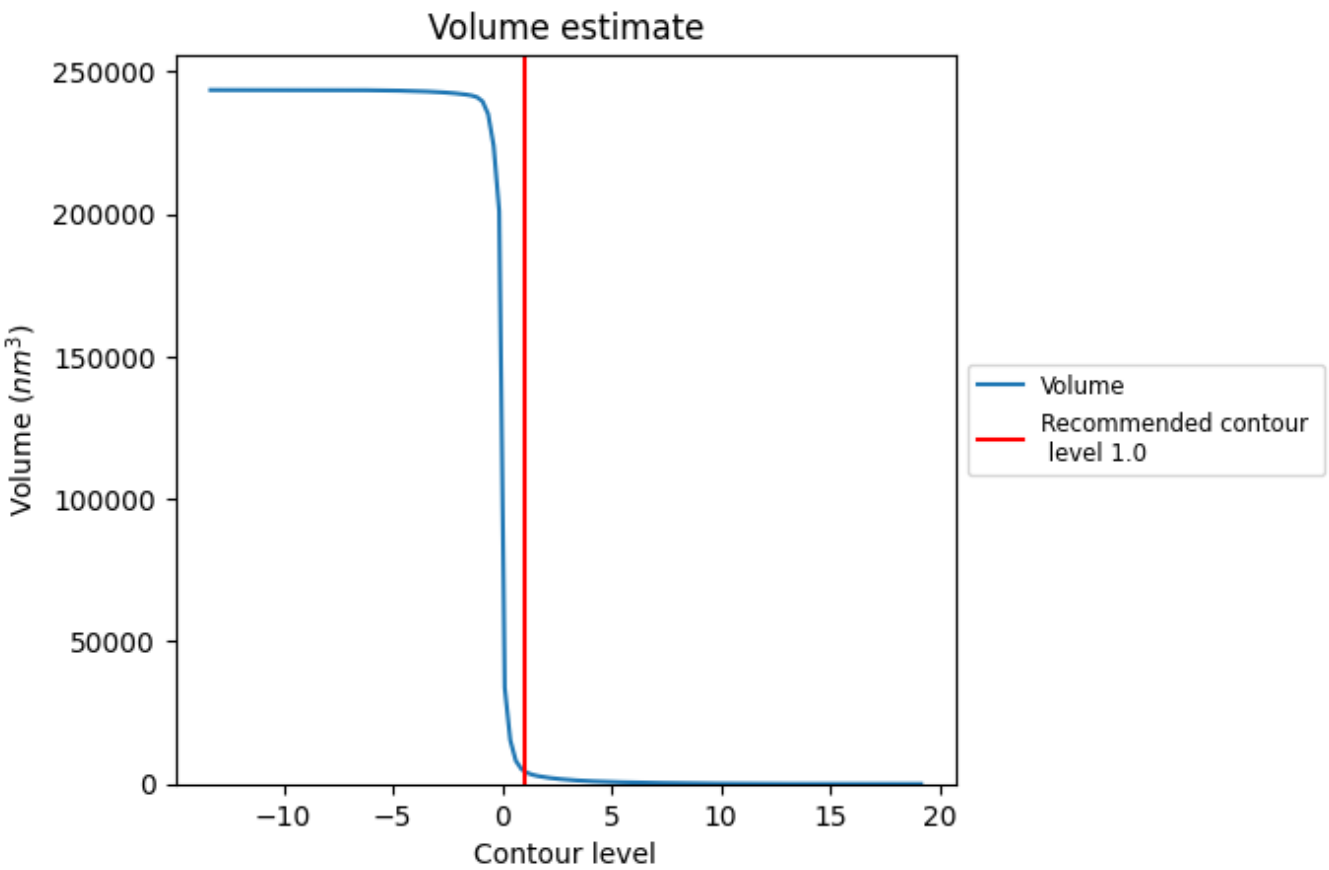
This section contains the results of statistical analysis of the map.

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.

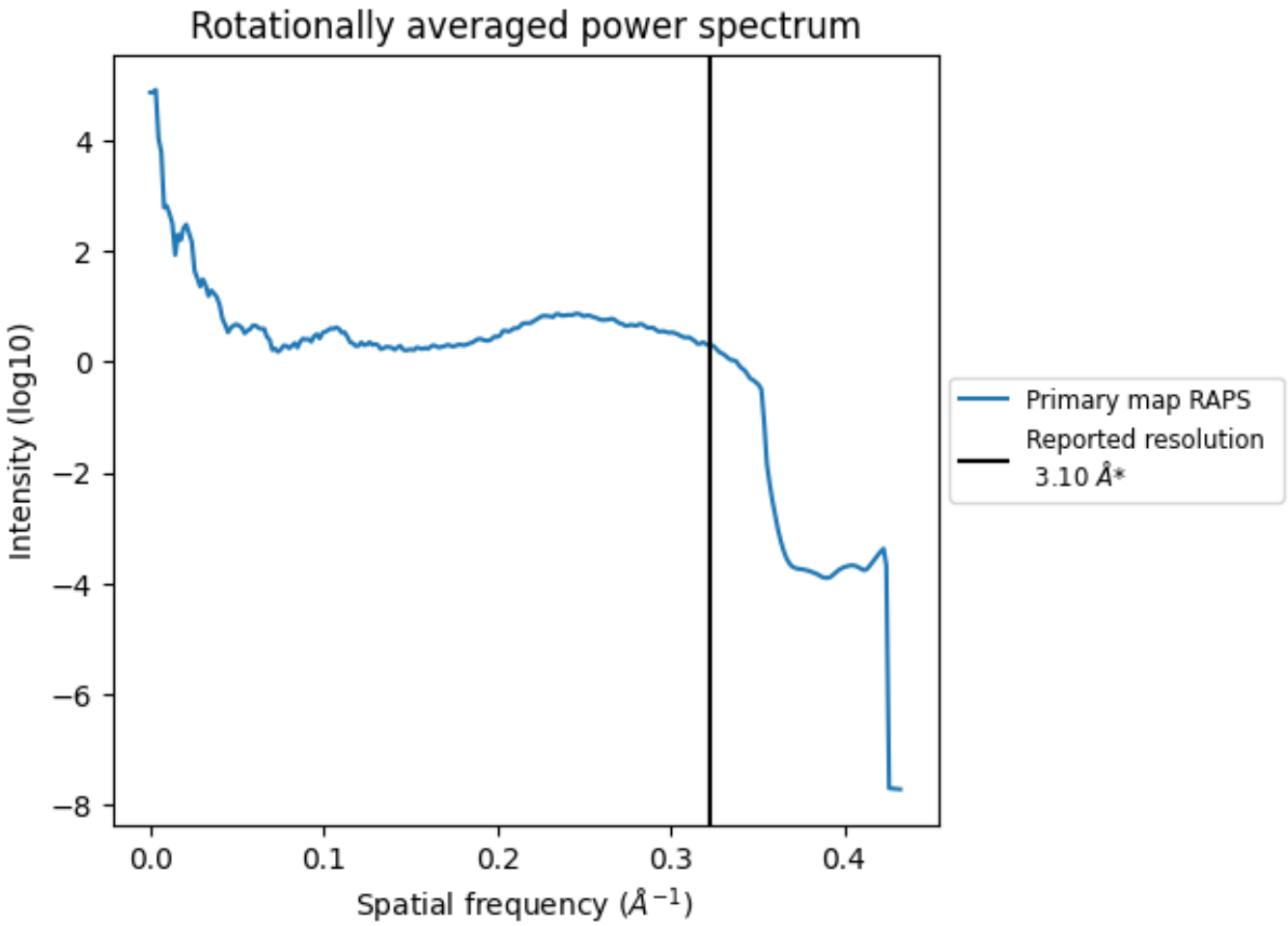
7.2 Volume estimate (i)



The volume at the recommended contour level is 4629 nm^3; this corresponds to an approximate mass of 4181 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)

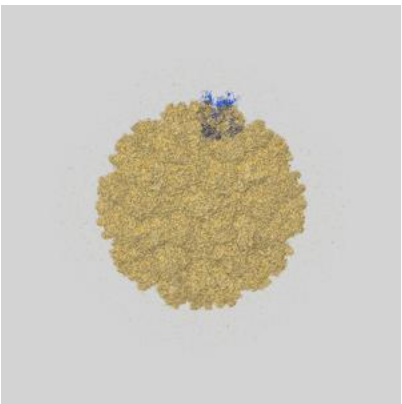
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

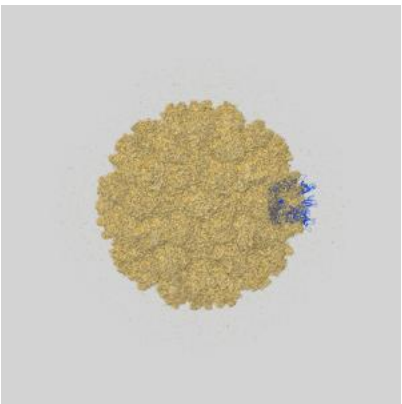
This section contains information regarding the fit between EMDB map EMD-20251 and PDB model 6P4K. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlays

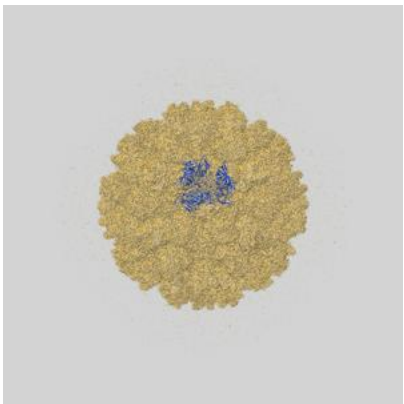
9.1.1 Map-model overlay (i)



X

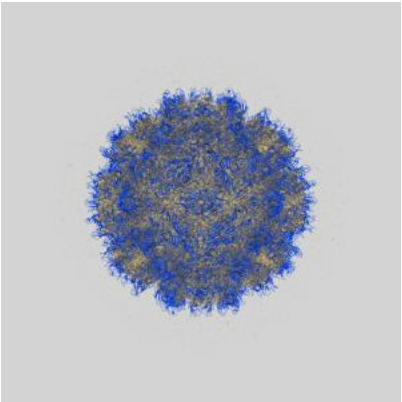


Y

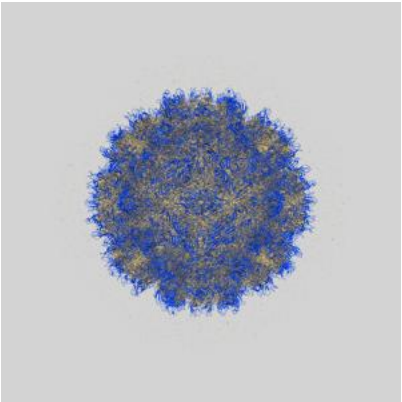


Z

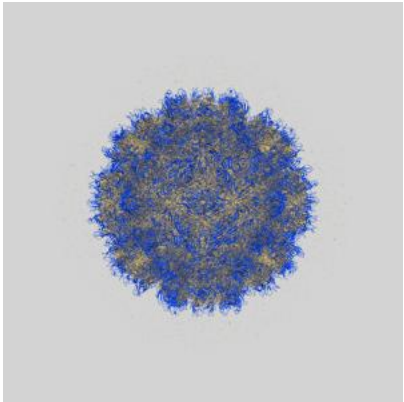
9.1.2 Map-model assembly overlay (i)



X



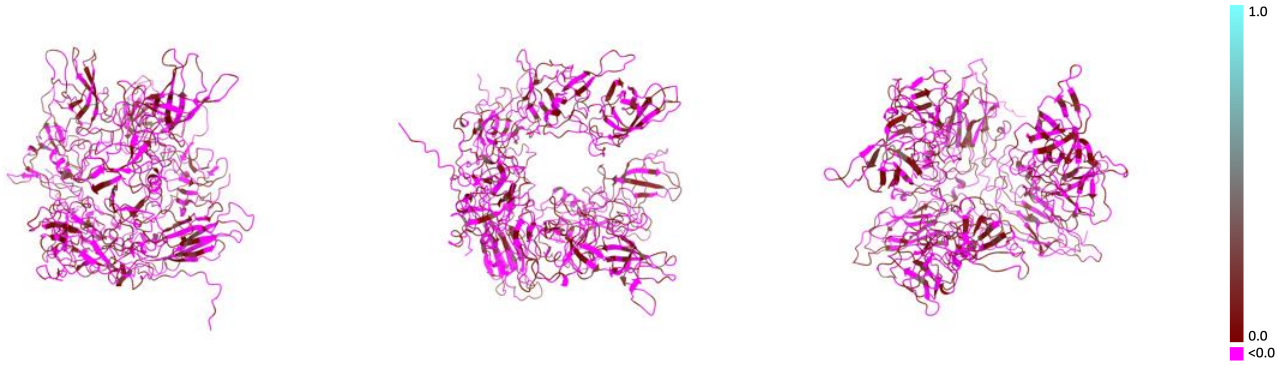
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.0 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.

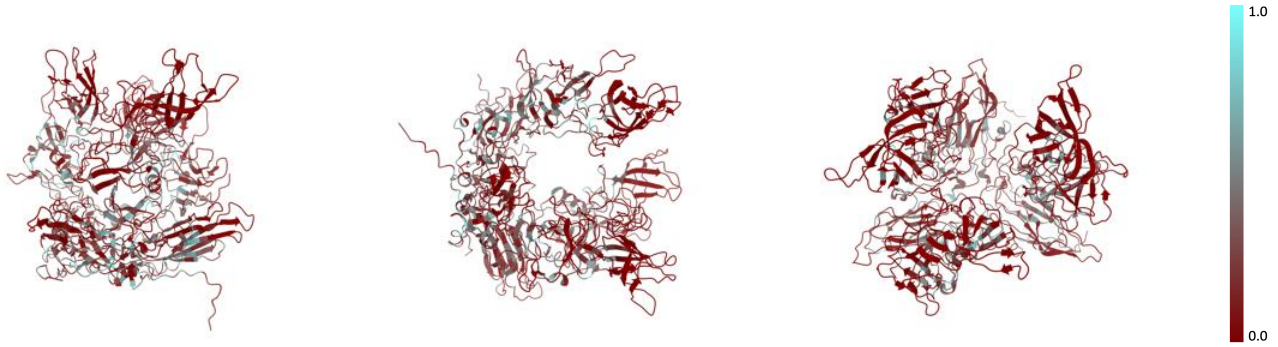
9.2 Q-score mapped to coordinate model (i)



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.

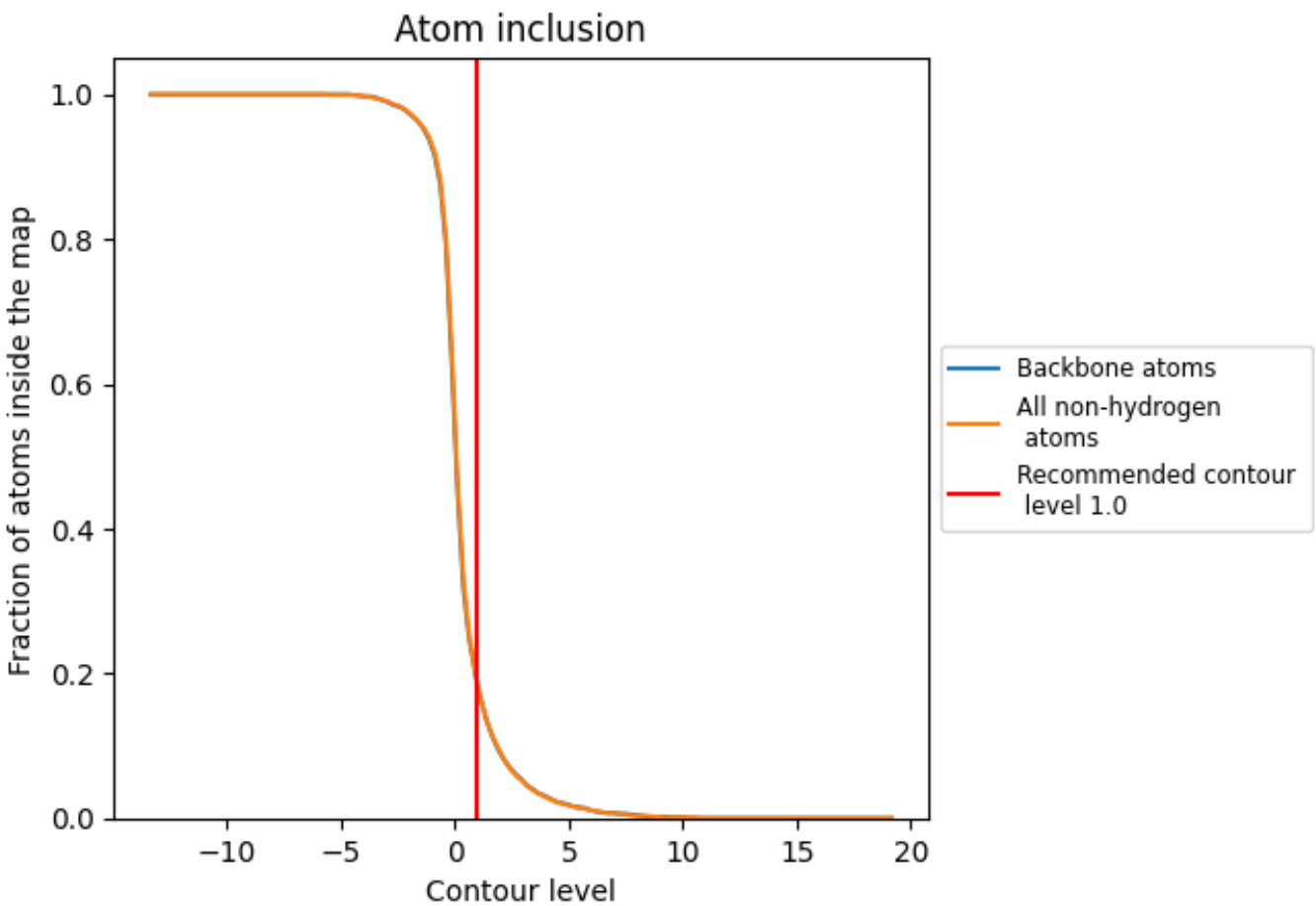
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.0).

9.4 Atom inclusion (i)



At the recommended contour level, 18% of all backbone atoms, 18% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1830	-0.0050
A	0.1790	-0.0030
B	0.1880	-0.0110
C	0.1810	-0.0000