Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 02:33 am BST

PDB ID	:	7P06 / pdb_00007p06
EMDB ID	:	EMD-13145
Title	:	Cryo-EM structure of Pdr5 from Saccharomyces cerevisiae in outward-facing conformation with ADP-orthovanadate/ATP
Authors	:	Szewczak-Harris, A.; Wagner, M.; Du, D.; Schmitt, L.; Luisi, B.F.
Deposited on	:	2021-06-29
Resolution	:	3.77 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 (i)) were used in the production of this report:

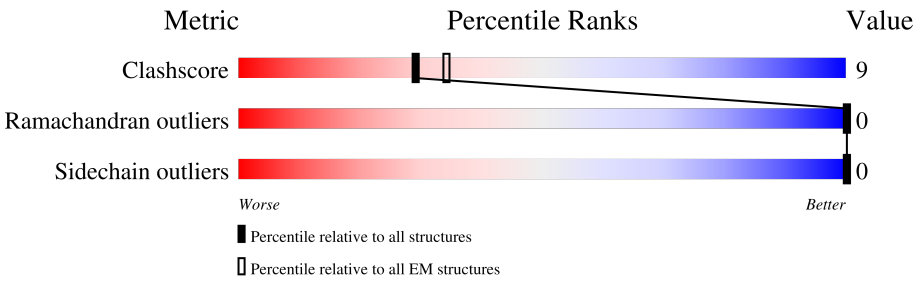
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

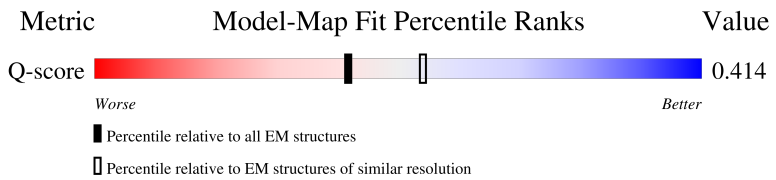
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.77 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10146 (3.27 - 4.27)

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	1511	6% 70% 19% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	AOV	A	1703	X	-	-	-

2 Entry composition (i)

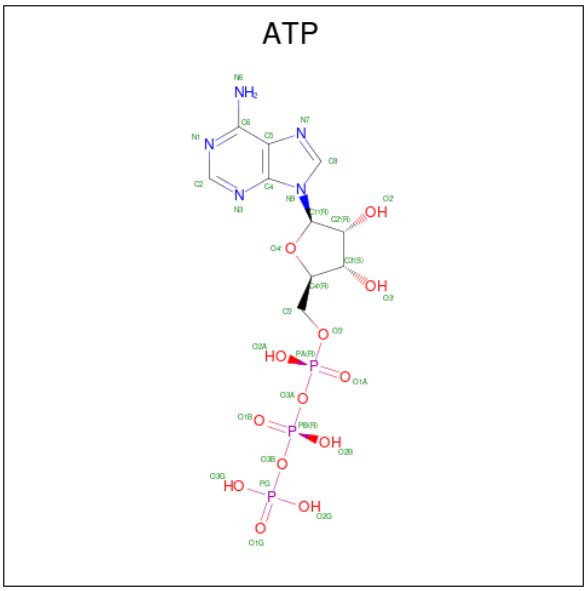
There are 4 unique types of molecules in this entry. The entry contains 21505 atoms, of which 10667 are hydrogens and 0 are deuteriums.

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 Pleiotropic ABC efflux transporter of multiple drugs.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	1350	21412	6978	10638	1781	1948	67	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

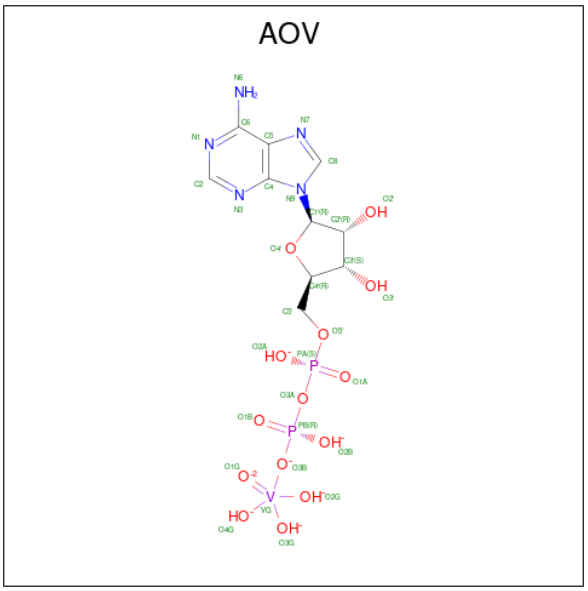


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	A	1	43	10	12	5	13	3	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0

- Molecule 4 is ADP ORTHOVANADATE (CCD ID: AOV) (formula: $C_{10}H_{17}N_5O_{14}P_2V$).



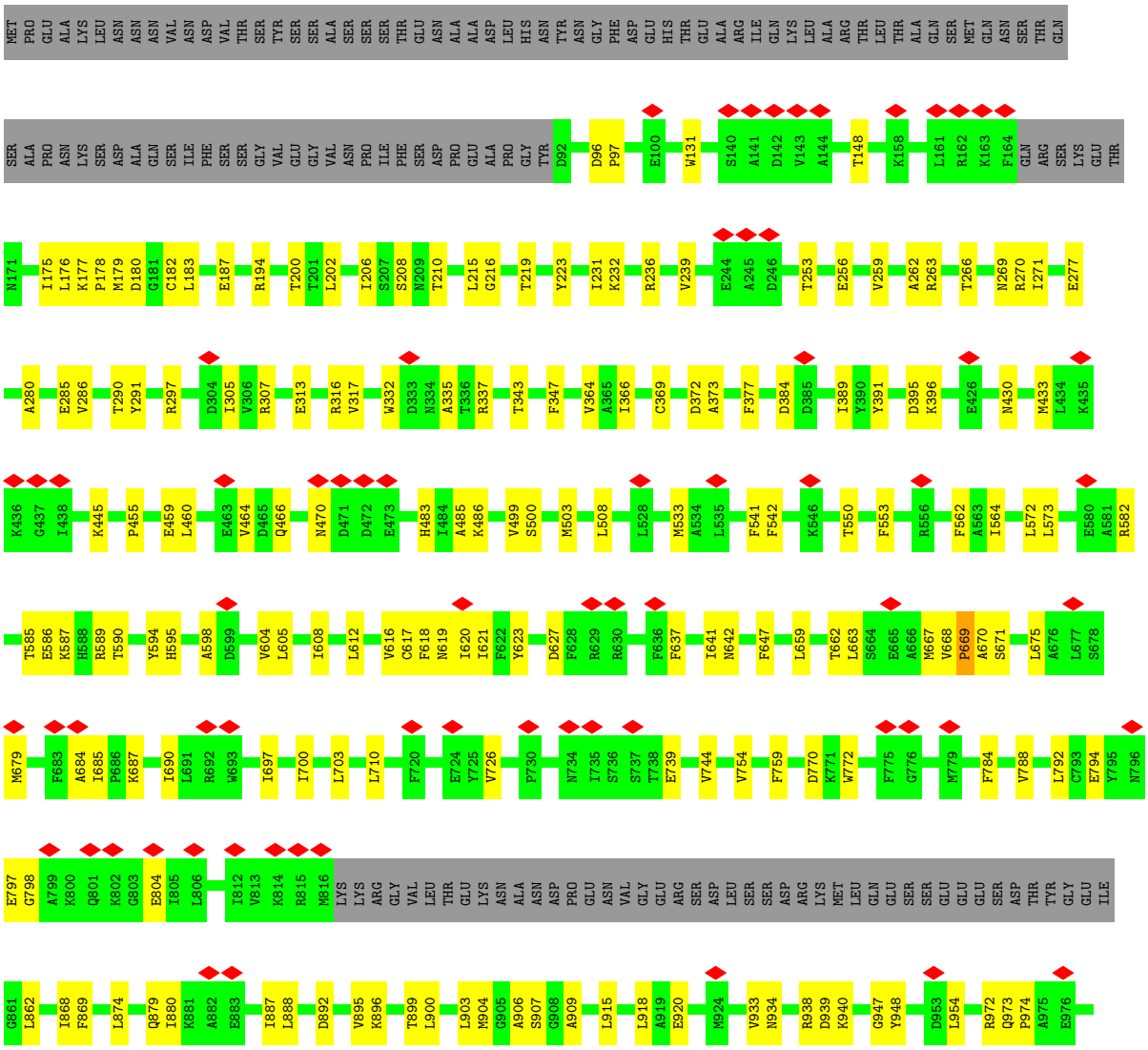
Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	V	
4	A	1	49	10	17	5	14	2	1	0

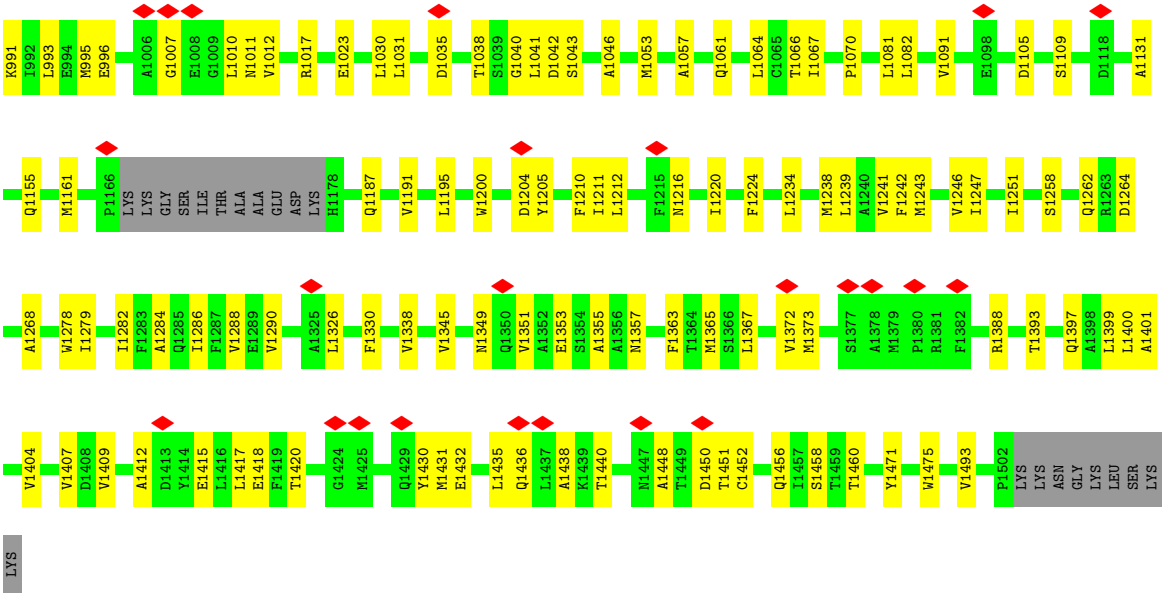
3 Residue-property plots (i)

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: Pleiotropic ABC efflux transporter of multiple drugs

Chain A: 6% 70% 19% 11%




K991
I992
L993
E994
M995
E996
A1006
G1007
E1008
G1009
L1010
N1011
V1012
R1017
E1023
L1030
L1031
D1035
T1038
S1039
G1040
L1041
D1042
S1043
A1046
M1053
A1057
Q1061
L1064
C1065
T1066
I1067
P1070
L1081
L1082
V1091
E1098
D1105
S1109
D1118
A1131
Q1155
M1161
P1166
LYS
LYS
GLY
SER
ILE
THR
ALA
ALA
GLU
ASP
LYS
H1178
Q1187
V1191
L1195
W1200
D1204
Y1205
F1210
I1211
L1212
F1215
N1216
I1220
F1224
L1234
M1238
L1239
A1240
V1241
F1242
M1243
V1246
I1247
I1251
S1258
Q1262
R1263
D1264
A1268
W1278
I1279
I1282
F1283
A1284
Q1285
I1286
F1287
V1288
E1289
V1290
A1325
L1326
F1330
V1338
V1345
N1349
Q1350
V1351
A1352
E1353
S1354
A1355
A1356
N1357
F1363
T1364
M1365
S1366
L1367
V1372
M1373
S1377
A1378
M1379
P1380
R1381
F1382
R1388
T1393
Q1397
A1398
L1399
L1400
A1401
V1404
V1407
D1408
V1409
A1412
D1413
Y1414
E1415
L1416
L1417
E1418
F1419
T1420
G1424
M1425
Q1429
Y1430
M1431
E1432
L1435
Q1436
L1437
A1438
K1439
T1440
N1447
A1448
T1449
D1450
T1451
C1452
Q1456
I1457
S1458
T1459
T1460
Y1471
W1475
V1493
P1502
LYS
LYS
ASN
GLY
LYS
LEU
SER
LYS
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55155	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 ($e^-/Å^2$)	48.13	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.06308	Depositor
Map size (Å)	299.92, 299.92, 299.92	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.652, 0.652, 0.652	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: MG, ATP, AOV

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	0.23	1/11052 (0.0%)	0.39	1/14976 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	LEU	C-N	-6.19	1.24	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	669	PRO	CA-N-CD	-5.94	103.68	112.00

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	10774	10638	10654	198	0
2	A	31	12	12	2	0
3	A	1	0	0	0	0
4	A	32	17	11	3	0
All	All	10838	10667	10677	199	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 9.

All (199) 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:739:GLU:OE2	1:A:1430:TYR:OH	1.85	0.94
1:A:1035:ASP:O	1:A:1066:THR:OG1	1.87	0.91
1:A:939:ASP:OD1	1:A:940:LYS:N	2.04	0.90
1:A:1241:VAL:HG13	1:A:1399:LEU:HD23	1.61	0.81
1:A:263:ARG:NH1	1:A:277:GLU:OE2	2.15	0.80
1:A:208:SER:O	1:A:232:LYS:NZ	2.17	0.78
1:A:909:ALA:O	4:A:1703:AOV:O2B	2.04	0.75
1:A:253:THR:OG1	1:A:256:GLU:OE1	2.02	0.74
1:A:206:ILE:O	1:A:223:TYR:OH	2.06	0.73
1:A:372:ASP:OD1	1:A:373:ALA:N	2.21	0.73
1:A:466:GLN:O	1:A:470:ASN:HB2	1.89	0.72
1:A:659:LEU:CD2	1:A:792:LEU:HD21	2.20	0.71
1:A:231:ILE:O	1:A:236:ARG:N	2.24	0.71
1:A:879:GLN:OE1	1:A:880:ILE:N	2.26	0.69
1:A:972:ARG:NH1	1:A:1023:GLU:OE1	2.24	0.69
1:A:179:MET:HE1	1:A:202:LEU:HD22	1.75	0.69
1:A:1418:GLU:OE2	1:A:1451:THR:OG1	2.11	0.68
1:A:290:THR:HG23	1:A:291:TYR:CD2	2.31	0.66
1:A:675:LEU:HD21	1:A:1220:ILE:HG13	1.78	0.65
1:A:671:SER:OG	1:A:1216:ASN:ND2	2.30	0.65
1:A:96:ASP:OD2	1:A:286:VAL:N	2.29	0.65
1:A:954:LEU:HD13	1:A:1268:ALA:HB1	1.77	0.65
1:A:430:ASN:ND2	1:A:433:MET:SD	2.71	0.64
1:A:1042:ASP:OD1	1:A:1043:SER:N	2.31	0.64
1:A:1286:ILE:O	1:A:1290:VAL:HG23	1.97	0.63
1:A:366:ILE:HD12	1:A:369:CYS:HB3	1.81	0.63
1:A:1238:MET:HA	1:A:1400:LEU:HD11	1.78	0.63
1:A:305:ILE:HD13	1:A:1264:ASP:HB3	1.79	0.63
1:A:991:LYS:NZ	1:A:996:GLU:OE1	2.28	0.62
1:A:1432:GLU:O	1:A:1436:GLN:NE2	2.33	0.62
1:A:804:GLU:OE1	1:A:1010:LEU:N	2.32	0.62
1:A:993:LEU:O	1:A:1017:ARG:NH2	2.33	0.62
1:A:906:ALA:HB2	1:A:1131:ALA:HB1	1.82	0.62
1:A:933:VAL:HG21	1:A:1030:LEU:HD11	1.81	0.61
1:A:675:LEU:HD21	1:A:1220:ILE:CG1	2.30	0.61
1:A:754:VAL:O	1:A:754:VAL:HG13	2.01	0.60
1:A:659:LEU:HD23	1:A:792:LEU:HD21	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1417:LEU:HD21	1:A:1456:GLN:OE1	2.01	0.60
4:A:1703:AOV:VG	4:A:1703:AOV:O1G	1.58	0.60
1:A:595:HIS:ND1	1:A:794:GLU:OE2	2.29	0.60
1:A:148:THR:HG1	1:A:1200:TRP:CD1	2.20	0.60
1:A:1251:ILE:HG23	1:A:1338:VAL:HG11	1.83	0.60
1:A:1345:VAL:O	1:A:1349:ASN:ND2	2.35	0.60
1:A:903:LEU:HD23	1:A:1066:THR:HG22	1.85	0.59
1:A:1242:PHE:CZ	1:A:1367:LEU:HD21	2.38	0.59
1:A:1224:PHE:CZ	1:A:1239:LEU:HD22	2.39	0.58
1:A:562:PHE:HB2	1:A:1373:MET:HE1	1.84	0.58
1:A:364:VAL:HG22	1:A:366:ILE:HG23	1.86	0.57
1:A:668:VAL:HB	1:A:669:PRO:HD2	1.85	0.57
1:A:1234:LEU:CD1	1:A:1404:VAL:HG11	2.35	0.57
1:A:685:ILE:HG23	1:A:685:ILE:O	2.06	0.56
1:A:892:ASP:OD2	1:A:1155:GLN:NE2	2.39	0.56
1:A:1251:ILE:CG2	1:A:1338:VAL:HG11	2.36	0.56
1:A:1241:VAL:HG11	1:A:1400:LEU:HD22	1.85	0.56
1:A:508:LEU:HD21	1:A:594:TYR:CE2	2.41	0.55
1:A:1393:THR:O	1:A:1397:GLN:HG3	2.06	0.55
1:A:920:GLU:OE1	1:A:938:ARG:NH2	2.39	0.55
1:A:572:LEU:HD11	1:A:670:ALA:HB1	1.89	0.55
1:A:1187:GLN:O	1:A:1191:VAL:HG12	2.06	0.55
1:A:266:THR:HG21	1:A:280:ALA:HB2	1.88	0.55
1:A:868:ILE:HG21	1:A:1161:MET:SD	2.47	0.55
1:A:194:ARG:NH1	1:A:1042:ASP:OD2	2.37	0.55
1:A:868:ILE:HG23	1:A:896:LYS:HB3	1.88	0.54
1:A:918:LEU:O	1:A:938:ARG:NH1	2.41	0.54
1:A:1030:LEU:HD23	1:A:1031:LEU:HG	1.90	0.53
1:A:562:PHE:CB	1:A:1373:MET:HE1	2.38	0.53
1:A:262:ALA:O	1:A:266:THR:HG23	2.08	0.53
1:A:933:VAL:O	1:A:933:VAL:HG13	2.08	0.53
1:A:954:LEU:HD13	1:A:1268:ALA:CB	2.39	0.52
1:A:1367:LEU:HD23	1:A:1367:LEU:O	2.09	0.52
1:A:1038:THR:OG1	1:A:1046:ALA:HB1	2.09	0.52
1:A:307:ARG:NH1	4:A:1703:AOV:O2A	2.41	0.52
1:A:96:ASP:OD1	1:A:97:PRO:HD3	2.08	0.52
1:A:1091:VAL:O	1:A:1091:VAL:HG22	2.10	0.52
1:A:641:ILE:HB	1:A:710:LEU:HD21	1.92	0.52
1:A:1038:THR:HA	1:A:1041:LEU:HD21	1.92	0.52
1:A:1345:VAL:HG21	1:A:1355:ALA:O	2.10	0.52
1:A:1191:VAL:HG13	1:A:1284:ALA:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:NH1	1:A:239:VAL:O	2.44	0.51
1:A:216:GLY:O	1:A:219:THR:HG22	2.11	0.51
1:A:904:MET:CE	1:A:1081:LEU:HD13	2.40	0.51
1:A:1409:VAL:HG22	1:A:1458:SER:O	2.11	0.50
1:A:993:LEU:HD23	1:A:995:MET:SD	2.52	0.50
1:A:316:ARG:HD3	1:A:343:THR:HG21	1.94	0.50
1:A:200:THR:HG21	2:A:1701:ATP:O3G	2.12	0.50
1:A:550:THR:CG2	1:A:744:VAL:HG21	2.41	0.50
1:A:269:ASN:ND2	1:A:485:ALA:O	2.45	0.50
1:A:1404:VAL:HG12	1:A:1404:VAL:O	2.11	0.50
1:A:208:SER:O	1:A:236:ARG:NH2	2.46	0.49
1:A:770:ASP:OD1	1:A:772:TRP:N	2.44	0.49
1:A:1431:MET:O	1:A:1435:LEU:HD23	2.13	0.49
1:A:384:ASP:HB2	1:A:389:ILE:HD11	1.95	0.49
1:A:1438:ALA:HB1	1:A:1440:THR:HG22	1.94	0.48
1:A:395:ASP:C	1:A:395:ASP:OD1	2.56	0.48
1:A:582:ARG:NH1	1:A:797:GLU:OE2	2.46	0.48
1:A:604:VAL:O	1:A:608:ILE:HG13	2.14	0.48
1:A:210:THR:HG21	1:A:215:LEU:HD11	1.95	0.48
1:A:483:HIS:O	1:A:486:LYS:N	2.43	0.48
1:A:533:MET:HE1	1:A:1365:MET:HG2	1.96	0.48
1:A:175:ILE:HD13	2:A:1701:ATP:O4'	2.13	0.48
1:A:903:LEU:CD1	1:A:1082:LEU:HD22	2.44	0.47
1:A:445:LYS:O	1:A:445:LYS:HD2	2.14	0.47
1:A:285:GLU:OE1	1:A:297:ARG:NH1	2.47	0.47
1:A:1278:TRP:CE2	1:A:1279:ILE:HG23	2.50	0.47
1:A:1258:SER:O	1:A:1262:GLN:OE1	2.32	0.47
1:A:562:PHE:CG	1:A:1373:MET:HE1	2.49	0.47
1:A:868:ILE:N	1:A:934:ASN:OD1	2.47	0.47
1:A:182:CYS:O	1:A:391:TYR:OH	2.29	0.47
1:A:1372:VAL:O	1:A:1372:VAL:HG22	2.15	0.47
1:A:564:ILE:CG2	1:A:703:LEU:HD12	2.45	0.47
1:A:868:ILE:HG22	1:A:869:PHE:N	2.28	0.47
1:A:1041:LEU:HD23	1:A:1041:LEU:H	1.80	0.47
1:A:1067:ILE:HG21	1:A:1070:PRO:HB3	1.97	0.46
1:A:605:LEU:HA	1:A:608:ILE:HD12	1.97	0.46
1:A:1415:GLU:N	1:A:1415:GLU:OE1	2.48	0.46
1:A:1401:ALA:HB1	1:A:1471:TYR:HA	1.98	0.46
1:A:915:LEU:HB3	1:A:948:TYR:HE1	1.80	0.46
1:A:1412:ALA:HB3	1:A:1415:GLU:OE1	2.16	0.46
1:A:1239:LEU:O	1:A:1243:MET:N	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:PHE:CZ	1:A:1367:LEU:HD12	2.51	0.46
1:A:183:LEU:HD11	1:A:187:GLU:O	2.16	0.45
1:A:553:PHE:CD1	1:A:759:PHE:CD2	3.05	0.45
1:A:499:VAL:HG22	1:A:503:MET:HB2	1.98	0.45
1:A:1326:LEU:HD11	1:A:1330:PHE:CE2	2.52	0.45
1:A:460:LEU:O	1:A:464:VAL:HG23	2.17	0.44
1:A:1212:LEU:HD21	1:A:1247:ILE:HD11	1.99	0.44
1:A:895:VAL:O	1:A:895:VAL:HG13	2.17	0.44
1:A:270:ARG:O	1:A:271:ILE:C	2.59	0.44
1:A:332:TRP:HB2	1:A:364:VAL:HG23	1.99	0.44
1:A:1407:VAL:O	1:A:1460:THR:OG1	2.26	0.44
1:A:900:LEU:HD12	1:A:1057:ALA:HB2	1.99	0.44
1:A:1326:LEU:HD11	1:A:1330:PHE:HE2	1.83	0.44
1:A:684:ALA:HB1	1:A:1239:LEU:HD11	1.99	0.44
1:A:1105:ASP:O	1:A:1109:SER:OG	2.22	0.44
1:A:617:CYS:SG	1:A:618:PHE:N	2.90	0.44
1:A:675:LEU:HD22	1:A:1216:ASN:CG	2.43	0.44
1:A:131:TRP:NE1	1:A:180:ASP:O	2.50	0.43
1:A:256:GLU:HA	1:A:259:VAL:HG12	1.99	0.43
1:A:573:LEU:HD11	1:A:1357:ASN:HA	1.99	0.43
1:A:899:THR:HG22	1:A:900:LEU:N	2.33	0.43
1:A:900:LEU:HD11	1:A:1053:MET:HB3	1.99	0.43
1:A:1204:ASP:OD1	1:A:1205:TYR:N	2.52	0.43
1:A:1195:LEU:HB3	1:A:1288:VAL:HG21	2.00	0.43
1:A:616:VAL:O	1:A:620:ILE:HG22	2.18	0.43
1:A:608:ILE:HG22	1:A:612:LEU:HD13	1.99	0.43
1:A:177:LYS:O	1:A:178:PRO:C	2.61	0.43
1:A:662:THR:HG22	1:A:663:LEU:N	2.32	0.43
1:A:623:TYR:CD2	1:A:627:ASP:HB2	2.53	0.43
1:A:659:LEU:HD21	1:A:792:LEU:HD21	1.96	0.43
1:A:1038:THR:OG1	1:A:1046:ALA:CB	2.66	0.43
1:A:337:ARG:HG3	1:A:1040:GLY:HA3	2.01	0.42
1:A:564:ILE:HG21	1:A:703:LEU:HD12	2.01	0.42
1:A:868:ILE:HG23	1:A:896:LYS:CB	2.48	0.42
1:A:96:ASP:N	1:A:97:PRO:CD	2.82	0.42
1:A:384:ASP:CB	1:A:389:ILE:HD11	2.49	0.42
1:A:500:SER:HB2	1:A:503:MET:HE3	2.01	0.42
1:A:1243:MET:O	1:A:1246:VAL:HG12	2.19	0.42
1:A:1351:VAL:HG12	1:A:1353:GLU:H	1.84	0.42
1:A:1448:ALA:HB3	1:A:1452:CYS:SG	2.59	0.42
1:A:619:ASN:ND2	1:A:642:ASN:OD1	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:LEU:O	1:A:1064:LEU:HD23	2.19	0.42
1:A:313:GLU:O	1:A:317:VAL:HG23	2.20	0.42
1:A:637:PHE:O	1:A:641:ILE:HG12	2.19	0.42
1:A:1388:ARG:O	1:A:1388:ARG:HD3	2.19	0.42
1:A:586:GLU:OE2	1:A:589:ARG:NH2	2.52	0.42
1:A:947:GLY:HA2	1:A:1023:GLU:OE2	2.20	0.42
1:A:973:GLN:HG2	1:A:974:PRO:HD2	2.02	0.42
1:A:1210:PHE:O	1:A:1211:ILE:C	2.61	0.42
1:A:687:LYS:O	1:A:690:ILE:HG12	2.19	0.42
1:A:697:ILE:HD13	1:A:700:ILE:HD11	2.01	0.42
1:A:874:LEU:C	1:A:874:LEU:HD23	2.45	0.42
1:A:1367:LEU:HD23	1:A:1367:LEU:C	2.45	0.42
1:A:455:PRO:O	1:A:459:GLU:OE1	2.38	0.41
1:A:1030:LEU:CD2	1:A:1031:LEU:HG	2.50	0.41
1:A:620:ILE:HG23	1:A:621:ILE:N	2.34	0.41
1:A:726:VAL:HG21	1:A:1417:LEU:CD1	2.50	0.41
1:A:1195:LEU:HG	1:A:1288:VAL:HG11	2.02	0.41
1:A:587:LYS:O	1:A:590:THR:OG1	2.30	0.41
1:A:784:PHE:O	1:A:788:VAL:HG23	2.21	0.41
1:A:862:LEU:HD23	1:A:1061:GLN:HE22	1.85	0.41
1:A:582:ARG:O	1:A:585:THR:HG22	2.21	0.41
1:A:804:GLU:OE2	1:A:1007:GLY:CA	2.69	0.41
1:A:1011:ASN:OD1	1:A:1012:VAL:N	2.54	0.41
1:A:1326:LEU:HD13	1:A:1475:TRP:CZ3	2.56	0.41
1:A:182:CYS:HB3	1:A:464:VAL:HG22	2.02	0.41
1:A:395:ASP:OD1	1:A:396:LYS:N	2.53	0.41
1:A:286:VAL:O	1:A:290:THR:HG22	2.21	0.41
1:A:316:ARG:NH1	1:A:907:SER:OG	2.48	0.41
1:A:335:ALA:HB1	1:A:347:PHE:CE2	2.56	0.41
1:A:366:ILE:HD11	1:A:377:PHE:CE2	2.56	0.41
1:A:595:HIS:O	1:A:598:ALA:HB3	2.21	0.41
1:A:1420:THR:HG23	1:A:1450:ASP:O	2.21	0.41
1:A:612:LEU:HD11	1:A:647:PHE:HZ	1.86	0.40
1:A:675:LEU:HG	1:A:679:MET:HE2	2.02	0.40
1:A:667:MET:HA	1:A:670:ALA:HB3	2.02	0.40
1:A:887:ILE:C	1:A:888:LEU:HD22	2.46	0.40
1:A:541:PHE:O	1:A:542:PHE:C	2.64	0.40
1:A:797:GLU:OE1	1:A:798:GLY:N	2.44	0.40
1:A:1282:ILE:HG21	1:A:1493:VAL:HG22	2.04	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	1342/1511 (89%)	1268 (94%)	74 (6%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1157/1297 (89%)	1157 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	248	HIS
1	A	518	ASN
1	A	1085	GLN
1	A	1178	HIS
1	A	1216	ASN
1	A	1313	ASN
1	A	1319	GLN
1	A	1436	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ATP	A	1701	-	29,33,33	1.29	5 (17%)	44,52,52	2.08	11 (25%)
4	AOV	A	1703	3	30,34,34	0.88	0	39,56,56	2.46	11 (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	ATP	A	1701	-	-	6/22/38/38	0/3/3/3
4	AOV	A	1703	3	1/1/7/7	5/16/39/39	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	ATP	C5-C4	3.96	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701	ATP	C5-N7	-2.46	1.34	1.39
2	A	1701	ATP	C8-N7	2.46	1.36	1.31
2	A	1701	ATP	C5-C6	2.37	1.47	1.41
2	A	1701	ATP	C4-N9	-2.10	1.33	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1703	AOV	O4'-C1'-N9	8.10	124.01	108.06
2	A	1701	ATP	C5-C4-N3	-5.92	119.02	126.75
4	A	1703	AOV	C5-C4-N3	-5.89	119.07	126.75
4	A	1703	AOV	N3-C4-N9	4.94	135.23	127.08
2	A	1701	ATP	PA-O3A-PB	-4.72	116.64	132.83
2	A	1701	ATP	N3-C4-N9	4.43	134.38	127.08
4	A	1703	AOV	C2'-C1'-N9	4.14	123.79	113.30
4	A	1703	AOV	C5-N7-C8	3.99	109.18	103.51
2	A	1701	ATP	C2-N3-C4	3.94	121.06	111.75
4	A	1703	AOV	N3-C2-N1	-3.85	122.58	128.60
2	A	1701	ATP	PB-O3B-PG	-3.77	119.88	132.83
4	A	1703	AOV	C2-N3-C4	3.70	120.48	111.75
2	A	1701	ATP	N3-C2-N1	-3.54	123.07	128.60
2	A	1701	ATP	C4-C5-N7	-3.33	106.57	110.62
4	A	1703	AOV	N9-C8-N7	-2.93	109.91	113.91
2	A	1701	ATP	C5-N7-C8	2.89	107.61	103.51
2	A	1701	ATP	C4-N9-C8	2.73	108.69	105.73
4	A	1703	AOV	C4-C5-N7	-2.52	107.55	110.62
2	A	1701	ATP	N9-C8-N7	-2.47	110.53	113.91
2	A	1701	ATP	C6-C5-N7	2.30	136.31	132.02
4	A	1703	AOV	C4'-O4'-C1'	-2.22	104.58	109.47
4	A	1703	AOV	O4'-C4'-C3'	2.17	109.41	105.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1703	AOV	C1'

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1701	ATP	C5'-O5'-PA-O1A
2	A	1701	ATP	C5'-O5'-PA-O2A
4	A	1703	AOV	C5'-O5'-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1703	AOV	C5'-O5'-PA-O2A
4	A	1703	AOV	O4'-C1'-N9-C8
4	A	1703	AOV	O4'-C1'-N9-C4
2	A	1701	ATP	PG-O3B-PB-O2B
2	A	1701	ATP	C5'-O5'-PA-O3A
4	A	1703	AOV	C5'-O5'-PA-O3A
2	A	1701	ATP	PG-O3B-PB-O1B
2	A	1701	ATP	PB-O3A-PA-O1A

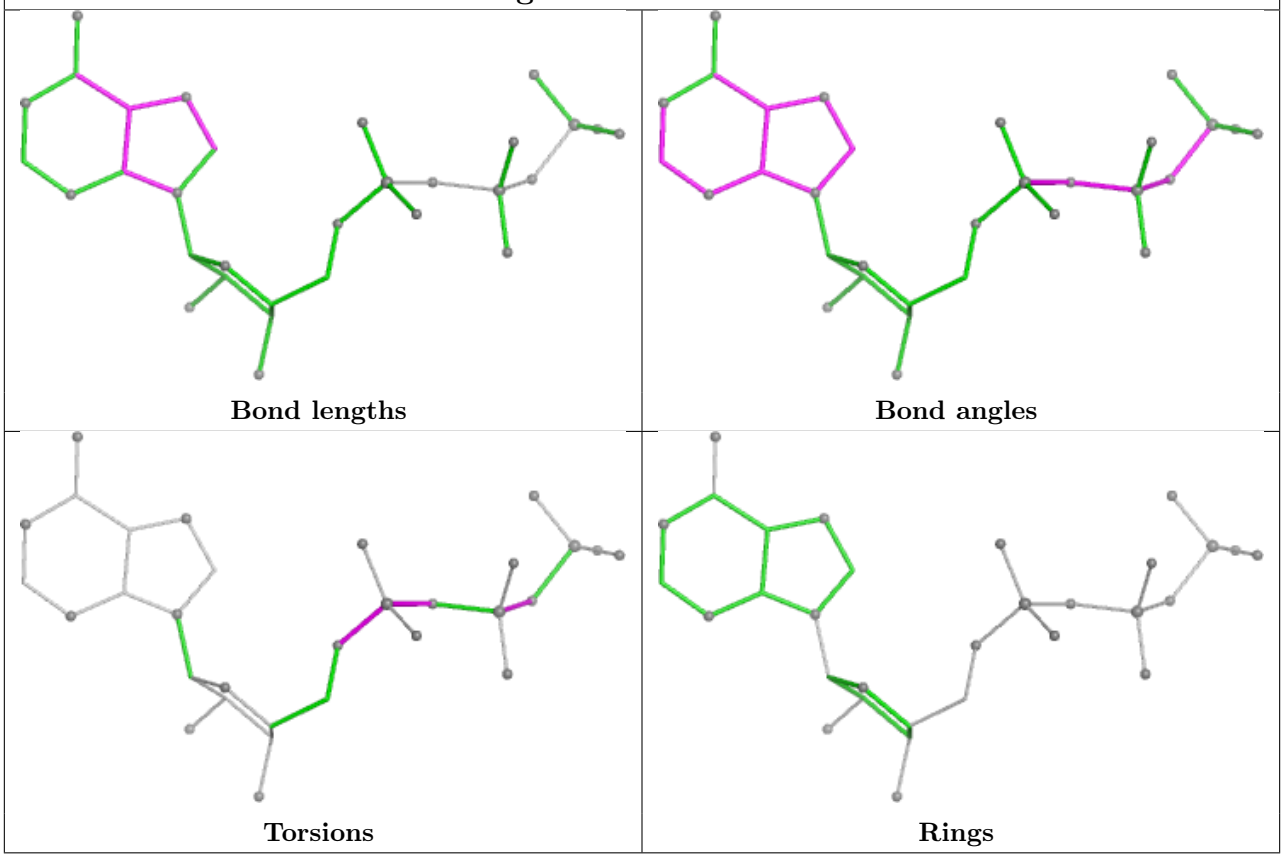
There are no ring outliers.

2 monomers are involved in 5 short contacts:

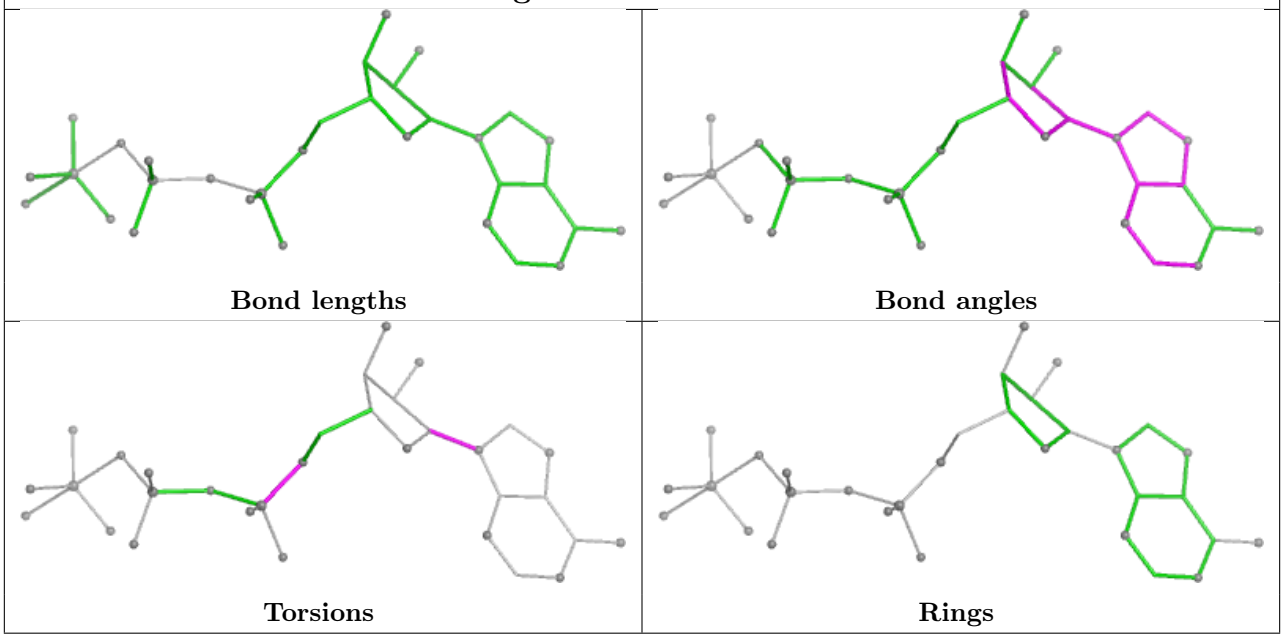
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1701	ATP	2	0
4	A	1703	AOV	3	0

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

Ligand ATP A 1701



Ligand AOV A 1703



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.

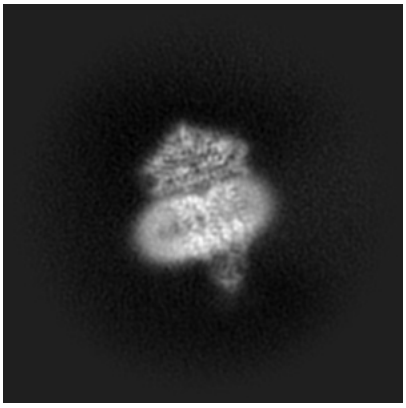
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13145. These allow visual inspection of the internal detail of the map and identification of artifacts.

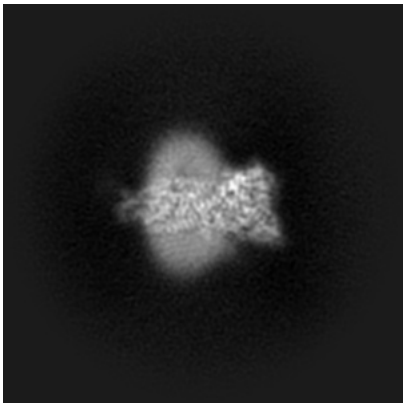
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

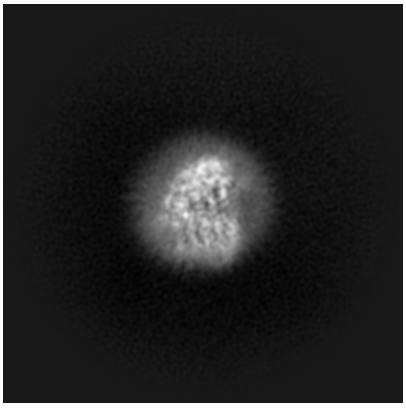
6.1.1 Primary map



X



Y

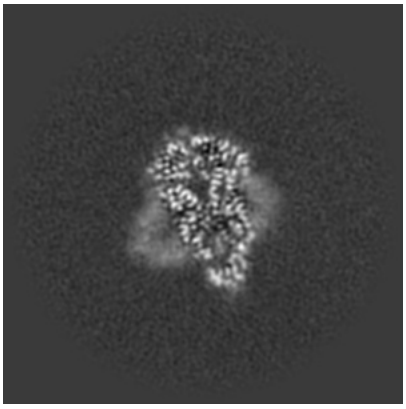


Z

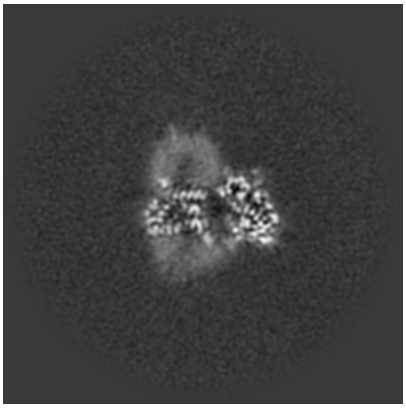
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

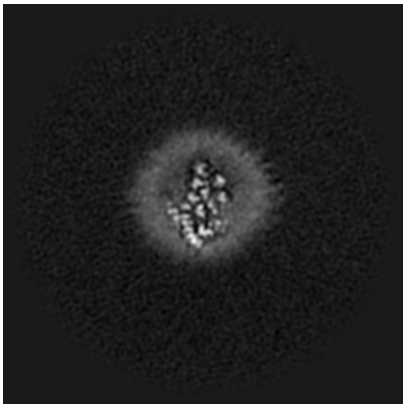
6.2.1 Primary map



X Index: 230



Y Index: 230

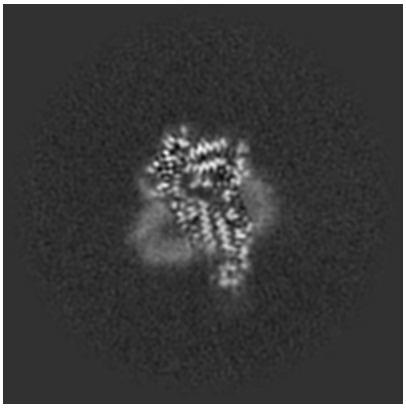


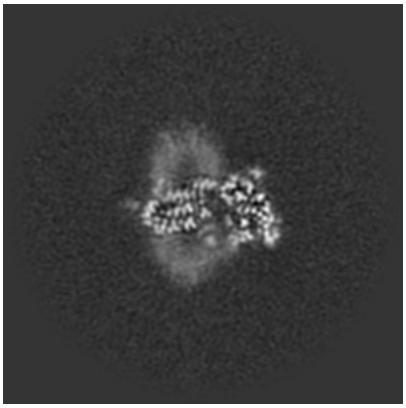
Z Index: 230

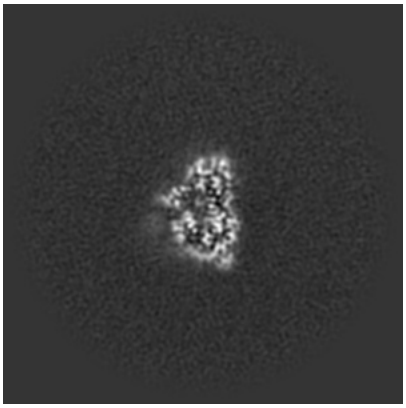
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 239

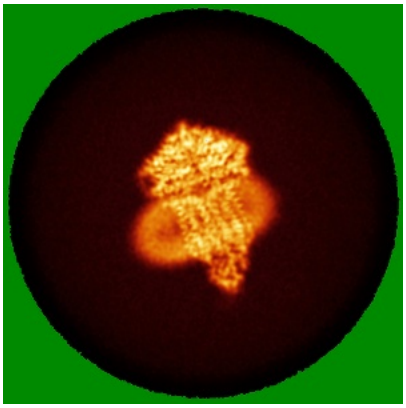

Y Index: 235

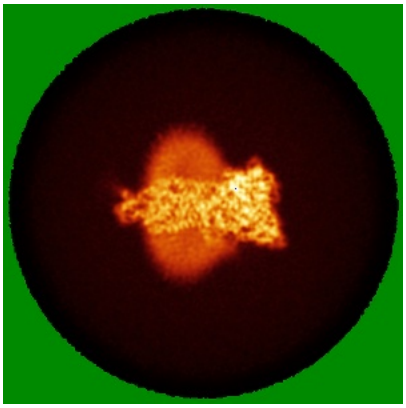

Z Index: 268

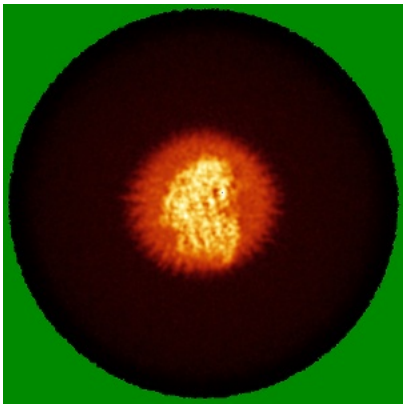
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.06308. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

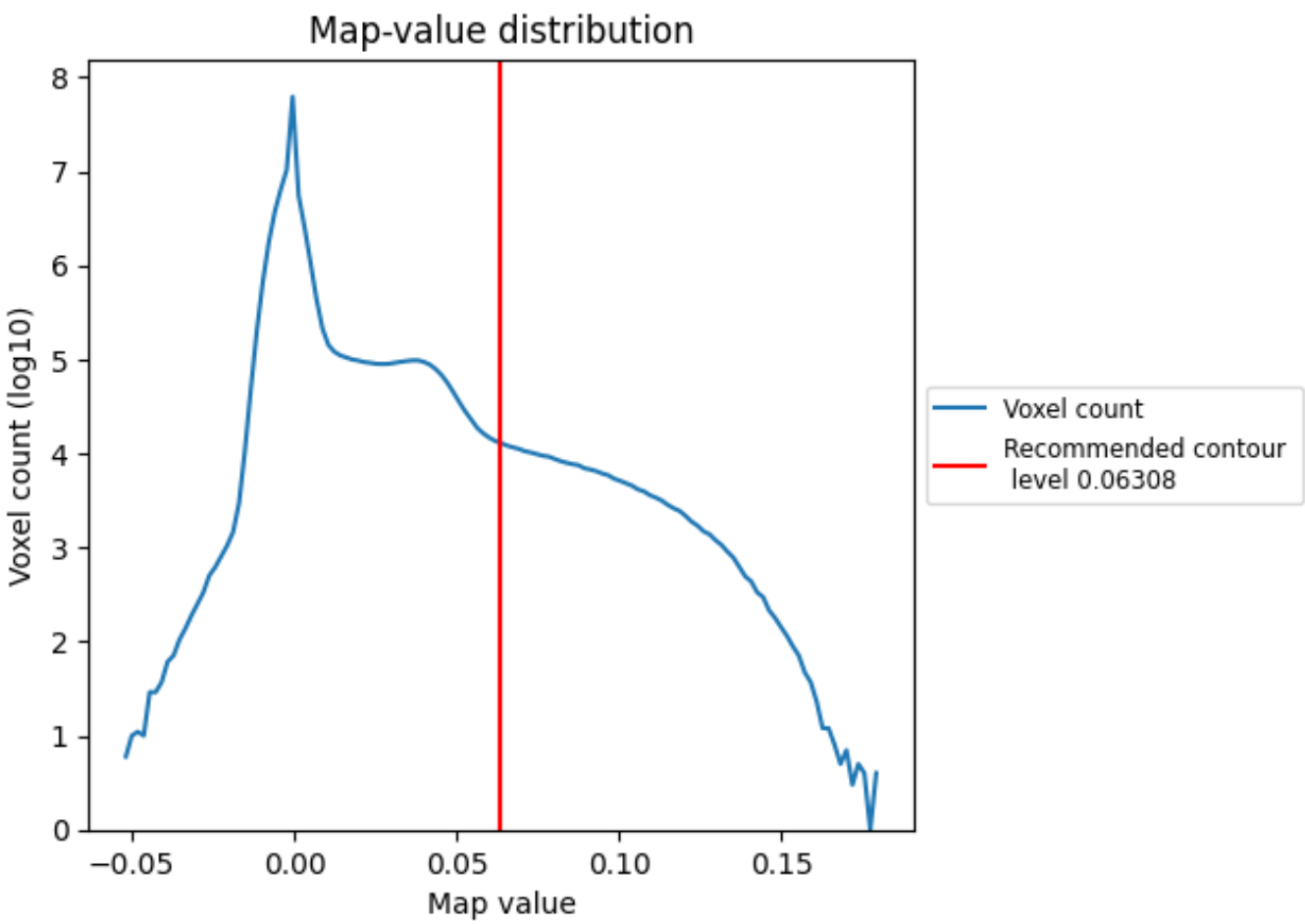
6.6 Mask visualisation (i)

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

7 Map analysis (i)

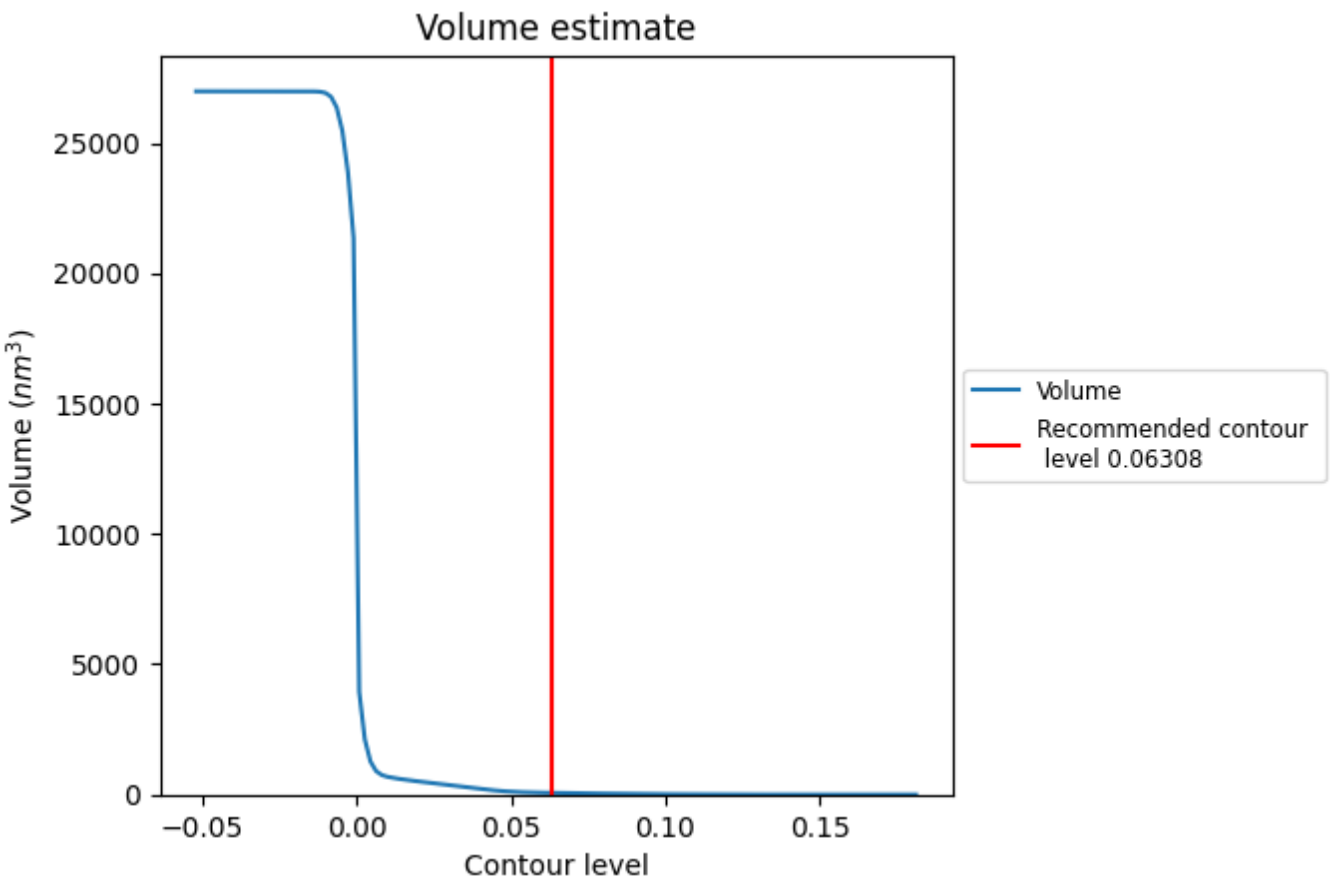
This section contains the results of statistical analysis of the map.

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.

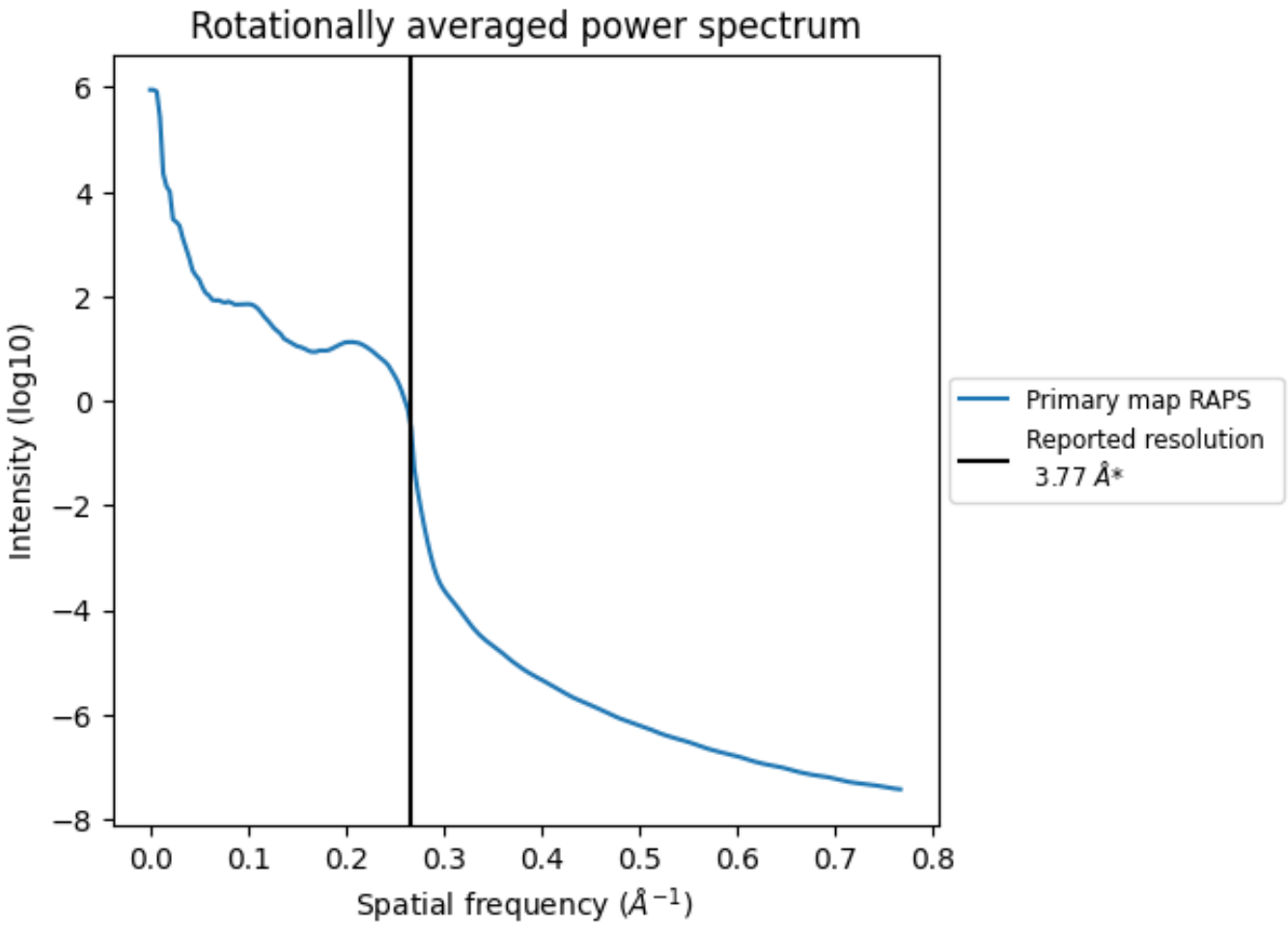
7.2 Volume estimate (i)



The volume at the recommended contour level is 65 nm^3; this corresponds to an approximate mass of 59 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 0.265 Å^{-1}

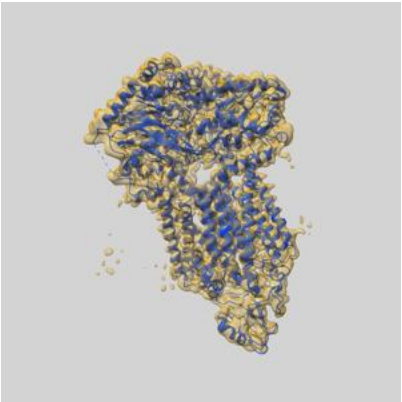
8 Fourier-Shell correlation (i)

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

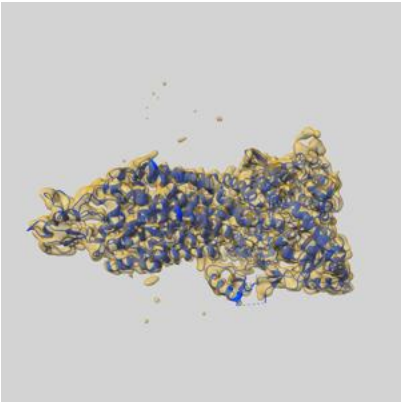
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13145 and PDB model 7P06. Per-residue inclusion information can be found in section 3 on page 6.

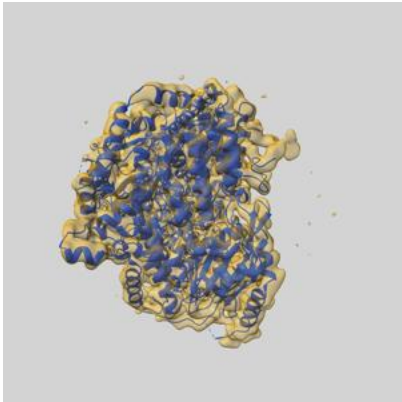
9.1 Map-model overlay (i)



X



Y



Z

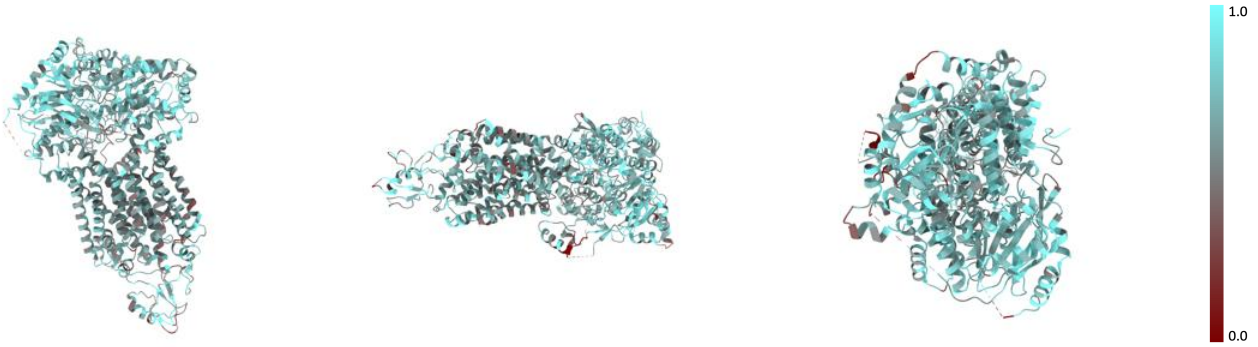
The images above show the 3D surface view of the map at the recommended contour level 0.06308 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

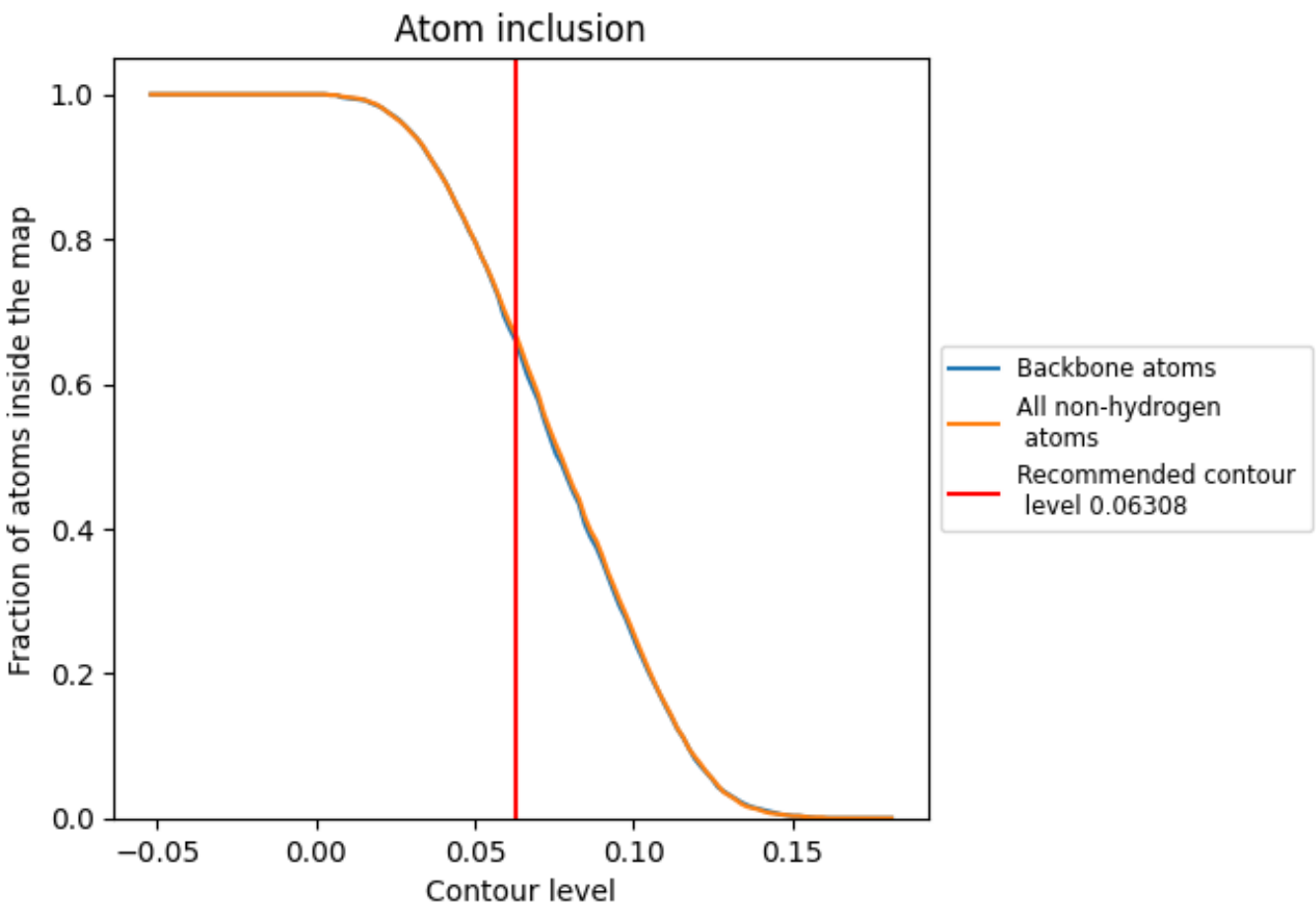
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06308).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 67% 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 (0.06308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6660	0.4140
A	0.6800	0.4140