



Full wwPDB EM Validation Report ⓘ

Jun 20, 2024 – 02:45 AM JST

PDB ID : 7WI4
EMDB ID : EMD-32521
Title : Cryo-EM structure of E.Coli FtsH protease cytosolic domains
Authors : Qiao, Z.; Gao, Y.G.
Deposited on : 2022-01-02
Resolution : 3.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92
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) : 2.37.1

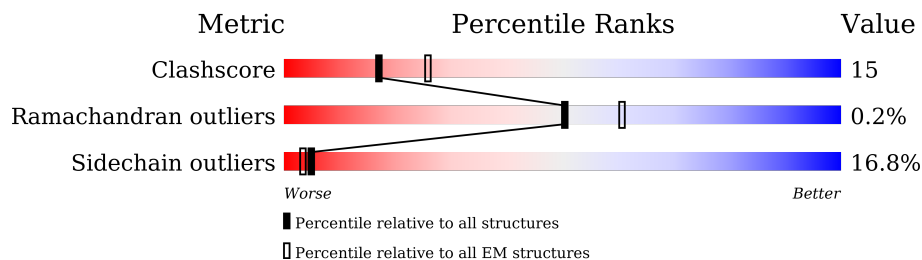
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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 $\leq 5\%$. 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	644	
1	B	644	
1	C	644	
1	D	644	
1	E	644	
1	F	644	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 19284 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.

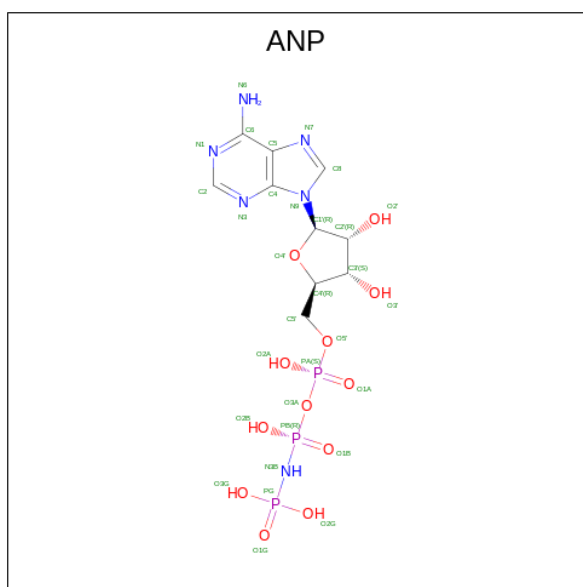
- Molecule 1 is a protein called ATP-dependent zinc metalloprotease FtsH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	410	3181	1996	571	594	20	5	0
1	D	410	3181	1996	571	594	20	5	0
1	E	410	3181	1996	571	594	20	5	0
1	F	410	3181	1996	571	594	20	5	0
1	B	410	3181	1996	571	594	20	5	0
1	C	410	3181	1996	571	594	20	5	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	GLN	GLU	engineered mutation	UNP P0AAI3
A	415	GLN	GLU	engineered mutation	UNP P0AAI3
D	252	GLN	GLU	engineered mutation	UNP P0AAI3
D	415	GLN	GLU	engineered mutation	UNP P0AAI3
E	252	GLN	GLU	engineered mutation	UNP P0AAI3
E	415	GLN	GLU	engineered mutation	UNP P0AAI3
F	252	GLN	GLU	engineered mutation	UNP P0AAI3
F	415	GLN	GLU	engineered mutation	UNP P0AAI3
B	252	GLN	GLU	engineered mutation	UNP P0AAI3
B	415	GLN	GLU	engineered mutation	UNP P0AAI3
C	252	GLN	GLU	engineered mutation	UNP P0AAI3
C	415	GLN	GLU	engineered mutation	UNP P0AAI3

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	D	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	E	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	F	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	B	1	Total	C	N	O	P	0
			31	10	6	12	3	
2	C	1	Total	C	N	O	P	0
			31	10	6	12	3	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	F	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	

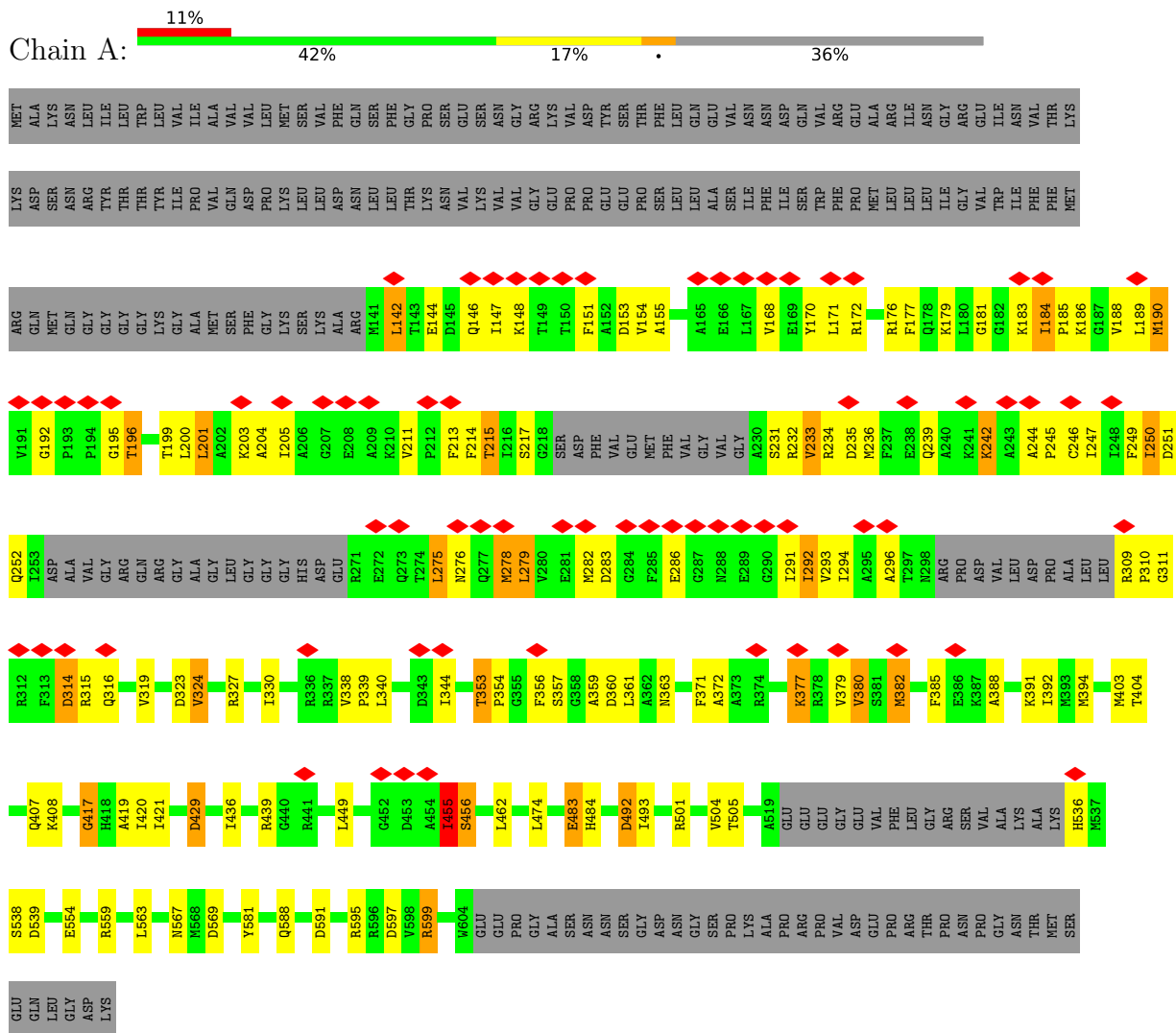
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Mg 1	0
4	D	1	Total 1	Mg 1	0
4	E	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0
4	B	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0

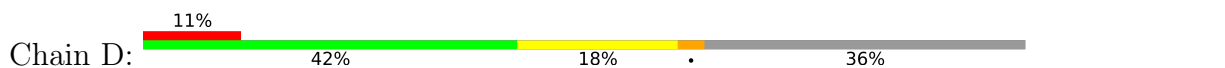
3 Residue-property plots i

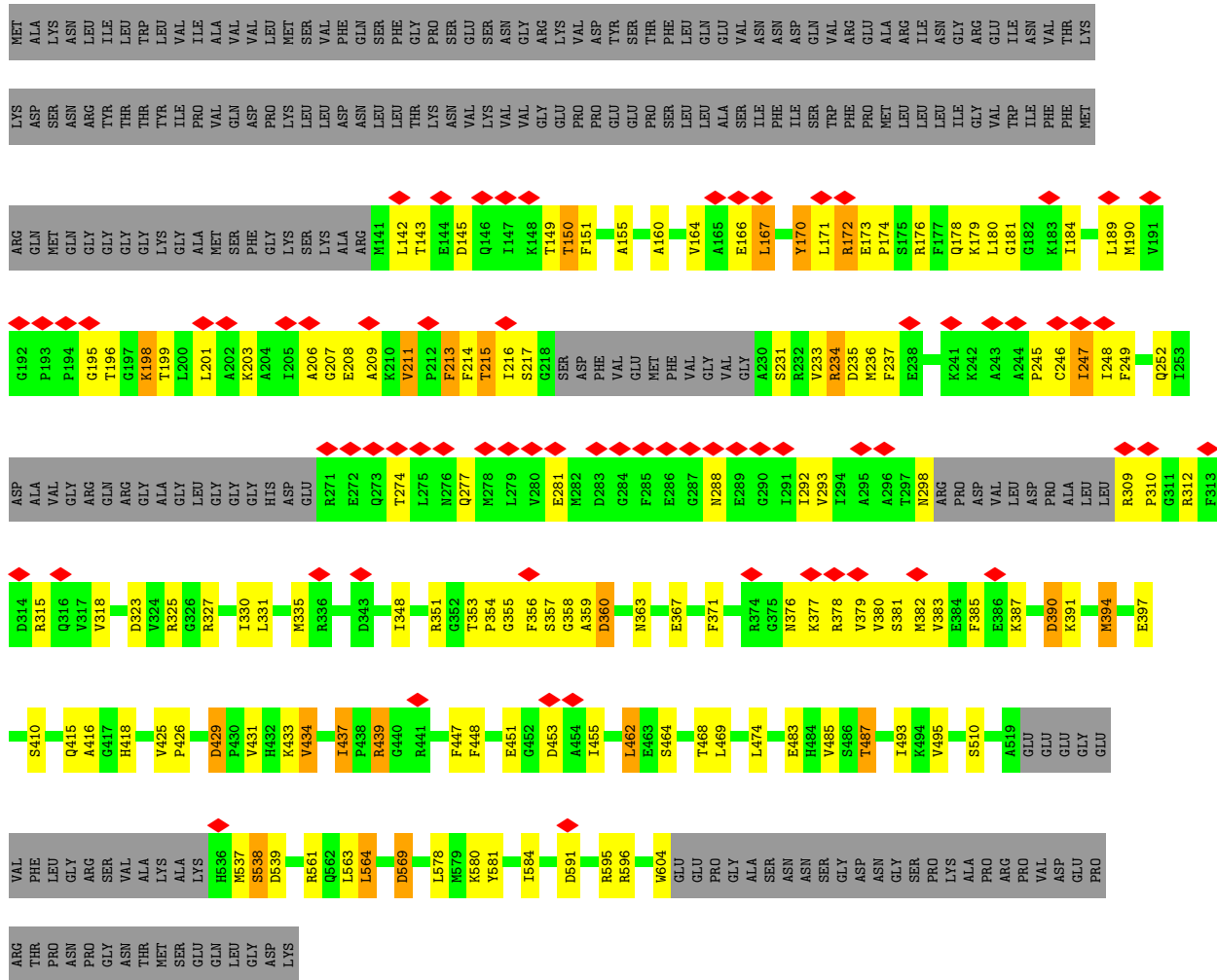
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: ATP-dependent zinc metalloprotease FtsH

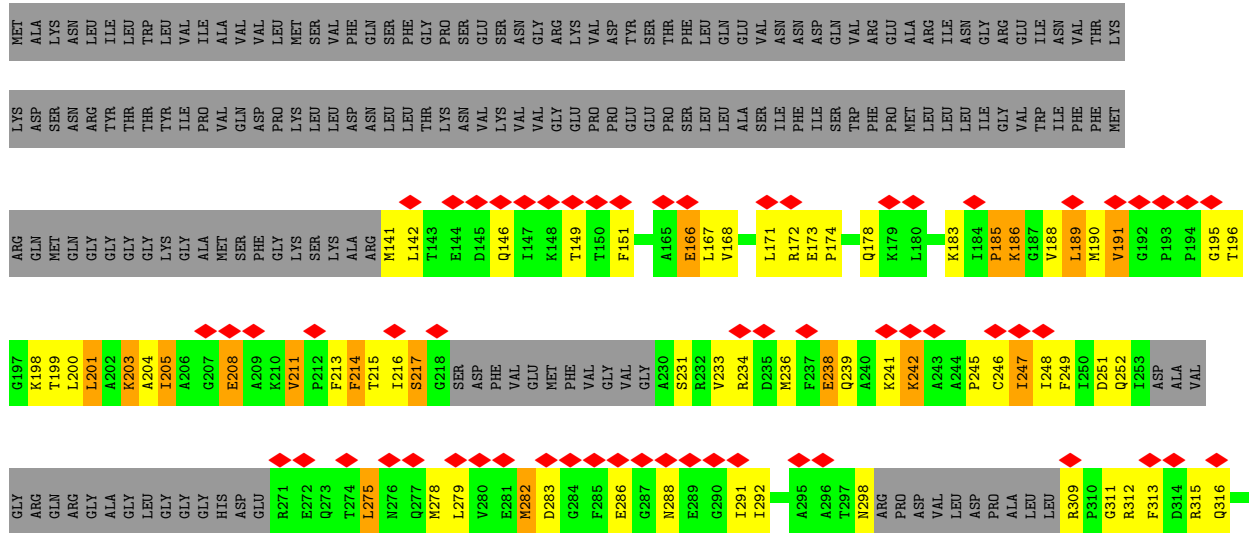


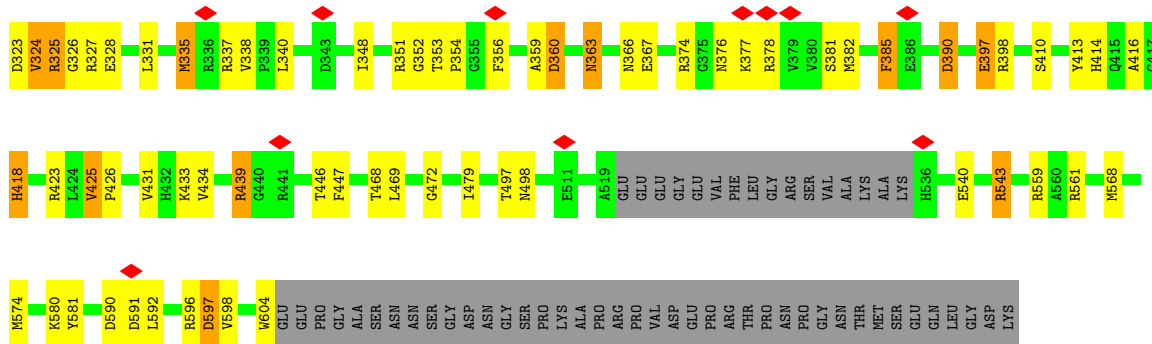
- Molecule 1: ATP-dependent zinc metalloprotease FtsH



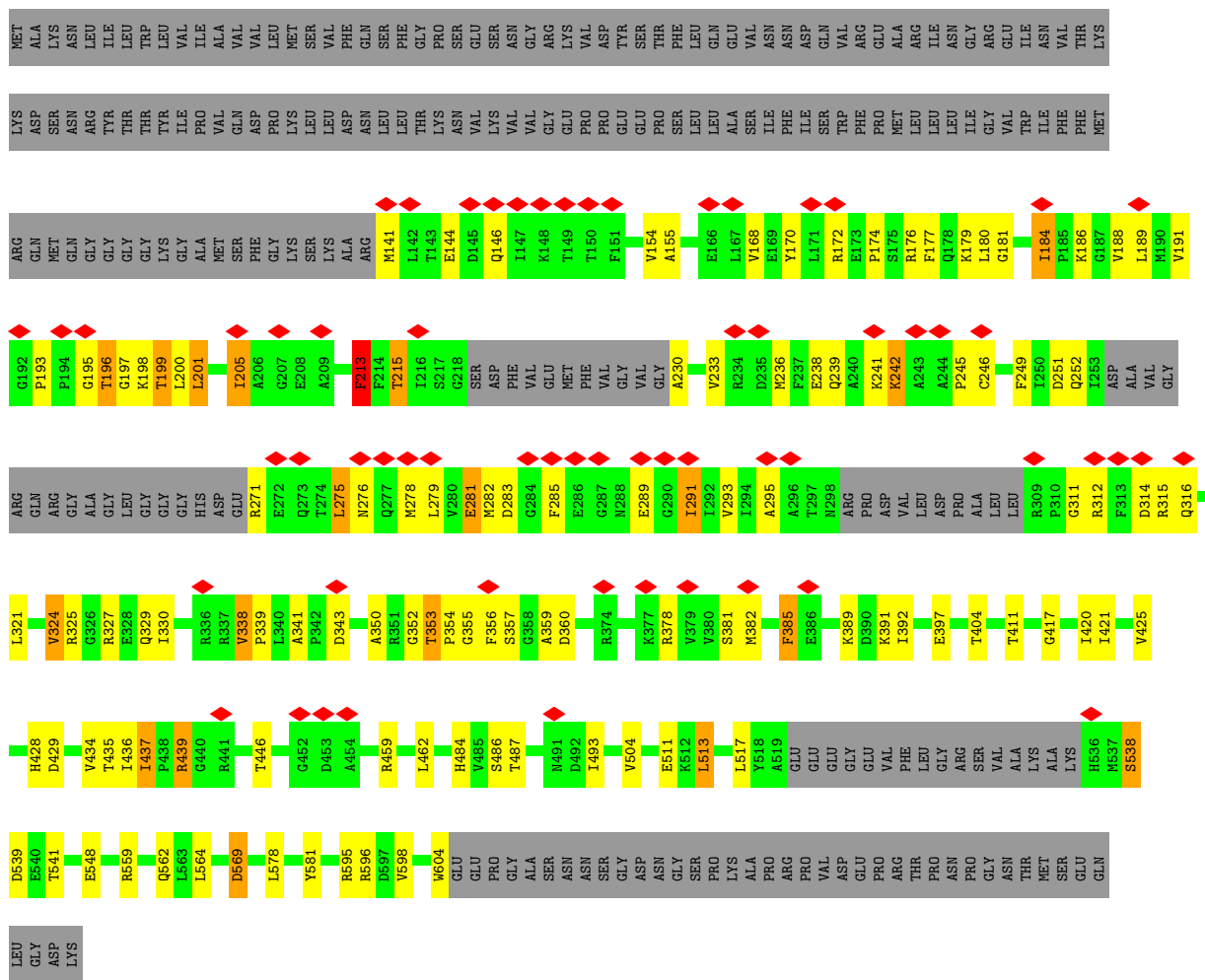
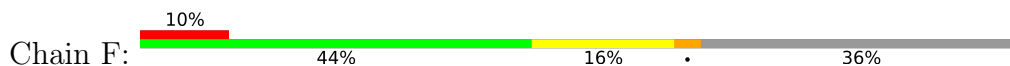


Molecule 1: ATP-dependent zinc metalloprotease FtsH

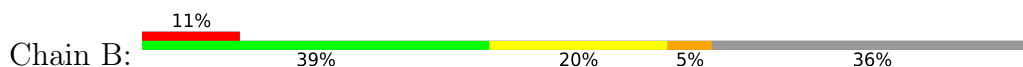


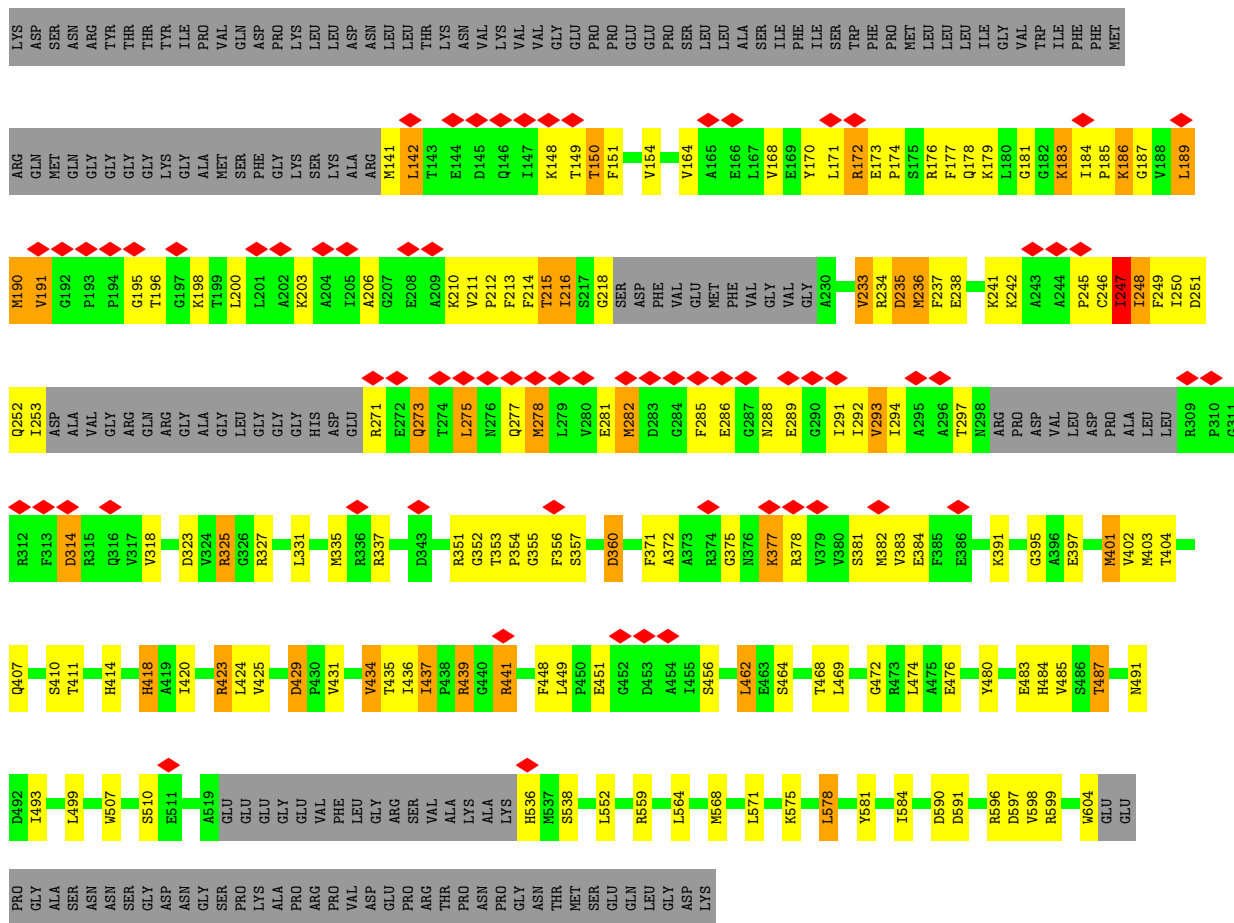


• Molecule 1: ATP-dependent zinc metalloprotease FtsH

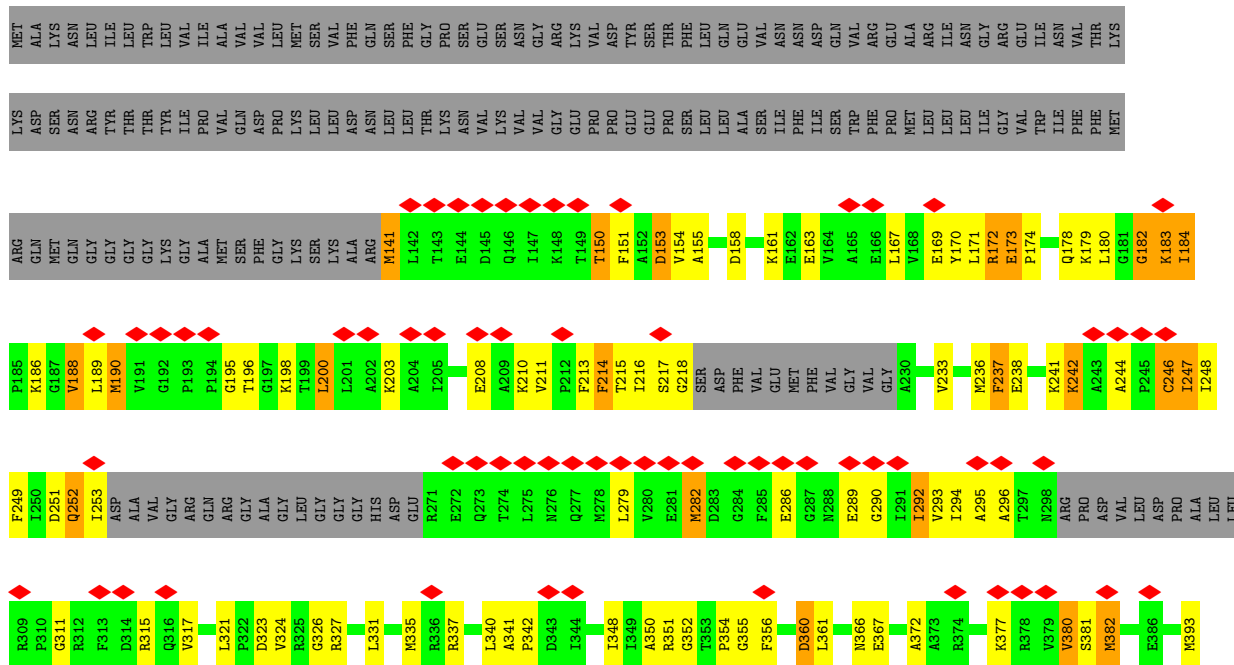


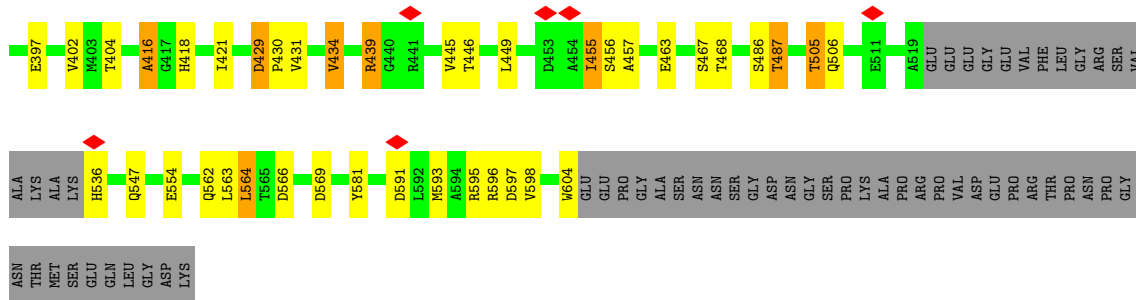
• Molecule 1: ATP-dependent zinc metalloprotease FtsH





● Molecule 1: ATP-dependent zinc metalloprotease FtsH





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32359	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.617	Depositor
Minimum map value	-0.003	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.172	Depositor
Map size (\AA)	219.648, 219.648, 219.648	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.3728, 1.3728, 1.3728	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, ANP

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	0.55	0/3254	0.54	0/4383
1	B	0.55	0/3254	0.54	0/4383
1	C	0.57	0/3254	0.55	1/4383 (0.0%)
1	D	0.56	0/3254	0.54	0/4383
1	E	0.57	0/3254	0.54	0/4383
1	F	0.56	0/3254	0.54	0/4383
All	All	0.56	0/19524	0.54	1/26298 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	D	0	2
1	F	0	5
All	All	0	10

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	ALA	C-N-CA	-5.44	110.87	122.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	417	GLY	Peptide
1	A	455	ILE	Peptide
1	B	247	ILE	Peptide
1	D	181	GLY	Peptide
1	D	415	GLN	Peptide
1	F	213	PHE	Peptide
1	F	215	THR	Peptide
1	F	251[A]	ASP	Peptide
1	F	251[B]	ASP	Peptide
1	F	417	GLY	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	3181	0	3231	100	0
1	B	3181	0	3231	117	0
1	C	3181	0	3230	91	0
1	D	3181	0	3231	92	0
1	E	3181	0	3231	100	0
1	F	3181	0	3231	92	0
2	A	31	0	13	8	0
2	B	31	0	13	3	0
2	C	31	0	12	5	0
2	D	31	0	13	7	0
2	E	31	0	13	5	0
2	F	31	0	13	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19284	0	19462	592	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 15.

All (592) 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:184:ILE:HD11	1:A:292:ILE:HG22	1.53	0.90
1:B:215:THR:HB	1:B:249:PHE:HB3	1.55	0.88
1:E:327:ARG:NH1	1:E:353:THR:O	2.07	0.87
1:C:141:MET:N	1:C:218:GLY:O	2.10	0.83
1:B:238:GLU:O	1:B:241:LYS:NZ	2.10	0.83
1:E:211:VAL:HB	1:E:245:PRO:HA	1.59	0.82
1:B:360:ASP:OD1	1:B:360:ASP:N	2.12	0.82
1:B:195:GLY:N	2:B:701:ANP:O3G	2.12	0.82
1:E:233:VAL:O	1:E:236:MET:N	2.13	0.82
2:B:701:ANP:O3G	2:B:701:ANP:O1B	1.97	0.80
1:E:434:VAL:HG12	1:E:446:THR:HG22	1.62	0.80
1:E:360:ASP:N	1:E:360:ASP:OD1	2.15	0.79
1:C:172:ARG:H	1:C:172:ARG:HH11	1.30	0.79
1:E:382:MET:HA	1:E:385:PHE:HB2	1.65	0.78
1:D:213:PHE:HB3	1:D:245:PRO:HG2	1.64	0.78
1:A:327:ARG:NH1	1:A:353:THR:O	2.17	0.77
1:E:195:GLY:N	2:E:701:ANP:O1G	2.17	0.77
1:E:217:SER:OG	1:E:252:GLN:NE2	2.13	0.77
1:A:233:VAL:O	1:A:236:MET:N	2.17	0.77
2:E:701:ANP:O2A	2:E:701:ANP:N3B	2.15	0.77
1:E:151:PHE:HA	1:E:204:ALA:HB1	1.65	0.76
1:B:246:CYS:HA	1:B:291:ILE:HA	1.66	0.76
1:F:199:THR:OG1	1:F:200:LEU:N	2.17	0.76
1:B:211:VAL:HG13	1:B:245:PRO:HG2	1.67	0.76
1:D:359:ALA:O	1:D:363[A]:ASN:ND2	2.19	0.75
1:B:314:ASP:OD1	1:B:314:ASP:N	2.19	0.75
1:C:188:VAL:HB	1:C:315:ARG:HB2	1.69	0.75
1:D:359:ALA:O	1:D:363[B]:ASN:ND2	2.20	0.75
1:B:277:GLN:NE2	1:B:281:GLU:OE1	2.19	0.75
1:D:360:ASP:OD1	1:D:360:ASP:N	2.20	0.74
1:B:170:TYR:CE2	1:B:185:PRO:HD2	2.23	0.73
1:D:231:SER:O	1:D:234:ARG:NH1	2.22	0.73
1:B:150:THR:OG1	1:B:151:PHE:N	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:O	1:A:242:LYS:NZ	2.22	0.72
1:B:189:LEU:HD12	1:B:191:VAL:HG22	1.71	0.72
1:F:381[A]:SER:OG	1:F:382:MET:N	2.20	0.72
1:F:381[B]:SER:OG	1:F:382:MET:N	2.20	0.72
1:C:195:GLY:N	2:C:701:ANP:O1G	2.22	0.72
2:A:701:ANP:O2B	2:A:701:ANP:O1G	2.07	0.72
1:F:233:VAL:O	1:F:236:MET:N	2.22	0.72
1:C:238:GLU:O	1:C:241:LYS:NZ	2.23	0.72
1:B:401:MET:SD	1:B:402:VAL:N	2.62	0.72
1:C:327:ARG:NH1	1:C:350:ALA:O	2.23	0.71
2:D:701:ANP:O2B	2:D:701:ANP:O1G	2.08	0.71
1:C:150:THR:OG1	1:C:151:PHE:N	2.22	0.70
1:A:353:THR:HG22	1:A:356:PHE:HD2	1.55	0.70
1:E:141:MET:HG2	1:E:214:PHE:HZ	1.57	0.70
1:D:150:THR:OG1	1:D:151:PHE:N	2.20	0.70
1:D:378:ARG:NH1	1:E:178:GLN:OE1	2.25	0.69
1:F:141:MET:SD	1:F:239:GLN:NE2	2.65	0.69
1:A:195:GLY:N	2:A:701:ANP:O1G	2.22	0.69
1:A:591:ASP:OD2	1:A:599:ARG:NH2	2.26	0.69
1:D:142:LEU:HA	1:D:214:PHE:CE1	2.28	0.69
1:A:181:GLY:O	1:A:183:LYS:N	2.23	0.68
1:C:155:ALA:O	2:C:701:ANP:N6	2.22	0.68
1:F:193:PRO:O	1:F:198:LYS:NZ	2.26	0.68
1:E:234:ARG:HH22	1:E:278:MET:HB3	1.56	0.68
1:D:487:THR:O	1:D:487:THR:OG1	2.10	0.68
1:F:195:GLY:N	2:F:701:ANP:O1G	2.18	0.68
1:C:213:PHE:HD2	1:C:247:ILE:HB	1.59	0.68
1:A:195:GLY:H	2:A:701:ANP:PG	2.17	0.68
1:A:382:MET:HA	1:A:385:PHE:HB2	1.75	0.67
1:A:569:ASP:OD2	1:A:595:ARG:NH1	2.28	0.67
1:E:359:ALA:O	1:E:363[B]:ASN:ND2	2.26	0.67
1:F:201:LEU:O	1:F:205:ILE:HG22	1.95	0.67
1:E:359:ALA:O	1:E:363[A]:ASN:ND2	2.26	0.67
1:B:434:VAL:HG23	1:B:584:ILE:HB	1.76	0.67
2:A:701:ANP:O1B	2:A:701:ANP:O2A	2.13	0.67
1:B:282:MET:SD	1:B:282:MET:N	2.68	0.67
1:F:215:THR:HB	1:F:249:PHE:HB3	1.76	0.66
1:B:286:GLU:HB3	1:B:289:GLU:H	1.61	0.66
1:B:233:VAL:O	1:B:236:MET:N	2.28	0.66
1:C:237:PHE:HD2	1:C:282:MET:HG2	1.62	0.65
1:B:184:ILE:HD11	1:B:292:ILE:HG22	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:MET:HA	1:A:385:PHE:HD1	1.61	0.65
1:C:242:LYS:O	1:C:242:LYS:NZ	2.24	0.65
1:D:376:ASN:O	1:D:377:LYS:NZ	2.30	0.64
1:A:170:TYR:CE2	1:A:185:PRO:HD2	2.33	0.64
1:D:195:GLY:N	2:D:701:ANP:O1G	2.21	0.64
1:B:281:GLU:O	1:B:285:PHE:HB2	1.98	0.64
1:C:282:MET:O	1:C:286:GLU:N	2.30	0.64
1:D:538:SER:OG	1:D:539:ASP:N	2.27	0.64
1:F:238:GLU:N	1:F:281:GLU:OE2	2.31	0.64
1:F:538:SER:OG	1:F:539:ASP:N	2.30	0.64
1:E:174:PRO:HG3	1:E:288:ASN:HB3	1.80	0.64
1:B:327:ARG:NH1	1:B:353:THR:O	2.31	0.64
2:F:701:ANP:O1B	2:F:701:ANP:O2A	2.12	0.63
1:A:282:MET:O	1:A:286:GLU:N	2.30	0.63
1:F:357:SER:OG	1:F:359:ALA:N	2.29	0.63
1:D:166:GLU:OE1	1:D:315:ARG:NH1	2.31	0.63
1:E:189:LEU:HD22	1:E:191:VAL:HG22	1.79	0.63
1:B:356:PHE:HB3	1:B:360:ASP:HB2	1.79	0.63
2:D:701:ANP:O2A	1:E:309:ARG:NH2	2.30	0.63
1:A:314:ASP:N	1:A:314:ASP:OD1	2.27	0.63
1:F:213:PHE:CD2	1:F:245:PRO:HG3	2.34	0.63
1:D:234:ARG:HA	1:D:237:PHE:HD1	1.63	0.62
2:B:701:ANP:O2A	2:B:701:ANP:N3B	2.29	0.62
1:A:215:THR:HB	1:A:249:PHE:HB3	1.82	0.62
1:B:213:PHE:HB3	1:B:247:ILE:HD12	1.81	0.62
1:C:381[A]:SER:OG	1:C:382:MET:N	2.32	0.62
1:C:487:THR:O	1:C:487:THR:OG1	2.11	0.62
1:E:381[A]:SER:OG	1:E:382:MET:N	2.32	0.62
1:D:215:THR:HB	1:D:249:PHE:HB3	1.82	0.62
1:F:197:GLY:N	2:F:701:ANP:O2B	2.32	0.62
1:B:375:GLY:O	1:B:377:LYS:NZ	2.32	0.62
1:B:423:ARG:NH2	1:B:590:ASP:OD1	2.32	0.62
1:E:234:ARG:NH1	1:E:278:MET:SD	2.74	0.61
1:D:142:LEU:HA	1:D:214:PHE:HE1	1.65	0.61
1:E:390:ASP:OD2	1:E:439:ARG:NH1	2.33	0.61
1:D:209:ALA:HB3	1:D:211:VAL:HG22	1.83	0.61
1:D:213:PHE:HD2	1:D:245:PRO:HB2	1.66	0.61
1:B:234:ARG:HA	1:B:237:PHE:HB2	1.83	0.61
1:F:155:ALA:HB3	1:F:330:ILE:HG12	1.82	0.61
1:D:170:TYR:CZ	1:D:184:ILE:HG12	2.36	0.61
1:F:486:SER:HG	1:B:456:SER:HG	1.45	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASP:OD1	1:B:235:ASP:N	2.24	0.61
1:B:271:ARG:N	1:B:273:GLN:OE1	2.34	0.60
1:A:339:PRO:HB2	1:A:379:VAL:HG21	1.83	0.60
1:E:381[B]:SER:OG	1:E:382:MET:N	2.32	0.60
1:B:381[A]:SER:OG	1:B:382:MET:N	2.35	0.60
1:B:431:VAL:HG22	1:B:448:PHE:HE1	1.65	0.60
1:C:188:VAL:HG13	1:C:294:ILE:HG22	1.82	0.60
1:F:324:VAL:HA	1:F:327:ARG:HG3	1.83	0.60
1:F:327:ARG:NH1	1:F:350:ALA:O	2.34	0.60
1:F:486:SER:OG	1:B:456:SER:OG	2.19	0.60
1:B:397:GLU:HB3	1:B:439:ARG:NH2	2.17	0.60
1:D:357:SER:OG	1:D:359:ALA:N	2.35	0.59
1:F:338:VAL:HG12	1:F:339:PRO:HD2	1.83	0.59
1:A:283:ASP:HA	1:A:286:GLU:HB2	1.83	0.59
1:D:381[A]:SER:OG	1:D:382:MET:N	2.34	0.59
1:C:381[B]:SER:OG	1:C:382:MET:N	2.33	0.59
1:A:356:PHE:HB3	1:A:360:ASP:HB3	1.82	0.59
1:C:180:LEU:C	1:C:182:GLY:H	2.06	0.59
1:B:170:TYR:CD1	1:B:177:PHE:HE2	2.21	0.59
1:F:327:ARG:NH2	1:F:354:PRO:HA	2.18	0.59
1:F:569:ASP:OD1	1:F:595:ARG:NH1	2.35	0.59
1:A:247:ILE:HG22	1:A:292:ILE:H	1.68	0.59
1:C:217:SER:HA	1:C:252:GLN:NE2	2.18	0.59
1:A:146:GLN:HG3	1:A:147:ILE:HG23	1.83	0.59
1:E:540:GLU:OE1	1:E:543:ARG:NH2	2.34	0.59
1:D:170:TYR:CD2	1:D:184:ILE:HG23	2.37	0.58
1:C:591:ASP:OD1	1:C:596:ARG:NH2	2.36	0.58
1:D:171:LEU:HD22	1:D:246:CYS:HB3	1.84	0.58
1:F:252:GLN:N	1:F:252:GLN:OE1	2.37	0.58
1:F:239:GLN:O	1:F:242:LYS:NZ	2.32	0.58
1:B:275:LEU:O	1:B:278:MET:HG3	2.03	0.58
1:A:357:SER:OG	1:A:359:ALA:N	2.36	0.58
1:F:188:VAL:HG13	1:F:315:ARG:HB3	1.84	0.58
1:C:248:ILE:HD13	1:C:292:ILE:O	2.04	0.58
1:A:168:VAL:HG22	1:A:205:ILE:HG23	1.85	0.58
1:A:278:MET:O	1:A:282:MET:HG2	2.03	0.58
1:F:378:ARG:O	1:B:179:LYS:NZ	2.31	0.58
1:B:378:ARG:O	1:C:179:LYS:NZ	2.35	0.58
1:C:372:ALA:HB2	1:C:380:VAL:HG13	1.85	0.57
1:A:247:ILE:HA	1:A:291:ILE:HG23	1.86	0.57
1:A:538:SER:OG	1:A:539:ASP:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ALA:HB1	1:D:201:LEU:HD11	1.87	0.57
1:B:381[B]:SER:OG	1:B:382:MET:N	2.35	0.57
1:C:217:SER:HA	1:C:252:GLN:HE22	1.70	0.57
1:D:353:THR:HB	1:D:356:PHE:CD2	2.40	0.57
1:D:429:ASP:N	1:D:429:ASP:OD1	2.34	0.57
1:B:429:ASP:OD1	1:B:429:ASP:N	2.35	0.57
1:C:562:GLN:NE2	1:C:566:ASP:OD2	2.38	0.57
1:C:327:ARG:HH22	1:C:354:PRO:HA	1.68	0.57
1:D:211:VAL:HB	1:D:245:PRO:HB3	1.87	0.57
2:D:701:ANP:O2A	2:D:701:ANP:O1B	2.23	0.57
1:E:275:LEU:HD23	1:E:312:ARG:HB2	1.85	0.57
1:B:236:MET:N	1:B:236:MET:SD	2.77	0.57
1:C:171:LEU:HD22	1:C:246:CYS:HB2	1.87	0.57
2:C:701:ANP:O1G	2:C:701:ANP:O2B	2.23	0.57
1:D:196:THR:O	1:D:196:THR:OG1	2.23	0.56
1:F:186:LYS:NZ	1:F:311:GLY:O	2.21	0.56
1:F:189:LEU:HD22	1:F:191:VAL:HB	1.87	0.56
1:F:434:VAL:HG12	1:F:446:THR:HG23	1.87	0.56
1:A:340:LEU:HB2	1:A:344:ILE:HD12	1.87	0.56
1:B:171:LEU:HB2	1:B:172:ARG:HH11	1.69	0.56
1:A:456:SER:HB3	1:C:487:THR:HG23	1.88	0.56
1:A:569:ASP:OD1	1:A:569:ASP:N	2.39	0.56
1:A:179:LYS:NZ	1:C:377:LYS:O	2.39	0.56
1:A:363[A]:ASN:ND2	1:D:310:PRO:HB3	2.21	0.56
1:D:178:GLN:HG3	1:D:179:LYS:HD2	1.86	0.56
1:A:382:MET:HA	1:A:385:PHE:CD1	2.41	0.56
1:D:234:ARG:HA	1:D:237:PHE:CD1	2.41	0.55
1:E:433:LYS:HG2	1:E:447:PHE:HD1	1.72	0.55
1:E:597:ASP:OD1	1:E:597:ASP:N	2.25	0.55
1:A:417:GLY:H	1:A:419:ALA:H	1.55	0.55
1:F:213:PHE:CG	1:F:245:PRO:HG3	2.42	0.55
1:E:149:THR:HB	1:E:203:LYS:HE3	1.89	0.55
1:F:179:LYS:O	1:F:181:GLY:N	2.39	0.55
1:F:437:ILE:HD11	1:F:439:ARG:HH11	1.72	0.55
1:F:170:TYR:CD2	1:F:177:PHE:HE1	2.24	0.55
1:F:282:MET:HB2	1:F:291:ILE:HG21	1.87	0.55
1:D:327:ARG:NH2	1:D:354:PRO:HA	2.22	0.55
1:A:190:MET:HE1	1:A:296:ALA:HB2	1.88	0.55
1:D:381[B]:SER:OG	1:D:382:MET:N	2.38	0.55
1:F:200:LEU:HD13	2:F:701:ANP:H3'	1.89	0.55
1:E:378:ARG:O	1:F:179:LYS:NZ	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:ASP:OD1	1:D:569:ASP:N	2.21	0.54
1:E:497:THR:HG21	1:F:517:LEU:HB3	1.87	0.54
1:F:356:PHE:HB3	1:F:360:ASP:HB3	1.88	0.54
1:C:421:ILE:HD11	1:C:564:LEU:HD12	1.89	0.54
1:B:211:VAL:HG13	1:B:247:ILE:HD13	1.88	0.54
1:B:218:GLY:N	1:B:252:GLN:OE1	2.39	0.54
1:E:171:LEU:HD22	1:E:246:CYS:HB3	1.90	0.54
1:A:188:VAL:HA	1:A:315:ARG:O	2.07	0.54
1:A:142:LEU:HA	1:A:214:PHE:CE1	2.43	0.54
1:F:352:GLY:O	1:F:354:PRO:HD3	2.08	0.54
1:B:275:LEU:H	1:B:275:LEU:HD22	1.73	0.54
1:C:249:PHE:CE2	1:C:251[B]:ASP:HB2	2.43	0.54
1:D:206:ALA:HB1	1:D:214:PHE:HA	1.90	0.53
1:C:249:PHE:CE2	1:C:251[A]:ASP:HB2	2.43	0.53
1:A:353:THR:HG22	1:A:356:PHE:CD2	2.41	0.53
1:E:356:PHE:HB3	1:E:360:ASP:HB2	1.90	0.53
1:F:242:LYS:HD2	1:F:242:LYS:O	2.08	0.53
1:A:196:THR:O	1:A:196:THR:OG1	2.20	0.53
1:A:213:PHE:HD2	1:A:245:PRO:HD3	1.73	0.53
1:D:434:VAL:HG23	1:D:584:ILE:HB	1.91	0.53
1:E:325:ARG:HH11	1:E:328:GLU:HB3	1.74	0.53
1:B:200:LEU:HD12	1:B:203:LYS:HB3	1.89	0.53
1:F:382:MET:HA	1:F:385:PHE:HB2	1.91	0.53
1:F:343:ASP:OD1	1:F:343:ASP:N	2.32	0.53
1:A:323:ASP:O	1:A:327:ARG:N	2.38	0.53
1:D:351:ARG:HD2	1:D:451:GLU:HA	1.89	0.53
1:C:327:ARG:NH2	1:C:354:PRO:HA	2.23	0.53
1:D:356:PHE:HB3	1:D:360:ASP:HB2	1.90	0.52
1:C:186:LYS:HD3	1:C:311:GLY:O	2.08	0.52
1:A:155:ALA:HB3	1:A:330:ILE:HG12	1.91	0.52
1:A:213:PHE:CD2	1:A:245:PRO:HD3	2.44	0.52
1:C:282:MET:SD	1:C:282:MET:N	2.82	0.52
1:D:213:PHE:CD2	1:D:245:PRO:HB2	2.44	0.52
1:D:360:ASP:HA	1:D:363[B]:ASN:HD22	1.74	0.52
1:B:237:PHE:HE2	1:B:278:MET:HB3	1.73	0.52
1:E:186:LYS:NZ	1:E:311:GLY:O	2.20	0.52
1:C:331:LEU:O	1:C:335:MET:HB2	2.10	0.52
1:D:215:THR:HB	1:D:249:PHE:CD2	2.45	0.52
1:C:286:GLU:OE1	1:C:289:GLU:HB2	2.09	0.52
1:C:397:GLU:HB3	1:C:439:ARG:NH2	2.25	0.52
1:B:148[B]:LYS:HG3	1:B:203:LYS:HZ1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:THR:HB	1:B:356:PHE:CD2	2.45	0.52
2:C:701:ANP:O1B	2:C:701:ANP:O2A	2.23	0.52
1:D:172:ARG:NH2	1:D:209:ALA:HB1	2.24	0.52
1:A:379:VAL:HG22	1:A:380:VAL:H	1.75	0.52
1:E:414:HIS:CD2	1:E:472:GLY:HA3	2.45	0.52
1:D:309:ARG:HG2	1:D:312:ARG:CZ	2.40	0.51
1:D:360:ASP:HA	1:D:363[A]:ASN:HD22	1.74	0.51
1:F:184:ILE:HD11	1:F:186:LYS:HG2	1.91	0.51
2:A:701:ANP:O2A	2:A:701:ANP:N3B	2.37	0.51
1:E:245:PRO:HG2	1:E:247:ILE:HG13	1.90	0.51
1:E:325:ARG:O	1:E:325:ARG:NE	2.43	0.51
1:D:170:TYR:CE2	1:D:184:ILE:HG23	2.45	0.51
1:C:237:PHE:CE2	1:C:279:LEU:HA	2.45	0.51
1:C:352:GLY:O	1:C:354:PRO:HD3	2.11	0.51
1:A:200:LEU:HD13	2:A:701:ANP:H2'	1.92	0.51
1:D:353:THR:O	1:D:353:THR:OG1	2.28	0.51
1:E:416:ALA:O	1:E:418:HIS:N	2.43	0.51
1:F:246:CYS:HB3	1:F:289:GLU:O	2.11	0.51
1:F:378:ARG:NH2	1:B:178:GLN:HE22	2.09	0.51
1:B:171:LEU:HA	1:B:246:CYS:SG	2.50	0.51
1:C:171:LEU:HD22	1:C:246:CYS:CB	2.41	0.51
1:C:244:ALA:HB1	1:C:247:ILE:HD11	1.93	0.51
1:A:199:THR:OG1	2:A:701:ANP:O1A	2.29	0.51
1:E:275:LEU:H	1:E:275:LEU:HD22	1.76	0.50
1:C:569:ASP:OD1	1:C:595:ARG:NH1	2.44	0.50
1:F:378:ARG:CZ	1:B:178:GLN:HE22	2.25	0.50
1:F:397:GLU:HG3	1:F:439:ARG:CZ	2.41	0.50
1:A:249:PHE:CZ	1:A:251[A]:ASP:HB2	2.47	0.50
1:F:170:TYR:CE1	1:F:184:ILE:HA	2.46	0.50
1:A:324:VAL:HG13	1:A:327:ARG:HH21	1.75	0.50
1:E:213:PHE:CD2	1:E:245:PRO:HD3	2.45	0.50
1:B:211:VAL:CG1	1:B:247:ILE:HD13	2.41	0.50
1:D:390:ASP:OD2	1:D:439:ARG:NH1	2.44	0.50
1:F:184:ILE:HG13	1:F:291:ILE:O	2.12	0.50
1:F:382:MET:HA	1:F:385:PHE:HD2	1.77	0.50
1:B:171:LEU:HD22	1:B:246:CYS:HB2	1.94	0.50
2:D:701:ANP:H2'	2:D:701:ANP:N3	2.26	0.50
1:C:324:VAL:HA	1:C:327:ARG:HG3	1.94	0.50
1:F:186:LYS:HE2	1:F:279:LEU:HD13	1.92	0.50
1:D:431:VAL:HG22	1:D:448:PHE:HE1	1.77	0.49
1:E:283:ASP:HA	1:E:286:GLU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:THR:O	1:B:487:THR:OG1	2.19	0.49
1:C:505:THR:HG22	1:C:506:GLN:HG3	1.94	0.49
1:A:214:PHE:HD2	1:A:215:THR:HG23	1.77	0.49
1:B:174:PRO:HG3	1:B:288:ASN:OD1	2.13	0.49
1:B:331:LEU:O	1:B:335:MET:HB2	2.12	0.49
1:D:416:ALA:O	1:D:418:HIS:N	2.45	0.49
1:E:171:LEU:HD13	1:E:246:CYS:HB2	1.94	0.49
1:B:597:ASP:OD1	1:B:597:ASP:N	2.46	0.49
1:E:231:SER:O	1:E:231:SER:OG	2.30	0.49
1:A:567:ASN:OD1	1:A:567:ASN:N	2.45	0.49
1:D:377:LYS:HA	1:D:377:LYS:HZ2	1.78	0.49
1:E:376:ASN:C	1:E:377:LYS:HZ3	2.15	0.49
1:F:236:MET:O	1:F:239:GLN:HB3	2.13	0.49
1:A:214:PHE:CD2	1:A:215:THR:HG23	2.48	0.49
1:A:249:PHE:CZ	1:A:251[B]:ASP:HB2	2.47	0.49
1:E:171:LEU:HB3	1:E:246:CYS:SG	2.52	0.49
1:D:327:ARG:HH21	1:D:355:GLY:H	1.59	0.48
1:D:382:MET:HA	1:D:385:PHE:HB2	1.95	0.48
1:A:286:GLU:OE2	1:A:291:ILE:HB	2.13	0.48
1:D:217:SER:OG	1:D:252:GLN:NE2	2.46	0.48
1:F:246:CYS:HA	1:F:289:GLU:HG3	1.96	0.48
2:F:701:ANP:O1B	2:F:701:ANP:O3G	2.31	0.48
1:E:199:THR:OG1	2:E:701:ANP:O1A	2.23	0.48
1:E:234:ARG:HH11	1:E:234:ARG:HA	1.79	0.48
1:E:238:GLU:OE2	1:E:278:MET:HB2	2.13	0.48
1:E:353:THR:HB	1:E:356:PHE:CD2	2.48	0.48
1:F:170:TYR:HE1	1:F:184:ILE:HA	1.78	0.48
1:F:275:LEU:HB3	1:F:312:ARG:HB2	1.95	0.48
1:B:170:TYR:CD1	1:B:177:PHE:CE2	3.01	0.48
1:A:231:SER:HB3	1:A:234:ARG:HH21	1.78	0.48
1:E:167:LEU:O	1:E:171:LEU:HG	2.13	0.48
1:C:429:ASP:OD1	1:C:429:ASP:N	2.46	0.48
1:A:275:LEU:H	1:A:275:LEU:HD12	1.79	0.48
1:F:356:PHE:HB3	1:F:360:ASP:CB	2.44	0.48
1:A:217:SER:OG	1:A:252:GLN:NE2	2.47	0.48
1:D:591:ASP:OD1	1:D:596:ARG:NH2	2.47	0.48
1:E:196:THR:O	1:E:196:THR:OG1	2.28	0.48
1:B:327:ARG:HH12	1:B:355:GLY:H	1.60	0.48
1:A:372:ALA:HB2	1:A:380:VAL:HG13	1.95	0.48
1:D:151:PHE:HB3	1:D:208:GLU:OE2	2.14	0.48
1:C:213:PHE:HB3	1:C:247:ILE:HD12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:GLU:HB2	1:A:484:HIS:CD2	2.49	0.48
1:B:214:PHE:CD2	1:B:215:THR:HG23	2.48	0.48
1:E:236:MET:O	1:E:239:GLN:HB2	2.13	0.47
1:F:230:ALA:HB3	1:F:271:ARG:HH21	1.79	0.47
1:F:486:SER:OG	1:F:487:THR:N	2.46	0.47
1:E:591:ASP:OD1	1:E:596:ARG:NH1	2.46	0.47
1:B:237:PHE:HB3	1:B:281:GLU:OE1	2.14	0.47
1:D:155:ALA:HB3	1:D:330:ILE:HG12	1.96	0.47
1:F:353:THR:HG22	1:F:356:PHE:CD2	2.50	0.47
1:D:433:LYS:HB3	1:D:447:PHE:HD1	1.80	0.47
1:B:253:ILE:HG23	1:B:297:THR:HB	1.95	0.47
1:A:215:THR:HB	1:A:249:PHE:HD2	1.80	0.47
1:D:217:SER:HG	1:D:252:GLN:CD	2.16	0.47
1:A:170:TYR:CD1	1:A:177:PHE:HE1	2.33	0.47
1:A:200:LEU:HD22	2:A:701:ANP:C5	2.44	0.47
1:A:309:ARG:NH1	1:A:310:PRO:O	2.48	0.47
1:D:195:GLY:H	2:D:701:ANP:PG	2.35	0.47
1:D:211:VAL:HB	1:D:245:PRO:CB	2.43	0.47
1:D:215:THR:HA	1:D:249:PHE:HB3	1.97	0.47
1:F:241:LYS:HD2	1:F:285:PHE:HB2	1.97	0.47
1:F:513:LEU:HD12	1:F:513:LEU:HA	1.73	0.47
1:B:237:PHE:HD2	1:B:282:MET:HE1	1.80	0.47
1:B:437:ILE:H	1:B:437:ILE:HG12	1.43	0.47
1:E:166:GLU:OE1	1:E:167:LEU:N	2.48	0.47
1:E:324:VAL:HA	1:E:327:ARG:HG3	1.95	0.47
1:B:491:ASN:N	1:B:491:ASN:OD1	2.46	0.47
1:A:356:PHE:HB3	1:A:360:ASP:CB	2.44	0.47
1:C:563:LEU:HD12	1:C:563:LEU:HA	1.68	0.47
1:A:429:ASP:N	1:A:429:ASP:OD1	2.47	0.46
1:E:282:MET:O	1:E:286:GLU:N	2.48	0.46
1:B:141:MET:HG2	1:B:214:PHE:HZ	1.78	0.46
1:B:591:ASP:OD1	1:B:596:ARG:HG3	2.15	0.46
1:C:178:GLN:HG3	1:C:179:LYS:HD2	1.97	0.46
1:D:149:THR:O	1:D:207:GLY:HA3	2.15	0.46
1:E:167:LEU:HD21	1:E:185:PRO:HG2	1.97	0.46
1:E:360:ASP:HA	1:E:363[B]:ASN:HD21	1.81	0.46
1:B:214:PHE:HD2	1:B:215:THR:HG23	1.79	0.46
1:C:356:PHE:HB3	1:C:360:ASP:HB3	1.95	0.46
1:E:360:ASP:HA	1:E:363[A]:ASN:HD21	1.81	0.46
1:F:177:PHE:O	1:F:180:LEU:HG	2.14	0.46
1:B:210:LYS:HB2	1:B:210:LYS:HE2	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLU:HG2	1:B:289:GLU:HB2	1.98	0.46
1:D:198:LYS:HB2	2:D:701:ANP:O1G	2.15	0.46
1:E:142:LEU:HA	1:E:214:PHE:HE1	1.81	0.46
1:C:141:MET:N	1:C:141:MET:SD	2.88	0.46
1:A:501:ARG:O	1:A:505:THR:OG1	2.32	0.46
1:F:382:MET:HA	1:F:385:PHE:CD2	2.50	0.46
1:B:395:GLY:O	1:B:439:ARG:NH1	2.48	0.46
1:B:435:THR:OG1	1:B:436:ILE:N	2.47	0.46
1:D:213:PHE:HE2	1:D:247:ILE:HG13	1.80	0.46
1:F:279:LEU:HD21	1:F:293:VAL:HG22	1.97	0.46
1:C:170:TYR:HE2	1:C:184:ILE:HB	1.81	0.46
1:C:216:ILE:O	1:C:252:GLN:NE2	2.48	0.46
1:E:211:VAL:CB	1:E:245:PRO:HA	2.40	0.46
1:E:215:THR:HA	1:E:249:PHE:HB3	1.98	0.46
1:D:143:THR:HG22	1:D:214:PHE:CE1	2.51	0.46
1:B:487:THR:HG22	1:C:457:ALA:O	2.16	0.46
1:D:170:TYR:CG	1:D:184:ILE:HG23	2.51	0.46
1:D:215:THR:HB	1:D:249:PHE:HD2	1.81	0.46
1:D:331:LEU:O	1:D:335:MET:HB2	2.15	0.46
1:F:200:LEU:HG	1:F:200:LEU:O	2.15	0.46
1:B:171:LEU:HB2	1:B:172:ARG:NH1	2.31	0.46
1:A:192:GLY:HA3	1:A:319:VAL:HG23	1.97	0.46
1:A:244:ALA:C	1:A:246:CYS:H	2.20	0.46
1:F:276:ASN:OD1	1:F:276:ASN:N	2.49	0.46
1:C:361:LEU:HD12	1:C:361:LEU:H	1.80	0.46
1:A:377:LYS:HZ2	1:A:377:LYS:HA	1.80	0.45
1:C:172:ARG:HD3	1:C:172:ARG:N	2.32	0.45
1:C:180:LEU:C	1:C:182:GLY:N	2.70	0.45
1:A:323:ASP:OD1	1:A:323:ASP:N	2.48	0.45
1:E:376:ASN:O	1:E:377:LYS:NZ	2.44	0.45
1:F:436:ILE:HD13	1:F:436:ILE:HA	1.80	0.45
1:B:190:MET:O	1:B:198:LYS:NZ	2.48	0.45
1:B:210:LYS:O	1:B:212:PRO:HD3	2.16	0.45
1:B:564:LEU:HD12	1:B:564:LEU:HA	1.72	0.45
1:A:151:PHE:HA	1:A:204:ALA:CB	2.47	0.45
1:A:327:ARG:HH12	1:A:354:PRO:HA	1.82	0.45
1:B:170:TYR:HD1	1:B:177:PHE:HE2	1.64	0.45
1:C:233:VAL:O	1:C:236:MET:N	2.50	0.45
1:D:462:LEU:HD12	1:D:462:LEU:HA	1.76	0.45
1:A:231:SER:C	1:A:233:VAL:H	2.20	0.45
1:D:143:THR:H	1:D:214:PHE:HE1	1.65	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:THR:O	1:F:196:THR:OG1	2.35	0.45
1:B:327:ARG:NH2	1:B:354:PRO:HA	2.31	0.45
1:A:449:LEU:HA	1:A:449:LEU:HD12	1.77	0.45
1:F:327:ARG:HH21	1:F:355:GLY:H	1.64	0.45
1:D:233:VAL:O	1:D:236:MET:N	2.50	0.45
1:F:174:PRO:O	1:F:176:ARG:N	2.50	0.45
1:B:187:GLY:HA2	1:B:293:VAL:O	2.17	0.45
1:D:170:TYR:CE1	1:D:184:ILE:HG12	2.51	0.45
1:D:216:ILE:HB	1:D:248:ILE:HG22	1.99	0.45
1:B:418:HIS:HE1	1:B:469:LEU:O	2.00	0.45
1:B:196:THR:HG22	1:B:357:SER:HB2	1.99	0.45
1:C:200:LEU:HA	1:C:200:LEU:HD22	1.67	0.45
1:A:246:CYS:O	1:A:247:ILE:HG23	2.16	0.44
1:E:213:PHE:HB3	1:E:245:PRO:HB3	1.98	0.44
1:D:235:ASP:OD1	1:D:236:MET:N	2.51	0.44
1:D:237:PHE:HB3	1:D:277:GLN:CD	2.38	0.44
1:F:195:GLY:H	2:F:701:ANP:PG	2.35	0.44
1:E:189:LEU:O	1:E:316:GLN:HA	2.17	0.44
1:E:324:VAL:HG23	1:E:327:ARG:HE	1.83	0.44
1:F:281:GLU:HG3	1:F:282:MET:N	2.33	0.44
1:C:321:LEU:HD12	1:C:355:GLY:HA2	2.00	0.44
1:C:434:VAL:HG13	1:C:446:THR:HG23	1.98	0.44
1:D:214:PHE:HD2	1:D:215:THR:HG23	1.81	0.44
1:E:423:ARG:NH2	1:E:590:ASP:OD1	2.48	0.44
1:F:511:GLU:OE1	1:F:511:GLU:N	2.45	0.44
1:B:171:LEU:HD13	1:B:211:VAL:HG21	1.99	0.44
1:B:186:LYS:HE3	1:B:314:ASP:HB2	1.99	0.44
1:D:323:ASP:OD1	1:D:323:ASP:N	2.51	0.44
1:E:425:VAL:HG22	1:E:426:PRO:HD2	2.00	0.44
1:B:170:TYR:HD1	1:B:177:PHE:CE2	2.35	0.44
1:B:449:LEU:HD12	1:B:449:LEU:HA	1.85	0.44
1:E:331:LEU:O	1:E:335:MET:HB2	2.17	0.44
1:E:352:GLY:C	1:E:354:PRO:HD3	2.39	0.44
1:E:469:LEU:HA	1:E:469:LEU:HD23	1.81	0.44
1:B:351:ARG:HH11	1:B:451:GLU:HA	1.82	0.44
1:A:279:LEU:HD13	1:A:282:MET:HB2	1.99	0.43
1:C:286:GLU:OE2	1:C:290:GLY:N	2.51	0.43
1:D:425:VAL:HG22	1:D:426:PRO:HD2	1.99	0.43
1:B:181:GLY:O	1:B:183:LYS:N	2.52	0.43
1:C:323:ASP:O	1:C:326:GLY:N	2.51	0.43
1:C:416:ALA:O	1:C:418:HIS:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ILE:HD12	1:A:456:SER:H	1.83	0.43
1:A:492:ASP:OD1	1:A:492:ASP:N	2.51	0.43
1:E:215:THR:HB	1:E:249:PHE:HB3	1.99	0.43
1:F:168:VAL:HG22	1:F:205:ILE:HG13	2.00	0.43
1:F:189:LEU:HA	1:F:295:ALA:O	2.18	0.43
1:C:186:LYS:HD2	1:C:311:GLY:HA2	1.99	0.43
1:E:239:GLN:O	1:E:242:LYS:HE2	2.17	0.43
1:A:483:GLU:OE1	1:A:484:HIS:NE2	2.51	0.43
1:E:397:GLU:HG2	1:E:439:ARG:HH12	1.83	0.43
1:F:189:LEU:O	1:F:316:GLN:HA	2.18	0.43
1:B:273:GLN:HE21	1:B:273:GLN:HB3	1.69	0.43
1:C:188:VAL:HA	1:C:315:ARG:O	2.18	0.43
1:C:348:ILE:HG12	1:C:351:ARG:HH21	1.83	0.43
1:A:436:ILE:HA	1:A:436:ILE:HD13	1.75	0.43
1:D:394:MET:HE2	1:D:394:MET:H	1.83	0.43
1:E:574:MET:HG3	1:E:592:LEU:HD13	2.00	0.43
1:F:198:LYS:HD3	1:F:198:LYS:HA	1.74	0.43
1:C:141:MET:N	1:C:214:PHE:HZ	2.17	0.43
1:C:190:MET:HA	1:C:317:VAL:O	2.19	0.43
1:C:195:GLY:N	2:C:701:ANP:O2B	2.51	0.43
1:C:455:ILE:HD12	1:C:456:SER:H	1.82	0.43
1:A:388:ALA:O	1:A:392:ILE:HG12	2.19	0.43
1:A:474:LEU:HD23	1:A:474:LEU:HA	1.78	0.43
1:E:242:LYS:HD2	1:E:242:LYS:O	2.19	0.43
1:E:286:GLU:HG2	1:E:291:ILE:HD12	2.00	0.43
1:F:436:ILE:HG12	1:F:578:LEU:HD12	2.01	0.43
1:B:184:ILE:HG12	1:B:185:PRO:O	2.19	0.43
1:A:403:MET:O	1:A:408:LYS:NZ	2.51	0.43
1:D:164:VAL:HG21	1:D:201:LEU:HD22	2.01	0.43
1:D:167:LEU:O	1:D:171:LEU:HG	2.19	0.43
1:E:188:VAL:HG23	1:E:292:ILE:HD12	2.01	0.43
1:F:238:GLU:O	1:F:241:LYS:NZ	2.30	0.43
1:A:144:GLU:HA	1:A:213:PHE:CE1	2.52	0.43
1:A:250:ILE:HD11	1:A:293:VAL:HG23	2.00	0.43
1:E:200:LEU:HD22	2:E:701:ANP:C5	2.49	0.43
1:E:286:GLU:CD	1:E:291:ILE:HB	2.40	0.43
1:B:198:LYS:HB3	1:B:198:LYS:HE3	1.53	0.43
1:B:206:ALA:O	1:B:211:VAL:HB	2.18	0.43
1:C:173:GLU:N	1:C:174:PRO:HD3	2.34	0.43
1:A:186:LYS:HD3	1:A:311:GLY:O	2.18	0.42
1:A:242:LYS:HD2	1:A:242:LYS:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:GLY:N	1:F:314:ASP:OD1	2.29	0.42
1:B:372:ALA:HB2	1:B:384:GLU:OE2	2.19	0.42
1:E:146:GLN:OE1	1:E:146:GLN:N	2.52	0.42
1:E:241:LYS:HE2	1:E:241:LYS:HB2	1.88	0.42
1:F:213:PHE:HD2	1:F:215:THR:HG22	1.84	0.42
1:F:325:ARG:HA	1:F:325:ARG:HD2	1.60	0.42
1:D:199:THR:O	1:D:203:LYS:HG2	2.18	0.42
1:E:205:ILE:O	1:E:208:GLU:N	2.50	0.42
1:E:323:ASP:O	1:E:326:GLY:N	2.53	0.42
1:E:352:GLY:O	1:E:354:PRO:HD3	2.19	0.42
1:B:241:LYS:HE2	1:B:241:LYS:HB2	1.85	0.42
1:E:186:LYS:HD2	1:E:186:LYS:HA	1.82	0.42
1:E:203:LYS:NZ	1:E:203:LYS:HB3	2.33	0.42
1:B:168:VAL:HA	1:B:171:LEU:HG	2.00	0.42
1:B:248:ILE:HG13	1:B:292:ILE:O	2.20	0.42
1:B:323:ASP:O	1:B:327:ARG:HG3	2.20	0.42
1:B:436:ILE:HG13	1:B:578:LEU:HD12	2.00	0.42
1:B:575:LYS:HE3	1:B:575:LYS:HB3	1.91	0.42
1:D:237:PHE:HZ	1:D:274:THR:HG22	1.84	0.42
1:A:339:PRO:CB	1:A:379:VAL:HG21	2.50	0.42
1:D:174:PRO:HG3	1:D:288:ASN:HB3	2.00	0.42
1:D:357:SER:OG	1:D:358:GLY:N	2.52	0.42
1:D:564:LEU:HD12	1:D:564:LEU:HA	1.66	0.42
1:E:249:PHE:CE2	1:E:251[A]:ASP:HB2	2.54	0.42
1:B:352:GLY:O	1:B:353:THR:OG1	2.28	0.42
1:B:420:ILE:HD12	1:B:571:LEU:HD12	2.02	0.42
1:B:469:LEU:HD23	1:B:469:LEU:HA	1.82	0.42
1:A:171:LEU:HD22	1:A:246:CYS:HB3	2.02	0.42
1:A:213:PHE:HB2	1:A:245:PRO:HD3	2.01	0.42
1:E:200:LEU:HD22	2:E:701:ANP:C4	2.49	0.42
1:F:186:LYS:HB3	1:F:279:LEU:HD13	2.01	0.42
1:C:190:MET:H	1:C:190:MET:HG2	1.47	0.42
1:A:276:ASN:OD1	1:A:276:ASN:N	2.50	0.42
1:E:216:ILE:HG21	1:E:248:ILE:HG23	2.01	0.42
1:B:327:ARG:HH22	1:B:355:GLY:H	1.68	0.42
1:F:196:THR:HG21	1:F:321:LEU:HD23	2.02	0.42
1:D:474:LEU:HD23	1:D:474:LEU:HA	1.90	0.42
1:C:198:LYS:HZ3	1:C:198:LYS:HB3	1.85	0.42
1:D:143:THR:N	1:D:214:PHE:HE1	2.17	0.41
1:B:200:LEU:HD12	1:B:200:LEU:HA	1.74	0.41
1:D:237:PHE:HB3	1:D:277:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:OG1	1:B:216:ILE:N	2.51	0.41
1:A:244:ALA:HB1	1:A:245:PRO:HD2	2.02	0.41
1:E:168:VAL:HG21	1:E:205:ILE:HG12	2.02	0.41
1:E:249:PHE:CE2	1:E:251[B]:ASP:HB2	2.54	0.41
1:B:282:MET:HB3	1:B:286:GLU:OE2	2.19	0.41
1:B:462:LEU:HD12	1:B:462:LEU:HA	1.73	0.41
1:C:172:ARG:HH11	1:C:172:ARG:N	2.08	0.41
1:C:203:LYS:HE3	1:C:203:LYS:HB3	1.88	0.41
1:A:170:TYR:CD1	1:A:177:PHE:CE1	3.09	0.41
1:A:190:MET:HE2	1:A:190:MET:HB2	1.80	0.41
1:A:201:LEU:H	1:A:201:LEU:HG	1.41	0.41
1:D:437:ILE:H	1:D:437:ILE:HG12	1.28	0.41
1:F:201:LEU:H	1:F:201:LEU:HG	1.31	0.41
1:B:142:LEU:HA	1:B:214:PHE:CE1	2.55	0.41
1:A:327:ARG:HG2	1:A:361:LEU:HD11	2.03	0.41
1:D:353:THR:HB	1:D:356:PHE:CG	2.56	0.41
1:C:153:ASP:OD1	1:C:153:ASP:N	2.53	0.41
1:C:163:GLU:OE2	1:C:315:ARG:NH2	2.54	0.41
1:A:231:SER:O	1:A:231:SER:OG	2.22	0.41
1:D:348:ILE:HD13	1:D:351:ARG:HH21	1.85	0.41
1:F:278:MET:HA	1:F:281:GLU:HB3	2.03	0.41
1:C:158:ASP:HA	1:C:161:LYS:HE3	2.03	0.41
1:C:189:LEU:HA	1:C:295:ALA:O	2.21	0.41
1:C:198:LYS:NZ	1:C:296:ALA:HB1	2.36	0.41
1:A:215:THR:HB	1:A:249:PHE:CD2	2.55	0.41
1:B:476:GLU:O	1:B:480:TYR:HB2	2.21	0.41
1:B:483:GLU:HG2	1:B:484:HIS:ND1	2.36	0.41
1:C:341:ALA:HB1	1:C:342:PRO:HD2	2.02	0.41
1:E:190:MET:HE1	1:E:201:LEU:HD21	2.03	0.41
1:E:413:TYR:CE2	1:E:479:ILE:HG21	2.55	0.41
1:F:144:GLU:HG3	1:F:146:GLN:HG2	2.03	0.41
1:B:179:LYS:HA	1:B:179:LYS:HD3	1.94	0.41
1:B:414:HIS:NE2	1:B:472:GLY:HA3	2.36	0.41
1:B:441:ARG:H	1:B:441:ARG:HD3	1.85	0.41
1:C:154:VAL:O	1:C:155:ALA:C	2.58	0.41
1:C:167:LEU:HG	1:C:171:LEU:HD21	2.03	0.41
1:C:198:LYS:HZ1	1:C:296:ALA:HB1	1.86	0.41
1:E:236:MET:HA	1:E:239:GLN:OE1	2.20	0.41
1:F:172:ARG:HD3	1:F:172:ARG:HA	1.70	0.41
1:F:389:LYS:O	1:F:392:ILE:HG13	2.21	0.41
1:B:403:MET:HB3	1:B:407:GLN:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LEU:HD23	1:B:474:LEU:HA	1.69	0.41
1:C:208:GLU:O	1:C:211:VAL:HG12	2.20	0.41
1:A:242:LYS:HB3	1:A:242:LYS:HE3	1.94	0.40
1:B:149:THR:OG1	1:B:203:LYS:HG3	2.21	0.40
1:A:247:ILE:HG22	1:A:292:ILE:HG23	2.03	0.40
1:E:233:VAL:O	1:E:234:ARG:C	2.60	0.40
1:F:429:ASP:OD1	1:F:429:ASP:N	2.53	0.40
1:B:142:LEU:HA	1:B:214:PHE:HE1	1.86	0.40
1:C:430:PRO:HD2	1:C:449:LEU:O	2.20	0.40
1:E:348:ILE:HG12	1:E:351:ARG:NH2	2.35	0.40
1:F:382:MET:O	1:F:385:PHE:HB2	2.21	0.40
1:C:215:THR:HG22	1:C:247:ILE:O	2.21	0.40
1:C:237:PHE:HB3	1:C:282:MET:HE2	2.03	0.40
1:B:203:LYS:HA	1:B:203:LYS:HD2	1.91	0.40
1:A:484:HIS:CD2	1:A:484:HIS:N	2.89	0.40
1:B:325:ARG:O	1:B:325:ARG:HD3	2.22	0.40
1:C:210:LYS:HB2	1:C:210:LYS:HE2	1.76	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	405/644 (63%)	362 (89%)	42 (10%)	1 (0%)	47 78
1	B	405/644 (63%)	380 (94%)	25 (6%)	0	100 100
1	C	405/644 (63%)	371 (92%)	32 (8%)	2 (0%)	29 61
1	D	405/644 (63%)	377 (93%)	28 (7%)	0	100 100
1	E	405/644 (63%)	371 (92%)	33 (8%)	1 (0%)	47 78
1	F	405/644 (63%)	362 (89%)	43 (11%)	0	100 100
All	All	2430/3864 (63%)	2223 (92%)	203 (8%)	4 (0%)	50 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	183	LYS
1	A	456	SER
1	E	185	PRO
1	C	182	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	337/527 (64%)	283 (84%)	54 (16%)	2 10
1	B	337/527 (64%)	267 (79%)	70 (21%)	1 3
1	C	337/527 (64%)	285 (85%)	52 (15%)	2 11
1	D	337/527 (64%)	276 (82%)	61 (18%)	1 6
1	E	337/527 (64%)	282 (84%)	55 (16%)	2 9
1	F	337/527 (64%)	293 (87%)	44 (13%)	4 15
All	All	2022/3162 (64%)	1686 (83%)	336 (17%)	5 8

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LEU
1	A	153	ASP
1	A	154	VAL
1	A	172	ARG
1	A	176	ARG
1	A	184	ILE
1	A	189	LEU
1	A	190	MET
1	A	196	THR
1	A	201	LEU
1	A	203	LYS
1	A	211	VAL
1	A	215	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	ARG
1	A	233	VAL
1	A	235	ASP
1	A	242	LYS
1	A	250	ILE
1	A	275	LEU
1	A	278	MET
1	A	279	LEU
1	A	292	ILE
1	A	294	ILE
1	A	314	ASP
1	A	316	GLN
1	A	324	VAL
1	A	338	VAL
1	A	353	THR
1	A	371	PHE
1	A	377	LYS
1	A	380	VAL
1	A	382	MET
1	A	391	LYS
1	A	394	MET
1	A	404	THR
1	A	407	GLN
1	A	420	ILE
1	A	421	ILE
1	A	429	ASP
1	A	439	ARG
1	A	455	ILE
1	A	462	LEU
1	A	483	GLU
1	A	492	ASP
1	A	493	ILE
1	A	504	VAL
1	A	536	HIS
1	A	554	GLU
1	A	559	ARG
1	A	563	LEU
1	A	581	TYR
1	A	588	GLN
1	A	597	ASP
1	A	599	ARG
1	D	145	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	150	THR
1	D	167	LEU
1	D	170	TYR
1	D	172	ARG
1	D	173	GLU
1	D	176	ARG
1	D	180	LEU
1	D	189	LEU
1	D	190	MET
1	D	198	LYS
1	D	211	VAL
1	D	213	PHE
1	D	215	THR
1	D	234	ARG
1	D	247	ILE
1	D	281	GLU
1	D	292	ILE
1	D	293	VAL
1	D	298	ASN
1	D	318	VAL
1	D	325	ARG
1	D	360	ASP
1	D	367	GLU
1	D	371	PHE
1	D	379	VAL
1	D	380	VAL
1	D	383	VAL
1	D	387	LYS
1	D	390	ASP
1	D	391	LYS
1	D	394	MET
1	D	397	GLU
1	D	410	SER
1	D	429	ASP
1	D	434	VAL
1	D	437	ILE
1	D	439	ARG
1	D	453	ASP
1	D	455	ILE
1	D	462	LEU
1	D	464	SER
1	D	468	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	469	LEU
1	D	483	GLU
1	D	485	VAL
1	D	487	THR
1	D	493	ILE
1	D	495	VAL
1	D	510	SER
1	D	537	MET
1	D	538	SER
1	D	561	ARG
1	D	563	LEU
1	D	564	LEU
1	D	569	ASP
1	D	578	LEU
1	D	580	LYS
1	D	581	TYR
1	D	595	ARG
1	D	604	TRP
1	E	166	GLU
1	E	172	ARG
1	E	173	GLU
1	E	183	LYS
1	E	186	LYS
1	E	189	LEU
1	E	191	VAL
1	E	198	LYS
1	E	201	LEU
1	E	203	LYS
1	E	205	ILE
1	E	208	GLU
1	E	211	VAL
1	E	214	PHE
1	E	217	SER
1	E	238	GLU
1	E	242	LYS
1	E	247	ILE
1	E	275	LEU
1	E	279	LEU
1	E	282	MET
1	E	298	ASN
1	E	313	PHE
1	E	315	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	324	VAL
1	E	325	ARG
1	E	335	MET
1	E	337	ARG
1	E	338	VAL
1	E	340	LEU
1	E	360	ASP
1	E	363[A]	ASN
1	E	363[B]	ASN
1	E	367	GLU
1	E	374	ARG
1	E	385	PHE
1	E	390	ASP
1	E	397	GLU
1	E	398	ARG
1	E	410	SER
1	E	418	HIS
1	E	425	VAL
1	E	431	VAL
1	E	439	ARG
1	E	468	THR
1	E	498	ASN
1	E	543	ARG
1	E	559	ARG
1	E	561	ARG
1	E	568	MET
1	E	580	LYS
1	E	581	TYR
1	E	597	ASP
1	E	598	VAL
1	E	604	TRP
1	F	154	VAL
1	F	184	ILE
1	F	196	THR
1	F	199	THR
1	F	201	LEU
1	F	205	ILE
1	F	213	PHE
1	F	242	LYS
1	F	275	LEU
1	F	281	GLU
1	F	283	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	291	ILE
1	F	324	VAL
1	F	329	GLN
1	F	338	VAL
1	F	353	THR
1	F	385	PHE
1	F	391	LYS
1	F	404	THR
1	F	411	THR
1	F	420	ILE
1	F	421	ILE
1	F	425	VAL
1	F	428	HIS
1	F	435	THR
1	F	437	ILE
1	F	439	ARG
1	F	459	ARG
1	F	462	LEU
1	F	484	HIS
1	F	493	ILE
1	F	504	VAL
1	F	513	LEU
1	F	538	SER
1	F	541	THR
1	F	548	GLU
1	F	559	ARG
1	F	562	GLN
1	F	564	LEU
1	F	569	ASP
1	F	581	TYR
1	F	596	ARG
1	F	598	VAL
1	F	604	TRP
1	B	142	LEU
1	B	150	THR
1	B	154	VAL
1	B	164	VAL
1	B	172	ARG
1	B	173	GLU
1	B	176	ARG
1	B	183	LYS
1	B	186	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	189	LEU
1	B	190	MET
1	B	191	VAL
1	B	215	THR
1	B	216	ILE
1	B	233	VAL
1	B	235	ASP
1	B	236	MET
1	B	242	LYS
1	B	247	ILE
1	B	248	ILE
1	B	250	ILE
1	B	251[A]	ASP
1	B	251[B]	ASP
1	B	273	GLN
1	B	275	LEU
1	B	278	MET
1	B	282	MET
1	B	293	VAL
1	B	294	ILE
1	B	314	ASP
1	B	318	VAL
1	B	325	ARG
1	B	337	ARG
1	B	360	ASP
1	B	371	PHE
1	B	377	LYS
1	B	383	VAL
1	B	391	LYS
1	B	401	MET
1	B	404	THR
1	B	410	SER
1	B	411	THR
1	B	418	HIS
1	B	423	ARG
1	B	424	LEU
1	B	425	VAL
1	B	429	ASP
1	B	434	VAL
1	B	437	ILE
1	B	439	ARG
1	B	441	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	462	LEU
1	B	464	SER
1	B	468	THR
1	B	485	VAL
1	B	487	THR
1	B	493	ILE
1	B	499	LEU
1	B	507	TRP
1	B	510	SER
1	B	536	HIS
1	B	538	SER
1	B	552	LEU
1	B	559	ARG
1	B	568	MET
1	B	578	LEU
1	B	581	TYR
1	B	598	VAL
1	B	599	ARG
1	B	604	TRP
1	C	141	MET
1	C	150	THR
1	C	153	ASP
1	C	169	GLU
1	C	172	ARG
1	C	173	GLU
1	C	183	LYS
1	C	184	ILE
1	C	188	VAL
1	C	190	MET
1	C	196	THR
1	C	200	LEU
1	C	214	PHE
1	C	237	PHE
1	C	242	LYS
1	C	246	CYS
1	C	247	ILE
1	C	252	GLN
1	C	253	ILE
1	C	282	MET
1	C	292	ILE
1	C	293	VAL
1	C	337	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	340	LEU
1	C	360	ASP
1	C	367	GLU
1	C	380	VAL
1	C	382	MET
1	C	393	MET
1	C	402	VAL
1	C	404	THR
1	C	429	ASP
1	C	431	VAL
1	C	434	VAL
1	C	439	ARG
1	C	445	VAL
1	C	455	ILE
1	C	463	GLU
1	C	467	SER
1	C	468	THR
1	C	486	SER
1	C	487	THR
1	C	505	THR
1	C	536	HIS
1	C	547	GLN
1	C	554	GLU
1	C	564	LEU
1	C	581	TYR
1	C	593	MET
1	C	597	ASP
1	C	598	VAL
1	C	604	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	329	GLN
1	F	239	GLN
1	B	178	GLN
1	B	273	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	ANP	D	701	4	29,33,33	1.15	2 (6%)	31,52,52	1.63	5 (16%)
2	ANP	B	701	-	29,33,33	1.26	3 (10%)	31,52,52	1.54	2 (6%)
2	ANP	C	701	4	29,33,33	1.12	1 (3%)	31,52,52	1.72	5 (16%)
2	ANP	E	701	4	29,33,33	1.15	2 (6%)	31,52,52	1.35	4 (12%)
2	ANP	F	701	4	29,33,33	1.23	2 (6%)	31,52,52	1.54	4 (12%)
2	ANP	A	701	4	29,33,33	1.25	2 (6%)	31,52,52	1.76	5 (16%)

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	ANP	D	701	4	-	6/14/38/38	0/3/3/3
2	ANP	B	701	-	-	4/14/38/38	0/3/3/3
2	ANP	C	701	4	-	5/14/38/38	0/3/3/3
2	ANP	E	701	4	-	4/14/38/38	0/3/3/3
2	ANP	F	701	4	-	9/14/38/38	0/3/3/3
2	ANP	A	701	4	-	4/14/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	ANP	PB-O3A	-4.74	1.53	1.59
2	B	701	ANP	PB-O3A	-4.68	1.53	1.59
2	A	701	ANP	PB-O3A	-4.67	1.53	1.59
2	D	701	ANP	PB-O3A	-4.21	1.53	1.59
2	E	701	ANP	PB-O3A	-4.09	1.53	1.59
2	C	701	ANP	PB-O3A	-3.85	1.54	1.59
2	B	701	ANP	PG-N3B	2.36	1.69	1.63
2	E	701	ANP	PG-N3B	2.26	1.69	1.63
2	A	701	ANP	PG-N3B	2.23	1.69	1.63
2	D	701	ANP	PG-N3B	2.19	1.69	1.63
2	B	701	ANP	PG-O1G	2.15	1.49	1.46
2	F	701	ANP	PG-O1G	2.02	1.49	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ANP	PB-O3A-PA	-7.50	106.21	132.62
2	B	701	ANP	PB-O3A-PA	-7.21	107.23	132.62
2	C	701	ANP	PB-O3A-PA	-7.19	107.28	132.62
2	F	701	ANP	PB-O3A-PA	-6.81	108.62	132.62
2	D	701	ANP	PB-O3A-PA	-6.44	109.93	132.62
2	E	701	ANP	PB-O3A-PA	-5.00	115.01	132.62
2	D	701	ANP	O3G-PG-O1G	-3.42	104.85	113.45
2	A	701	ANP	O3G-PG-O1G	-3.23	105.34	113.45
2	C	701	ANP	O2B-PB-O3A	2.95	114.49	104.64
2	A	701	ANP	O1G-PG-N3B	-2.75	107.72	111.77
2	C	701	ANP	O1B-PB-N3B	-2.54	108.02	111.77
2	C	701	ANP	O1G-PG-N3B	-2.43	108.19	111.77
2	D	701	ANP	O1G-PG-N3B	-2.37	108.28	111.77
2	E	701	ANP	O1B-PB-N3B	-2.34	108.33	111.77
2	A	701	ANP	C5-C6-N6	2.27	123.80	120.35
2	B	701	ANP	C5-C6-N6	2.27	123.80	120.35
2	E	701	ANP	O3G-PG-O1G	-2.27	107.75	113.45
2	E	701	ANP	C5-C6-N6	2.26	123.79	120.35
2	D	701	ANP	C5-C6-N6	2.26	123.79	120.35
2	C	701	ANP	C5-C6-N6	2.23	123.74	120.35
2	F	701	ANP	C5-C6-N6	2.23	123.73	120.35
2	F	701	ANP	O2B-PB-O3A	2.18	111.92	104.64
2	F	701	ANP	O1G-PG-N3B	-2.16	108.58	111.77
2	A	701	ANP	O2B-PB-O3A	2.03	111.41	104.64
2	D	701	ANP	O2B-PB-O3A	2.02	111.39	104.64

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ANP	PG-N3B-PB-O1B
2	D	701	ANP	PG-N3B-PB-O1B
2	D	701	ANP	O4'-C4'-C5'-O5'
2	D	701	ANP	C3'-C4'-C5'-O5'
2	E	701	ANP	PB-N3B-PG-O1G
2	E	701	ANP	C3'-C4'-C5'-O5'
2	F	701	ANP	PB-N3B-PG-O1G
2	F	701	ANP	PG-N3B-PB-O1B
2	F	701	ANP	PG-N3B-PB-O3A
2	F	701	ANP	C5'-O5'-PA-O1A
2	F	701	ANP	C5'-O5'-PA-O2A
2	F	701	ANP	O4'-C4'-C5'-O5'
2	F	701	ANP	C3'-C4'-C5'-O5'
2	B	701	ANP	PB-N3B-PG-O1G
2	B	701	ANP	C5'-O5'-PA-O1A
2	B	701	ANP	C5'-O5'-PA-O2A
2	C	701	ANP	PG-N3B-PB-O1B
2	C	701	ANP	PG-N3B-PB-O3A
2	C	701	ANP	C5'-O5'-PA-O2A
2	C	701	ANP	C5'-O5'-PA-O3A
2	A	701	ANP	O4'-C4'-C5'-O5'
2	A	701	ANP	C3'-C4'-C5'-O5'
2	E	701	ANP	O4'-C4'-C5'-O5'
2	F	701	ANP	PB-O3A-PA-O1A
2	A	701	ANP	C4'-C5'-O5'-PA
2	F	701	ANP	C5'-O5'-PA-O3A
2	D	701	ANP	C4'-C5'-O5'-PA
2	D	701	ANP	PB-O3A-PA-O2A
2	C	701	ANP	PB-O3A-PA-O2A
2	E	701	ANP	PB-O3A-PA-O1A
2	B	701	ANP	C5'-O5'-PA-O3A
2	D	701	ANP	C5'-O5'-PA-O1A

There are no ring outliers.

6 monomers are involved in 34 short contacts:

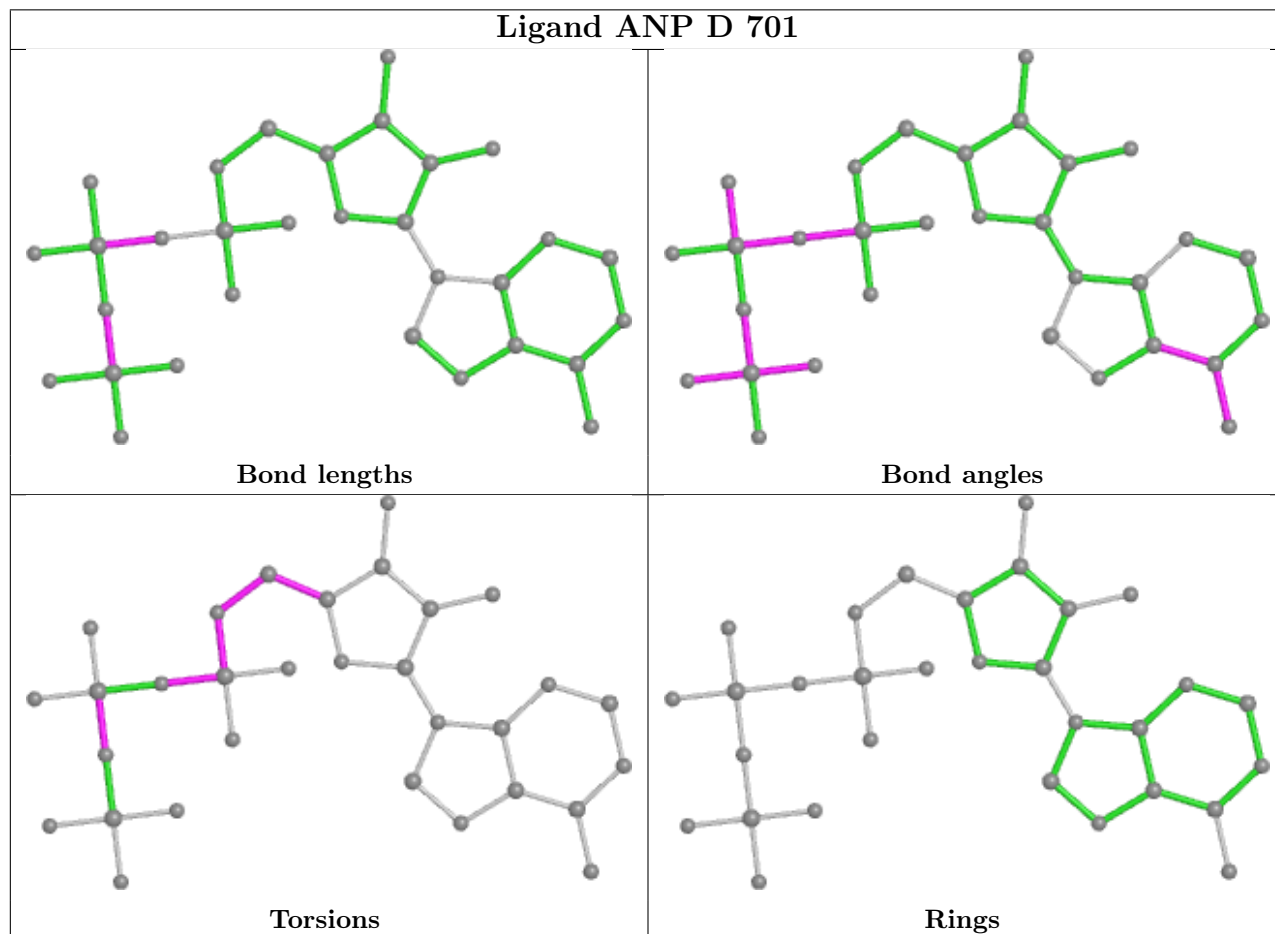
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	ANP	7	0
2	B	701	ANP	3	0
2	C	701	ANP	5	0

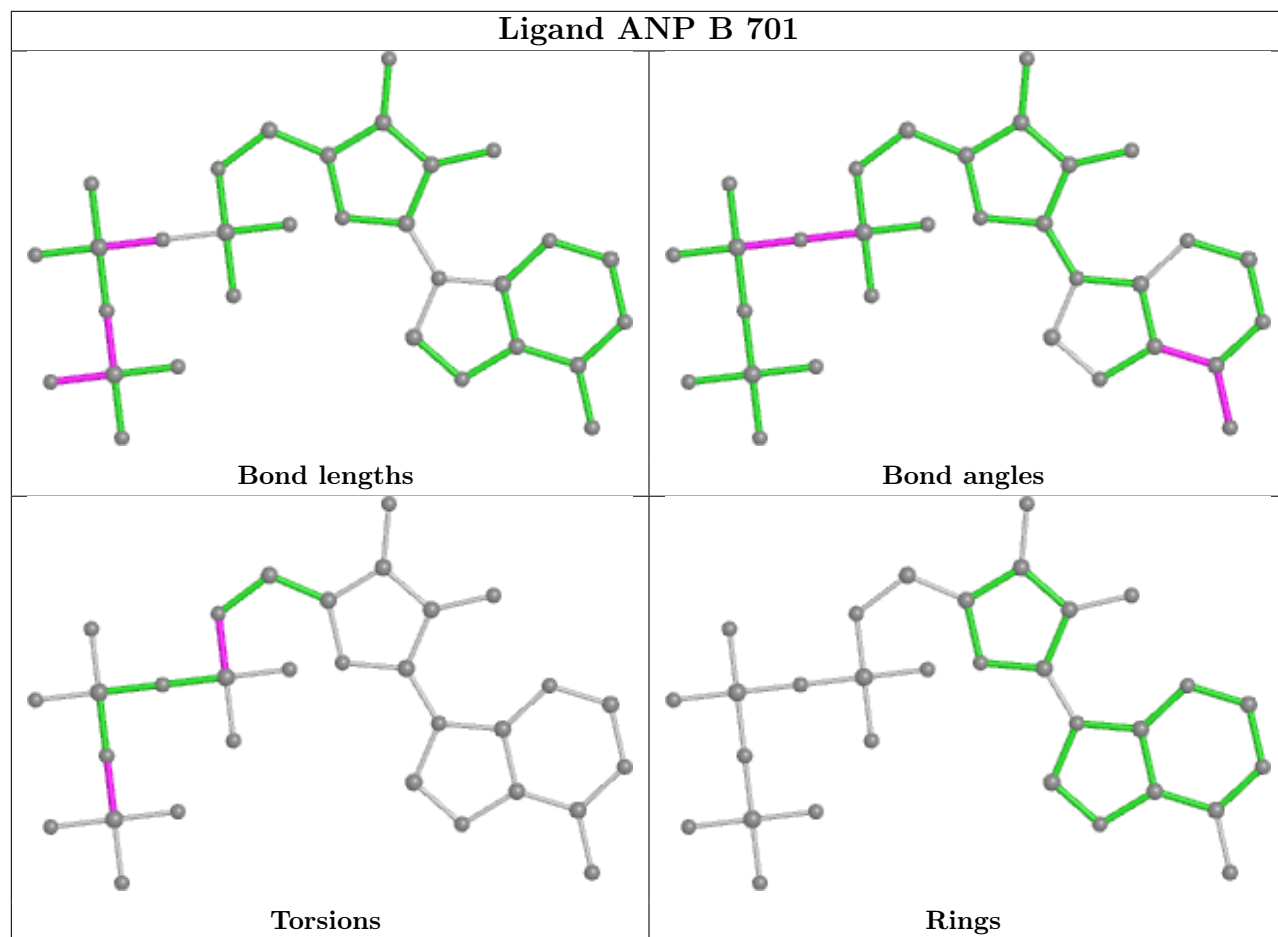
Continued on next page...

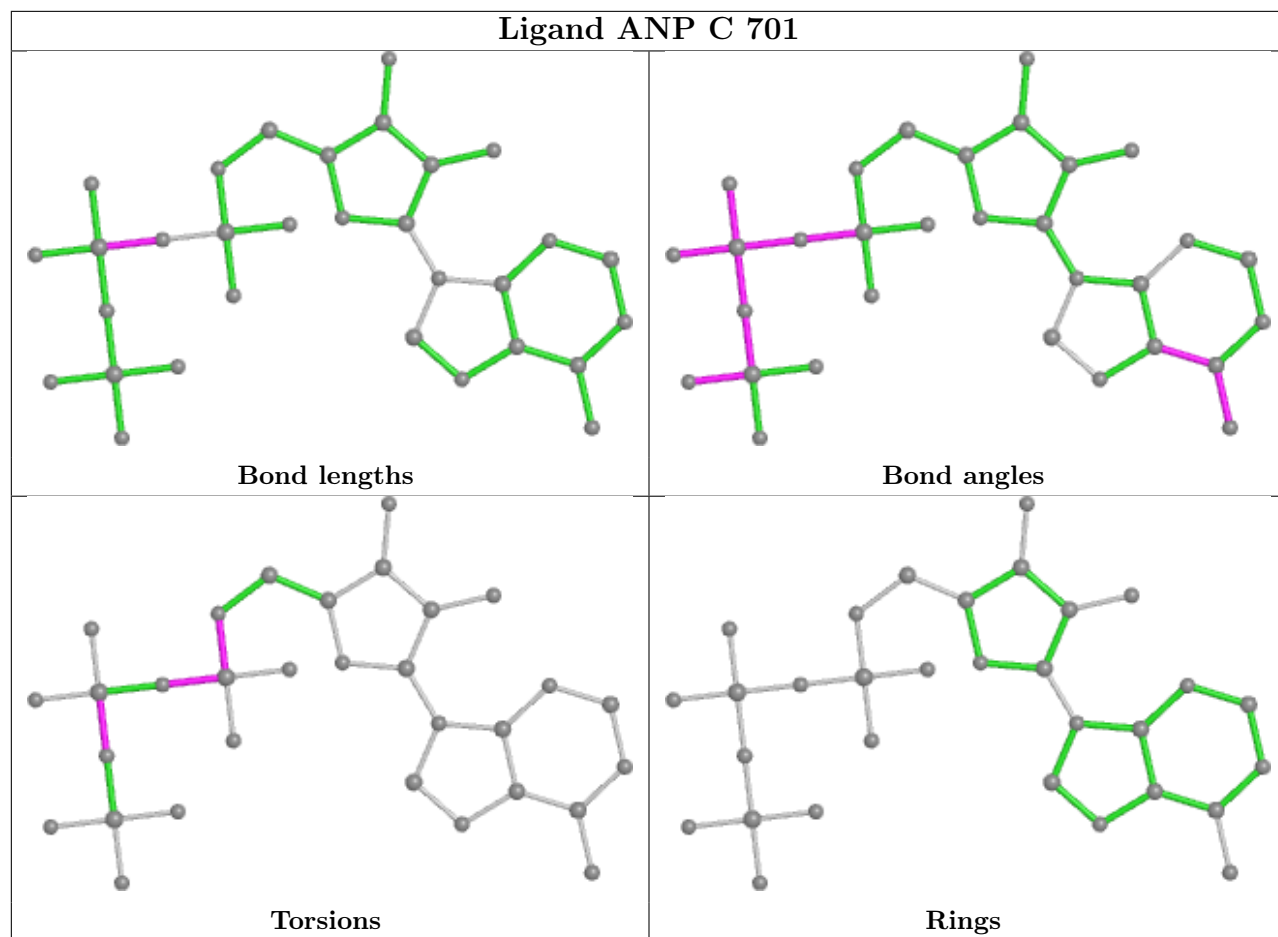
Continued from previous page...

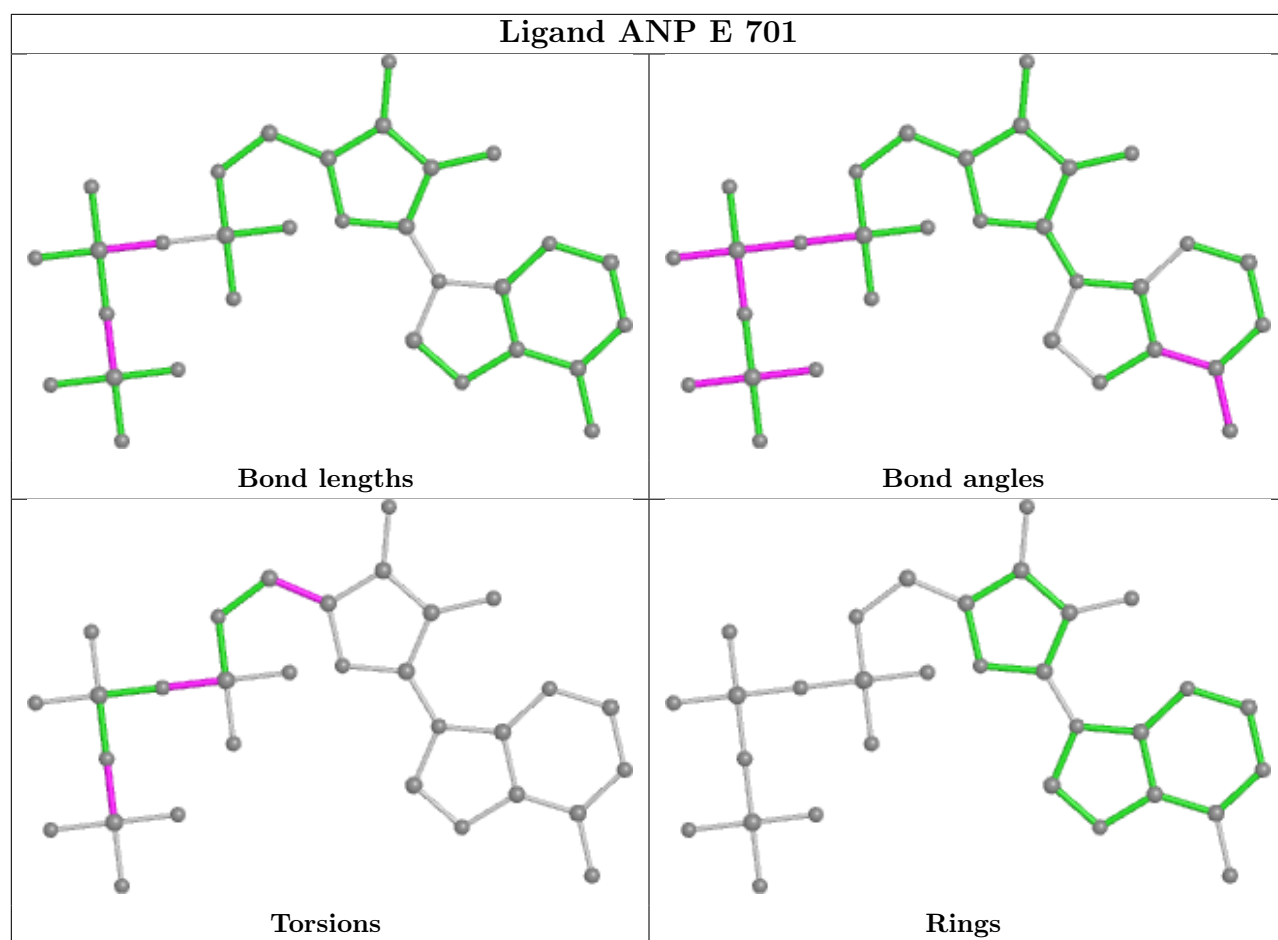
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	ANP	5	0
2	F	701	ANP	6	0
2	A	701	ANP	8	0

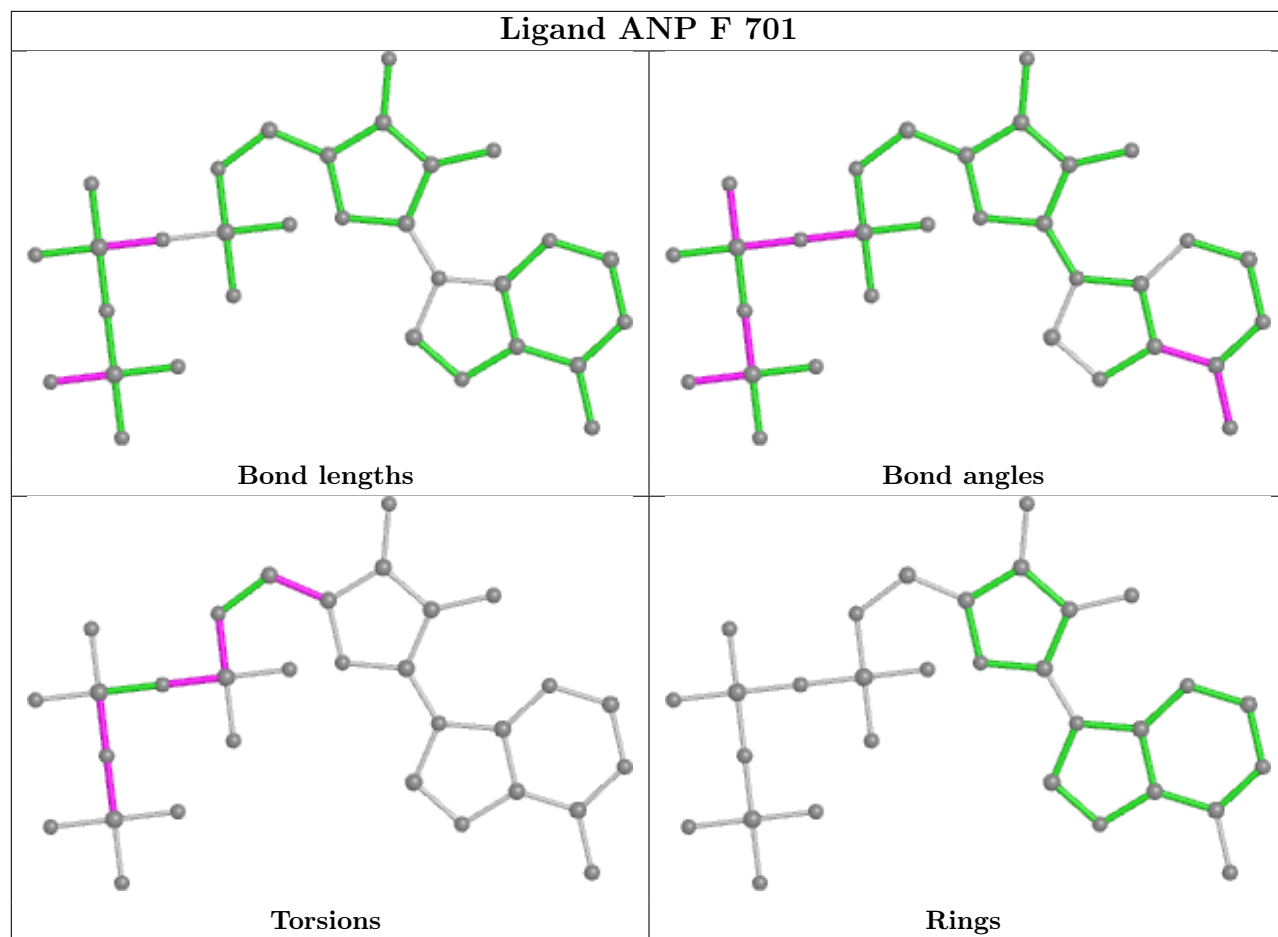
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

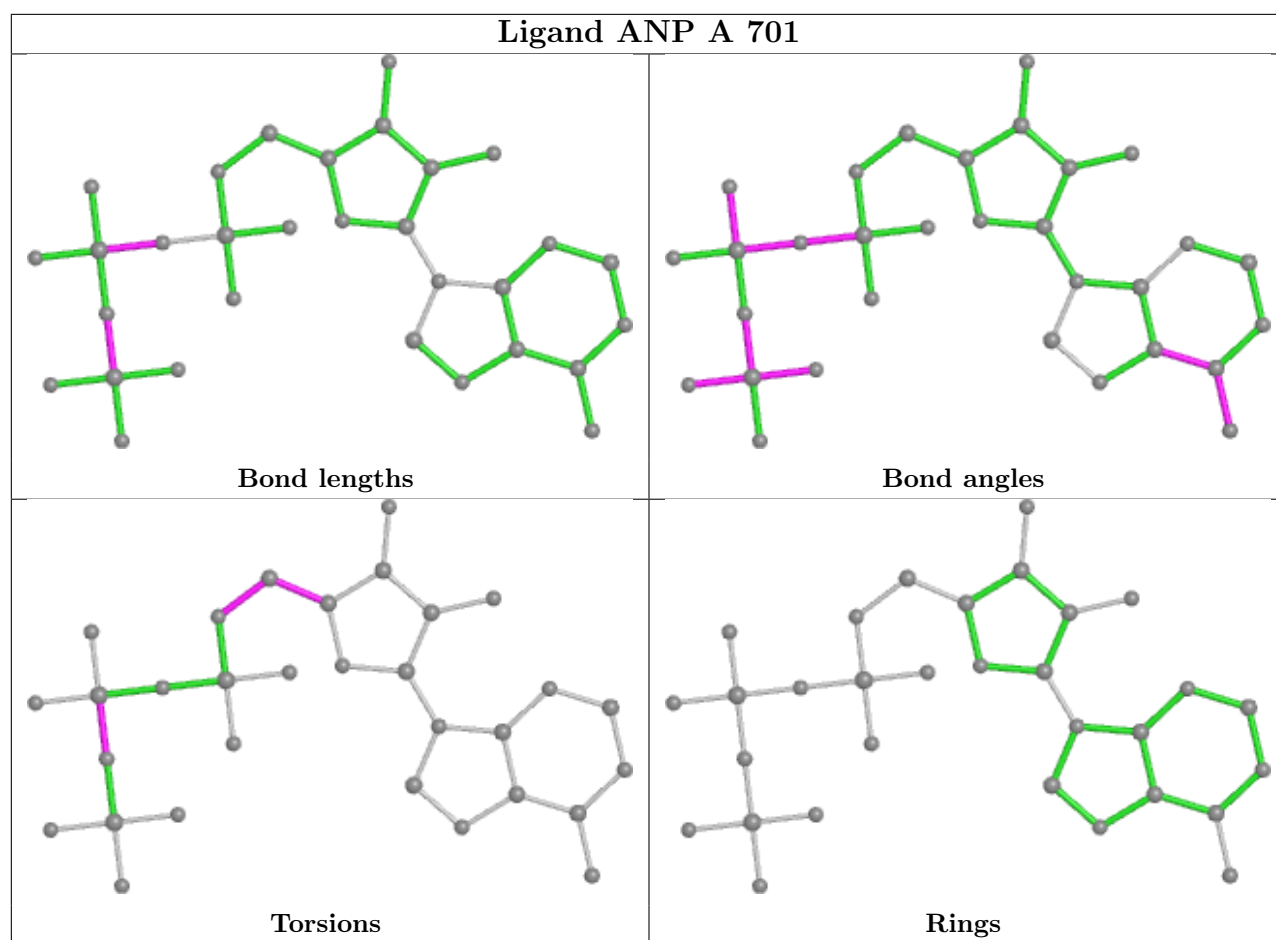












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

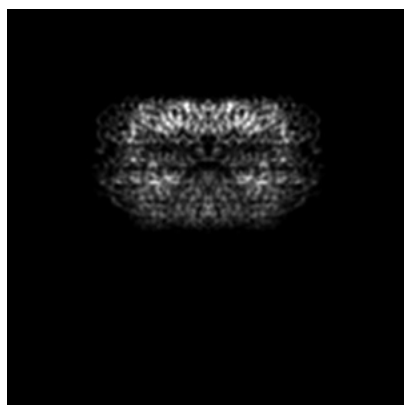
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32521. These allow visual inspection of the internal detail of the map and identification of artifacts.

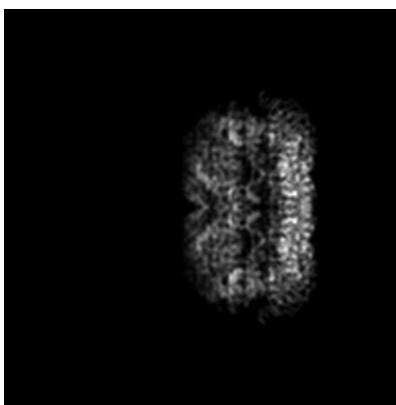
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

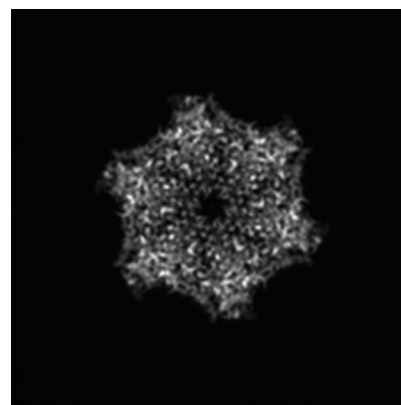
6.1.1 Primary map



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: 80



Y Index: 80



Z Index: 80

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: 64



Y Index: 72



Z Index: 113

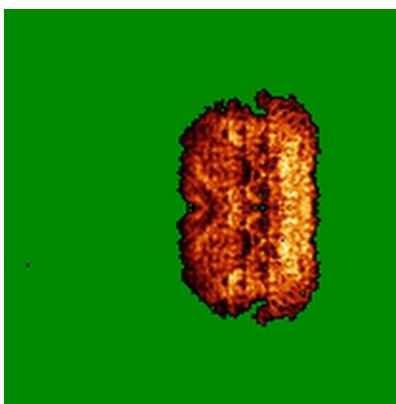
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

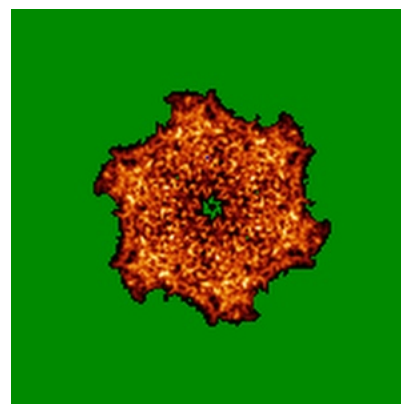
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.172. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

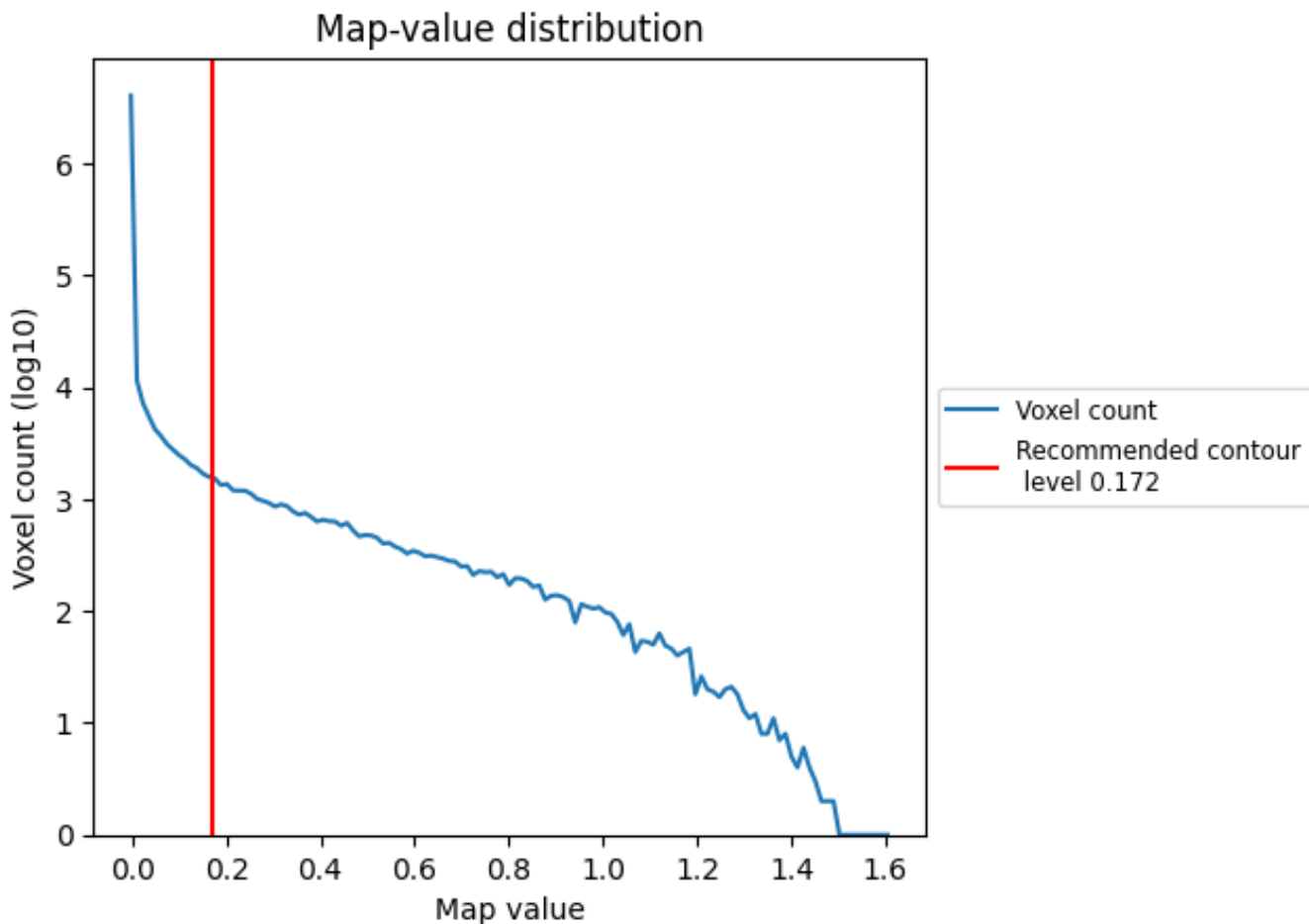
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

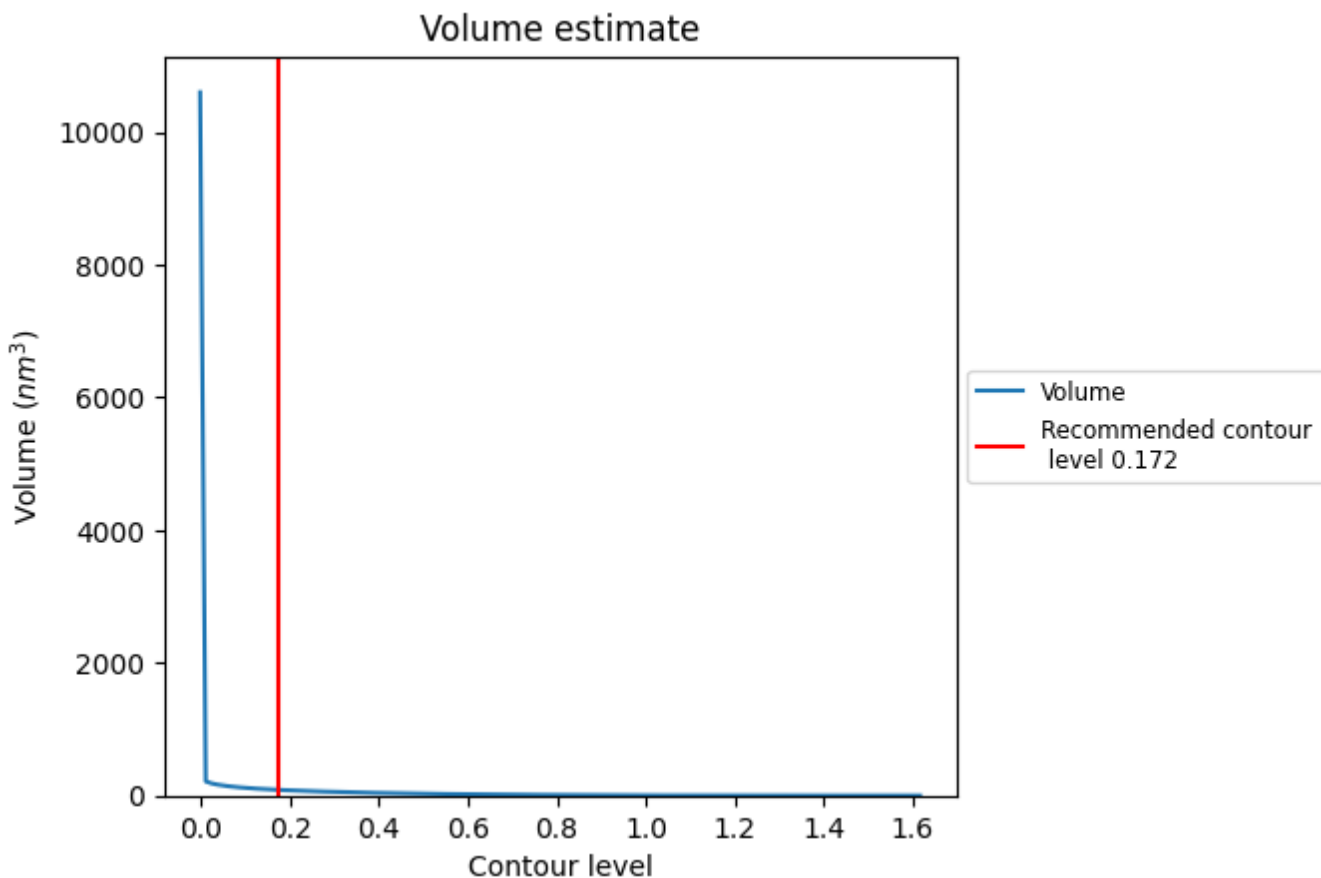
This section contains the results of statistical analysis of the map.

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.

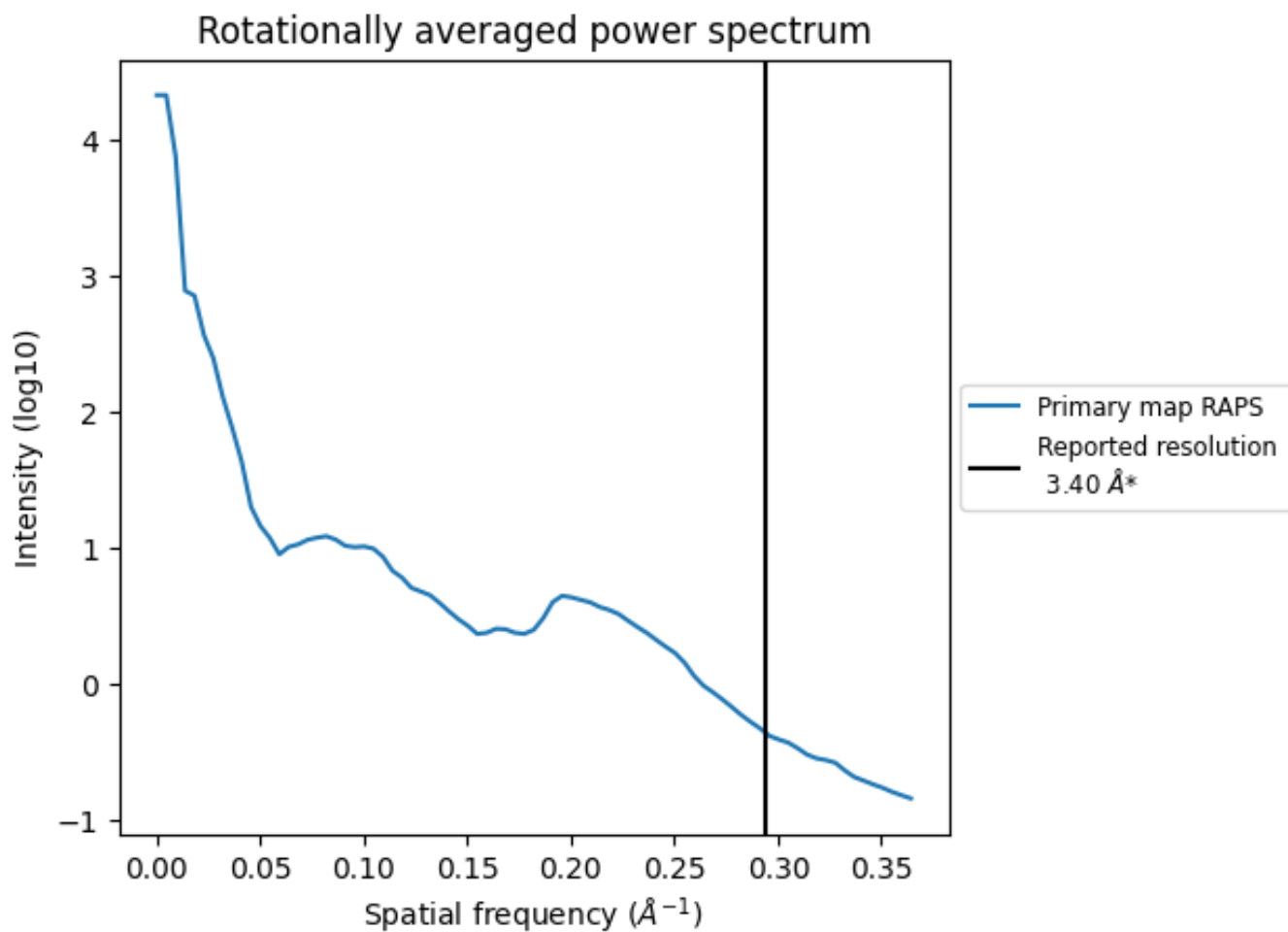
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 78 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 0.294 Å⁻¹

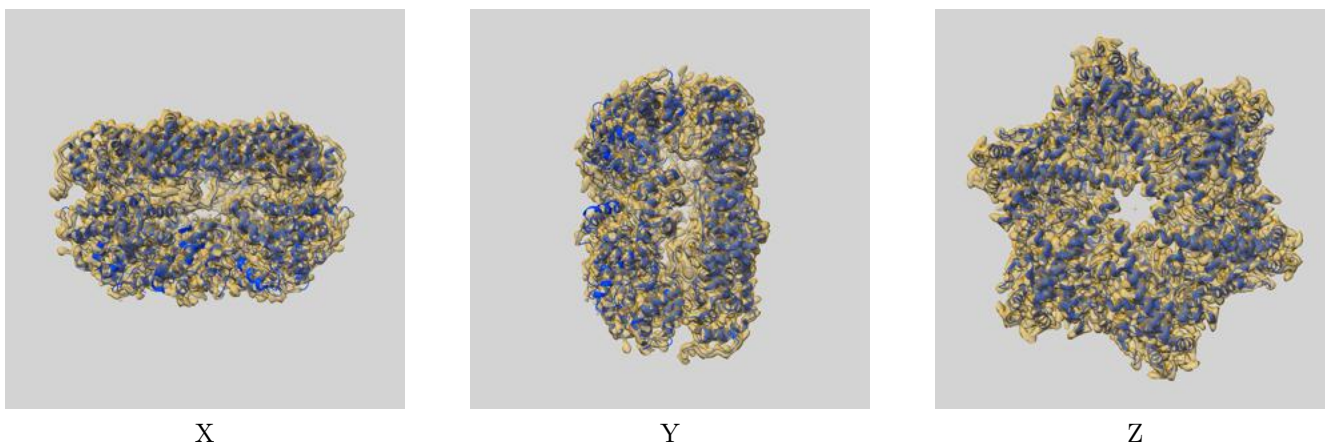
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

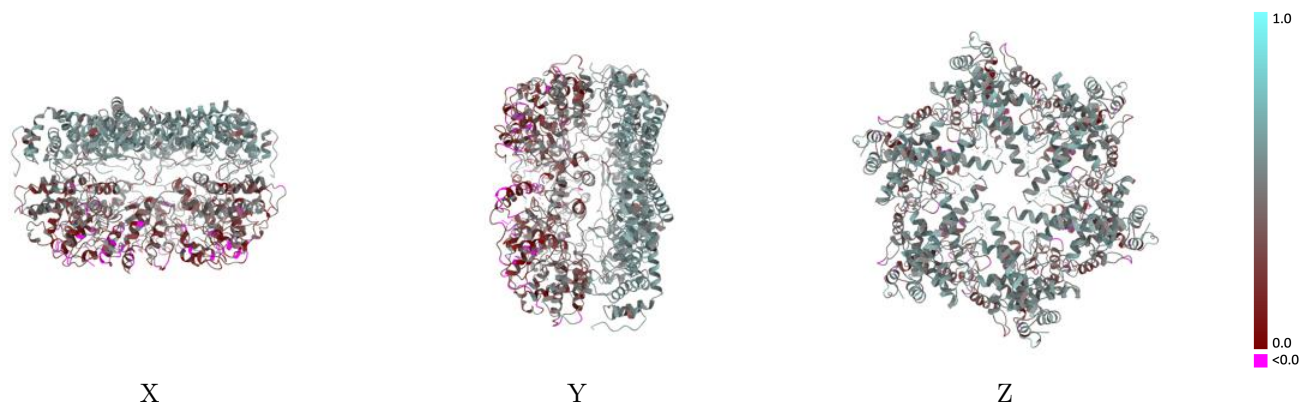
This section contains information regarding the fit between EMDB map EMD-32521 and PDB model 7WI4. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



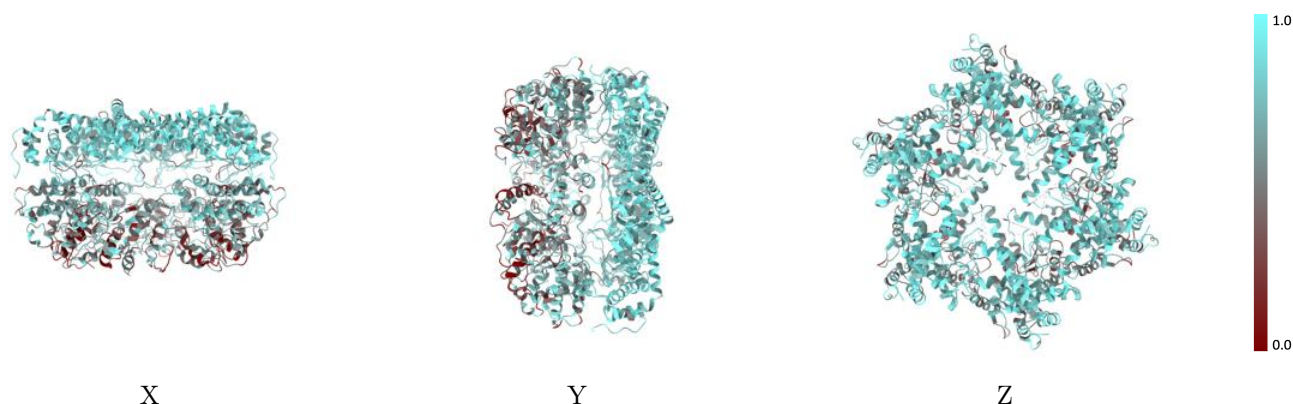
The images above show the 3D surface view of the map at the recommended contour level 0.172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



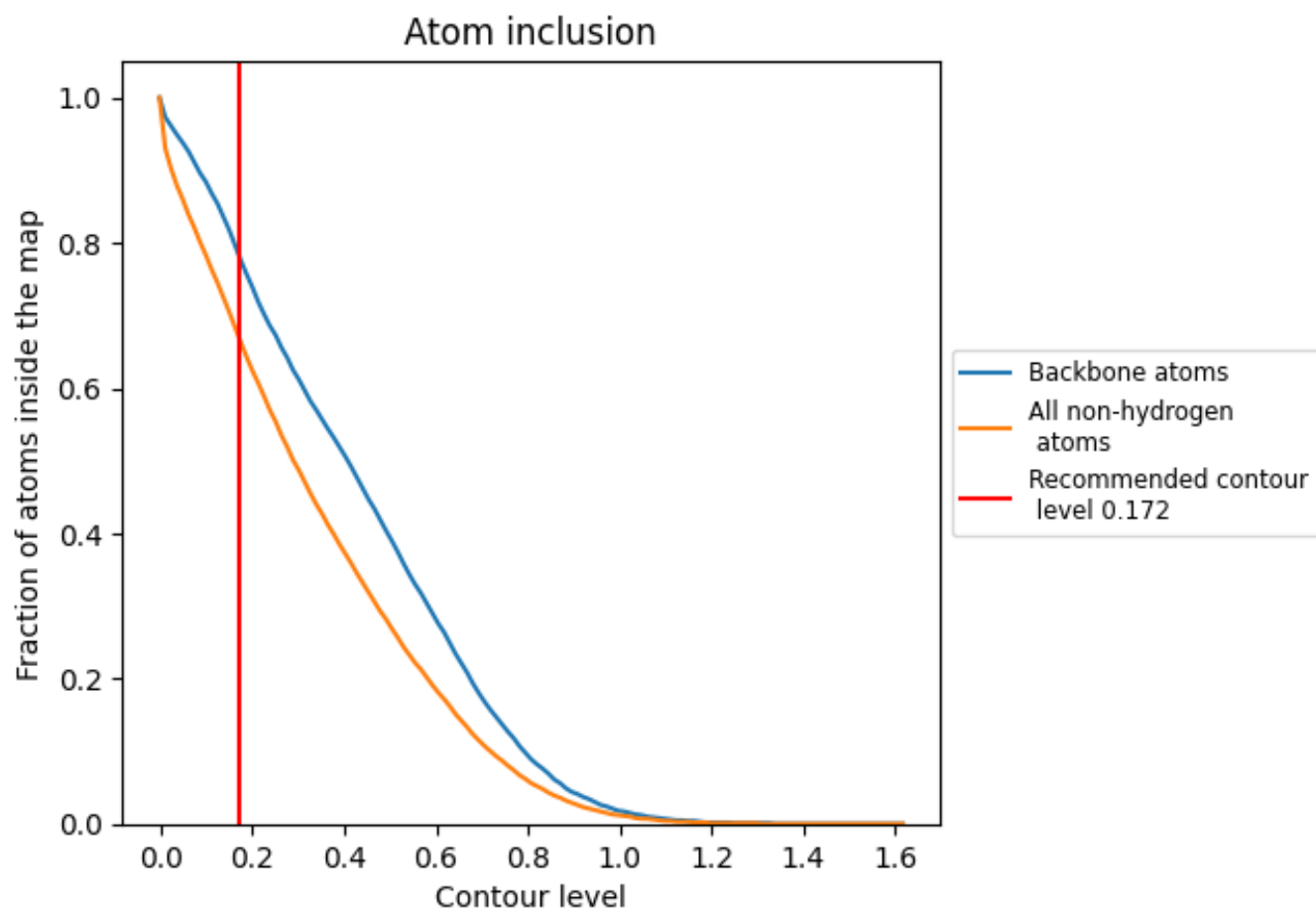
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.172).















9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6670	 0.4320
A	 0.6650	 0.4350
B	 0.6630	 0.4270
C	 0.6640	 0.4340
D	 0.6620	 0.4290
E	 0.6730	 0.4340
F	 0.6760	 0.4360

