



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:14 AM UTC

PDB ID : 6TD5 / pdb_00006td5
EMDB ID : EMD-10463
Title : Leishmania tarentolae proteasome 20S subunit complexed with LXE408 and bortezomib
Authors : Srinivas, H.
Deposited on : 2019-11-07
Resolution : 3.20 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:

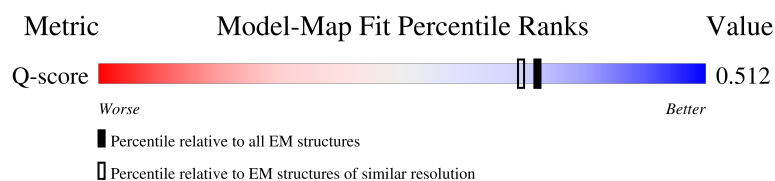
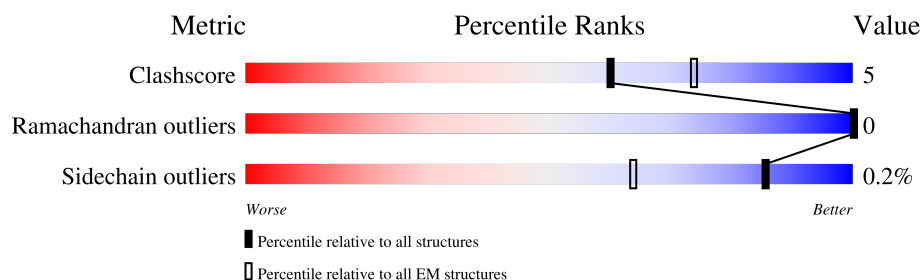
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.20 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	15020 (2.70 - 3.70)

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	250	
1	a	250	
2	B	231	
2	b	231	

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Mol	Chain	Length	Quality of chain
3	C	285	
3	c	285	
4	D	248	
4	d	248	
5	E	344	
5	e	344	
6	F	428	
6	f	428	
7	G	238	
7	g	238	
8	H	229	
8	h	229	
9	I	225	
9	i	225	
10	J	205	
10	j	205	
11	K	206	
11	k	206	
12	L	203	
12	l	203	
13	M	339	
13	m	339	
14	N	220	
14	n	220	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 49408 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 Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		
1	a	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		

- Molecule 2 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		
2	b	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		

- Molecule 3 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		
3	c	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		

- Molecule 4 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		
4	d	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		

- Molecule 5 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	235	Total	C	N	O	S	0	0
			1802	1119	315	356	12		
5	e	235	Total	C	N	O	S	0	0
			1802	1119	315	356	12		

- Molecule 6 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		
6	f	238	Total	C	N	O	S	0	0
			1869	1173	325	359	12		

- Molecule 7 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1741	1085	308	338	10		
7	g	230	Total	C	N	O	S	0	0
			1741	1085	308	338	10		

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total	C	N	O	S	0	0
			1709	1062	295	340	12		
8	h	229	Total	C	N	O	S	0	0
			1709	1062	295	340	12		

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		
9	i	219	Total	C	N	O	S	0	0
			1659	1037	292	318	12		

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1557	980	259	302	16		

- Molecule 11 is a protein called Proteasome subunit family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		
11	k	206	Total	C	N	O	S	0	0
			1612	1012	280	304	16		

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	201	Total	C	N	O	S	0	0
			1573	995	276	295	7		
12	l	201	Total	C	N	O	S	0	0
			1573	995	276	295	7		

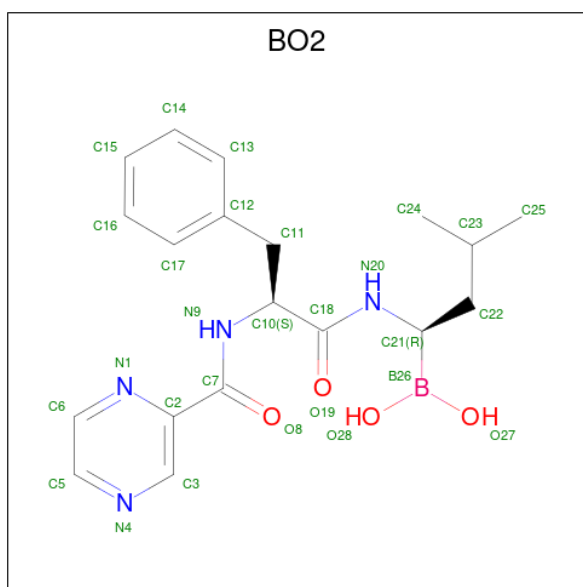
- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		
13	m	214	Total	C	N	O	S	0	0
			1702	1079	287	324	12		

- Molecule 14 is a protein called Proteasome subunit beta.

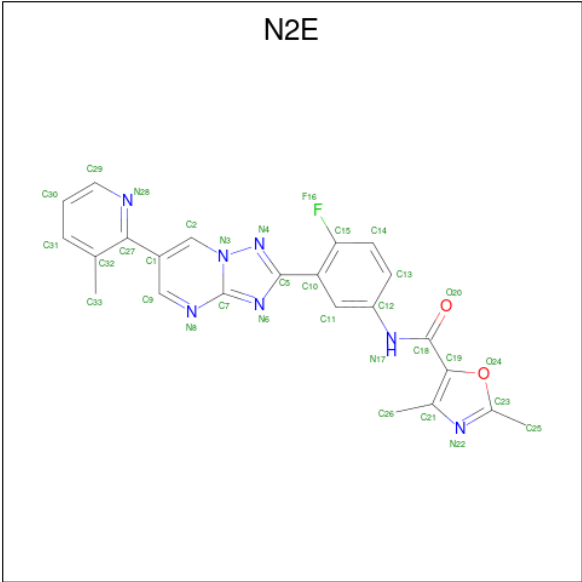
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		
14	n	218	Total	C	N	O	S	0	0
			1712	1083	292	323	14		

- Molecule 15 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (CCD ID: BO2) (formula: C₁₉H₂₅BN₄O₄).



Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	I	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	L	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	h	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	i	1	Total	B	C	N	O	0
			28	1	19	4	4	
15	l	1	Total	B	C	N	O	0
			28	1	19	4	4	

- Molecule 16 is {N}-[4-fluoranyl-3-[6-(3-methylpyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-2-yl]phenyl]-2,4-dimethyl-1,3-oxazole-5-carboxamide (CCD ID: N2E) (formula: C₂₃H₁₈FN₇O₂).

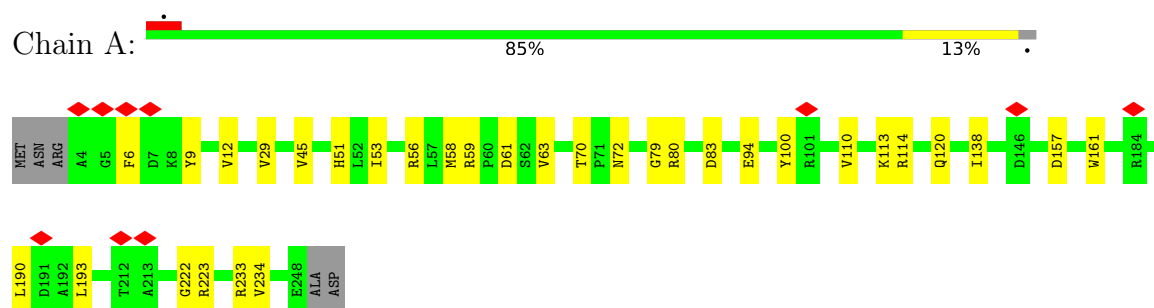


Mol	Chain	Residues	Atoms					AltConf
16	L	1	Total	C	F	N	O	0
			33	23	1	7	2	
16	1	1	Total	C	F	N	O	0
			33	23	1	7	2	

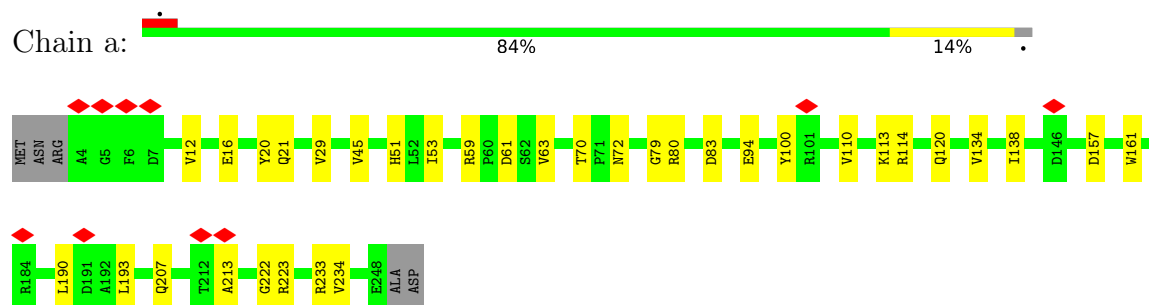
3 Residue-property plots [i](#)

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

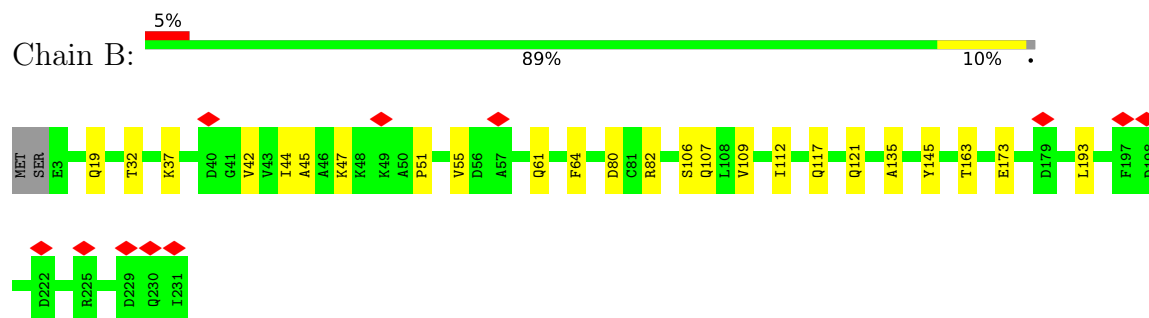
- Molecule 1: Proteasome subunit alpha type



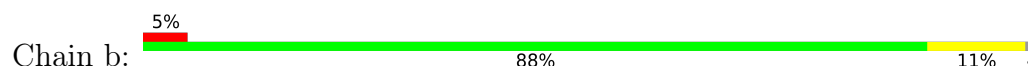
- Molecule 1: Proteasome subunit alpha type

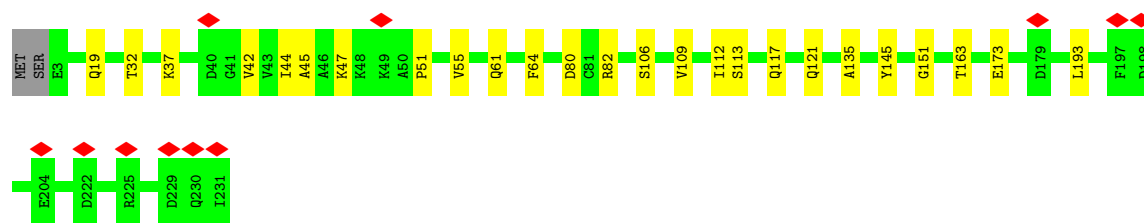


- Molecule 2: Proteasome subunit alpha type

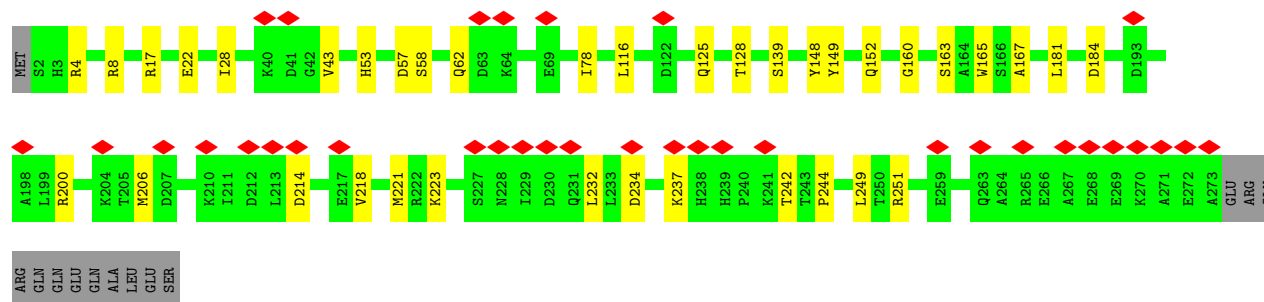
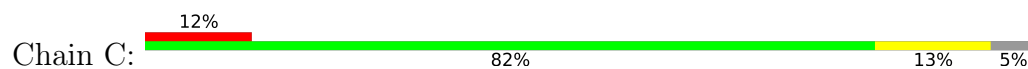


- Molecule 2: Proteasome subunit alpha type

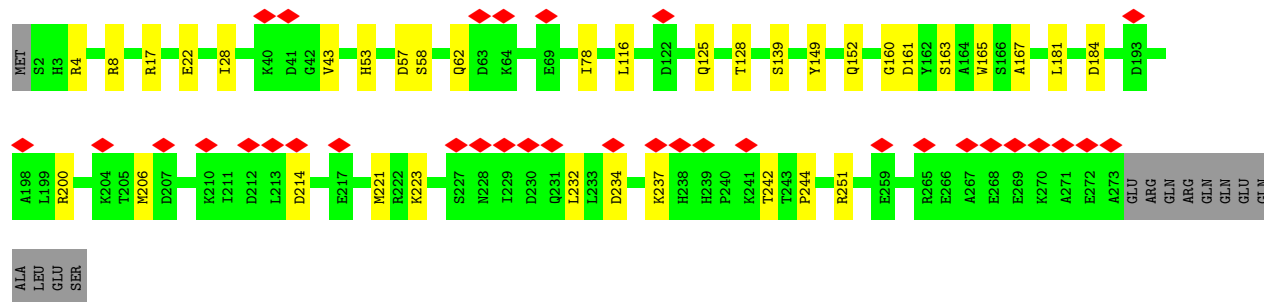
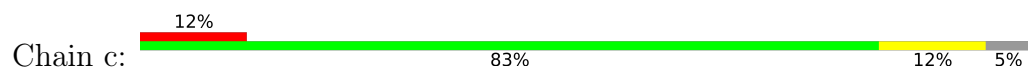




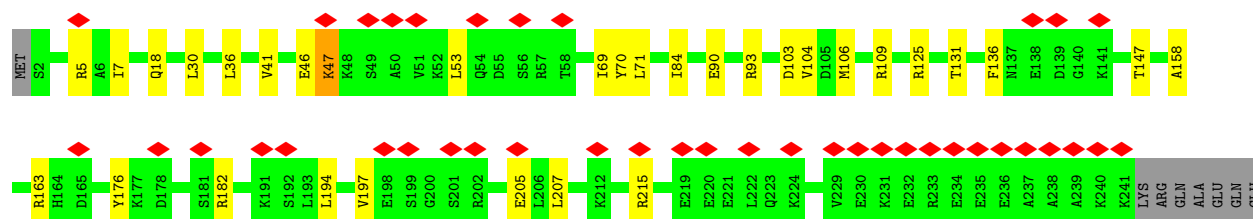
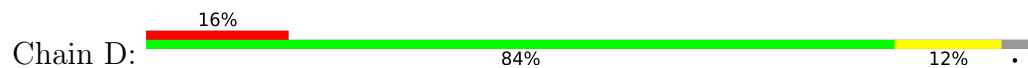
• Molecule 3: Proteasome subunit alpha type



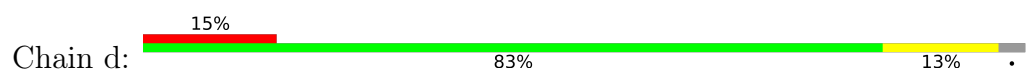
• Molecule 3: Proteasome subunit alpha type

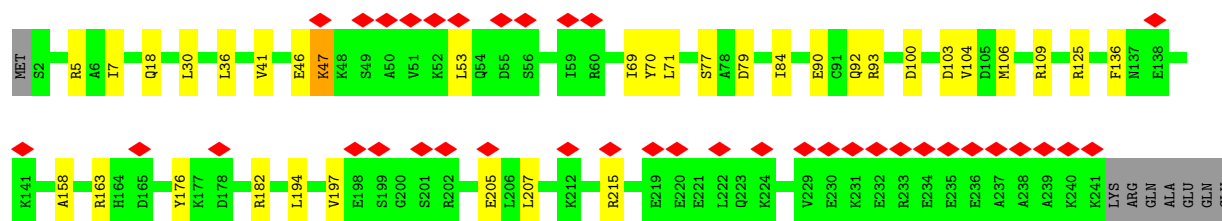


• Molecule 4: Proteasome endopeptidase complex

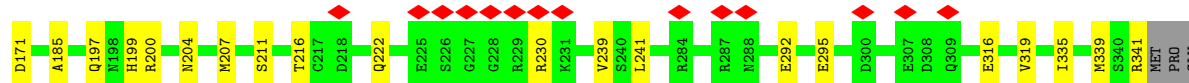
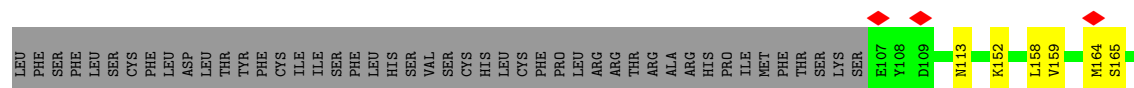


• Molecule 4: Proteasome endopeptidase complex

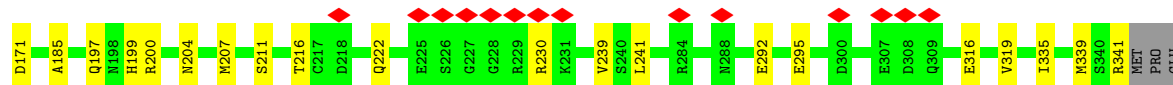
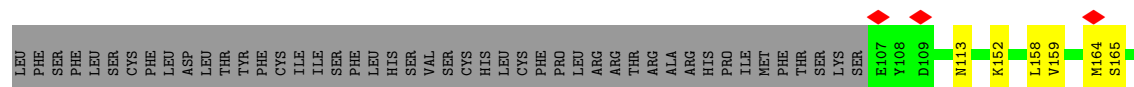
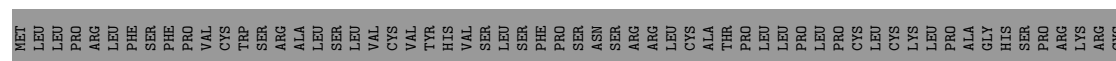




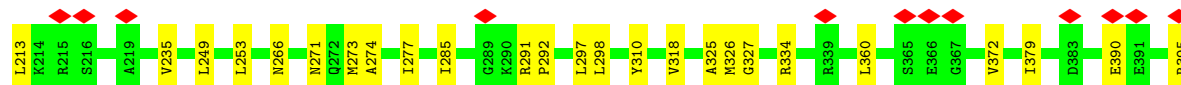
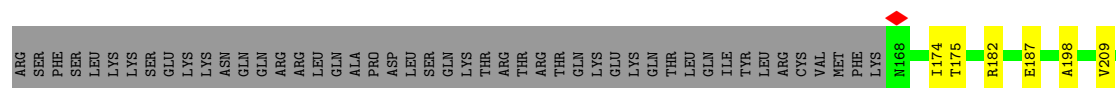
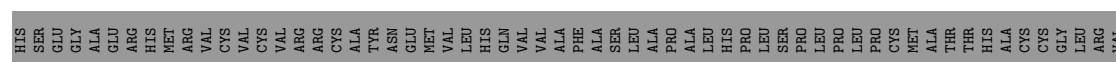
• Molecule 5: Proteasome subunit alpha type

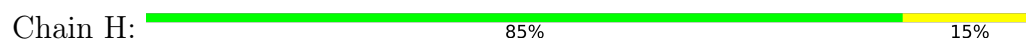


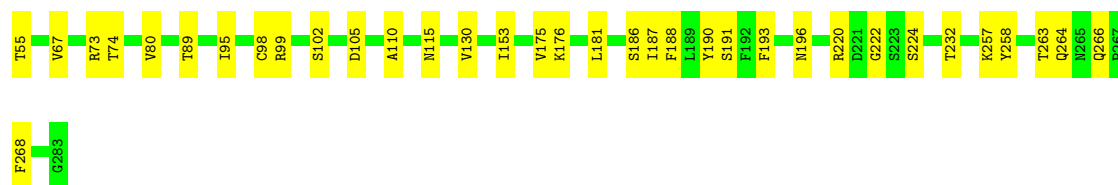
• Molecule 5: Proteasome subunit alpha type



• Molecule 6: Proteasome subunit alpha type

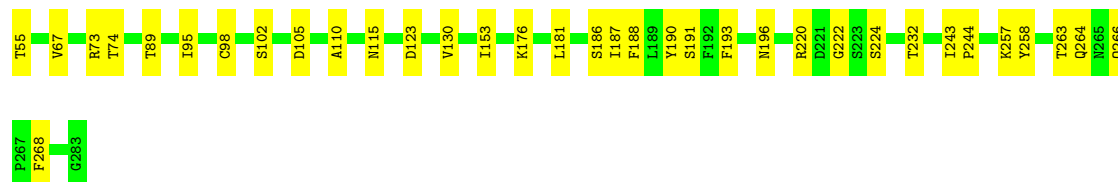






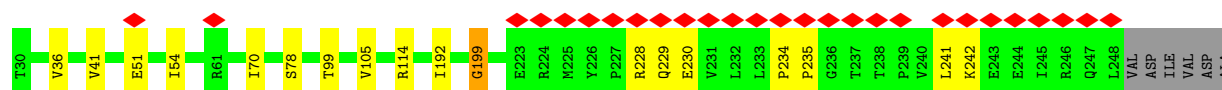
- Molecule 8: Proteasome subunit beta

Chain h: 85% 15%



- Molecule 9: Proteasome subunit beta

Chain I: 12% 89% 8%



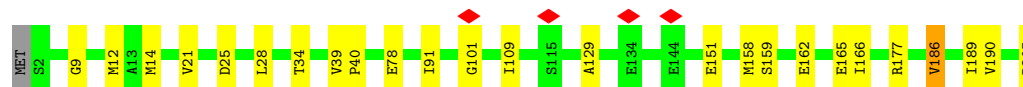
- Molecule 9: Proteasome subunit beta

Chain i: 11% 88% 9%



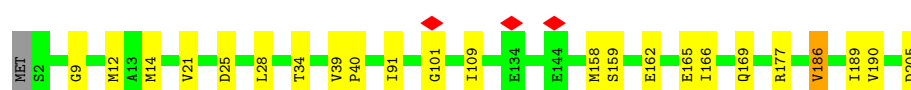
- Molecule 10: Proteasome subunit beta

Chain J: 87% 12%



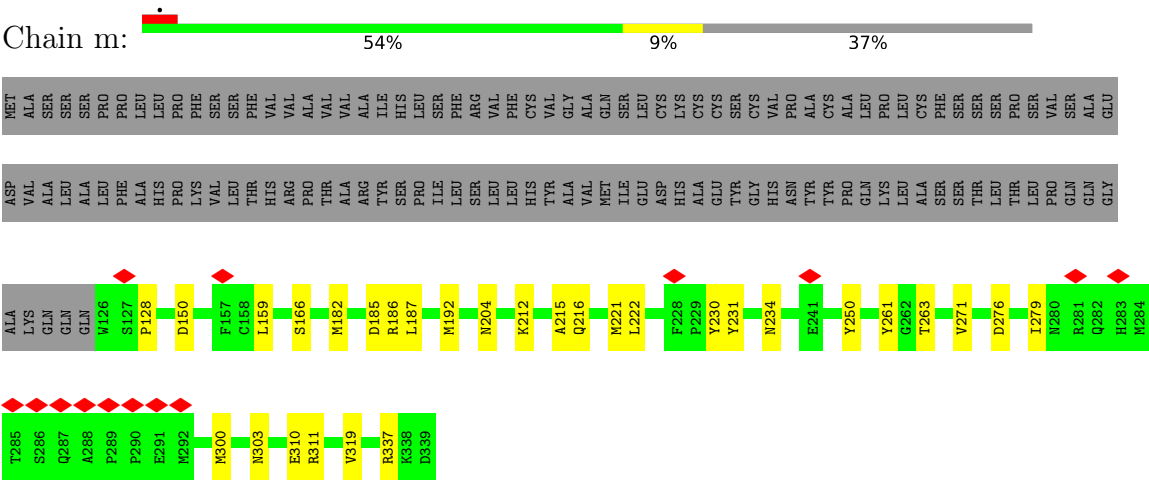
- Molecule 10: Proteasome subunit beta

Chain j: 88% 11%

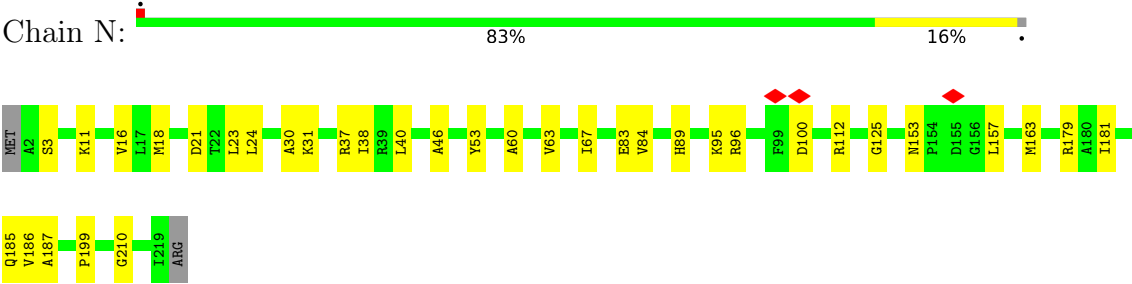


- Molecule 11: Proteasome subunit family protein

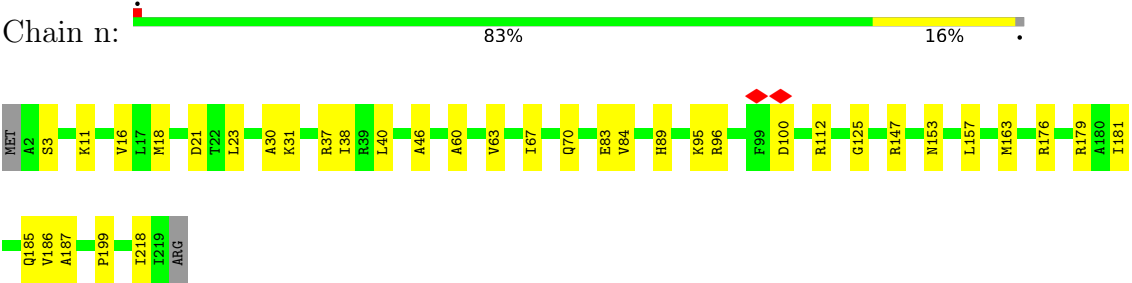
Chain K: 9% 87% 13%



• Molecule 14: Proteasome subunit beta



• Molecule 14: Proteasome subunit beta



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	127000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	258.0, 258.0, 258.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	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: N2E, BO2

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	0.22	0/1893	0.54	0/2567
1	a	0.22	0/1893	0.54	0/2567
2	B	0.24	0/1786	0.56	0/2421
2	b	0.24	0/1786	0.56	0/2421
3	C	0.21	0/2202	0.56	4/2982 (0.1%)
3	c	0.22	0/2202	0.56	4/2982 (0.1%)
4	D	0.22	0/1911	0.59	1/2573 (0.0%)
4	d	0.22	0/1911	0.59	1/2573 (0.0%)
5	E	0.20	0/1831	0.53	0/2476
5	e	0.20	0/1831	0.53	0/2476
6	F	0.21	0/1907	0.53	2/2575 (0.1%)
6	f	0.21	0/1907	0.53	2/2575 (0.1%)
7	G	0.23	0/1773	0.55	3/2398 (0.1%)
7	g	0.23	0/1773	0.55	1/2398 (0.0%)
8	H	0.25	0/1741	0.50	0/2359
8	h	0.25	0/1741	0.50	0/2359
9	I	0.24	0/1685	0.60	2/2284 (0.1%)
9	i	0.24	0/1685	0.60	2/2284 (0.1%)
10	J	0.22	0/1583	0.53	0/2135
10	j	0.22	0/1583	0.53	0/2135
11	K	0.20	0/1643	0.53	0/2222
11	k	0.20	0/1643	0.53	0/2222
12	L	0.24	0/1607	0.55	0/2175
12	l	0.23	0/1607	0.54	0/2175
13	M	0.23	0/1743	0.52	0/2354
13	m	0.23	0/1743	0.52	0/2354
14	N	0.25	0/1748	0.54	2/2363 (0.1%)
14	n	0.25	0/1748	0.54	2/2363 (0.1%)
All	All	0.23	0/50106	0.55	26/67768 (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
4	D	0	1
4	d	0	1
10	J	0	1
10	j	0	1
All	All	0	4

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	199	GLY	CA-C-N	6.21	133.40	121.54
9	i	199	GLY	C-N-CA	6.21	133.40	121.54
9	I	199	GLY	CA-C-N	6.20	133.38	121.54
9	I	199	GLY	C-N-CA	6.20	133.38	121.54
4	D	53	LEU	N-CA-C	-5.70	106.13	114.39
4	d	53	LEU	N-CA-C	-5.66	106.19	114.39
7	G	231	MET	N-CA-C	-5.53	107.78	114.75
7	g	231	MET	N-CA-C	-5.52	107.79	114.75
6	f	390	GLU	CA-C-N	5.21	128.63	120.82
6	f	390	GLU	C-N-CA	5.21	128.63	120.82
6	F	390	GLU	CA-C-N	5.19	128.61	120.82
6	F	390	GLU	C-N-CA	5.19	128.61	120.82
3	C	62	GLN	CA-C-N	5.19	130.19	122.82
3	C	62	GLN	C-N-CA	5.19	130.19	122.82
3	c	62	GLN	CA-C-N	5.17	130.16	122.82
3	c	62	GLN	C-N-CA	5.17	130.16	122.82
3	C	206	MET	CA-C-N	5.13	131.35	121.54
3	C	206	MET	C-N-CA	5.13	131.35	121.54
3	c	206	MET	CA-C-N	5.12	131.32	121.54
3	c	206	MET	C-N-CA	5.12	131.32	121.54
14	N	112	ARG	CA-C-N	5.07	130.03	122.82
14	N	112	ARG	C-N-CA	5.07	130.03	122.82
14	n	112	ARG	CA-C-N	5.05	130.00	122.82
14	n	112	ARG	C-N-CA	5.05	130.00	122.82
7	G	42	CYS	CA-C-N	5.01	131.10	121.54
7	G	42	CYS	C-N-CA	5.01	131.10	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	47	LYS	Peptide
10	J	101	GLY	Peptide
4	d	47	LYS	Peptide
10	j	101	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	1861	0	1874	21	0
1	a	1861	0	1874	22	0
2	B	1753	0	1741	16	0
2	b	1753	0	1741	15	0
3	C	2155	0	2102	21	0
3	c	2155	0	2102	21	0
4	D	1882	0	1881	18	0
4	d	1882	0	1881	22	0
5	E	1802	0	1784	18	0
5	e	1802	0	1784	18	0
6	F	1869	0	1823	19	0
6	f	1869	0	1823	19	0
7	G	1741	0	1702	23	0
7	g	1741	0	1702	25	0
8	H	1709	0	1664	26	0
8	h	1709	0	1664	27	0
9	I	1659	0	1681	12	0
9	i	1659	0	1681	15	0
10	J	1557	0	1552	16	0
10	j	1557	0	1552	13	0
11	K	1612	0	1571	16	0
11	k	1612	0	1571	18	0
12	L	1573	0	1532	17	0
12	l	1573	0	1532	19	0
13	M	1702	0	1638	21	0
13	m	1702	0	1638	20	0
14	N	1712	0	1668	20	0
14	n	1712	0	1668	22	0
15	H	28	0	25	1	0
15	I	28	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	L	28	0	25	1	0
15	h	28	0	25	1	0
15	i	28	0	24	0	0
15	l	28	0	22	0	0
16	L	33	0	0	0	0
16	l	33	0	0	0	0
All	All	49408	0	48571	445	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 5.

All (445) 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)
6:f:266:ASN:ND2	14:n:83:GLU:OE2	2.11	0.83
4:d:46:GLU:OE2	4:d:163:ARG:NH2	2.14	0.81
4:D:46:GLU:OE2	4:D:163:ARG:NH2	2.14	0.80
4:d:90:GLU:OE2	4:d:93:ARG:NH2	2.19	0.76
4:D:90:GLU:OE2	4:D:93:ARG:NH2	2.18	0.76
2:b:173:GLU:OE2	3:c:53:HIS:NE2	2.19	0.75
3:c:128:THR:O	4:d:125:ARG:NH1	2.20	0.74
6:F:266:ASN:ND2	14:N:83:GLU:OE2	2.18	0.74
12:l:131:MET:HE1	12:l:288:ARG:HH12	1.54	0.73
3:c:4:ARG:HH12	7:g:10:GLN:HG3	1.53	0.72
12:l:106:ARG:HH12	12:l:208:PRO:C	1.97	0.72
3:c:184:ASP:OD2	3:c:200:ARG:NH2	2.24	0.70
3:C:184:ASP:OD2	3:C:200:ARG:NH2	2.24	0.70
3:C:128:THR:O	4:D:125:ARG:NH1	2.24	0.70
1:a:100:TYR:O	9:i:114:ARG:NH1	2.25	0.69
1:a:223:ARG:HH11	1:a:234:VAL:HG12	1.58	0.69
1:A:223:ARG:HH11	1:A:234:VAL:HG12	1.58	0.67
3:c:234:ASP:HB3	3:c:237:LYS:HB3	1.77	0.66
8:H:193:PHE:O	8:h:257:LYS:NZ	2.29	0.65
3:C:234:ASP:HB3	3:C:237:LYS:HB3	1.77	0.65
2:B:173:GLU:OE2	3:C:53:HIS:NE2	2.31	0.63
8:H:257:LYS:NZ	8:h:193:PHE:O	2.32	0.62
9:I:192:ILE:HG12	9:I:199:GLY:HA2	1.82	0.61
5:e:152:LYS:NZ	5:e:316:GLU:OE2	2.34	0.61
9:i:192:ILE:HG12	9:i:199:GLY:HA2	1.82	0.61
5:E:152:LYS:NZ	5:E:316:GLU:OE2	2.34	0.61
12:L:196:MET:H	12:L:215:ASP:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:70:THR:HG23	1:a:72:ASN:H	1.66	0.60
12:l:196:MET:H	12:l:215:ASP:HB3	1.66	0.60
1:A:70:THR:HG23	1:A:72:ASN:H	1.66	0.59
7:G:72:ARG:NH2	8:h:268:PHE:O	2.34	0.59
7:G:150:VAL:HG21	7:G:163:VAL:HG21	1.84	0.59
12:L:239:ASP:HB3	11:k:180:ARG:HH11	1.68	0.59
13:M:263:THR:HG21	13:M:271:VAL:HB	1.84	0.59
8:H:190:TYR:OH	14:N:31:LYS:NZ	2.30	0.59
2:B:44:ILE:HD11	2:B:135:ALA:HB3	1.85	0.59
13:m:263:THR:HG21	13:m:271:VAL:HB	1.84	0.58
9:I:229:GLN:OE1	13:m:303:ASN:ND2	2.36	0.58
14:N:23:LEU:HD11	14:N:30:ALA:HB1	1.85	0.58
8:H:264:GLN:HE22	8:h:176:LYS:H	1.51	0.58
8:H:187:ILE:HD12	8:h:187:ILE:HD12	1.86	0.58
7:g:150:VAL:HG21	7:g:163:VAL:HG21	1.84	0.58
5:E:171:ASP:OD1	5:E:197:GLN:NE2	2.37	0.57
7:g:78:ILE:HD11	7:g:82:LEU:HD12	1.87	0.57
2:b:44:ILE:HD11	2:b:135:ALA:HB3	1.85	0.57
8:h:190:TYR:OH	14:n:31:LYS:NZ	2.34	0.57
3:C:4:ARG:HH12	7:G:10:GLN:HG3	1.70	0.57
7:g:175:GLU:HB3	7:g:196:ILE:HD12	1.86	0.57
14:n:21:ASP:OD1	14:n:37:ARG:NH1	2.37	0.57
3:C:223:LYS:NZ	3:C:242:THR:OG1	2.37	0.57
7:G:78:ILE:HD11	7:G:82:LEU:HD12	1.86	0.57
14:N:21:ASP:OD1	14:N:37:ARG:NH1	2.37	0.57
3:c:223:LYS:NZ	3:c:242:THR:OG1	2.37	0.57
5:e:200:ARG:O	12:l:156:ARG:NH2	2.38	0.57
8:h:73:ARG:NH1	8:h:222:GLY:O	2.38	0.57
5:e:171:ASP:OD1	5:e:197:GLN:NE2	2.37	0.57
14:n:23:LEU:HD11	14:n:30:ALA:HB1	1.85	0.57
10:j:40:PRO:HB3	10:j:186:VAL:HG11	1.87	0.57
13:M:162:ARG:NH2	9:i:193:PHE:O	2.38	0.56
13:M:303:ASN:ND2	9:i:229:GLN:OE1	2.38	0.56
7:G:175:GLU:HB3	7:G:196:ILE:HD12	1.86	0.56
10:J:40:PRO:HB3	10:J:186:VAL:HG11	1.87	0.56
1:A:100:TYR:O	9:I:114:ARG:NH1	2.38	0.56
8:H:73:ARG:NH1	8:H:222:GLY:O	2.38	0.56
8:H:176:LYS:H	8:h:264:GLN:HE22	1.52	0.56
5:E:159:VAL:HG11	5:E:164:MET:HE2	1.88	0.56
5:E:200:ARG:O	12:L:156:ARG:NH2	2.38	0.56
8:H:268:PHE:O	7:g:72:ARG:NH2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:140:TYR:OH	11:K:155:ASP:OD1	2.24	0.55
5:e:159:VAL:HG11	5:e:164:MET:HE2	1.88	0.55
7:g:180:ASP:OD2	7:g:183:SER:OG	2.21	0.55
1:A:110:VAL:HG21	9:I:99:THR:HG22	1.88	0.55
7:G:190:VAL:HG13	7:G:213:VAL:HG11	1.89	0.55
4:d:109:ARG:NH1	12:l:169:ASN:OD1	2.39	0.55
11:k:140:TYR:OH	11:k:155:ASP:OD1	2.24	0.55
7:g:190:VAL:HG13	7:g:213:VAL:HG11	1.89	0.55
12:l:106:ARG:NH1	12:l:208:PRO:HB2	2.22	0.54
4:D:47:LYS:HD3	4:D:205:GLU:HB2	1.89	0.54
4:d:47:LYS:HD3	4:d:205:GLU:HB2	1.89	0.54
13:M:128:PRO:O	14:N:96:ARG:NH2	2.40	0.54
10:J:151:GLU:HG3	13:m:311:ARG:HE	1.73	0.54
3:c:149:TYR:HB2	3:c:152:GLN:HE21	1.73	0.53
3:C:149:TYR:HB2	3:C:152:GLN:HE21	1.73	0.53
9:i:241:LEU:HD13	9:i:242:LYS:HG3	1.91	0.53
4:d:30:LEU:HB3	4:d:46:GLU:HB3	1.90	0.53
6:f:325:ALA:O	6:f:334:ARG:NH2	2.42	0.53
1:a:100:TYR:HB2	8:h:115:ASN:HD22	1.74	0.53
5:e:113:ASN:HB3	6:f:291:ARG:HB3	1.88	0.53
12:l:100:THR:N	12:l:268:ALA:O	2.42	0.53
8:h:263:THR:OG1	8:h:266:GLN:NE2	2.42	0.53
1:a:12:VAL:HG13	2:b:19:GLN:HE22	1.73	0.53
1:A:56:ARG:NH2	7:G:177:GLU:OE1	2.39	0.53
1:A:80:ARG:HD3	1:A:83:ASP:OD2	2.09	0.53
1:A:113:LYS:HE3	2:B:82:ARG:HH21	1.72	0.53
6:F:325:ALA:O	6:F:334:ARG:NH2	2.42	0.53
1:A:29:VAL:HA	1:A:79:GLY:HA2	1.91	0.52
14:N:38:ILE:HG21	14:N:187:ALA:HB2	1.91	0.52
4:d:92:GLN:NE2	11:k:63:CYS:O	2.43	0.52
6:f:174:ILE:HD11	6:f:285:ILE:HA	1.90	0.52
6:F:174:ILE:HD11	6:F:285:ILE:HA	1.90	0.52
1:a:80:ARG:HD3	1:a:83:ASP:OD2	2.09	0.52
5:E:204:ASN:HB2	13:M:216:GLN:HG2	1.92	0.52
5:E:199:HIS:HB2	5:E:207:MET:HE3	1.92	0.52
8:H:263:THR:OG1	8:H:266:GLN:NE2	2.42	0.52
11:k:40:ASP:OD1	11:k:69:ARG:NH1	2.43	0.52
14:n:38:ILE:HG21	14:n:187:ALA:HB2	1.91	0.52
4:D:30:LEU:HB3	4:D:46:GLU:HB3	1.90	0.52
13:M:283:HIS:O	10:j:169:GLN:NE2	2.39	0.52
9:I:241:LEU:HD13	9:I:242:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:91:ILE:HD11	10:J:109:ILE:HD11	1.91	0.52
1:a:113:LYS:HE3	2:b:82:ARG:HH21	1.74	0.52
11:K:182:VAL:HG12	11:K:184:ILE:H	1.74	0.51
12:L:102:THR:HG21	12:L:143:THR:HB	1.93	0.51
8:H:188:PHE:O	8:h:191:SER:OG	2.23	0.51
8:H:55:THR:N	8:H:224:SER:HG	2.08	0.51
11:k:182:VAL:HG12	11:k:184:ILE:H	1.74	0.51
6:F:209:VAL:HG22	6:F:379:ILE:HG12	1.93	0.51
11:K:40:ASP:OD1	11:K:69:ARG:NH1	2.43	0.51
10:J:28:LEU:HB2	10:J:39:VAL:HG11	1.93	0.51
5:e:204:ASN:O	13:m:212:LYS:NZ	2.43	0.51
10:j:91:ILE:HD11	10:j:109:ILE:HD11	1.91	0.51
2:B:107:GLN:HG3	10:J:78:GLU:HG2	1.93	0.51
6:F:298:LEU:HG	6:F:326:MET:HE2	1.92	0.51
8:H:196:ASN:HD21	8:h:196:ASN:HD21	1.59	0.51
12:L:243:ARG:NH2	12:L:245:ASP:O	2.44	0.51
14:N:185:GLN:HE21	14:N:199:PRO:HG3	1.76	0.51
5:e:199:HIS:HB2	5:e:207:MET:HE3	1.92	0.51
12:l:243:ARG:NH2	12:l:245:ASP:O	2.44	0.51
14:n:185:GLN:HE21	14:n:199:PRO:HG3	1.76	0.51
5:E:113:ASN:HB3	6:F:291:ARG:HB3	1.93	0.51
1:a:29:VAL:HA	1:a:79:GLY:HA2	1.91	0.51
6:f:285:ILE:HG22	6:f:292:PRO:HG3	1.93	0.51
6:F:285:ILE:HG22	6:F:292:PRO:HG3	1.93	0.50
14:N:89:HIS:NE2	14:N:125:GLY:O	2.42	0.50
6:f:298:LEU:HG	6:f:326:MET:HE2	1.93	0.50
13:m:166:SER:O	13:m:186:ARG:NE	2.39	0.50
2:B:61:GLN:HG3	2:B:64:PHE:HE1	1.77	0.50
3:C:214:ASP:OD1	3:C:251:ARG:NH2	2.44	0.50
13:M:250:TYR:O	13:M:264:ARG:NH1	2.26	0.50
3:C:163:SER:OG	3:C:165:TRP:NE1	2.45	0.50
3:c:223:LYS:HA	3:c:244:PRO:HA	1.93	0.50
6:f:209:VAL:HG22	6:f:379:ILE:HG12	1.93	0.50
10:j:28:LEU:HB2	10:j:39:VAL:HG11	1.93	0.50
12:l:102:THR:HG23	12:l:115:VAL:HG12	1.93	0.50
3:c:214:ASP:OD1	3:c:251:ARG:NH2	2.44	0.50
3:c:163:SER:OG	3:c:165:TRP:NE1	2.45	0.50
11:k:65:LEU:HD11	11:k:82:THR:HG23	1.93	0.50
14:N:67:ILE:HD11	14:N:84:VAL:HG21	1.94	0.50
3:C:223:LYS:HA	3:C:244:PRO:HA	1.93	0.50
2:b:117:GLN:NE2	2:b:121:GLN:OE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:51:GLU:OE2	9:i:54:ILE:HD11	2.12	0.50
13:M:261:TYR:OH	13:M:276:ASP:OD1	2.27	0.49
13:m:128:PRO:O	14:n:96:ARG:NH2	2.45	0.49
2:b:61:GLN:HG3	2:b:64:PHE:HE1	1.77	0.49
14:N:11:LYS:HG2	14:N:16:VAL:HG22	1.94	0.49
10:J:9:GLY:HA2	10:J:25:ASP:OD2	2.12	0.49
8:h:98:CYS:HB2	8:h:153:ILE:HB	1.95	0.49
4:D:70:TYR:HD2	4:D:207:LEU:HD21	1.78	0.49
8:H:98:CYS:HB2	8:H:153:ILE:HB	1.95	0.49
10:j:9:GLY:HA2	10:j:25:ASP:OD2	2.12	0.49
11:K:65:LEU:HD11	11:K:82:THR:HG23	1.93	0.49
4:d:194:LEU:HA	4:d:197:VAL:HG12	1.95	0.49
7:g:54:HIS:HB2	7:g:208:LEU:HB3	1.95	0.49
8:h:55:THR:N	8:h:224:SER:HG	2.09	0.49
4:D:109:ARG:NH1	12:L:169:ASN:OD1	2.46	0.49
9:I:78:SER:HB2	10:J:129:ALA:HB1	1.94	0.49
11:K:146:GLY:HA2	11:K:149:PHE:HD2	1.77	0.49
11:K:121:VAL:HG11	11:K:125:GLN:HE21	1.78	0.48
10:j:21:VAL:HG12	10:j:189:ILE:HG22	1.94	0.48
11:k:146:GLY:HA2	11:k:149:PHE:HD2	1.77	0.48
4:D:131:THR:HG1	4:D:147:THR:HG1	1.59	0.48
5:e:204:ASN:HB2	13:m:216:GLN:HG2	1.95	0.48
12:L:148:ALA:HA	15:L:401:BO2:H243	1.94	0.48
4:d:70:TYR:HD2	4:d:207:LEU:HD21	1.78	0.48
4:D:194:LEU:HA	4:D:197:VAL:HG12	1.95	0.48
10:J:21:VAL:HG12	10:J:189:ILE:HG22	1.94	0.48
11:k:121:VAL:HG11	11:k:125:GLN:HE21	1.78	0.48
14:n:11:LYS:HG2	14:n:16:VAL:HG22	1.94	0.48
14:n:67:ILE:HD11	14:n:84:VAL:HG21	1.94	0.48
7:G:54:HIS:HB2	7:G:208:LEU:HB3	1.95	0.48
2:B:32:THR:OG1	2:B:163:THR:O	2.31	0.48
6:F:235:VAL:HG21	6:F:273:MET:HE1	1.94	0.48
6:F:274:ALA:HB1	6:F:318:VAL:HG21	1.95	0.48
2:b:45:ALA:HB1	2:b:193:LEU:HD11	1.95	0.48
11:K:60:TYR:O	11:K:64:ASN:ND2	2.47	0.48
14:N:95:LYS:NZ	14:N:100:ASP:O	2.46	0.48
6:F:271:ASN:ND2	6:F:310:TYR:OH	2.47	0.48
9:I:51:GLU:OE2	9:I:54:ILE:HD11	2.12	0.48
8:H:67:VAL:HG22	8:H:232:THR:HG22	1.96	0.48
6:f:174:ILE:HG23	6:f:175:THR:HG23	1.95	0.48
2:B:117:GLN:NE2	2:B:121:GLN:OE1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:ALA:HB1	3:C:181:LEU:HD13	1.96	0.47
7:G:215:TRP:HE1	7:G:220:SER:HB3	1.79	0.47
6:f:274:ALA:HB1	6:f:318:VAL:HG21	1.95	0.47
10:j:158:MET:HE1	10:j:166:ILE:HG13	1.96	0.47
8:H:73:ARG:NH1	8:H:224:SER:O	2.47	0.47
12:L:270:GLY:HA3	10:j:205:ASP:OD1	2.13	0.47
14:N:210:GLY:HA3	9:i:152:PRO:HG3	1.96	0.47
6:f:235:VAL:HG21	6:f:273:MET:HE1	1.94	0.47
9:i:235:PRO:HA	10:j:165:GLU:HG3	1.96	0.47
14:n:23:LEU:HD22	14:n:181:ILE:HG23	1.97	0.47
10:J:158:MET:HE1	10:J:166:ILE:HG13	1.96	0.47
3:c:43:VAL:HG13	3:c:221:MET:HB3	1.96	0.47
3:c:78:ILE:HD13	3:c:116:LEU:HD22	1.95	0.47
6:F:174:ILE:HG23	6:F:175:THR:HG23	1.94	0.47
12:L:102:THR:HG23	12:L:115:VAL:HG12	1.96	0.47
8:h:73:ARG:NH1	8:h:224:SER:O	2.47	0.47
11:k:60:TYR:O	11:k:64:ASN:ND2	2.47	0.47
13:m:279:ILE:HG13	13:m:300:MET:HE1	1.96	0.47
3:C:43:VAL:HG13	3:C:221:MET:HB3	1.96	0.47
6:F:372:VAL:HG11	6:F:395:ARG:HG2	1.96	0.47
11:K:180:ARG:HH11	12:l:239:ASP:HB3	1.80	0.47
11:K:195:THR:HG23	11:K:197:ASN:H	1.79	0.47
13:M:279:ILE:HG13	13:M:300:MET:HE1	1.97	0.47
2:b:113:SER:OG	2:b:151:GLY:O	2.28	0.47
7:g:137:ILE:HG12	7:g:150:VAL:HG22	1.96	0.47
2:B:45:ALA:HB1	2:B:193:LEU:HD11	1.95	0.47
3:C:78:ILE:HD13	3:C:116:LEU:HD22	1.95	0.47
4:d:158:ALA:HB3	5:e:158:LEU:HD13	1.97	0.47
2:B:37:LYS:NZ	3:C:57:ASP:OD2	2.42	0.47
14:N:23:LEU:HD22	14:N:181:ILE:HG23	1.96	0.47
2:b:37:LYS:HG2	2:b:42:VAL:HG22	1.96	0.47
8:h:67:VAL:HG22	8:h:232:THR:HG22	1.96	0.47
11:k:195:THR:HG23	11:k:197:ASN:H	1.79	0.47
13:m:159:LEU:O	14:n:147:ARG:NH2	2.39	0.47
10:J:177:ARG:NE	13:m:276:ASP:OD2	2.43	0.47
2:b:32:THR:OG1	2:b:163:THR:O	2.31	0.47
9:I:228:ARG:HD2	9:I:230:GLU:OE2	2.15	0.47
12:L:265:ARG:NH2	10:j:34:THR:O	2.48	0.47
8:h:220:ARG:NH2	8:h:258:TYR:OH	2.48	0.47
1:A:94:GLU:OE2	1:A:114:ARG:HD3	2.15	0.47
5:E:292:GLU:O	5:E:341:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:171:ASP:OD2	5:e:200:ARG:NH2	2.47	0.47
6:f:271:ASN:ND2	6:f:310:TYR:OH	2.47	0.47
10:j:12:MET:HE1	10:j:14:MET:HE3	1.96	0.47
13:m:261:TYR:OH	13:m:276:ASP:OD1	2.27	0.47
10:J:12:MET:HE1	10:J:14:MET:HE3	1.96	0.46
4:d:100:ASP:OD2	12:l:177:ALA:HB2	2.16	0.46
2:B:37:LYS:HG2	2:B:42:VAL:HG22	1.96	0.46
13:M:166:SER:O	13:M:186:ARG:NE	2.39	0.46
3:c:167:ALA:HB1	3:c:181:LEU:HD13	1.96	0.46
6:f:372:VAL:HG11	6:f:395:ARG:HG2	1.96	0.46
7:g:9:ASP:O	7:g:23:GLN:NE2	2.44	0.46
7:G:137:ILE:HG12	7:G:150:VAL:HG22	1.96	0.46
3:C:28:ILE:HD13	3:C:139:SER:HB2	1.98	0.46
6:F:253:LEU:HD11	6:F:277:ILE:HG12	1.98	0.46
12:L:261:HIS:HD2	11:k:155:ASP:HB3	1.80	0.46
13:M:310:GLU:OE2	13:M:337:ARG:HD2	2.16	0.46
1:A:12:VAL:HG13	2:B:19:GLN:HE22	1.80	0.46
8:H:80:VAL:HB	14:n:176:ARG:HA	1.97	0.46
6:f:249:LEU:HD13	6:f:297:LEU:HD11	1.97	0.46
12:l:116:ASP:OD1	12:l:132:LYS:NZ	2.48	0.46
5:E:165:SER:HA	5:E:316:GLU:OE2	2.16	0.46
6:F:198:ALA:HA	6:F:327:GLY:HA3	1.97	0.46
1:a:110:VAL:HG21	9:i:99:THR:HG22	1.97	0.46
4:d:36:LEU:O	4:d:176:TYR:OH	2.28	0.46
5:e:165:SER:HA	5:e:316:GLU:OE2	2.16	0.46
6:f:253:LEU:HD11	6:f:277:ILE:HG12	1.98	0.46
13:m:310:GLU:OE2	13:m:337:ARG:HD2	2.16	0.46
14:n:95:LYS:NZ	14:n:100:ASP:O	2.46	0.46
4:d:69:ILE:HG12	4:d:104:VAL:HG22	1.97	0.46
7:g:215:TRP:HE1	7:g:220:SER:HB3	1.79	0.46
5:E:335:ILE:HG22	5:E:339:MET:HE3	1.98	0.46
13:M:182:MET:HB2	13:M:231:TYR:HD2	1.81	0.46
14:N:40:LEU:HA	14:N:46:ALA:HA	1.98	0.46
3:c:8:ARG:HG2	4:d:5:ARG:HH22	1.81	0.46
12:L:164:LEU:HD23	12:L:167:LEU:HD12	1.98	0.46
4:d:92:GLN:HG3	11:k:67:LEU:HB2	1.98	0.46
7:g:115:ARG:NH1	8:h:123:ASP:OD2	2.47	0.46
12:l:164:LEU:HD23	12:l:167:LEU:HD12	1.98	0.46
1:A:190:LEU:HA	1:A:193:LEU:HD13	1.98	0.45
5:e:335:ILE:HG22	5:e:339:MET:HE3	1.98	0.45
9:i:228:ARG:HD2	9:i:230:GLU:OE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:SER:HA	2:B:145:TYR:HE2	1.81	0.45
1:a:222:GLY:HA2	1:a:233:ARG:HA	1.98	0.45
14:n:18:MET:HE3	14:n:38:ILE:HD12	1.99	0.45
3:C:148:TYR:HB3	11:K:75:ARG:HD2	1.97	0.45
1:A:222:GLY:HA2	1:A:233:ARG:HA	1.98	0.45
5:e:211:SER:OG	13:m:204:ASN:OD1	2.25	0.45
13:m:192:MET:HB3	13:m:221:MET:HE1	1.98	0.45
4:D:69:ILE:HG12	4:D:104:VAL:HG22	1.97	0.45
8:H:220:ARG:NH2	8:H:258:TYR:OH	2.48	0.45
8:h:74:THR:HG22	15:h:301:BO2:H252	1.98	0.45
14:n:40:LEU:HA	14:n:46:ALA:HA	1.98	0.45
2:b:106:SER:HA	2:b:145:TYR:HE2	1.81	0.45
13:m:182:MET:HB2	13:m:231:TYR:HD2	1.81	0.45
6:F:249:LEU:HD13	6:F:297:LEU:HD11	1.97	0.45
13:M:192:MET:HB3	13:M:221:MET:HE1	1.98	0.45
3:c:28:ILE:HD13	3:c:139:SER:HB2	1.98	0.45
1:A:83:ASP:OD1	7:G:121:HIS:NE2	2.32	0.45
5:E:185:ALA:HB2	5:E:239:VAL:HG21	1.99	0.45
5:e:222:GLN:OE1	5:e:230:ARG:NH2	2.49	0.45
14:n:89:HIS:NE2	14:n:125:GLY:O	2.42	0.45
5:E:222:GLN:OE1	5:E:230:ARG:NH2	2.49	0.45
8:H:74:THR:HG22	15:H:301:BO2:H252	1.98	0.45
8:H:95:ILE:HG12	8:H:130:VAL:HG22	1.99	0.45
11:K:155:ASP:HB3	12:l:261:HIS:HD2	1.81	0.45
1:a:94:GLU:OE2	1:a:114:ARG:HD3	2.15	0.45
13:M:311:ARG:HA	9:i:55:VAL:HB	1.98	0.45
2:b:51:PRO:HD2	2:b:55:VAL:HG21	1.99	0.45
6:f:198:ALA:HA	6:f:327:GLY:HA3	1.98	0.45
8:h:95:ILE:HG12	8:h:130:VAL:HG22	1.99	0.45
1:a:100:TYR:HB2	8:h:115:ASN:ND2	2.32	0.44
1:a:120:GLN:NE2	2:b:80:ASP:OD1	2.38	0.44
5:e:216:THR:HG21	5:e:241:LEU:HD12	1.99	0.44
5:E:204:ASN:O	13:M:212:LYS:NZ	2.50	0.44
3:C:8:ARG:HG2	4:D:5:ARG:HH22	1.81	0.44
6:F:182:ARG:NH2	6:F:187:GLU:OE1	2.51	0.44
14:N:18:MET:HE3	14:N:38:ILE:HD12	1.99	0.44
1:a:190:LEU:HA	1:a:193:LEU:HD13	1.98	0.44
14:n:3:SER:HB2	14:n:179:ARG:HH22	1.82	0.44
5:e:185:ALA:HB2	5:e:239:VAL:HG21	1.99	0.44
7:g:13:ASP:OD2	7:g:127:PHE:HB3	2.18	0.44
7:G:13:ASP:OD2	7:G:127:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:104:ASN:HB3	11:k:143:HIS:CD2	2.52	0.44
13:m:222:LEU:HD11	13:m:234:ASN:HD22	1.82	0.44
11:K:104:ASN:HB3	11:K:143:HIS:CD2	2.52	0.44
7:G:22:PHE:O	7:G:26:TYR:N	2.43	0.44
10:J:34:THR:O	12:l:265:ARG:NH2	2.51	0.44
1:a:21:GLN:HE22	7:g:15:PHE:H	1.66	0.44
2:B:51:PRO:HD2	2:B:55:VAL:HG21	1.99	0.43
4:D:158:ALA:HB3	5:E:158:LEU:HD13	2.00	0.43
13:M:222:LEU:HD11	13:M:234:ASN:HD22	1.82	0.43
14:N:3:SER:HB2	14:N:179:ARG:HH22	1.82	0.43
1:a:51:HIS:NE2	1:a:63:VAL:O	2.50	0.43
5:E:216:THR:HG21	5:E:241:LEU:HD12	1.99	0.43
6:f:182:ARG:NH2	6:f:187:GLU:OE1	2.50	0.43
12:L:131:MET:HE1	12:L:288:ARG:HH12	1.81	0.43
10:J:205:ASP:OD1	12:l:118:ARG:NH1	2.51	0.43
13:M:150:ASP:HA	13:M:319:VAL:HA	2.00	0.43
7:G:67:ILE:HD12	7:G:212:GLU:HG2	2.01	0.43
1:A:157:ASP:OD2	1:A:161:TRP:HB2	2.18	0.43
3:C:125:GLN:HB2	3:C:160:GLY:HA3	2.00	0.43
7:G:9:ASP:O	7:G:23:GLN:NE2	2.44	0.43
1:a:157:ASP:OD2	1:a:161:TRP:HB2	2.18	0.43
3:c:125:GLN:HB2	3:c:160:GLY:HA3	2.01	0.43
7:g:67:ILE:HD12	7:g:212:GLU:HG2	2.01	0.43
13:m:150:ASP:HA	13:m:319:VAL:HA	2.00	0.43
1:A:120:GLN:NE2	2:B:80:ASP:OD1	2.38	0.43
5:E:171:ASP:OD2	5:E:200:ARG:NH2	2.46	0.43
13:M:272:GLU:OE2	10:j:177:ARG:NH2	2.52	0.43
13:M:337:ARG:HH22	9:i:200:THR:HG22	1.83	0.43
14:N:153:ASN:HD21	14:N:157:LEU:HD23	1.84	0.43
11:k:21:LEU:HD11	11:k:28:LYS:HG2	2.01	0.43
7:g:137:ILE:HD11	7:g:165:LEU:HD12	2.01	0.43
7:G:70:VAL:H	7:G:75:GLY:HA2	1.83	0.43
12:L:106:ARG:O	12:L:242:TYR:OH	2.35	0.43
11:k:168:LEU:HD11	11:k:202:ILE:HG21	2.01	0.43
14:N:163:MET:HE1	14:N:186:VAL:HG21	2.00	0.42
7:g:22:PHE:O	7:g:26:TYR:N	2.43	0.42
8:h:102:SER:HB3	8:h:105:ASP:HB2	2.01	0.42
9:I:70:ILE:HG12	9:I:105:VAL:HG22	2.01	0.42
5:e:292:GLU:O	5:e:341:ARG:NH1	2.47	0.42
13:m:215:ALA:O	13:m:250:TYR:OH	2.34	0.42
14:n:153:ASN:HD21	14:n:157:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:HIS:NE2	1:A:63:VAL:O	2.50	0.42
8:H:89:THR:HG21	8:H:110:ALA:HB1	2.01	0.42
3:c:161:ASP:OD1	4:d:77:SER:OG	2.29	0.42
7:g:70:VAL:H	7:g:75:GLY:HA2	1.84	0.42
7:G:172:ALA:HB2	7:G:200:VAL:HG21	2.02	0.42
2:b:109:VAL:HA	2:b:112:ILE:HG12	2.02	0.42
7:g:20:ARG:NH2	7:g:25:GLU:OE1	2.52	0.42
2:B:109:VAL:HA	2:B:112:ILE:HG12	2.02	0.42
11:K:21:LEU:HD11	11:K:28:LYS:HG2	2.01	0.42
8:h:181:LEU:HB3	8:h:186:SER:HB2	2.01	0.42
12:L:239:ASP:O	11:k:180:ARG:NH1	2.52	0.42
2:b:32:THR:H	2:b:47:LYS:HE2	1.85	0.42
7:G:137:ILE:HD11	7:G:165:LEU:HD12	2.00	0.42
8:H:102:SER:HB3	8:H:105:ASP:HB2	2.02	0.42
10:J:205:ASP:OD1	12:l:270:GLY:HA3	2.19	0.42
11:K:50:GLU:HG2	11:K:53:PRO:HD2	2.02	0.42
11:K:168:LEU:HD11	11:K:202:ILE:HG21	2.01	0.42
9:i:70:ILE:HG12	9:i:105:VAL:HG22	2.01	0.42
10:j:159:SER:HB3	10:j:162:GLU:HG2	2.02	0.42
11:k:50:GLU:HG2	11:k:53:PRO:HD2	2.02	0.42
4:D:103:ASP:HB2	4:D:106:MET:HG3	2.02	0.42
1:a:59:ARG:HG2	1:a:61:ASP:OD1	2.20	0.42
4:d:103:ASP:HB2	4:d:106:MET:HG3	2.02	0.42
4:D:71:LEU:HD22	4:D:84:ILE:HD11	2.02	0.42
7:G:20:ARG:NH2	7:G:25:GLU:OE1	2.52	0.42
12:L:265:ARG:HD3	11:k:155:ASP:OD2	2.20	0.42
6:f:213:LEU:HB2	6:f:360:LEU:HD11	2.01	0.42
14:n:60:ALA:HA	14:n:63:VAL:HG22	2.02	0.42
6:F:213:LEU:HB2	6:F:360:LEU:HD11	2.01	0.41
6:F:273:MET:HE3	6:F:273:MET:HB2	1.80	0.41
4:d:71:LEU:HD22	4:d:84:ILE:HD11	2.02	0.41
7:g:197:LEU:HA	7:g:200:VAL:HG12	2.03	0.41
14:n:163:MET:HE1	14:n:186:VAL:HG21	2.00	0.41
3:C:57:ASP:OD1	3:C:58:SER:N	2.54	0.41
13:M:185:ASP:HB3	13:M:230:TYR:HD1	1.86	0.41
14:N:60:ALA:HA	14:N:63:VAL:HG22	2.02	0.41
3:c:57:ASP:OD1	3:c:58:SER:N	2.54	0.41
8:H:175:VAL:HA	8:h:264:GLN:HE22	1.85	0.41
8:H:181:LEU:HB3	8:H:186:SER:HB2	2.01	0.41
8:h:89:THR:HG21	8:h:110:ALA:HB1	2.01	0.41
8:h:243:ILE:HA	8:h:244:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:36:VAL:HG22	9:i:41:VAL:HG12	2.03	0.41
1:A:100:TYR:HB2	8:H:115:ASN:HD22	1.86	0.41
3:C:218:VAL:HG23	3:C:249:LEU:HB2	2.03	0.41
6:F:174:ILE:HD12	6:F:292:PRO:HD3	2.03	0.41
6:f:174:ILE:HD12	6:f:292:PRO:HD3	2.02	0.41
1:a:29:VAL:HG21	1:a:134:VAL:HG23	2.03	0.41
7:g:172:ALA:HB2	7:g:200:VAL:HG21	2.02	0.41
13:m:185:ASP:HB3	13:m:230:TYR:HD1	1.85	0.41
4:D:41:VAL:HG23	4:D:136:PHE:HE1	1.85	0.41
5:E:211:SER:OG	13:M:203:ASN:O	2.39	0.41
3:c:4:ARG:NH1	7:g:10:GLN:HG3	2.29	0.41
1:A:6:PHE:HD2	1:A:9:TYR:H	1.69	0.41
1:A:45:VAL:HG11	1:A:138:ILE:HB	2.02	0.41
1:A:59:ARG:HG2	1:A:61:ASP:OD1	2.20	0.41
3:C:17:ARG:HB3	3:C:22:GLU:OE2	2.21	0.41
4:D:36:LEU:O	4:D:176:TYR:OH	2.29	0.41
7:G:197:LEU:HA	7:G:200:VAL:HG12	2.03	0.41
9:I:36:VAL:HG22	9:I:41:VAL:HG12	2.03	0.41
9:I:235:PRO:HA	10:J:165:GLU:HG3	2.03	0.41
10:J:159:SER:HB3	10:J:162:GLU:HG2	2.02	0.41
1:a:45:VAL:HG11	1:a:138:ILE:HB	2.02	0.41
3:c:17:ARG:HB3	3:c:22:GLU:OE2	2.21	0.41
3:c:125:GLN:NE2	4:d:79:ASP:OD1	2.54	0.41
7:g:66:ARG:NH2	7:g:80:GLY:O	2.52	0.41
13:m:166:SER:HB2	13:m:187:LEU:HD21	2.03	0.41
4:D:7:ILE:HG22	4:D:18:GLN:HG3	2.02	0.41
4:D:182:ARG:NH2	4:D:215:ARG:HH21	2.19	0.41
11:K:180:ARG:NH1	12:l:239:ASP:O	2.53	0.41
14:N:24:LEU:HD11	14:N:53:TYR:HB2	2.03	0.41
1:a:16:GLU:OE2	1:a:20:TYR:OH	2.20	0.41
4:d:182:ARG:NH2	4:d:215:ARG:HH21	2.19	0.41
5:e:295:GLU:OE2	5:e:319:VAL:HG11	2.21	0.41
2:B:32:THR:H	2:B:47:LYS:HE2	1.85	0.40
8:H:99:ARG:HH12	14:n:218:ILE:HD12	1.85	0.40
4:d:41:VAL:HG23	4:d:136:PHE:HE1	1.85	0.40
6:f:272:GLN:NE2	14:n:70:GLN:HE22	2.19	0.40
7:g:51:GLU:HB2	7:g:197:LEU:HD23	2.03	0.40
1:A:58:MET:HE2	7:G:160:TYR:HE1	1.86	0.40
7:g:215:TRP:CZ3	7:g:227:VAL:HG12	2.56	0.40
7:G:215:TRP:CZ3	7:G:227:VAL:HG12	2.56	0.40
1:a:207:GLN:HG2	1:a:213:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:295:GLU:OE2	5:E:319:VAL:HG11	2.21	0.40
8:H:191:SER:OG	8:h:188:PHE:O	2.31	0.40
12:L:118:ARG:NH1	12:L:269:SER:O	2.54	0.40
9:i:234:PRO:HA	9:i:235:PRO:HD3	1.94	0.40
12:l:106:ARG:NH1	12:l:209:SER:HA	2.37	0.40
7:G:51:GLU:HB2	7:G:197:LEU:HD23	2.03	0.40
9:I:234:PRO:HA	9:I:235:PRO:HD3	1.94	0.40
4:d:7:ILE:HG22	4:d:18:GLN:HG3	2.03	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	243/250 (97%)	233 (96%)	10 (4%)	0	100	100
1	a	243/250 (97%)	233 (96%)	10 (4%)	0	100	100
2	B	227/231 (98%)	215 (95%)	12 (5%)	0	100	100
2	b	227/231 (98%)	215 (95%)	12 (5%)	0	100	100
3	C	270/285 (95%)	258 (96%)	12 (4%)	0	100	100
3	c	270/285 (95%)	258 (96%)	12 (4%)	0	100	100
4	D	238/248 (96%)	229 (96%)	9 (4%)	0	100	100
4	d	238/248 (96%)	229 (96%)	9 (4%)	0	100	100
5	E	233/344 (68%)	228 (98%)	5 (2%)	0	100	100
5	e	233/344 (68%)	228 (98%)	5 (2%)	0	100	100
6	F	236/428 (55%)	228 (97%)	8 (3%)	0	100	100
6	f	236/428 (55%)	228 (97%)	8 (3%)	0	100	100
7	G	228/238 (96%)	220 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
8	H	227/229 (99%)	219 (96%)	8 (4%)	0	100	100
8	h	227/229 (99%)	219 (96%)	8 (4%)	0	100	100
9	I	217/225 (96%)	205 (94%)	12 (6%)	0	100	100
9	i	217/225 (96%)	205 (94%)	12 (6%)	0	100	100
10	J	202/205 (98%)	189 (94%)	13 (6%)	0	100	100
10	j	202/205 (98%)	189 (94%)	13 (6%)	0	100	100
11	K	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
11	k	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
12	L	199/203 (98%)	186 (94%)	13 (6%)	0	100	100
12	l	199/203 (98%)	186 (94%)	13 (6%)	0	100	100
13	M	212/339 (62%)	202 (95%)	10 (5%)	0	100	100
13	m	212/339 (62%)	201 (95%)	11 (5%)	0	100	100
14	N	216/220 (98%)	207 (96%)	9 (4%)	0	100	100
14	n	216/220 (98%)	207 (96%)	9 (4%)	0	100	100
All	All	6304/7302 (86%)	6029 (96%)	275 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	193/197 (98%)	192 (100%)	1 (0%)	81	85
1	a	193/197 (98%)	192 (100%)	1 (0%)	81	85
2	B	188/190 (99%)	188 (100%)	0	100	100
2	b	188/190 (99%)	188 (100%)	0	100	100
3	C	229/241 (95%)	228 (100%)	1 (0%)	84	86
3	c	229/241 (95%)	228 (100%)	1 (0%)	84	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	201/208 (97%)	201 (100%)	0	100	100
4	d	201/208 (97%)	201 (100%)	0	100	100
5	E	197/301 (65%)	197 (100%)	0	100	100
5	e	197/301 (65%)	197 (100%)	0	100	100
6	F	200/363 (55%)	200 (100%)	0	100	100
6	f	200/363 (55%)	200 (100%)	0	100	100
7	G	185/190 (97%)	185 (100%)	0	100	100
7	g	185/190 (97%)	185 (100%)	0	100	100
8	H	184/184 (100%)	184 (100%)	0	100	100
8	h	184/184 (100%)	184 (100%)	0	100	100
9	I	180/185 (97%)	180 (100%)	0	100	100
9	i	180/185 (97%)	180 (100%)	0	100	100
10	J	167/168 (99%)	165 (99%)	2 (1%)	63	79
10	j	167/168 (99%)	165 (99%)	2 (1%)	63	79
11	K	172/172 (100%)	172 (100%)	0	100	100
11	k	172/172 (100%)	172 (100%)	0	100	100
12	L	162/164 (99%)	162 (100%)	0	100	100
12	l	162/164 (99%)	162 (100%)	0	100	100
13	M	181/288 (63%)	181 (100%)	0	100	100
13	m	181/288 (63%)	181 (100%)	0	100	100
14	N	181/183 (99%)	181 (100%)	0	100	100
14	n	181/183 (99%)	181 (100%)	0	100	100
All	All	5240/6068 (86%)	5232 (100%)	8 (0%)	85	89

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

Mol	Chain	Res	Type
1	A	53	ILE
3	C	232	LEU
10	J	186	VAL
10	J	190	VAL
1	a	53	ILE
3	c	232	LEU
10	j	186	VAL

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Mol	Chain	Res	Type
10	j	190	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	72	ASN
1	A	99	GLN
2	B	19	GLN
2	B	107	GLN
2	B	143	HIS
3	C	65	ASN
4	D	54	GLN
4	D	115	GLN
4	D	116	GLN
4	D	137	ASN
4	D	187	HIS
4	D	210	GLN
5	E	286	HIS
6	F	168	ASN
6	F	206	ASN
6	F	271	ASN
6	F	272	GLN
6	F	308	HIS
7	G	226	HIS
8	H	216	HIS
8	H	264	GLN
8	H	266	GLN
10	J	43	HIS
11	K	22	ASN
11	K	84	ASN
11	K	104	ASN
11	K	125	GLN
11	K	136	GLN
12	L	128	GLN
12	L	184	ASN
12	L	191	ASN
12	L	279	HIS
12	L	296	HIS
13	M	191	GLN
13	M	216	GLN
13	M	303	ASN

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Mol	Chain	Res	Type
14	N	185	GLN
1	a	21	GLN
1	a	72	ASN
1	a	99	GLN
2	b	19	GLN
2	b	107	GLN
2	b	143	HIS
3	c	65	ASN
4	d	115	GLN
4	d	116	GLN
4	d	137	ASN
4	d	210	GLN
5	e	197	GLN
5	e	286	HIS
6	f	168	ASN
6	f	206	ASN
6	f	271	ASN
6	f	272	GLN
6	f	281	HIS
6	f	305	GLN
6	f	308	HIS
7	g	226	HIS
8	h	115	ASN
8	h	196	ASN
8	h	216	HIS
8	h	264	GLN
8	h	266	GLN
10	j	43	HIS
11	k	22	ASN
11	k	84	ASN
11	k	104	ASN
11	k	125	GLN
11	k	136	GLN
12	l	128	GLN
12	l	184	ASN
12	l	191	ASN
12	l	222	GLN
12	l	279	HIS
13	m	216	GLN
13	m	303	ASN
14	n	185	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	N2E	L	402	-	35,37,37	2.22	11 (31%)	45,54,54	4.56	23 (51%)
15	BO2	H	301	8	25,29,29	0.44	0	33,38,38	1.25	7 (21%)
15	BO2	I	301	9	25,29,29	0.42	0	33,38,38	1.21	4 (12%)
16	N2E	l	402	-	35,37,37	2.23	11 (31%)	45,54,54	4.56	23 (51%)
15	BO2	i	301	9	25,29,29	0.42	0	33,38,38	1.20	4 (12%)
15	BO2	h	301	8	25,29,29	0.45	0	33,38,38	1.25	7 (21%)
15	BO2	L	401	12	25,29,29	0.41	0	33,38,38	1.33	7 (21%)
15	BO2	l	401	12	25,29,29	0.47	0	33,38,38	1.21	6 (18%)

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
16	N2E	L	402	-	-	3/14/16/16	0/5/5/5
15	BO2	H	301	8	-	4/23/28/28	0/2/2/2
15	BO2	I	301	9	-	10/23/28/28	0/2/2/2
16	N2E	l	402	-	-	3/14/16/16	0/5/5/5
15	BO2	i	301	9	-	10/23/28/28	0/2/2/2
15	BO2	h	301	8	-	4/23/28/28	0/2/2/2
15	BO2	L	401	12	-	12/23/28/28	0/2/2/2
15	BO2	l	401	12	-	7/23/28/28	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	l	402	N2E	C7-N6	-5.34	1.25	1.33
16	L	402	N2E	C7-N6	-5.33	1.25	1.33
16	l	402	N2E	C7-N3	-5.25	1.29	1.38
16	L	402	N2E	C7-N3	-5.23	1.29	1.38
16	l	402	N2E	C7-N8	5.10	1.43	1.35
16	L	402	N2E	C7-N8	5.09	1.43	1.35
16	l	402	N2E	C27-C1	3.99	1.52	1.48
16	L	402	N2E	C27-C1	3.91	1.52	1.48
16	l	402	N2E	C5-N4	-3.87	1.28	1.33
16	L	402	N2E	C5-N4	-3.83	1.28	1.33
16	l	402	N2E	C2-N3	-3.10	1.30	1.36
16	L	402	N2E	C2-N3	-3.09	1.30	1.36
16	L	402	N2E	C5-N6	2.98	1.43	1.37
16	l	402	N2E	C5-N6	2.96	1.43	1.37
16	l	402	N2E	C23-N22	-2.87	1.25	1.29
16	L	402	N2E	C23-N22	-2.78	1.25	1.29
16	L	402	N2E	C9-N8	-2.72	1.27	1.32
16	l	402	N2E	C9-N8	-2.69	1.27	1.32
16	L	402	N2E	C21-N22	2.43	1.42	1.38
16	l	402	N2E	C21-N22	2.42	1.42	1.38
16	l	402	N2E	O24-C23	-2.21	1.34	1.37
16	L	402	N2E	O24-C23	-2.21	1.34	1.37

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	l	402	N2E	C5-N4-N3	17.05	111.71	101.98
16	L	402	N2E	C5-N4-N3	16.98	111.68	101.98
16	l	402	N2E	C7-N3-N4	-11.95	105.03	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	402	N2E	C7-N3-N4	-11.87	105.06	110.04
16	l	402	N2E	N4-C5-N6	-11.83	102.98	114.71
16	L	402	N2E	N4-C5-N6	-11.83	102.99	114.71
16	L	402	N2E	C7-N6-C5	9.39	108.35	103.10
16	l	402	N2E	C7-N6-C5	9.35	108.33	103.10
16	L	402	N2E	C1-C9-N8	-8.22	117.92	125.38
16	l	402	N2E	C1-C9-N8	-8.20	117.94	125.38
16	l	402	N2E	C2-N3-N4	5.84	132.95	125.20
16	L	402	N2E	C2-N3-N4	5.83	132.94	125.20
16	L	402	N2E	O24-C23-N22	-4.62	109.32	114.87
16	l	402	N2E	O24-C23-N22	-4.59	109.37	114.87
16	L	402	N2E	C32-C27-N28	-3.97	119.17	123.12
16	l	402	N2E	C32-C27-N28	-3.92	119.21	123.12
16	L	402	N2E	C29-N28-C27	3.46	123.52	116.80
16	l	402	N2E	C29-N28-C27	3.43	123.47	116.80
16	L	402	N2E	C9-N8-C7	3.40	119.81	115.60
16	l	402	N2E	C9-N8-C7	3.36	119.76	115.60
16	L	402	N2E	C32-C27-C1	3.35	128.25	122.98
16	l	402	N2E	C32-C27-C1	3.35	128.24	122.98
16	L	402	N2E	C14-C15-C10	-3.24	119.58	123.07
16	l	402	N2E	C14-C15-C10	-3.21	119.61	123.07
15	L	401	BO2	B26-C21-C22	-3.08	106.50	112.31
16	l	402	N2E	C10-C5-N4	2.99	129.27	123.64
16	L	402	N2E	C10-C5-N4	2.98	129.25	123.64
15	I	301	BO2	C6-N1-C2	2.90	120.67	116.93
16	l	402	N2E	C26-C21-N22	2.87	125.08	119.32
16	L	402	N2E	C26-C21-N22	2.85	125.03	119.32
15	i	301	BO2	C6-N1-C2	2.84	120.59	116.93
15	H	301	BO2	C6-N1-C2	2.81	120.55	116.93
15	h	301	BO2	C6-N1-C2	2.80	120.54	116.93
16	L	402	N2E	C11-C10-C15	2.78	120.28	116.83
16	l	402	N2E	C11-C10-C15	2.77	120.27	116.83
16	l	402	N2E	C1-C27-N28	-2.76	112.53	115.30
15	L	401	BO2	C6-N1-C2	2.75	120.47	116.93
16	L	402	N2E	C1-C27-N28	-2.73	112.57	115.30
15	I	301	BO2	C7-C2-N1	2.72	120.60	117.42
15	i	301	BO2	C7-C2-N1	2.65	120.52	117.42
15	l	401	BO2	C6-N1-C2	2.62	120.31	116.93
16	L	402	N2E	C10-C5-N6	2.60	127.77	122.08
16	l	402	N2E	C10-C5-N6	2.59	127.75	122.08
16	L	402	N2E	O24-C23-C25	2.44	122.39	117.49
16	l	402	N2E	O24-C23-C25	2.42	122.34	117.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	h	301	BO2	C7-C2-N1	2.39	120.21	117.42
15	H	301	BO2	C7-C2-N1	2.38	120.21	117.42
16	l	402	N2E	C33-C32-C31	-2.37	115.70	120.28
15	l	401	BO2	B26-C21-C22	-2.37	107.83	112.31
16	L	402	N2E	C33-C32-C31	-2.36	115.72	120.28
16	l	402	N2E	N3-C7-N6	2.35	111.94	109.74
15	L	401	BO2	C21-N20-C18	2.34	128.90	122.99
16	L	402	N2E	N3-C7-N6	2.33	111.93	109.74
15	H	301	BO2	C5-N4-C3	2.32	120.92	116.85
15	i	301	BO2	C5-N4-C3	2.32	120.91	116.85
16	L	402	N2E	C30-C29-N28	-2.31	119.76	123.42
16	l	402	N2E	C30-C29-N28	-2.29	119.79	123.42
15	I	301	BO2	C5-N4-C3	2.28	120.85	116.85
15	h	301	BO2	C5-N4-C3	2.28	120.85	116.85
15	L	401	BO2	C7-C2-N1	2.24	120.03	117.42
15	h	301	BO2	B26-C21-C22	-2.22	108.12	112.31
15	L	401	BO2	C5-N4-C3	2.22	120.73	116.85
15	H	301	BO2	B26-C21-C22	-2.20	108.15	112.31
16	L	402	N2E	O20-C18-C19	-2.20	118.47	121.51
16	l	402	N2E	C33-C32-C27	2.19	126.46	123.34
16	l	402	N2E	O20-C18-C19	-2.17	118.50	121.51
15	l	401	BO2	C5-N4-C3	2.16	120.63	116.85
16	L	402	N2E	C33-C32-C27	2.16	126.42	123.34
15	I	301	BO2	C5-C6-N1	-2.14	119.17	122.19
15	l	401	BO2	C2-C3-N4	-2.13	119.17	121.97
15	H	301	BO2	C5-C6-N1	-2.12	119.20	122.19
15	H	301	BO2	C2-C3-N4	-2.12	119.20	121.97
15	i	301	BO2	C5-C6-N1	-2.11	119.21	122.19
15	h	301	BO2	C5-C6-N1	-2.10	119.23	122.19
15	h	301	BO2	C2-C3-N4	-2.09	119.23	121.97
15	L	401	BO2	C5-C6-N1	-2.09	119.25	122.19
15	l	401	BO2	C5-C6-N1	-2.08	119.25	122.19
15	h	301	BO2	C2-C7-N9	2.06	119.14	115.19
15	H	301	BO2	C2-C7-N9	2.05	119.13	115.19
15	l	401	BO2	C21-C22-C23	-2.01	112.75	115.32
15	L	401	BO2	C2-C3-N4	-2.01	119.34	121.97

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	BO2	C3-C2-C7-O8

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Mol	Chain	Res	Type	Atoms
15	H	301	BO2	C3-C2-C7-N9
15	I	301	BO2	N1-C2-C7-O8
15	I	301	BO2	N1-C2-C7-N9
15	I	301	BO2	C3-C2-C7-O8
15	I	301	BO2	C3-C2-C7-N9
15	I	301	BO2	O19-C18-N20-C21
15	I	301	BO2	B26-C21-C22-C23
15	I	301	BO2	C21-C22-C23-C24
15	I	301	BO2	C21-C22-C23-C25
15	L	401	BO2	C3-C2-C7-O8
15	L	401	BO2	C3-C2-C7-N9
15	L	401	BO2	C10-C18-N20-C21
15	L	401	BO2	O19-C18-N20-C21
15	L	401	BO2	B26-C21-C22-C23
15	h	301	BO2	C3-C2-C7-O8
15	h	301	BO2	C3-C2-C7-N9
15	i	301	BO2	N1-C2-C7-O8
15	i	301	BO2	N1-C2-C7-N9
15	i	301	BO2	C3-C2-C7-O8
15	i	301	BO2	C3-C2-C7-N9
15	i	301	BO2	O19-C18-N20-C21
15	i	301	BO2	B26-C21-C22-C23
15	i	301	BO2	C21-C22-C23-C24
15	i	301	BO2	C21-C22-C23-C25
15	l	401	BO2	N1-C2-C7-O8
15	l	401	BO2	N1-C2-C7-N9
15	l	401	BO2	C3-C2-C7-O8
15	l	401	BO2	C3-C2-C7-N9
15	I	301	BO2	C10-C18-N20-C21
15	i	301	BO2	C10-C18-N20-C21
15	H	301	BO2	N1-C2-C7-O8
15	L	401	BO2	N1-C2-C7-O8
15	h	301	BO2	N1-C2-C7-O8
15	H	301	BO2	N1-C2-C7-N9
15	L	401	BO2	N1-C2-C7-N9
15	h	301	BO2	N1-C2-C7-N9
15	I	301	BO2	N20-C21-C22-C23
15	i	301	BO2	N20-C21-C22-C23
15	L	401	BO2	N20-C21-C22-C23
15	L	401	BO2	N9-C10-C18-N20
15	L	401	BO2	N9-C10-C18-O19
15	l	401	BO2	O8-C7-N9-C10

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Mol	Chain	Res	Type	Atoms
15	l	401	BO2	N9-C10-C11-C12
16	L	402	N2E	C15-C10-C5-N6
16	l	402	N2E	C15-C10-C5-N6
16	L	402	N2E	C11-C10-C5-N6
16	l	402	N2E	C11-C10-C5-N6
16	L	402	N2E	C2-C1-C27-C32
16	l	402	N2E	C2-C1-C27-C32
15	L	401	BO2	C11-C10-C18-O19
15	l	401	BO2	C2-C7-N9-C10
15	L	401	BO2	C11-C10-C18-N20

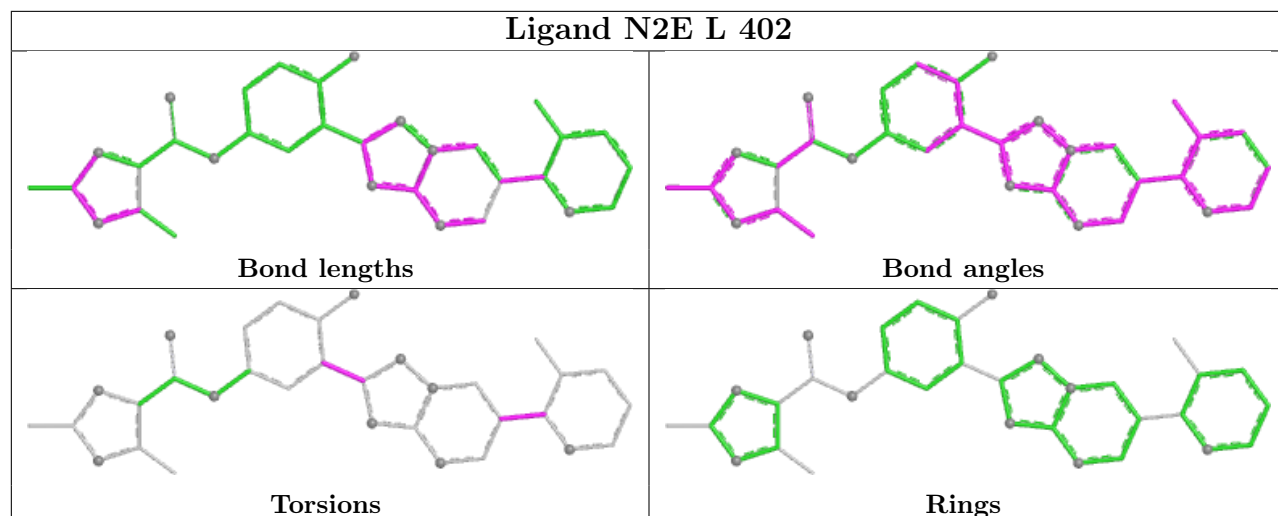
There are no ring outliers.

3 monomers are involved in 3 short contacts:

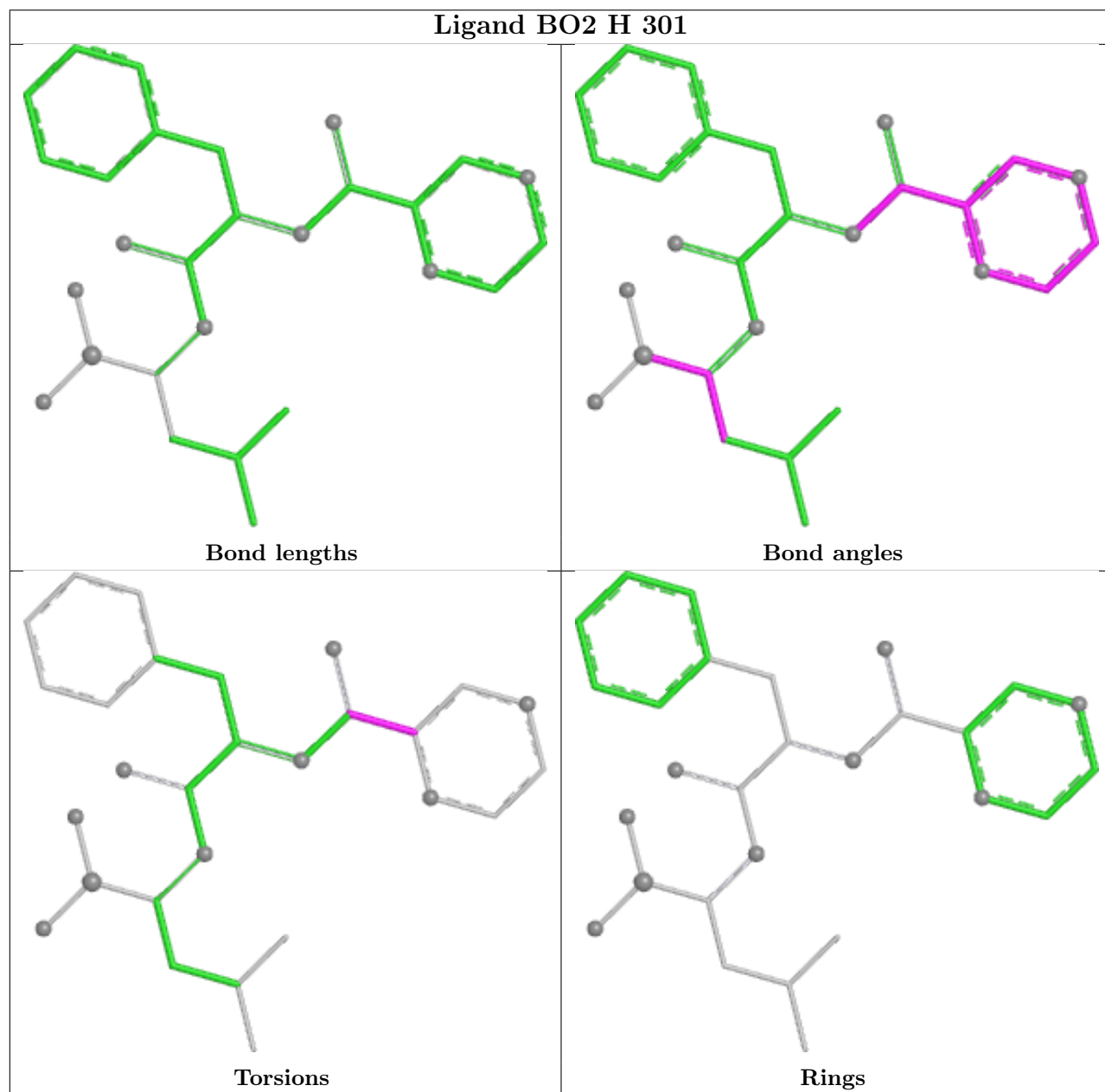
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	301	BO2	1	0
15	h	301	BO2	1	0
15	L	401	BO2	1	0

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

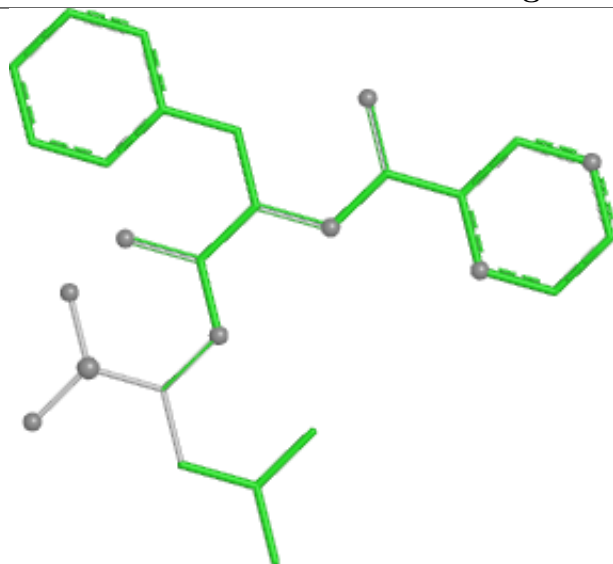
Ligand N2E L 402



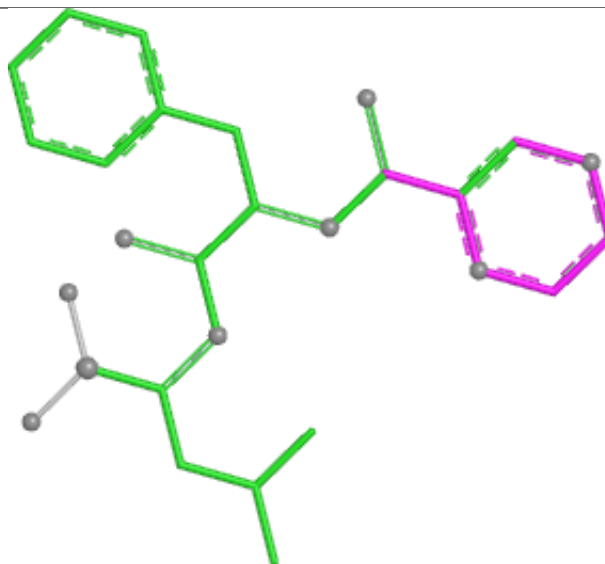
Ligand BO2 H 301



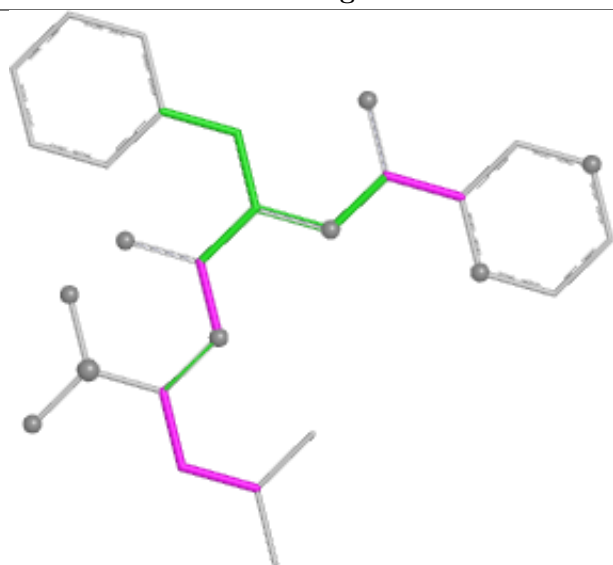
Ligand BO2 I 301



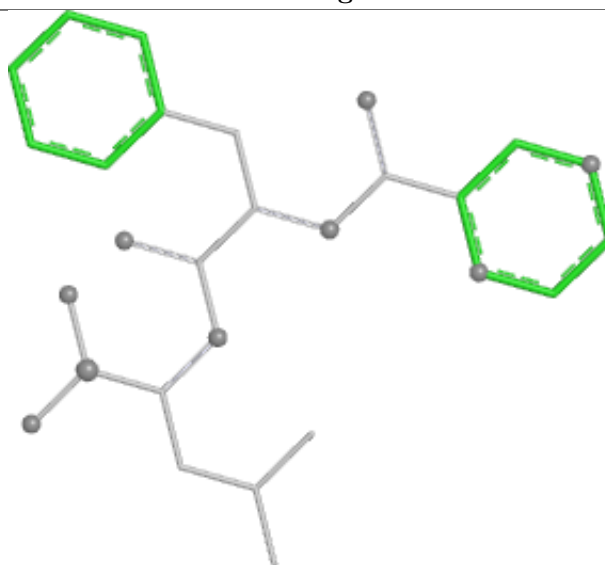
Bond lengths



Bond angles

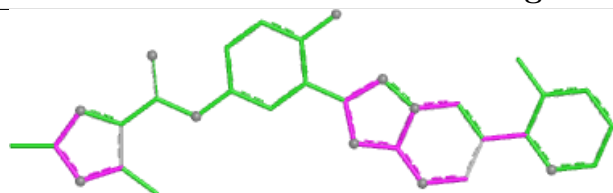


Torsions

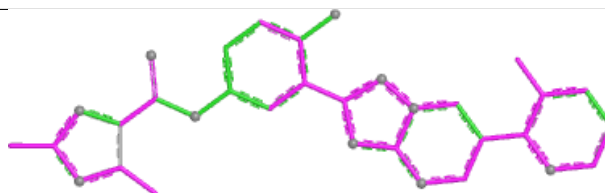


Rings

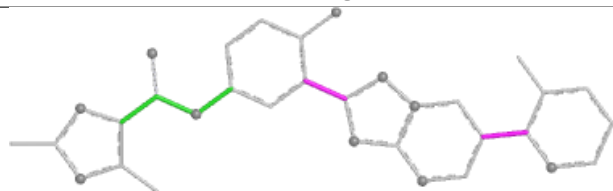
Ligand N2E I 402



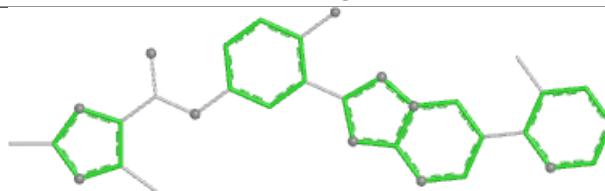
Bond lengths



Bond angles

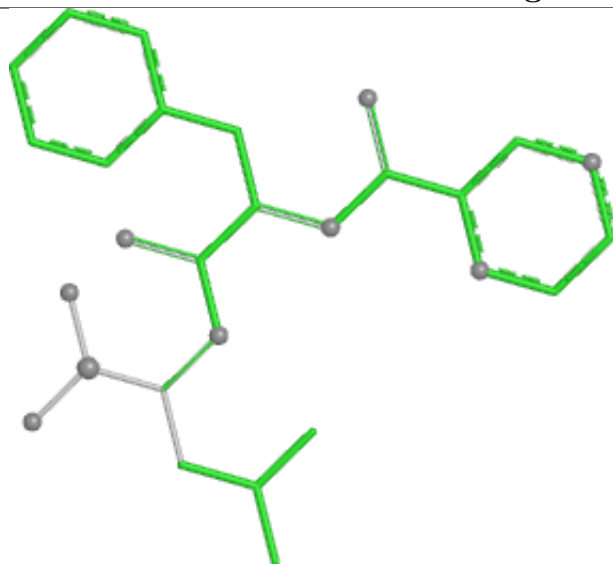


Torsions

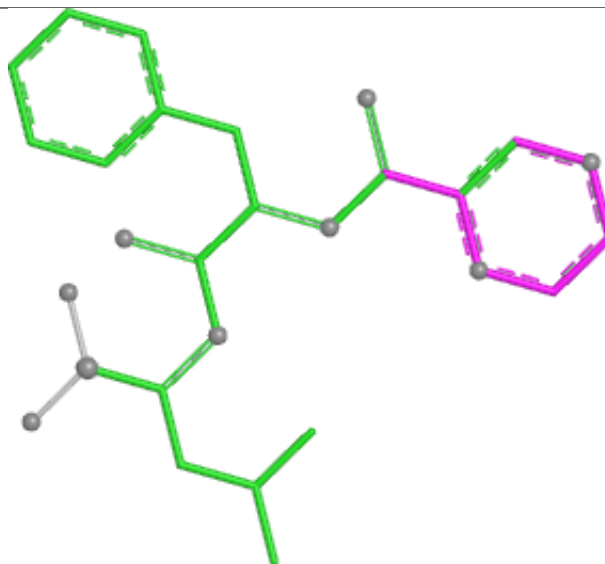


Rings

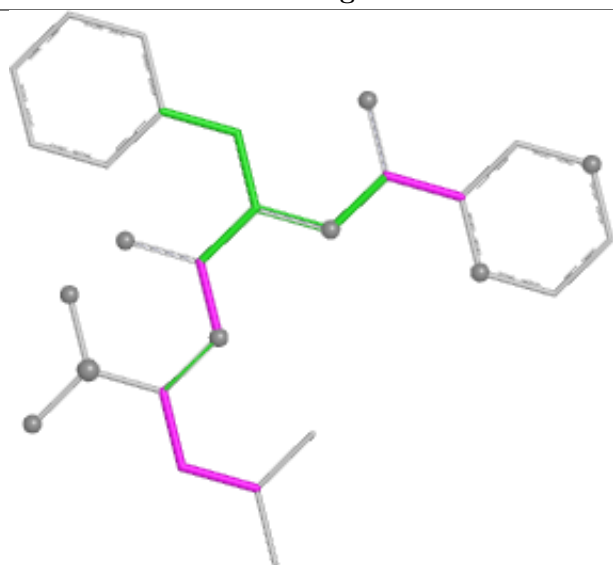
Ligand BO2 i 301



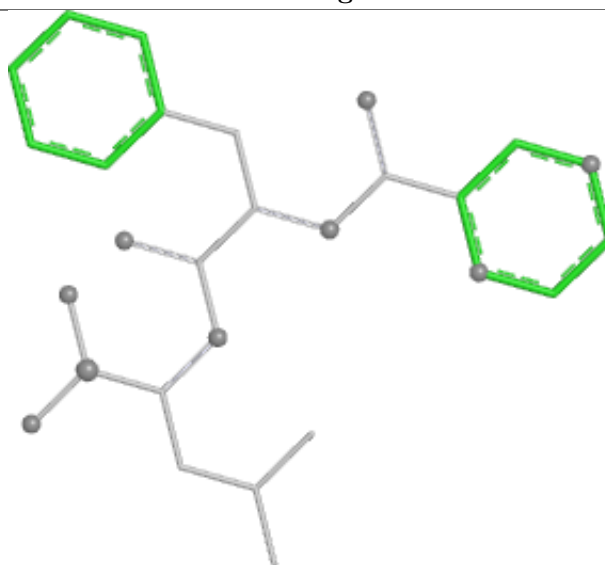
Bond lengths



Bond angles

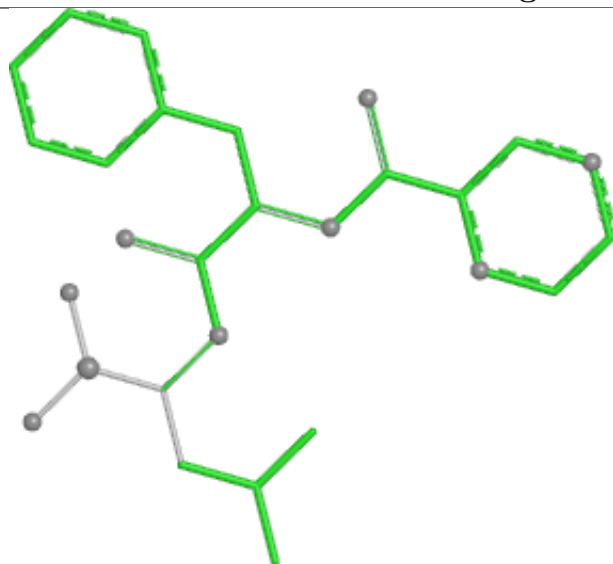


Torsions

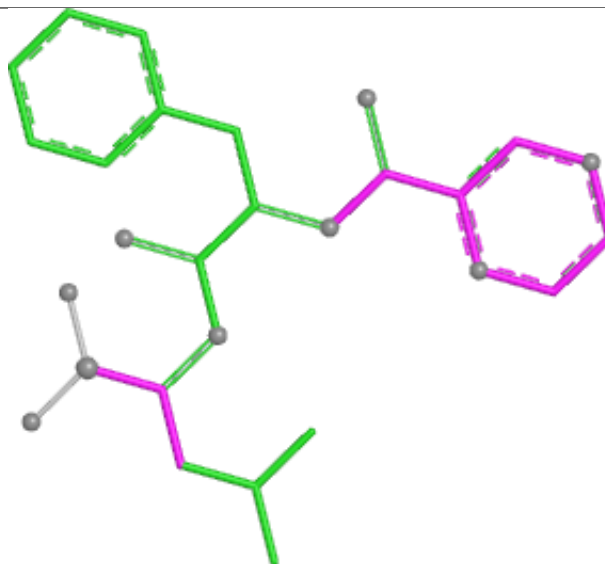


Rings

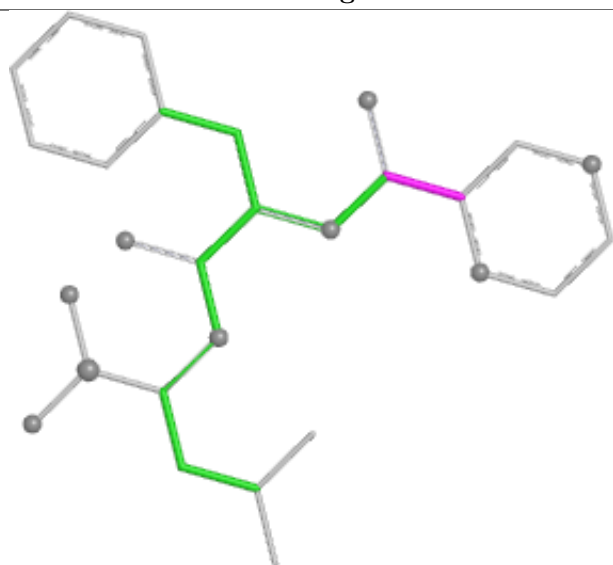
Ligand BO2 h 301



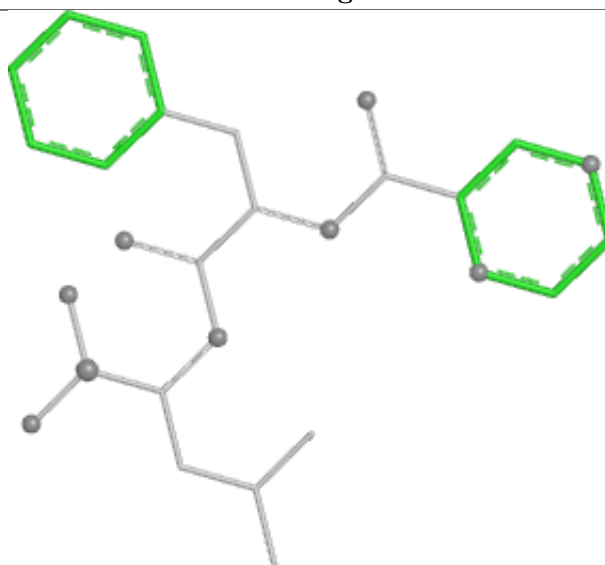
Bond lengths



Bond angles

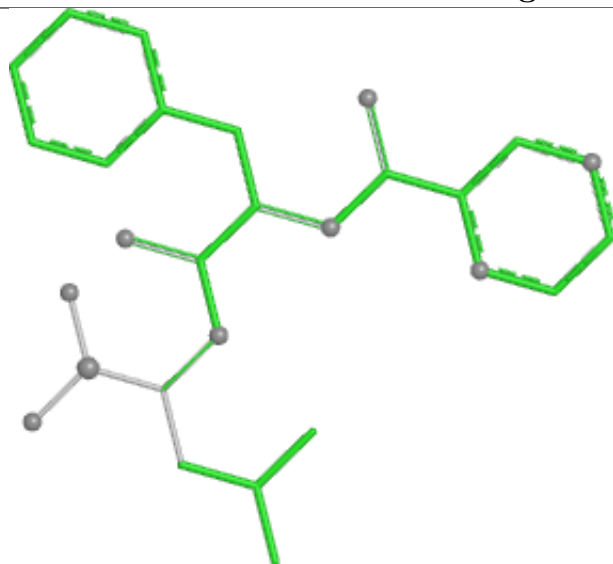


Torsions

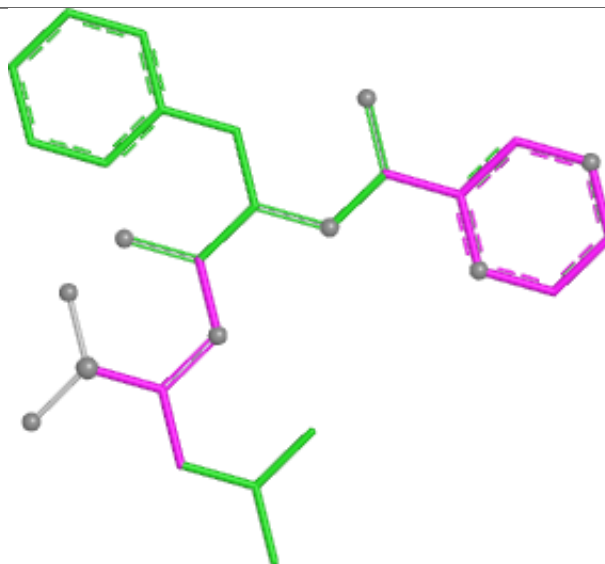


Rings

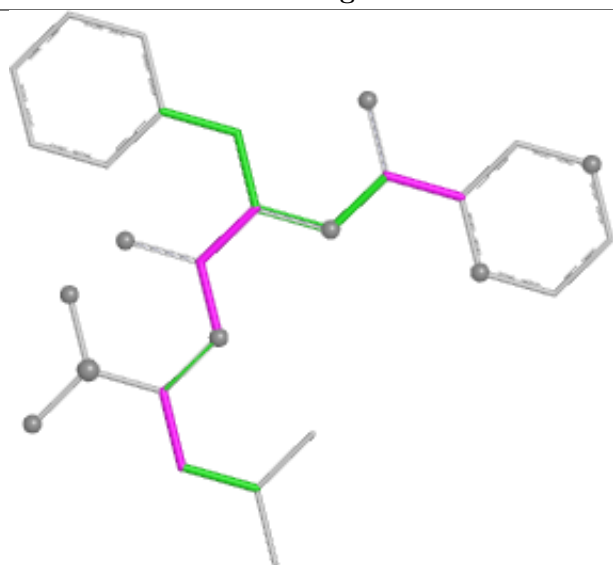
Ligand BO2 L 401



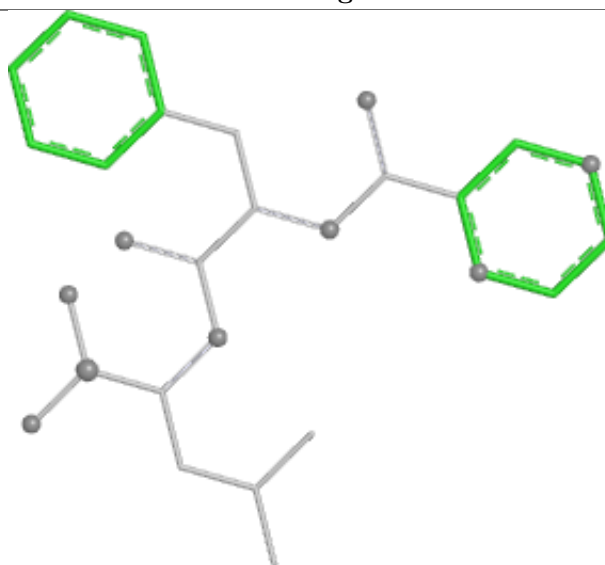
Bond lengths



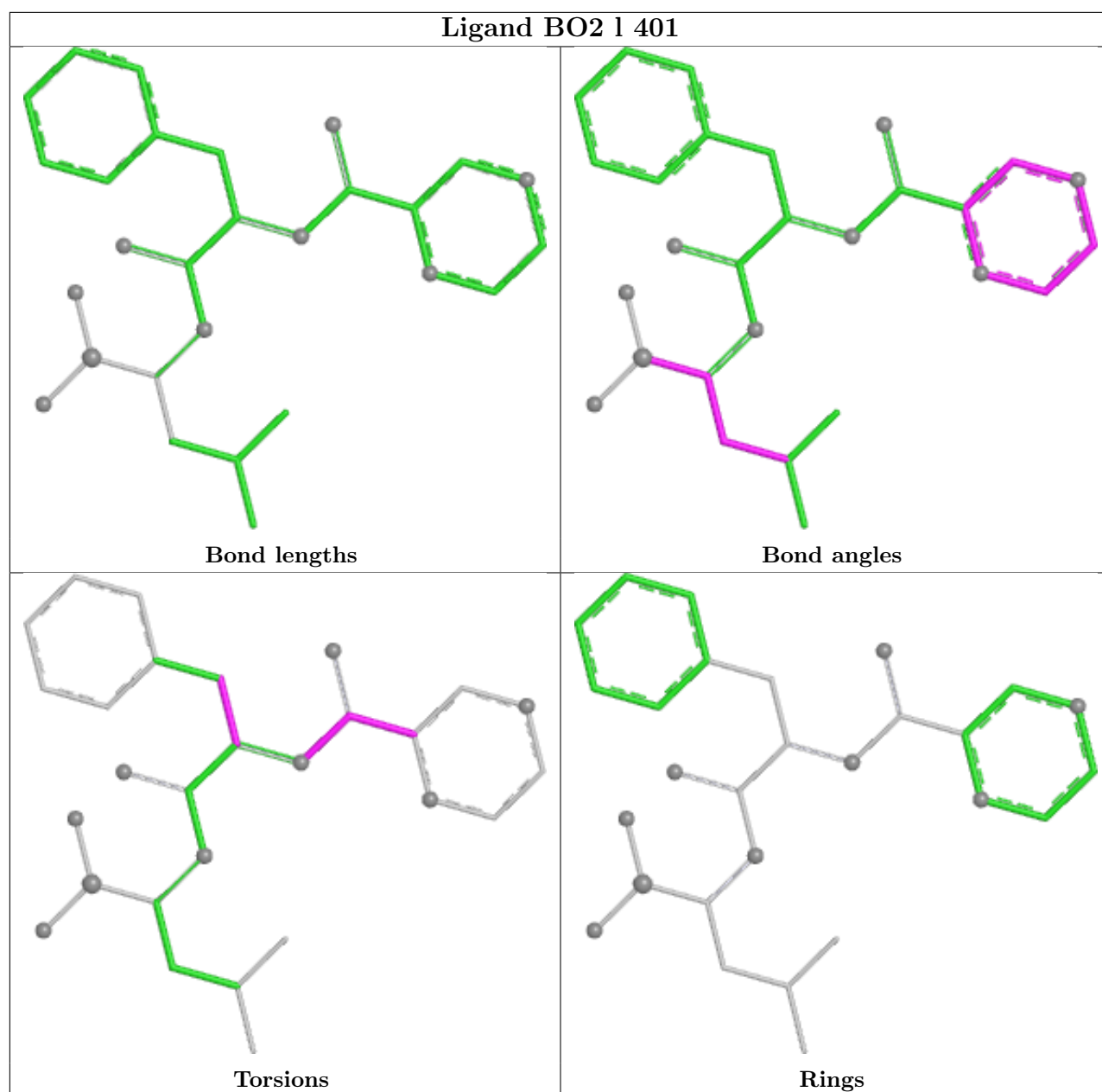
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

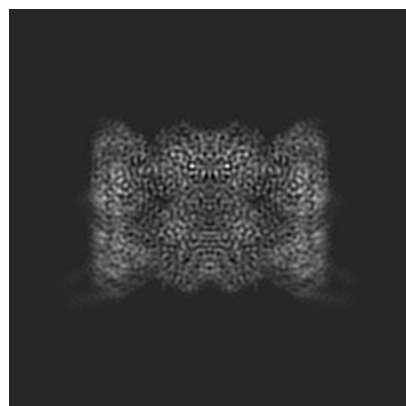
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10463. These allow visual inspection of the internal detail of the map and identification of artifacts.

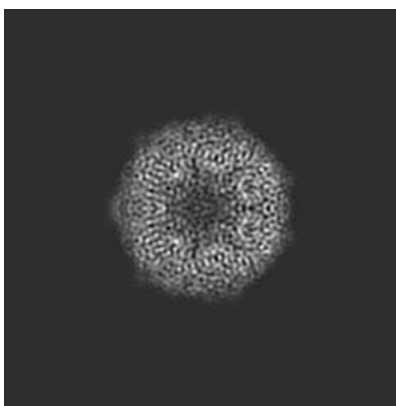
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

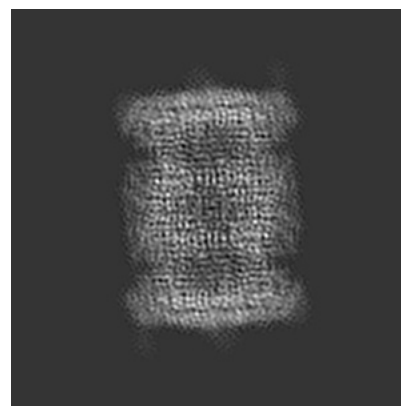
6.1.1 Primary map



X

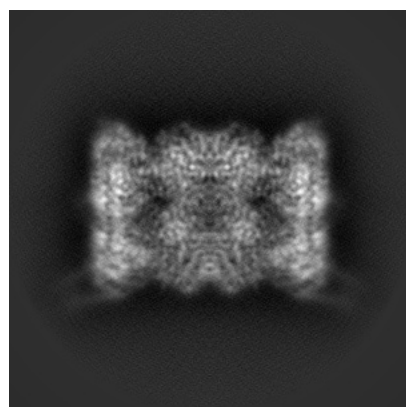


Y

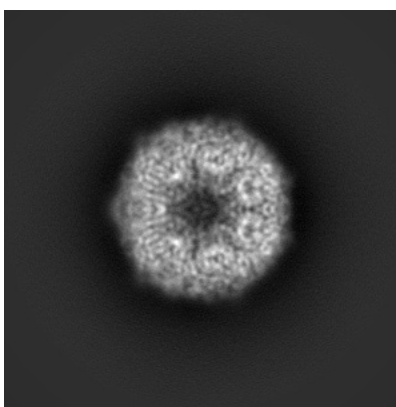


Z

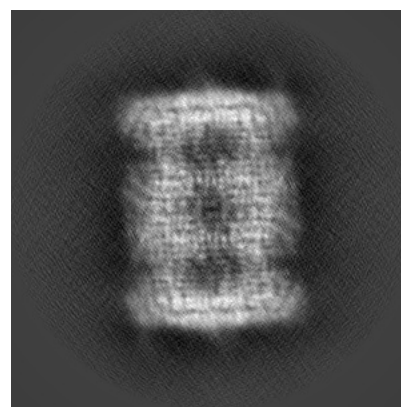
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 150

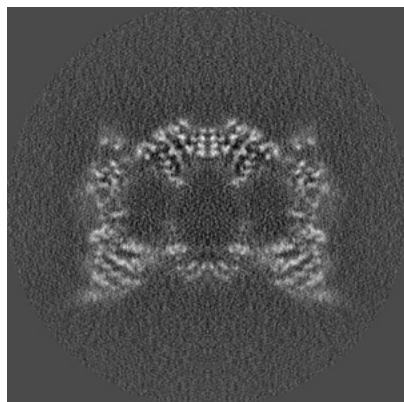


Y Index: 150

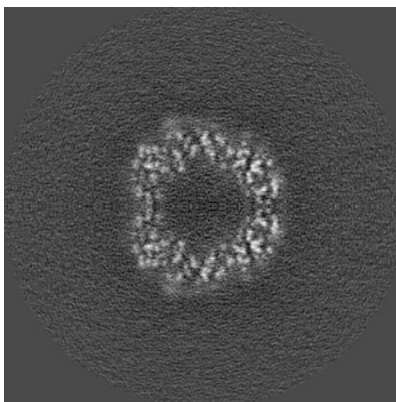


Z Index: 150

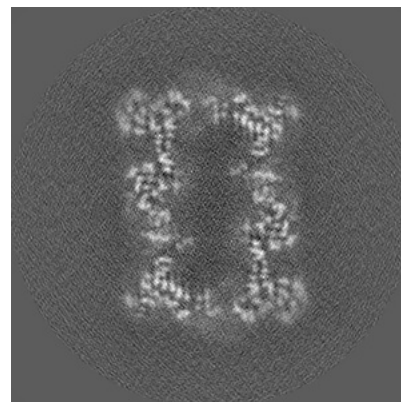
6.2.2 Raw map



X Index: 150



Y Index: 150

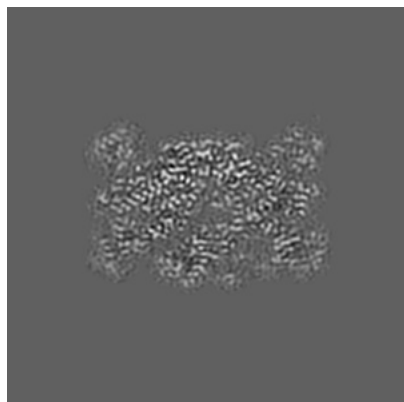


Z Index: 150

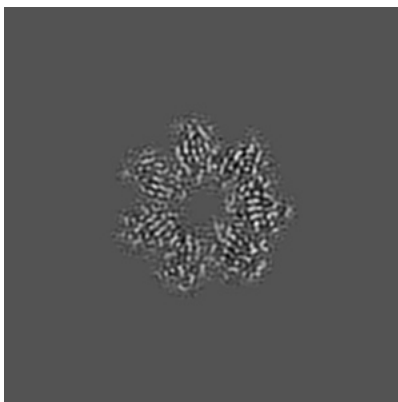
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

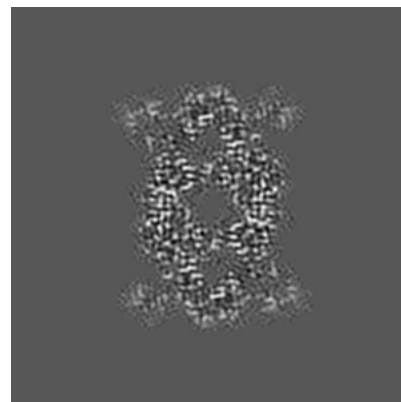
6.3.1 Primary map



X Index: 183

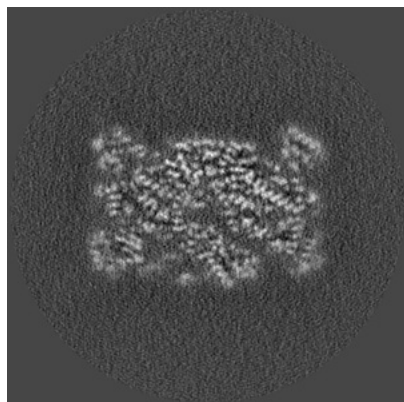


Y Index: 129

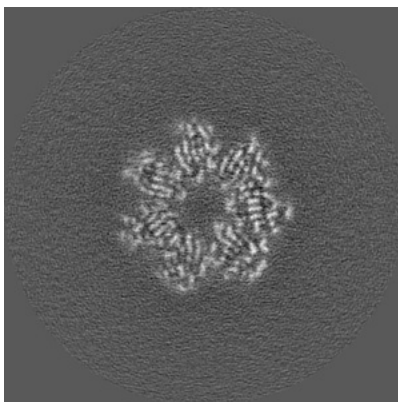


Z Index: 176

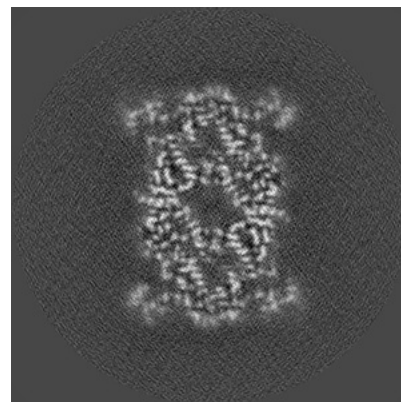
6.3.2 Raw map



X Index: 117



Y Index: 129

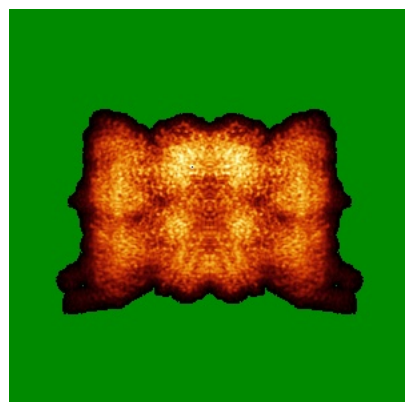


Z Index: 177

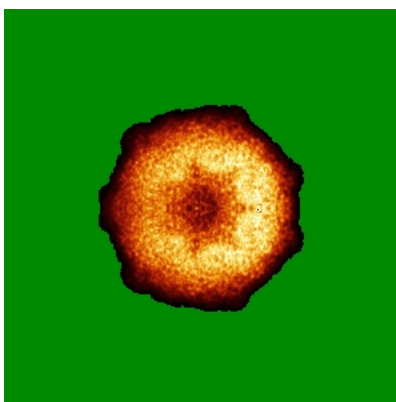
The images above show the largest variance slices of the map in three orthogonal directions.

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

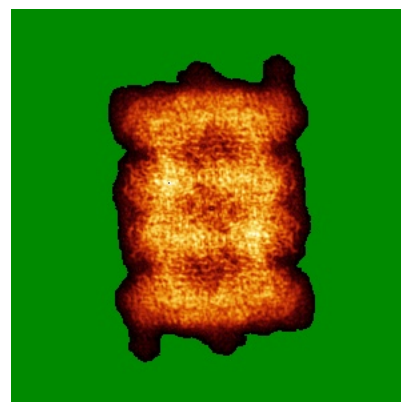
6.4.1 Primary map



X

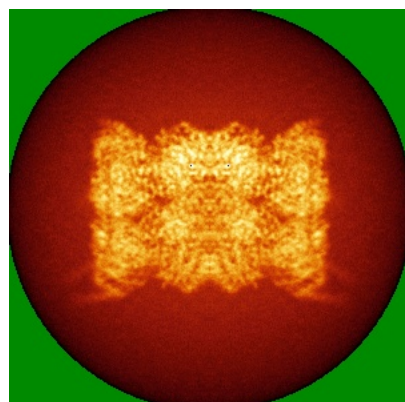


Y

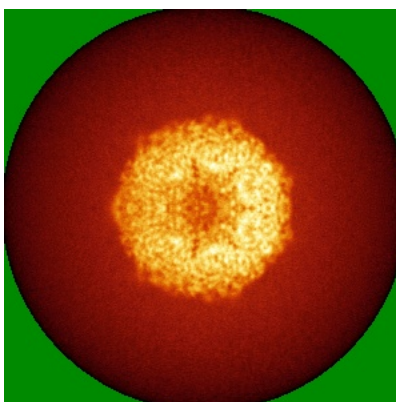


Z

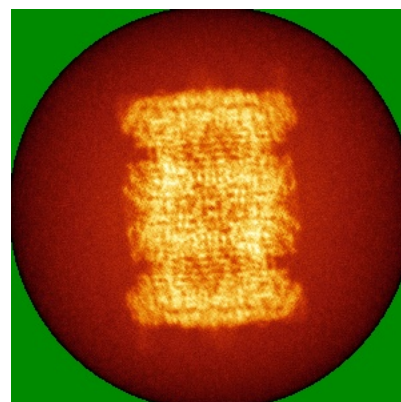
6.4.2 Raw map



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.

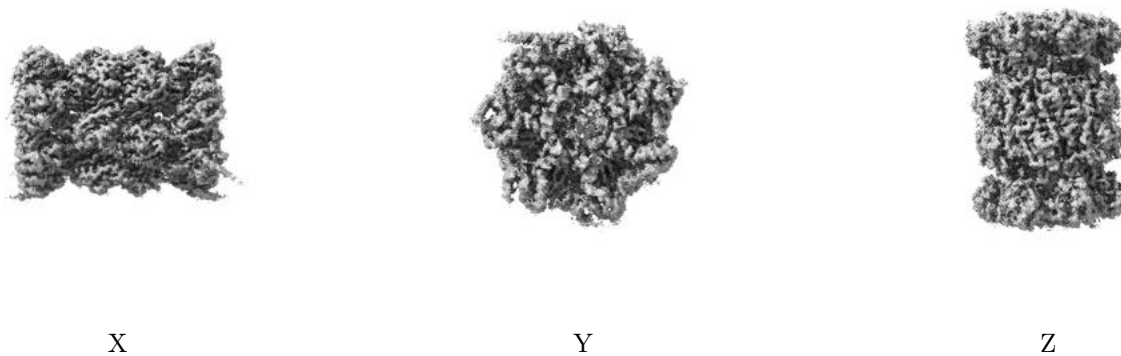
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

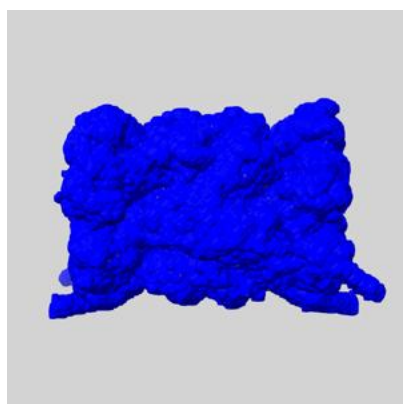
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

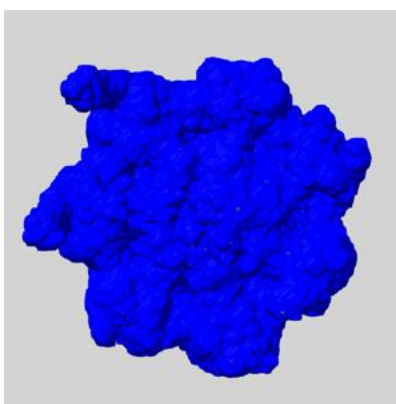
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

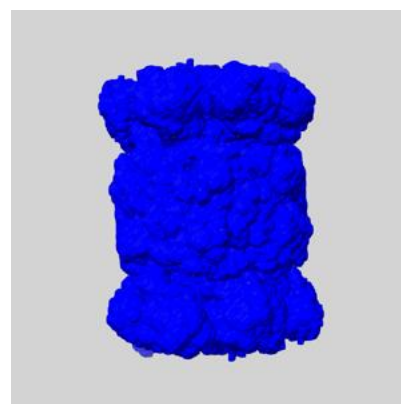
6.6.1 emd_10463_msk_1.map [i](#)



X



Y

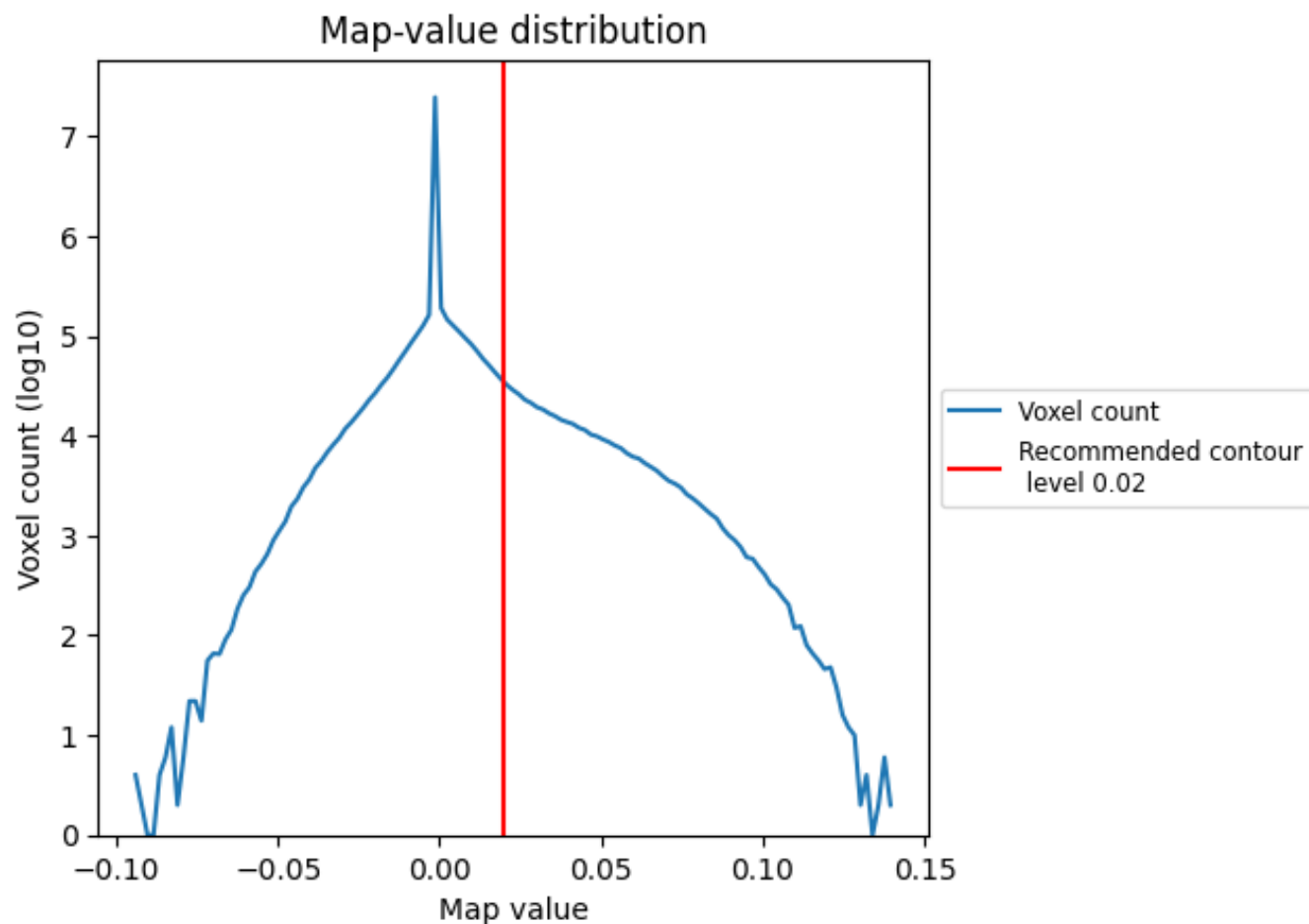


Z

7 Map analysis [i](#)

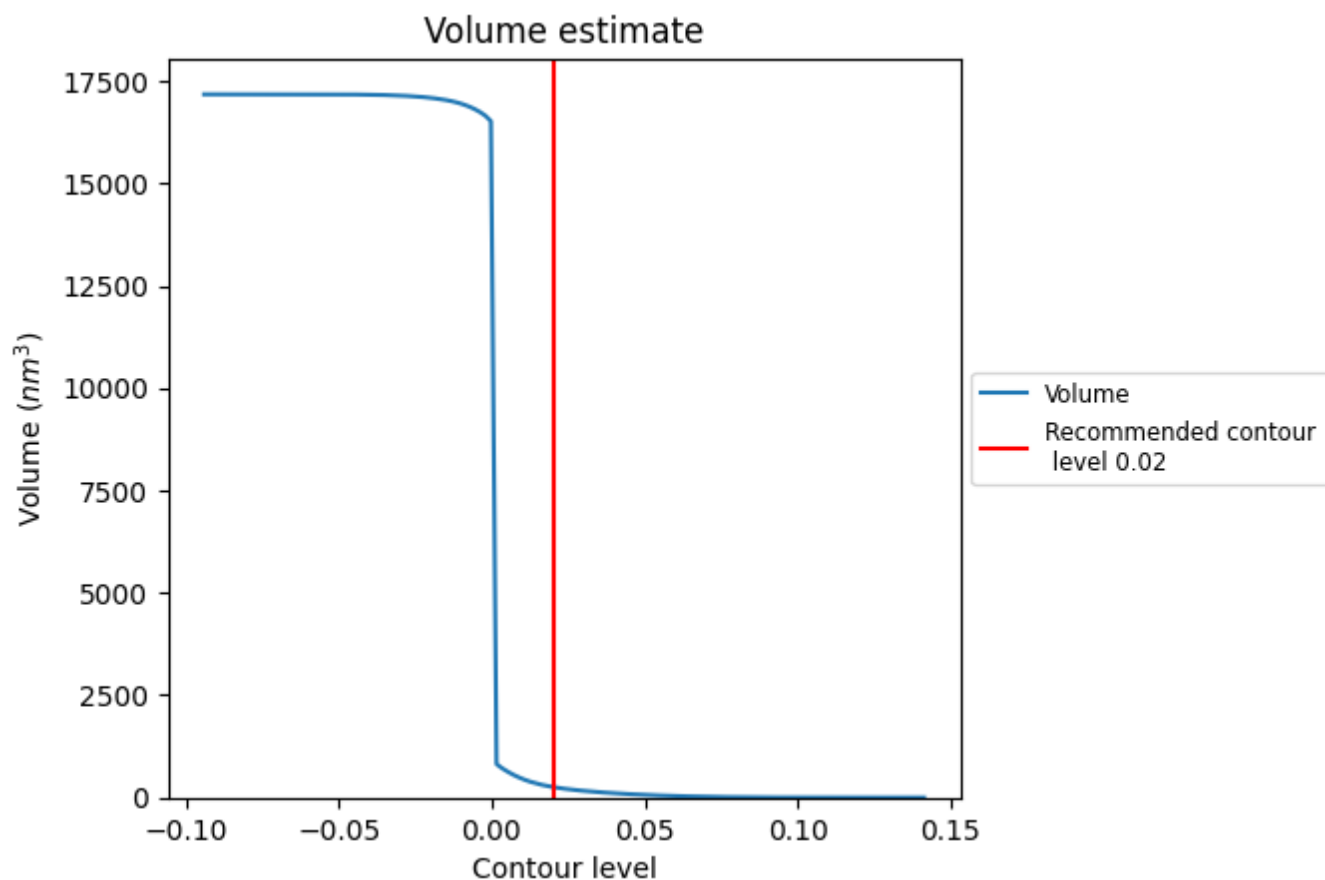
This section contains the results of statistical analysis of the map.

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.

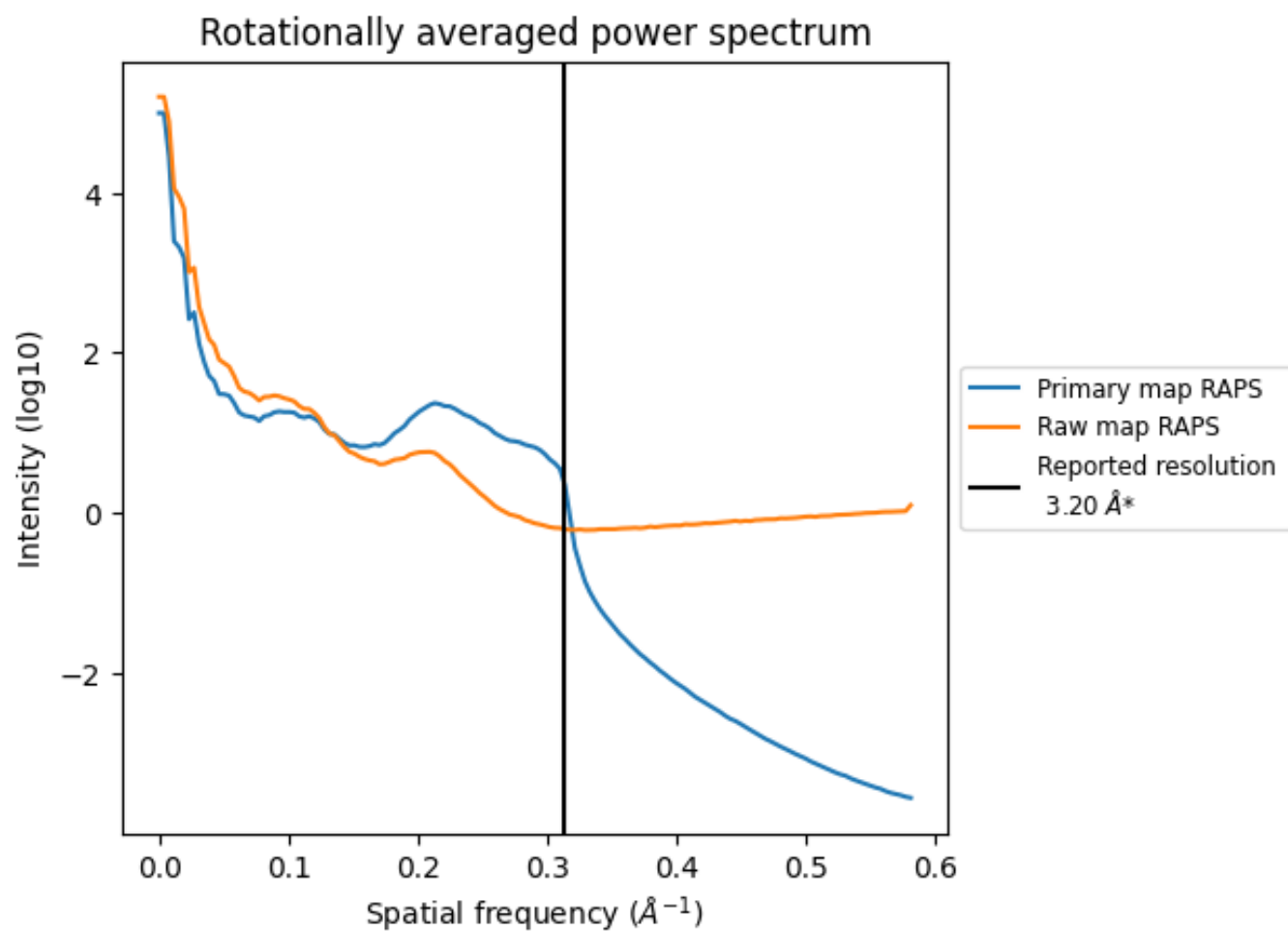
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm³; this corresponds to an approximate mass of 232 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 ⓘ

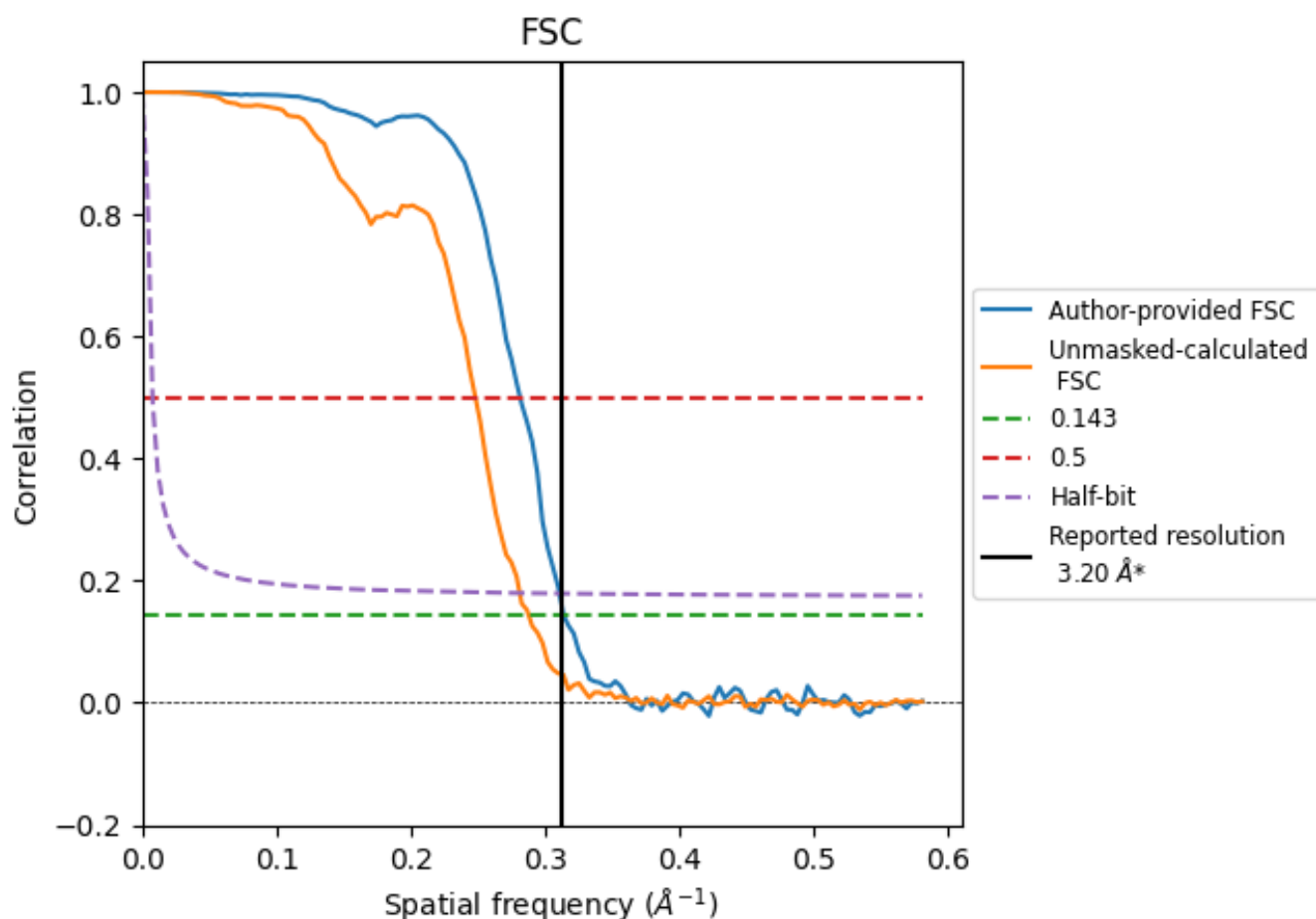


*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

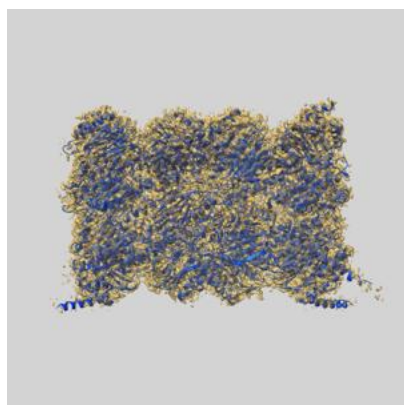
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.18	3.55	3.22
Unmasked-calculated*	3.47	4.03	3.55

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

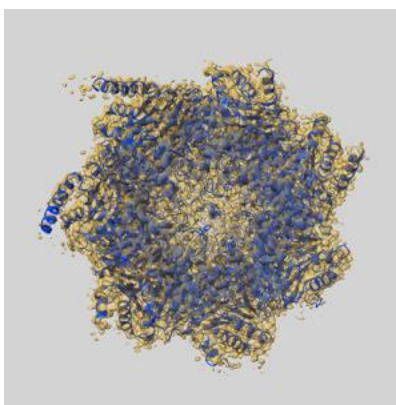
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10463 and PDB model 6TD5. Per-residue inclusion information can be found in section [3](#) on page [9](#).

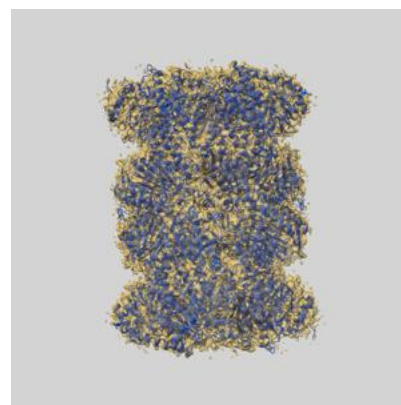
9.1 Map-model overlay [i](#)



X



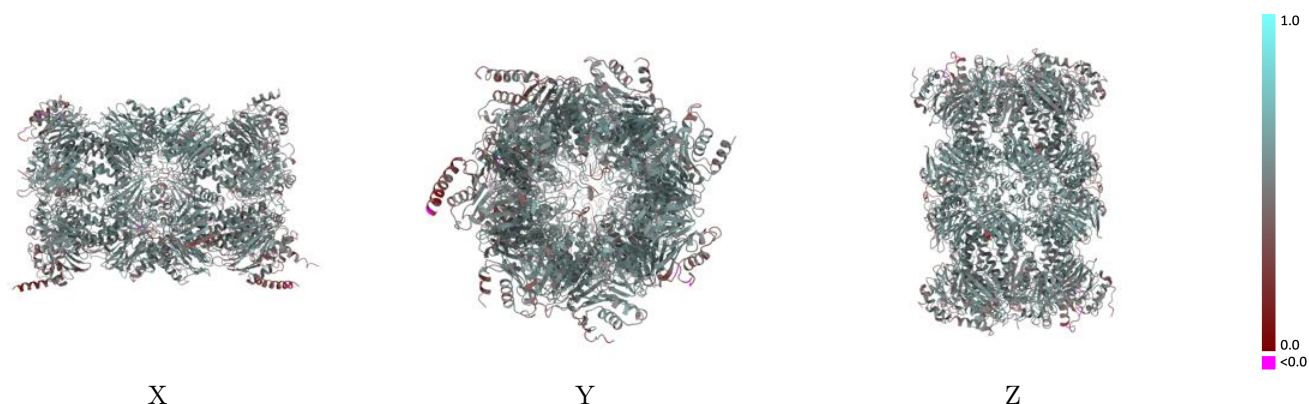
Y



Z

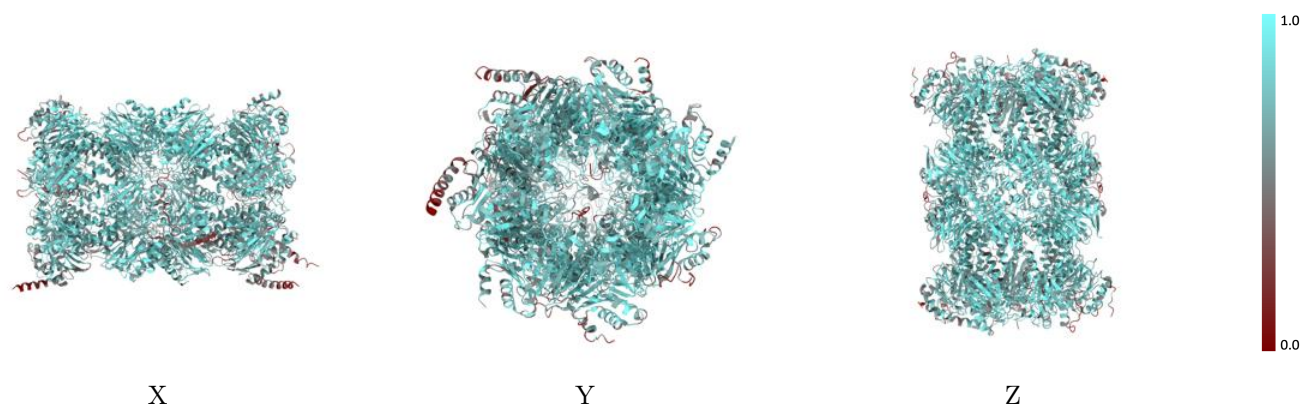
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



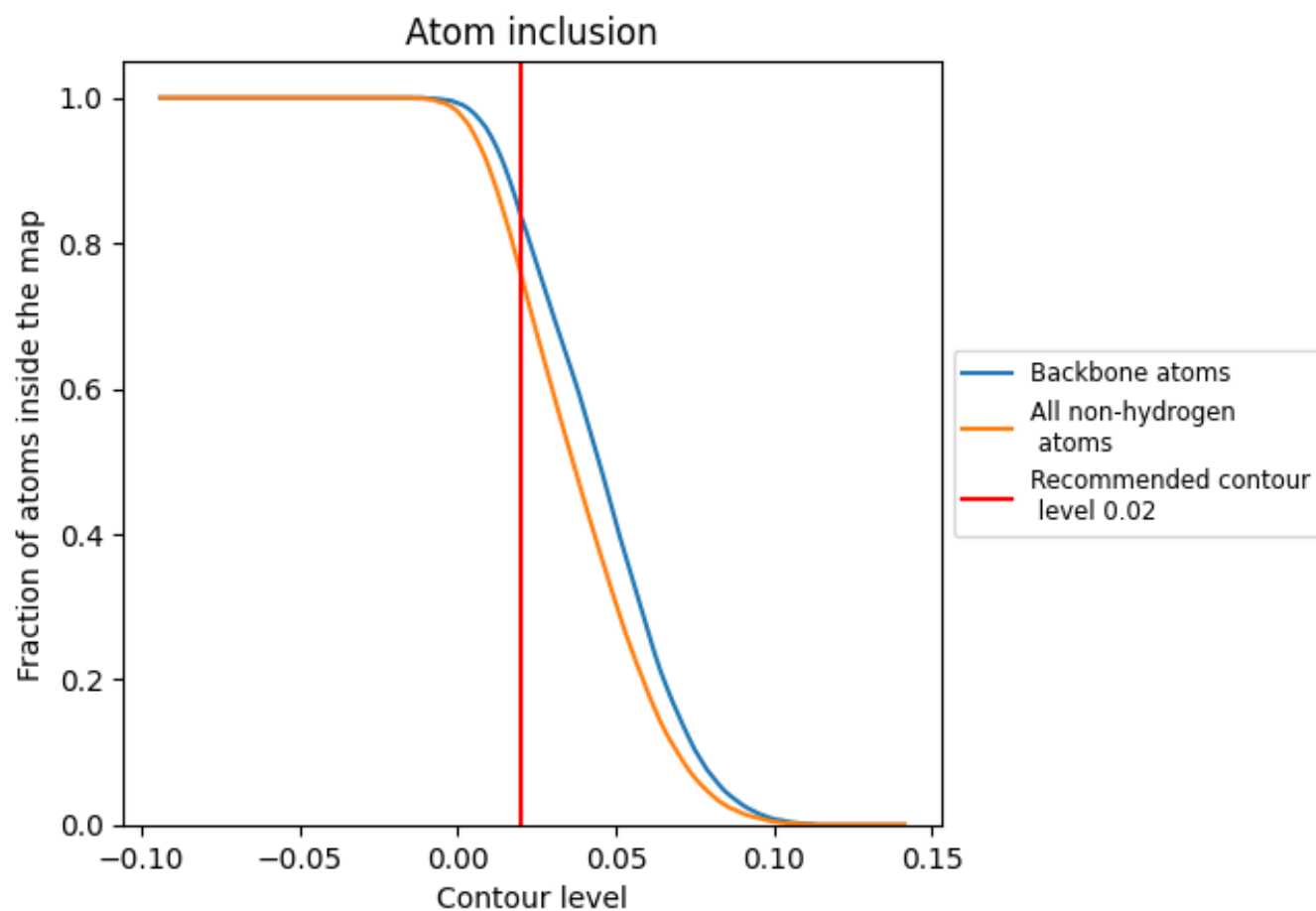
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7560	 0.5120
A	 0.7690	 0.5110
B	 0.7510	 0.5140
C	 0.6890	 0.4860
D	 0.6370	 0.4490
E	 0.7220	 0.5000
F	 0.7530	 0.5130
G	 0.7310	 0.4910
H	 0.8650	 0.5640
I	 0.7540	 0.5150
J	 0.7980	 0.5310
K	 0.7170	 0.5060
L	 0.8030	 0.5280
M	 0.7860	 0.5190
N	 0.8370	 0.5490
a	 0.7680	 0.5110
b	 0.7550	 0.5160
c	 0.6900	 0.4850
d	 0.6420	 0.4500
e	 0.7220	 0.4960
f	 0.7540	 0.5150
g	 0.7300	 0.4920
h	 0.8670	 0.5670
i	 0.7550	 0.5130
j	 0.7980	 0.5310
k	 0.7230	 0.5060
l	 0.8020	 0.5240
m	 0.7800	 0.5180
n	 0.8350	 0.5510

