W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 01:30 PM EST

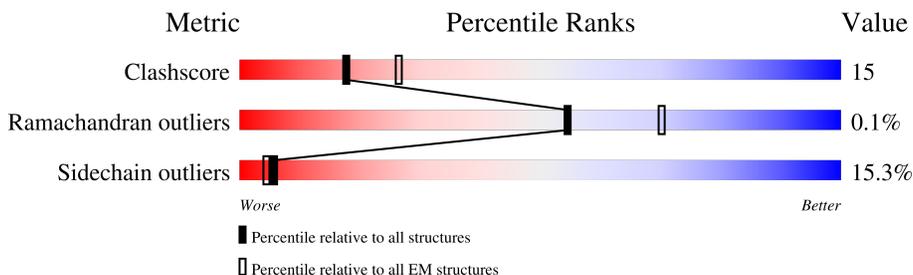|		
PDB ID	:	7M7F
EMDB ID	:	EMD-23711
Title	:	6-Deoxyerythronolide B synthase (DEBS) module 1 in complex with antibody fragment 1B2: State 1
Authors	:	Cogan, D.P.; Zhang, K.; Chiu, W.; Khosla, C.
Deposited on	:	2021-03-28
Resolution	:	3.20 Å(reported)

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	Percentile Ranks	Value
Clashscore		15
Ramachandran outliers		0.1%
Sidechain outliers		15.3%

Worse — *Better*

■ Percentile relative to all structures
▯ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1784	11% / 47% 27% • 22%
1	B	1784	6% / 34% 19% • 44%
2	C	249	44% 31% 6% • 18%
2	E	249	44% 32% 6% 18%
3	D	236	44% 39% • 13%
3	F	236	44% 40% • 13%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 23971 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 EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	999	Total	C	N	O	S	0	0
			7417	4613	1363	1414	27		
1	A	1390	Total	C	N	O	S	0	0
			10319	6413	1899	1972	35		

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP Q5UNP6
B	2	ALA	-	expression tag	UNP Q5UNP6
B	3	SER	-	expression tag	UNP Q5UNP6
B	4	THR	-	expression tag	UNP Q5UNP6
B	5	ASP	-	expression tag	UNP Q5UNP6
B	6	SER	-	expression tag	UNP Q5UNP6
B	7	GLU	-	expression tag	UNP Q5UNP6
B	8	LYS	-	expression tag	UNP Q5UNP6
B	9	VAL	-	expression tag	UNP Q5UNP6
B	10	ALA	-	expression tag	UNP Q5UNP6
B	11	GLU	-	expression tag	UNP Q5UNP6
B	12	TYR	-	expression tag	UNP Q5UNP6
B	13	LEU	-	expression tag	UNP Q5UNP6
B	14	ARG	-	expression tag	UNP Q5UNP6
B	15	ARG	-	expression tag	UNP Q5UNP6
B	16	ALA	-	expression tag	UNP Q5UNP6
B	17	THR	-	expression tag	UNP Q5UNP6
B	18	LEU	-	expression tag	UNP Q5UNP6
B	19	ASP	-	expression tag	UNP Q5UNP6
B	20	LEU	-	expression tag	UNP Q5UNP6
B	21	ARG	-	expression tag	UNP Q5UNP6
B	22	ALA	-	expression tag	UNP Q5UNP6
B	23	ALA	-	expression tag	UNP Q5UNP6
B	24	ARG	-	expression tag	UNP Q5UNP6
B	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ARG	-	expression tag	UNP Q5UNP6
B	27	ILE	-	expression tag	UNP Q5UNP6
B	28	ARG	-	expression tag	UNP Q5UNP6
B	29	GLU	-	expression tag	UNP Q5UNP6
B	30	LEU	-	expression tag	UNP Q5UNP6
B	31	GLU	-	expression tag	UNP Q5UNP6
B	1486	THR	-	linker	UNP Q5UNP6
B	1487	SER	-	linker	UNP Q5UNP6
B	1488	GLU	-	linker	UNP Q5UNP6
B	1489	LEU	-	linker	UNP Q5UNP6
B	1490	GLY	-	linker	UNP Q5UNP6
B	1768	SER	-	expression tag	UNP Q03133
B	1769	SER	-	expression tag	UNP Q03133
B	1770	VAL	-	expression tag	UNP Q03133
B	1771	ASP	-	expression tag	UNP Q03133
B	1772	LYS	-	expression tag	UNP Q03133
B	1773	LEU	-	expression tag	UNP Q03133
B	1774	ALA	-	expression tag	UNP Q03133
B	1775	ALA	-	expression tag	UNP Q03133
B	1776	ALA	-	expression tag	UNP Q03133
B	1777	LEU	-	expression tag	UNP Q03133
B	1778	GLU	-	expression tag	UNP Q03133
B	1779	HIS	-	expression tag	UNP Q03133
B	1780	HIS	-	expression tag	UNP Q03133
B	1781	HIS	-	expression tag	UNP Q03133
B	1782	HIS	-	expression tag	UNP Q03133
B	1783	HIS	-	expression tag	UNP Q03133
B	1784	HIS	-	expression tag	UNP Q03133
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	1486	THR	-	linker	UNP Q5UNP6
A	1487	SER	-	linker	UNP Q5UNP6
A	1488	GLU	-	linker	UNP Q5UNP6
A	1489	LEU	-	linker	UNP Q5UNP6
A	1490	GLY	-	linker	UNP Q5UNP6
A	1768	SER	-	expression tag	UNP Q03133
A	1769	SER	-	expression tag	UNP Q03133
A	1770	VAL	-	expression tag	UNP Q03133
A	1771	ASP	-	expression tag	UNP Q03133
A	1772	LYS	-	expression tag	UNP Q03133
A	1773	LEU	-	expression tag	UNP Q03133
A	1774	ALA	-	expression tag	UNP Q03133
A	1775	ALA	-	expression tag	UNP Q03133
A	1776	ALA	-	expression tag	UNP Q03133
A	1777	LEU	-	expression tag	UNP Q03133
A	1778	GLU	-	expression tag	UNP Q03133
A	1779	HIS	-	expression tag	UNP Q03133
A	1780	HIS	-	expression tag	UNP Q03133
A	1781	HIS	-	expression tag	UNP Q03133
A	1782	HIS	-	expression tag	UNP Q03133
A	1783	HIS	-	expression tag	UNP Q03133
A	1784	HIS	-	expression tag	UNP Q03133

- Molecule 2 is a protein called 1B2 (heavy chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		
2	E	205	Total	C	N	O	S	0	0
			1539	978	257	298	6		

- Molecule 3 is a protein called 1B2 (light chain).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	206	Total	C	N	O	S	0	0
			1568	983	262	317	6		
3	F	206	Total	C	N	O	S	0	0
			1568	984	262	316	6		

- Molecule 4 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanylethyl)-beta-alaninamide (three-letter code: PN7) (formula: $C_{11}H_{23}N_2O_7PS$).
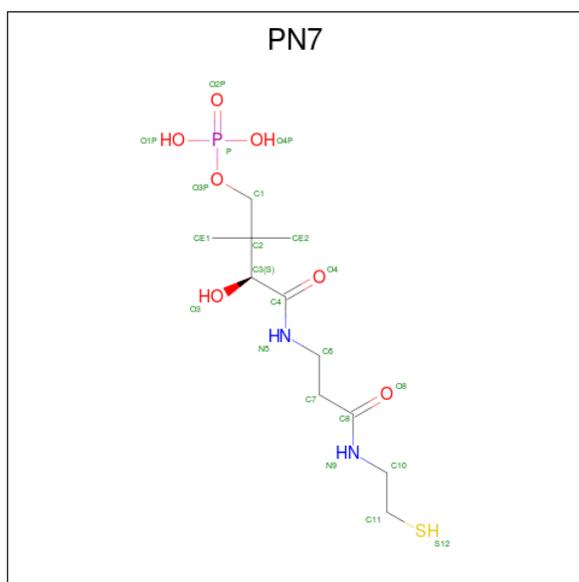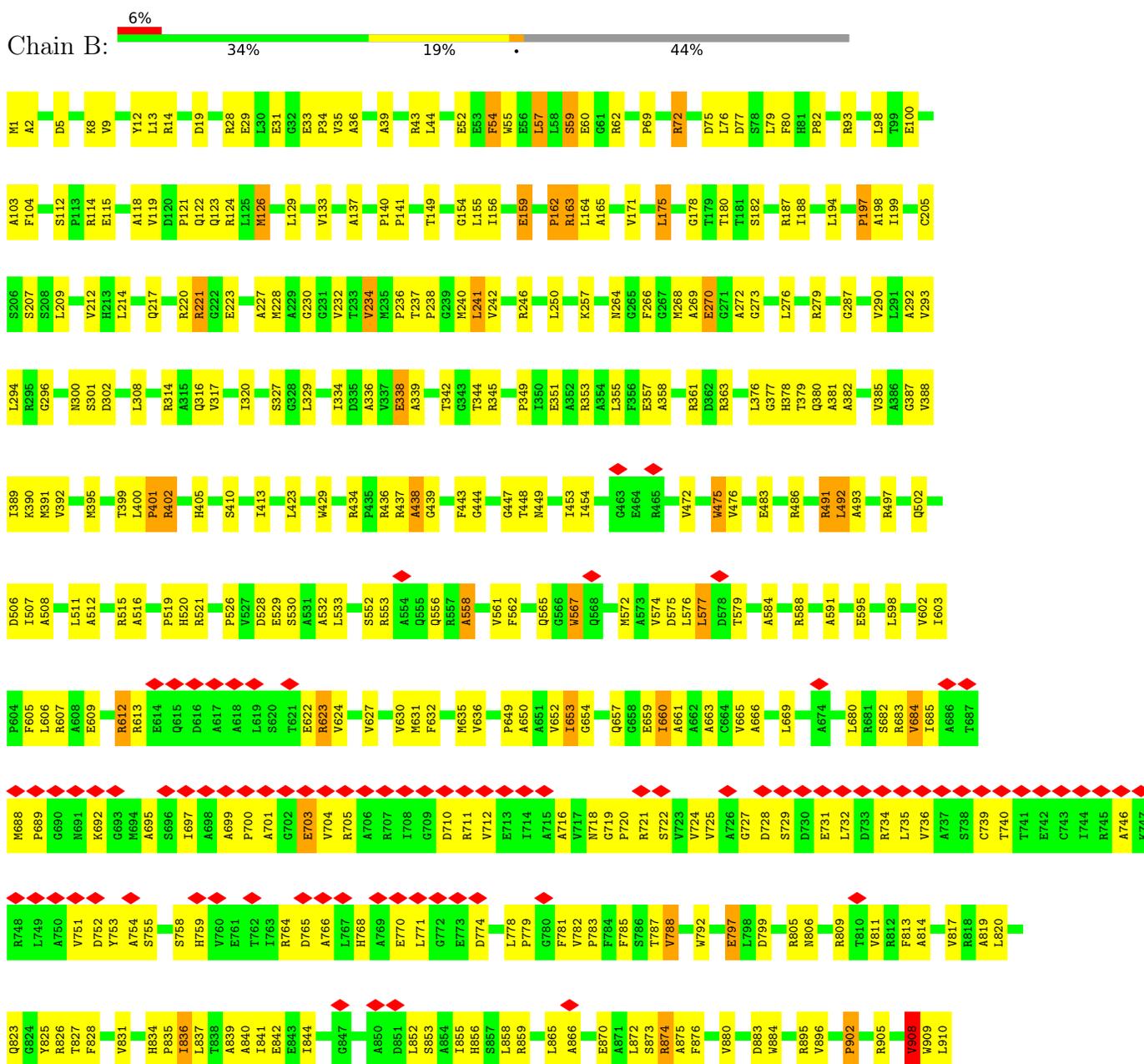

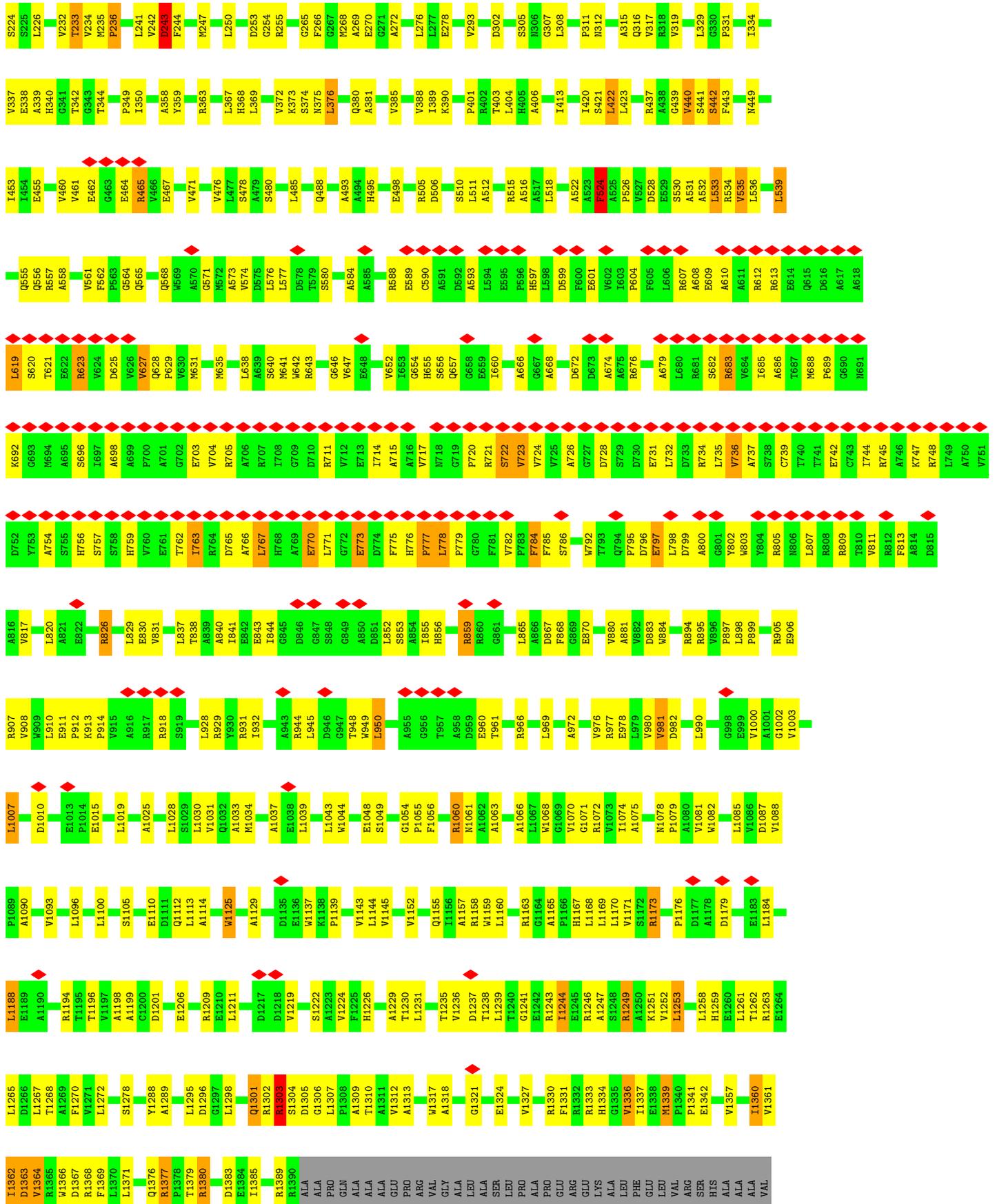| Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

3 Residue-property plots ⓘ

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.
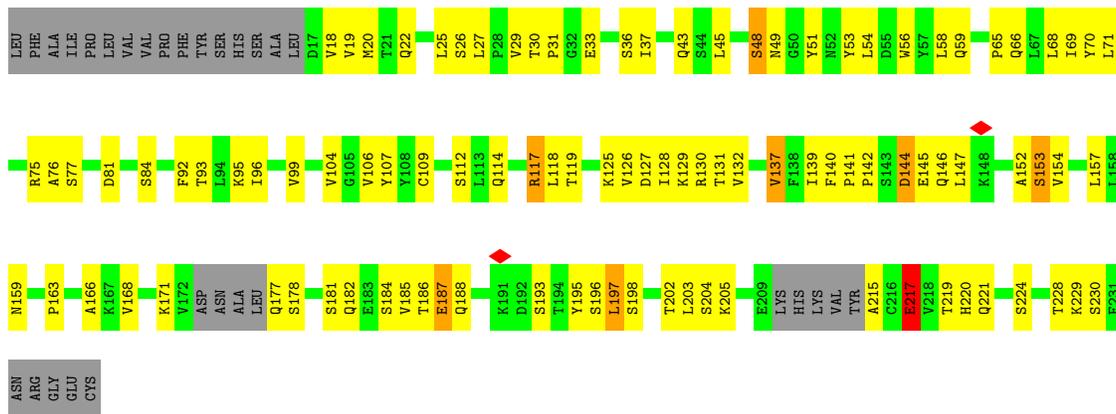
• Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

E911 P912

Labeled residues (with outlier markers):

L1404 A1405 S1406 L1407 P1408 A1409 P1410 E1411 R1412 E1413 K1414 A1415 L1416 R1421 V1427 L1428 A1431 S1432 A1433 E1434 R1435 V1436 P1437 Q1440 V1447 D1448 S1449 L1450 S1451 A1452 L1453 E1454 L1455 R1456 L1459 T1463 G1464 V1465 R1466

T1471 D1474 H1475 L1485 L1489 G1490

• Molecule 1: EryAI,6-deoxyerythronolide-B synthase EryA3, modules 5 and 6 chimera

Chain A: 11% | 47% | 27% | 22%

M1 A2 S3 T4 D5 S6 E7 K8 Y12 L13 R14 R15 A16 T17 E29 E33 V38 A39 C42 R43 L44 F54 L57 R62 D63 A64 V65 P69 I70 D71 R86 S87 Q92 R93 F97 L98 A103 F108 A116 L117 A118 V119 D120 Q123

R124 L125 M126 L129 S130 W131 E132 V133 A137 G138 I139 P140 P141 T149 V153 G154 L155 I156 P157 Q158 E159 P162 R163 V171 Y174 L175 M176 T177 G178 T179 T180 V183 A184 I188 L194 P197 S200 V201 D202 T203 S207 S208 L209 R220 R221

LEU GLY HIS ALA SER ALA GLU ARG VAL PRO ALA ASP GLN ALA PHE ALA GLU LEU GLY VAL ASP SER LEU SER ALA LEU GLU LEU ARG ASN ARG LEU GLY ALA THR GLY VAL ARG LEU PRO THR THR VAL PHE HIS PRO ASP VAL ARG THR LEU ALA ALA HIS LEU THR SER

GLU LEU GLY SER GLY THR PRO ALA ARG GLU ALA SER ALA LEU ARG ASP GLY TYR ARG GLN ALA GLY VAL SER GLY ARG VAL ALA SER TYR LEU ASP LEU ILE ALA GLY LEU SER ASP PHE ARG GLU HIS PHE ASP GLY SER ASP GLY PHE SER LEU GLU VAL ASP MET ALA ASP

GLY PRO GLY VAL THR ILE CYS ALA GLY ALA THR ALA ILE SER GLY PRO HIS GLU THR ARG LEU ALA GLY ALA LEU ARG GLY ILE ALA PRO VAL ARG ALA VAL PRO GLN GLY TYR GLU GLU GLU LEU PRO SER MET ALA VAL ALA ALA VAL GLN

ALA ASP ALA VAL ILE ARG GLN GLY LYS PRO VAL VAL GLY HIS SER ALA GLY LEU MET ALA TYR ALA LEU ALA THR GLU LEU ASP ALA ARG GLY HIS PRO ARG GLY VAL VAL ILE ASP TYR PRO GLY LEU GLN GLN ASP ALA MET ALA TRP LEU

GLU GLU LEU ALA THR THR PHE ASP GLU THR THR VAL ARG MET ASP THR ARG LEU THR ALA LEU GLY ALA TYR ASP ARG LEU GLY GLN TRP PRO ARG GLU THR GLY LEU PRO THR LEU VAL SER ALA GLY PRO MET GLY PRO TRP PRO ASP SER TRP LYS

PRO THR TRP PRO PHE GLU HIS ASP THR VAL ALA VAL PRO GLY ASP PHE HIS MET VAL GLN GLU HIS ALA ASP ALA ILE ALA ARG HIS ILE ASP ALA TRP LEU GLY GLY ASN SER SER VAL ASP LYS ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 2: 1B2 (heavy chain)

Chain C:

• Molecule 2: 1B2 (heavy chain)

Chain E:

• Molecule 3: 1B2 (light chain)

Chain D:

44%   39%   13%

LEU PHE ALA ILE PRO LEU VAL VAL PRO PHE TYR SER HIS SER ALA LEU D17 V18 V19 M20 T21 Q22 L25 S26 L27 P28 V29 T30 P31 G32 E33 S36 I37 Q43 S44 L45 S48 N49 G50 Y51 N52 Y53 L54 D55 W56 Y57 L58 Q59 P65 Q66 L67 L68 I69 Y70 L71

R75 A76 S77 D81 S84 F92 T93 L94 K95 I96 V99 V104 G105 V106 Y107 Y108 C109 S112 L113 Q114 R117 L118 T119 K125 V126 D127 I128 K129 R130 T131 V132 V137 F138 I139 F140 P141 P142 S143 D144 E145 Q146 L147 K148 A152 S153 V154 L157 L158

N159 P163 A166 K167 V168 K171 V172 ASP ASN ALA LEU Q177 S178 S181 Q182 E183 S184 V185 T186 E187 Q188 K191 D192 S193 T194 Y195 S196 L197 S198 T202 L203 S204 K205 E209 LYS HIS LYS VAL TYR A215 C216 E217 V218 T219 H220 Q221 S224 T228 K229 S230 F231

ASN ARG GLY GLU CYS

- Molecule 3: 1B2 (light chain)

Chain F:

44%   40%   13%

LEU PHE ALA ILE PRO LEU VAL VAL PRO PHE TYR SER HIS SER ALA LEU D17 V18 V19 M20 T21 Q22 L25 S26 L27 P28 V29 T30 P31 G32 E33 S36 I37 Q43 S44 L45 S48 N49 Y53 L54 D55 W56 Y57 L58 Q59 K60 P65 Q66 L67 L68 I69 Y70 L71

N74 R75 A76 S77 G78 V79 P80 D81 S84 G85 S86 T90 D91 F92 T93 L94 V99 E102 D103 V106 Y107 Y108 C109 S112 T115 P116 R117 L118 T119 K125 V126 D127 I128 K129 R130 T131 V132 A133 A134 P135 S136 V137 F138 I139 F140 P141 P142 S143 D144 E145 Q146 L147

K148 A152 S153 V154 V155 C156 L157 L158 A166 K167 W170 K171 V172 ASP ASN ALA LEU GLN S178 G179 N180 S181 S184 V185 T186 E187 Q188 D189 S190 K191 D192 S193 T194 Y195 S198 L201 T202 L203 S204 K205 K210 HIS LYS VAL TYR A215 C216 E217 V218 T219 H220 Q221

S224 T228 K229 S230 F231 ASN ARG GLY GLU CYS

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	172352	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.734	Depositor
Minimum map value	-4.602	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.53	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PN7

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	0.67	24/10522 (0.2%)	0.85	27/14323 (0.2%)
1	B	0.66	21/7566 (0.3%)	0.86	28/10293 (0.3%)
2	C	0.62	3/1575 (0.2%)	0.86	5/2141 (0.2%)
2	E	0.59	1/1575 (0.1%)	0.87	4/2141 (0.2%)
3	D	0.46	1/1601 (0.1%)	0.68	1/2175 (0.0%)
3	F	0.54	3/1601 (0.2%)	0.76	5/2174 (0.2%)
All	All	0.64	53/24440 (0.2%)	0.84	70/33247 (0.2%)

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	1
2	C	0	1
2	E	0	3
3	F	0	1
All	All	0	6

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	SER	CA-CB	-16.15	1.28	1.52
1	A	442	SER	CA-CB	-14.72	1.30	1.52
1	A	441	SER	CA-CB	-10.75	1.36	1.52
1	A	374	SER	CA-CB	-9.77	1.38	1.52
1	B	230	GLY	C-O	-8.63	1.09	1.23

The worst 5 of 70 bond angle outliers are listed below:

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	162	PRO	N-CA-CB	-16.54	83.45	103.30
1	A	159	GLU	CB-CA-C	-16.14	78.12	110.40
1	B	883	ASP	CB-CA-C	-15.95	78.51	110.40
1	A	43	ARG	CB-CA-C	-13.60	83.20	110.40
1	A	157	PRO	N-CA-CB	-12.39	88.43	103.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1301	GLN	Mainchain
2	C	155	GLU	Peptide
2	E	155	GLU	Peptide
2	E	21	ARG	Sidechain
2	E	96	ALA	Mainchain

5.2 Too-close contacts ⓘ

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	10319	0	10164	311	0
1	B	7417	0	7306	208	0
2	C	1539	0	1511	59	0
2	E	1539	0	1511	61	0
3	D	1568	0	1528	54	0
3	F	1568	0	1533	62	0
4	B	21	0	22	2	0
All	All	23971	0	23575	714	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.

The worst 5 of 714 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:777:PRO:HB3	1:A:796:ASP:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:86:GLN:HA	2:C:86:GLN:HE21	1.38	0.87
1:B:567:TRP:HB3	1:B:834:HIS:HB3	1.68	0.74
1:A:1019:LEU:HD13	1:A:1244:ILE:HG22	1.70	0.73
2:E:108:ASP:CG	3:F:67:LEU:CD2	2.60	0.70

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1388/1784 (78%)	1264 (91%)	123 (9%)	1 (0%)	51	83
1	B	995/1784 (56%)	915 (92%)	78 (8%)	2 (0%)	47	79
2	C	199/249 (80%)	179 (90%)	20 (10%)	0	100	100
2	E	199/249 (80%)	176 (88%)	23 (12%)	0	100	100
3	D	200/236 (85%)	184 (92%)	16 (8%)	0	100	100
3	F	200/236 (85%)	187 (94%)	13 (6%)	0	100	100
All	All	3181/4538 (70%)	2905 (91%)	273 (9%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1449	SER
1	B	720	PRO
1	A	779	PRO

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	1028/1325 (78%)	884 (86%)	144 (14%)	3	16
1	B	746/1325 (56%)	653 (88%)	93 (12%)	4	21
2	C	170/203 (84%)	132 (78%)	38 (22%)	1	4
2	E	170/203 (84%)	136 (80%)	34 (20%)	1	6
3	D	182/208 (88%)	146 (80%)	36 (20%)	1	7
3	F	182/208 (88%)	147 (81%)	35 (19%)	1	8
All	All	2478/3472 (71%)	2098 (85%)	380 (15%)	6	13

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1371	LEU
3	D	95	LYS
2	C	5	GLN
2	C	112	GLN
3	D	181	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	86	GLN
2	C	112	GLN
3	F	188	GLN
2	C	206	ASN
3	D	188	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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
4	PN7	B	1801	1	13,20,21	2.33	4 (30%)	18,26,29	1.41	4 (22%)

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
4	PN7	B	1801	1	-	10/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1801	PN7	C4-N5	5.34	1.45	1.33
4	B	1801	PN7	C8-N9	5.21	1.45	1.33
4	B	1801	PN7	O4-C4	-2.28	1.18	1.23
4	B	1801	PN7	O8-C8	-2.10	1.19	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1801	PN7	C6-C7-C8	2.45	116.44	112.36
4	B	1801	PN7	C6-N5-C4	-2.29	118.50	122.59
4	B	1801	PN7	CE2-C2-C3	2.14	112.52	108.82
4	B	1801	PN7	C11-C10-N9	-2.02	107.68	112.31

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1801	PN7	C1-C2-C3-O3
4	B	1801	PN7	C1-C2-C3-C4
4	B	1801	PN7	CE1-C2-C3-O3
4	B	1801	PN7	CE1-C2-C3-C4
4	B	1801	PN7	CE2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1801	PN7	2	0

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

Ligand PN7 B 1801

Bond lengths

Bond angles

Torsions

Rings
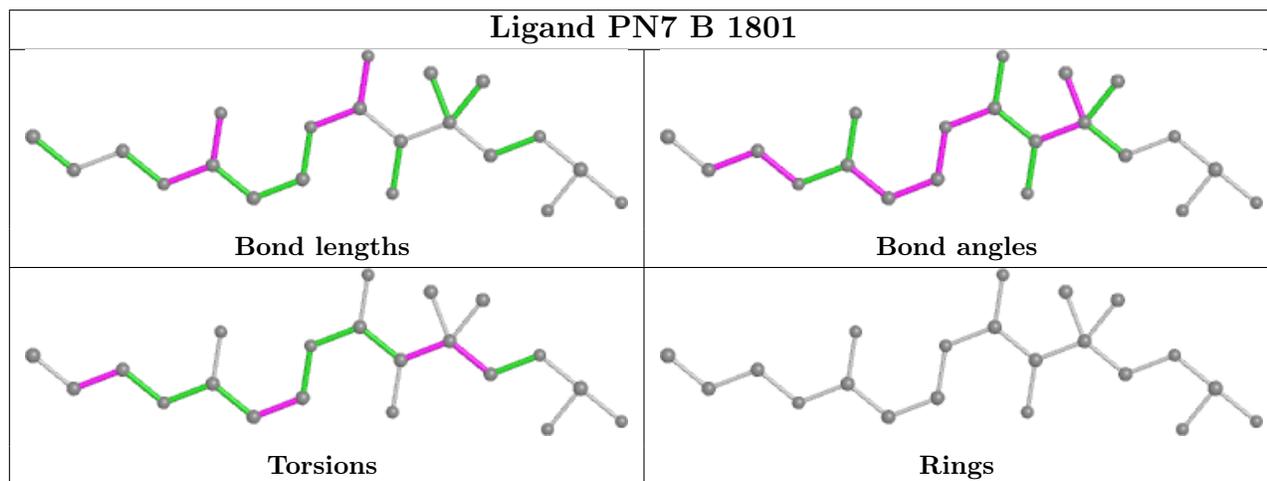
5.7   Other polymers ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-23711. 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 ⓘ

6.1.1 Primary map

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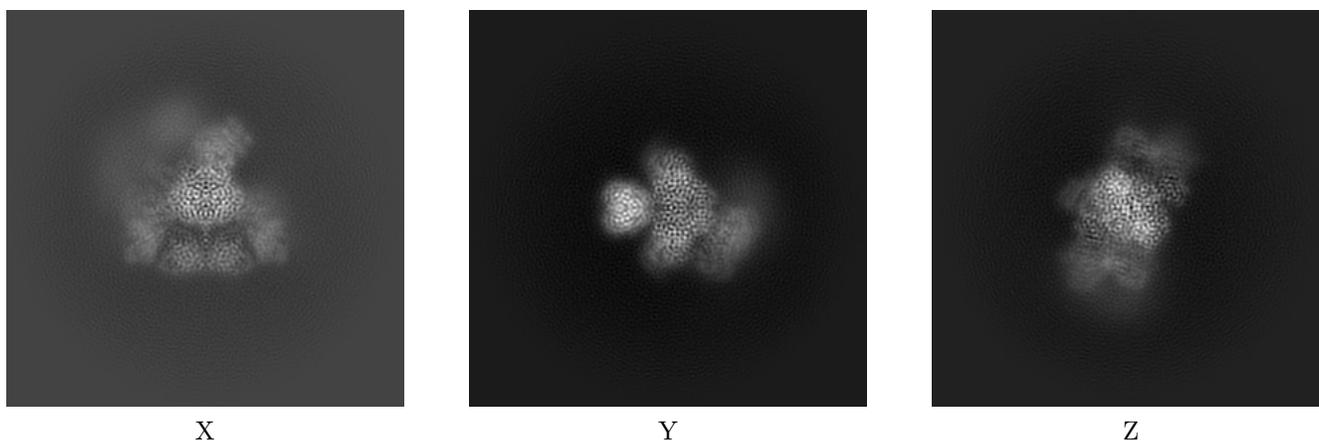
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

6.2.1 Primary map

X Index: 168	Y Index: 168	Z Index: 168
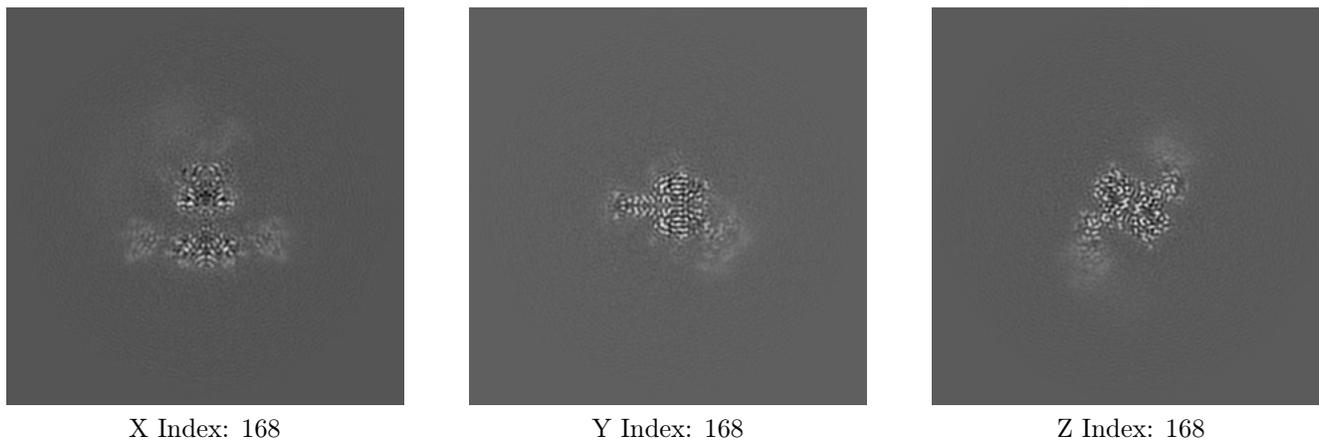
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
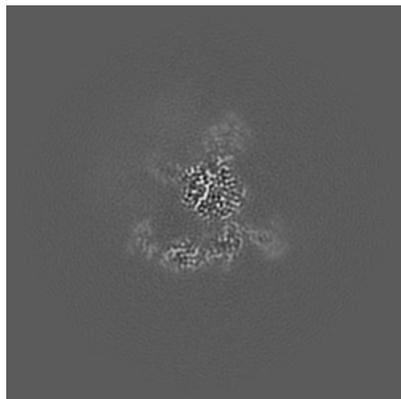
6.3.1   Primary map
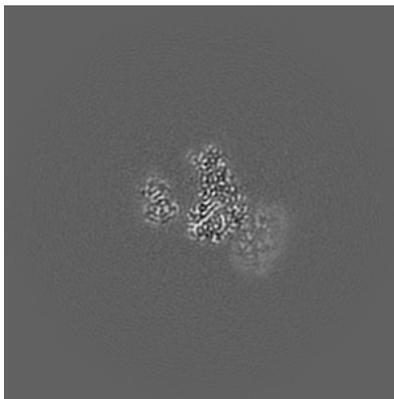
| X Index: 157 | Y Index: 181 | Z Index: 173 |
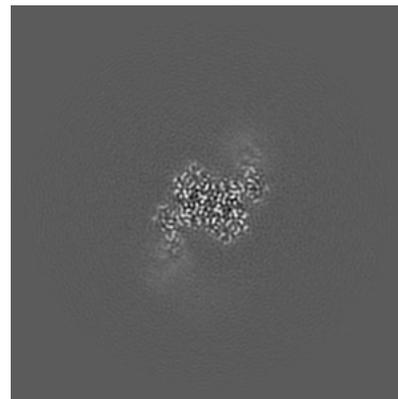
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views ⓘ

6.4.1   Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.53. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
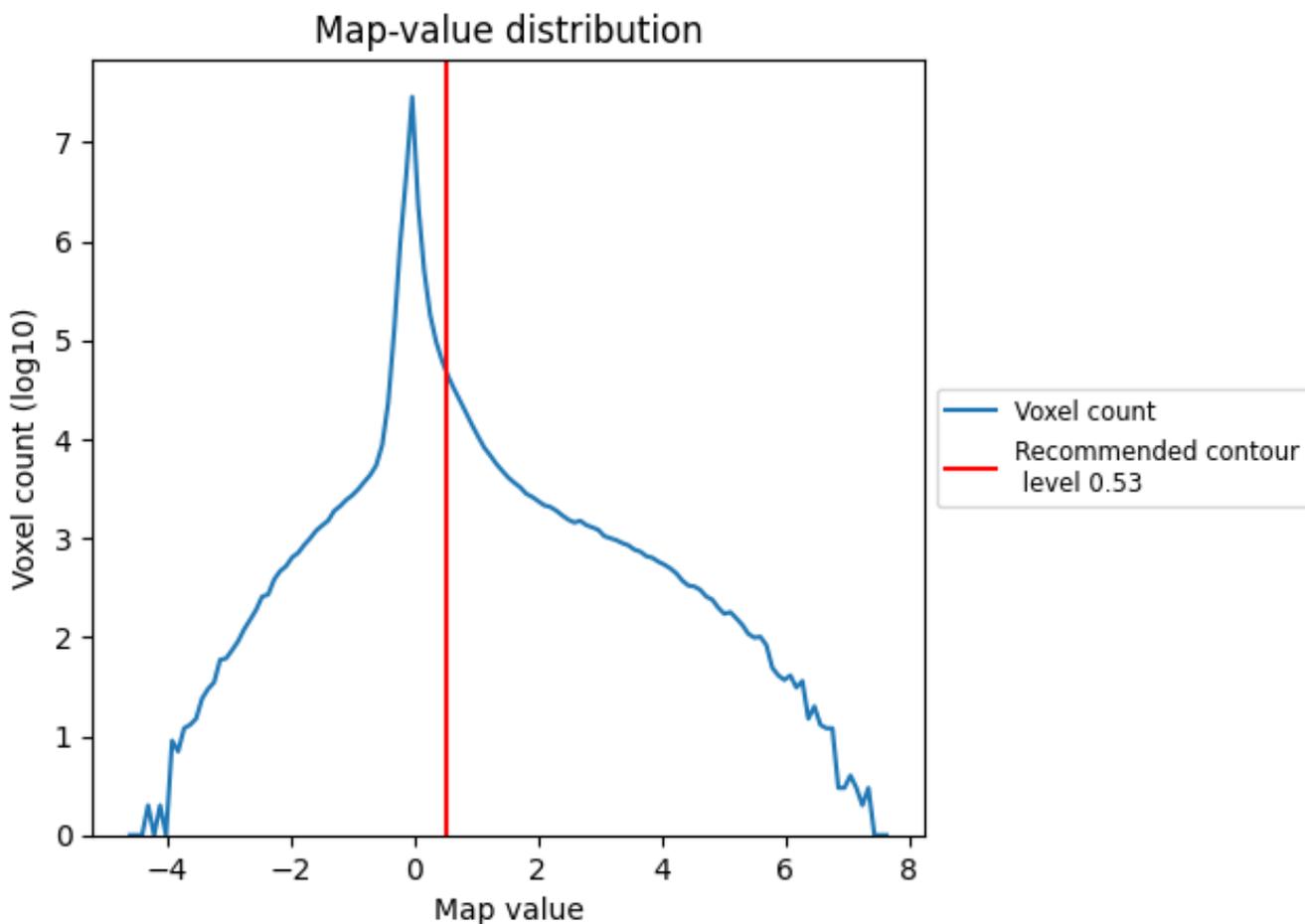
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
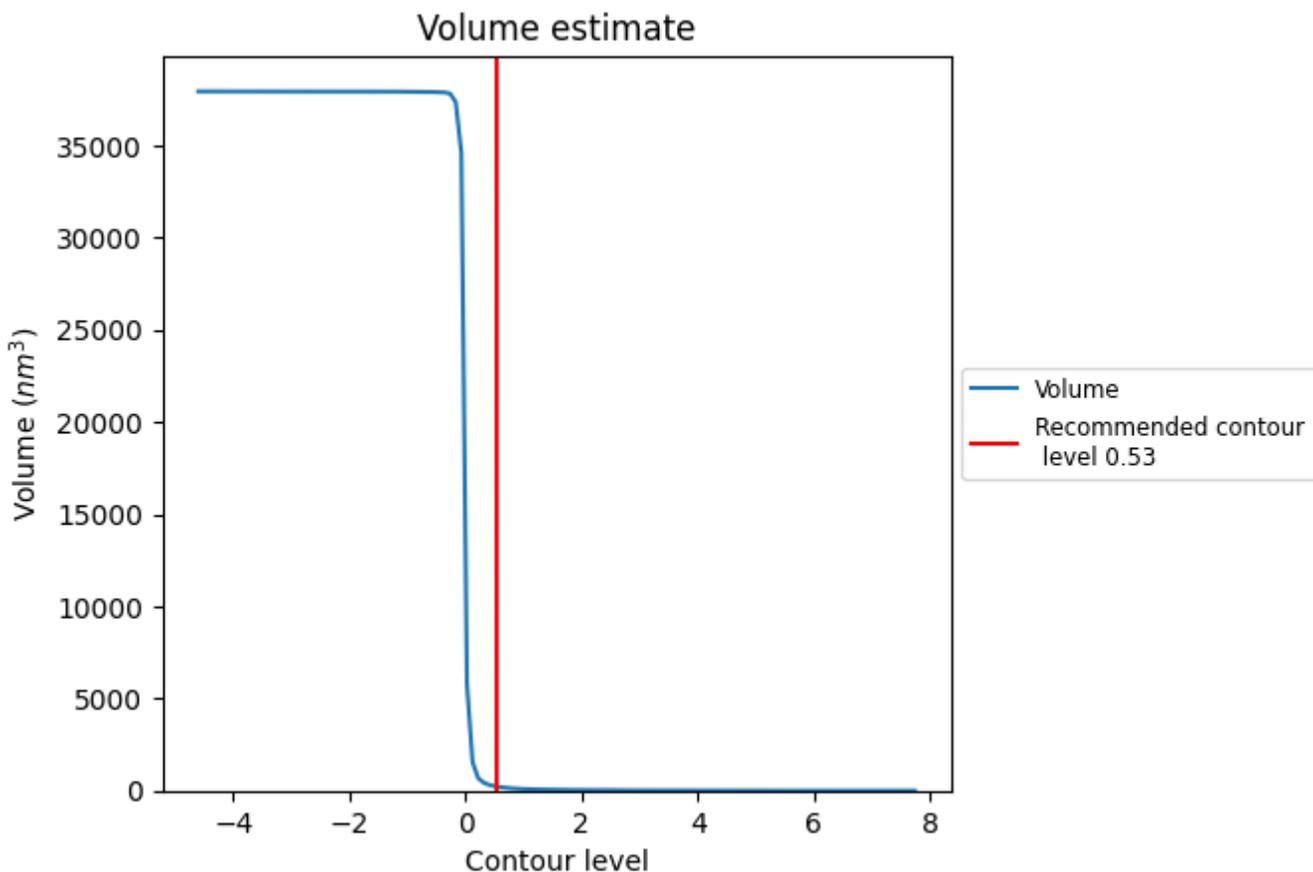
The volume at the recommended contour level is 226 nm^3; this corresponds to an approximate mass of 204 kDa.

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 ⓘ
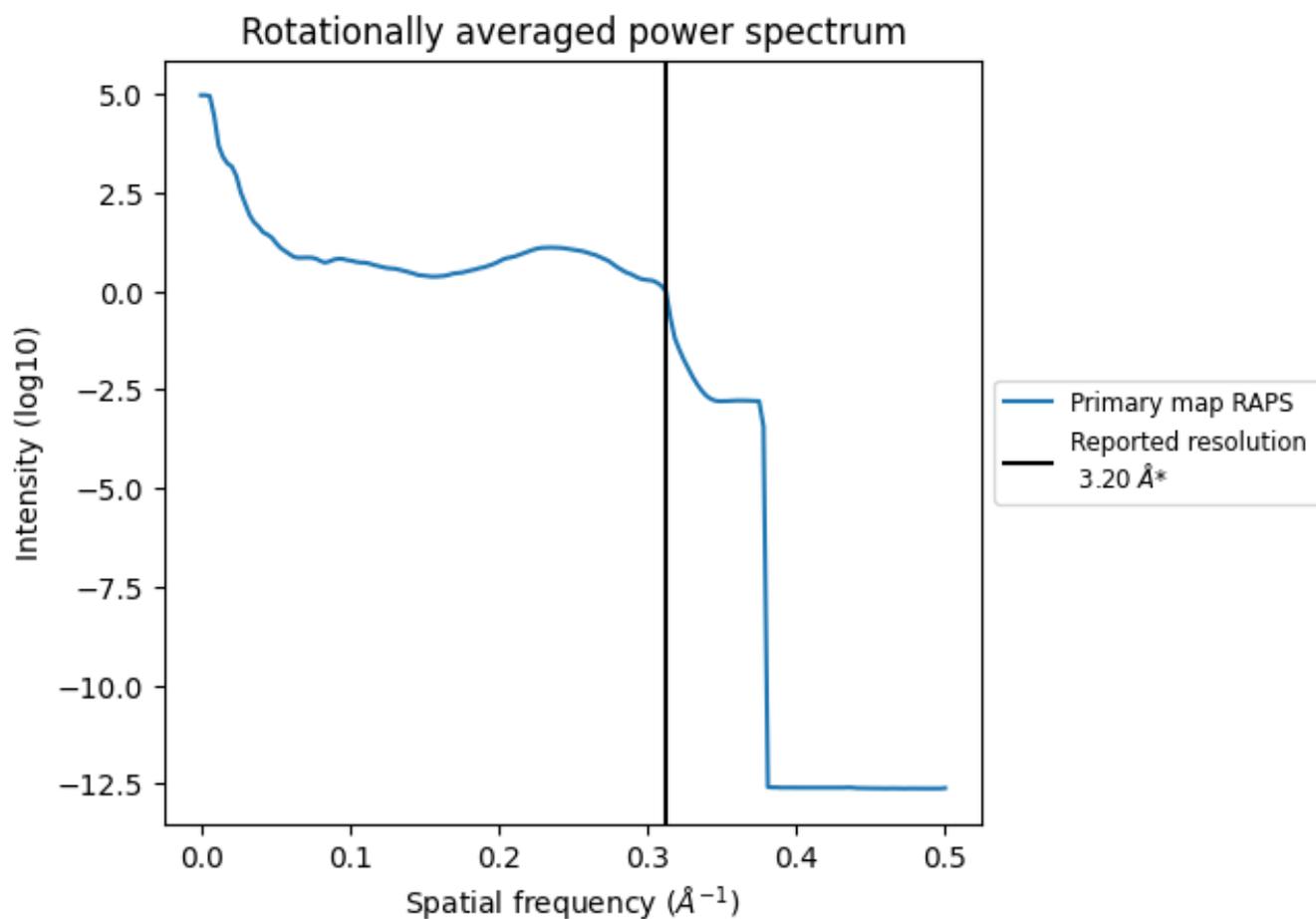
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23711 and PDB model 7M7F. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay ⓘ

X   Y   Z
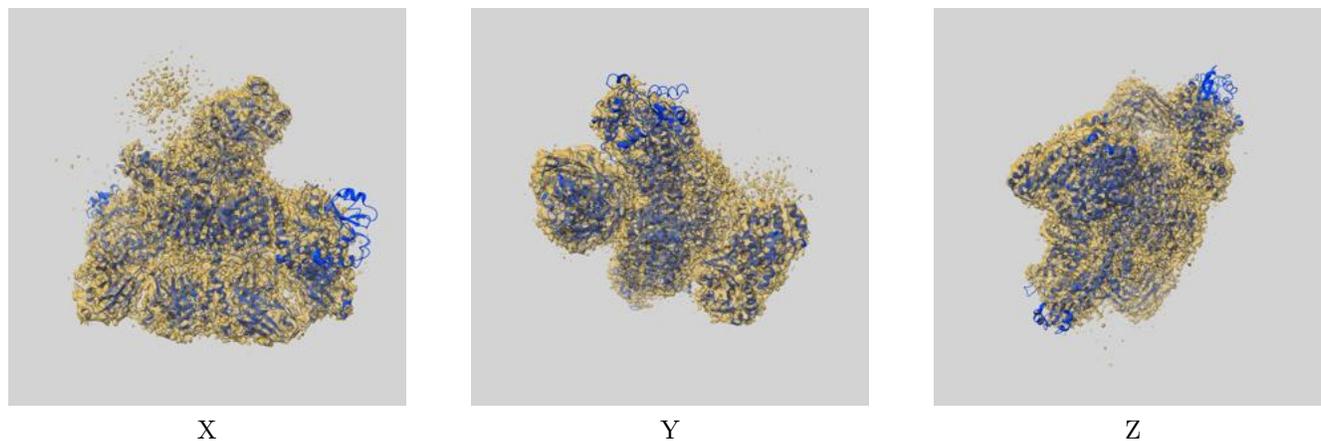
The images above show the 3D surface view of the map at the recommended contour level 0.53 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ
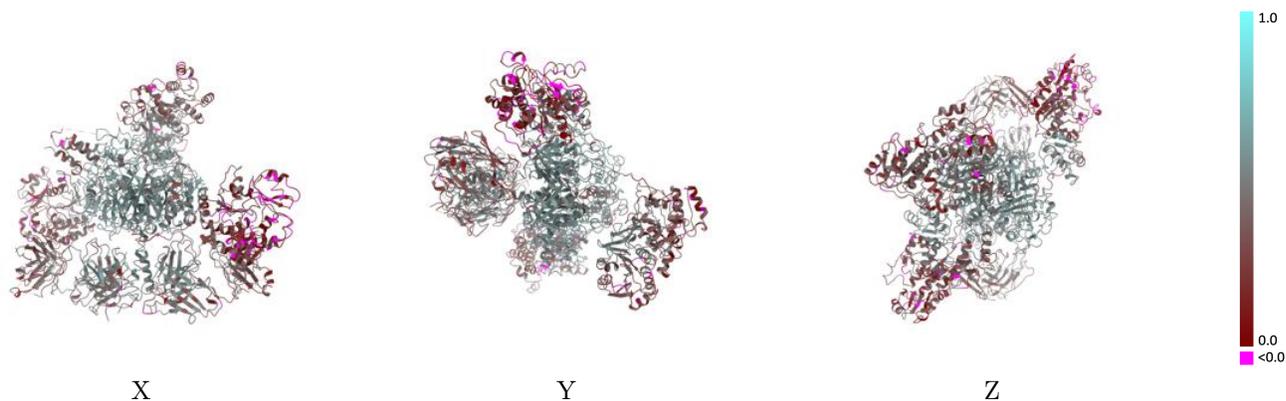

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model ⓘ
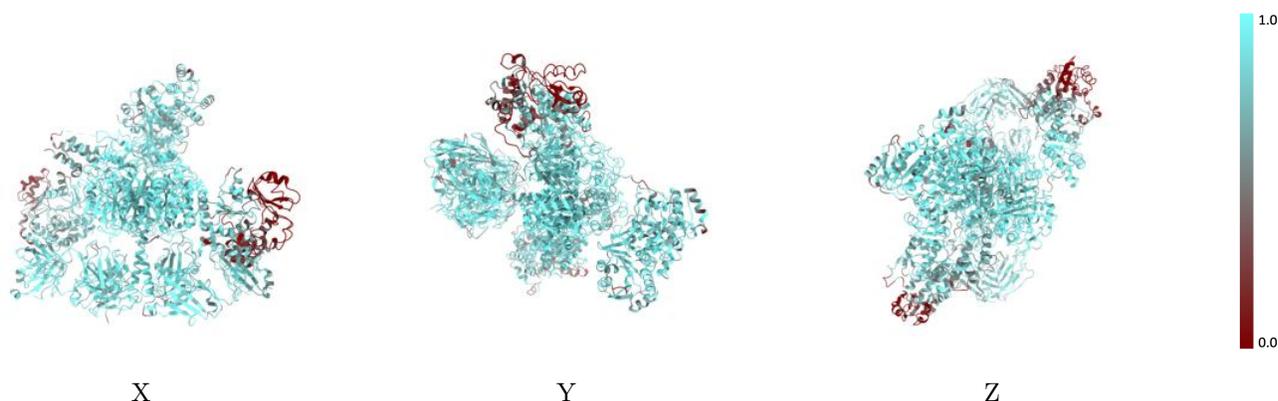
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.53).

9.4 Atom inclusion (i)
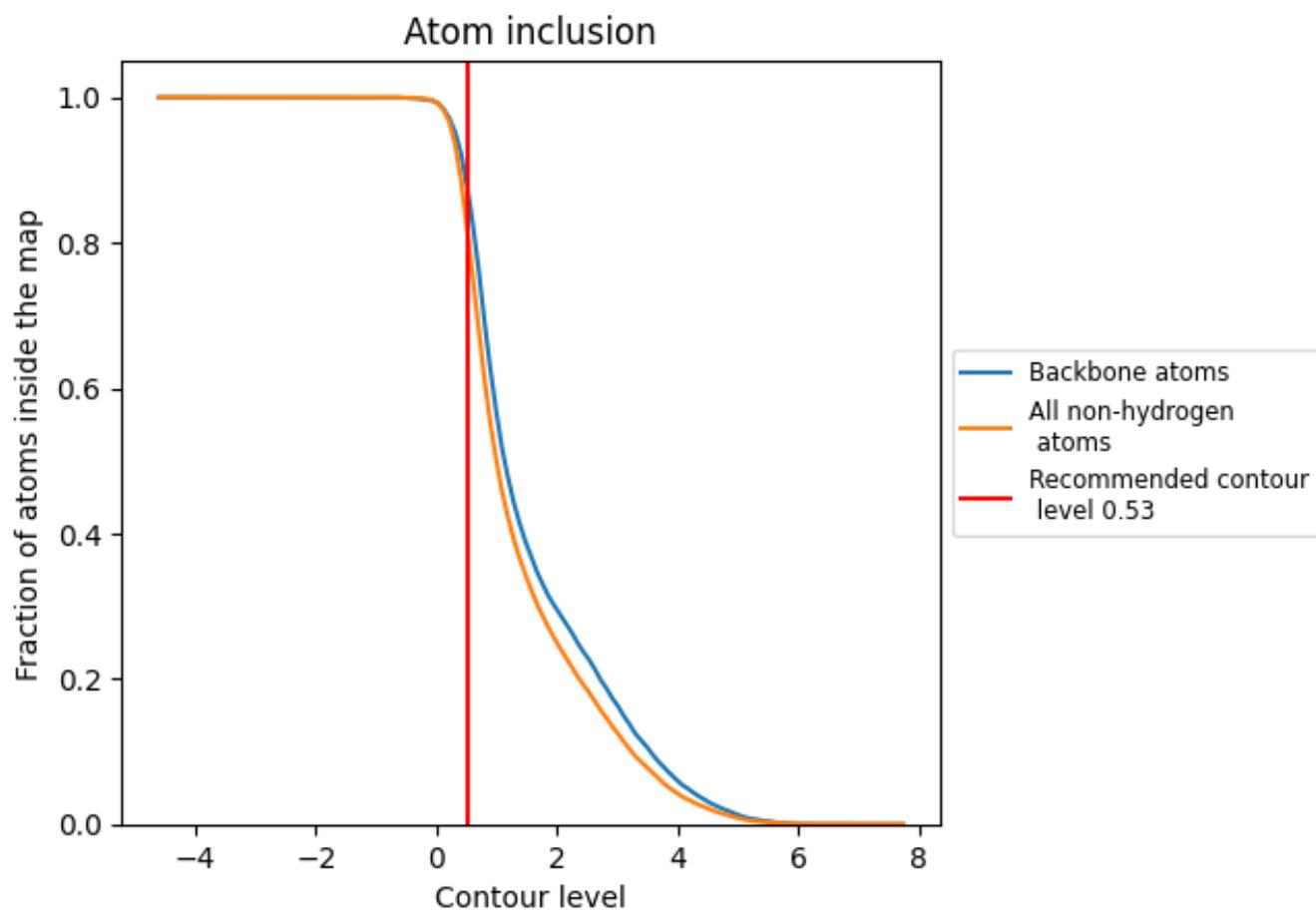
At the recommended contour level, 87% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.53) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8035	0.4030
A	0.7706	0.3800
B	0.8075	0.4320
C	0.8312	0.3850
D	0.8633	0.4110
E	0.8637	0.4200
F	0.8522	0.4070

1.0

0.0
<0.0