



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:15 PM UTC

PDB ID : 8TYQ / pdb_00008tyq
EMDB ID : EMD-41728
Title : Structure of the C-terminal half of LRRK2 bound to GZD-824 (G2019S mutant)
Authors : Villagran-Suarez, A.; Sanz-Murillo, M.; Alegrio-Louro, J.; Leschziner, A.
Deposited on : 2023-08-25
Resolution : 2.99 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

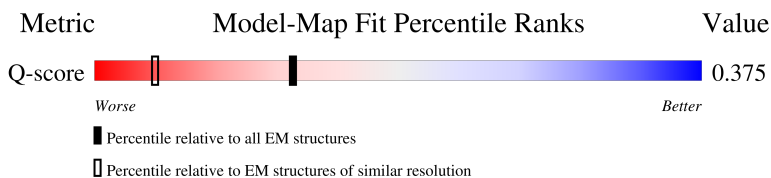
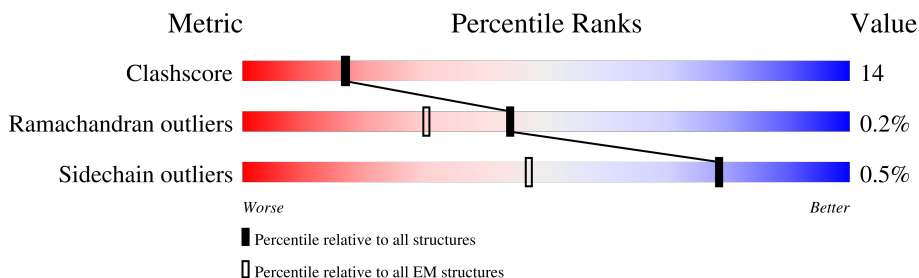
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

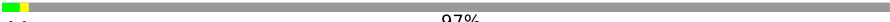
The reported resolution of this entry is 2.99 Å.

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	13287 (2.49 - 3.49)

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	1406	 .. 97%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8529 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 Leucine-rich repeat serine/threonine-protein kinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	957	Total	C	N	O	S	1	0
			7645	4914	1301	1382	48		

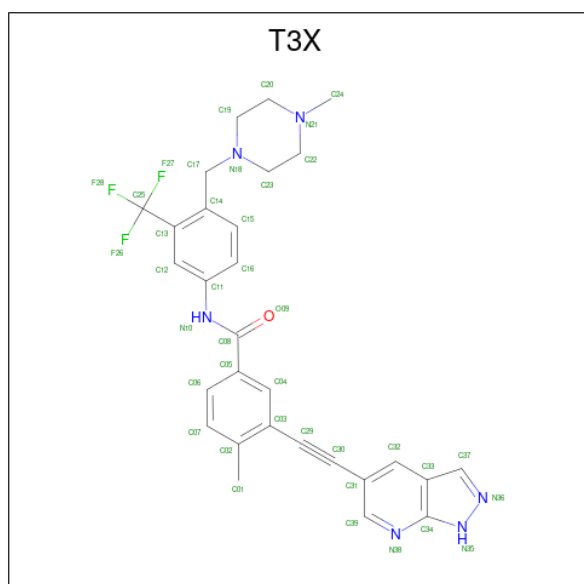
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2019	SER	GLY	engineered mutation	UNP Q5S007

- Molecule 2 is a protein called Designed Ankyrin Repeats Protein E11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	S	0	0
			845	541	142	161	1		

- Molecule 3 is 4-methyl-N-{4-[(4-methylpiperazin-1-yl)methyl]-3-(trifluoromethyl)phenyl}-3-[(1H-pyrazolo[3,4-b]pyridin-5-yl)ethynyl]benzamide (CCD ID: T3X) (formula: C₂₉H₂₇F₃N₆O) (labeled as "Ligand of Interest" by depositor).

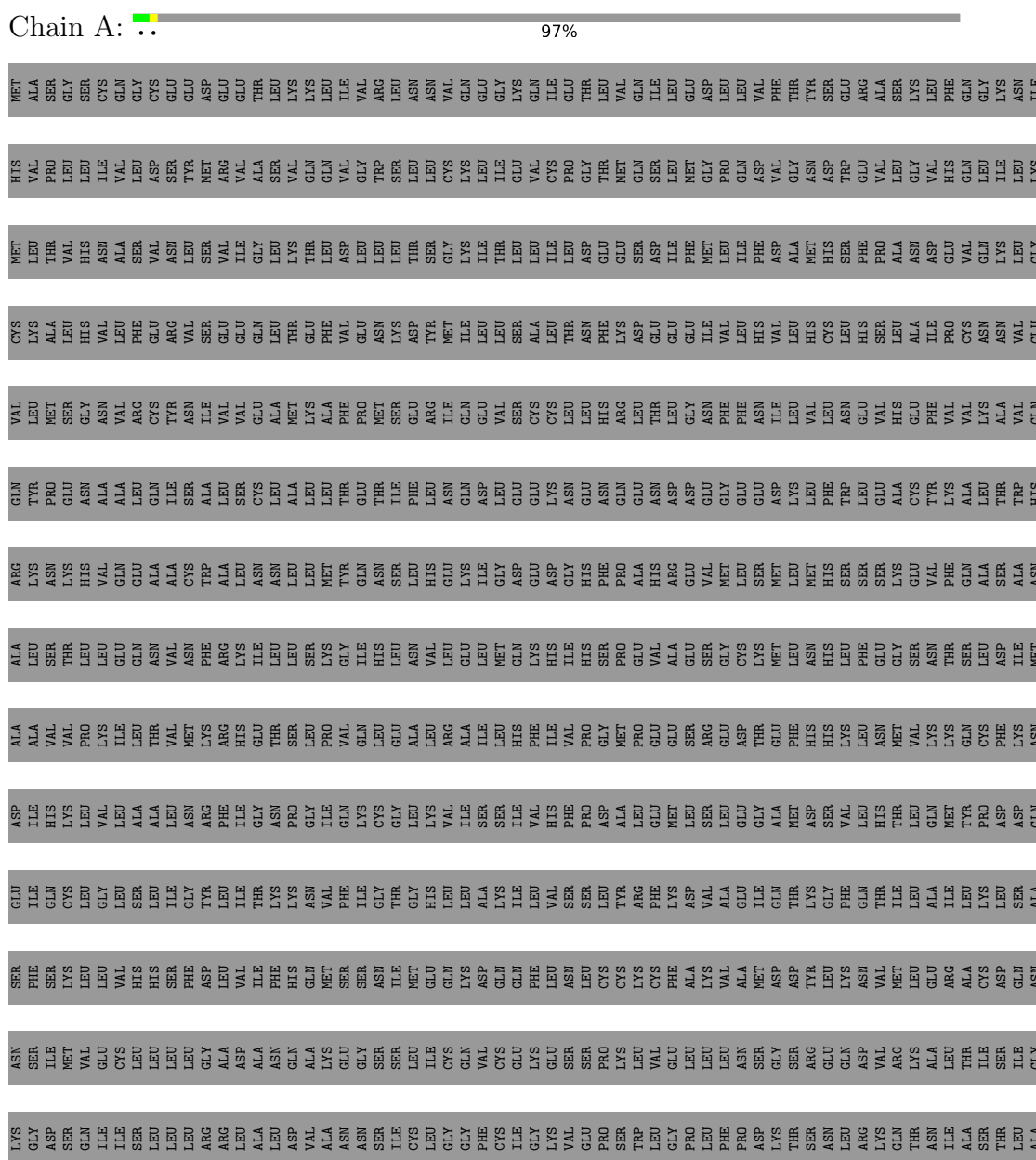


Mol	Chain	Residues	Atoms					AltConf
			Total	C	F	N	O	
3	A	1	39	29	3	6	1	0

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: Leucine-rich repeat serine/threonine-protein kinase 2



L1390	PHE	PRO	LEU	ILE	LYS	ASN	SER	SER	ARG
W1393	LEU	PRO	ASP	SER	CYS	ALA	SER	PHE	MET
D1394	GLN	GLU	MET	SER	PRO	THR	LEU	VAL	LEU
F1395	GLN	ILE	SER	SER	THR	THR	LEU	VAL	ILE
ALA	ARG	GLY	SER	SER	LEU	PHE	GLN	LYS	TYR
GLY	LEU	CYS	ASN	ASN	LYS	PRO	HIS	LYS	TYR
ARG	LYS	LEU	ASP	ASN	PHE	GLN	MET	SER	GLN
E1399	LYS	GLU	ILE	PHE	ASN	THR	ILE	VAL	VAL
Y1402	ALA	ASN	GLN	LEU	LEU	LYS	SER	GLY	GLU
SER	VAL	THR	TYR	GLU	TYR	CYS	ASP	VAL	VAL
THR	ASN	LEU	PRO	CYS	PRO	ASN	SER	SER	VAL
HIS	ARG	ASP	PRO	LYS	GLN	THR	ILE	GLY	GLU
PRO	ARG	VAL	ALA	VAL	LEU	LEU	ILE	GLU	GLY
	M1335	VAL	VAL	GLU	ASP	ASP	ALA	ASP	ALA
	K1336	SER	HIS	GLU	SER	ARG	GLU	VAL	VAL
	L1337	TYR	TRP	SER	PHE	THR	LEU	LEU	GLY
	M1338	ASN	LYS	PHE	VAL	THR	ALA	ARG	TYR
	I1339	LEU	SER	SER	PRO	HIS	SER	ASP	ARG
	V1340	GLU	LEU	ALA	GLU	LEU	GLU	ASP	GLY
	G1341	LEU	ASN	ARG	ASN	ASP	ARG	VAL	VAL
	M1342	ARG	LEU	MET	THR	HIS	LEU	LEU	GLY
		PHE	GLU	ASN	ASP	THR	ILE	THR	THR
	T1348	PRO	LEU	LEU	VAL	LYS	CYS	SER	PHE
		ASN	LEU	ALA	VAL	VAL	VAL	SER	GLU
	L1351	GLU	PHE	ALA	GLU	GLU	LEU	PRO	ASP
	Q1352	MET	SER	MET	THR	THR	PHE	ASN	VAL
	L1354	GLY	HIS	PRO	LYS	LYS	SER	ASN	VAL
	MET	LYS	ASN	PHE	GLU	PHE	LEU	GLN	SER
	LYS	LEU	GLN	LEU	GLN	PRO	ALA	ARG	LYS
	THR	SER	ILE	PRO	ILE	SER	ASN	HIS	PHE
	LYS	LYS	SER	PRO	ILE	GLU	GLU	SER	ASP
	LYS	ILE	ILE	SER	LEU	LEU	LEU	ASN	GLU
	SER	TRP	LEU	MET	GLU	ARG	TRP	SER	THR
	ASP	ASP	ASP	THR	LYS	ASP	LEU	LEU	THR
	LEU	LEU	LEU	ILE	ASN	MET	GLY	GLY	THR
	GLY	PRO	SER	LEU	LYS	SER	ASP	PHE	PHE
	MET	LEU	GLU	LYS	ILE	CYS	THR	ILE	ILE
	GLN	ASP	LYS	LEU	SER	ILE	ALA	ASP	PRO
	SER	GLU	ALA	SER	GLY	ALA	GLN	SER	ASP
	ALA	LEU	TYR	GLN	ILE	ASN	GLN	HIS	ASP
	THR	HIS	TRP	LYS	SER	ASP	LEU	GLY	MET
	VAL	ASN	SER	PHE	PRO	VAL	CYS	ASP	ASP
	G1370	ASN	TRP	LYS	ASN	ASP	CYS	ASP	ASP
	I1371	PHE	ARG	SER	LEU	SER	ILE	LEU	SER
	D1372	ASP	VAL	CYS	ARG	ARG	VAL	LEU	VAL
		PHE	GLU	ILE	LEU	ASN	VAL	ARG	ALA
		LYS	LYS	PRO	LYS	ASP	LYS	LYS	ALA
	I1378	HIS	LEU	GLU	ILE	THR	ARG	ARG	GLN
	GLN	ILE	HIS	GLY	LEU	GLY	ILE	LYS	SER
	ILE	LEU	LEU	ILE	LEU	ILE	PRO	ILE	ASP
	ARG	SER	SER	LEU	ILE	SER	HIS	LYS	ASP
	ASP	CYS	LYS	ILE	ILE	THR	LEU	LEU	ASP
	LYS	LYS	HIS	ASN	ASN	VAL	LYS	SER	ASP
	ARG	ALA	ASN	LEU	ASN	VAL	LEU	ASP	GLY
	LYS	LYS	LYS	PRO	LEU	SER	LEU	ASP	GLY
	THR	ASP	LEU	HIS	SER	ASP	GLU	ASP	SER
	ARG	ILE	LYS	GLU	THR	PRO	LEU	SER	SER
	ASP	ILE	LYS	ARG	ASN	THR	ASN	LEU	GLU
	I1388	ILE	ILE	GLU	GLU	THR	GLN	GLY	GLY
	V1389	ARG	ILE	SER	HIS	VAL	VAL	ARG	ARG

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	261641	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.157	Depositor
Minimum map value	-1.097	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.124	Depositor
Map size (Å)	299.2, 299.2, 299.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93500006, 0.93500006, 0.93500006	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: T3X

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	0.30	2/7779 (0.0%)	0.57	16/10498 (0.2%)
2	B	0.15	0/866	0.33	0/1187
All	All	0.29	2/8645 (0.0%)	0.55	16/11685 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2208	PRO	N-CD	-15.46	1.26	1.47
1	A	1695	TYR	C-N	-7.08	1.23	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1699	TYR	CB-CA-C	-15.56	79.48	109.66
1	A	1700	PHE	CA-C-N	9.74	132.02	119.84
1	A	1700	PHE	C-N-CA	9.74	132.02	119.84
1	A	1699	TYR	CA-C-O	-9.11	110.81	121.46
1	A	2208	PRO	N-CD-CG	7.05	113.78	103.20
1	A	1696	GLU	N-CA-CB	-7.02	98.99	110.43
1	A	1694	LEU	CA-C-N	-6.72	112.72	122.19
1	A	1694	LEU	C-N-CA	-6.72	112.72	122.19
1	A	1700	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	1947	MET	CA-C-O	-6.17	114.43	121.40
1	A	1697	MET	CB-CA-C	6.11	118.06	108.84
1	A	1695	TYR	O-C-N	-5.99	116.39	123.22
1	A	1696	GLU	CA-C-O	-5.67	114.25	120.43
1	A	1695	TYR	N-CA-C	-5.54	100.27	109.46
1	A	1562	LEU	CB-CA-C	-5.51	110.20	116.54
1	A	1697	MET	N-CA-C	-5.34	101.93	110.10

There are no chirality outliers.

There are no planarity outliers.

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	7645	0	7826	224	0
2	B	845	0	808	19	0
3	A	39	0	0	3	0
All	All	8529	0	8634	238	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 14.

All (238) 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:1902:GLU:HG2	1:A:1949:LEU:HD23	1.51	0.93
1:A:1699:TYR:O	1:A:1701:PRO:HD3	1.77	0.83
1:A:2216:VAL:HG12	1:A:2226:VAL:HG22	1.62	0.80
1:A:1866:ARG:HA	1:A:1869:MET:HE1	1.64	0.79
1:A:1730:ASN:HB3	1:A:1741:ASN:HB3	1.66	0.76
1:A:1895:ARG:HG3	1:A:1949:LEU:HD21	1.66	0.76
1:A:1695:TYR:OH	1:A:1781:VAL:HG13	1.87	0.75
1:A:1675:ASP:HB3	1:A:1735:ARG:HE	1.52	0.75
1:A:1696:GLU:HB2	1:A:1809:LYS:HG3	1.70	0.74
1:A:2243:ASP:OD1	1:A:2244:SER:N	2.21	0.73
1:A:1695:TYR:HB3	1:A:1808:LEU:HD11	1.72	0.72
1:A:1816:PHE:HA	1:A:1850:ILE:HD11	1.72	0.72
1:A:1921:LEU:HD21	1:A:1945:LEU:HD21	1.69	0.72
1:A:1701:PRO:HG2	1:A:1795:LEU:HD11	1.72	0.71
1:A:1446:PRO:HB3	1:A:1483:ARG:HG3	1.71	0.70
1:A:2171:CYS:SG	1:A:2180:SER:OG	2.48	0.70
1:A:2141:THR:HG22	1:A:2142:ARG:HG2	1.74	0.69
1:A:1697:MET:HE3	1:A:1808:LEU:HD13	1.74	0.68
1:A:1937:ALA:HB3	1:A:1946:VAL:HG13	1.75	0.68
1:A:2155:MET:HB3	1:A:2169:LEU:HD23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1771:ARG:NH1	1:A:1862:ALA:O	2.29	0.66
1:A:1811:TRP:CE3	1:A:1824:LYS:HD2	2.30	0.66
1:A:1699:TYR:HB2	1:A:1701:PRO:HD3	1.78	0.66
1:A:1699:TYR:HD2	1:A:1701:PRO:HG3	1.60	0.66
1:A:2153:GLU:HG2	1:A:2456:ARG:HE	1.60	0.66
1:A:2420:GLN:NE2	1:A:2498:ILE:O	2.27	0.65
1:A:1697:MET:HB3	1:A:1808:LEU:HD13	1.79	0.64
1:A:1968:ARG:NH2	1:A:2102:ALA:O	2.31	0.63
1:A:1739:TYR:HE2	1:A:1741:ASN:HB2	1.63	0.63
1:A:1771:ARG:NH2	1:A:1864:LEU:O	2.26	0.62
1:A:2152:VAL:HG23	1:A:2473:LEU:HD21	1.82	0.62
1:A:1832:LYS:NZ	1:A:1836:GLU:OE2	2.29	0.61
1:A:1739:TYR:CE2	1:A:1741:ASN:HB2	2.36	0.61
1:A:1700:PHE:CE2	1:A:1761:SER:HB2	2.36	0.61
2:B:123:ALA:HB1	2:B:155:ALA:HB2	1.82	0.61
1:A:1699:TYR:C	1:A:1701:PRO:HD3	2.25	0.61
1:A:2411:SER:O	2:B:113:HIS:NE2	2.34	0.60
1:A:2169:LEU:HB2	1:A:2180:SER:HB2	1.84	0.60
1:A:1941:ARG:HB2	1:A:1942:PRO:HD2	1.84	0.60
1:A:2139:CYS:HB2	1:A:2500:LEU:HD13	1.83	0.59
1:A:1692:ILE:HG12	1:A:1766:THR:HG22	1.84	0.59
1:A:2274:ILE:O	1:A:2288:LEU:N	2.36	0.59
1:A:1422:SER:O	1:A:1461:GLN:NE2	2.35	0.59
1:A:2267:THR:OG1	1:A:2269:ASP:OD1	2.19	0.59
1:A:1466:MET:HE1	1:A:1485:TYR:CE2	2.38	0.58
1:A:1415:TYR:HB2	1:A:1447:VAL:HA	1.84	0.58
1:A:1709:ILE:HA	1:A:1738:ILE:HD11	1.84	0.58
1:A:1684:HIS:HB3	1:A:1689:GLU:HG3	1.84	0.58
1:A:2477:ARG:HG2	1:A:2489:ILE:HG12	1.86	0.58
1:A:1697:MET:CE	1:A:1808:LEU:HD13	2.34	0.57
1:A:1354:LEU:HD11	1:A:1500:LEU:HB3	1.87	0.57
1:A:1697:MET:CE	1:A:1795:LEU:HD13	2.35	0.57
1:A:1423:LYS:HB2	1:A:1427:GLU:HB2	1.87	0.56
1:A:1633:LYS:HA	1:A:1637:LYS:HB3	1.86	0.56
1:A:1697:MET:HE1	1:A:1788:MET:CE	2.36	0.56
1:A:1748:CYS:HB2	1:A:1776:LEU:HD23	1.88	0.56
2:B:102:LEU:HD11	2:B:134:LEU:HD23	1.87	0.56
1:A:2323:ILE:HD11	1:A:2365:ILE:HD13	1.88	0.56
1:A:1963:LYS:HD3	1:A:2069:THR:HG21	1.87	0.56
1:A:2413:ARG:O	1:A:2430:GLY:N	2.39	0.56
1:A:1433:PRO:HB3	1:A:1702:MET:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1602:TRP:HB2	1:A:1607:MET:HE3	1.87	0.56
1:A:1813:LEU:HD13	1:A:1822:HIS:HB3	1.88	0.55
1:A:1935:LEU:HD13	1:A:1947:MET:HE2	1.87	0.55
1:A:1962:ASP:OD1	1:A:1965:SER:OG	2.24	0.55
2:B:54:HIS:NE2	2:B:83:PHE:O	2.38	0.55
1:A:1734:TRP:NE1	1:A:1736:GLN:O	2.39	0.55
1:A:1986:HIS:NE2	1:A:2055:ASP:OD2	2.33	0.55
1:A:1339:ILE:HD12	1:A:1416:LEU:HD23	1.87	0.55
1:A:1560:ASN:HD21	1:A:1564:LEU:HA	1.72	0.55
1:A:1924:LEU:HD13	1:A:1947:MET:HE1	1.88	0.55
1:A:1809:LYS:HD2	1:A:1811:TRP:HE1	1.71	0.55
1:A:1860:ILE:HG23	1:A:1940:ILE:HG21	1.89	0.54
1:A:2445:ILE:HD13	1:A:2501:PRO:HB3	1.88	0.54
1:A:1904:ALA:O	1:A:1946:VAL:HA	2.08	0.54
1:A:2411:SER:HA	2:B:113:HIS:HD2	1.73	0.54
1:A:1458:ASP:OD2	1:A:1460:LYS:NZ	2.36	0.53
1:A:1371:ILE:N	1:A:1604:CYS:SG	2.71	0.53
1:A:1861:LEU:HB2	1:A:1940:ILE:HD11	1.92	0.52
2:B:124:LEU:HB2	2:B:154:LEU:HD23	1.91	0.52
1:A:2222:GLY:HA2	1:A:2245:VAL:HG23	1.91	0.52
1:A:2316:TRP:CZ3	1:A:2363:LEU:HD11	2.45	0.52
1:A:2205:VAL:HG22	1:A:2250:CYS:SG	2.50	0.51
1:A:2363:LEU:HB2	1:A:2376:TRP:HB2	1.92	0.51
1:A:1971:GLN:NE2	1:A:2066:ILE:O	2.43	0.51
2:B:69:LEU:HD11	2:B:101:LEU:HD23	1.92	0.51
1:A:1813:LEU:HA	1:A:1823:GLN:O	2.10	0.51
1:A:2445:ILE:HG21	1:A:2501:PRO:HB3	1.92	0.51
1:A:2241:MET:SD	1:A:2241:MET:N	2.83	0.51
1:A:2151:ILE:H	1:A:2173:HIS:HB3	1.76	0.51
2:B:62:LEU:HD21	2:B:96:GLU:HB2	1.92	0.51
1:A:1767:VAL:HG21	1:A:1777:LEU:HB2	1.92	0.51
1:A:2006:TYR:CZ	1:A:2008:ASN:HB2	2.46	0.51
1:A:1447:VAL:HB	1:A:1482:ILE:HD13	1.93	0.51
1:A:1335:MET:HG2	1:A:1336:LYS:N	2.25	0.51
1:A:1662:ILE:HD12	1:A:1731:ARG:HH12	1.75	0.51
1:A:1782:ASP:OD1	1:A:1918:ARG:NH1	2.44	0.51
1:A:1950:ALA:HA	1:A:2003:PHE:HD1	1.75	0.51
1:A:2246:THR:OG1	1:A:2300:LEU:O	2.28	0.51
1:A:1462:ARG:O	1:A:1466:MET:HG2	2.11	0.50
1:A:1680:ILE:HG21	1:A:1749:LEU:HD22	1.93	0.50
1:A:1969:THR:O	1:A:1973:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1827:LEU:HD12	1:A:1859:LEU:HD21	1.94	0.50
1:A:2411:SER:HA	2:B:113:HIS:CD2	2.46	0.50
1:A:1695:TYR:CZ	1:A:1810:LYS:NZ	2.78	0.50
1:A:1709:ILE:HG12	1:A:1738:ILE:HD11	1.94	0.50
1:A:2388:ASP:HB3	1:A:2391:HIS:HB3	1.93	0.50
1:A:1693:ARG:HH12	1:A:1827:LEU:HD11	1.77	0.50
1:A:1959:LEU:HD23	1:A:1966:LEU:HD11	1.93	0.49
1:A:1885:LEU:HD21	3:A:2601:T3X:C33	2.41	0.49
1:A:1981:GLY:HA2	1:A:1984:TYR:HB2	1.94	0.49
1:A:2434:ILE:HG23	1:A:2458:MET:HE1	1.92	0.49
1:A:2264:LEU:HB3	1:A:2272:LEU:HD11	1.94	0.49
1:A:2363:LEU:O	1:A:2375:VAL:HA	2.12	0.49
2:B:84:THR:HB	2:B:85:PRO:HD2	1.95	0.49
1:A:1660:LEU:H	1:A:1668:LEU:N	2.11	0.49
1:A:1693:ARG:HH22	1:A:1827:LEU:HG	1.78	0.48
1:A:1895:ARG:CG	1:A:1949:LEU:HD21	2.42	0.48
1:A:1691:ILE:HD11	1:A:1769:SER:HA	1.95	0.48
1:A:1348:THR:O	1:A:1352:GLN:HG2	2.13	0.48
1:A:2266:GLY:HA3	1:A:2300:LEU:HD22	1.96	0.48
1:A:1695:TYR:OH	1:A:1810:LYS:NZ	2.47	0.48
1:A:2429:THR:OG1	1:A:2433:HIS:HB2	2.14	0.48
1:A:1337:LEU:HD13	1:A:1414:LEU:HD23	1.96	0.48
1:A:1701:PRO:HB2	1:A:1792:PHE:CD1	2.49	0.48
1:A:1927:LEU:HB3	1:A:1932:LEU:HD13	1.96	0.48
2:B:45:THR:HB	2:B:49:GLY:HA2	1.95	0.48
1:A:2214:TRP:HE1	1:A:2281:LYS:HB3	1.79	0.47
1:A:1815:SER:OG	1:A:1817:ASN:O	2.32	0.47
1:A:1610:ILE:HD12	1:A:1635:LEU:HD22	1.95	0.47
1:A:1950:ALA:HA	1:A:2003:PHE:CD1	2.50	0.47
1:A:2346:TYR:CZ	2:B:50:VAL:HG21	2.50	0.47
1:A:1687:ASN:ND2	1:A:1820:GLU:O	2.47	0.47
1:A:1750:VAL:HG22	1:A:1763:LEU:HD11	1.96	0.47
1:A:1775:ILE:HD12	1:A:1863:ASP:HB2	1.97	0.47
1:A:2239:GLU:HG3	1:A:2286:ALA:HA	1.96	0.47
1:A:2394:ARG:HD2	2:B:80:HIS:HB3	1.97	0.47
1:A:2420:GLN:HE21	1:A:2498:ILE:HG13	1.78	0.47
1:A:1814:TYR:HE1	1:A:1825:ILE:HG13	1.80	0.47
1:A:2420:GLN:NE2	1:A:2498:ILE:HG13	2.29	0.47
1:A:1852:ILE:HB	1:A:1860:ILE:HD11	1.97	0.47
1:A:1708:LEU:O	1:A:1712:LEU:HG	2.15	0.47
1:A:1859:LEU:HA	1:A:1914:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2355:ILE:HG13	1:A:2356:THR:HG22	1.97	0.46
1:A:1697:MET:SD	1:A:1808:LEU:HD13	2.55	0.46
1:A:1890:PHE:CE2	3:A:2601:T3X:C37	2.98	0.46
1:A:1985:LEU:HD13	1:A:1992:TYR:HB2	1.98	0.46
2:B:86:LEU:HD11	2:B:98:VAL:HG13	1.96	0.46
1:A:2360:ASP:OD1	1:A:2419:LEU:HD21	2.16	0.46
2:B:50:VAL:HG13	2:B:54:HIS:CB	2.45	0.46
1:A:1371:ILE:HG22	1:A:1393:TRP:HB3	1.98	0.46
1:A:1791:TRP:C	1:A:1792:PHE:HD2	2.24	0.46
1:A:2243:ASP:OD1	1:A:2268:ALA:HB3	2.16	0.46
1:A:1870:LEU:HD11	1:A:1875:LEU:HD13	1.97	0.46
1:A:2244:SER:O	1:A:2268:ALA:N	2.45	0.46
1:A:1791:TRP:C	1:A:1793:PRO:HD3	2.41	0.46
1:A:2426:TRP:CD2	1:A:2470:MET:HE3	2.51	0.46
1:A:1979:ALA:HB2	1:A:2059:PHE:CZ	2.51	0.46
1:A:1860:ILE:O	1:A:1862:ALA:N	2.49	0.45
1:A:2136:GLU:HG3	1:A:2448:ILE:HD12	1.98	0.45
1:A:1372:ASP:OD1	1:A:1605:LYS:NZ	2.48	0.45
1:A:2146:LEU:HD12	1:A:2491:SER:OG	2.16	0.45
1:A:2215:ILE:HG23	1:A:2227:ILE:HB	1.98	0.45
1:A:1658:ILE:O	1:A:1670:PRO:HD3	2.16	0.45
1:A:2228:ASN:HB3	1:A:2231:ASP:O	2.16	0.45
1:A:1699:TYR:HB2	1:A:1701:PRO:CD	2.44	0.45
2:B:65:VAL:HG21	2:B:97:ILE:HD12	1.99	0.45
1:A:1421:LEU:HD13	1:A:1454:LEU:HD23	1.98	0.45
1:A:2104:TRP:NE1	1:A:2137:LEU:O	2.36	0.44
1:A:1533:ILE:H	1:A:1562:LEU:HD21	1.82	0.44
1:A:1812:ALA:O	1:A:1824:LYS:HA	2.18	0.44
1:A:1827:LEU:O	1:A:1831:MET:HB2	2.17	0.44
1:A:2227:ILE:HG13	1:A:2235:ARG:HG3	1.98	0.44
1:A:1423:LYS:O	1:A:1426:ALA:HB3	2.17	0.44
1:A:1697:MET:HE1	1:A:1788:MET:HE1	1.98	0.44
1:A:2053:GLN:HB3	1:A:2122:ARG:HH11	1.82	0.44
1:A:1734:TRP:CZ2	1:A:1737:GLY:HA3	2.53	0.44
1:A:1339:ILE:HG13	1:A:1351:LEU:HD21	1.99	0.44
1:A:1700:PHE:O	1:A:1701:PRO:C	2.59	0.44
1:A:1737:GLY:HA2	1:A:1751:GLY:HA2	2.00	0.44
1:A:2174:THR:HG23	1:A:2176:ARG:H	1.82	0.44
1:A:2135:ALA:HB3	1:A:2504:VAL:HG22	2.00	0.43
1:A:2248:LEU:CD2	1:A:2265:VAL:HG22	2.48	0.43
1:A:2423:THR:HA	1:A:2439:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1694:LEU:CD1	1:A:1811:TRP:HB2	2.49	0.43
1:A:2106:MET:HE2	1:A:2106:MET:HB3	1.83	0.43
1:A:1695:TYR:HD2	1:A:1808:LEU:HD21	1.83	0.43
1:A:1337:LEU:HB2	1:A:1390:LEU:HD13	2.01	0.43
1:A:2441:THR:O	1:A:2441:THR:OG1	2.31	0.43
1:A:1700:PHE:CD2	1:A:1761:SER:HB2	2.53	0.43
1:A:1705:TRP:CZ3	1:A:1708:LEU:HD23	2.53	0.43
2:B:50:VAL:HG13	2:B:54:HIS:HB2	2.00	0.43
1:A:1903:VAL:CG2	1:A:1946:VAL:HG23	2.48	0.43
1:A:2214:TRP:HZ3	1:A:2228:ASN:HB2	1.83	0.43
1:A:2339:ARG:O	1:A:2342:GLN:HB3	2.18	0.43
1:A:1340:VAL:HG12	1:A:1395:PHE:CG	2.53	0.43
2:B:150:THR:OG1	2:B:153:ASP:OD2	2.26	0.43
1:A:2423:THR:HB	1:A:2439:LEU:HB2	2.00	0.43
1:A:1772:LYS:O	1:A:1775:ILE:HG22	2.18	0.43
1:A:1775:ILE:HD12	1:A:1775:ILE:HA	1.94	0.43
1:A:1893:VAL:HG22	1:A:1906:LYS:HB2	2.00	0.43
1:A:1976:LEU:HD21	1:A:2511:ILE:HD11	2.00	0.43
1:A:2321:THR:O	1:A:2338:THR:OG1	2.35	0.43
1:A:2171:CYS:HB2	1:A:2178:GLN:HB2	2.01	0.42
1:A:2454:SER:HB3	1:A:2475:TYR:HB2	2.00	0.42
2:B:112:ASP:OD1	2:B:116:TRP:N	2.44	0.42
1:A:1694:LEU:HD23	1:A:1764:LYS:HG2	2.01	0.42
1:A:1921:LEU:CD2	1:A:1945:LEU:HD21	2.44	0.42
1:A:1931:SER:OG	1:A:1980:ASP:O	2.27	0.42
1:A:2146:LEU:HD22	1:A:2189:TYR:HD1	1.84	0.42
1:A:2327:SER:HB3	1:A:2333:GLN:OE1	2.20	0.42
1:A:2452:CYS:HG	1:A:2492:CYS:HG	1.65	0.42
1:A:1673:LEU:HB2	1:A:1735:ARG:HG3	2.02	0.42
1:A:2207:LEU:HA	1:A:2208:PRO:HD2	1.78	0.42
1:A:1694:LEU:HD12	1:A:1811:TRP:HB2	2.01	0.42
1:A:2382:LYS:HD2	1:A:2382:LYS:HA	1.78	0.42
1:A:1692:ILE:HG21	1:A:1813:LEU:HD12	2.02	0.42
1:A:1811:TRP:CD2	1:A:1824:LYS:HD2	2.54	0.42
1:A:2146:LEU:HD22	1:A:2189:TYR:CD1	2.54	0.42
1:A:1753:GLU:O	1:A:1762:PHE:HB2	2.19	0.42
1:A:2459:MET:HE3	1:A:2459:MET:HB3	1.89	0.42
1:A:1552:ARG:HG2	1:A:1568:GLU:OE2	2.20	0.42
1:A:1705:TRP:HZ2	1:A:1752:SER:HB2	1.85	0.41
1:A:2155:MET:HG3	1:A:2459:MET:HE1	2.02	0.41
1:A:1863:ASP:CG	1:A:1918:ARG:HH21	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1697:MET:HE1	1:A:1788:MET:HE3	2.03	0.41
1:A:1552:ARG:HE	1:A:1568:GLU:HG3	1.86	0.41
1:A:1950:ALA:HB3	3:A:2601:T3X:C34	2.51	0.41
1:A:2194:VAL:HG12	1:A:2235:ARG:NH2	2.35	0.41
1:A:1573:VAL:O	1:A:1576:LEU:HG	2.21	0.41
1:A:1907:ILE:HD13	1:A:1944:MET:HB3	2.03	0.41
1:A:1907:ILE:HD13	1:A:1907:ILE:HA	1.96	0.40
1:A:1999:ASN:HB3	1:A:2016:ALA:O	2.21	0.40
1:A:1685:CYS:N	1:A:1689:GLU:OE1	2.50	0.40
1:A:1687:ASN:OD1	1:A:1822:HIS:NE2	2.54	0.40
1:A:2156:VAL:HG13	1:A:2168:TRP:HB2	2.03	0.40
1:A:1814:TYR:CE1	1:A:1825:ILE:HG13	2.56	0.40
1:A:1931:SER:HB3	1:A:2514:ARG:NH2	2.37	0.40

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	908/1406 (65%)	871 (96%)	35 (4%)	2 (0%)	43	76
2	B	-	105 (97%)	3 (3%)	0	100	100
All	All	1016/1406 (72%)	976 (96%)	38 (4%)	2 (0%)	44	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1701	PRO
1	A	1700	PHE

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	857/1278 (67%)	852 (99%)	5 (1%)	78	88
2	B	-	85 (100%)	0	100	100
All	All	942/1278 (74%)	937 (100%)	5 (0%)	78	89

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

Mol	Chain	Res	Type
1	A	1694	LEU
1	A	1697	MET
1	A	1810	LYS
1	A	1946	VAL
1	A	1949	LEU

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

Mol	Chain	Res	Type
1	A	1342	ASN
1	A	1352	GLN
1	A	2051	ASN
1	A	2422	ASN
1	A	2433	HIS
1	A	2476	ASN
1	A	2499	ASN
2	B	80	HIS
2	B	109	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	T3X	A	2601	-	43,43,43	3.82	17 (39%)	61,62,62	7.91	22 (36%)

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
3	T3X	A	2601	-	-	4/23/33/33	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	T3X	C37-N36	-8.87	1.26	1.32
3	A	2601	T3X	C34-N35	8.61	1.41	1.35
3	A	2601	T3X	N35-N36	-8.49	1.30	1.36
3	A	2601	T3X	C22-N21	-7.13	1.29	1.46
3	A	2601	T3X	C23-N18	-6.93	1.28	1.46
3	A	2601	T3X	C24-N21	-6.91	1.30	1.46
3	A	2601	T3X	C17-N18	-6.75	1.34	1.47
3	A	2601	T3X	C20-N21	-6.30	1.31	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2601	T3X	C19-N18	-6.05	1.30	1.46
3	A	2601	T3X	C32-C33	-4.82	1.32	1.40
3	A	2601	T3X	C03-C29	4.04	1.51	1.43
3	A	2601	T3X	C17-C14	3.94	1.58	1.51
3	A	2601	T3X	C08-N10	3.88	1.47	1.35
3	A	2601	T3X	C11-N10	3.67	1.49	1.41
3	A	2601	T3X	C31-C30	3.13	1.51	1.44
3	A	2601	T3X	O09-C08	-3.05	1.16	1.23
3	A	2601	T3X	C34-N38	-2.45	1.31	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2601	T3X	C34-N35-N36	47.28	122.32	111.26
3	A	2601	T3X	C37-N36-N35	-22.91	94.07	106.02
3	A	2601	T3X	C33-C37-N36	17.80	124.62	111.68
3	A	2601	T3X	C33-C34-N35	-15.30	100.56	107.21
3	A	2601	T3X	N35-C34-N38	12.32	136.67	125.83
3	A	2601	T3X	C34-C33-C37	-10.81	98.42	104.25
3	A	2601	T3X	C33-C34-N38	-6.56	122.77	126.66
3	A	2601	T3X	C32-C33-C34	5.56	122.66	118.20
3	A	2601	T3X	C14-C17-N18	4.56	120.85	112.75
3	A	2601	T3X	O09-C08-C05	-3.71	113.54	120.90
3	A	2601	T3X	C33-C32-C31	-3.44	115.97	120.66
3	A	2601	T3X	C22-N21-C20	-3.23	104.40	109.54
3	A	2601	T3X	C05-C08-N10	3.12	123.49	115.90
3	A	2601	T3X	C32-C31-C39	2.83	120.99	118.28
3	A	2601	T3X	F28-C25-C13	-2.51	108.20	112.65
3	A	2601	T3X	C05-C04-C03	-2.49	118.38	120.60
3	A	2601	T3X	C39-C31-C30	-2.47	116.72	120.90
3	A	2601	T3X	C32-C33-C37	2.37	138.93	135.46
3	A	2601	T3X	C15-C14-C13	-2.35	116.52	118.75
3	A	2601	T3X	C17-N18-C23	2.10	115.58	111.07
3	A	2601	T3X	F27-C25-C13	-2.07	108.97	112.65
3	A	2601	T3X	C20-C19-N18	2.05	114.77	110.65

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2601	T3X	C14-C17-N18-C19
3	A	2601	T3X	C14-C17-N18-C23

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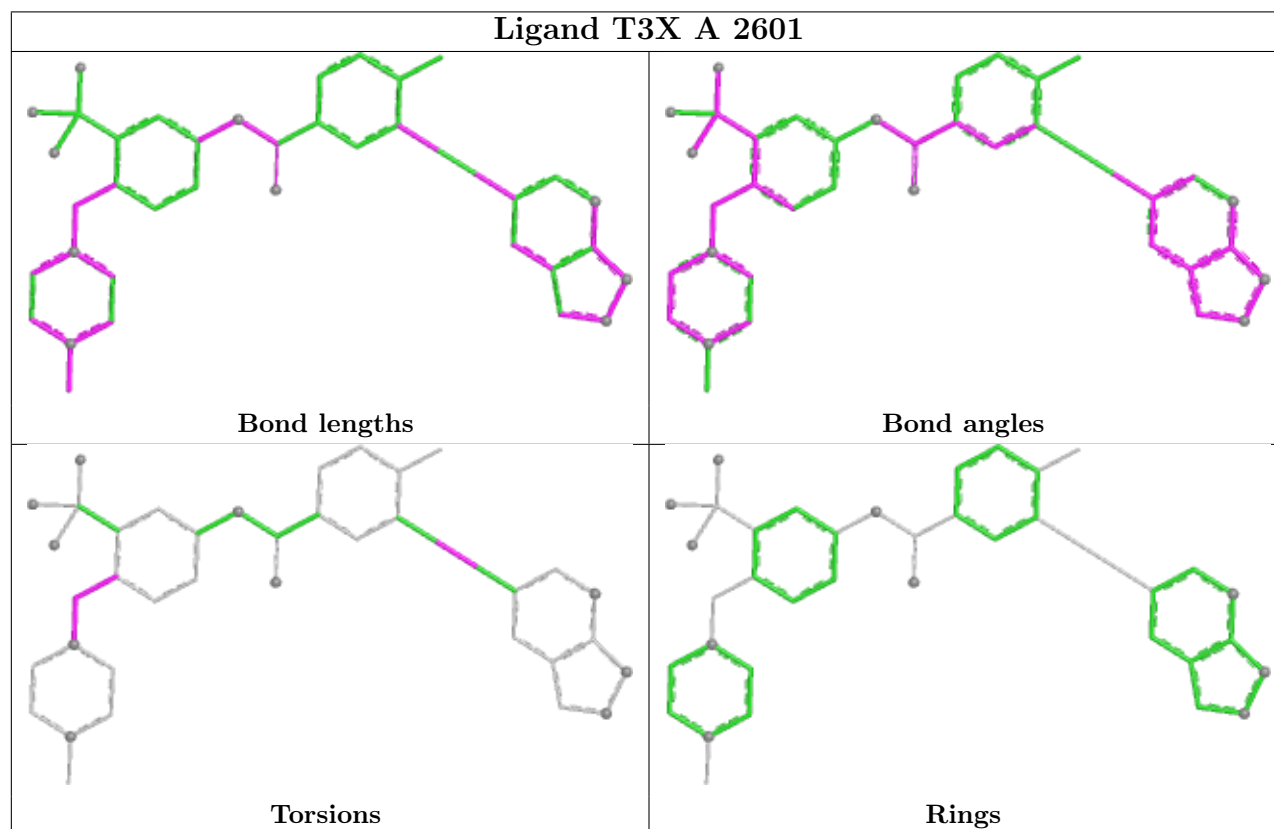
Mol	Chain	Res	Type	Atoms
3	A	2601	T3X	C03-C29-C30-C31
3	A	2601	T3X	C13-C14-C17-N18

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	T3X	3	0

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



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

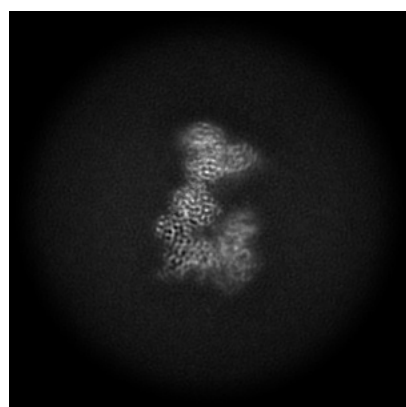
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41728. These allow visual inspection of the internal detail of the map and identification of artifacts.

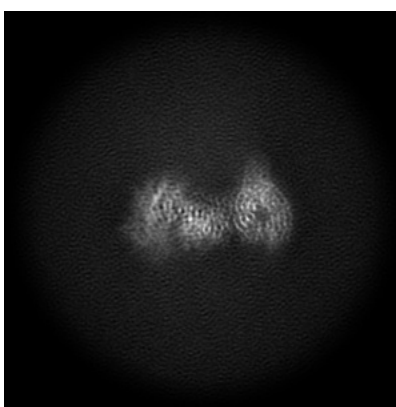
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

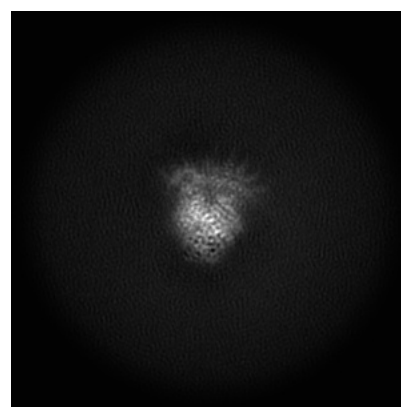
6.1.1 Primary map



X



Y

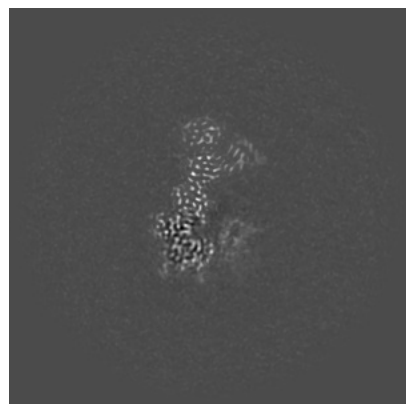


Z

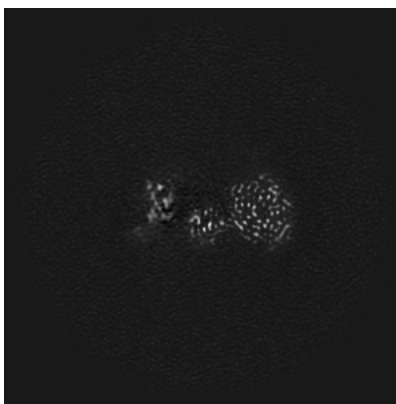
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

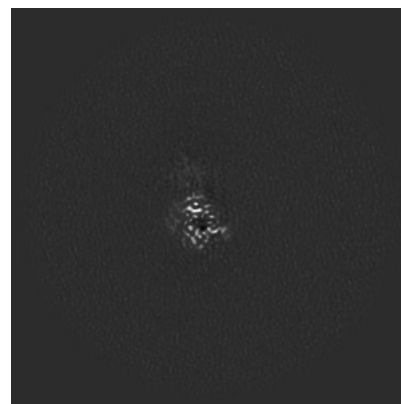
6.2.1 Primary map



X Index: 160



Y Index: 160

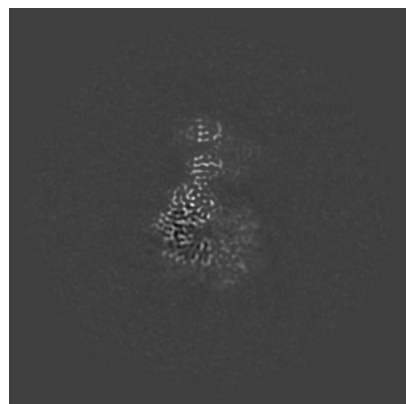


Z Index: 160

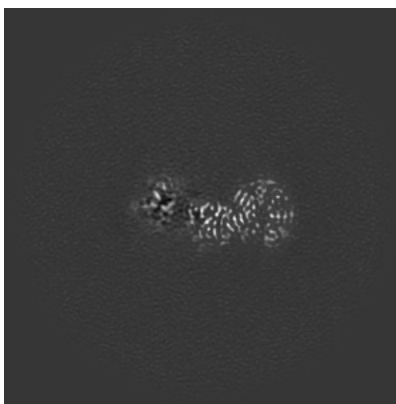
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

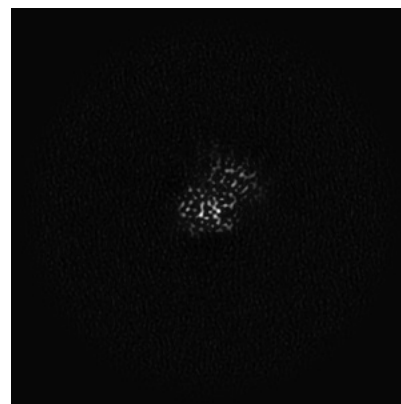
6.3.1 Primary map



X Index: 153



Y Index: 152

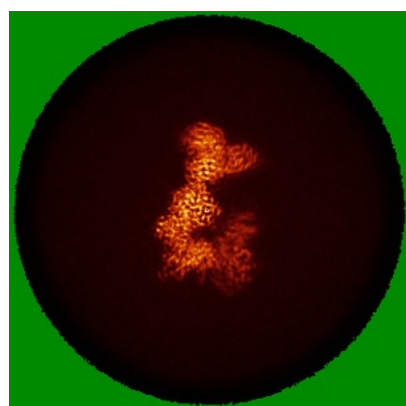


Z Index: 195

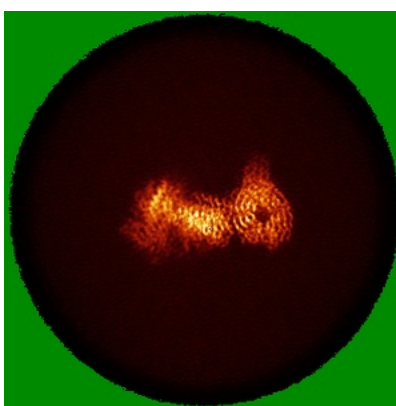
The images above show the largest variance slices of the map in three orthogonal directions.

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

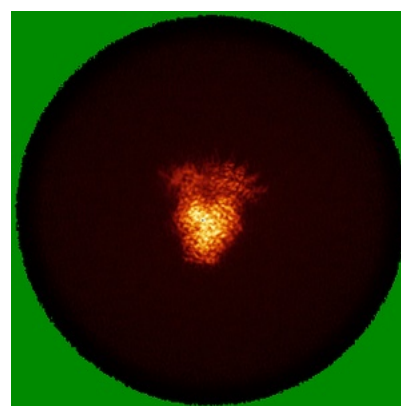
6.4.1 Primary map



X



Y

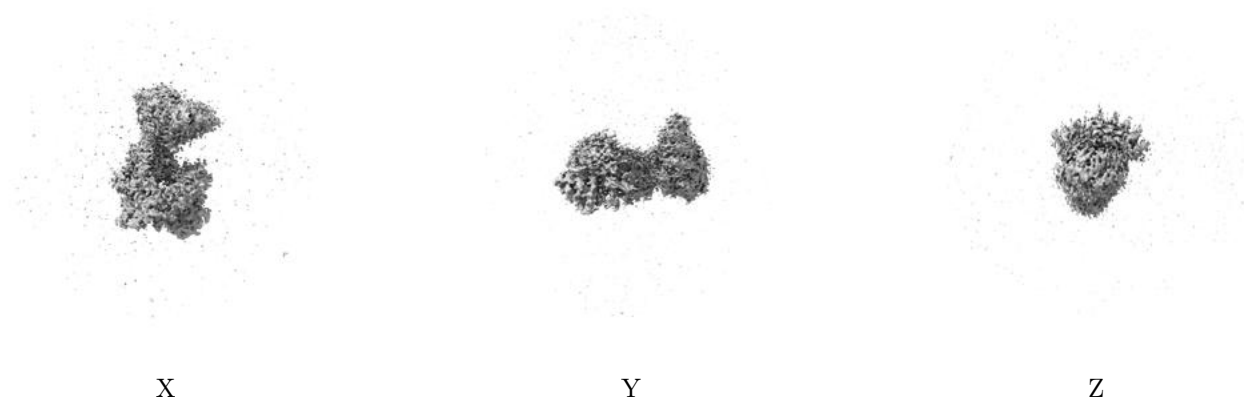


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.124. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

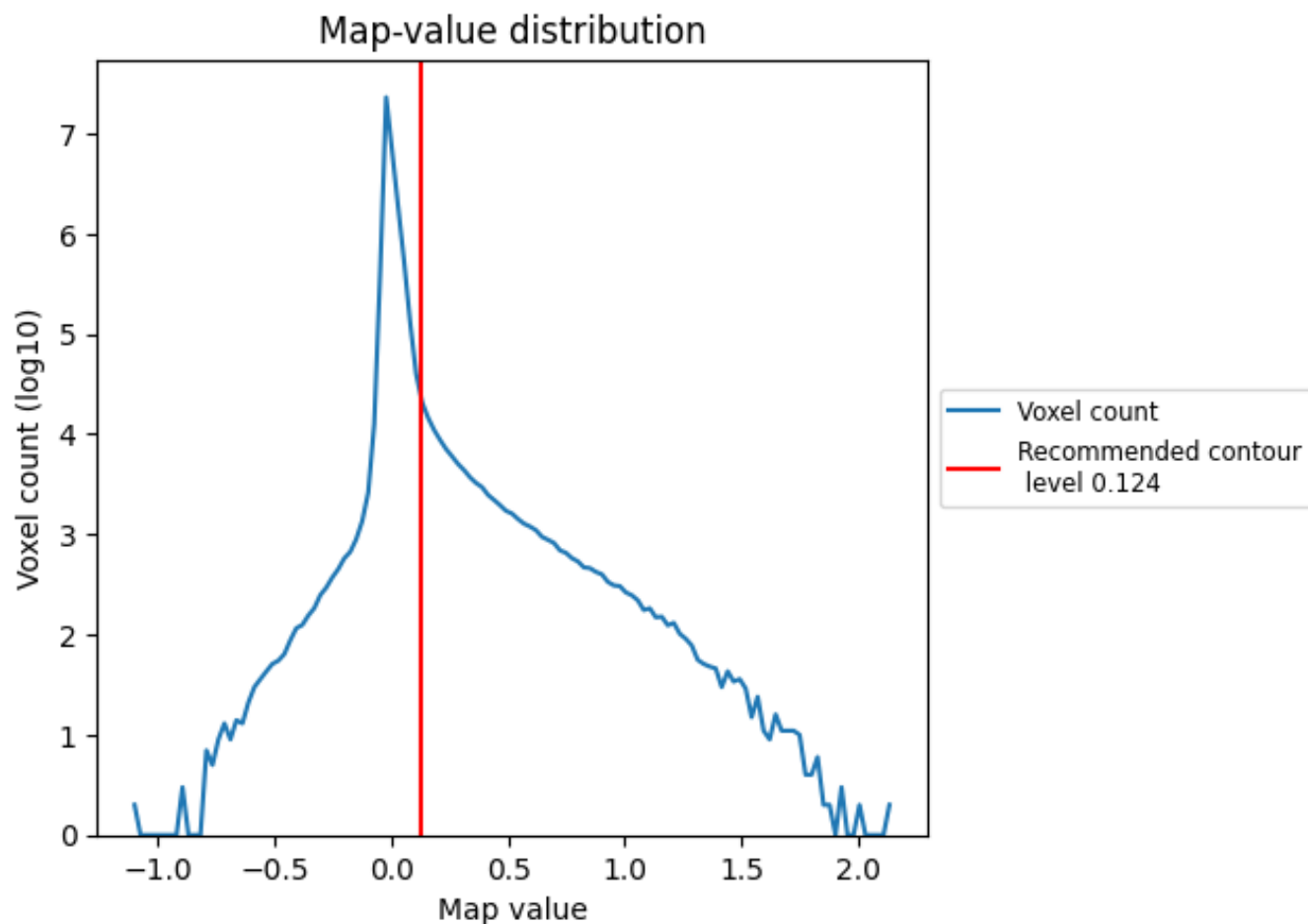
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

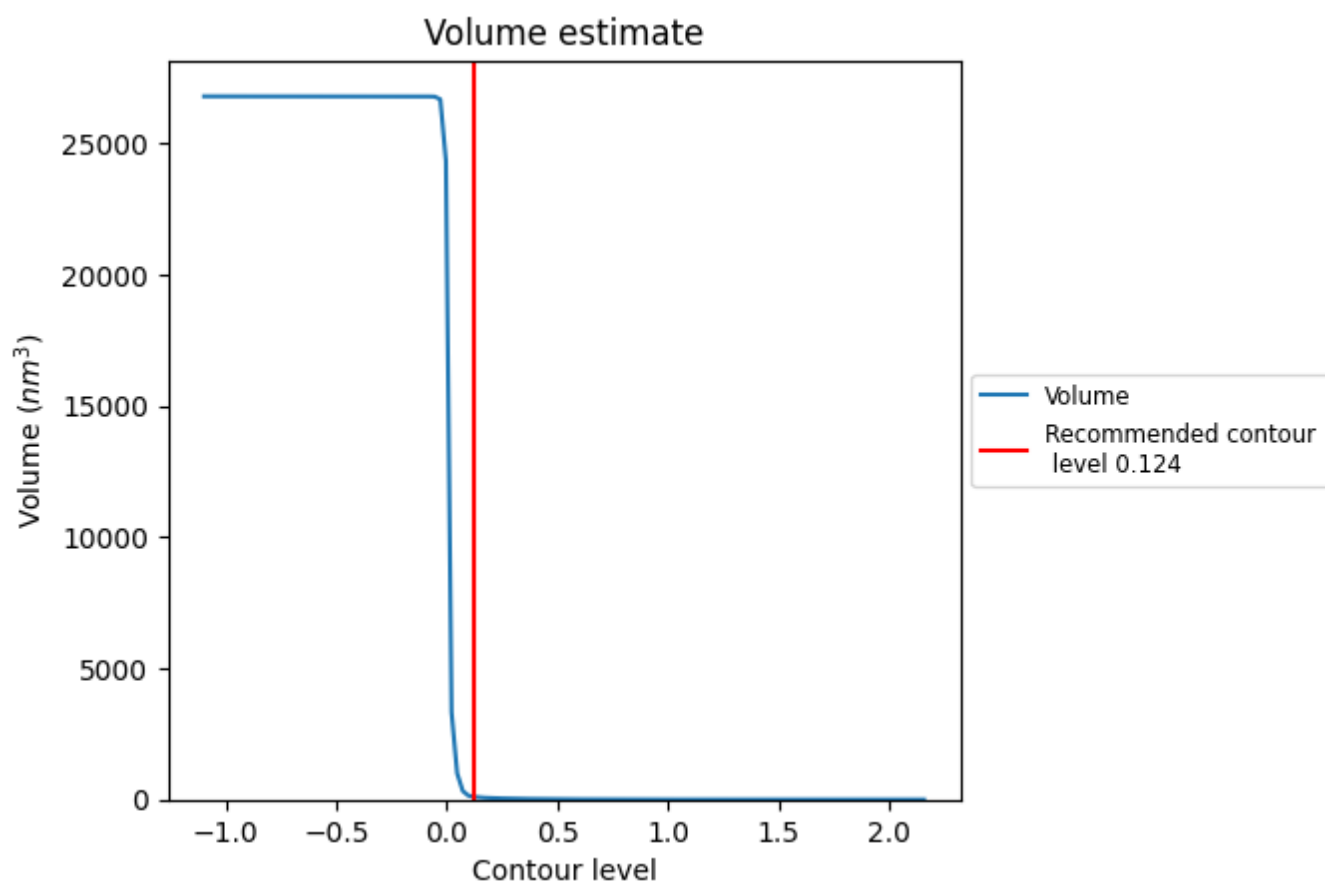
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

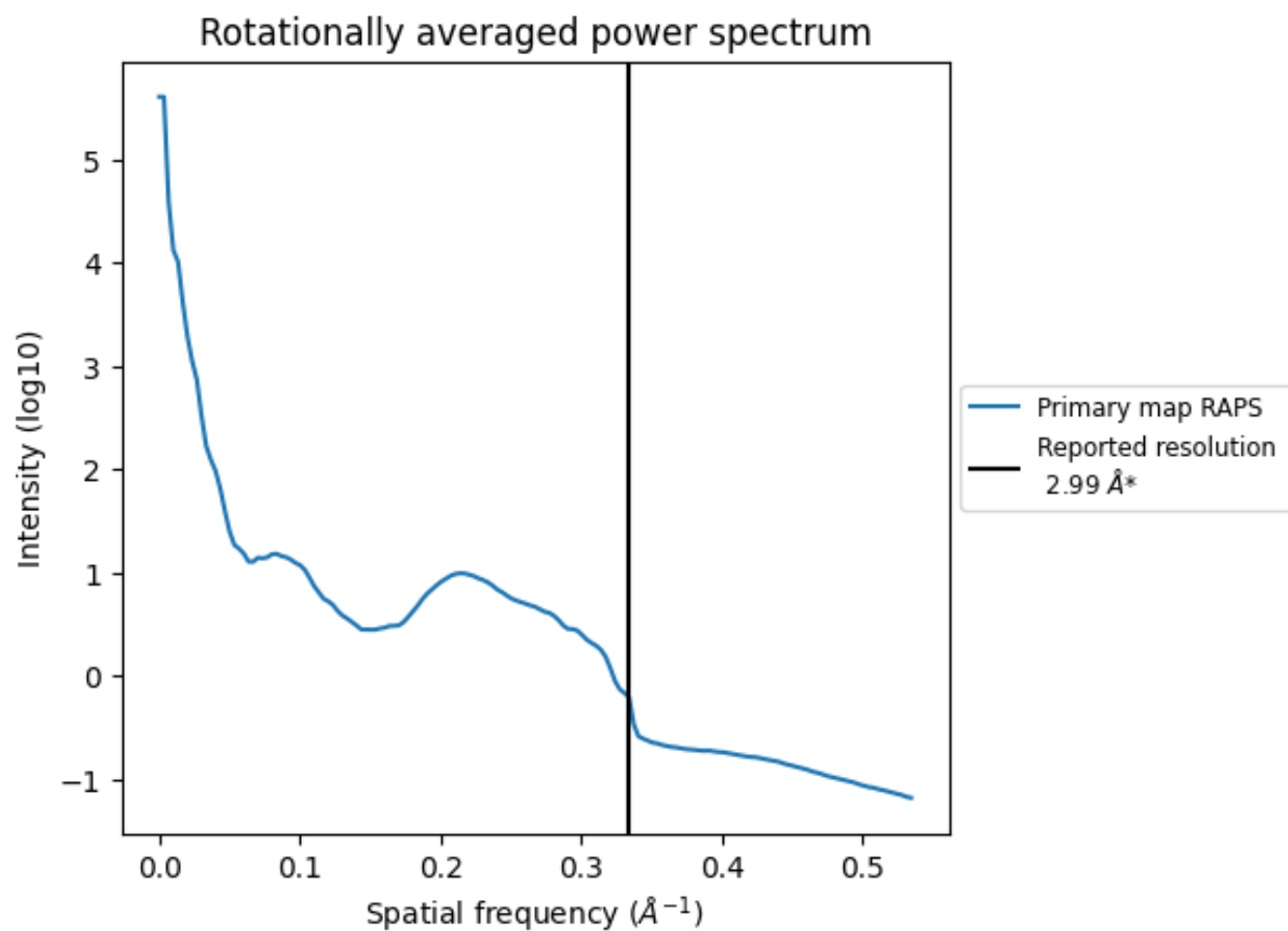
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm^3 ; this corresponds to an approximate mass of 91 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 0.334 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

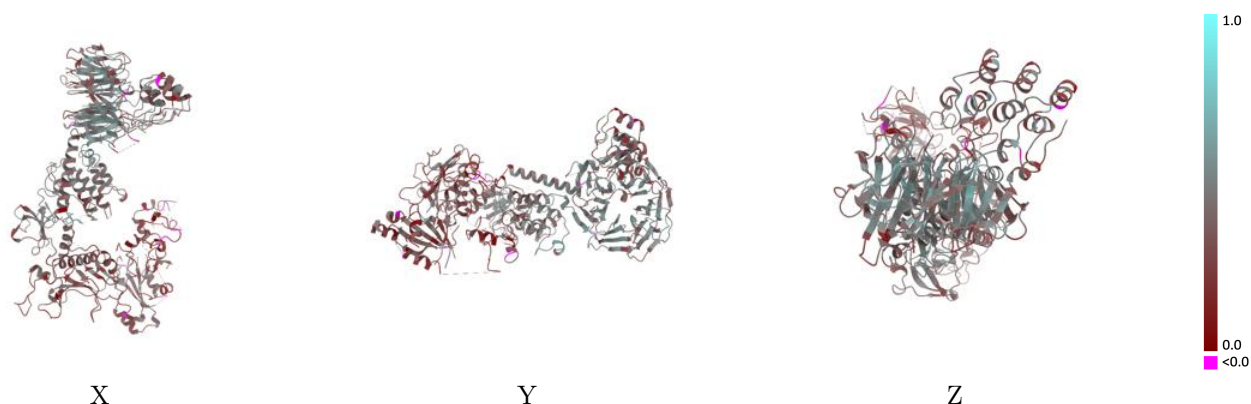
This section contains information regarding the fit between EMDB map EMD-41728 and PDB model 8TYQ. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



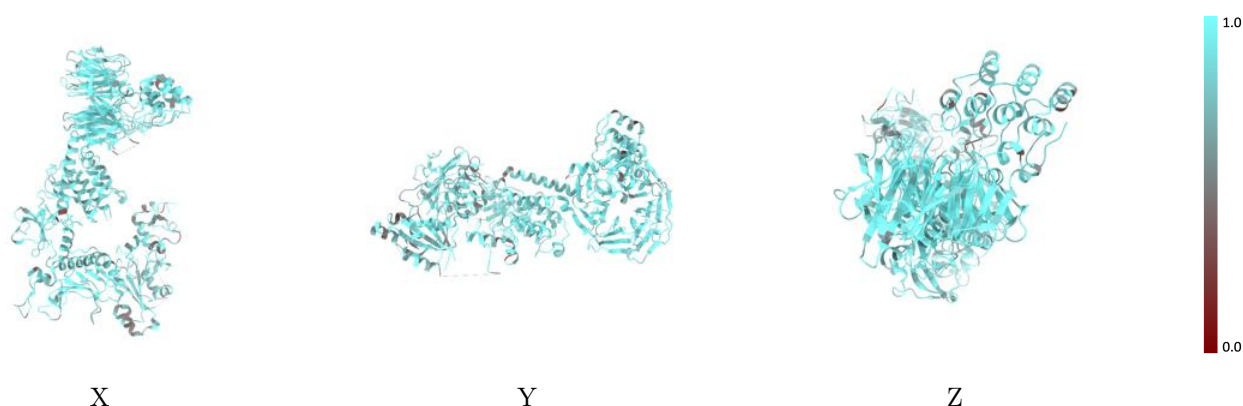
The images above show the 3D surface view of the map at the recommended contour level 0.124 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



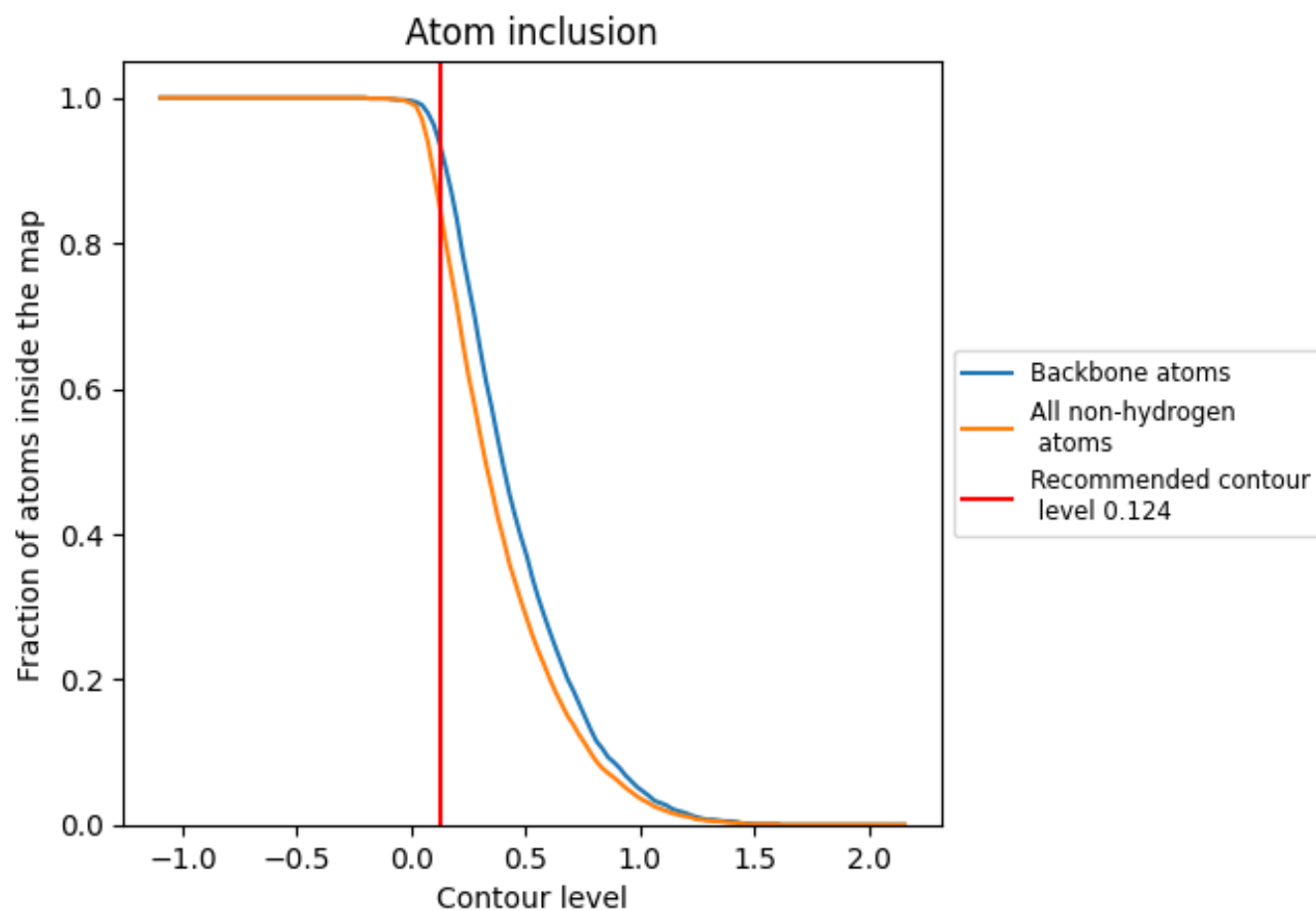
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.124).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.124) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.3750
A	0.8540	0.3730
B	0.8250	0.3850

