



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 08:43 PM UTC

PDB ID : 9HUX / pdb_00009hux
EMDB ID : EMD-52419
Title : CryoEM map of the large glutamate dehydrogenase composed of 180 kDa subunits from Mycobacterium smegmatis obtained in the presence of NAD⁺ and L-glutamate. Open Tetramer.
Authors : Lazaro, M.; Chamorro, N.; Lopez-Alonso, J.P.; Charro, D.; Rasia, R.M.; Jimenez-Oses, G.; Valle, M.; Lisa, M.N.
Deposited on : 2024-12-23
Resolution : 3.88 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

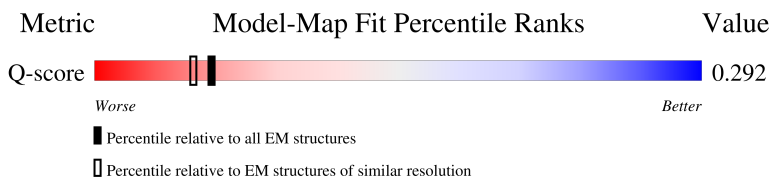
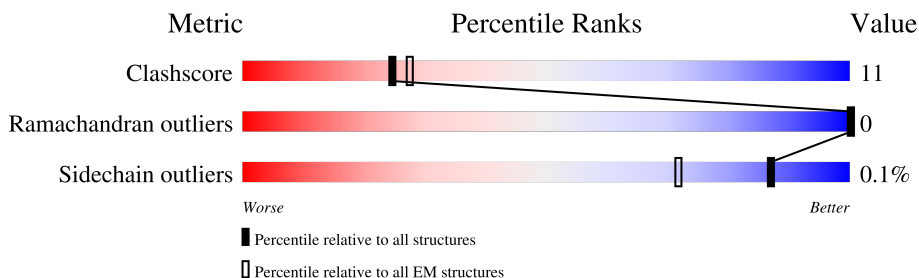
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 3.88 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	8773 (3.38 - 4.38)

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	1611	
1	B	1611	
1	C	1611	

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Mol	Chain	Length	Quality of chain
1	D	1611	<div><div></div><div>51%</div><div>16%</div><div>33%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33576 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 NAD-specific glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	B	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	C	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		
1	D	1075	Total	C	N	O	S	0	0
			8350	5240	1496	1594	20		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP A0R1C2
A	-15	HIS	-	expression tag	UNP A0R1C2
A	-14	HIS	-	expression tag	UNP A0R1C2
A	-13	HIS	-	expression tag	UNP A0R1C2
A	-12	HIS	-	expression tag	UNP A0R1C2
A	-11	HIS	-	expression tag	UNP A0R1C2
A	-10	HIS	-	expression tag	UNP A0R1C2
A	-9	GLU	-	expression tag	UNP A0R1C2
A	-8	ASN	-	expression tag	UNP A0R1C2
A	-7	LEU	-	expression tag	UNP A0R1C2
A	-6	TYR	-	expression tag	UNP A0R1C2
A	-5	PHE	-	expression tag	UNP A0R1C2
A	-4	GLN	-	expression tag	UNP A0R1C2
A	-3	GLY	-	expression tag	UNP A0R1C2
A	-2	ALA	-	expression tag	UNP A0R1C2
A	-1	ALA	-	expression tag	UNP A0R1C2
A	0	SER	-	expression tag	UNP A0R1C2
B	-16	MET	-	initiating methionine	UNP A0R1C2
B	-15	HIS	-	expression tag	UNP A0R1C2
B	-14	HIS	-	expression tag	UNP A0R1C2
B	-13	HIS	-	expression tag	UNP A0R1C2
B	-12	HIS	-	expression tag	UNP A0R1C2

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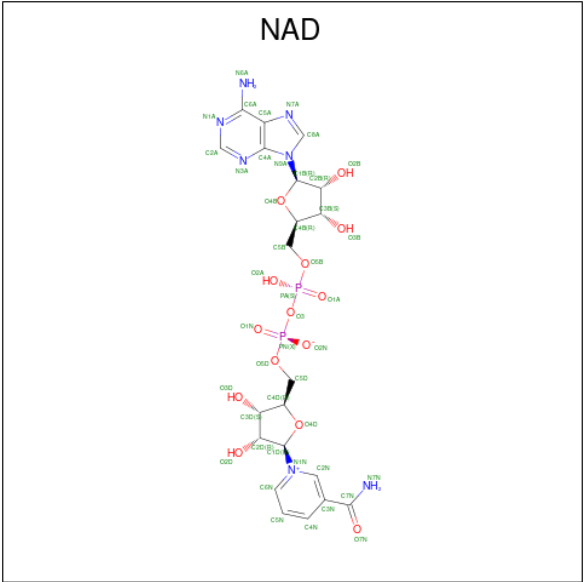
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0R1C2
B	-10	HIS	-	expression tag	UNP A0R1C2
B	-9	GLU	-	expression tag	UNP A0R1C2
B	-8	ASN	-	expression tag	UNP A0R1C2
B	-7	LEU	-	expression tag	UNP A0R1C2
B	-6	TYR	-	expression tag	UNP A0R1C2
B	-5	PHE	-	expression tag	UNP A0R1C2
B	-4	GLN	-	expression tag	UNP A0R1C2
B	-3	GLY	-	expression tag	UNP A0R1C2
B	-2	ALA	-	expression tag	UNP A0R1C2
B	-1	ALA	-	expression tag	UNP A0R1C2
B	0	SER	-	expression tag	UNP A0R1C2
C	-16	MET	-	initiating methionine	UNP A0R1C2
C	-15	HIS	-	expression tag	UNP A0R1C2
C	-14	HIS	-	expression tag	UNP A0R1C2
C	-13	HIS	-	expression tag	UNP A0R1C2
C	-12	HIS	-	expression tag	UNP A0R1C2
C	-11	HIS	-	expression tag	UNP A0R1C2
C	-10	HIS	-	expression tag	UNP A0R1C2
C	-9	GLU	-	expression tag	UNP A0R1C2
C	-8	ASN	-	expression tag	UNP A0R1C2
C	-7	LEU	-	expression tag	UNP A0R1C2
C	-6	TYR	-	expression tag	UNP A0R1C2
C	-5	PHE	-	expression tag	UNP A0R1C2
C	-4	GLN	-	expression tag	UNP A0R1C2
C	-3	GLY	-	expression tag	UNP A0R1C2
C	-2	ALA	-	expression tag	UNP A0R1C2
C	-1	ALA	-	expression tag	UNP A0R1C2
C	0	SER	-	expression tag	UNP A0R1C2
D	-16	MET	-	initiating methionine	UNP A0R1C2
D	-15	HIS	-	expression tag	UNP A0R1C2
D	-14	HIS	-	expression tag	UNP A0R1C2
D	-13	HIS	-	expression tag	UNP A0R1C2
D	-12	HIS	-	expression tag	UNP A0R1C2
D	-11	HIS	-	expression tag	UNP A0R1C2
D	-10	HIS	-	expression tag	UNP A0R1C2
D	-9	GLU	-	expression tag	UNP A0R1C2
D	-8	ASN	-	expression tag	UNP A0R1C2
D	-7	LEU	-	expression tag	UNP A0R1C2
D	-6	TYR	-	expression tag	UNP A0R1C2
D	-5	PHE	-	expression tag	UNP A0R1C2
D	-4	GLN	-	expression tag	UNP A0R1C2

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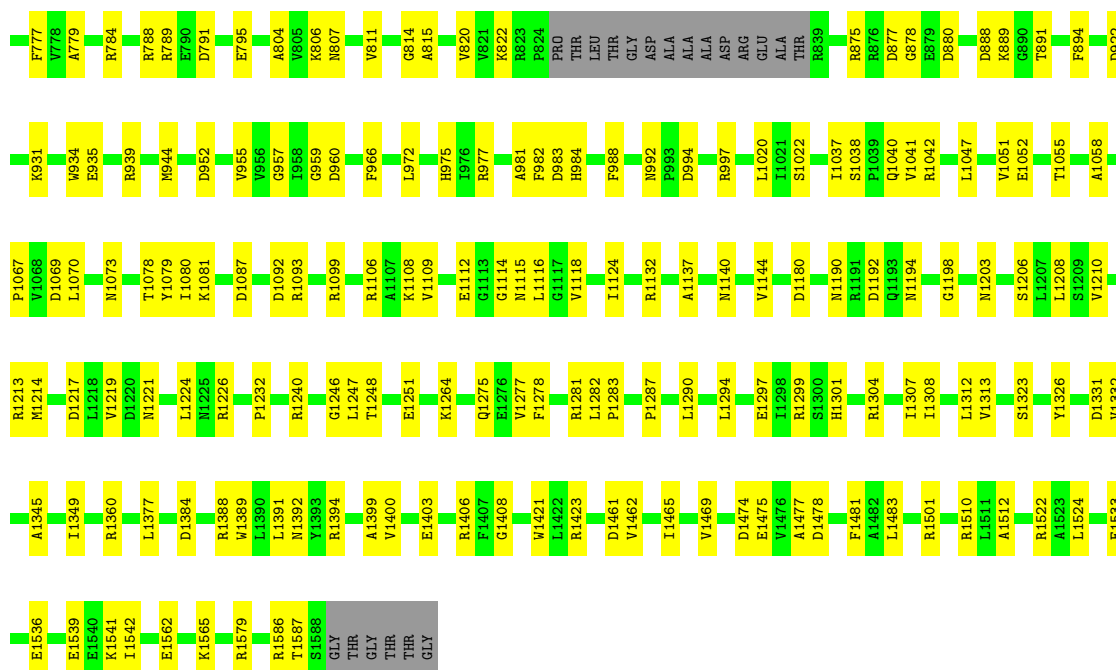
Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP A0R1C2
D	-2	ALA	-	expression tag	UNP A0R1C2
D	-1	ALA	-	expression tag	UNP A0R1C2
D	0	SER	-	expression tag	UNP A0R1C2

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂) (labeled as "Ligand of Interest" by depositor).

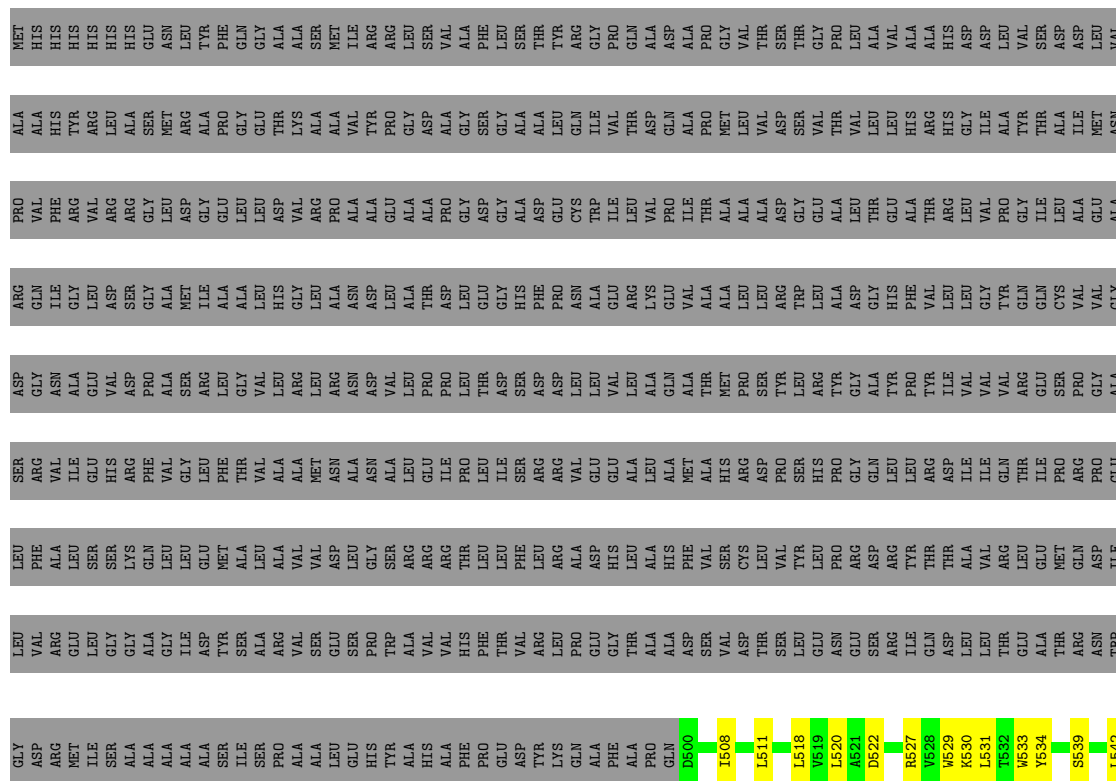


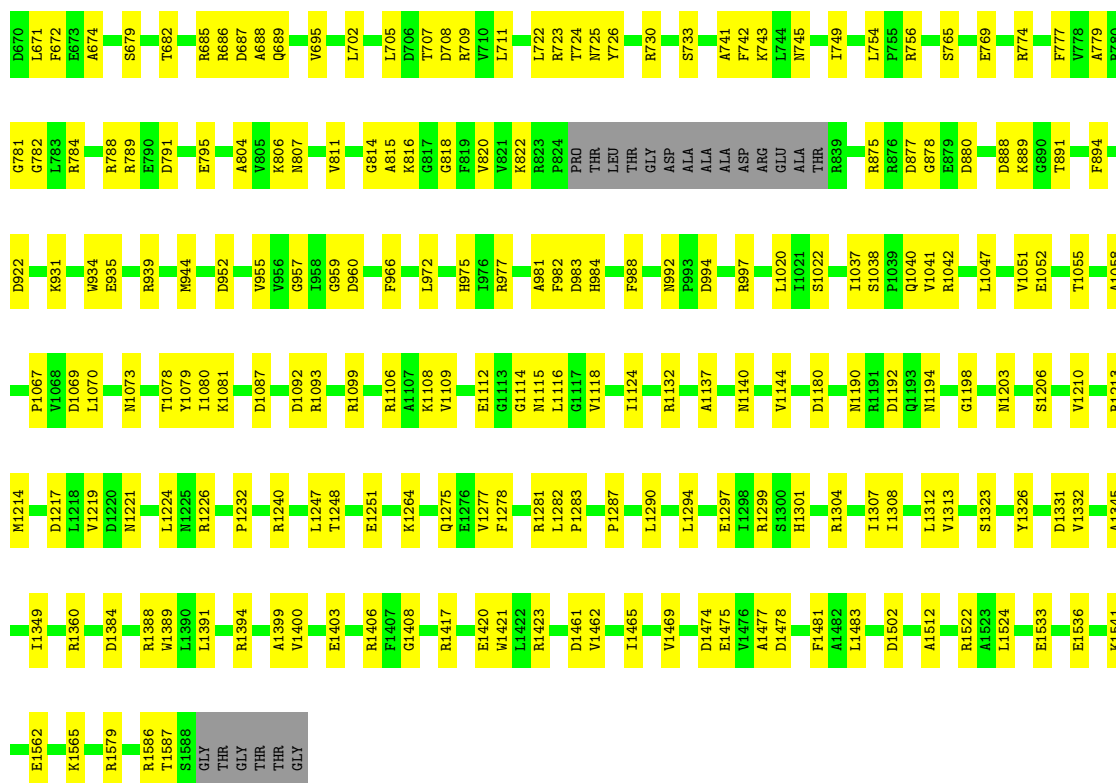
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	Total 44	21	7	14	2	0
2	B	1	Total 44	21	7	14	2	0
2	C	1	Total 44	21	7	14	2	0
2	D	1	Total 44	21	7	14	2	0



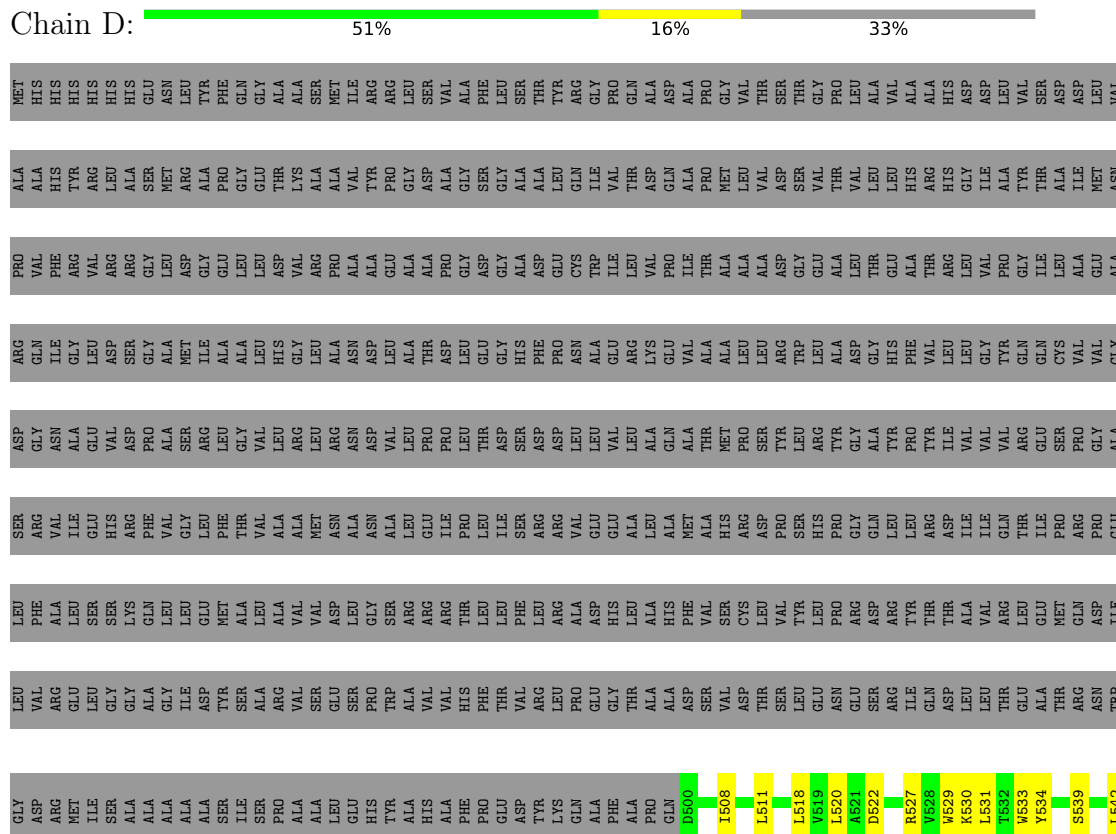


• Molecule 1: NAD-specific glutamate dehydrogenase





● Molecule 1: NAD-specific glutamate dehydrogenase



E1539	I1349	D1217	D1069		V778	S856
E1540	R1360	L1218	L1070	W934	A779	V657
K1541		V1219		E935		
I1542	L1377	D1220	M1073		R784	T664
		M1221		R939		T665
E1562			Y1079		R788	
D1384		L1224	I1090	M944	R789	R689
		M1225	K1081		E790	D670
R1388		R1226		D952	D791	L671
W1389			D1087			E558
L1390		P1232		V955	E795	F672
L1391			D1092	V956		F673
N1392		R1240	R1093	G957	A804	A674
R1394		G1246	R1099	F958	V805	R685
		L1247		K959	R806	R686
A1399		T1248	R1106	D960	N807	D687
V1400			A1187	F966	V811	A688
		E1251	K1108			Q689
E1403			V1109	L972	G814	V695
		K1264			A815	
R1406			E1112	H975		L702
F1407		Q1275	G1113	I976	V820	
G1408		E1276	G1114	A977	V821	L705
		V1277	N1115		K822	D706
W1421		F1278	L1116	A981	R823	T707
L1422			G1117	F982	P824	D708
R1423		R1281	V1118	D983	PH0	R709
		L1282		H984	W710	
D1461		P1283	T1124		LEU	L711
V1462				F988	THR	
		P1287	R1132		GLY	L722
I1465				N992	ASP	H587
V1469		L1290	A1137	P993	ALA	R723
				D994	ALA	T724
		L1294	N1140		ALA	N725
D1474				A997	ASP	Y726
E1475		E1297	V1144		ARG	R730
V1476		I1298		L1020	GLU	
A1477		R1299	D1180	I1021	ALA	R612
D1478		S1300		S1022	THR	S733
		H1301	N1190		R839	
F1481			R1191	I1037		A741
A1482		R1304	D1192	R875		F742
L1483			Q1193	S1038	R876	K743
		I1307	N1194	Q1040	D877	L744
R1501		I1308		V1041	G878	N745
			G1198	R1042		
R1510		L1312	N1203	L1047	D880	I749
A1512		V1313				L754
		S1323	S1206	V1051	D888	P755
R1522			L1207	K889		V634
A1523		Y1326	L1208	E1052	G890	L635
L1524			S1209	T891		R636
E1533		D1331	V1210	T1055		S765
		V1332		F894		E769
			R1213	A1058		
E1536		A1345	M1214	D922		R774
						F777

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37641	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 ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	439.41602, 439.41602, 439.41602	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2924, 1.2924, 1.2924	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.07	0/8502	0.20	0/11541
1	B	0.07	0/8502	0.20	0/11541
1	C	0.07	0/8502	0.20	0/11541
1	D	0.07	0/8502	0.20	0/11541
All	All	0.07	0/34008	0.20	0/46164

There are no bond length outliers.

There are no bond angle outliers.

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	8350	0	8301	182	0
1	B	8350	0	8301	183	0
1	C	8350	0	8301	179	0
1	D	8350	0	8301	177	0
2	A	44	0	26	6	0
2	B	44	0	26	7	0
2	C	44	0	26	7	0
2	D	44	0	26	7	0
All	All	33576	0	33308	710	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 11.

All (710) 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:B:960:ASP:HB2	1:B:983:ASP:OD2	1.48	1.14
1:D:960:ASP:HB2	1:D:983:ASP:OD2	1.48	1.14
1:A:960:ASP:HB2	1:A:983:ASP:OD2	1.48	1.13
1:C:960:ASP:HB2	1:C:983:ASP:OD2	1.48	1.13
1:B:960:ASP:CB	1:B:983:ASP:OD2	2.25	0.85
1:D:960:ASP:CB	1:D:983:ASP:OD2	2.25	0.85
1:C:960:ASP:CB	1:C:983:ASP:OD2	2.25	0.83
1:A:960:ASP:CB	1:A:983:ASP:OD2	2.25	0.83
1:A:1115:ASN:HD22	1:A:1116:LEU:N	1.85	0.74
1:C:1115:ASN:HD22	1:C:1116:LEU:N	1.86	0.74
1:B:1115:ASN:HD22	1:B:1116:LEU:N	1.86	0.74
1:D:1115:ASN:HD22	1:D:1116:LEU:N	1.86	0.74
1:B:1037:ILE:HB	1:B:1052:GLU:HA	1.71	0.73
1:D:1037:ILE:HB	1:D:1052:GLU:HA	1.71	0.73
1:A:671:LEU:HD12	1:A:686:ARG:HH22	1.55	0.72
1:C:671:LEU:HD12	1:C:686:ARG:HH22	1.55	0.72
1:D:671:LEU:HD12	1:D:686:ARG:HH22	1.55	0.71
1:A:1037:ILE:HB	1:A:1052:GLU:HA	1.71	0.71
1:B:671:LEU:HD12	1:B:686:ARG:HH22	1.55	0.71
1:C:1037:ILE:HB	1:C:1052:GLU:HA	1.71	0.71
1:B:1115:ASN:HD22	1:B:1115:ASN:C	2.00	0.69
1:B:1512:ALA:O	1:C:1579:ARG:NH2	2.24	0.69
1:D:1115:ASN:HD22	1:D:1115:ASN:C	2.00	0.69
1:C:1115:ASN:HD22	1:C:1115:ASN:C	2.00	0.69
1:A:1115:ASN:HD22	1:A:1115:ASN:C	2.00	0.69
1:A:1073:ASN:HB3	1:A:1112:GLU:HA	1.75	0.68
1:C:1092:ASP:O	1:C:1099:ARG:NH2	2.27	0.68
1:A:1092:ASP:O	1:A:1099:ARG:NH2	2.27	0.68
1:C:1073:ASN:HB3	1:C:1112:GLU:HA	1.76	0.68
1:D:952:ASP:HA	1:D:975:HIS:HB3	1.76	0.67
1:B:952:ASP:HA	1:B:975:HIS:HB3	1.76	0.67
1:D:1092:ASP:O	1:D:1099:ARG:NH2	2.27	0.67
1:B:1092:ASP:O	1:B:1099:ARG:NH2	2.27	0.67
1:A:952:ASP:HA	1:A:975:HIS:HB3	1.76	0.66
1:C:765:SER:O	1:C:822:LYS:NZ	2.29	0.66
1:C:952:ASP:HA	1:C:975:HIS:HB3	1.76	0.66
1:D:1042:ARG:HH21	1:D:1047:LEU:H	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:SER:O	1:A:822:LYS:NZ	2.29	0.66
1:B:1042:ARG:HH21	1:B:1047:LEU:H	1.42	0.66
1:B:1073:ASN:HB3	1:B:1112:GLU:HA	1.75	0.66
1:D:1073:ASN:HB3	1:D:1112:GLU:HA	1.75	0.66
1:C:1042:ARG:HH21	1:C:1047:LEU:H	1.42	0.66
1:A:1042:ARG:HH21	1:A:1047:LEU:H	1.42	0.65
1:B:674:ALA:HB3	1:B:686:ARG:HH21	1.60	0.65
1:D:674:ALA:HB3	1:D:686:ARG:HH21	1.60	0.65
1:C:983:ASP:CG	1:C:984:HIS:H	2.03	0.65
1:A:983:ASP:CG	1:A:984:HIS:H	2.03	0.65
1:D:765:SER:O	1:D:822:LYS:NZ	2.29	0.65
1:B:765:SER:O	1:B:822:LYS:NZ	2.29	0.64
1:D:983:ASP:CG	1:D:984:HIS:H	2.03	0.64
1:B:983:ASP:CG	1:B:984:HIS:H	2.03	0.64
1:A:530:LYS:HG3	1:A:576:GLN:HE22	1.62	0.64
1:C:530:LYS:HG3	1:C:576:GLN:HE22	1.62	0.64
1:A:1512:ALA:O	1:D:1579:ARG:NH2	2.29	0.64
1:C:674:ALA:HB3	1:C:686:ARG:HH21	1.60	0.64
1:D:530:LYS:HG3	1:D:576:GLN:HE22	1.62	0.64
1:A:674:ALA:HB3	1:A:686:ARG:HH21	1.60	0.64
1:B:530:LYS:HG3	1:B:576:GLN:HE22	1.62	0.64
1:C:520:LEU:HD11	1:C:529:TRP:HB3	1.79	0.64
1:D:944:MET:HG3	1:D:1132:ARG:HE	1.63	0.64
1:A:1394:ARG:NH1	1:A:1403:GLU:OE1	2.32	0.63
1:B:944:MET:HG3	1:B:1132:ARG:HE	1.64	0.63
1:C:1394:ARG:NH1	1:C:1403:GLU:OE1	2.32	0.63
1:A:520:LEU:HD11	1:A:529:TRP:HB3	1.79	0.63
1:A:546:LEU:HD13	1:B:546:LEU:HD13	1.81	0.63
1:B:527:ARG:NH2	1:B:585:ILE:O	2.30	0.63
1:D:527:ARG:NH2	1:D:585:ILE:O	2.30	0.63
1:B:520:LEU:HD11	1:B:529:TRP:HB3	1.78	0.62
1:D:520:LEU:HD11	1:D:529:TRP:HB3	1.79	0.62
1:D:1301:HIS:O	1:D:1304:ARG:NH1	2.32	0.62
1:A:779:ALA:HB1	1:A:815:ALA:HB2	1.82	0.62
1:C:779:ALA:HB1	1:C:815:ALA:HB2	1.82	0.62
1:B:1301:HIS:O	1:B:1304:ARG:NH1	2.32	0.62
1:A:1579:ARG:NH2	1:D:1512:ALA:O	2.31	0.62
1:B:1394:ARG:NH1	1:B:1403:GLU:OE1	2.32	0.62
1:D:1394:ARG:NH1	1:D:1403:GLU:OE1	2.32	0.62
1:A:1301:HIS:O	1:A:1304:ARG:NH1	2.32	0.62
1:B:724:THR:HG22	1:B:726:TYR:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1301:HIS:O	1:C:1304:ARG:NH1	2.32	0.62
1:D:724:THR:HG22	1:D:726:TYR:H	1.65	0.62
1:A:1080:ILE:HD13	1:A:1118:VAL:HG22	1.82	0.62
1:C:546:LEU:HD13	1:D:546:LEU:HD13	1.81	0.61
1:C:1080:ILE:HD13	1:C:1118:VAL:HG22	1.82	0.61
1:A:527:ARG:NH2	1:A:585:ILE:O	2.30	0.61
1:A:1190:ASN:O	1:A:1194:ASN:ND2	2.33	0.61
1:B:1080:ILE:HD13	1:B:1118:VAL:HG22	1.82	0.61
1:C:1190:ASN:O	1:C:1194:ASN:ND2	2.33	0.61
1:A:664:THR:HG21	1:A:711:LEU:HD13	1.83	0.61
1:A:944:MET:HG3	1:A:1132:ARG:HE	1.63	0.61
1:C:527:ARG:NH2	1:C:585:ILE:O	2.30	0.61
1:C:664:THR:HG21	1:C:711:LEU:HD13	1.83	0.61
1:C:944:MET:HG3	1:C:1132:ARG:HE	1.63	0.61
1:D:1080:ILE:HD13	1:D:1118:VAL:HG22	1.82	0.61
1:D:779:ALA:HB1	1:D:815:ALA:HB2	1.82	0.61
1:B:779:ALA:HB1	1:B:815:ALA:HB2	1.82	0.61
1:D:664:THR:HG21	1:D:711:LEU:HD13	1.83	0.60
1:D:1190:ASN:O	1:D:1194:ASN:ND2	2.33	0.60
1:A:1217:ASP:OD1	1:A:1221:ASN:ND2	2.35	0.60
1:B:664:THR:HG21	1:B:711:LEU:HD13	1.83	0.60
1:B:1190:ASN:O	1:B:1194:ASN:ND2	2.33	0.60
1:C:1217:ASP:OD1	1:C:1221:ASN:ND2	2.35	0.60
1:A:724:THR:HG22	1:A:726:TYR:H	1.65	0.60
1:C:724:THR:HG22	1:C:726:TYR:H	1.65	0.60
1:C:508:ILE:O	1:C:566:ARG:NH1	2.35	0.60
1:A:508:ILE:O	1:A:566:ARG:NH1	2.35	0.60
1:B:1217:ASP:OD1	1:B:1221:ASN:ND2	2.35	0.60
1:B:508:ILE:O	1:B:566:ARG:NH1	2.35	0.60
1:D:508:ILE:O	1:D:566:ARG:NH1	2.35	0.60
1:C:981:ALA:HB3	1:C:988:PHE:HB3	1.84	0.60
1:D:1217:ASP:OD1	1:D:1221:ASN:ND2	2.35	0.60
1:A:981:ALA:HB3	1:A:988:PHE:HB3	1.84	0.59
1:A:1423:ARG:NH2	1:A:1478:ASP:OD1	2.35	0.59
1:D:1536:GLU:O	1:D:1541:LYS:NZ	2.33	0.59
1:C:1423:ARG:NH2	1:C:1478:ASP:OD1	2.35	0.59
1:A:997:ARG:HD2	1:A:1020:LEU:HD22	1.85	0.59
1:B:1536:GLU:O	1:B:1541:LYS:NZ	2.33	0.59
1:C:997:ARG:HD2	1:C:1020:LEU:HD22	1.85	0.59
1:D:981:ALA:HB3	1:D:988:PHE:HB3	1.84	0.59
1:C:1192:ASP:OD1	1:C:1360:ARG:NH1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:ASP:OD1	1:A:1360:ARG:NH1	2.35	0.59
1:B:981:ALA:HB3	1:B:988:PHE:HB3	1.85	0.59
1:D:565:ARG:HH22	1:D:570:LEU:N	2.01	0.59
1:B:565:ARG:HH22	1:B:570:LEU:N	2.01	0.58
1:B:788:ARG:NH2	1:B:791:ASP:O	2.36	0.58
1:B:997:ARG:HD2	1:B:1020:LEU:HD22	1.85	0.58
1:D:788:ARG:NH2	1:D:791:ASP:O	2.36	0.58
1:D:997:ARG:HD2	1:D:1020:LEU:HD22	1.85	0.58
1:A:565:ARG:HH22	1:A:570:LEU:N	2.01	0.58
1:C:565:ARG:HH22	1:C:570:LEU:N	2.01	0.58
1:A:788:ARG:NH2	1:A:791:ASP:O	2.36	0.58
1:B:558:GLU:HG3	1:B:560:ARG:HH12	1.69	0.58
1:C:788:ARG:NH2	1:C:791:ASP:O	2.36	0.58
1:D:558:GLU:HG3	1:D:560:ARG:HH12	1.69	0.58
1:B:1421:TRP:HB2	1:B:1481:PHE:HD2	1.68	0.58
1:A:983:ASP:OD1	1:A:984:HIS:N	2.36	0.57
1:A:1421:TRP:HB2	1:A:1481:PHE:HD2	1.68	0.57
1:C:983:ASP:OD1	1:C:984:HIS:N	2.36	0.57
1:D:1421:TRP:HB2	1:D:1481:PHE:HD2	1.68	0.57
1:C:1421:TRP:HB2	1:C:1481:PHE:HD2	1.68	0.57
1:A:1536:GLU:O	1:A:1541:LYS:NZ	2.33	0.57
1:B:1287:PRO:HD2	1:B:1290:LEU:HD12	1.87	0.57
1:C:1536:GLU:O	1:C:1541:LYS:NZ	2.34	0.57
1:D:1287:PRO:HD2	1:D:1290:LEU:HD12	1.87	0.57
1:A:1287:PRO:HD2	1:A:1290:LEU:HD12	1.87	0.56
1:C:542:LEU:HB3	1:C:546:LEU:HD11	1.88	0.56
1:C:1287:PRO:HD2	1:C:1290:LEU:HD12	1.87	0.56
1:A:542:LEU:HB3	1:A:546:LEU:HD11	1.88	0.56
1:B:1192:ASP:OD1	1:B:1360:ARG:NH1	2.35	0.56
1:B:616:ASP:OD2	1:B:636:ARG:NE	2.37	0.56
1:D:542:LEU:HB3	1:D:546:LEU:HD11	1.88	0.56
1:B:542:LEU:HB3	1:B:546:LEU:HD11	1.88	0.56
1:D:616:ASP:OD2	1:D:636:ARG:NE	2.37	0.56
1:D:1192:ASP:OD1	1:D:1360:ARG:NH1	2.35	0.56
1:D:983:ASP:OD1	1:D:984:HIS:N	2.36	0.56
1:A:558:GLU:HG3	1:A:560:ARG:HH12	1.69	0.55
1:B:749:ILE:O	1:B:756:ARG:NH1	2.39	0.55
1:B:983:ASP:OD1	1:B:984:HIS:N	2.37	0.55
1:C:807:ASN:HD22	1:C:814:GLY:HA2	1.72	0.55
1:D:749:ILE:O	1:D:756:ARG:NH1	2.39	0.55
1:B:607:ALA:HB1	1:B:612:ARG:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:GLU:HG3	1:C:560:ARG:HH12	1.69	0.55
1:D:607:ALA:HB1	1:D:612:ARG:HB2	1.89	0.55
1:A:807:ASN:HD22	1:A:814:GLY:HA2	1.72	0.55
1:A:722:LEU:HD11	1:A:745:ASN:HB2	1.89	0.55
1:C:722:LEU:HD11	1:C:745:ASN:HB2	1.89	0.55
1:A:607:ALA:HB1	1:A:612:ARG:HB2	1.89	0.55
1:A:749:ILE:O	1:A:756:ARG:NH1	2.39	0.55
1:C:607:ALA:HB1	1:C:612:ARG:HB2	1.89	0.55
1:C:749:ILE:O	1:C:756:ARG:NH1	2.39	0.55
1:B:1331:ASP:OD2	1:B:1388:ARG:NH2	2.35	0.54
1:B:955:VAL:HG22	1:B:1070:LEU:HB3	1.89	0.54
1:D:955:VAL:HG22	1:D:1070:LEU:HB3	1.89	0.54
1:C:616:ASP:OD2	1:C:636:ARG:NE	2.37	0.54
1:A:955:VAL:HG22	1:A:1070:LEU:HB3	1.89	0.54
1:D:1115:ASN:HD21	1:D:1116:LEU:HD23	1.73	0.54
1:A:774:ARG:NH1	1:A:880:ASP:OD2	2.40	0.54
1:B:807:ASN:HD22	1:B:814:GLY:HA2	1.72	0.54
1:B:1115:ASN:HD21	1:B:1116:LEU:HD23	1.73	0.54
1:C:955:VAL:HG22	1:C:1070:LEU:HB3	1.89	0.54
1:D:1331:ASP:OD2	1:D:1388:ARG:NH2	2.35	0.54
1:A:616:ASP:OD2	1:A:636:ARG:NE	2.37	0.54
1:B:722:LEU:HD11	1:B:745:ASN:HB2	1.89	0.54
1:D:511:LEU:HD11	1:D:534:TYR:HB3	1.89	0.54
1:B:511:LEU:HD11	1:B:534:TYR:HB3	1.89	0.54
1:C:774:ARG:NH1	1:C:880:ASP:OD2	2.41	0.54
1:D:722:LEU:HD11	1:D:745:ASN:HB2	1.89	0.54
1:D:807:ASN:HD22	1:D:814:GLY:HA2	1.72	0.54
1:A:685:ARG:NH1	1:A:689:GLN:OE1	2.41	0.54
1:C:685:ARG:NH1	1:C:689:GLN:OE1	2.41	0.54
1:D:952:ASP:OD1	1:D:975:HIS:ND1	2.41	0.54
1:B:952:ASP:OD1	1:B:975:HIS:ND1	2.41	0.53
1:B:774:ARG:NH1	1:B:880:ASP:OD2	2.40	0.53
1:C:671:LEU:HD22	1:C:695:VAL:HG21	1.90	0.53
1:A:671:LEU:HD22	1:A:695:VAL:HG21	1.90	0.53
1:D:1423:ARG:NH2	1:D:1478:ASP:OD1	2.35	0.53
1:B:685:ARG:NH1	1:B:689:GLN:OE1	2.41	0.53
1:D:774:ARG:NH1	1:D:880:ASP:OD2	2.40	0.53
1:D:1214:MET:HE2	1:D:1326:TYR:HB3	1.91	0.53
1:B:1214:MET:HE2	1:B:1326:TYR:HB3	1.91	0.53
1:C:1483:LEU:HD11	1:C:1524:LEU:HB3	1.90	0.53
1:A:1115:ASN:HD21	1:A:1116:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1483:LEU:HD11	1:A:1524:LEU:HB3	1.90	0.53
1:B:1423:ARG:NH2	1:B:1478:ASP:OD1	2.35	0.53
1:C:952:ASP:OD1	1:C:975:HIS:ND1	2.41	0.53
1:C:1394:ARG:HH12	1:C:1406:ARG:HH12	1.56	0.53
1:D:685:ARG:NH1	1:D:689:GLN:OE1	2.41	0.53
1:A:511:LEU:HD11	1:A:534:TYR:HB3	1.89	0.53
1:A:1394:ARG:HH12	1:A:1406:ARG:HH12	1.56	0.53
1:B:804:ALA:HA	1:B:814:GLY:HA3	1.91	0.53
1:C:556:VAL:HA	1:C:579:ILE:HG22	1.90	0.53
1:A:556:VAL:HA	1:A:579:ILE:HG22	1.90	0.53
1:B:604:ALA:O	1:B:608:ILE:HG13	2.09	0.53
1:C:511:LEU:HD11	1:C:534:TYR:HB3	1.89	0.53
1:A:952:ASP:OD1	1:A:975:HIS:ND1	2.41	0.53
1:B:1394:ARG:HH12	1:B:1406:ARG:HH12	1.56	0.53
1:C:1115:ASN:HD21	1:C:1116:LEU:HD23	1.73	0.53
1:D:604:ALA:O	1:D:608:ILE:HG13	2.09	0.53
1:A:804:ALA:HA	1:A:814:GLY:HA3	1.91	0.52
1:A:1214:MET:HE2	1:A:1326:TYR:HB3	1.91	0.52
1:B:671:LEU:HD22	1:B:695:VAL:HG21	1.90	0.52
1:C:804:ALA:HA	1:C:814:GLY:HA3	1.91	0.52
1:C:1214:MET:HE2	1:C:1326:TYR:HB3	1.91	0.52
1:D:804:ALA:HA	1:D:814:GLY:HA3	1.91	0.52
1:D:1394:ARG:HH12	1:D:1406:ARG:HH12	1.56	0.52
1:D:671:LEU:HD22	1:D:695:VAL:HG21	1.90	0.52
1:B:556:VAL:HA	1:B:579:ILE:HG22	1.90	0.52
1:B:1087:ASP:OD1	1:B:1099:ARG:NH1	2.42	0.52
1:C:1087:ASP:OD1	1:C:1099:ARG:NH1	2.42	0.52
1:D:556:VAL:HA	1:D:579:ILE:HG22	1.90	0.52
1:D:1087:ASP:OD1	1:D:1099:ARG:NH1	2.42	0.52
1:C:1331:ASP:OD2	1:C:1388:ARG:NH2	2.35	0.52
1:D:1483:LEU:HD11	1:D:1524:LEU:HB3	1.90	0.52
1:B:1483:LEU:HD11	1:B:1524:LEU:HB3	1.90	0.52
1:D:1210:VAL:HG12	1:D:1214:MET:HE3	1.92	0.52
1:A:1087:ASP:OD1	1:A:1099:ARG:NH1	2.42	0.52
1:B:1210:VAL:HG12	1:B:1214:MET:HE3	1.92	0.52
1:B:1389:TRP:NE1	1:B:1461:ASP:OD1	2.34	0.52
1:D:672:PHE:HZ	1:D:724:THR:HG21	1.74	0.52
1:B:672:PHE:HZ	1:B:724:THR:HG21	1.74	0.52
1:A:672:PHE:HZ	1:A:724:THR:HG21	1.74	0.52
1:A:723:ARG:HB2	1:A:743:LYS:HB3	1.92	0.52
1:A:1331:ASP:OD2	1:A:1388:ARG:NH2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:ARG:HH22	1:D:570:LEU:H	1.58	0.52
1:A:604:ALA:O	1:A:608:ILE:HG13	2.09	0.51
1:B:565:ARG:HH22	1:B:570:LEU:H	1.58	0.51
1:C:723:ARG:HB2	1:C:743:LYS:HB3	1.92	0.51
1:C:604:ALA:O	1:C:608:ILE:HG13	2.09	0.51
1:C:672:PHE:HZ	1:C:724:THR:HG21	1.74	0.51
1:D:1389:TRP:NE1	1:D:1461:ASP:OD1	2.34	0.51
1:A:983:ASP:OD2	2:A:1601:NAD:O2B	2.29	0.51
1:B:723:ARG:HB2	1:B:743:LYS:HB3	1.92	0.51
1:B:983:ASP:OD2	2:B:1601:NAD:O2B	2.29	0.51
1:B:1579:ARG:NH2	1:C:1512:ALA:O	2.42	0.51
1:C:983:ASP:OD2	2:C:1601:NAD:O2B	2.29	0.51
1:D:806:LYS:HE3	1:D:1144:VAL:HG21	1.93	0.51
1:D:983:ASP:OD2	2:D:1601:NAD:O2B	2.29	0.51
1:B:806:LYS:HE3	1:B:1144:VAL:HG21	1.93	0.51
1:D:723:ARG:HB2	1:D:743:LYS:HB3	1.92	0.51
1:A:806:LYS:HE3	1:A:1144:VAL:HG21	1.93	0.51
1:B:557:LEU:HD11	1:B:580:SER:HB2	1.93	0.51
1:C:806:LYS:HE3	1:C:1144:VAL:HG21	1.93	0.51
1:A:788:ARG:HH22	1:A:795:GLU:HB2	1.76	0.51
1:A:875:ARG:NH1	1:A:878:GLY:O	2.44	0.51
1:B:1421:TRP:O	1:B:1423:ARG:NH1	2.44	0.51
1:C:788:ARG:HH22	1:C:795:GLU:HB2	1.76	0.51
1:C:1421:TRP:O	1:C:1423:ARG:NH1	2.44	0.51
1:D:1421:TRP:O	1:D:1423:ARG:NH1	2.44	0.51
1:A:1421:TRP:O	1:A:1423:ARG:NH1	2.44	0.51
1:C:875:ARG:NH1	1:C:878:GLY:O	2.44	0.51
1:D:557:LEU:HD11	1:D:580:SER:HB2	1.93	0.50
1:B:518:LEU:HD23	1:B:531:LEU:HD21	1.93	0.50
1:B:875:ARG:NH1	1:B:878:GLY:O	2.44	0.50
1:D:518:LEU:HD23	1:D:531:LEU:HD21	1.93	0.50
1:D:875:ARG:NH1	1:D:878:GLY:O	2.44	0.50
1:A:1214:MET:HE1	1:A:1323:SER:HA	1.94	0.50
1:B:997:ARG:HB3	1:B:1020:LEU:HD13	1.94	0.50
1:B:1465:ILE:HD11	1:B:1522:ARG:HG3	1.94	0.50
1:C:1214:MET:HE1	1:C:1323:SER:HA	1.94	0.50
1:D:997:ARG:HB3	1:D:1020:LEU:HD13	1.94	0.50
1:D:1465:ILE:HD11	1:D:1522:ARG:HG3	1.94	0.50
1:C:1210:VAL:HG12	1:C:1214:MET:HE3	1.92	0.50
1:C:1240:ARG:NH1	1:C:1251:GLU:OE1	2.34	0.50
1:A:1210:VAL:HG12	1:A:1214:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1465:ILE:HD11	1:A:1522:ARG:HG3	1.94	0.50
1:A:539:SER:HB3	1:A:573:TRP:CE2	2.47	0.50
1:A:1240:ARG:NH1	1:A:1251:GLU:OE1	2.34	0.50
1:B:788:ARG:HH22	1:B:795:GLU:HB2	1.76	0.50
1:C:539:SER:HB3	1:C:573:TRP:CE2	2.47	0.50
1:A:959:GLY:N	1:A:982:PHE:O	2.32	0.50
1:B:1214:MET:HE1	1:B:1323:SER:HA	1.94	0.50
1:C:1038:SER:OG	1:C:1040:GLN:OE1	2.27	0.50
1:C:1465:ILE:HD11	1:C:1522:ARG:HG3	1.94	0.50
1:D:1214:MET:HE1	1:D:1323:SER:HA	1.94	0.50
1:B:539:SER:HB3	1:B:573:TRP:CE2	2.47	0.50
1:C:1081:LYS:HB2	1:C:1099:ARG:HD2	1.94	0.50
1:D:539:SER:HB3	1:D:573:TRP:CE2	2.47	0.50
1:D:788:ARG:HH22	1:D:795:GLU:HB2	1.76	0.50
1:B:1055:THR:HG23	1:B:1058:ALA:H	1.77	0.50
1:C:1349:ILE:HG23	1:C:1408:GLY:HA2	1.94	0.50
1:A:634:VAL:HG13	1:A:742:PHE:HZ	1.77	0.49
1:A:1038:SER:OG	1:A:1040:GLN:OE1	2.28	0.49
1:A:1081:LYS:HB2	1:A:1099:ARG:HD2	1.94	0.49
1:C:634:VAL:HG13	1:C:742:PHE:HZ	1.77	0.49
1:D:1055:THR:HG23	1:D:1058:ALA:H	1.77	0.49
1:A:1349:ILE:HG23	1:A:1408:GLY:HA2	1.94	0.49
1:B:533:TRP:HB3	1:B:575:TYR:HB2	1.93	0.49
1:C:557:LEU:HD11	1:C:580:SER:HB2	1.93	0.49
1:C:565:ARG:HH22	1:C:570:LEU:H	1.58	0.49
1:C:959:GLY:N	1:C:982:PHE:O	2.32	0.49
1:A:557:LEU:HD11	1:A:580:SER:HB2	1.93	0.49
1:A:784:ARG:HE	1:A:889:LYS:HG2	1.77	0.49
1:C:518:LEU:HD23	1:C:531:LEU:HD21	1.93	0.49
1:D:784:ARG:HE	1:D:889:LYS:HG2	1.77	0.49
1:D:1349:ILE:HG23	1:D:1408:GLY:HA2	1.94	0.49
1:A:533:TRP:HB3	1:A:575:TYR:HB2	1.93	0.49
1:B:1349:ILE:HG23	1:B:1408:GLY:HA2	1.94	0.49
1:C:784:ARG:HE	1:C:889:LYS:HG2	1.77	0.49
1:D:533:TRP:HB3	1:D:575:TYR:HB2	1.93	0.49
1:A:518:LEU:HD23	1:A:531:LEU:HD21	1.93	0.49
1:A:565:ARG:HH22	1:A:570:LEU:H	1.58	0.49
1:B:784:ARG:HE	1:B:889:LYS:HG2	1.77	0.49
1:C:789:ARG:HG3	1:C:820:VAL:HG21	1.94	0.49
1:D:1081:LYS:HB2	1:D:1099:ARG:HD2	1.94	0.49
1:A:789:ARG:HG3	1:A:820:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:TRP:HB3	1:C:575:TYR:HB2	1.93	0.49
1:C:997:ARG:HB3	1:C:1020:LEU:HD13	1.94	0.49
1:A:997:ARG:HB3	1:A:1020:LEU:HD13	1.94	0.49
1:B:1081:LYS:HB2	1:B:1099:ARG:HD2	1.94	0.49
1:D:1282:LEU:HD13	1:D:1308:ILE:HG13	1.94	0.49
1:A:1055:THR:HG23	1:A:1058:ALA:H	1.77	0.49
1:D:983:ASP:CG	1:D:984:HIS:N	2.71	0.49
1:B:1282:LEU:HD13	1:B:1308:ILE:HG13	1.95	0.49
1:B:522:ASP:OD1	1:B:522:ASP:N	2.46	0.49
1:B:983:ASP:CG	1:B:984:HIS:N	2.71	0.49
1:B:1067:PRO:HG3	1:B:1106:ARG:HE	1.78	0.49
1:C:806:LYS:HA	1:C:1137:ALA:HB1	1.94	0.49
1:C:1055:THR:HG23	1:C:1058:ALA:H	1.77	0.49
1:D:522:ASP:OD1	1:D:522:ASP:N	2.45	0.49
1:B:554:VAL:HG21	1:B:579:ILE:HD12	1.95	0.48
1:B:1087:ASP:O	1:B:1093:ARG:NH2	2.39	0.48
1:A:806:LYS:HA	1:A:1137:ALA:HB1	1.95	0.48
1:A:994:ASP:OD2	1:A:997:ARG:NE	2.46	0.48
1:A:1474:ASP:OD1	1:A:1475:GLU:N	2.46	0.48
1:B:983:ASP:OD1	2:B:1601:NAD:O2B	2.32	0.48
1:C:994:ASP:OD2	1:C:997:ARG:NE	2.46	0.48
1:C:1474:ASP:OD1	1:C:1475:GLU:N	2.46	0.48
1:D:554:VAL:HG21	1:D:579:ILE:HD12	1.95	0.48
1:D:1087:ASP:O	1:D:1093:ARG:NH2	2.39	0.48
1:D:1115:ASN:ND2	1:D:1116:LEU:HD23	2.28	0.48
1:A:1282:LEU:HD13	1:A:1308:ILE:HG13	1.95	0.48
1:B:702:LEU:HD13	1:B:708:ASP:HA	1.96	0.48
1:C:554:VAL:HG21	1:C:579:ILE:HD12	1.95	0.48
1:C:1067:PRO:HG3	1:C:1106:ARG:HE	1.78	0.48
1:C:1282:LEU:HD13	1:C:1308:ILE:HG13	1.94	0.48
1:D:983:ASP:OD1	2:D:1601:NAD:O2B	2.32	0.48
1:D:1067:PRO:HG3	1:D:1106:ARG:HE	1.79	0.48
1:A:554:VAL:HG21	1:A:579:ILE:HD12	1.95	0.48
1:A:631:GLN:HB3	1:A:669:ILE:HD12	1.95	0.48
1:A:1067:PRO:HG3	1:A:1106:ARG:HE	1.78	0.48
1:B:1115:ASN:ND2	1:B:1116:LEU:HD23	2.28	0.48
1:B:1512:ALA:HB1	1:C:1579:ARG:HE	1.77	0.48
1:C:631:GLN:HB3	1:C:669:ILE:HD12	1.95	0.48
1:D:702:LEU:HD13	1:D:708:ASP:HA	1.96	0.48
1:A:1115:ASN:ND2	1:A:1116:LEU:HD23	2.28	0.48
1:B:992:ASN:O	1:B:1022:SER:OG	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:922:ASP:OD1	1:D:922:ASP:N	2.42	0.48
1:D:992:ASN:O	1:D:1022:SER:OG	2.32	0.48
1:B:806:LYS:HA	1:B:1137:ALA:HB1	1.94	0.48
1:D:789:ARG:HG3	1:D:820:VAL:HG21	1.94	0.48
1:A:983:ASP:OD1	2:A:1601:NAD:H1B	2.14	0.48
1:B:630:GLN:HB3	1:B:726:TYR:HE1	1.79	0.48
1:B:789:ARG:HG3	1:B:820:VAL:HG21	1.94	0.48
1:B:983:ASP:OD1	2:B:1601:NAD:H1B	2.14	0.48
1:C:983:ASP:CG	1:C:984:HIS:N	2.71	0.48
1:C:983:ASP:OD1	2:C:1601:NAD:H1B	2.14	0.48
1:C:1332:VAL:HG11	1:C:1391:LEU:HD23	1.96	0.48
1:D:983:ASP:OD1	2:D:1601:NAD:H1B	2.14	0.48
1:A:1038:SER:HB3	1:A:1041:VAL:HG23	1.96	0.48
1:B:634:VAL:HG13	1:B:742:PHE:HZ	1.77	0.48
1:B:922:ASP:OD1	1:B:922:ASP:N	2.42	0.48
1:C:1038:SER:HB3	1:C:1041:VAL:HG23	1.96	0.48
1:C:1115:ASN:ND2	1:C:1116:LEU:HD23	2.28	0.48
1:D:634:VAL:HG13	1:D:742:PHE:HZ	1.77	0.48
1:D:806:LYS:HA	1:D:1137:ALA:HB1	1.95	0.48
1:A:922:ASP:OD1	1:A:922:ASP:N	2.42	0.48
1:A:1332:VAL:HG11	1:A:1391:LEU:HD23	1.96	0.48
1:B:1203:ASN:OD1	1:B:1206:SER:OG	2.32	0.48
1:D:630:GLN:HB3	1:D:726:TYR:HE1	1.79	0.48
1:A:983:ASP:CG	1:A:984:HIS:N	2.71	0.47
1:D:1203:ASN:OD1	1:D:1206:SER:OG	2.32	0.47
1:D:1586:ARG:HG3	1:D:1587:THR:HG23	1.96	0.47
1:B:1038:SER:HB3	1:B:1041:VAL:HG23	1.96	0.47
1:B:1586:ARG:HG3	1:B:1587:THR:HG23	1.96	0.47
1:C:922:ASP:OD1	1:C:922:ASP:N	2.42	0.47
1:D:959:GLY:N	1:D:982:PHE:O	2.32	0.47
1:D:631:GLN:HB3	1:D:669:ILE:HD12	1.95	0.47
1:D:1038:SER:HB3	1:D:1041:VAL:HG23	1.96	0.47
1:B:631:GLN:HB3	1:B:669:ILE:HD12	1.95	0.47
1:B:769:GLU:HB2	1:B:822:LYS:NZ	2.30	0.47
1:C:702:LEU:HD13	1:C:708:ASP:HA	1.95	0.47
1:A:702:LEU:HD13	1:A:708:ASP:HA	1.95	0.47
1:C:630:GLN:HB3	1:C:726:TYR:HE1	1.79	0.47
1:D:649:TYR:HE2	1:D:709:ARG:HD3	1.79	0.47
1:A:630:GLN:HB3	1:A:726:TYR:HE1	1.79	0.47
1:A:769:GLU:HB2	1:A:822:LYS:NZ	2.30	0.47
1:A:983:ASP:OD1	2:A:1601:NAD:O2B	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:ASN:OD1	1:A:1206:SER:OG	2.32	0.47
1:B:649:TYR:HE2	1:B:709:ARG:HD3	1.80	0.47
1:B:959:GLY:N	1:B:982:PHE:O	2.32	0.47
1:C:769:GLU:HB2	1:C:822:LYS:NZ	2.30	0.47
1:C:1203:ASN:OD1	1:C:1206:SER:OG	2.32	0.47
1:C:1389:TRP:NE1	1:C:1461:ASP:OD1	2.34	0.47
1:D:769:GLU:HB2	1:D:822:LYS:NZ	2.30	0.47
1:A:1389:TRP:NE1	1:A:1461:ASP:OD1	2.34	0.47
1:C:983:ASP:OD1	2:C:1601:NAD:O2B	2.32	0.47
1:D:1332:VAL:HG11	1:D:1391:LEU:HD23	1.96	0.47
1:B:1332:VAL:HG11	1:B:1391:LEU:HD23	1.96	0.47
1:A:1108:LYS:HG2	1:A:1109:VAL:HG23	1.98	0.46
1:A:1275:GLN:HG3	1:A:1277:VAL:HG12	1.98	0.46
1:B:657:VAL:HG13	1:B:707:THR:HG23	1.97	0.46
1:C:1275:GLN:HG3	1:C:1277:VAL:HG12	1.98	0.46
1:D:657:VAL:HG13	1:D:707:THR:HG23	1.97	0.46
1:D:1474:ASP:OD1	1:D:1475:GLU:N	2.46	0.46
1:B:994:ASP:OD2	1:B:997:ARG:NE	2.46	0.46
1:B:1474:ASP:OD1	1:B:1475:GLU:N	2.46	0.46
1:C:1108:LYS:HG2	1:C:1109:VAL:HG23	1.98	0.46
1:D:994:ASP:OD2	1:D:997:ARG:NE	2.46	0.46
1:B:1115:ASN:C	1:B:1115:ASN:ND2	2.70	0.46
1:B:1240:ARG:NH1	1:B:1251:GLU:OE1	2.34	0.46
1:D:730:ARG:HB2	1:D:733:SER:HB3	1.96	0.46
1:D:811:VAL:HG21	1:D:1307:ILE:HG12	1.97	0.46
1:D:1275:GLN:HG3	1:D:1277:VAL:HG12	1.97	0.46
1:A:1384:ASP:HB3	1:A:1388:ARG:HH12	1.80	0.46
1:A:1586:ARG:HG3	1:A:1587:THR:HG23	1.96	0.46
1:B:730:ARG:HB2	1:B:733:SER:HB3	1.96	0.46
1:B:811:VAL:HG21	1:B:1307:ILE:HG12	1.97	0.46
1:C:1384:ASP:HB3	1:C:1388:ARG:HH12	1.80	0.46
1:C:1586:ARG:HG3	1:C:1587:THR:HG23	1.96	0.46
1:A:649:TYR:HE2	1:A:709:ARG:HD3	1.79	0.46
1:B:1275:GLN:HG3	1:B:1277:VAL:HG12	1.98	0.46
1:C:1403:GLU:OE1	1:C:1406:ARG:NH1	2.49	0.46
1:D:1240:ARG:NH1	1:D:1251:GLU:OE1	2.34	0.46
1:D:1281:ARG:HH11	1:D:1312:LEU:HD23	1.80	0.46
1:A:1403:GLU:OE1	1:A:1406:ARG:NH1	2.49	0.46
1:B:1281:ARG:HH11	1:B:1312:LEU:HD23	1.80	0.46
1:C:992:ASN:O	1:C:1022:SER:OG	2.32	0.46
1:D:1115:ASN:C	1:D:1115:ASN:ND2	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:ASN:OD1	1:A:741:ALA:N	2.42	0.46
1:B:705:LEU:HD23	1:B:705:LEU:H	1.81	0.46
1:B:1275:GLN:HB3	1:B:1278:PHE:HD2	1.81	0.46
1:C:649:TYR:HE2	1:C:709:ARG:HD3	1.79	0.46
1:C:730:ARG:HB2	1:C:733:SER:HB3	1.96	0.46
1:C:1079:TYR:OH	2:C:1601:NAD:N1A	2.49	0.46
1:D:1275:GLN:HB3	1:D:1278:PHE:HD2	1.81	0.46
1:A:730:ARG:HB2	1:A:733:SER:HB3	1.97	0.46
1:A:939:ARG:HE	1:A:1198:GLY:HA3	1.81	0.46
1:A:992:ASN:O	1:A:1022:SER:OG	2.32	0.46
1:A:1079:TYR:OH	2:A:1601:NAD:N1A	2.49	0.46
1:C:1275:GLN:HB3	1:C:1278:PHE:HD2	1.81	0.46
1:D:705:LEU:HD23	1:D:705:LEU:H	1.81	0.46
1:D:939:ARG:HE	1:D:1198:GLY:HA3	1.81	0.46
1:A:1275:GLN:HB3	1:A:1278:PHE:HD2	1.81	0.45
1:B:939:ARG:HE	1:B:1198:GLY:HA3	1.81	0.45
1:C:1281:ARG:HH11	1:C:1312:LEU:HD23	1.80	0.45
1:A:811:VAL:HG21	1:A:1307:ILE:HG12	1.97	0.45
1:A:1281:ARG:HH11	1:A:1312:LEU:HD23	1.80	0.45
1:A:1462:VAL:HG11	1:A:1477:ALA:HB2	1.99	0.45
1:A:1533:GLU:O	1:A:1541:LYS:NZ	2.50	0.45
1:C:811:VAL:HG21	1:C:1307:ILE:HG12	1.97	0.45
1:C:939:ARG:HE	1:C:1198:GLY:HA3	1.82	0.45
1:C:983:ASP:CG	2:C:1601:NAD:HO2A	2.24	0.45
1:C:1533:GLU:O	1:C:1541:LYS:NZ	2.50	0.45
1:D:1073:ASN:O	1:D:1114:GLY:N	2.48	0.45
1:B:1038:SER:OG	1:B:1040:GLN:OE1	2.27	0.45
1:B:1078:THR:OG1	1:B:1116:LEU:O	2.32	0.45
1:B:1462:VAL:HG11	1:B:1477:ALA:HB2	1.99	0.45
1:C:1115:ASN:C	1:C:1115:ASN:ND2	2.70	0.45
1:C:1462:VAL:HG11	1:C:1477:ALA:HB2	1.99	0.45
1:D:1384:ASP:HB3	1:D:1388:ARG:HH12	1.80	0.45
1:D:1462:VAL:HG11	1:D:1477:ALA:HB2	1.99	0.45
1:A:1180:ASP:OD1	1:A:1180:ASP:N	2.50	0.45
1:B:1384:ASP:HB3	1:B:1388:ARG:HH12	1.80	0.45
1:C:725:ASN:OD1	1:C:741:ALA:N	2.42	0.45
1:C:1180:ASP:OD1	1:C:1180:ASP:N	2.50	0.45
1:A:686:ARG:NH1	1:A:688:ALA:HA	2.31	0.45
1:B:1108:LYS:HG2	1:B:1109:VAL:HG23	1.98	0.45
1:C:686:ARG:NH1	1:C:688:ALA:HA	2.31	0.45
1:C:1345:ALA:HB2	1:C:1400:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1108:LYS:HG2	1:D:1109:VAL:HG23	1.98	0.45
1:A:657:VAL:HG13	1:A:707:THR:HG23	1.97	0.45
1:A:1115:ASN:C	1:A:1115:ASN:ND2	2.70	0.45
1:A:1345:ALA:HB2	1:A:1400:VAL:HG13	1.99	0.45
1:D:1038:SER:OG	1:D:1040:GLN:OE1	2.27	0.45
1:B:1180:ASP:OD1	1:B:1180:ASP:N	2.50	0.45
1:D:1180:ASP:OD1	1:D:1180:ASP:N	2.50	0.45
1:B:1399:ALA:O	1:B:1403:GLU:HG2	2.17	0.45
1:C:518:LEU:HB3	1:C:531:LEU:HD11	1.99	0.45
1:C:657:VAL:HG13	1:C:707:THR:HG23	1.97	0.45
1:C:705:LEU:HD23	1:C:705:LEU:H	1.81	0.45
1:D:1079:TYR:OH	2:D:1601:NAD:N1A	2.49	0.45
1:A:705:LEU:H	1:A:705:LEU:HD23	1.81	0.45
1:A:1073:ASN:O	1:A:1114:GLY:N	2.48	0.45
1:B:617:ARG:NH1	1:B:656:SER:OG	2.50	0.45
1:B:1079:TYR:OH	2:B:1601:NAD:N1A	2.49	0.45
1:B:1264:LYS:HG3	1:B:1313:VAL:HG21	1.99	0.45
1:C:1073:ASN:O	1:C:1114:GLY:N	2.48	0.45
1:D:617:ARG:NH1	1:D:656:SER:OG	2.50	0.45
1:D:957:GLY:HA3	1:D:966:PHE:HE2	1.82	0.45
1:D:1264:LYS:HG3	1:D:1313:VAL:HG21	1.99	0.45
1:D:1399:ALA:O	1:D:1403:GLU:HG2	2.17	0.45
1:A:1092:ASP:HB3	1:A:1099:ARG:HH21	1.82	0.44
1:A:1219:VAL:HG22	1:A:1224:LEU:HB3	1.99	0.44
1:B:686:ARG:NH1	1:B:688:ALA:HA	2.31	0.44
1:B:1073:ASN:O	1:B:1114:GLY:N	2.48	0.44
1:B:1345:ALA:HB2	1:B:1400:VAL:HG13	1.99	0.44
1:D:686:ARG:NH1	1:D:688:ALA:HA	2.31	0.44
1:D:1232:PRO:HG2	1:D:1247:LEU:HD22	1.98	0.44
1:A:774:ARG:NH2	1:A:777:PHE:O	2.50	0.44
1:A:1399:ALA:O	1:A:1403:GLU:HG2	2.17	0.44
1:B:723:ARG:HD2	1:B:743:LYS:HD3	1.99	0.44
1:B:957:GLY:HA3	1:B:966:PHE:HE2	1.82	0.44
1:B:1219:VAL:HG22	1:B:1224:LEU:HB3	1.99	0.44
1:C:723:ARG:HD2	1:C:743:LYS:HD3	1.99	0.44
1:C:1092:ASP:HB3	1:C:1099:ARG:HH21	1.82	0.44
1:C:1219:VAL:HG22	1:C:1224:LEU:HB3	2.00	0.44
1:C:1399:ALA:O	1:C:1403:GLU:HG2	2.17	0.44
1:D:1345:ALA:HB2	1:D:1400:VAL:HG13	1.99	0.44
1:A:518:LEU:HB3	1:A:531:LEU:HD11	1.99	0.44
1:A:617:ARG:NH1	1:A:656:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:ARG:HD2	1:A:743:LYS:HD3	1.99	0.44
1:B:934:TRP:CD1	1:B:972:LEU:HD22	2.53	0.44
1:B:1232:PRO:HG2	1:B:1247:LEU:HD22	1.98	0.44
1:C:617:ARG:NH1	1:C:656:SER:OG	2.50	0.44
1:C:774:ARG:NH2	1:C:777:PHE:O	2.50	0.44
1:C:1226:ARG:NH2	1:C:1232:PRO:O	2.48	0.44
1:D:527:ARG:HH21	1:D:587:HIS:CE1	2.35	0.44
1:D:723:ARG:HD2	1:D:743:LYS:HD3	1.99	0.44
1:D:1219:VAL:HG22	1:D:1224:LEU:HB3	2.00	0.44
1:A:1226:ARG:NH2	1:A:1232:PRO:O	2.48	0.44
1:A:1232:PRO:HG2	1:A:1247:LEU:HD22	1.98	0.44
1:C:527:ARG:HH21	1:C:587:HIS:CE1	2.35	0.44
1:D:934:TRP:CD1	1:D:972:LEU:HD22	2.53	0.44
1:A:565:ARG:NE	1:A:566:ARG:O	2.45	0.44
1:B:527:ARG:HH21	1:B:587:HIS:CE1	2.35	0.44
1:B:774:ARG:NH2	1:B:777:PHE:O	2.50	0.44
1:C:621:LEU:HD13	1:C:665:THR:HG21	2.00	0.44
1:C:1232:PRO:HG2	1:C:1247:LEU:HD22	1.98	0.44
1:D:725:ASN:OD1	1:D:741:ALA:N	2.42	0.44
1:D:774:ARG:NH2	1:D:777:PHE:O	2.50	0.44
1:D:1403:GLU:OE1	1:D:1406:ARG:NH1	2.49	0.44
1:A:527:ARG:HH21	1:A:587:HIS:CE1	2.35	0.44
1:A:621:LEU:HD13	1:A:665:THR:HG21	2.00	0.44
1:B:1403:GLU:OE1	1:B:1406:ARG:NH1	2.49	0.44
1:C:565:ARG:NE	1:C:566:ARG:O	2.45	0.44
1:D:977:ARG:NH2	1:D:992:ASN:OD1	2.51	0.44
1:B:977:ARG:NH2	1:B:992:ASN:OD1	2.51	0.44
1:D:1283:PRO:HG3	1:D:1299:ARG:HH12	1.83	0.44
1:B:725:ASN:OD1	1:B:741:ALA:N	2.42	0.44
1:B:1283:PRO:HG3	1:B:1299:ARG:HH12	1.83	0.44
1:A:934:TRP:CD1	1:A:972:LEU:HD22	2.53	0.43
1:A:1283:PRO:HG3	1:A:1299:ARG:HH12	1.83	0.43
1:B:983:ASP:CG	2:B:1601:NAD:O2B	2.61	0.43
1:B:1037:ILE:HG23	1:B:1042:ARG:HH11	1.83	0.43
1:C:934:TRP:CD1	1:C:972:LEU:HD22	2.53	0.43
1:D:983:ASP:CG	2:D:1601:NAD:O2B	2.61	0.43
1:D:1037:ILE:HG23	1:D:1042:ARG:HH11	1.83	0.43
1:A:1264:LYS:HG3	1:A:1313:VAL:HG21	1.99	0.43
1:B:1092:ASP:HB3	1:B:1099:ARG:HH21	1.82	0.43
1:C:957:GLY:HA3	1:C:966:PHE:HE2	1.82	0.43
1:C:1264:LYS:HG3	1:C:1313:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1283:PRO:HG3	1:C:1299:ARG:HH12	1.84	0.43
1:D:1092:ASP:HB3	1:D:1099:ARG:HH21	1.82	0.43
1:A:957:GLY:HA3	1:A:966:PHE:HE2	1.82	0.43
1:D:685:ARG:NH1	1:D:686:ARG:O	2.52	0.43
1:A:983:ASP:CG	2:A:1601:NAD:O2B	2.61	0.43
1:B:621:LEU:HD13	1:B:665:THR:HG21	2.00	0.43
1:B:685:ARG:NH1	1:B:686:ARG:O	2.52	0.43
1:C:522:ASP:OD1	1:C:522:ASP:N	2.46	0.43
1:C:983:ASP:CG	2:C:1601:NAD:O2B	2.61	0.43
1:D:621:LEU:HD13	1:D:665:THR:HG21	2.00	0.43
1:D:1294:LEU:HB3	1:D:1297:GLU:HB2	2.01	0.43
1:B:687:ASP:OD1	1:B:687:ASP:N	2.51	0.43
1:B:983:ASP:OD1	2:B:1601:NAD:C1B	2.67	0.43
1:B:1533:GLU:O	1:B:1541:LYS:NZ	2.50	0.43
1:D:563:THR:HB	1:D:573:TRP:CE3	2.53	0.43
1:A:522:ASP:OD1	1:A:522:ASP:N	2.46	0.43
1:A:1078:THR:OG1	1:A:1116:LEU:O	2.32	0.43
1:B:1294:LEU:HB3	1:B:1297:GLU:HB2	2.01	0.43
1:C:1078:THR:OG1	1:C:1116:LEU:O	2.32	0.43
1:D:983:ASP:OD1	2:D:1601:NAD:C1B	2.67	0.43
1:A:977:ARG:NH2	1:A:992:ASN:OD1	2.51	0.43
1:D:640:LYS:NZ	1:D:651:GLN:OE1	2.51	0.43
1:D:1533:GLU:O	1:D:1541:LYS:NZ	2.50	0.43
1:A:563:THR:HB	1:A:573:TRP:CE3	2.53	0.43
1:A:784:ARG:HA	1:A:888:ASP:CG	2.44	0.43
1:A:1384:ASP:HB3	1:A:1388:ARG:NH1	2.34	0.43
1:B:518:LEU:HB3	1:B:531:LEU:HD11	1.99	0.43
1:B:563:THR:HB	1:B:573:TRP:CE3	2.53	0.43
1:B:640:LYS:NZ	1:B:651:GLN:OE1	2.51	0.43
1:C:784:ARG:HA	1:C:888:ASP:CG	2.44	0.43
1:C:977:ARG:NH2	1:C:992:ASN:OD1	2.51	0.43
1:D:518:LEU:HB3	1:D:531:LEU:HD11	1.99	0.43
1:A:685:ARG:NH1	1:A:686:ARG:O	2.52	0.42
1:C:563:THR:HB	1:C:573:TRP:CE3	2.53	0.42
1:C:685:ARG:NH1	1:C:686:ARG:O	2.52	0.42
1:C:1384:ASP:HB3	1:C:1388:ARG:NH1	2.34	0.42
1:A:1562:GLU:HA	1:A:1565:LYS:HE3	2.02	0.42
1:C:1562:GLU:HA	1:C:1565:LYS:HE3	2.02	0.42
1:A:983:ASP:OD1	2:A:1601:NAD:C1B	2.67	0.42
1:A:1294:LEU:HB3	1:A:1297:GLU:HB2	2.01	0.42
1:C:983:ASP:OD1	2:C:1601:NAD:C1B	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1294:LEU:HB3	1:C:1297:GLU:HB2	2.01	0.42
1:A:931:LYS:O	1:A:935:GLU:HG2	2.20	0.42
1:C:931:LYS:O	1:C:935:GLU:HG2	2.20	0.42
1:D:1465:ILE:O	1:D:1469:VAL:HG12	2.20	0.42
1:B:1465:ILE:O	1:B:1469:VAL:HG12	2.20	0.42
1:D:565:ARG:NE	1:D:566:ARG:O	2.45	0.42
1:D:1384:ASP:HB3	1:D:1388:ARG:NH1	2.34	0.42
1:B:784:ARG:HA	1:B:888:ASP:CG	2.44	0.42
1:B:1210:VAL:HG22	1:B:1213:ARG:HH21	1.85	0.42
1:B:1384:ASP:HB3	1:B:1388:ARG:NH1	2.34	0.42
1:C:1465:ILE:O	1:C:1469:VAL:HG12	2.20	0.42
1:D:1210:VAL:HG22	1:D:1213:ARG:HH21	1.85	0.42
1:A:960:ASP:HB2	1:A:983:ASP:CG	2.37	0.42
1:A:1037:ILE:HG23	1:A:1042:ARG:HH11	1.83	0.42
1:A:1465:ILE:O	1:A:1469:VAL:HG12	2.20	0.42
1:C:1037:ILE:HG23	1:C:1042:ARG:HH11	1.83	0.42
1:D:784:ARG:HA	1:D:888:ASP:CG	2.44	0.42
1:A:565:ARG:HH21	1:A:566:ARG:C	2.28	0.42
1:B:565:ARG:NE	1:B:566:ARG:O	2.45	0.42
1:B:1226:ARG:NH2	1:B:1232:PRO:O	2.48	0.42
1:C:679:SER:O	1:C:682:THR:OG1	2.31	0.42
1:C:1087:ASP:O	1:C:1093:ARG:NH2	2.39	0.42
1:A:687:ASP:OD1	1:A:687:ASP:N	2.51	0.42
1:A:1087:ASP:O	1:A:1093:ARG:NH2	2.39	0.42
1:B:788:ARG:HH12	1:B:795:GLU:HB2	1.85	0.42
1:B:891:THR:HB	1:B:894:PHE:HB2	2.02	0.42
1:C:565:ARG:HH21	1:C:566:ARG:C	2.28	0.42
1:D:891:THR:HB	1:D:894:PHE:HB2	2.02	0.42
1:D:1226:ARG:NH2	1:D:1232:PRO:O	2.48	0.42
1:A:679:SER:O	1:A:682:THR:OG1	2.31	0.41
1:A:1210:VAL:HG22	1:A:1213:ARG:HH21	1.85	0.41
1:B:931:LYS:O	1:B:935:GLU:HG2	2.20	0.41
1:D:931:LYS:O	1:D:935:GLU:HG2	2.20	0.41
1:B:877:ASP:OD1	1:B:877:ASP:N	2.53	0.41
1:B:1562:GLU:HA	1:B:1565:LYS:HE3	2.02	0.41
1:C:687:ASP:OD1	1:C:687:ASP:N	2.51	0.41
1:C:960:ASP:HB2	1:C:983:ASP:CG	2.37	0.41
1:D:788:ARG:HH12	1:D:795:GLU:HB2	1.86	0.41
1:D:877:ASP:OD1	1:D:877:ASP:N	2.53	0.41
1:D:1562:GLU:HA	1:D:1565:LYS:HE3	2.02	0.41
1:C:1210:VAL:HG22	1:C:1213:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:960:ASP:N	2:D:1601:NAD:O3B	2.53	0.41
1:A:1417:ARG:NE	1:A:1420:GLU:OE1	2.53	0.41
1:B:960:ASP:N	2:B:1601:NAD:O3B	2.53	0.41
1:C:1114:GLY:O	1:C:1140:ASN:ND2	2.54	0.41
1:C:1417:ARG:NE	1:C:1420:GLU:OE1	2.53	0.41
1:A:754:LEU:HD13	1:A:756:ARG:HG2	2.03	0.41
1:A:781:GLY:HA3	1:A:815:ALA:O	2.21	0.41
1:B:1069:ASP:HA	1:B:1108:LYS:HB3	2.02	0.41
1:B:1124:ILE:HG23	1:B:1248:THR:HG21	2.03	0.41
1:D:1069:ASP:HA	1:D:1108:LYS:HB3	2.02	0.41
1:A:782:GLY:O	1:A:816:LYS:NZ	2.54	0.41
1:A:1512:ALA:HB1	1:D:1579:ARG:HE	1.86	0.41
1:C:754:LEU:HD13	1:C:756:ARG:HG2	2.03	0.41
1:C:781:GLY:HA3	1:C:815:ALA:O	2.21	0.41
1:C:782:GLY:O	1:C:816:LYS:NZ	2.54	0.41
1:A:556:VAL:O	1:B:541:SER:OG	2.35	0.41
1:A:877:ASP:N	1:A:877:ASP:OD1	2.53	0.41
1:A:1114:GLY:O	1:A:1140:ASN:ND2	2.54	0.41
1:B:1114:GLY:O	1:B:1140:ASN:ND2	2.54	0.41
1:B:1203:ASN:HB2	1:B:1377:LEU:HD11	2.03	0.41
1:B:1388:ARG:O	1:B:1392:ASN:ND2	2.39	0.41
1:B:1501:ARG:HG2	1:B:1510:ARG:HD3	2.02	0.41
1:D:687:ASP:N	1:D:687:ASP:OD1	2.51	0.41
1:D:1114:GLY:O	1:D:1140:ASN:ND2	2.54	0.41
1:D:1124:ILE:HG23	1:D:1248:THR:HG21	2.03	0.41
1:A:788:ARG:HH12	1:A:795:GLU:HB2	1.85	0.41
1:B:621:LEU:HA	1:B:624:ARG:HB2	2.03	0.41
1:C:877:ASP:OD1	1:C:877:ASP:N	2.53	0.41
1:D:553:GLY:O	1:D:582:HIS:ND1	2.54	0.41
1:D:621:LEU:HA	1:D:624:ARG:HB2	2.03	0.41
1:D:1501:ARG:HG2	1:D:1510:ARG:HD3	2.02	0.41
1:B:553:GLY:O	1:B:582:HIS:ND1	2.54	0.40
1:C:621:LEU:HA	1:C:624:ARG:HB2	2.03	0.40
1:C:788:ARG:HH12	1:C:795:GLU:HB2	1.85	0.40
1:D:1203:ASN:HB2	1:D:1377:LEU:HD11	2.03	0.40
1:A:621:LEU:HA	1:A:624:ARG:HB2	2.03	0.40
1:C:1069:ASP:HA	1:C:1108:LYS:HB3	2.02	0.40
1:D:1539:GLU:HA	1:D:1542:ILE:HB	2.02	0.40
1:A:1069:ASP:HA	1:A:1108:LYS:HB3	2.02	0.40
1:B:560:ARG:HD3	1:B:560:ARG:HA	1.92	0.40
1:B:565:ARG:HH21	1:B:566:ARG:C	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1388:ARG:O	1:D:1392:ASN:ND2	2.39	0.40
1:A:891:THR:HB	1:A:894:PHE:HB2	2.02	0.40
1:A:1124:ILE:HG23	1:A:1248:THR:HG21	2.03	0.40
1:B:754:LEU:HD13	1:B:756:ARG:HG2	2.03	0.40
1:B:1208:LEU:HD13	1:B:1246:GLY:HA2	2.03	0.40
1:C:784:ARG:O	1:C:818:GLY:HA2	2.22	0.40
1:C:891:THR:HB	1:C:894:PHE:HB2	2.02	0.40
1:C:1124:ILE:HG23	1:C:1248:THR:HG21	2.03	0.40
1:C:1502:ASP:OD1	1:C:1502:ASP:N	2.53	0.40
1:D:1208:LEU:HD13	1:D:1246:GLY:HA2	2.03	0.40
1:A:541:SER:OG	1:B:556:VAL:O	2.33	0.40
1:A:558:GLU:OE2	1:B:561:PRO:HG3	2.22	0.40
1:A:669:ILE:HD13	1:A:669:ILE:HA	1.97	0.40
1:A:784:ARG:O	1:A:818:GLY:HA2	2.22	0.40
1:A:1502:ASP:OD1	1:A:1502:ASP:N	2.53	0.40
1:B:1539:GLU:HA	1:B:1542:ILE:HB	2.03	0.40
1:D:754:LEU:HD13	1:D:756:ARG:HG2	2.03	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	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
1	B	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
1	C	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
1	D	1071/1611 (66%)	1041 (97%)	30 (3%)	0	100	100
All	All	4284/6444 (66%)	4164 (97%)	120 (3%)	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	877/1294 (68%)	876 (100%)	1 (0%)	88	89
1	B	877/1294 (68%)	876 (100%)	1 (0%)	88	89
1	C	877/1294 (68%)	876 (100%)	1 (0%)	88	89
1	D	877/1294 (68%)	876 (100%)	1 (0%)	88	89
All	All	3508/5176 (68%)	3504 (100%)	4 (0%)	87	89

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1051	VAL
1	B	1051	VAL
1	C	1051	VAL
1	D	1051	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	631	GLN
1	A	644	GLN
1	A	680	GLN
1	A	745	ASN
1	A	803	GLN
1	A	807	ASN
1	A	1073	ASN
1	A	1115	ASN
1	A	1190	ASN
1	A	1295	HIS
1	A	1449	HIS
1	A	1456	GLN
1	B	644	GLN
1	B	680	GLN
1	B	803	GLN

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Mol	Chain	Res	Type
1	B	807	ASN
1	B	1073	ASN
1	B	1115	ASN
1	B	1190	ASN
1	B	1295	HIS
1	B	1449	HIS
1	B	1456	GLN
1	C	644	GLN
1	C	680	GLN
1	C	803	GLN
1	C	807	ASN
1	C	1073	ASN
1	C	1115	ASN
1	C	1190	ASN
1	C	1295	HIS
1	C	1449	HIS
1	C	1456	GLN
1	D	644	GLN
1	D	680	GLN
1	D	803	GLN
1	D	807	ASN
1	D	1073	ASN
1	D	1115	ASN
1	D	1190	ASN
1	D	1295	HIS
1	D	1449	HIS
1	D	1456	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

4 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
2	NAD	B	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.58	0
2	NAD	C	1601	-	46,48,48	0.63	1 (2%)	64,73,73	0.59	1 (1%)
2	NAD	A	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.58	0
2	NAD	D	1601	-	46,48,48	0.64	1 (2%)	64,73,73	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAD	B	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	C	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	A	1601	-	-	1/30/62/62	0/5/5/5
2	NAD	D	1601	-	-	1/30/62/62	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	NAD	C2N-N1N	2.84	1.38	1.35
2	B	1601	NAD	C2N-N1N	2.84	1.38	1.35
2	D	1601	NAD	C2N-N1N	2.80	1.38	1.35
2	C	1601	NAD	C2N-N1N	2.77	1.38	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1601	NAD	C6N-N1N-C2N	-2.04	120.14	121.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

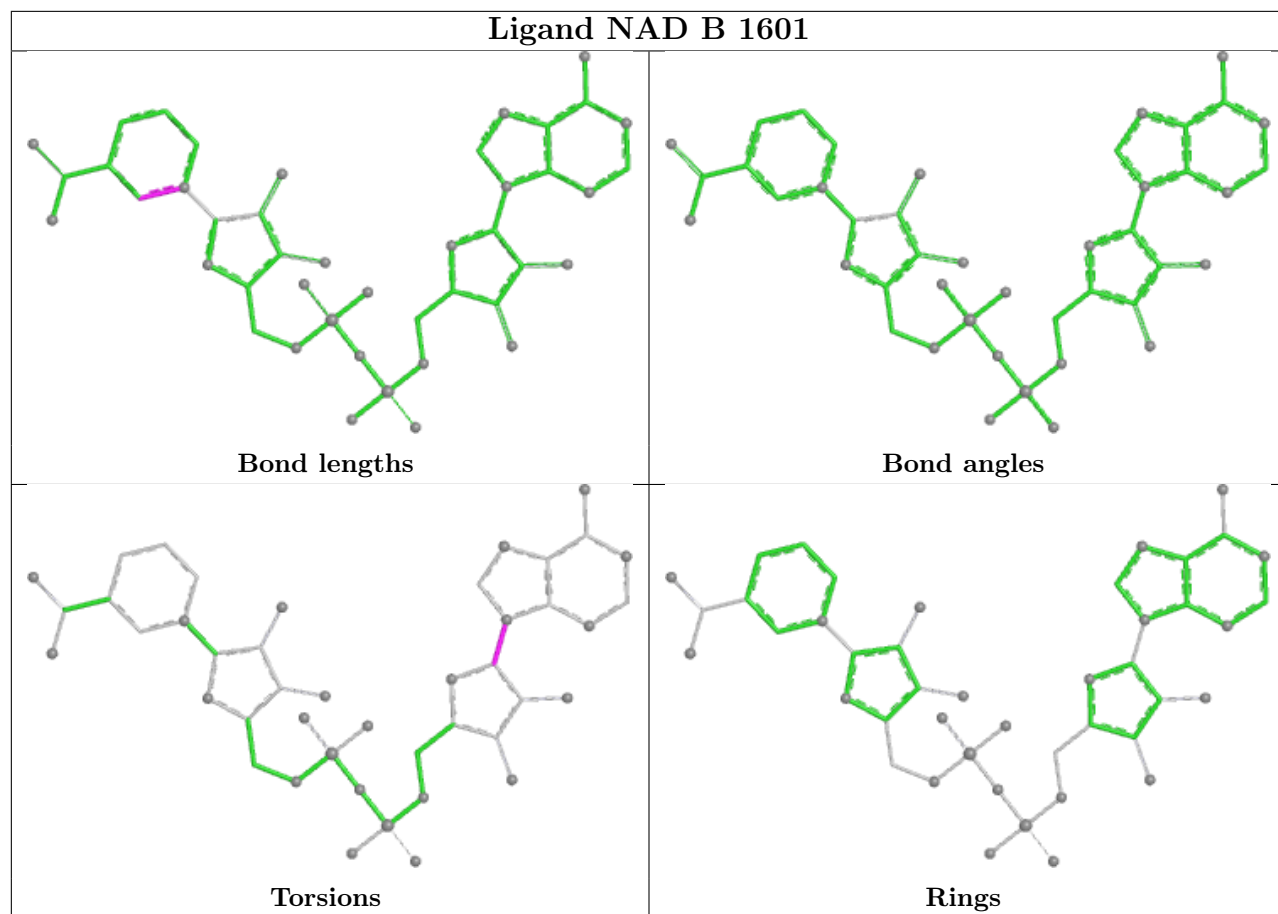
Mol	Chain	Res	Type	Atoms
2	A	1601	NAD	C2B-C1B-N9A-C8A
2	B	1601	NAD	C2B-C1B-N9A-C8A
2	C	1601	NAD	C2B-C1B-N9A-C8A
2	D	1601	NAD	C2B-C1B-N9A-C8A

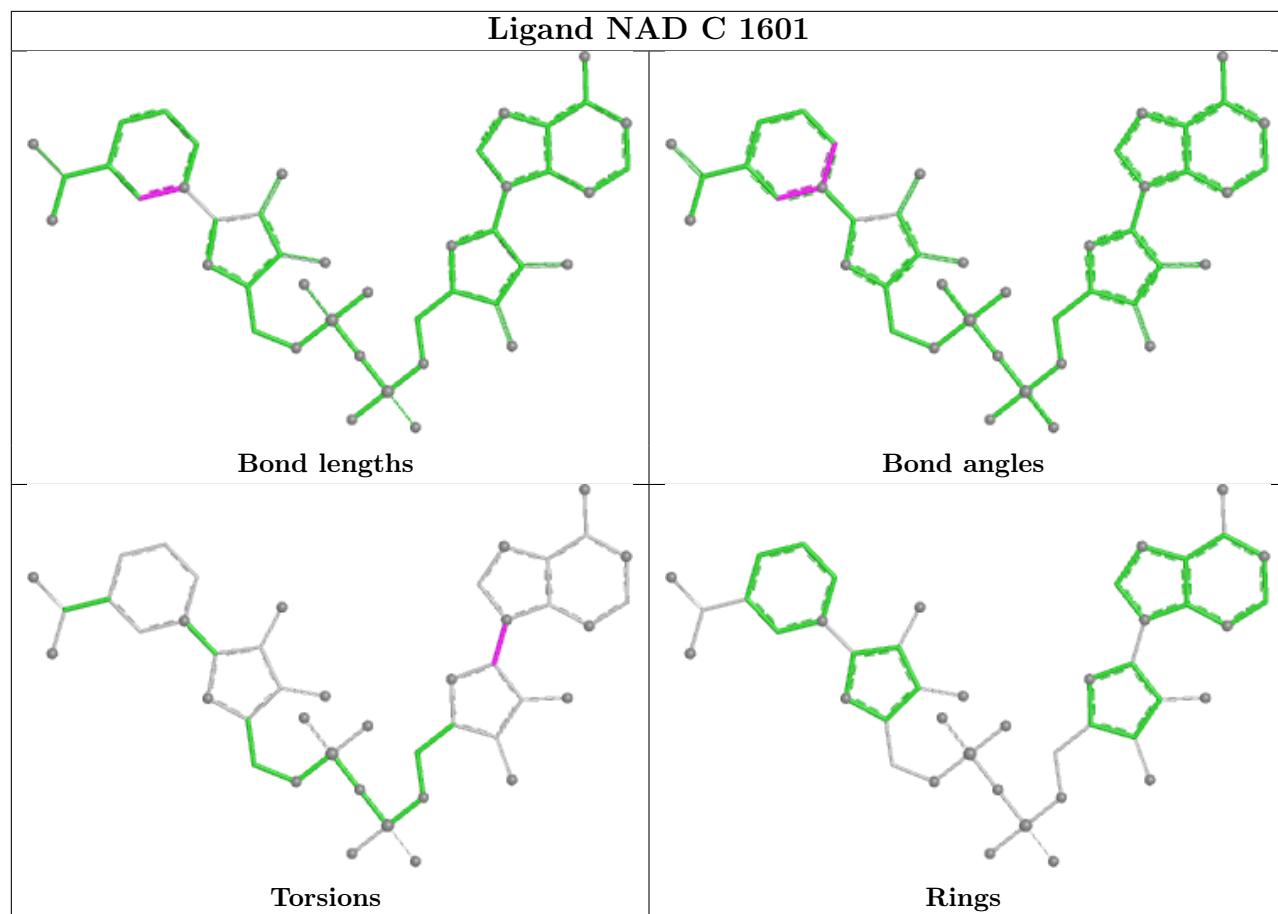
There are no ring outliers.

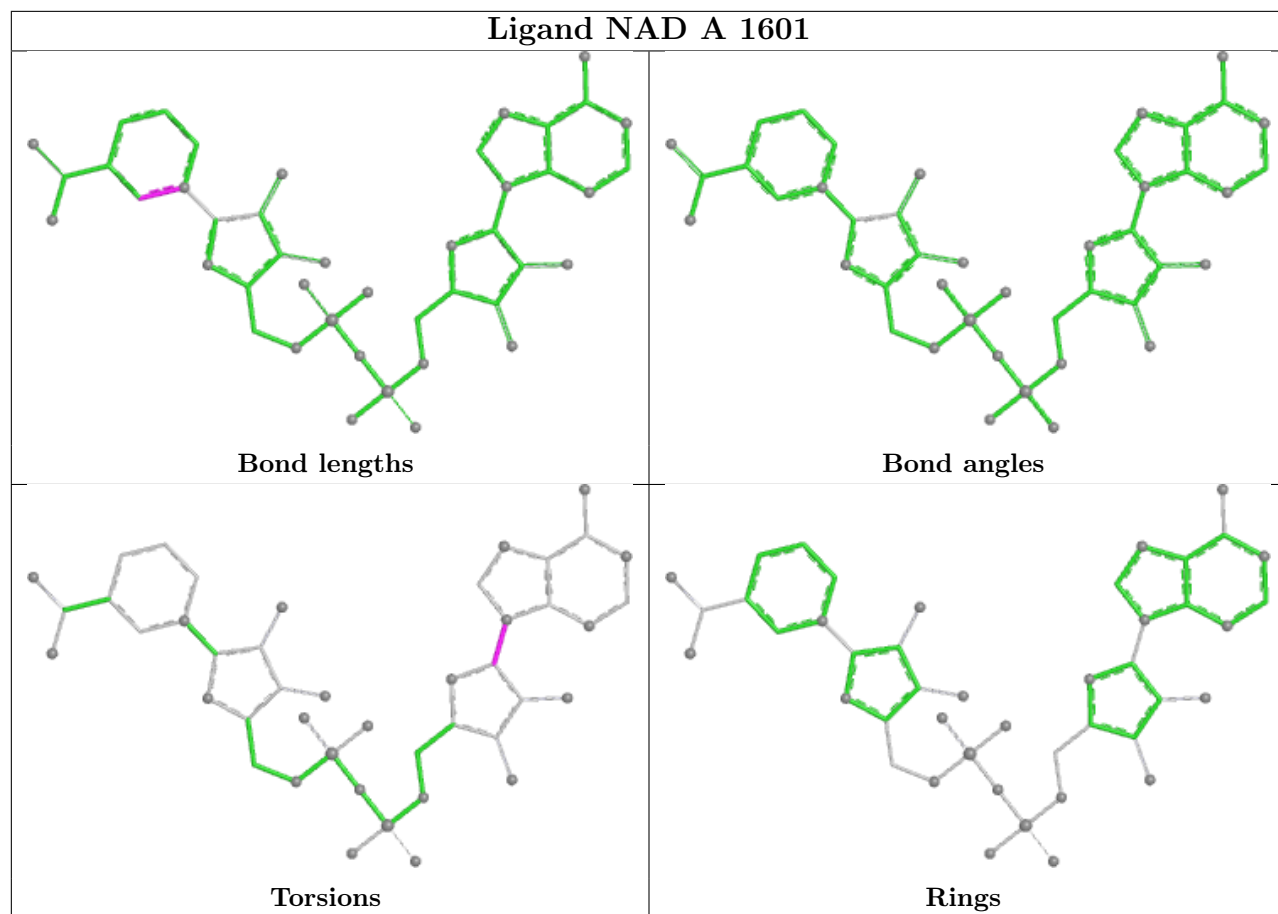
4 monomers are involved in 27 short contacts:

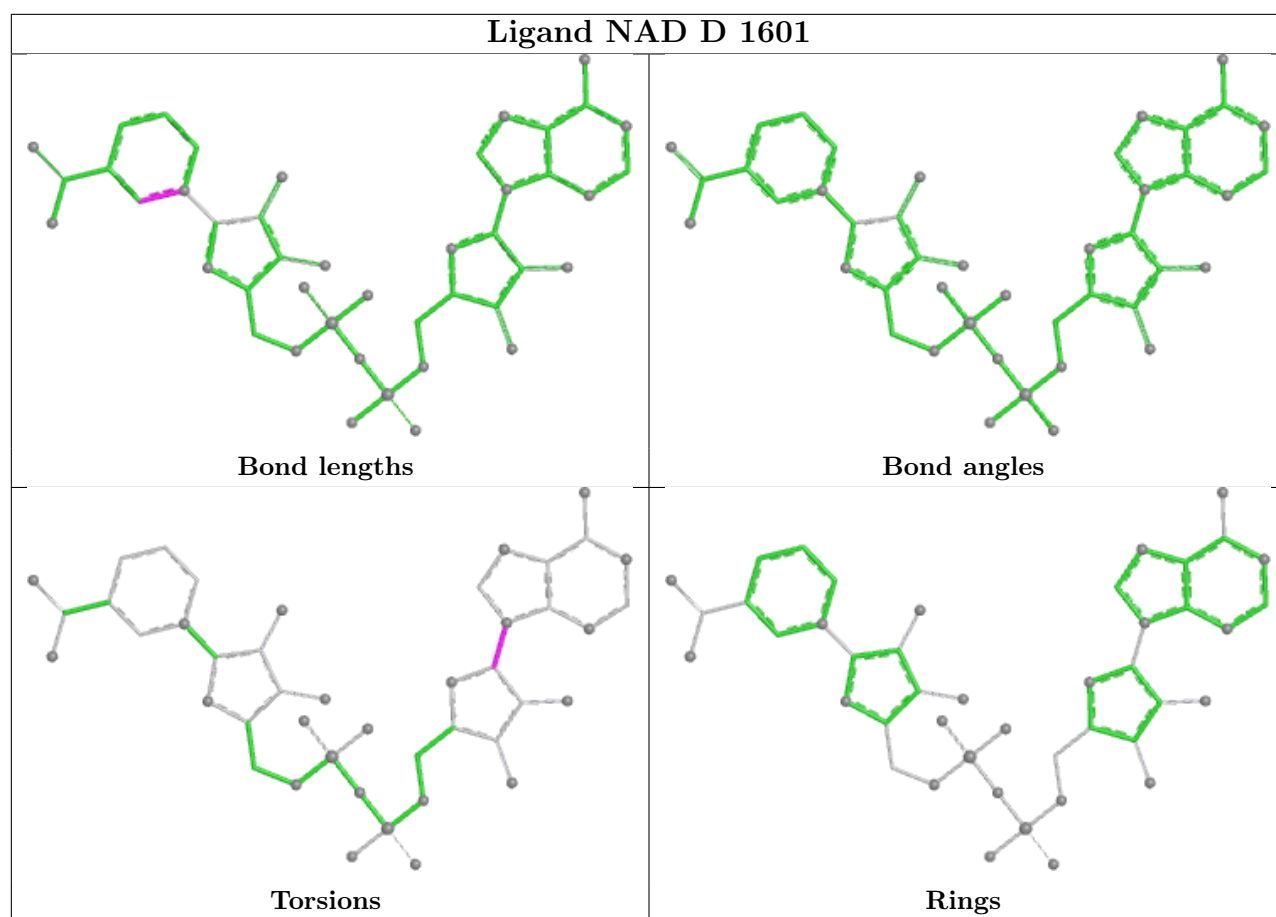
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1601	NAD	7	0
2	C	1601	NAD	7	0
2	A	1601	NAD	6	0
2	D	1601	NAD	7	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

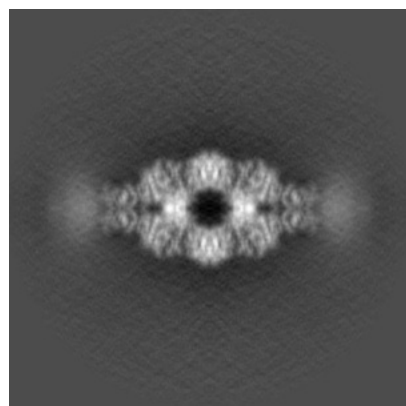
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52419. These allow visual inspection of the internal detail of the map and identification of artifacts.

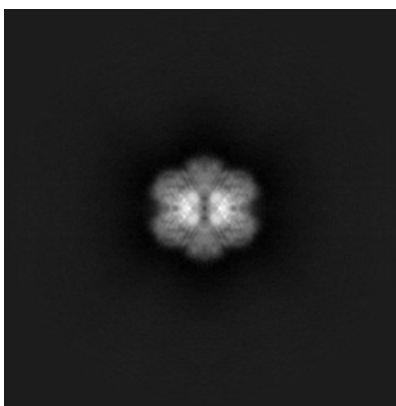
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

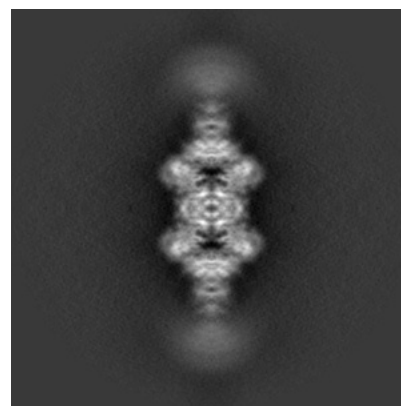
6.1.1 Primary map



X

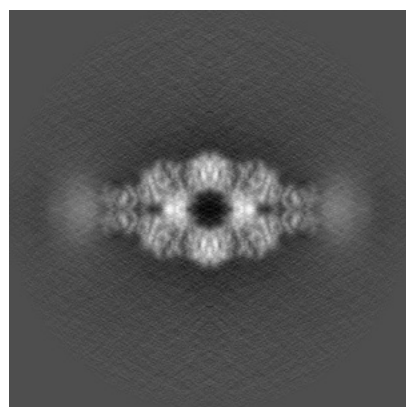


Y

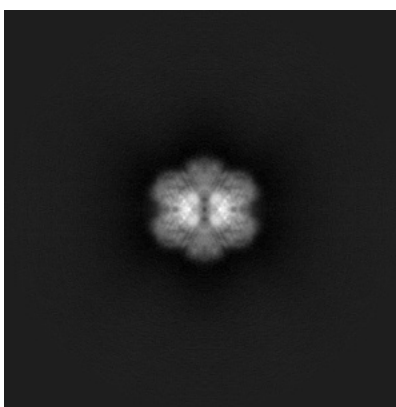


Z

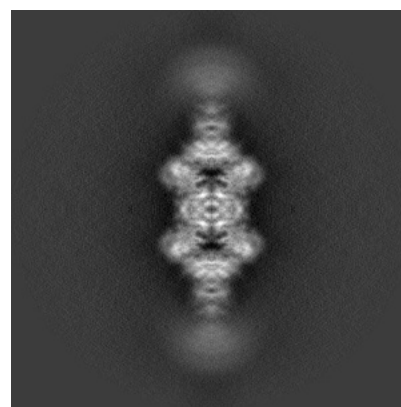
6.1.2 Raw map



X



Y

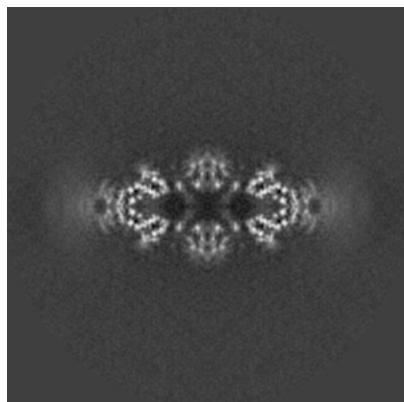


Z

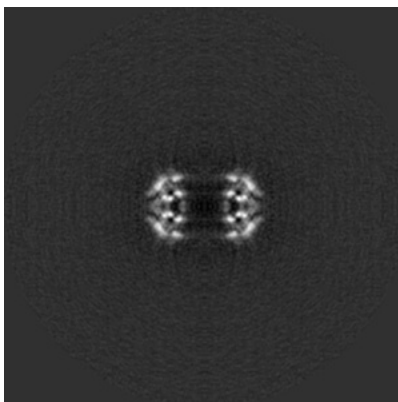
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

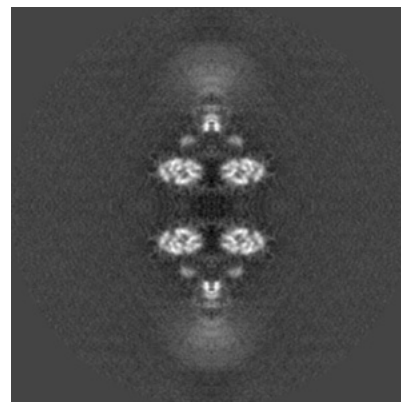
6.2.1 Primary map



X Index: 170

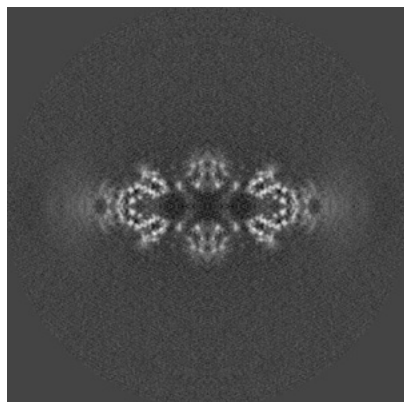


Y Index: 170

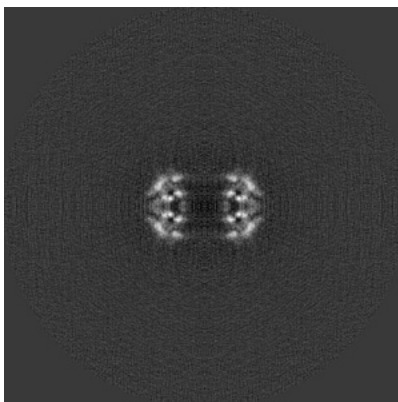


Z Index: 170

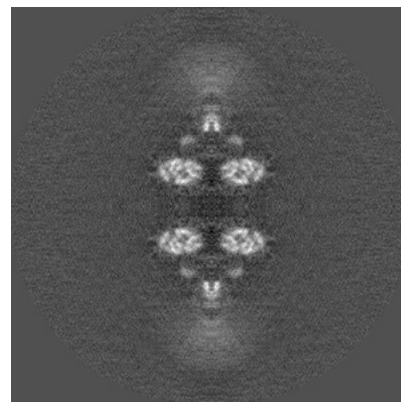
6.2.2 Raw map



X Index: 170



Y Index: 170

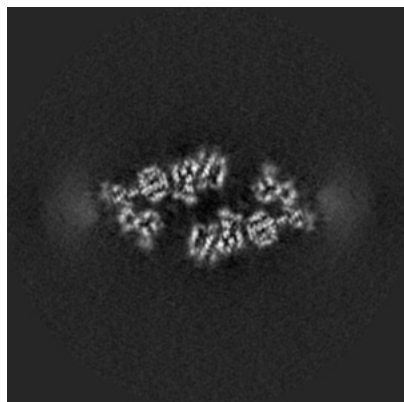


Z Index: 170

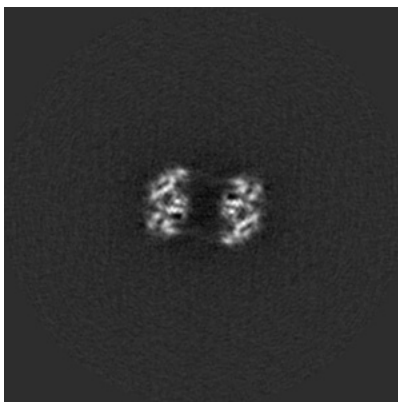
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

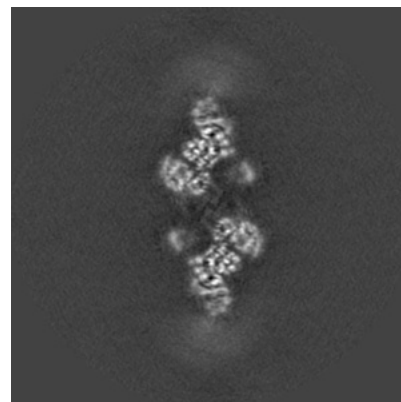
6.3.1 Primary map



X Index: 163

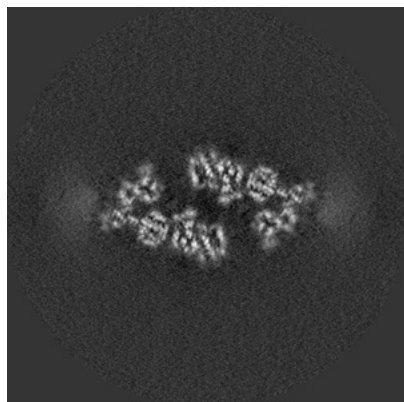


Y Index: 165

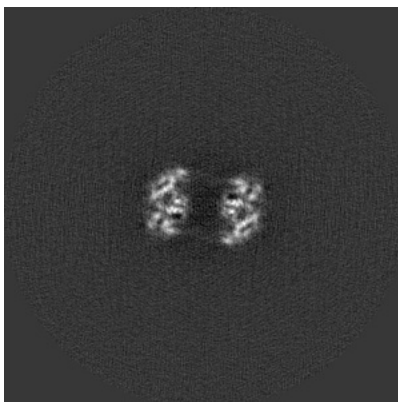


Z Index: 158

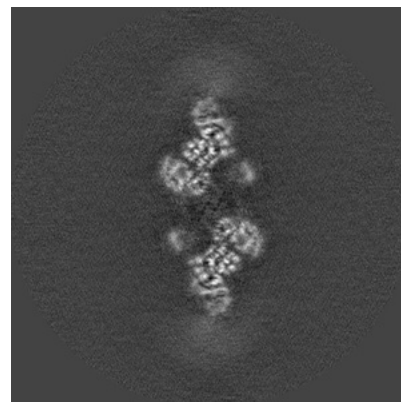
6.3.2 Raw map



X Index: 177



Y Index: 165

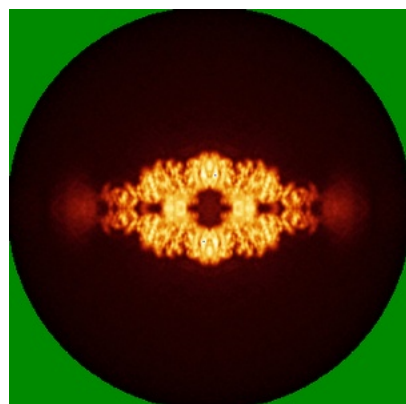


Z Index: 158

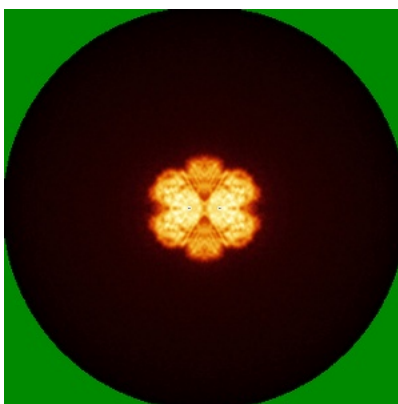
The images above show the largest variance slices of the map in three orthogonal directions.

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

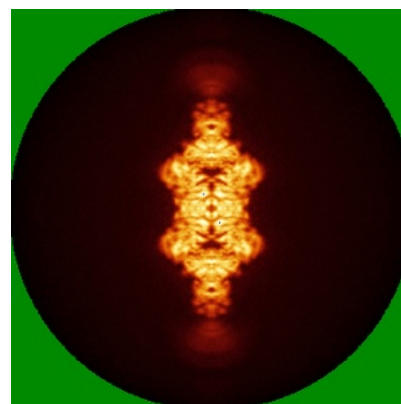
6.4.1 Primary map



X

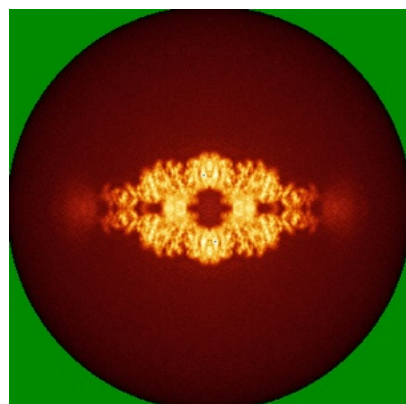


Y

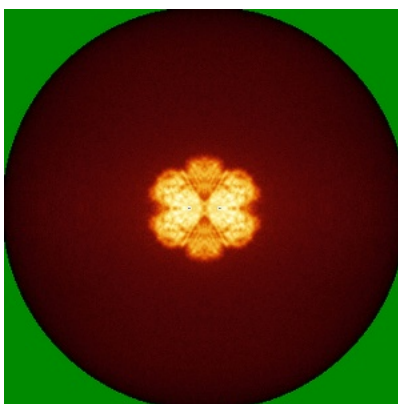


Z

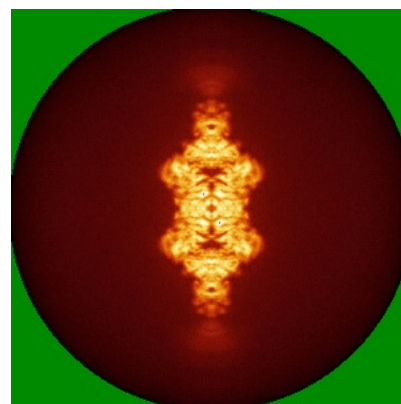
6.4.2 Raw map



X



Y

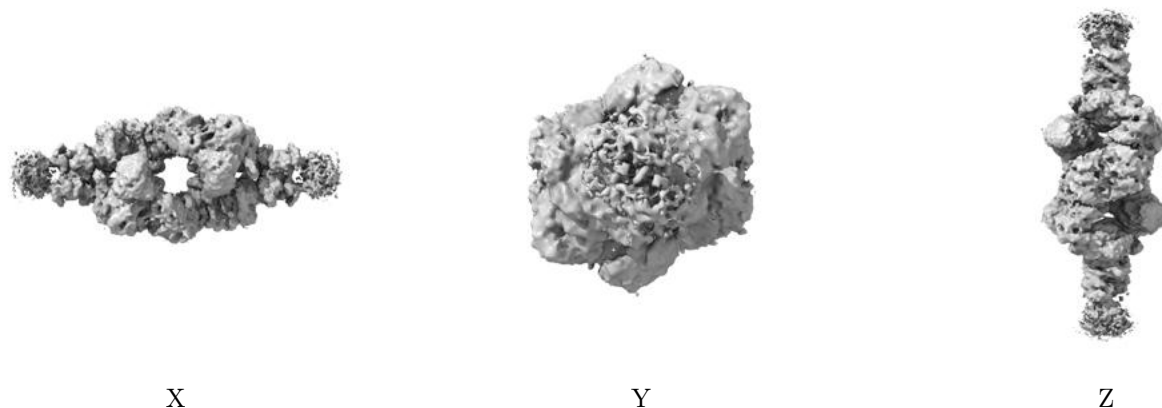


Z

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.

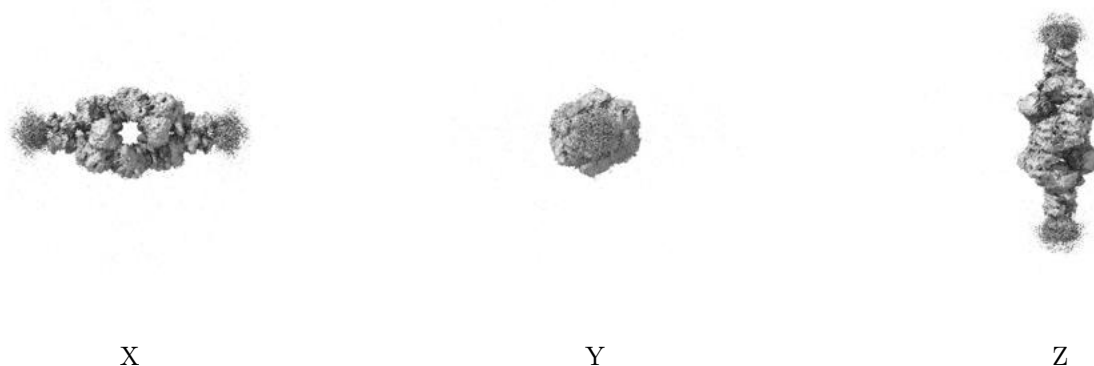
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

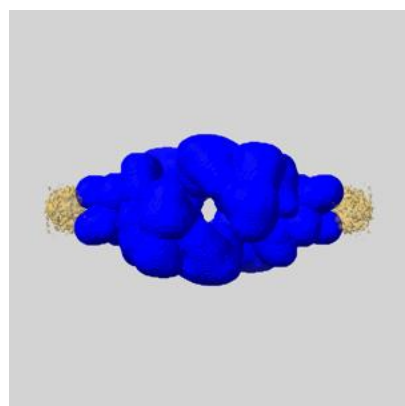
6.6 Mask visualisation [i](#)

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

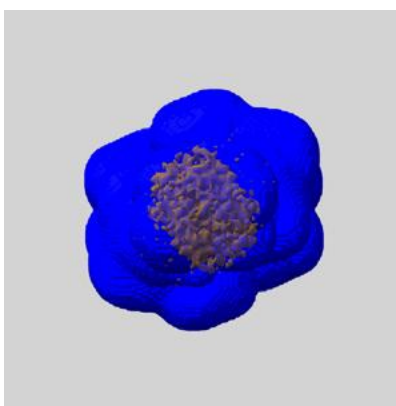
A mask typically either:

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

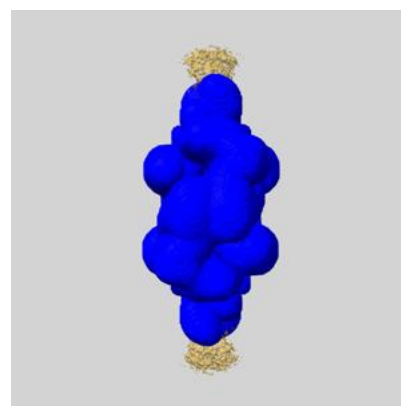
6.6.1 emd_52419_msk_1.map [i](#)



X



Y

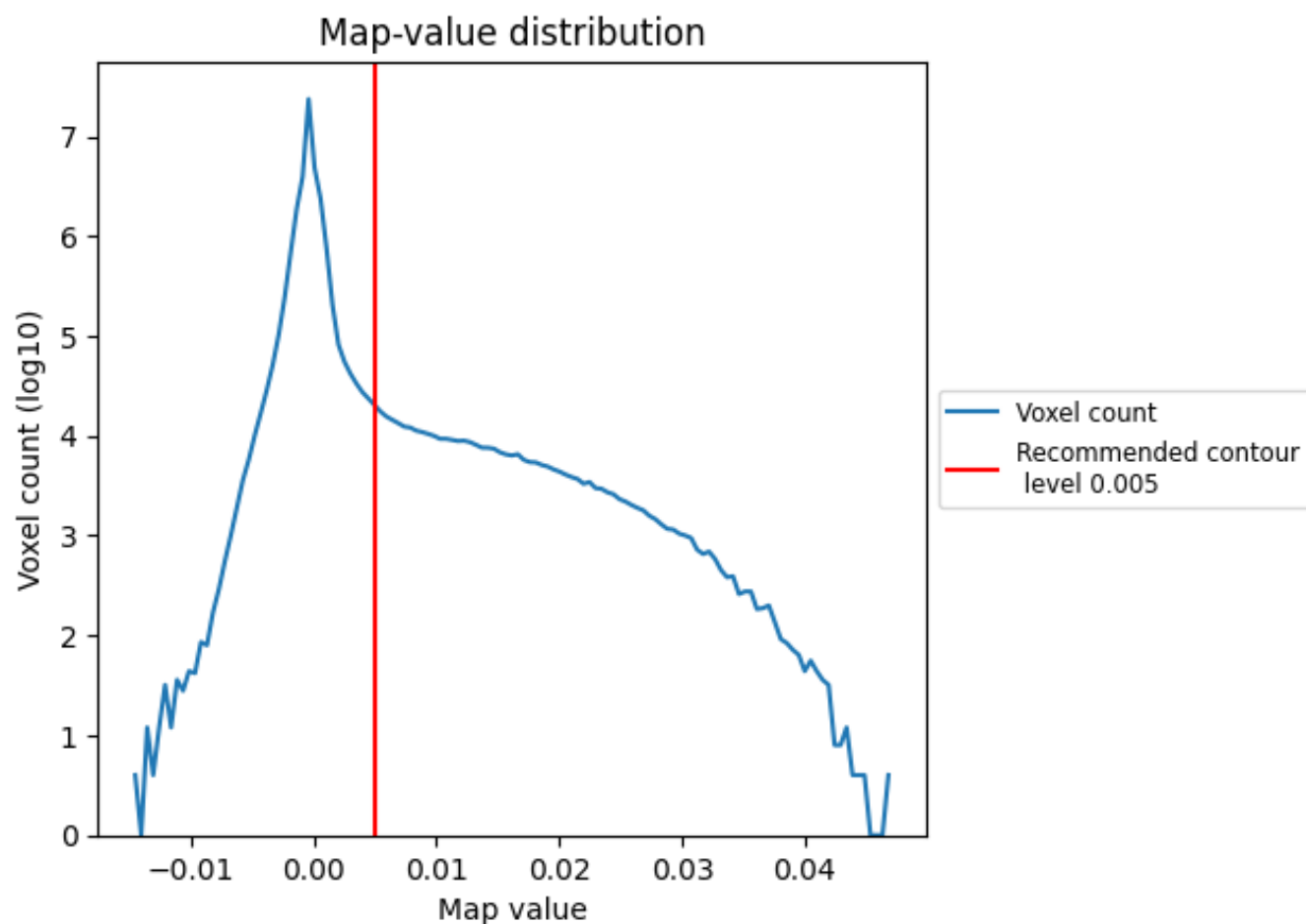


Z

7 Map analysis [i](#)

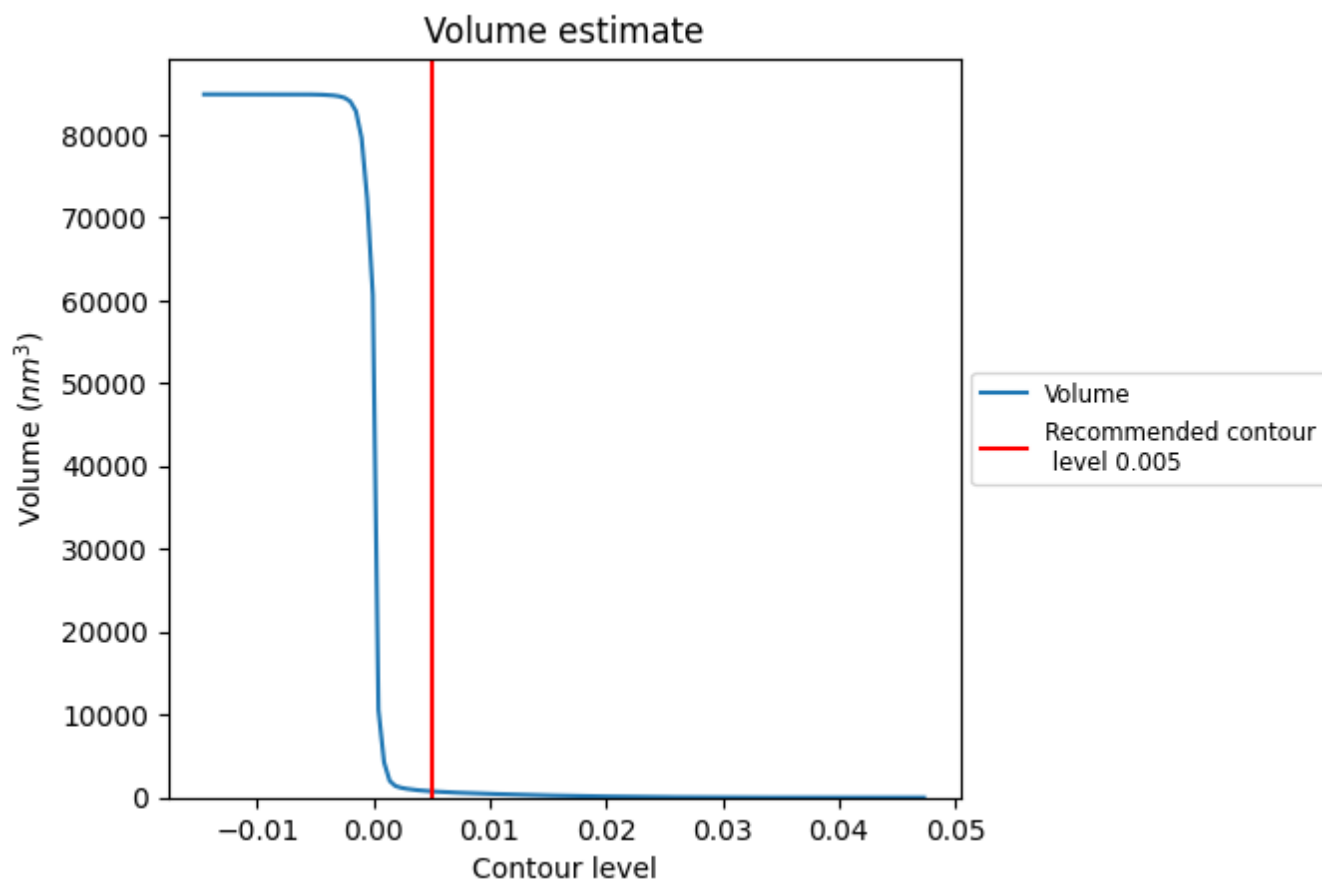
This section contains the results of statistical analysis of the map.

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.

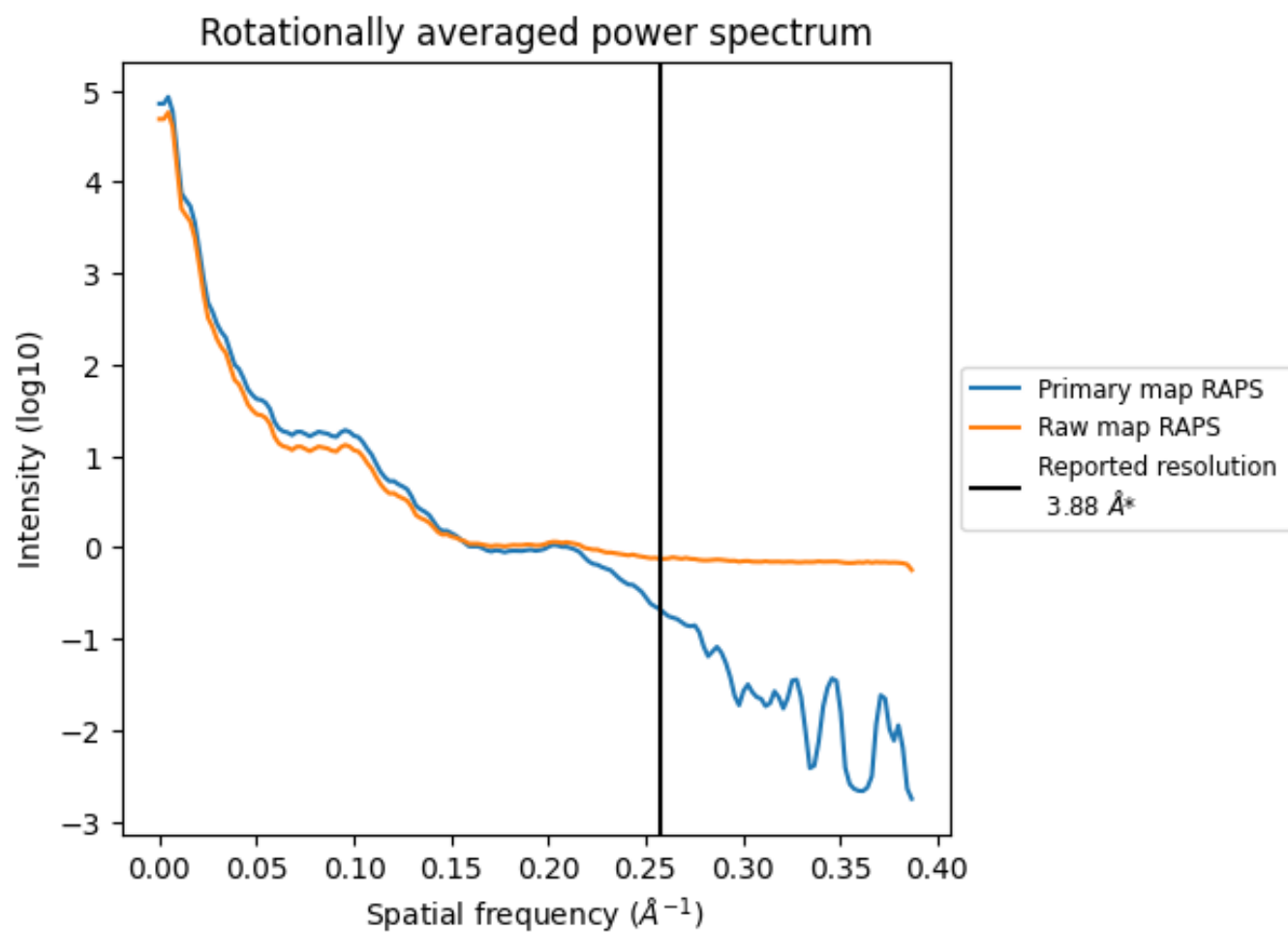
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 751 nm^3 ; this corresponds to an approximate mass of 679 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

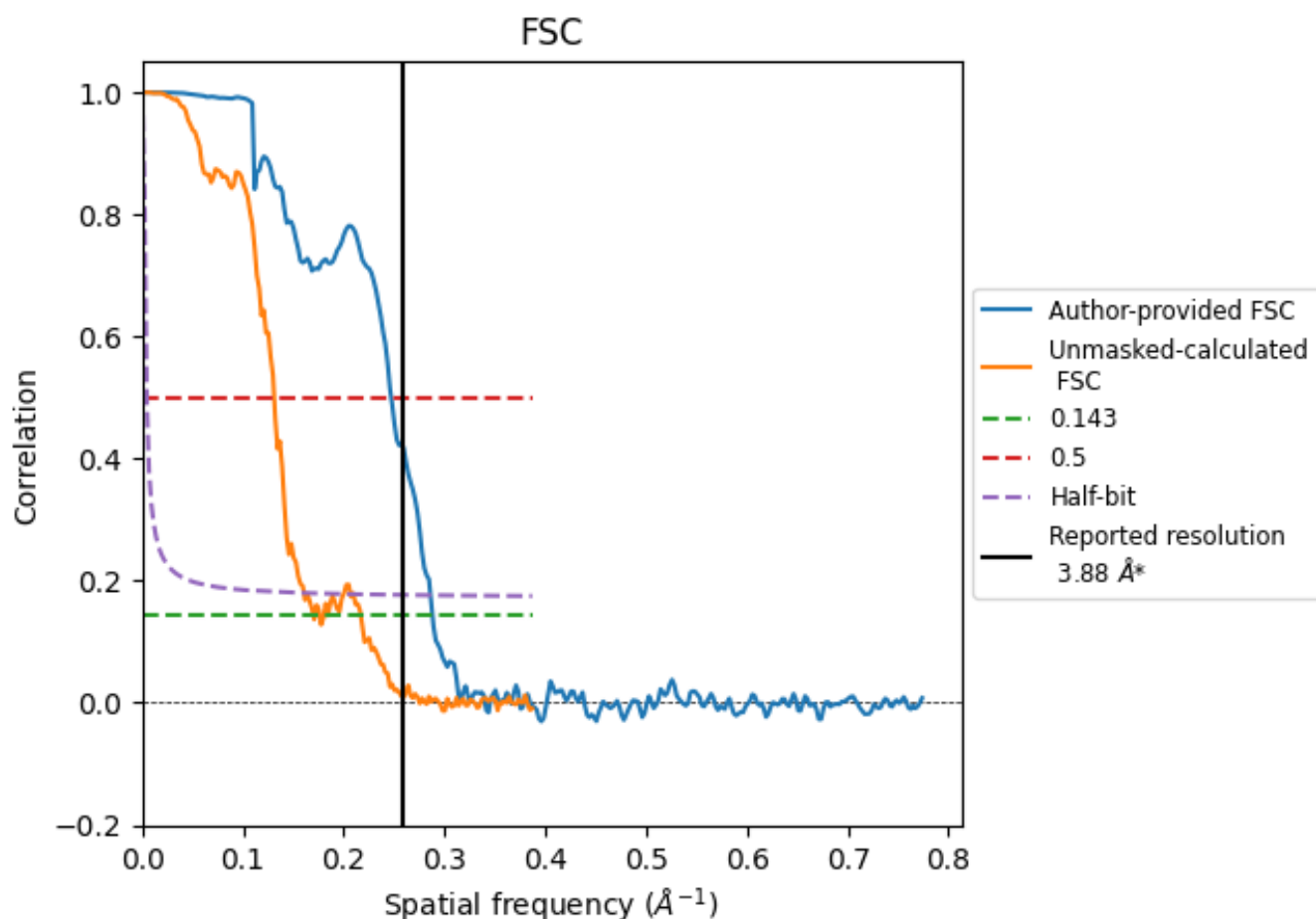


*Reported resolution corresponds to spatial frequency of 0.258 \AA^{-1}

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 0.258 \AA^{-1}

8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.88	-	-
Author-provided FSC curve	3.47	4.05	3.50
Unmasked-calculated*	5.89	7.64	6.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.47 differs from the reported value 3.88 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.89 differs from the reported value 3.88 by more than 10 %

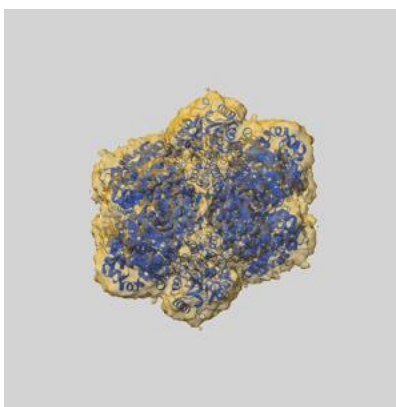
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52419 and PDB model 9HUX. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

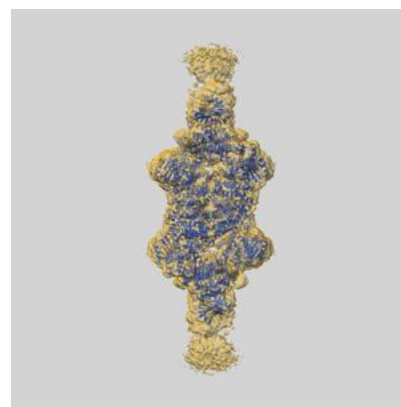
9.1 Map-model overlay [i](#)



X



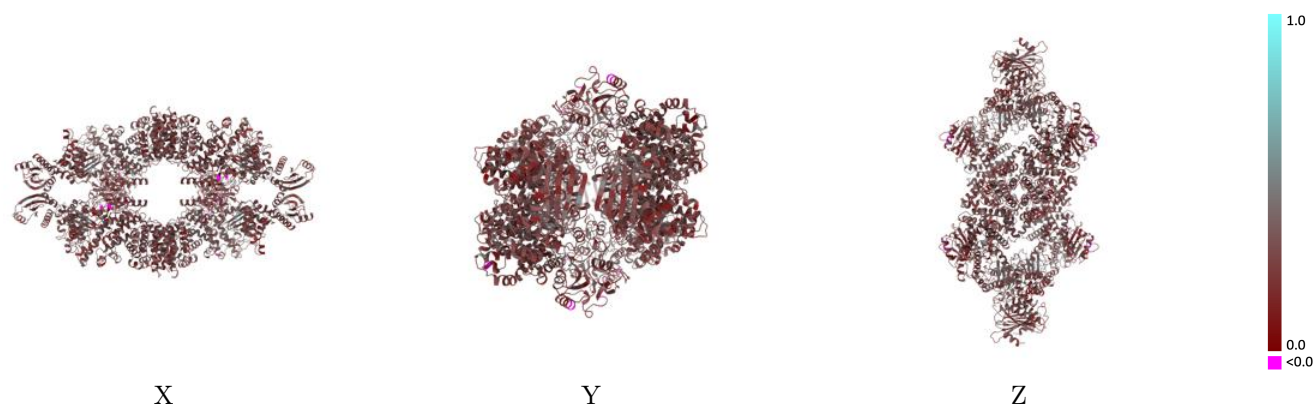
Y



Z

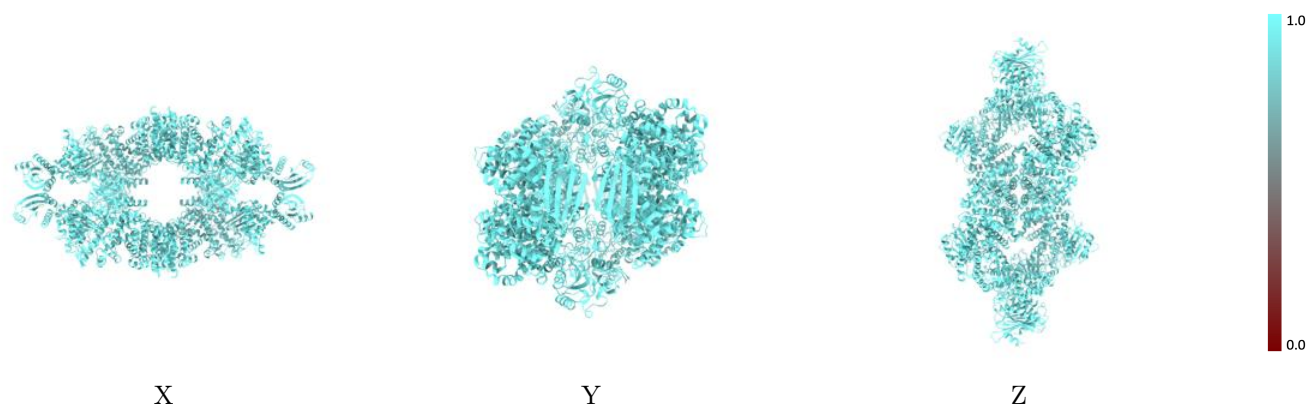
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



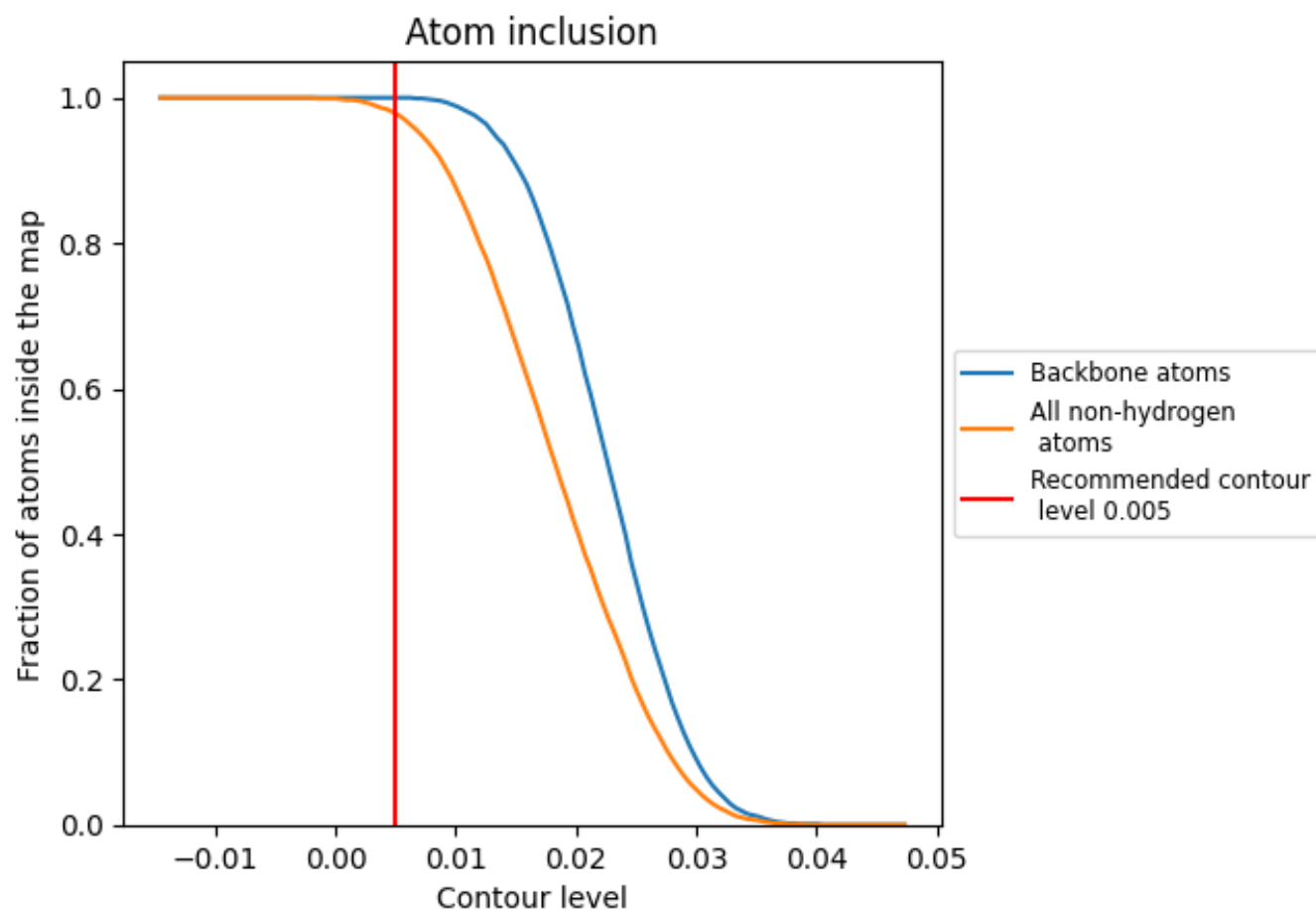
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9780	<div></div> 0.2920
A	<div></div> 0.9780	<div></div> 0.2920
B	<div></div> 0.9790	<div></div> 0.2920
C	<div></div> 0.9780	<div></div> 0.2930
D	<div></div> 0.9780	<div></div> 0.2930

