



Full wwPDB EM Validation Report ⓘ

Aug 15, 2026 – 12:41 PM EDT

PDB ID : 9ZCY / pdb_00009zcy
EMDB ID : EMD-74045
Title : Cryo-EM structure of apo-ATR-ATRIP
Authors : Li, B.; Pavletich, N.P.
Deposited on : 2025-11-24
Resolution : 2.50 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.dev133
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) : 2.50

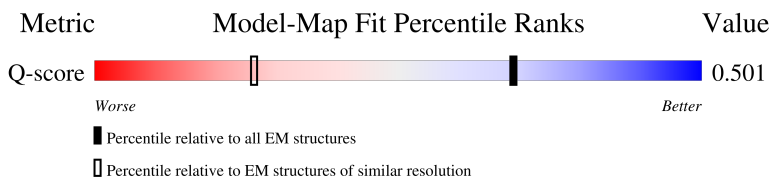
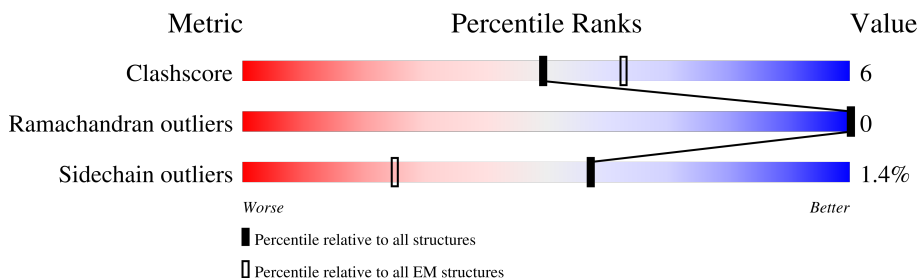
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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	2663	 83% 12% • 5%
1	B	2663	 82% 12% • 5%
2	C	810	 40% 7% 52%
2	D	810	 40% 7% 52%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46442 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 Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2522	Total 20210	C 12962	N 3428	O 3678	S 142	0	0
1	B	2522	Total 20210	C 12962	N 3428	O 3678	S 142	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q13535
A	-17	ASP	-	expression tag	UNP Q13535
A	-16	TYR	-	expression tag	UNP Q13535
A	-15	LYS	-	expression tag	UNP Q13535
A	-14	ASP	-	expression tag	UNP Q13535
A	-13	ASP	-	expression tag	UNP Q13535
A	-12	ASP	-	expression tag	UNP Q13535
A	-11	ASP	-	expression tag	UNP Q13535
A	-10	LYS	-	expression tag	UNP Q13535
A	-9	GLU	-	expression tag	UNP Q13535
A	-8	ASN	-	expression tag	UNP Q13535
A	-7	LEU	-	expression tag	UNP Q13535
A	-6	TYR	-	expression tag	UNP Q13535
A	-5	PHE	-	expression tag	UNP Q13535
A	-4	GLN	-	expression tag	UNP Q13535
A	-3	GLY	-	expression tag	UNP Q13535
A	-2	GLY	-	expression tag	UNP Q13535
A	-1	GLY	-	expression tag	UNP Q13535
A	0	ARG	-	expression tag	UNP Q13535
B	-18	MET	-	initiating methionine	UNP Q13535
B	-17	ASP	-	expression tag	UNP Q13535
B	-16	TYR	-	expression tag	UNP Q13535
B	-15	LYS	-	expression tag	UNP Q13535
B	-14	ASP	-	expression tag	UNP Q13535
B	-13	ASP	-	expression tag	UNP Q13535
B	-12	ASP	-	expression tag	UNP Q13535

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	ASP	-	expression tag	UNP Q13535
B	-10	LYS	-	expression tag	UNP Q13535
B	-9	GLU	-	expression tag	UNP Q13535
B	-8	ASN	-	expression tag	UNP Q13535
B	-7	LEU	-	expression tag	UNP Q13535
B	-6	TYR	-	expression tag	UNP Q13535
B	-5	PHE	-	expression tag	UNP Q13535
B	-4	GLN	-	expression tag	UNP Q13535
B	-3	GLY	-	expression tag	UNP Q13535
B	-2	GLY	-	expression tag	UNP Q13535
B	-1	GLY	-	expression tag	UNP Q13535
B	0	ARG	-	expression tag	UNP Q13535

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	389	Total	C	N	O	S	0	0
			2976	1891	523	537	25		
2	D	389	Total	C	N	O	S	0	0
			2976	1891	523	537	25		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	initiating methionine	UNP Q8WXE1
C	-17	ASP	-	expression tag	UNP Q8WXE1
C	-16	TYR	-	expression tag	UNP Q8WXE1
C	-15	LYS	-	expression tag	UNP Q8WXE1
C	-14	ASP	-	expression tag	UNP Q8WXE1
C	-13	ASP	-	expression tag	UNP Q8WXE1
C	-12	ASP	-	expression tag	UNP Q8WXE1
C	-11	ASP	-	expression tag	UNP Q8WXE1
C	-10	LYS	-	expression tag	UNP Q8WXE1
C	-9	GLU	-	expression tag	UNP Q8WXE1
C	-8	ASN	-	expression tag	UNP Q8WXE1
C	-7	LEU	-	expression tag	UNP Q8WXE1
C	-6	TYR	-	expression tag	UNP Q8WXE1
C	-5	PHE	-	expression tag	UNP Q8WXE1
C	-4	GLN	-	expression tag	UNP Q8WXE1
C	-3	GLY	-	expression tag	UNP Q8WXE1
C	-2	GLY	-	expression tag	UNP Q8WXE1
C	-1	GLY	-	expression tag	UNP Q8WXE1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ARG	-	expression tag	UNP Q8WXE1
D	-18	MET	-	initiating methionine	UNP Q8WXE1
D	-17	ASP	-	expression tag	UNP Q8WXE1
D	-16	TYR	-	expression tag	UNP Q8WXE1
D	-15	LYS	-	expression tag	UNP Q8WXE1
D	-14	ASP	-	expression tag	UNP Q8WXE1
D	-13	ASP	-	expression tag	UNP Q8WXE1
D	-12	ASP	-	expression tag	UNP Q8WXE1
D	-11	ASP	-	expression tag	UNP Q8WXE1
D	-10	LYS	-	expression tag	UNP Q8WXE1
D	-9	GLU	-	expression tag	UNP Q8WXE1
D	-8	ASN	-	expression tag	UNP Q8WXE1
D	-7	LEU	-	expression tag	UNP Q8WXE1
D	-6	TYR	-	expression tag	UNP Q8WXE1
D	-5	PHE	-	expression tag	UNP Q8WXE1
D	-4	GLN	-	expression tag	UNP Q8WXE1
D	-3	GLY	-	expression tag	UNP Q8WXE1
D	-2	GLY	-	expression tag	UNP Q8WXE1
D	-1	GLY	-	expression tag	UNP Q8WXE1
D	0	ARG	-	expression tag	UNP Q8WXE1

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

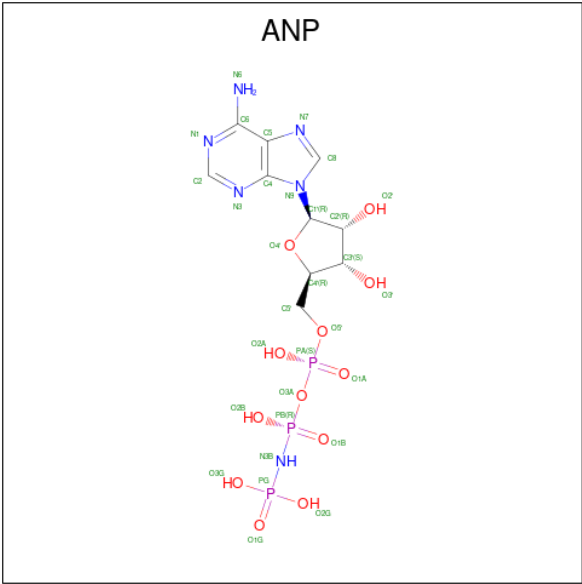
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID:

ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).

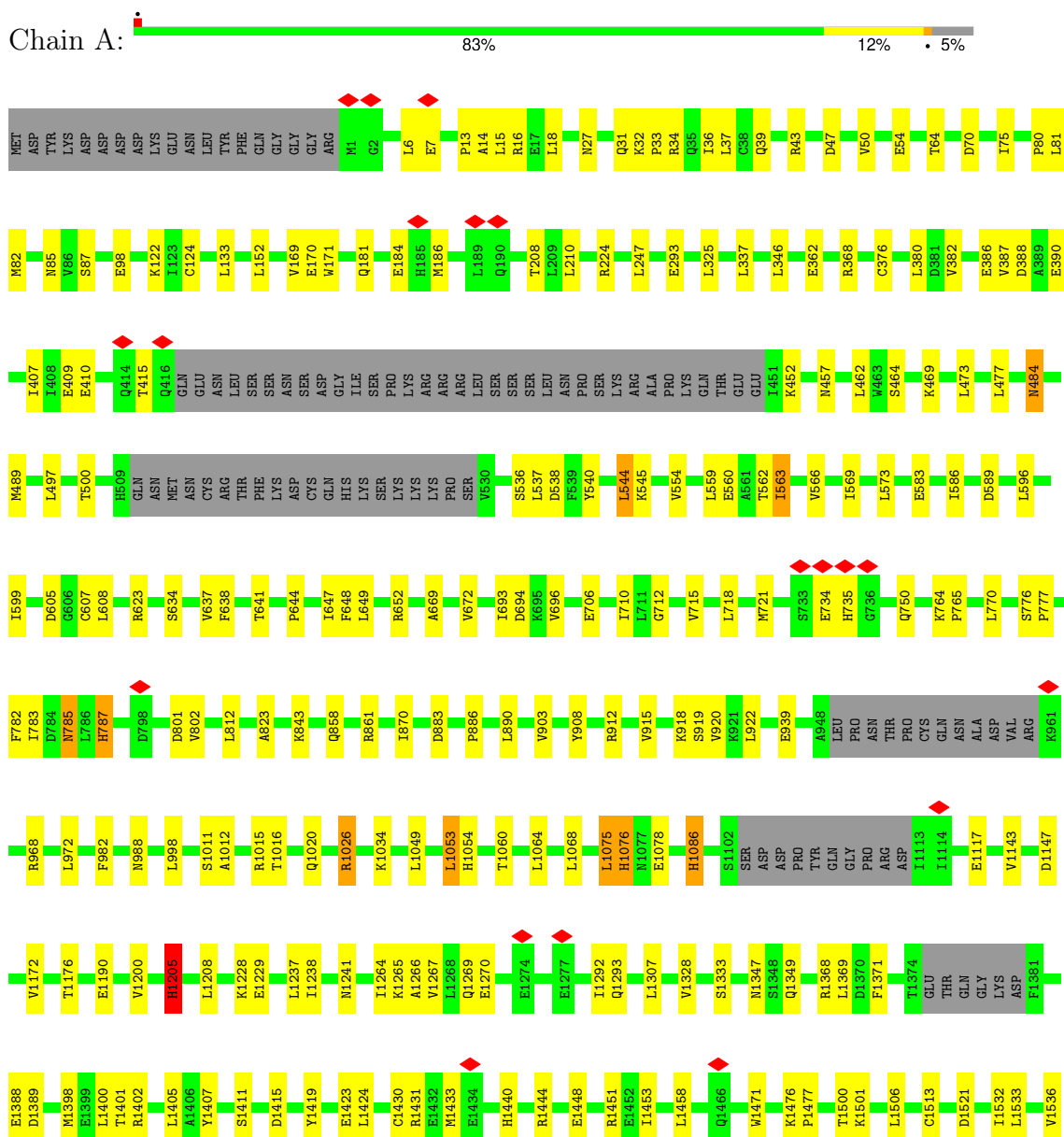


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			31	10	6	12	3	
5	B	1	Total	C	N	O	P	0
			31	10	6	12	3	

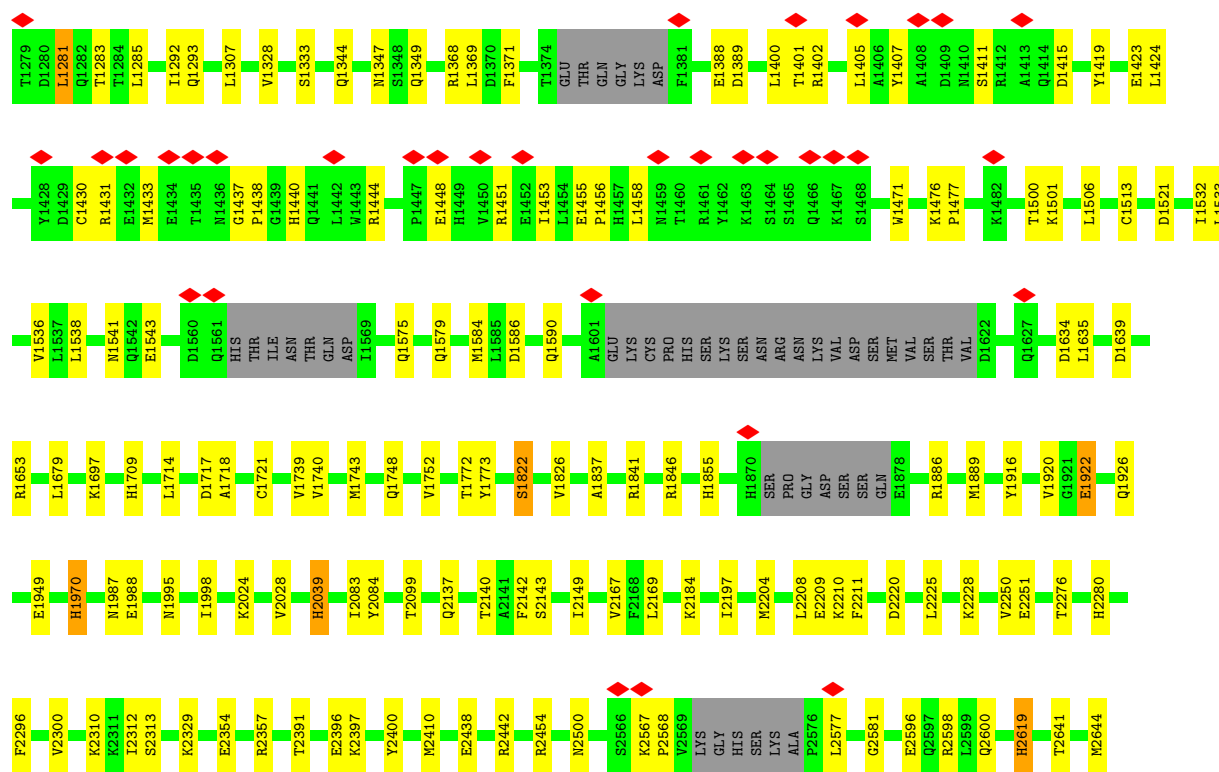
3 Residue-property plots

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: Serine/threonine-protein kinase ATR

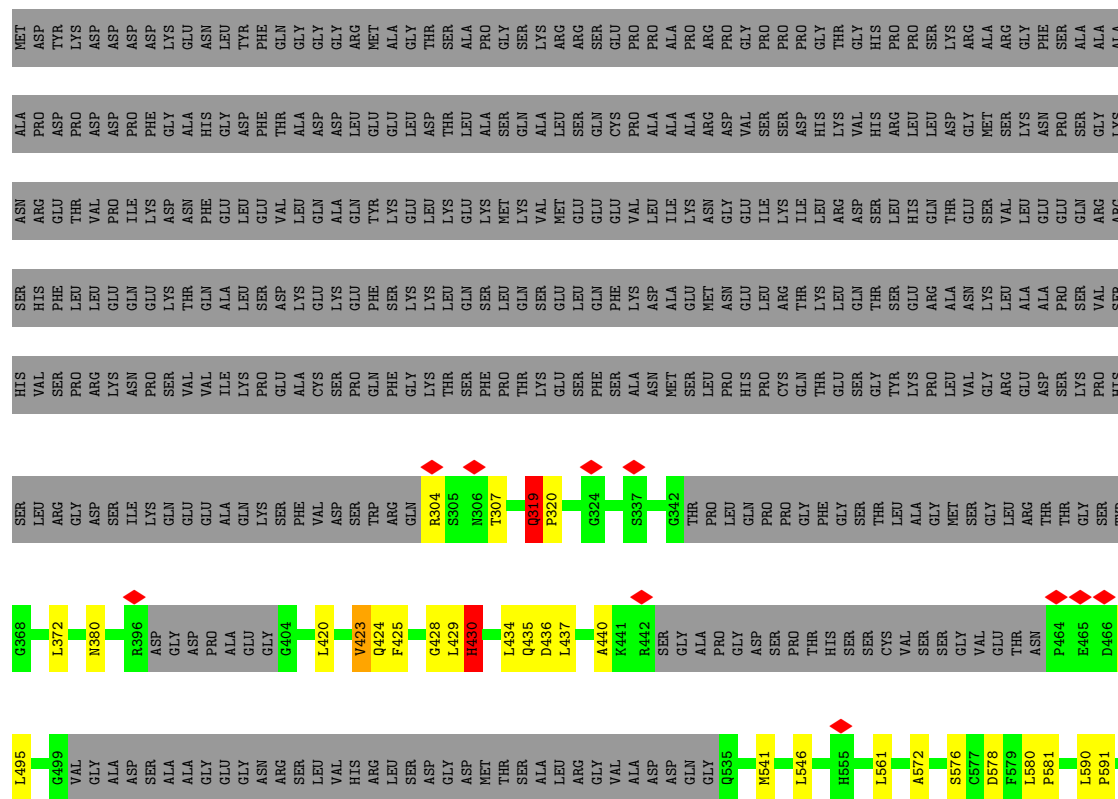






• Molecule 2: ATR-interacting protein

Chain C:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1697213	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 ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.110	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	340.48, 340.48, 340.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	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: ZN, ANP, MG

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	0.20	7/20630 (0.0%)	0.37	17/27883 (0.1%)
1	B	0.21	8/20630 (0.0%)	0.39	17/27883 (0.1%)
2	C	0.20	1/3028 (0.0%)	0.41	2/4112 (0.0%)
2	D	0.20	1/3028 (0.0%)	0.41	2/4112 (0.0%)
All	All	0.20	17/47316 (0.0%)	0.38	38/63990 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
2	C	0	2
2	D	0	2
All	All	0	20

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	919	SER	C-N	7.81	1.43	1.33
1	B	1086	HIS	CE1-NE2	-5.17	1.27	1.32
1	B	1970	HIS	CE1-NE2	-5.16	1.27	1.32
1	A	2039	HIS	CE1-NE2	-5.16	1.27	1.32
1	A	787	HIS	CE1-NE2	-5.14	1.27	1.32
2	C	430	HIS	CE1-NE2	-5.13	1.27	1.32
2	D	430	HIS	CE1-NE2	-5.13	1.27	1.32
1	B	787	HIS	CE1-NE2	-5.12	1.27	1.32
1	A	2619	HIS	CE1-NE2	-5.09	1.27	1.32
1	A	1086	HIS	CE1-NE2	-5.08	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1076	HIS	CE1-NE2	-5.07	1.27	1.32
1	B	1076	HIS	CE1-NE2	-5.07	1.27	1.32
1	B	2619	HIS	CE1-NE2	-5.07	1.27	1.32
1	B	1205	HIS	CE1-NE2	-5.06	1.27	1.32
1	B	2039	HIS	CE1-NE2	-5.06	1.27	1.32
1	A	1205	HIS	CE1-NE2	-5.04	1.27	1.32
1	A	1970	HIS	CE1-NE2	-5.00	1.27	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	919	SER	CA-C-N	-9.20	110.87	123.10
1	A	919	SER	C-N-CA	-9.20	110.87	123.10
1	B	919	SER	O-C-N	-7.94	113.05	122.58
1	B	919	SER	CA-C-N	7.88	134.18	122.98
1	B	919	SER	C-N-CA	7.88	134.18	122.98
1	B	787	HIS	ND1-CG-CD2	-6.48	99.62	106.10
1	A	1086	HIS	ND1-CG-CD2	-6.48	99.62	106.10
1	A	1205	HIS	ND1-CG-CD2	-6.47	99.63	106.10
2	C	430	HIS	ND1-CG-CD2	-6.46	99.64	106.10
1	A	787	HIS	ND1-CG-CD2	-6.46	99.64	106.10
1	B	1205	HIS	ND1-CG-CD2	-6.46	99.64	106.10
1	A	2619	HIS	ND1-CG-CD2	-6.44	99.66	106.10
1	B	1086	HIS	ND1-CG-CD2	-6.44	99.66	106.10
1	B	1076	HIS	ND1-CG-CD2	-6.44	99.66	106.10
1	A	1076	HIS	ND1-CG-CD2	-6.42	99.68	106.10
1	B	2619	HIS	ND1-CG-CD2	-6.41	99.69	106.10
2	D	430	HIS	ND1-CG-CD2	-6.41	99.69	106.10
1	B	1970	HIS	ND1-CG-CD2	-6.40	99.70	106.10
1	A	1970	HIS	ND1-CG-CD2	-6.37	99.73	106.10
1	B	2039	HIS	ND1-CG-CD2	-6.34	99.76	106.10
1	A	2039	HIS	ND1-CG-CD2	-6.34	99.76	106.10
1	A	919	SER	O-C-N	5.68	132.04	122.21
1	B	1076	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	B	1205	HIS	CE1-NE2-CD2	-5.34	103.66	109.00
1	B	1970	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
1	B	1086	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
2	C	430	HIS	CE1-NE2-CD2	-5.33	103.67	109.00
1	B	2619	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
1	A	1970	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
1	A	2619	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
1	B	787	HIS	CE1-NE2-CD2	-5.31	103.69	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
2	D	430	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	B	2039	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
1	A	1205	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
1	A	1076	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
1	A	1086	HIS	CE1-NE2-CD2	-5.28	103.72	109.00
1	A	2039	HIS	CE1-NE2-CD2	-5.23	103.77	109.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1076	HIS	Sidechain
1	A	1086	HIS	Sidechain
1	A	1205	HIS	Sidechain
1	A	171	TRP	Peptide
1	A	1970	HIS	Sidechain
1	A	2039	HIS	Sidechain
1	A	2619	HIS	Sidechain
1	A	787	HIS	Sidechain
1	B	1076	HIS	Sidechain
1	B	1086	HIS	Sidechain
1	B	1205	HIS	Sidechain
1	B	171	TRP	Peptide
1	B	1970	HIS	Sidechain
1	B	2039	HIS	Sidechain
1	B	2619	HIS	Sidechain
1	B	787	HIS	Sidechain
2	C	319	GLN	Peptide
2	C	430	HIS	Sidechain
2	D	319	GLN	Peptide
2	D	430	HIS	Sidechain

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	20210	0	20491	216	0
1	B	20210	0	20491	229	0
2	C	2976	0	3063	46	0
2	D	2976	0	3063	45	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	31	0	13	0	0
5	B	31	0	13	0	0
All	All	46442	0	47134	531	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 6.

All (531) 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:1281:LEU:HD12	1:B:1281:LEU:O	1.77	0.84
1:B:536:SER:OG	1:B:538:ASP:OD1	1.97	0.82
1:A:536:SER:OG	1:A:538:ASP:OD1	1.97	0.81
2:D:597:GLU:OE2	2:D:597:GLU:N	2.14	0.81
2:C:597:GLU:N	2:C:597:GLU:OE2	2.14	0.80
1:B:1401:THR:O	1:B:1405:LEU:HD23	1.82	0.80
1:B:1117:GLU:N	1:B:1117:GLU:OE1	2.14	0.80
1:A:1401:THR:O	1:A:1405:LEU:HD23	1.82	0.80
1:A:1117:GLU:N	1:A:1117:GLU:OE1	2.14	0.79
1:B:1272:ARG:CB	1:B:1272:ARG:HH11	1.96	0.78
2:D:436:ASP:OD1	2:D:437:LEU:N	2.18	0.77
2:C:436:ASP:OD1	2:C:437:LEU:N	2.18	0.77
1:A:1292:ILE:HD11	1:A:1307:LEU:HD22	1.67	0.76
1:B:1841:ARG:O	1:B:1846:ARG:NH1	2.22	0.73
1:A:1841:ARG:O	1:A:1846:ARG:NH1	2.22	0.72
1:B:2251:GLU:OE2	1:B:2251:GLU:N	2.22	0.72
1:B:1278:SER:HA	1:B:1283:THR:HG21	1.72	0.72
1:B:1272:ARG:HH11	1:B:1272:ARG:HB2	1.55	0.71
1:A:2251:GLU:N	1:A:2251:GLU:OE2	2.22	0.70
2:D:682:CYS:O	2:D:686:VAL:HG23	1.90	0.70
2:C:682:CYS:O	2:C:686:VAL:HG23	1.90	0.69
1:B:2500:ASN:OD1	1:B:2598:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2500:ASN:OD1	1:A:2598:ARG:NH2	2.26	0.69
2:C:372:LEU:HD13	2:C:372:LEU:O	1.93	0.69
1:B:1272:ARG:O	1:B:1276:SER:N	2.22	0.69
1:B:1448:GLU:OE1	1:B:1451:ARG:NH1	2.27	0.68
2:D:372:LEU:O	2:D:372:LEU:HD13	1.93	0.68
1:A:1407:TYR:OH	1:A:1521:ASP:OD1	2.10	0.67
1:B:1272:ARG:HH11	1:B:1272:ARG:CG	2.06	0.67
1:A:1448:GLU:OE1	1:A:1451:ARG:NH1	2.27	0.67
1:A:1049:LEU:O	1:A:1053:LEU:HD22	1.94	0.67
1:B:1049:LEU:O	1:B:1053:LEU:HD22	1.94	0.67
1:A:712:GLY:N	1:A:785:ASN:OD1	2.27	0.67
1:A:477:LEU:HD22	1:A:489:MET:HE2	1.77	0.67
2:D:694:LEU:HD12	2:D:720:LEU:HD23	1.77	0.67
1:A:537:LEU:HD23	1:A:537:LEU:O	1.95	0.67
1:A:2410:MET:HA	1:A:2410:MET:HE3	1.76	0.67
1:B:712:GLY:N	1:B:785:ASN:OD1	2.27	0.67
1:A:124:CYS:SG	1:A:208:THR:HG23	2.35	0.67
1:B:2410:MET:HE3	1:B:2410:MET:HA	1.76	0.66
1:B:537:LEU:O	1:B:537:LEU:HD23	1.95	0.66
1:B:124:CYS:SG	1:B:208:THR:HG23	2.35	0.66
2:C:694:LEU:HD12	2:C:720:LEU:HD23	1.77	0.65
1:B:477:LEU:HD22	1:B:489:MET:HE2	1.77	0.65
1:B:1238:ILE:CD1	1:B:1264:ILE:HG23	2.27	0.65
1:B:1238:ILE:HD11	1:B:1264:ILE:HG23	1.79	0.65
1:A:1012:ALA:O	1:A:1016:THR:HG23	1.98	0.64
1:B:1012:ALA:O	1:B:1016:THR:HG23	1.98	0.64
1:B:988:ASN:ND2	1:B:1020:GLN:OE1	2.31	0.64
1:A:1034:LYS:NZ	1:A:1078:GLU:OE1	2.30	0.64
1:A:181:GLN:OE1	1:A:181:GLN:N	2.31	0.64
1:A:988:ASN:ND2	1:A:1020:GLN:OE1	2.31	0.64
1:B:750:GLN:OE1	1:B:750:GLN:N	2.31	0.64
2:D:546:LEU:HD12	2:D:561:LEU:HD12	1.79	0.64
1:A:1238:ILE:HD11	1:A:1264:ILE:HG23	1.79	0.63
1:B:181:GLN:N	1:B:181:GLN:OE1	2.31	0.63
1:A:2184:LYS:NZ	1:A:2220:ASP:OD2	2.31	0.63
2:C:546:LEU:HD12	2:C:561:LEU:HD12	1.79	0.63
1:B:2184:LYS:NZ	1:B:2220:ASP:OD2	2.31	0.62
1:A:750:GLN:N	1:A:750:GLN:OE1	2.31	0.62
1:B:1229:GLU:N	1:B:1229:GLU:OE2	2.30	0.62
1:B:1586:ASP:OD2	1:B:1653:ARG:NH2	2.32	0.62
1:B:376:CYS:O	1:B:380:LEU:HD13	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:CYS:O	1:A:380:LEU:HD13	2.00	0.62
1:B:1407:TYR:OH	1:B:1521:ASP:OD1	2.10	0.62
1:A:1229:GLU:OE2	1:A:1229:GLU:N	2.30	0.61
1:A:1238:ILE:CD1	1:A:1264:ILE:HG23	2.30	0.61
1:A:390:GLU:N	1:A:390:GLU:OE1	2.33	0.61
1:B:224:ARG:NH2	2:D:572:ALA:O	2.34	0.61
1:A:770:LEU:HD22	1:A:812:LEU:HD22	1.82	0.61
1:A:1333:SER:OG	1:A:1369:LEU:O	2.16	0.61
1:B:390:GLU:N	1:B:390:GLU:OE1	2.33	0.61
1:B:18:LEU:HD21	1:B:81:LEU:HD12	1.83	0.61
1:B:13:PRO:O	1:B:16:ARG:HG2	2.01	0.60
1:B:770:LEU:HD22	1:B:812:LEU:HD22	1.82	0.60
1:A:13:PRO:O	1:A:16:ARG:HG2	2.01	0.60
1:B:583:GLU:OE2	1:B:586:ILE:HG23	2.02	0.60
1:A:18:LEU:HD21	1:A:81:LEU:HD12	1.83	0.59
1:B:1281:LEU:HD12	1:B:1281:LEU:C	2.27	0.59
1:A:583:GLU:OE2	1:A:586:ILE:HG23	2.02	0.59
1:A:1987:ASN:OD1	1:A:1988:GLU:N	2.36	0.59
1:B:1987:ASN:OD1	1:B:1988:GLU:N	2.36	0.59
1:A:224:ARG:NH2	2:C:572:ALA:O	2.36	0.58
1:B:783:ILE:HG21	1:B:823:ALA:HB1	1.86	0.58
1:B:540:TYR:O	1:B:544:LEU:HD12	2.03	0.58
1:A:783:ILE:HG21	1:A:823:ALA:HB1	1.86	0.58
1:B:85:ASN:OD1	1:B:87:SER:OG	2.21	0.58
1:A:469:LYS:O	1:A:473:LEU:HD23	2.03	0.58
1:B:469:LYS:O	1:B:473:LEU:HD23	2.02	0.58
1:A:477:LEU:CD2	1:A:489:MET:HE2	2.34	0.58
1:B:2596:GLU:OE1	1:B:2600:GLN:NE2	2.36	0.58
1:A:540:TYR:O	1:A:544:LEU:HD12	2.03	0.58
1:A:85:ASN:OD1	1:A:87:SER:OG	2.21	0.57
1:A:224:ARG:NH1	2:C:615:ASP:OD2	2.35	0.57
1:A:1748:GLN:O	1:A:1752:VAL:HG23	2.04	0.57
1:B:477:LEU:CD2	1:B:489:MET:HE2	2.34	0.57
2:C:617:ASP:N	2:C:617:ASP:OD2	2.37	0.57
1:B:1748:GLN:O	1:B:1752:VAL:HG23	2.04	0.57
1:A:2596:GLU:OE1	1:A:2600:GLN:NE2	2.36	0.57
1:A:1709:HIS:CE1	1:A:1718:ALA:HB2	2.41	0.56
1:B:1709:HIS:CE1	1:B:1718:ALA:HB2	2.41	0.56
2:D:617:ASP:OD2	2:D:617:ASP:N	2.37	0.56
2:D:694:LEU:CD1	2:D:720:LEU:HD23	2.35	0.56
1:A:1532:ILE:O	1:A:1536:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:694:LEU:CD1	2:C:720:LEU:HD23	2.35	0.56
1:B:718:LEU:HD23	1:B:718:LEU:O	2.06	0.56
1:B:2149:ILE:HD11	1:B:2197:ILE:HD12	1.87	0.56
2:D:304:ARG:O	2:D:307:THR:OG1	2.17	0.56
1:B:1532:ILE:O	1:B:1536:VAL:HG23	2.06	0.56
1:A:1538:LEU:HD11	1:A:1625:ASP:HB3	1.88	0.56
1:B:908:TYR:OH	1:B:912:ARG:NH2	2.39	0.55
1:A:80:PRO:HB3	1:A:133:LEU:HD11	1.88	0.55
1:B:1281:LEU:CD1	1:B:1285:LEU:HG	2.36	0.55
1:B:1292:ILE:HD11	1:B:1307:LEU:HD22	1.88	0.55
1:A:908:TYR:OH	1:A:912:ARG:NH2	2.40	0.55
1:A:2149:ILE:HD11	1:A:2197:ILE:HD12	1.87	0.55
2:C:764:ASP:O	2:C:764:ASP:OD2	2.25	0.55
1:A:718:LEU:HD23	1:A:718:LEU:O	2.06	0.55
1:B:770:LEU:HD21	1:B:782:PHE:CD2	2.42	0.55
2:D:735:LYS:O	2:D:735:LYS:HD3	2.07	0.55
2:D:764:ASP:O	2:D:764:ASP:OD2	2.25	0.54
1:A:770:LEU:HD21	1:A:782:PHE:CD2	2.42	0.54
1:B:1252:ILE:CG2	1:B:1268:LEU:HD11	2.37	0.54
1:A:2225:LEU:HD23	1:A:2225:LEU:O	2.07	0.54
1:A:2329:LYS:O	1:A:2329:LYS:HG2	2.08	0.54
2:C:735:LYS:O	2:C:735:LYS:HD3	2.07	0.54
1:B:80:PRO:HB3	1:B:133:LEU:HD11	1.88	0.54
1:A:915:VAL:HG11	1:A:922:LEU:HD23	1.90	0.54
1:A:1440:HIS:O	1:A:1444:ARG:HG3	2.08	0.54
2:D:707:PRO:O	2:D:709:ARG:NH1	2.40	0.54
1:B:2329:LYS:O	1:B:2329:LYS:HG2	2.08	0.54
2:C:707:PRO:O	2:C:709:ARG:NH1	2.40	0.53
1:A:1267:VAL:O	1:A:1270:GLU:HG3	2.08	0.53
1:B:186:MET:HE2	1:B:186:MET:HA	1.90	0.53
1:B:2225:LEU:O	1:B:2225:LEU:HD23	2.07	0.53
2:C:760:ARG:NH2	2:C:774:ASP:OD1	2.41	0.53
2:C:672:LEU:O	2:C:674:PRO:HD2	2.09	0.53
1:A:1709:HIS:NE2	1:A:1714:LEU:O	2.41	0.53
2:D:760:ARG:NH2	2:D:774:ASP:OD1	2.41	0.53
1:A:1369:LEU:HD13	1:A:1371:PHE:CZ	2.44	0.53
1:A:693:ILE:HA	1:A:696:VAL:HG12	1.91	0.53
1:B:1388:GLU:O	1:B:1388:GLU:HG3	2.09	0.53
1:B:1369:LEU:HD13	1:B:1371:PHE:CZ	2.44	0.53
1:A:386:GLU:OE1	1:A:387:VAL:N	2.42	0.53
1:B:386:GLU:OE1	1:B:387:VAL:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1440:HIS:O	1:B:1444:ARG:HG3	2.08	0.53
1:A:186:MET:HE2	1:A:186:MET:HA	1.89	0.52
1:B:484:ASN:OD1	1:B:484:ASN:N	2.42	0.52
1:B:1389:ASP:OD1	1:B:1389:ASP:C	2.52	0.52
1:B:337:LEU:HD13	1:B:337:LEU:O	2.10	0.52
1:B:734:GLU:OE1	1:B:735:HIS:N	2.43	0.52
1:A:1389:ASP:C	1:A:1389:ASP:OD1	2.52	0.52
2:D:672:LEU:O	2:D:674:PRO:HD2	2.09	0.52
1:A:210:LEU:HD23	1:A:247:LEU:HB3	1.90	0.52
1:A:559:LEU:O	1:A:562:THR:HG22	2.10	0.52
1:A:1369:LEU:HD13	1:A:1371:PHE:HZ	1.75	0.52
1:B:2641:THR:HG22	1:B:2644:MET:HB3	1.92	0.52
1:A:734:GLU:OE1	1:A:735:HIS:N	2.43	0.52
1:A:1922:GLU:OE2	1:A:1926:GLN:NE2	2.42	0.52
1:B:559:LEU:O	1:B:562:THR:HG22	2.10	0.52
1:B:693:ILE:HA	1:B:696:VAL:HG12	1.91	0.52
1:B:1717:ASP:O	1:B:1717:ASP:OD2	2.28	0.52
1:A:2641:THR:HG22	1:A:2644:MET:HB3	1.92	0.51
1:B:210:LEU:HD23	1:B:247:LEU:HB3	1.90	0.51
1:B:415:THR:HG21	1:B:452:LYS:NZ	2.25	0.51
1:B:1922:GLU:OE2	1:B:1926:GLN:NE2	2.43	0.51
1:B:1709:HIS:NE2	1:B:1714:LEU:O	2.42	0.51
2:D:319:GLN:OE1	2:D:319:GLN:HA	2.09	0.51
1:B:554:VAL:O	1:B:623:ARG:NH2	2.43	0.51
1:A:484:ASN:OD1	1:A:484:ASN:N	2.43	0.51
1:A:337:LEU:HD13	1:A:337:LEU:O	2.10	0.51
1:A:554:VAL:O	1:A:623:ARG:NH2	2.43	0.51
1:B:1369:LEU:HD13	1:B:1371:PHE:HZ	1.75	0.51
1:B:2250:VAL:HG21	1:B:2296:PHE:HE1	1.74	0.51
2:C:319:GLN:HA	2:C:319:GLN:OE1	2.09	0.51
1:A:1717:ASP:O	1:A:1717:ASP:OD2	2.28	0.51
2:C:319:GLN:HG3	2:C:320:PRO:HD3	1.92	0.51
1:B:224:ARG:NH1	2:D:615:ASP:OD2	2.39	0.51
1:B:1190:GLU:OE2	1:B:1190:GLU:O	2.29	0.51
1:A:2250:VAL:HG21	1:A:2296:PHE:HE1	1.74	0.51
1:A:415:THR:HG21	1:A:452:LYS:NZ	2.25	0.50
1:A:1266:ALA:O	1:A:1269:GLN:HG3	2.11	0.50
1:A:1388:GLU:HG3	1:A:1388:GLU:O	2.09	0.50
1:A:2577:LEU:O	1:A:2581:GLY:N	2.37	0.50
1:B:1208:LEU:HD23	1:B:1208:LEU:O	2.11	0.50
1:A:1190:GLU:OE2	1:A:1190:GLU:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:319:GLN:HG3	2:D:320:PRO:HD3	1.92	0.50
1:B:2137:GLN:O	1:B:2140:THR:OG1	2.29	0.50
1:B:2396:GLU:OE1	1:B:2442:ARG:NH1	2.44	0.50
1:A:545:LYS:HE3	1:A:545:LYS:HA	1.94	0.50
1:B:1252:ILE:HG21	1:B:1268:LEU:HD11	1.94	0.50
1:B:1252:ILE:CG2	1:B:1268:LEU:CD1	2.89	0.50
1:A:1208:LEU:HD23	1:A:1208:LEU:O	2.11	0.50
1:B:608:LEU:O	1:B:608:LEU:HD23	2.12	0.50
1:A:32:LYS:HD2	1:A:32:LYS:C	2.37	0.49
1:A:1634:ASP:OD2	1:A:1634:ASP:C	2.55	0.49
1:A:388:ASP:O	1:A:388:ASP:OD2	2.31	0.49
1:B:47:ASP:HB2	1:B:50:VAL:HG22	1.94	0.49
2:D:711:ASP:OD2	2:D:715:ARG:NH1	2.45	0.49
1:A:605:ASP:OD1	1:A:607:CYS:N	2.45	0.49
1:A:608:LEU:HD23	1:A:608:LEU:O	2.12	0.49
1:A:1501:LYS:HB2	1:A:1536:VAL:HG13	1.94	0.49
1:B:605:ASP:OD1	1:B:607:CYS:N	2.44	0.49
1:B:32:LYS:C	1:B:32:LYS:HD2	2.37	0.49
1:B:1252:ILE:HG22	1:B:1268:LEU:CD1	2.42	0.49
1:B:1238:ILE:HD11	1:B:1264:ILE:HD12	1.94	0.49
1:A:1739:VAL:HG12	1:A:1743:MET:HE3	1.95	0.49
1:B:388:ASP:O	1:B:388:ASP:OD2	2.30	0.49
1:A:939:GLU:C	1:A:939:GLU:OE1	2.55	0.49
1:A:1419:TYR:CE1	1:A:1423:GLU:OE1	2.66	0.49
2:C:437:LEU:C	2:C:437:LEU:HD23	2.38	0.49
2:C:711:ASP:OD2	2:C:715:ARG:NH1	2.45	0.49
1:B:484:ASN:HD22	1:B:489:MET:HE1	1.77	0.49
1:B:801:ASP:OD1	1:B:802:VAL:HG13	2.13	0.49
1:B:1739:VAL:HG12	1:B:1743:MET:HE3	1.95	0.49
2:D:437:LEU:C	2:D:437:LEU:HD23	2.38	0.49
1:A:15:LEU:HD23	1:A:15:LEU:C	2.38	0.49
1:B:545:LYS:HE3	1:B:545:LYS:HA	1.94	0.49
1:A:1054:HIS:C	1:A:1054:HIS:CD2	2.91	0.49
1:B:647:ILE:HG13	1:B:648:PHE:N	2.28	0.49
1:B:939:GLU:OE1	1:B:939:GLU:C	2.55	0.49
1:B:1634:ASP:OD2	1:B:1634:ASP:C	2.55	0.49
1:A:47:ASP:HB2	1:A:50:VAL:HG22	1.94	0.49
2:C:434:LEU:HD12	2:C:435:GLN:N	2.28	0.48
1:B:484:ASN:ND2	1:B:489:MET:HE1	2.28	0.48
1:B:1328:VAL:HG22	1:B:1368:ARG:O	2.13	0.48
1:A:75:ILE:HD11	1:A:82:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ASN:ND2	1:A:489:MET:HE1	2.28	0.48
1:A:801:ASP:OD1	1:A:802:VAL:HG13	2.13	0.48
1:A:1064:LEU:HD12	1:A:1068:LEU:HD13	1.95	0.48
1:A:1328:VAL:HG22	1:A:1368:ARG:O	2.13	0.48
1:B:15:LEU:C	1:B:15:LEU:HD23	2.38	0.48
1:B:75:ILE:HD11	1:B:82:MET:SD	2.53	0.48
1:B:1886:ARG:HA	1:B:1889:MET:HE3	1.95	0.48
1:A:647:ILE:HG13	1:A:648:PHE:N	2.28	0.48
1:B:388:ASP:OD2	1:B:388:ASP:C	2.56	0.48
1:B:1419:TYR:CE1	1:B:1423:GLU:OE1	2.66	0.48
1:A:1575:GLN:O	1:A:1579:GLN:HG3	2.14	0.48
1:A:293:GLU:C	1:A:293:GLU:OE2	2.57	0.48
1:A:1405:LEU:HD22	1:A:1453:ILE:HD12	1.96	0.48
1:B:1501:LYS:HB2	1:B:1536:VAL:HG13	1.94	0.48
1:B:1575:GLN:O	1:B:1579:GLN:HG3	2.14	0.48
1:A:1639:ASP:OD1	1:A:1639:ASP:N	2.45	0.48
1:B:1249:LEU:HB2	1:B:1271:TYR:CE2	2.49	0.48
1:A:484:ASN:HD22	1:A:489:MET:HE1	1.77	0.48
2:D:434:LEU:HD12	2:D:435:GLN:N	2.28	0.48
1:B:43:ARG:NH1	1:B:43:ARG:HB3	2.29	0.48
1:B:1639:ASP:OD1	1:B:1639:ASP:N	2.45	0.48
1:A:43:ARG:HH11	1:A:43:ARG:HB3	1.79	0.48
1:A:783:ILE:HD11	1:A:812:LEU:HD21	1.96	0.48
1:B:1405:LEU:HD22	1:B:1453:ILE:HD12	1.96	0.48
2:D:319:GLN:O	2:D:320:PRO:C	2.56	0.48
1:A:1431:ARG:NH1	1:A:1458:LEU:O	2.47	0.47
1:A:388:ASP:OD2	1:A:388:ASP:C	2.56	0.47
2:C:319:GLN:O	2:C:320:PRO:C	2.56	0.47
1:B:1054:HIS:C	1:B:1054:HIS:CD2	2.91	0.47
1:B:1740:VAL:HG13	1:B:1752:VAL:HG13	1.96	0.47
1:A:43:ARG:HB3	1:A:43:ARG:NH1	2.29	0.47
1:A:1886:ARG:HA	1:A:1889:MET:HE3	1.95	0.47
1:B:54:GLU:OE1	1:B:64:THR:OG1	2.31	0.47
1:B:184:GLU:OE2	1:B:184:GLU:N	2.44	0.47
1:B:81:LEU:C	1:B:81:LEU:HD13	2.40	0.47
1:B:1064:LEU:HD12	1:B:1068:LEU:HD13	1.95	0.47
1:A:81:LEU:C	1:A:81:LEU:HD13	2.40	0.47
1:B:293:GLU:OE2	1:B:293:GLU:C	2.56	0.47
1:B:783:ILE:HD11	1:B:812:LEU:CD2	2.45	0.47
1:A:886:PRO:O	1:A:890:LEU:HD13	2.14	0.47
2:C:636:TYR:CE2	2:C:686:VAL:HG22	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ARG:HB3	1:B:43:ARG:HH11	1.79	0.47
1:B:1269:GLN:HA	1:B:1272:ARG:NH1	2.28	0.47
1:B:2577:LEU:O	1:B:2581:GLY:N	2.37	0.47
2:D:636:TYR:CZ	2:D:686:VAL:HG22	2.50	0.47
2:D:636:TYR:CE2	2:D:686:VAL:HG22	2.50	0.47
2:D:670:SER:N	2:D:671:PRO:CD	2.78	0.47
1:A:33:PRO:HA	1:A:36:ILE:HG22	1.97	0.47
1:B:647:ILE:CG1	1:B:648:PHE:N	2.78	0.47
1:B:783:ILE:HD11	1:B:812:LEU:HD21	1.96	0.47
1:B:1431:ARG:NH1	1:B:1458:LEU:O	2.47	0.47
1:B:2024:LYS:O	1:B:2028:VAL:HG23	2.15	0.47
2:C:424:GLN:O	2:C:425:PHE:C	2.58	0.47
1:B:33:PRO:HA	1:B:36:ILE:HG22	1.97	0.47
1:B:186:MET:HE2	1:B:186:MET:CA	2.45	0.47
1:B:1697:LYS:O	1:B:1697:LYS:HG2	2.15	0.46
1:A:2024:LYS:O	1:A:2028:VAL:HG23	2.15	0.46
2:C:670:SER:N	2:C:671:PRO:CD	2.78	0.46
1:B:1281:LEU:HD11	1:B:1285:LEU:HG	1.97	0.46
2:D:436:ASP:OD1	2:D:436:ASP:C	2.57	0.46
1:A:1697:LYS:HG2	1:A:1697:LYS:O	2.15	0.46
1:B:734:GLU:O	1:B:735:HIS:HB2	2.14	0.46
1:B:1281:LEU:HD12	1:B:1285:LEU:HG	1.98	0.46
1:B:2354:GLU:OE2	1:B:2357:ARG:NH2	2.44	0.46
1:A:54:GLU:OE1	1:A:64:THR:OG1	2.31	0.46
1:A:186:MET:HE2	1:A:186:MET:CA	2.45	0.46
1:A:1200:VAL:HG13	1:A:1237:LEU:HD21	1.97	0.46
2:C:436:ASP:OD1	2:C:436:ASP:C	2.58	0.46
2:C:636:TYR:CZ	2:C:686:VAL:HG22	2.50	0.46
1:B:473:LEU:CD1	1:B:489:MET:HG2	2.46	0.46
1:A:647:ILE:CG1	1:A:648:PHE:N	2.78	0.46
1:B:886:PRO:O	1:B:890:LEU:HD13	2.14	0.46
1:A:721:MET:O	1:A:721:MET:HG2	2.16	0.46
1:A:734:GLU:O	1:A:735:HIS:HB2	2.14	0.46
1:A:1740:VAL:HG13	1:A:1752:VAL:HG13	1.96	0.46
2:D:424:GLN:O	2:D:425:PHE:C	2.58	0.46
1:A:409:GLU:OE1	1:A:410:GLU:N	2.49	0.46
1:B:325:LEU:HD11	1:B:346:LEU:CD1	2.46	0.46
1:B:1220:LEU:HD11	1:B:1256:PRO:HD3	1.98	0.46
2:C:719:CYS:O	2:C:723:THR:OG1	2.29	0.46
2:D:436:ASP:O	2:D:440:ALA:N	2.48	0.46
2:D:735:LYS:HA	2:D:735:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLU:OE1	1:B:410:GLU:N	2.49	0.46
1:B:1949:GLU:OE1	1:B:1949:GLU:N	2.49	0.46
1:B:2391:THR:HG23	1:B:2400:TYR:CE1	2.51	0.46
1:A:184:GLU:OE2	1:A:184:GLU:N	2.44	0.46
1:A:1347:ASN:OD1	1:A:1349:GLN:N	2.49	0.46
1:A:2391:THR:HG23	1:A:2400:TYR:CE1	2.51	0.46
1:B:1200:VAL:CG1	1:B:1237:LEU:HD21	2.46	0.46
1:B:1292:ILE:CD1	1:B:1307:LEU:HD22	2.46	0.46
1:A:783:ILE:HD11	1:A:812:LEU:CD2	2.45	0.45
1:A:2137:GLN:O	1:A:2140:THR:OG1	2.29	0.45
1:A:380:LEU:HD11	1:A:462:LEU:HD11	1.99	0.45
2:C:420:LEU:HD12	2:C:495:LEU:HD23	1.98	0.45
1:B:559:LEU:O	1:B:560:GLU:C	2.59	0.45
1:B:764:LYS:N	1:B:765:PRO:CD	2.79	0.45
1:B:1347:ASN:OD1	1:B:1349:GLN:N	2.49	0.45
1:B:1433:MET:SD	1:B:1433:MET:N	2.90	0.45
1:A:1200:VAL:CG1	1:A:1237:LEU:HD21	2.46	0.45
1:A:1949:GLU:N	1:A:1949:GLU:OE1	2.49	0.45
1:B:1228:LYS:O	1:B:1228:LYS:HD3	2.16	0.45
1:A:325:LEU:HD11	1:A:346:LEU:CD1	2.46	0.45
1:A:473:LEU:CD1	1:A:489:MET:HG2	2.46	0.45
2:C:711:ASP:OD2	2:C:711:ASP:C	2.59	0.45
1:B:1333:SER:OG	1:B:1369:LEU:O	2.16	0.45
1:A:764:LYS:N	1:A:765:PRO:CD	2.79	0.45
1:B:54:GLU:OE1	1:B:64:THR:N	2.50	0.45
1:B:1411:SER:O	1:B:1415:ASP:OD2	2.35	0.45
1:A:1228:LYS:O	1:A:1228:LYS:HD3	2.16	0.45
1:A:1264:ILE:O	1:A:1265:LYS:C	2.59	0.45
1:A:1411:SER:O	1:A:1415:ASP:OD2	2.35	0.45
1:A:1433:MET:SD	1:A:1433:MET:N	2.90	0.45
1:B:721:MET:HG2	1:B:721:MET:O	2.16	0.45
2:D:590:LEU:N	2:D:591:PRO:CD	2.79	0.45
1:A:918:LYS:HB3	1:A:920:VAL:HG22	1.97	0.45
2:C:304:ARG:O	2:C:307:THR:OG1	2.16	0.45
2:C:423:VAL:O	2:C:424:GLN:C	2.60	0.45
1:B:1200:VAL:HG13	1:B:1237:LEU:HD21	1.97	0.45
1:B:1822:SER:O	1:B:1826:VAL:HG23	2.17	0.45
2:D:711:ASP:OD2	2:D:711:ASP:C	2.58	0.45
1:A:2396:GLU:OE1	1:A:2442:ARG:NH1	2.44	0.45
2:C:590:LEU:N	2:C:591:PRO:CD	2.80	0.45
2:C:735:LYS:HE2	2:C:735:LYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1533:LEU:HD22	1:B:1584:MET:HE2	1.99	0.45
1:B:1772:THR:HG23	1:B:1773:TYR:N	2.32	0.45
2:D:580:LEU:N	2:D:581:PRO:CD	2.79	0.45
1:A:81:LEU:HD13	1:A:81:LEU:O	2.17	0.45
1:A:1143:VAL:HG12	1:A:1147:ASP:HB2	1.99	0.45
2:C:580:LEU:N	2:C:581:PRO:CD	2.80	0.45
1:B:81:LEU:HD13	1:B:81:LEU:O	2.17	0.45
1:A:1772:THR:HG23	1:A:1773:TYR:N	2.32	0.44
2:D:752:MET:O	2:D:756:SER:OG	2.23	0.44
1:A:1822:SER:O	1:A:1826:VAL:HG23	2.17	0.44
1:A:2142:PHE:CD1	1:A:2167:VAL:HG11	2.52	0.44
2:C:576:SER:OG	2:C:578:ASP:OD1	2.23	0.44
2:D:423:VAL:O	2:D:424:GLN:C	2.59	0.44
1:B:2142:PHE:CD1	1:B:2167:VAL:HG11	2.52	0.44
1:B:2228:LYS:O	1:B:2310:LYS:NZ	2.45	0.44
1:A:54:GLU:OE1	1:A:64:THR:N	2.50	0.44
1:A:407:ILE:O	1:A:410:GLU:HG3	2.18	0.44
1:A:2567:LYS:N	1:A:2568:PRO:HD2	2.33	0.44
1:B:544:LEU:HD11	1:B:573:LEU:CD1	2.48	0.44
1:A:559:LEU:O	1:A:560:GLU:C	2.59	0.44
1:A:1238:ILE:HD11	1:A:1264:ILE:HD12	1.99	0.44
1:A:1533:LEU:HD22	1:A:1584:MET:HE2	1.99	0.44
1:B:706:GLU:O	1:B:710:ILE:HG23	2.17	0.44
1:B:1011:SER:O	1:B:1015:ARG:HG3	2.17	0.44
1:B:2410:MET:HE3	1:B:2410:MET:CA	2.44	0.44
1:B:2567:LYS:N	1:B:2568:PRO:HD2	2.33	0.44
2:D:420:LEU:HD12	2:D:495:LEU:HD23	1.98	0.44
1:A:473:LEU:O	1:A:477:LEU:HD23	2.18	0.44
1:B:968:ARG:O	1:B:972:LEU:HD23	2.18	0.44
1:B:1272:ARG:HB2	1:B:1272:ARG:NH1	2.26	0.44
1:B:1506:LEU:HD23	1:B:1506:LEU:O	2.18	0.44
2:D:728:HIS:HB2	2:D:772:ALA:HB1	2.00	0.44
2:D:758:LEU:O	2:D:762:LEU:HD22	2.18	0.44
1:A:644:PRO:O	1:A:652:ARG:NH2	2.50	0.44
1:A:861:ARG:HB3	1:A:861:ARG:NH1	2.33	0.44
1:B:380:LEU:HD11	1:B:462:LEU:HD11	1.99	0.44
1:B:407:ILE:O	1:B:410:GLU:HG3	2.18	0.44
1:B:693:ILE:HD12	1:B:694:ASP:N	2.33	0.44
1:B:861:ARG:HB3	1:B:861:ARG:NH1	2.33	0.44
1:A:544:LEU:HD11	1:A:573:LEU:CD1	2.48	0.44
1:A:1011:SER:O	1:A:1015:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:PRO:O	1:B:652:ARG:NH2	2.50	0.44
1:B:1272:ARG:CG	1:B:1272:ARG:NH1	2.72	0.44
2:D:728:HIS:NE2	2:D:732:GLN:OE1	2.51	0.44
2:C:728:HIS:NE2	2:C:732:GLN:OE1	2.51	0.43
2:C:758:LEU:O	2:C:762:LEU:HD22	2.18	0.43
1:A:497:LEU:O	1:A:500:THR:HG22	2.18	0.43
1:A:706:GLU:O	1:A:710:ILE:HG23	2.17	0.43
1:A:968:ARG:O	1:A:972:LEU:HD23	2.18	0.43
1:B:1344:GLN:NE2	1:B:1837:ALA:O	2.52	0.43
1:A:2365:TYR:HH	1:A:2493:VAL:HA	1.83	0.43
1:B:1072:PHE:HZ	1:B:1101:ALA:HB2	1.83	0.43
1:B:1272:ARG:HH11	1:B:1272:ARG:HG2	1.82	0.43
1:A:918:LYS:CB	1:A:920:VAL:HG22	2.48	0.43
2:C:728:HIS:HB2	2:C:772:ALA:HB1	2.00	0.43
1:B:473:LEU:O	1:B:477:LEU:HD23	2.18	0.43
1:B:497:LEU:O	1:B:500:THR:HG22	2.18	0.43
1:A:693:ILE:HD12	1:A:694:ASP:N	2.33	0.43
1:B:1143:VAL:HG12	1:B:1147:ASP:HB2	1.99	0.43
1:B:1471:TRP:CD1	1:B:1500:THR:HG21	2.53	0.43
1:A:1506:LEU:O	1:A:1506:LEU:HD23	2.18	0.43
1:A:2169:LEU:HD22	1:A:2204:MET:HE2	2.01	0.43
1:A:2410:MET:HE3	1:A:2410:MET:CA	2.44	0.43
1:A:1405:LEU:HD22	1:A:1453:ILE:CD1	2.49	0.43
1:B:1405:LEU:HD22	1:B:1453:ILE:CD1	2.49	0.43
1:B:1543:GLU:CD	1:B:1543:GLU:H	2.26	0.43
1:A:1543:GLU:CD	1:A:1543:GLU:H	2.26	0.43
1:B:870:ILE:HD11	1:B:903:VAL:HG13	2.01	0.43
2:D:428:GLY:N	2:D:541:MET:HE1	2.34	0.43
2:C:436:ASP:O	2:C:440:ALA:N	2.48	0.42
1:A:1471:TRP:CD1	1:A:1500:THR:HG21	2.53	0.42
2:D:576:SER:OG	2:D:578:ASP:OD1	2.23	0.42
2:D:738:MET:HE2	2:D:738:MET:C	2.44	0.42
2:C:738:MET:C	2:C:738:MET:HE2	2.44	0.42
1:B:152:LEU:HD23	1:B:152:LEU:C	2.45	0.42
1:A:1265:LYS:O	1:A:1266:ALA:C	2.62	0.42
1:B:91:GLU:H	1:B:91:GLU:CD	2.24	0.42
1:B:2397:LYS:NZ	1:B:2438:GLU:OE2	2.50	0.42
1:A:497:LEU:CD1	1:A:569:ILE:HG23	2.50	0.42
2:C:428:GLY:N	2:C:541:MET:HE1	2.34	0.42
1:B:497:LEU:CD1	1:B:569:ILE:HG23	2.50	0.42
1:A:152:LEU:C	1:A:152:LEU:HD23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:ALA:O	1:B:672:VAL:HG22	2.20	0.42
1:B:2169:LEU:HD22	1:B:2204:MET:HE2	2.01	0.42
1:B:2276:THR:O	1:B:2280:HIS:HB2	2.20	0.42
1:A:362:GLU:OE2	1:A:368:ARG:NH1	2.53	0.42
1:A:649:LEU:C	1:A:649:LEU:HD13	2.45	0.42
1:A:776:SER:N	1:A:777:PRO:HD2	2.35	0.42
2:C:666:LEU:O	2:C:672:LEU:HD12	2.20	0.42
1:A:39:GLN:C	1:A:39:GLN:CD	2.87	0.42
1:A:669:ALA:O	1:A:672:VAL:HG22	2.20	0.42
1:A:1026:ARG:NH2	1:A:1060:THR:O	2.53	0.42
1:A:2228:LYS:O	1:A:2310:LYS:NZ	2.45	0.42
1:A:457:ASN:O	1:A:464:SER:OG	2.38	0.42
1:A:972:LEU:HD11	1:A:1020:GLN:HG3	2.02	0.42
1:A:2151:HIS:O	1:A:2193:ARG:NH1	2.49	0.42
1:A:2208:LEU:O	1:A:2209:GLU:C	2.63	0.41
1:A:2209:GLU:O	1:A:2210:LYS:C	2.63	0.41
1:A:2276:THR:O	1:A:2280:HIS:HB2	2.20	0.41
1:B:280:LEU:HD12	1:B:342:LEU:HD13	2.02	0.41
1:B:776:SER:N	1:B:777:PRO:HD2	2.35	0.41
1:B:843:LYS:NZ	1:B:883:ASP:O	2.51	0.41
1:B:922:LEU:HD22	1:B:982:PHE:HA	2.02	0.41
1:B:1208:LEU:HD21	1:B:1237:LEU:HD22	2.02	0.41
1:A:563:ILE:O	1:A:566:VAL:HG22	2.20	0.41
1:A:870:ILE:HD11	1:A:903:VAL:HG13	2.01	0.41
1:B:649:LEU:HD13	1:B:649:LEU:C	2.45	0.41
1:A:1541:ASN:OD1	1:A:1543:GLU:OE1	2.39	0.41
1:A:2329:LYS:O	1:A:2329:LYS:CG	2.69	0.41
1:B:1541:ASN:OD1	1:B:1543:GLU:OE1	2.39	0.41
1:A:1634:ASP:OD2	1:A:1635:LEU:N	2.53	0.41
1:A:2397:LYS:NZ	1:A:2438:GLU:OE2	2.50	0.41
2:C:380:ASN:OD1	2:D:319:GLN:HG2	2.21	0.41
1:B:537:LEU:HD23	1:B:537:LEU:C	2.45	0.41
1:B:563:ILE:O	1:B:566:VAL:HG22	2.20	0.41
2:D:666:LEU:O	2:D:672:LEU:HD12	2.20	0.41
1:B:362:GLU:OE2	1:B:368:ARG:NH1	2.53	0.41
1:B:1026:ARG:NH2	1:B:1060:THR:O	2.53	0.41
1:B:1634:ASP:OD2	1:B:1635:LEU:N	2.53	0.41
1:B:1855:HIS:CD2	1:B:1855:HIS:C	2.98	0.41
1:A:1264:ILE:O	1:A:1267:VAL:HG12	2.20	0.41
1:A:1476:LYS:HB2	1:A:1477:PRO:HD3	2.02	0.41
1:B:39:GLN:CD	1:B:39:GLN:C	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1916:TYR:CE1	1:B:1920:VAL:HG21	2.55	0.41
1:B:2209:GLU:O	1:B:2210:LYS:C	2.63	0.41
1:A:169:VAL:HG12	1:A:170:GLU:O	2.21	0.41
1:A:1855:HIS:CD2	1:A:1855:HIS:C	2.98	0.41
1:A:2225:LEU:HD23	1:A:2225:LEU:C	2.46	0.41
1:B:70:ASP:OD1	1:B:122:LYS:NZ	2.54	0.41
1:B:1437:GLY:O	1:B:1438:PRO:C	2.64	0.41
1:B:2208:LEU:O	1:B:2209:GLU:C	2.63	0.41
1:B:2410:MET:HA	1:B:2410:MET:CE	2.49	0.41
2:D:429:LEU:O	2:D:430:HIS:C	2.64	0.41
1:A:1034:LYS:HB3	1:A:1075:LEU:HD22	2.02	0.41
1:A:1205:HIS:HD2	1:A:1241:ASN:ND2	2.19	0.41
1:B:169:VAL:HG12	1:B:170:GLU:O	2.21	0.41
1:B:1077:ASN:ND2	1:B:1130:ILE:HA	2.36	0.41
1:B:1205:HIS:HD2	1:B:1241:ASN:ND2	2.19	0.41
1:B:1476:LYS:HB2	1:B:1477:PRO:HD3	2.02	0.41
1:A:6:LEU:HG	1:A:7:GLU:H	1.85	0.41
1:A:27:ASN:O	1:A:31:GLN:HG2	2.21	0.41
1:A:70:ASP:OD1	1:A:122:LYS:NZ	2.54	0.41
1:A:1049:LEU:HD23	1:A:1053:LEU:CD2	2.50	0.41
1:A:1208:LEU:HD21	1:A:1237:LEU:HD22	2.02	0.41
1:A:1538:LEU:HD12	1:A:1538:LEU:HA	1.96	0.41
1:B:6:LEU:HG	1:B:7:GLU:H	1.85	0.41
1:B:1049:LEU:HD23	1:B:1053:LEU:CD2	2.50	0.41
1:B:1400:LEU:CD1	1:B:1424:LEU:HD12	2.51	0.41
1:B:1455:GLU:HB3	1:B:1456:PRO:HD3	2.03	0.41
1:B:2329:LYS:O	1:B:2329:LYS:CG	2.68	0.41
2:D:719:CYS:O	2:D:723:THR:OG1	2.29	0.41
1:A:922:LEU:HD22	1:A:982:PHE:HA	2.02	0.41
1:A:2211:PHE:O	1:A:2212:VAL:C	2.64	0.41
1:A:2354:GLU:OE2	1:A:2357:ARG:NH2	2.44	0.41
2:C:428:GLY:O	2:C:429:LEU:C	2.64	0.41
1:A:34:ARG:HG3	1:A:82:MET:HE3	2.03	0.40
1:A:409:GLU:C	1:A:409:GLU:CD	2.90	0.40
1:A:638:PHE:O	1:A:641:THR:OG1	2.39	0.40
1:A:1172:VAL:O	1:A:1176:THR:HG23	2.22	0.40
1:A:1916:TYR:CE1	1:A:1920:VAL:HG21	2.55	0.40
1:B:34:ARG:HG3	1:B:82:MET:HE3	2.03	0.40
1:B:457:ASN:O	1:B:464:SER:OG	2.38	0.40
1:B:1995:ASN:O	1:B:1998:ILE:HG22	2.21	0.40
1:A:14:ALA:CB	1:A:32:LYS:HE2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:LEU:HA	1:A:599:ILE:HD12	2.03	0.40
2:C:762:LEU:HD22	2:C:762:LEU:H	1.87	0.40
1:B:39:GLN:OE1	1:B:40:PHE:N	2.54	0.40
1:B:409:GLU:CD	1:B:409:GLU:C	2.89	0.40
1:B:2210:LYS:O	1:B:2211:PHE:C	2.64	0.40
1:A:634:SER:O	1:A:637:VAL:HG12	2.20	0.40
1:A:1400:LEU:CD1	1:A:1424:LEU:HD12	2.51	0.40
1:B:634:SER:O	1:B:637:VAL:HG12	2.21	0.40
1:B:2300:VAL:HG22	1:B:2312:ILE:HG22	2.03	0.40
1:A:843:LYS:NZ	1:A:883:ASP:O	2.51	0.40
1:A:1398:MET:HE3	1:A:1398:MET:HB3	1.97	0.40
1:B:1172:VAL:O	1:B:1176:THR:HG23	2.22	0.40
1:A:382:VAL:O	1:A:382:VAL:HG12	2.22	0.40
1:A:537:LEU:HD23	1:A:537:LEU:C	2.46	0.40
2:C:429:LEU:O	2:C:430:HIS:C	2.63	0.40
1:B:415:THR:HG21	1:B:452:LYS:HZ2	1.87	0.40
1:B:2083:ILE:HG23	1:B:2084:TYR:N	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	2502/2663 (94%)	2410 (96%)	92 (4%)	0	100	100
1	B	2502/2663 (94%)	2412 (96%)	90 (4%)	0	100	100
2	C	379/810 (47%)	350 (92%)	29 (8%)	0	100	100
2	D	379/810 (47%)	352 (93%)	27 (7%)	0	100	100
All	All	5762/6946 (83%)	5524 (96%)	238 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2249/2379 (94%)	2223 (99%)	26 (1%)	63	83
1	B	2249/2379 (94%)	2216 (98%)	33 (2%)	57	80
2	C	340/694 (49%)	333 (98%)	7 (2%)	47	74
2	D	340/694 (49%)	333 (98%)	7 (2%)	47	74
All	All	5178/6146 (84%)	5105 (99%)	73 (1%)	57	81

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	98	GLU
1	A	484	ASN
1	A	544	LEU
1	A	563	ILE
1	A	589	ASP
1	A	715	VAL
1	A	785	ASN
1	A	858	GLN
1	A	998	LEU
1	A	1026	ARG
1	A	1053	LEU
1	A	1075	LEU
1	A	1293	GLN
1	A	1402	ARG
1	A	1430	CYS
1	A	1513	CYS
1	A	1538	LEU
1	A	1590	GLN
1	A	1721	CYS
1	A	1822	SER
1	A	1922	GLU
1	A	2099	THR
1	A	2143	SER

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Mol	Chain	Res	Type
1	A	2313	SER
1	A	2454	ARG
2	C	319	GLN
2	C	423	VAL
2	C	467	SER
2	C	691	THR
2	C	716	THR
2	C	732	GLN
2	C	756	SER
1	B	37	LEU
1	B	98	GLU
1	B	484	ASN
1	B	535	MET
1	B	544	LEU
1	B	563	ILE
1	B	715	VAL
1	B	785	ASN
1	B	858	GLN
1	B	998	LEU
1	B	1026	ARG
1	B	1053	LEU
1	B	1075	LEU
1	B	1175	MET
1	B	1270	GLU
1	B	1272	ARG
1	B	1273	LYS
1	B	1277	GLU
1	B	1281	LEU
1	B	1293	GLN
1	B	1402	ARG
1	B	1430	CYS
1	B	1513	CYS
1	B	1538	LEU
1	B	1590	GLN
1	B	1679	LEU
1	B	1721	CYS
1	B	1822	SER
1	B	1922	GLU
1	B	2099	THR
1	B	2143	SER
1	B	2313	SER
1	B	2454	ARG

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Mol	Chain	Res	Type
2	D	319	GLN
2	D	423	VAL
2	D	467	SER
2	D	691	THR
2	D	716	THR
2	D	732	GLN
2	D	756	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	167	HIS
1	A	200	GLN
1	A	279	HIS
1	A	498	GLN
1	A	506	HIS
1	A	744	ASN
1	A	935	GLN
1	A	967	GLN
1	A	1031	ASN
1	A	1039	HIS
1	A	1058	ASN
1	A	1076	HIS
1	A	1205	HIS
1	A	1302	HIS
1	A	1314	ASN
1	A	1334	GLN
1	A	1457	HIS
1	A	1520	HIS
1	A	1531	HIS
1	A	1705	GLN
1	A	1936	HIS
1	A	1937	HIS
1	A	1942	ASN
1	A	1995	ASN
1	A	2039	HIS
1	A	2085	GLN
1	A	2361	HIS
1	A	2578	ASN
1	A	2635	GLN
2	C	424	GLN

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Mol	Chain	Res	Type
2	C	483	GLN
2	C	484	HIS
2	C	588	GLN
2	C	626	HIS
2	C	695	HIS
2	C	697	GLN
1	B	74	HIS
1	B	167	HIS
1	B	200	GLN
1	B	231	GLN
1	B	498	GLN
1	B	506	HIS
1	B	744	ASN
1	B	935	GLN
1	B	967	GLN
1	B	1031	ASN
1	B	1039	HIS
1	B	1058	ASN
1	B	1086	HIS
1	B	1205	HIS
1	B	1314	ASN
1	B	1457	HIS
1	B	1520	HIS
1	B	1531	HIS
1	B	1587	HIS
1	B	1705	GLN
1	B	1936	HIS
1	B	1937	HIS
1	B	1942	ASN
1	B	1970	HIS
1	B	1995	ASN
1	B	2039	HIS
1	B	2085	GLN
1	B	2361	HIS
1	B	2578	ASN
1	B	2635	GLN
2	D	424	GLN
2	D	626	HIS
2	D	695	HIS
2	D	697	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 ⓘ

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ANP	B	2704	4	33,33,33	0.93	4 (12%)	45,52,52	0.57	0
5	ANP	A	2704	4	33,33,33	0.93	4 (12%)	45,52,52	0.57	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
5	ANP	B	2704	4	-	5/18/38/38	0/3/3/3
5	ANP	A	2704	4	-	4/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2704	ANP	PG-O1G	2.58	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2704	ANP	PG-O1G	2.52	1.50	1.46
5	B	2704	ANP	PG-N3B	2.45	1.69	1.63
5	A	2704	ANP	PG-N3B	2.45	1.69	1.63
5	B	2704	ANP	PB-O1B	2.40	1.49	1.46
5	A	2704	ANP	PB-O1B	2.40	1.49	1.46
5	B	2704	ANP	PB-O3A	-2.33	1.56	1.59
5	A	2704	ANP	PB-O3A	-2.32	1.56	1.59

There are no bond angle outliers.

There are no chirality outliers.

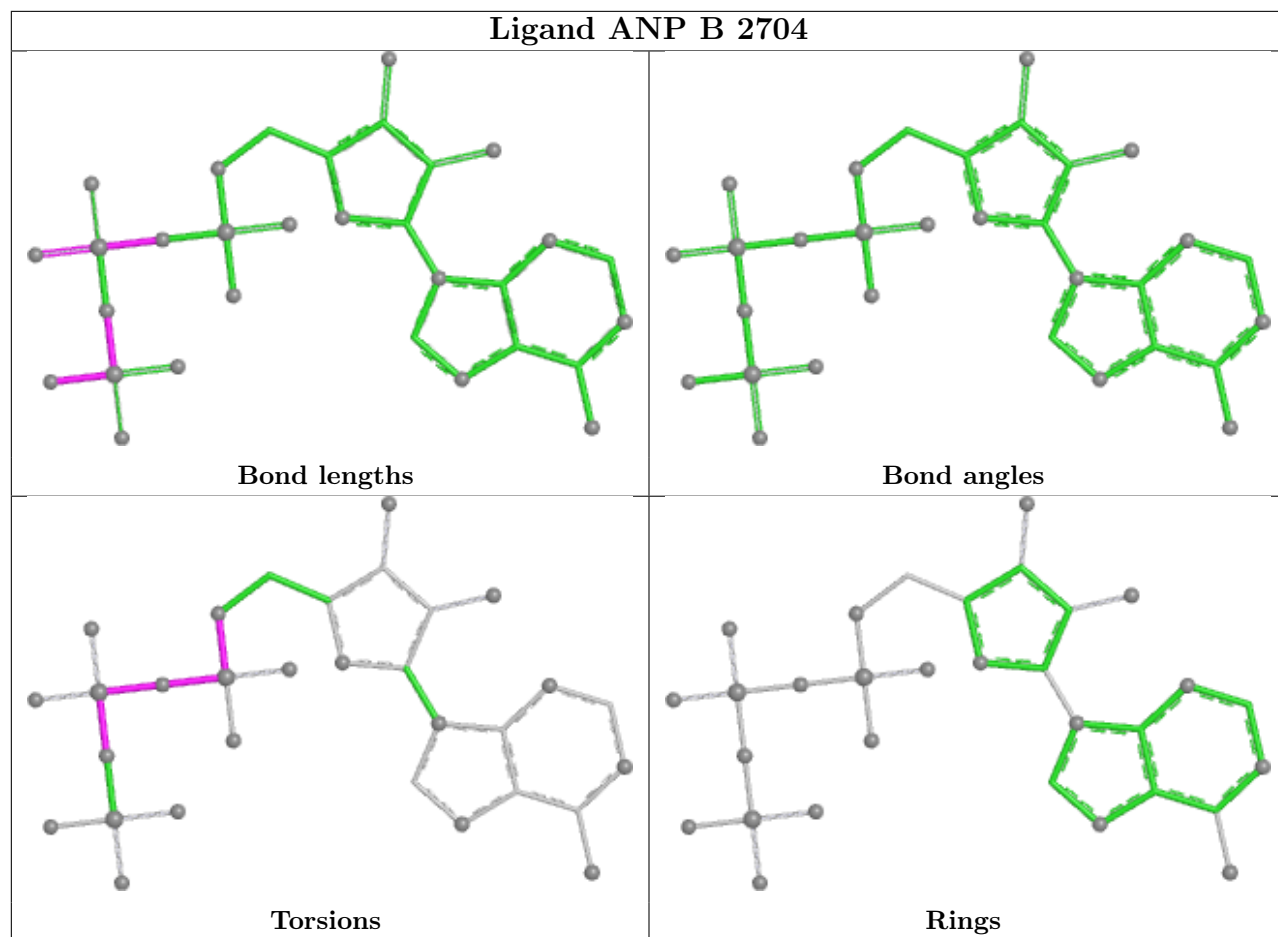
All (9) torsion outliers are listed below:

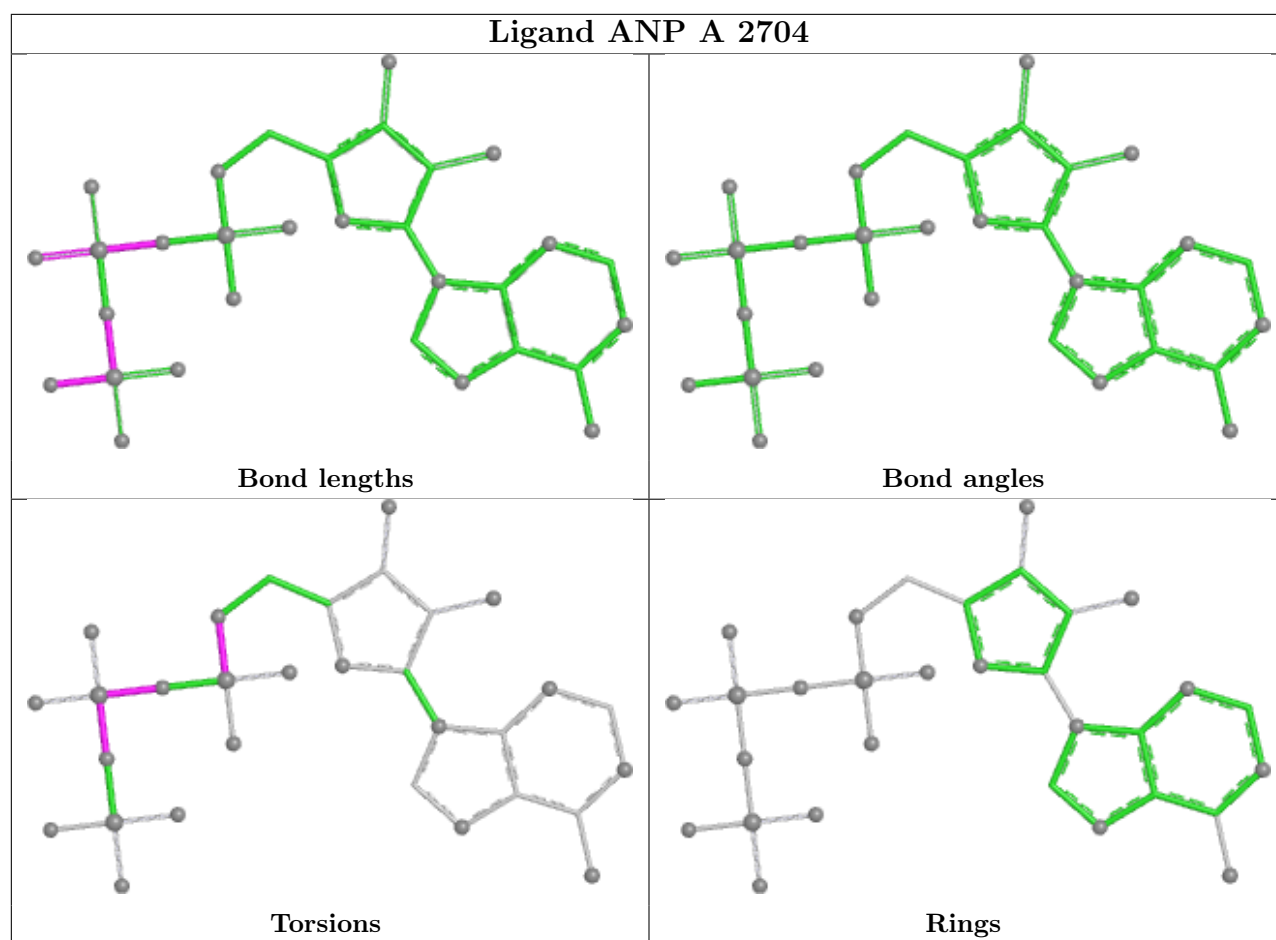
Mol	Chain	Res	Type	Atoms
5	A	2704	ANP	PG-N3B-PB-O1B
5	A	2704	ANP	C5'-O5'-PA-O1A
5	B	2704	ANP	PG-N3B-PB-O1B
5	B	2704	ANP	PA-O3A-PB-O2B
5	B	2704	ANP	C5'-O5'-PA-O1A
5	A	2704	ANP	PA-O3A-PB-O2B
5	B	2704	ANP	PB-O3A-PA-O2A
5	A	2704	ANP	PA-O3A-PB-O1B
5	B	2704	ANP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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.

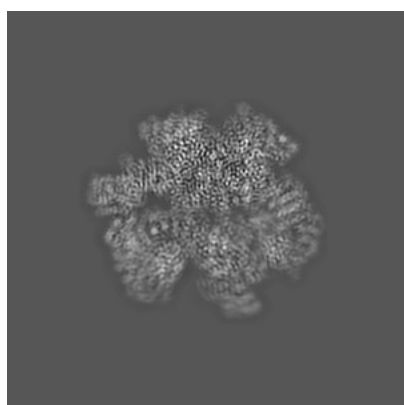
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74045. These allow visual inspection of the internal detail of the map and identification of artifacts.

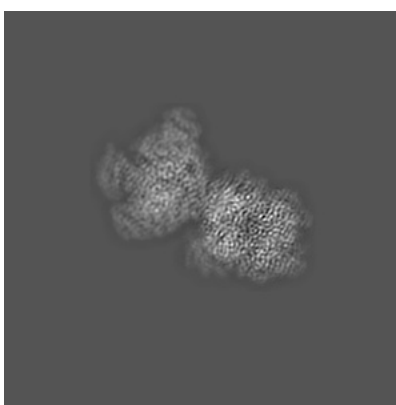
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

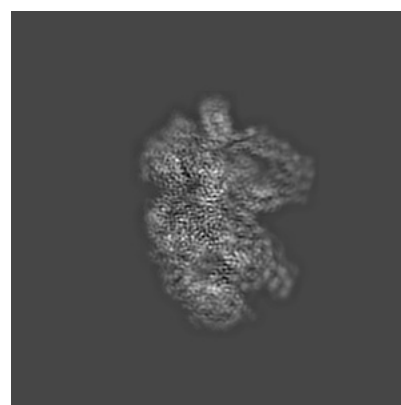
6.1.1 Primary map



X



Y

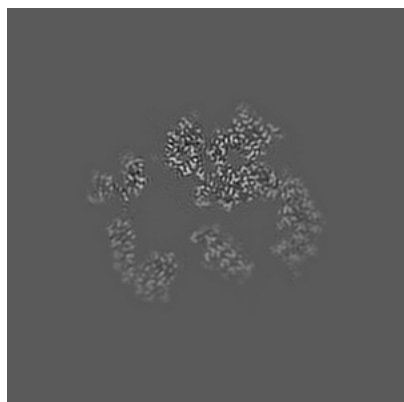


Z

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

6.2 Central slices [i](#)

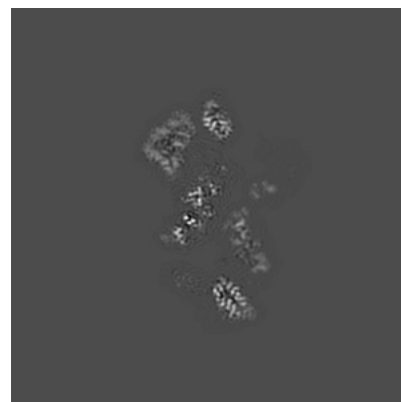
6.2.1 Primary map



X Index: 160



Y Index: 160

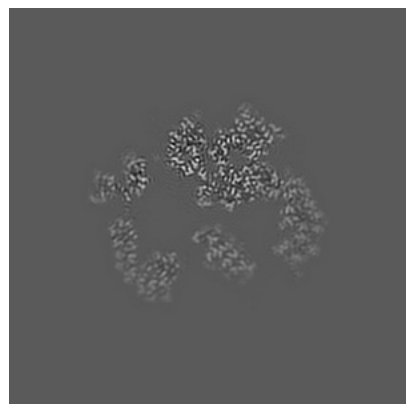


Z Index: 160

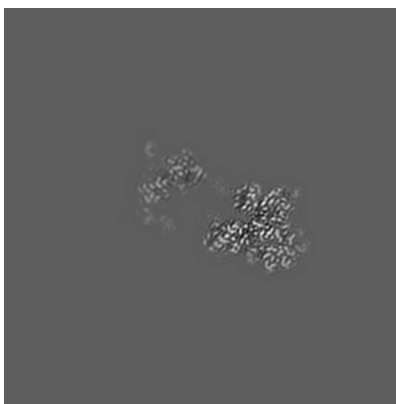
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

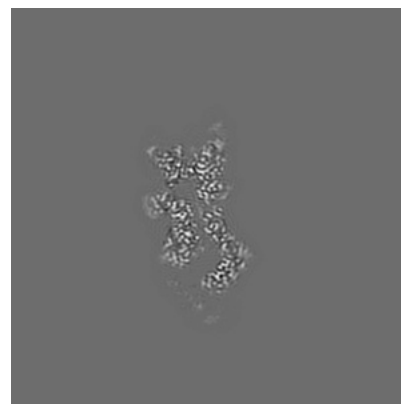
6.3.1 Primary map



X Index: 160



Y Index: 139

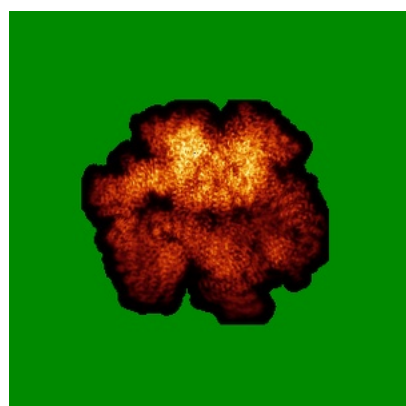


Z Index: 189

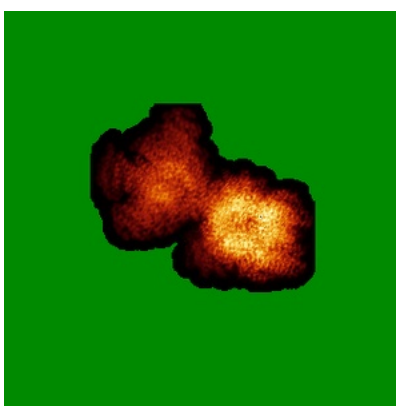
The images above show the largest variance slices of the map in three orthogonal directions.

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

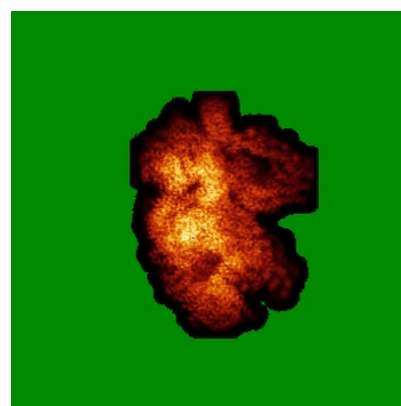
6.4.1 Primary map



X



Y

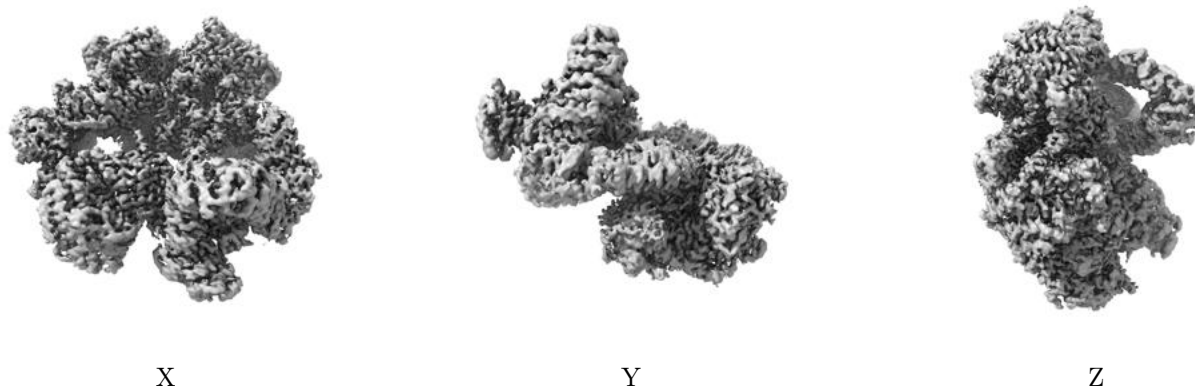


Z

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 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

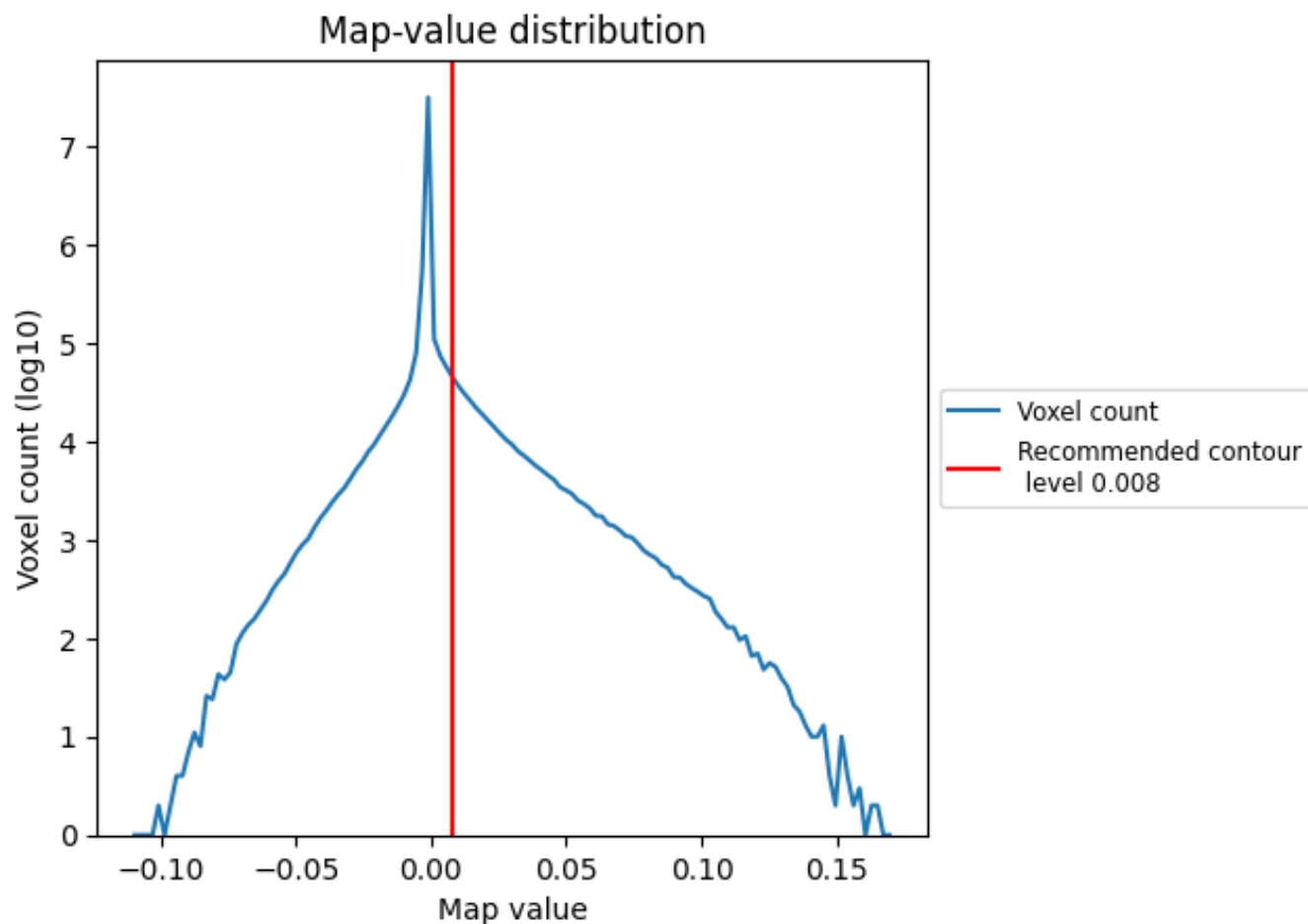
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

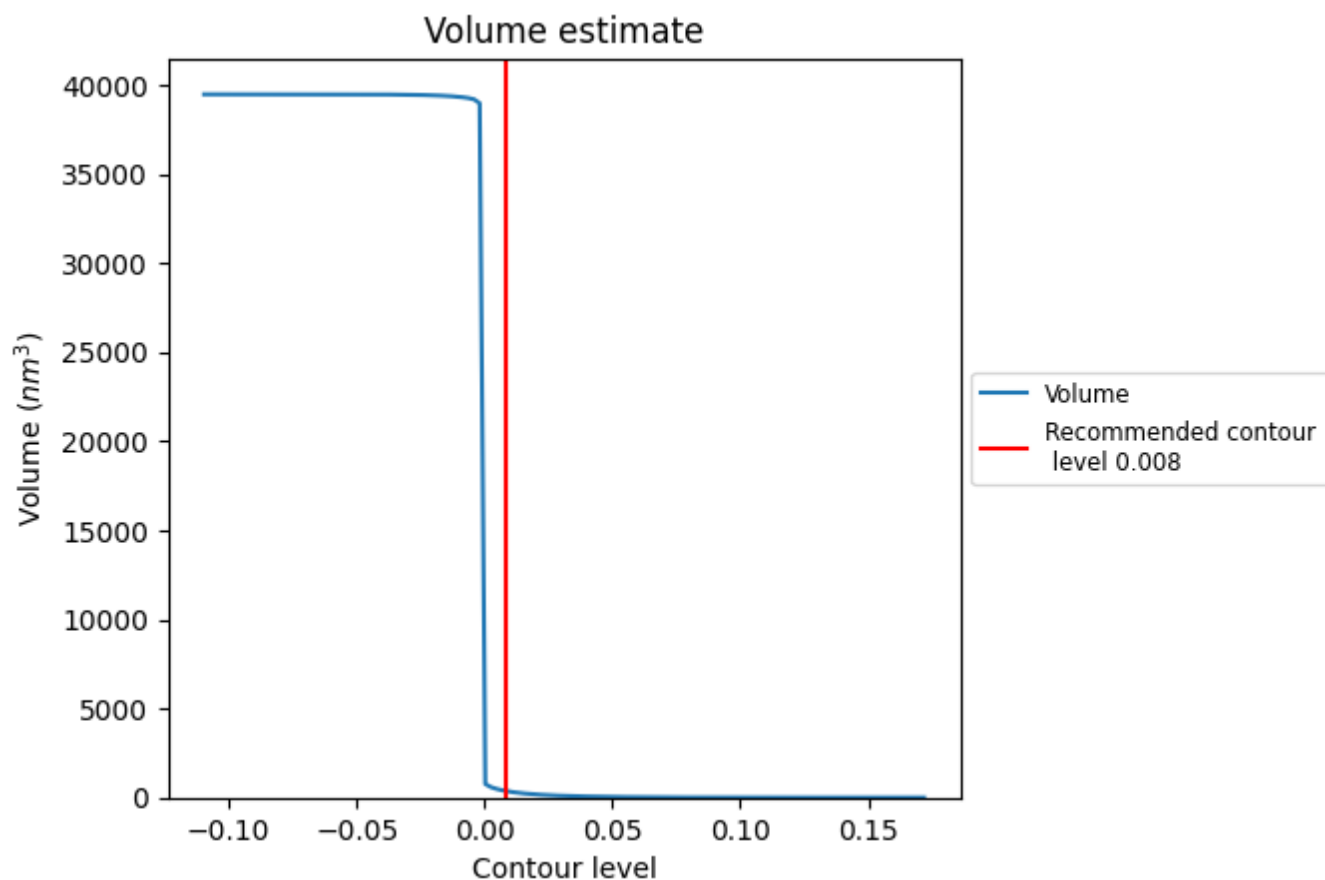
This section contains the results of statistical analysis of the map.

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.

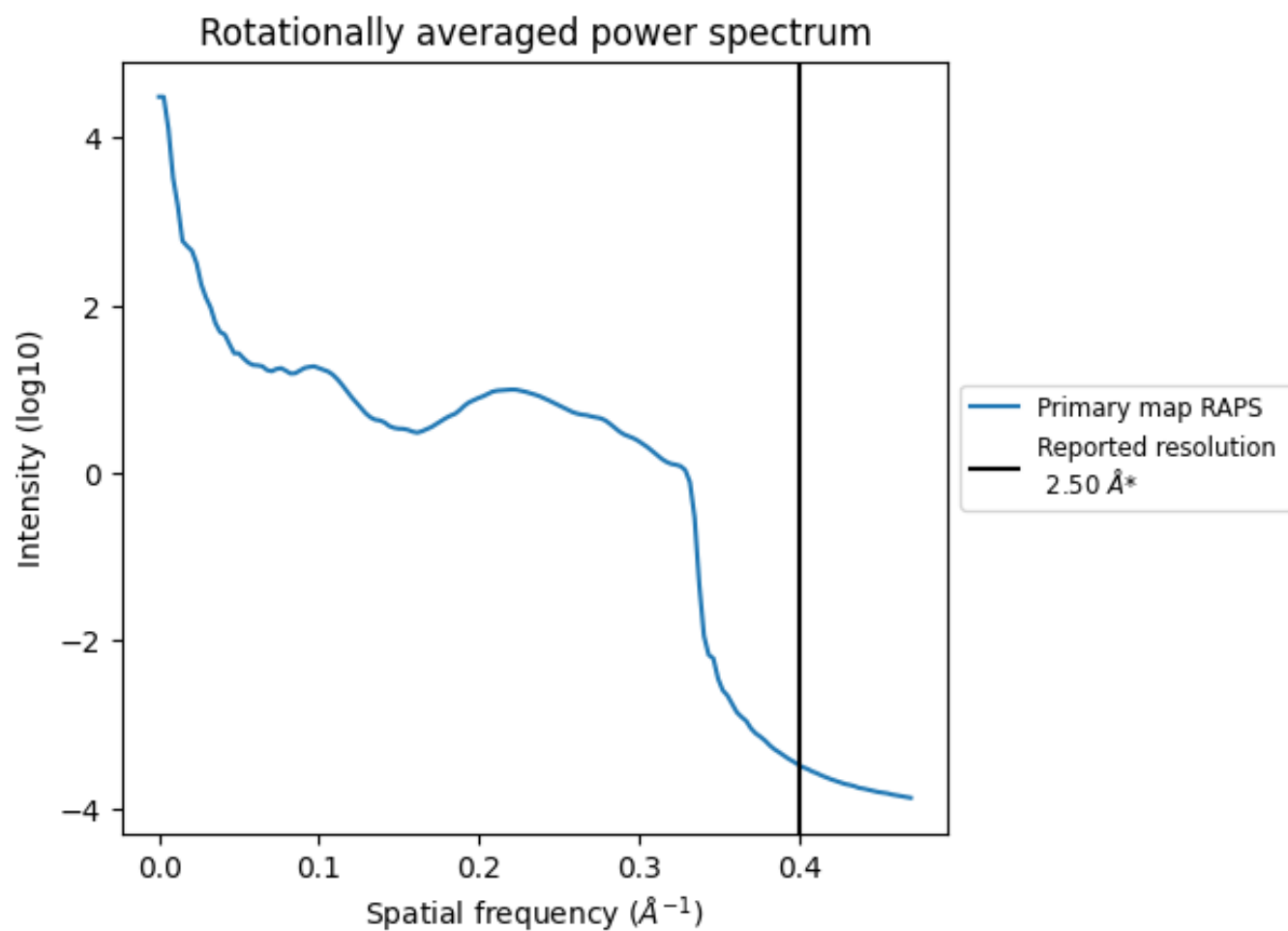
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 379 nm³; this corresponds to an approximate mass of 342 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 0.400 Å⁻¹

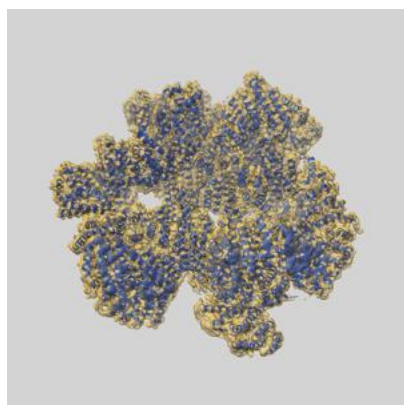
8 Fourier-Shell correlation ⓘ

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

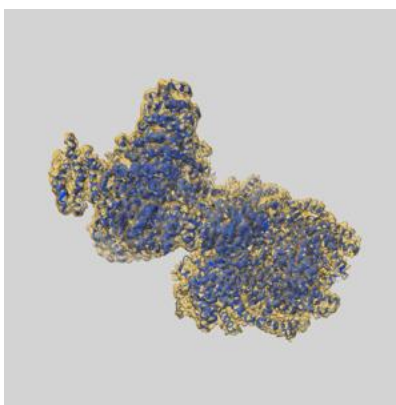
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74045 and PDB model 9ZCY. Per-residue inclusion information can be found in section 3 on page 7.

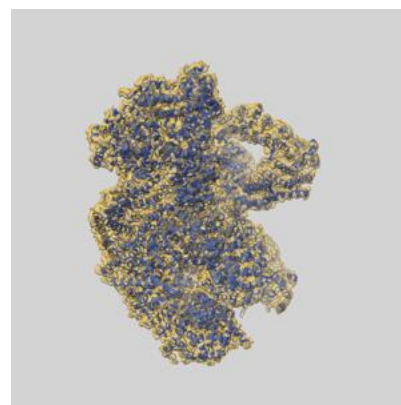
9.1 Map-model overlay [i](#)



X



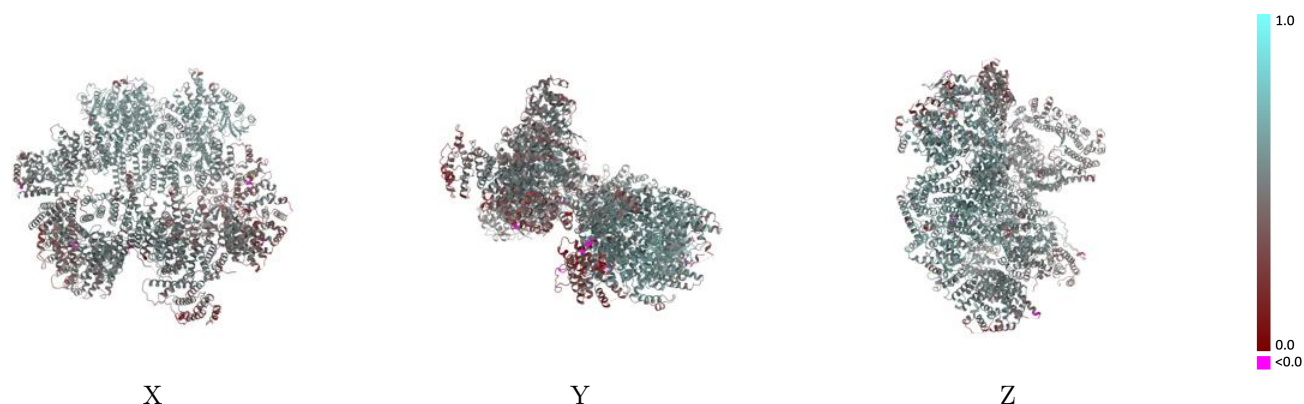
Y



Z

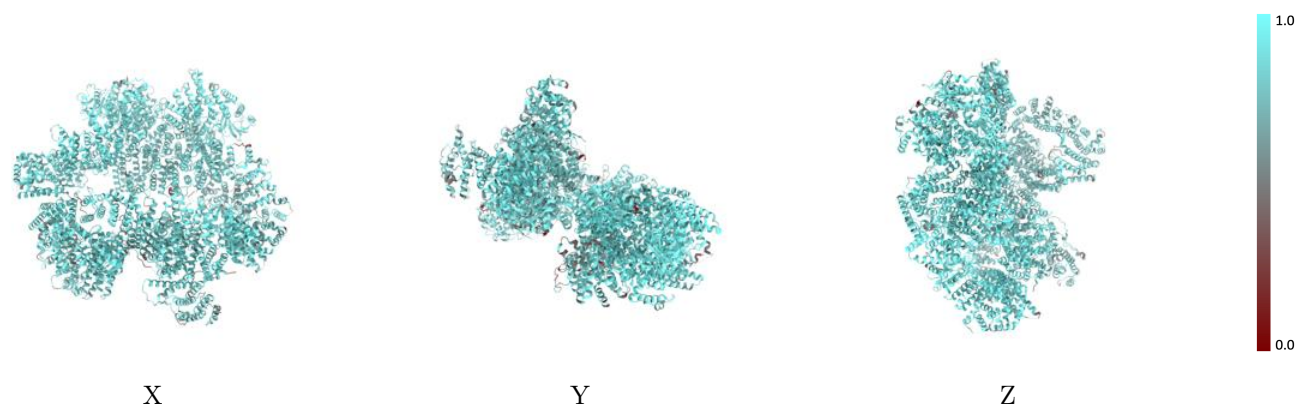
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



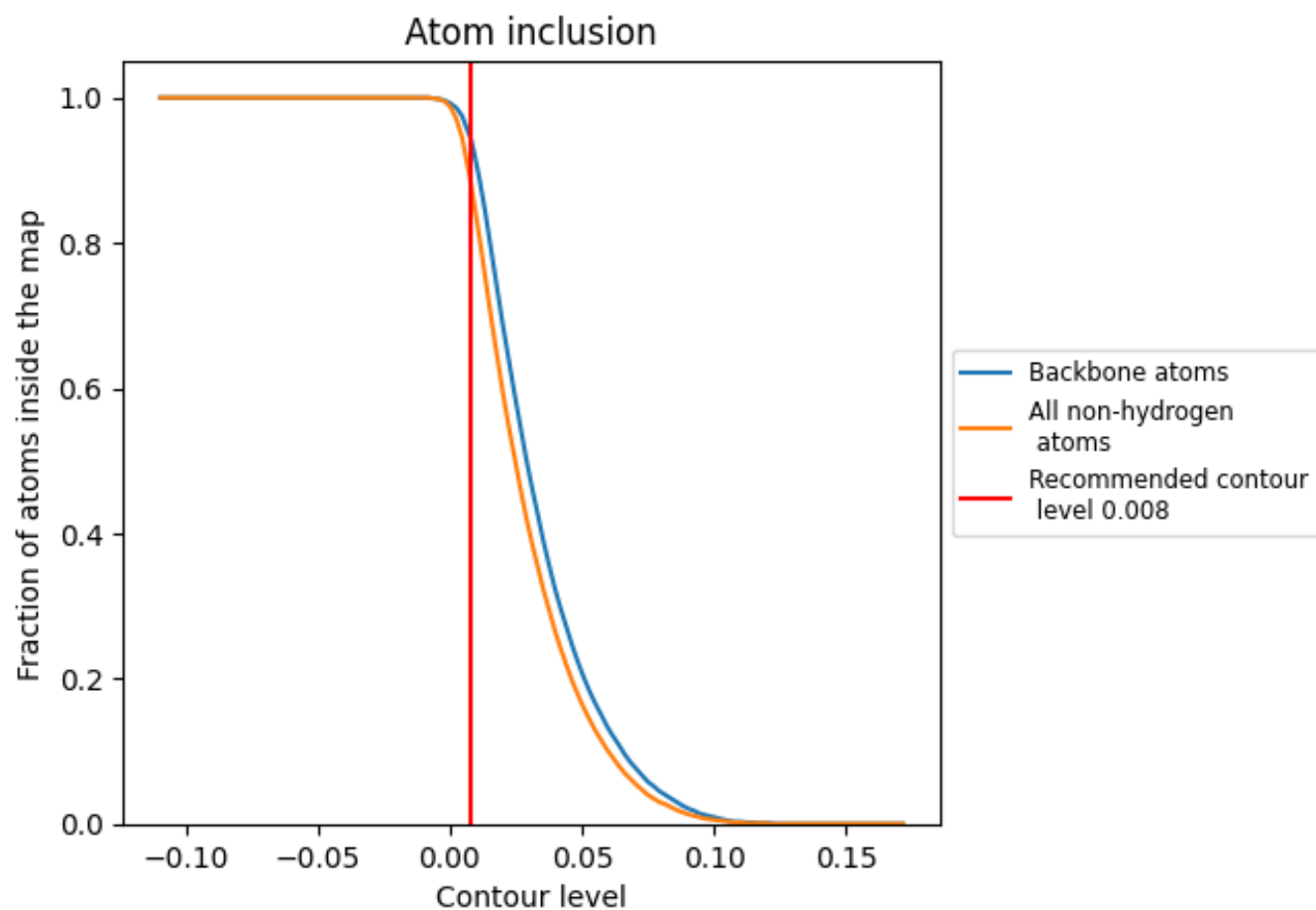
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.008).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 88% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8830	0.5010
A	0.9110	0.5280
B	0.8620	0.4780
C	0.8630	0.4930
D	0.8580	0.4810

