



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 7CPX / pdb_00007cpx
EMDB ID : EMD-30434
Title : Lovastatin nonaketide synthase
Authors : Wang, J.; Wang, Z.
Deposited on : 2020-08-08
Resolution : 2.91 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

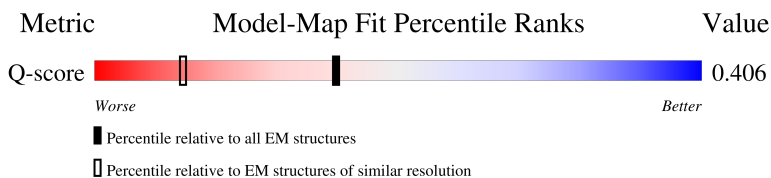
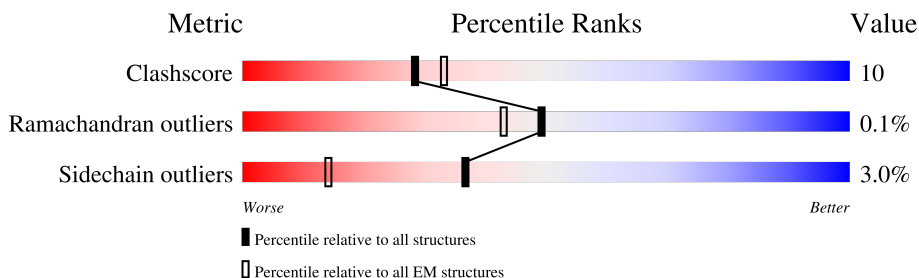
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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	12972 (2.41 - 3.41)

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	3046	
1	B	3046	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 70118 atoms, of which 34718 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.

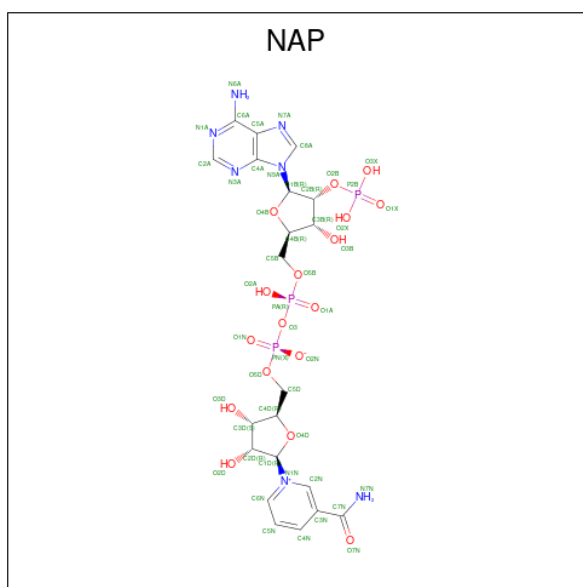
- Molecule 1 is a protein called Lovastatin nonaketide synthase, polyketide synthase component.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2262	Total	C	H	N	O	S	0	0
			34986	11177	17334	3061	3325	89		
1	B	2262	Total	C	H	N	O	S	0	0
			34986	11177	17334	3061	3325	89		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1884	GLN	GLY	engineered mutation	UNP Q9Y8A5
A	1885	ALA	GLN	engineered mutation	UNP Q9Y8A5
A	3039	HIS	-	expression tag	UNP Q9Y8A5
A	3040	VAL	-	expression tag	UNP Q9Y8A5
A	3041	HIS	-	expression tag	UNP Q9Y8A5
A	3042	HIS	-	expression tag	UNP Q9Y8A5
A	3043	HIS	-	expression tag	UNP Q9Y8A5
A	3044	HIS	-	expression tag	UNP Q9Y8A5
A	3045	HIS	-	expression tag	UNP Q9Y8A5
A	3046	HIS	-	expression tag	UNP Q9Y8A5
B	1884	GLN	GLY	engineered mutation	UNP Q9Y8A5
B	1885	ALA	GLN	engineered mutation	UNP Q9Y8A5
B	3039	HIS	-	expression tag	UNP Q9Y8A5
B	3040	VAL	-	expression tag	UNP Q9Y8A5
B	3041	HIS	-	expression tag	UNP Q9Y8A5
B	3042	HIS	-	expression tag	UNP Q9Y8A5
B	3043	HIS	-	expression tag	UNP Q9Y8A5
B	3044	HIS	-	expression tag	UNP Q9Y8A5
B	3045	HIS	-	expression tag	UNP Q9Y8A5
B	3046	HIS	-	expression tag	UNP Q9Y8A5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

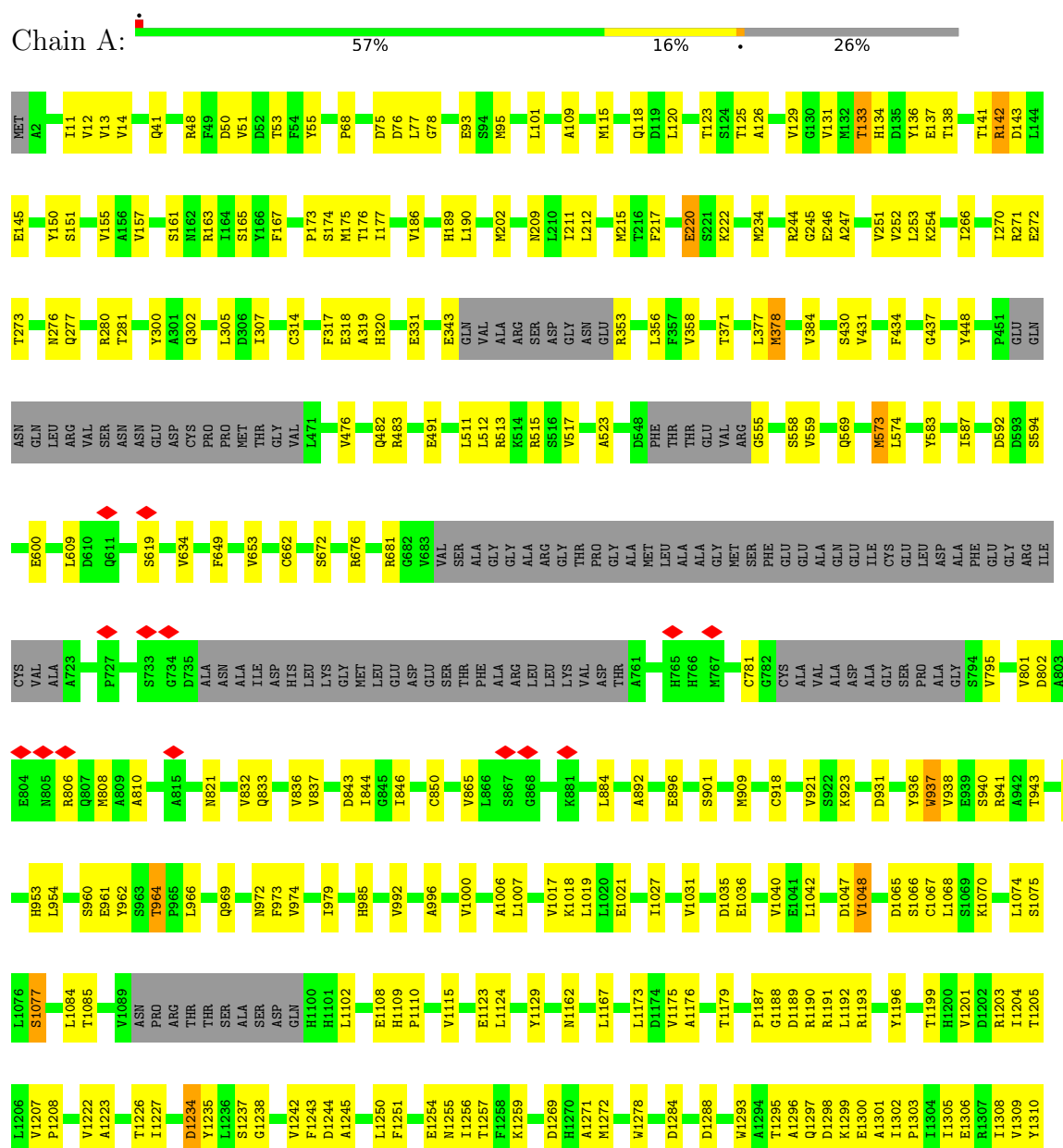


Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0
2	B	1	Total 73	C 21	H 25	N 7	O 17	P 3	0

3 Residue-property plots

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

- Molecule 1: Lovastatin nonaketide synthase, polyketide synthase component





SER	ASN	ALA	ALA	ALA	ALA	ARG	ARG	ASP	ALA	ALA	VAL	VAL	R2378	L2344	SER	L1953	E1797	E1683	L1563	R1436
GLN	GLN	MET	GLY	ASP	THR	VAL	VAL	GLU	ASP	ILE	ASP	ILE	Q2387	V2245	L2083	S1954	W1800	EL683	W1567	E1444
PRO	PRO	ALA	THR	ASP	THR	GLY	GLY	ASP	THR	THR	GLY	THR	Q2387	M2250	Y2087	THR	C1801	F1691	C1576	G1448
PRO	PRO	ALA	ARG	THR	ARG	LEU	LEU	GLU	THR	LEU	LEU	ASP	T2392	N2251	W2088	LYS	R1804	M1692	T1577	G1453
LEU	LEU	LEU	ARG	PRO	HIS	ALA	ALA	PRO	GLU	ASN	ALA	ALA	T2393	N2253	E2089	CYS	T1807	F1583	T1483	T1483
PHE	PHE	ASN	VAL	GLY	ALA	LYS	LYS	GLY	ALA	ASN	LYS	LYS	T2394	N2254	H2090	GLY	T1809	L1701	K1484	K1484
ASN	ASN	VAL	GLY	GLY	GLY	ALA	ALA	GLY	GLY	GLY	GLY	GLY	L2395	E2255	L2094	V1961	P1809	L1580	V1485	V1485
VAL	VAL	GLY	GLY	GLY	GLY	VAL	VAL	M2396	L2256	R2096	R2096	R2096	M2396	L2256	A2095	D1962	R1809	F1702	V1486	V1486
THR	THR	THR	THR	THR	THR	THR	THR	E2400	M2261	L2309	L2309	L2309	E2400	M2261	R1812	D1963	R1812	L1705	F1595	L1462
GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	L2401	V2262	L2099	L2099	L2099	L2401	V2262	D1813	P1970	D1813	T1706	S1600	L1462
PRO	PRO	PRO	PRO	PRO	PRO	PRO	PRO	T2402	L2263	L2309	L2309	L2309	T2402	L2263	R1816	P1971	R1816	K1714	Y1469	Y1469
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	G2404	V2267	L2309	L2309	L2309	G2404	V2267	R1824	C1974	R1824	L1715	T1470	T1470
THR	THR	THR	THR	THR	THR	THR	THR	P2422	V2270	L2309	L2309	L2309	P2422	V2270	I1827	C1975	I1827	L1716	D1471	D1471
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	R2423	H2274	L2309	L2309	L2309	R2423	H2274	M1830	A1992	M1830	T1723	F1487	F1487
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L2424	S2278	L2309	L2309	L2309	L2424	S2278	L1840	GLY	L1840	W1725	R1490	R1490
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	N2426	D2287	L2309	L2309	L2309	N2426	D2287	R1844	ASN	R1844	T1612	M1491	M1491
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	K2428	L2295	L2309	L2309	L2309	K2428	L2295	F1615	ARG	F1615	S1613	I1498	I1498
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	E2431	V2296	L2309	L2309	L2309	E2431	V2296	T1856	SER	T1856	S1616	R1499	R1499
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Y2432	A2297	L2309	L2309	L2309	Y2432	A2297	V1738	VAL	V1738	T1617	L1514	L1514
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ARG	A2300	L2309	L2309	L2309	ARG	A2300	T1740	ALA	T1740	I1515	I1516	I1516
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	N2311	L2309	L2309	L2309	GLY	N2311	L1744	GLY	L1744	D1621	D1621	D1621
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	Q2315	L2309	L2309	L2309	ALA	Q2315	Q1864	ASP	Q1864	A1622	L1521	L1521
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	Q2315	L2309	L2309	L2309	ALA	Q2315	Q1865	ALA	Q1865	T1623	H1522	H1522
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	Q2315	L2309	L2309	L2309	ALA	Q2315	L2168	ALA	L2168	E1625	T1524	T1524
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	A2316	L2309	L2309	L2309	ALA	A2316	M1866	LYS	M1866	Y1626	P1525	P1525
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	Q2319	L2309	L2309	L2309	ALA	Q2319	C1877	S2008	C1877	LEU	D1526	D1526
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	Q2320	L2309	L2309	L2309	ALA	Q2320	V1883	R2015	V1883	ASP	T1530	T1530
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	R2321	L2309	L2309	L2309	ALA	R2321	Q1884	Q2030	Q1884	ALA	T1530	T1530
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	V2322	L2309	L2309	L2309	ALA	V2322	F1888	D2034	F1888	LEU	R1535	R1535
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	T2330	L2309	L2309	L2309	ALA	T2330	L1891	M2049	L1891	SER	L1538	L1538
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	T2331	L2309	L2309	L2309	ALA	T2331	ALA	ASP	ALA	GLY	P1539	P1539
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	D2332	L2309	L2309	L2309	ALA	D2332	THR	ALA	THR	THR	P1540	P1540
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	R2355	L2309	L2309	L2309	ALA	R2355	R1911	A2061	R1911	VAL	G1541	G1541
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	D2359	L2309	L2309	L2309	ALA	D2359	R1919	T2066	R1919	LYS	G1542	G1542
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	S2360	L2309	L2309	L2309	ALA	S2360	A1927	LEU	A1927	ASP	Q1543	Q1543
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	V2361	L2309	L2309	L2309	ALA	V2361	Y1773	SER	Y1773	ASP	M1544	M1544
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2362	L2309	L2309	L2309	ALA	E2362	L1777	SER	L1777	SER	V1545	V1545
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	E1780	P1642	E1780	LYS	L1546	L1546
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	E1781	P1642	E1781	VAL	L1547	L1547
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	Y1941	P1646	Y1941	GLY	E1548	E1548
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1942	V1646	T1942	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	H1551
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	E2365	L2309	L2309	L2309	ALA	E2365	T1943	V1646	T1943	THR	H1551	

LEU
GLN
SER
SER
ARG
TYR
GLU
ALA
HIS
HIS
PRO
GLN
ALA
PHE
LEU
GLU
SER
TYR
MET
SER
LEU
LEU
SER
MET
PHE
SER
MET
ASN
PRO
ALA
LEU
LYS
LEU
ALA
HIS
VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	205047	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.177	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0075	Depositor
Map size ($\text{\AA}$)	350.0, 350.0, 350.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	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: NAP

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	0.12	0/18071	0.32	6/24587 (0.0%)
1	B	0.12	0/18071	0.32	6/24587 (0.0%)
All	All	0.12	0/36142	0.32	12/49174 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1622	ALA	CA-C-N	5.96	132.91	121.54
1	B	1622	ALA	C-N-CA	5.96	132.91	121.54
1	A	1622	ALA	CA-C-N	5.93	132.87	121.54
1	A	1622	ALA	C-N-CA	5.93	132.87	121.54
1	B	947	LEU	CA-C-N	5.13	131.15	122.12
1	B	947	LEU	C-N-CA	5.13	131.15	122.12
1	A	947	LEU	CA-C-N	5.12	131.13	122.12
1	A	947	LEU	C-N-CA	5.12	131.13	122.12
1	B	1794	GLN	CA-C-N	5.04	134.09	121.80
1	B	1794	GLN	C-N-CA	5.04	134.09	121.80
1	A	1794	GLN	CA-C-N	5.02	134.05	121.80
1	A	1794	GLN	C-N-CA	5.02	134.05	121.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17652	17334	17276	340	0
1	B	17652	17334	17276	342	0
2	A	48	25	25	0	0
2	B	48	25	25	0	0
All	All	35400	34718	34602	665	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 10.

All (665) 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:1234:ASP:OD1	1:B:1844:ARG:NH1	2.12	0.82
1:A:1234:ASP:OD1	1:A:1844:ARG:NH1	2.12	0.82
1:B:1176:ALA:O	1:B:1179:THR:OG1	2.01	0.78
1:A:2315:GLN:NE2	1:A:2332:ASP:OD2	2.17	0.78
1:A:2431:GLU:OE1	1:A:2432:TYR:N	2.17	0.78
1:B:2431:GLU:OE1	1:B:2432:TYR:N	2.17	0.77
1:B:2315:GLN:NE2	1:B:2332:ASP:OD2	2.17	0.77
1:B:2252:ASN:OD1	1:B:2253:ASN:ND2	2.18	0.76
1:A:2252:ASN:OD1	1:A:2253:ASN:ND2	2.18	0.76
1:A:1237:SER:OG	1:A:1255:ASN:OD1	2.04	0.76
1:A:2387:GLN:O	1:A:2387:GLN:NE2	2.19	0.75
1:B:1567:TRP:O	1:B:1577:THR:OG1	2.04	0.75
1:B:2387:GLN:O	1:B:2387:GLN:NE2	2.19	0.75
1:A:1567:TRP:O	1:A:1577:THR:OG1	2.04	0.75
1:A:1176:ALA:O	1:A:1179:THR:OG1	2.01	0.74
1:B:320:HIS:N	1:B:331:GLU:OE2	2.21	0.74
1:A:1188:GLY:O	1:A:2355:ARG:NH2	2.21	0.74
1:B:1188:GLY:O	1:B:2355:ARG:NH2	2.21	0.74
1:A:1490:ARG:NH2	1:A:2428:LYS:O	2.21	0.73
1:B:1129:TYR:OH	1:B:1196:TYR:N	2.21	0.73
1:B:1490:ARG:NH2	1:B:2428:LYS:O	2.20	0.73
1:A:1129:TYR:OH	1:A:1196:TYR:N	2.21	0.73
1:B:1237:SER:OG	1:B:1255:ASN:OD1	2.05	0.73
1:B:220:GLU:OE1	1:B:220:GLU:N	2.22	0.72
1:A:1471:ASP:OD1	1:A:1472:ILE:N	2.22	0.72
1:A:320:HIS:N	1:A:331:GLU:OE2	2.21	0.72
1:A:220:GLU:N	1:A:220:GLU:OE1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1471:ASP:OD1	1:B:1472:ILE:N	2.22	0.72
1:A:2148:ASP:O	1:A:2179:HIS:NE2	2.23	0.72
1:B:676:ARG:NE	1:B:781:CYS:SG	2.63	0.71
1:B:2148:ASP:O	1:B:2179:HIS:NE2	2.23	0.71
1:B:1271:ALA:O	1:B:1812:ARG:NH1	2.24	0.70
1:A:676:ARG:NE	1:A:781:CYS:SG	2.63	0.70
1:B:2250:MET:O	1:B:2254:MET:N	2.24	0.70
1:A:1271:ALA:O	1:A:1812:ARG:NH1	2.24	0.70
1:A:1306:GLU:OE2	1:A:1556:ARG:NE	2.23	0.70
1:B:1306:GLU:OE2	1:B:1556:ARG:NE	2.23	0.70
1:A:2250:MET:O	1:A:2254:MET:N	2.25	0.69
1:A:300:TYR:OH	1:A:314:CYS:SG	2.52	0.68
1:A:1297:GLN:O	1:A:1301:ALA:N	2.27	0.68
1:B:300:TYR:OH	1:B:314:CYS:SG	2.52	0.67
1:B:2315:GLN:HA	1:B:2330:THR:HG21	1.76	0.67
1:A:318:GLU:N	1:A:430:SER:O	2.28	0.67
1:B:1297:GLN:O	1:B:1301:ALA:N	2.27	0.67
1:B:1366:ILE:HG23	1:B:1379:VAL:HG22	1.77	0.67
1:A:141:THR:O	1:B:215:MET:HE1	1.96	0.67
1:A:1366:ILE:HG23	1:A:1379:VAL:HG22	1.77	0.66
1:A:1326:GLN:NE2	1:A:1563:LEU:O	2.28	0.66
1:A:50:ASP:O	1:A:53:THR:OG1	2.10	0.66
1:A:137:GLU:O	1:A:141:THR:OG1	2.13	0.66
1:B:318:GLU:N	1:B:430:SER:O	2.28	0.66
1:B:1326:GLN:NE2	1:B:1563:LEU:O	2.28	0.66
1:B:50:ASP:O	1:B:53:THR:OG1	2.10	0.66
1:B:1284:ASP:OD1	1:B:1804:ARG:NH2	2.29	0.65
1:A:483:ARG:NH1	1:A:931:ASP:OD1	2.29	0.65
1:B:483:ARG:NH1	1:B:931:ASP:OD1	2.29	0.65
1:A:215:MET:HE1	1:B:141:THR:O	1.95	0.65
1:A:574:LEU:HG	1:A:634:VAL:HG22	1.78	0.65
1:A:1284:ASP:OD1	1:A:1804:ARG:NH2	2.29	0.65
1:A:2167:ASP:OD1	1:A:2170:ARG:NH2	2.30	0.65
1:A:2315:GLN:HA	1:A:2330:THR:HG21	1.76	0.65
1:A:482:GLN:N	1:A:482:GLN:OE1	2.30	0.64
1:B:1031:VAL:HG13	1:B:1040:VAL:HG11	1.79	0.64
1:B:482:GLN:OE1	1:B:482:GLN:N	2.30	0.64
1:B:574:LEU:HG	1:B:634:VAL:HG22	1.78	0.64
1:A:1749:ARG:NH1	1:A:2300:GLY:O	2.31	0.64
1:A:190:LEU:HD21	1:B:175:MET:HE2	1.80	0.64
1:B:161:SER:OG	1:B:174:SER:O	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2263:LEU:O	1:B:2267:VAL:N	2.28	0.64
1:B:137:GLU:O	1:B:141:THR:OG1	2.13	0.64
1:B:13:VAL:HG13	1:B:251:VAL:HG13	1.79	0.63
1:B:209:ASN:ND2	1:B:245:GLY:O	2.31	0.63
1:A:209:ASN:ND2	1:A:245:GLY:O	2.31	0.63
1:A:1840:LEU:HD23	1:A:2129:ILE:HD13	1.81	0.63
1:B:1749:ARG:NH1	1:B:2300:GLY:O	2.31	0.63
1:B:1840:LEU:HD23	1:B:2129:ILE:HD13	1.81	0.63
1:B:1238:GLY:O	1:B:1256:ILE:HG22	1.99	0.63
1:A:175:MET:HE2	1:B:190:LEU:HD21	1.80	0.62
1:A:161:SER:OG	1:A:174:SER:O	2.11	0.62
1:B:2167:ASP:OD1	1:B:2170:ARG:NH2	2.30	0.62
1:A:2237:GLY:O	1:A:2287:ASP:N	2.31	0.62
1:A:13:VAL:HG13	1:A:251:VAL:HG13	1.79	0.62
1:A:1031:VAL:HG13	1:A:1040:VAL:HG11	1.79	0.62
1:A:2263:LEU:O	1:A:2267:VAL:N	2.28	0.62
1:B:1609:LEU:O	1:B:1613:SER:OG	2.14	0.62
1:A:1238:GLY:O	1:A:1256:ILE:HG22	1.99	0.61
1:A:1609:LEU:O	1:A:1613:SER:OG	2.14	0.61
1:A:134:HIS:O	1:A:134:HIS:ND1	2.33	0.61
1:A:1284:ASP:O	1:A:1600:SER:OG	2.16	0.60
1:A:129:VAL:O	1:A:177:ILE:N	2.33	0.60
1:A:559:VAL:HG21	1:A:846:ILE:HD12	1.82	0.60
1:A:1435:HIS:O	1:A:1809:ARG:NE	2.34	0.60
1:A:115:MET:HE1	1:A:254:LYS:HD2	1.84	0.60
1:B:320:HIS:NE2	1:B:434:PHE:O	2.34	0.60
1:A:1429:LEU:HD23	1:A:1545:VAL:HG13	1.84	0.60
1:B:1429:LEU:HD23	1:B:1545:VAL:HG13	1.84	0.60
1:B:1435:HIS:O	1:B:1809:ARG:NE	2.34	0.60
1:B:115:MET:HE1	1:B:254:LYS:HD2	1.83	0.60
1:B:129:VAL:O	1:B:177:ILE:N	2.33	0.60
1:B:1189:ASP:OD1	1:B:1190:ARG:N	2.35	0.60
1:B:1381:LEU:HD11	1:B:1409:LEU:HA	1.84	0.60
1:B:134:HIS:O	1:B:134:HIS:ND1	2.33	0.59
1:A:320:HIS:NE2	1:A:434:PHE:O	2.34	0.59
1:B:559:VAL:HG21	1:B:846:ILE:HD12	1.82	0.59
1:B:1284:ASP:O	1:B:1600:SER:OG	2.16	0.59
1:A:1381:LEU:HD11	1:A:1409:LEU:HA	1.84	0.59
1:B:1115:VAL:HG13	1:B:1187:PRO:HD3	1.84	0.59
1:A:1115:VAL:HG13	1:A:1187:PRO:HD3	1.84	0.59
1:B:1522:HIS:N	1:B:1548:GLU:OE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1969:ASN:N	1:B:1992:ALA:O	2.33	0.59
1:B:569:GLN:N	1:B:569:GLN:OE1	2.35	0.58
1:A:1189:ASP:OD1	1:A:1190:ARG:N	2.35	0.58
1:B:1199:THR:HG21	1:B:1259:LYS:HB3	1.85	0.58
1:A:343:GLU:N	1:A:343:GLU:OE1	2.36	0.58
1:B:343:GLU:N	1:B:343:GLU:OE1	2.36	0.58
1:B:1017:VAL:HG23	1:B:1208:PRO:HG3	1.86	0.58
1:B:1793:THR:HG21	1:B:2422:PRO:HB3	1.85	0.58
1:A:1522:HIS:N	1:A:1548:GLU:OE2	2.36	0.58
1:B:377:LEU:HA	1:B:431:VAL:HG21	1.85	0.58
1:B:2237:GLY:O	1:B:2287:ASP:N	2.31	0.58
1:A:1199:THR:HG21	1:A:1259:LYS:HB3	1.85	0.58
1:B:574:LEU:HD11	1:B:634:VAL:HA	1.85	0.58
1:A:175:MET:HE3	1:B:186:VAL:HG13	1.85	0.58
1:A:377:LEU:HA	1:A:431:VAL:HG21	1.85	0.58
1:B:1498:ILE:O	1:B:1530:THR:HG22	2.04	0.58
1:A:133:THR:HG21	1:A:244:ARG:NH1	2.19	0.57
1:A:186:VAL:HG13	1:B:175:MET:HE3	1.85	0.57
1:A:2090:HIS:NE2	1:A:2094:LEU:HD11	2.19	0.57
1:A:1793:THR:HG21	1:A:2422:PRO:HB3	1.85	0.57
1:A:1498:ILE:O	1:A:1530:THR:HG22	2.04	0.57
1:A:138:THR:O	1:A:142:ARG:N	2.38	0.57
1:B:2090:HIS:NE2	1:B:2094:LEU:HD11	2.20	0.57
1:A:120:LEU:O	1:A:123:THR:HG22	2.05	0.57
1:A:574:LEU:HD11	1:A:634:VAL:HA	1.85	0.57
1:A:1017:VAL:HG23	1:A:1208:PRO:HG3	1.86	0.57
1:A:1191:ARG:N	1:A:2362:GLU:OE2	2.37	0.57
1:A:523:ALA:HB3	1:A:892:ALA:HB1	1.87	0.57
1:B:1191:ARG:N	1:B:2362:GLU:OE2	2.37	0.57
1:B:133:THR:HG21	1:B:244:ARG:NH1	2.19	0.57
1:B:1123:GLU:OE2	1:B:1190:ARG:N	2.38	0.57
1:A:569:GLN:OE1	1:A:569:GLN:N	2.35	0.56
1:A:1123:GLU:OE2	1:A:1190:ARG:N	2.38	0.56
1:A:1189:ASP:O	1:A:2360:SER:OG	2.22	0.56
1:A:1702:PHE:CD2	1:A:2263:LEU:HD21	2.40	0.56
1:B:138:THR:O	1:B:142:ARG:N	2.38	0.56
1:A:189:HIS:ND1	1:A:273:THR:O	2.39	0.56
1:B:1309:VAL:HG23	1:B:1352:LEU:O	2.05	0.56
1:B:48:ARG:NH2	1:B:246:GLU:OE2	2.39	0.56
1:B:300:TYR:HH	1:B:314:CYS:HG	1.54	0.56
1:B:1801:CYS:HG	1:B:2392:THR:HG1	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:O	1:B:123:THR:HG22	2.05	0.56
1:A:211:ILE:HG23	1:A:217:PHE:HE1	1.71	0.56
1:B:523:ALA:HB3	1:B:892:ALA:HB1	1.87	0.56
1:A:653:VAL:HG12	1:A:662:CYS:SG	2.46	0.56
1:A:1234:ASP:OD1	1:A:1235:TYR:N	2.39	0.56
1:A:1309:VAL:HG23	1:A:1352:LEU:O	2.05	0.56
1:B:1234:ASP:OD1	1:B:1235:TYR:N	2.39	0.56
1:A:48:ARG:NH2	1:A:246:GLU:OE2	2.39	0.55
1:A:2359:ASP:N	1:A:2404:GLY:O	2.35	0.55
1:B:972:ASN:OD1	1:B:973:PHE:N	2.39	0.55
1:B:1691:PHE:HB2	1:B:1723:THR:HG23	1.88	0.55
1:A:559:VAL:HG23	1:A:844:ILE:HG23	1.89	0.55
1:B:123:THR:HG23	1:B:125:THR:H	1.71	0.55
1:A:1745:ARG:NH1	1:A:2297:ALA:O	2.35	0.55
1:A:1969:ASN:N	1:A:1992:ALA:O	2.33	0.55
1:A:972:ASN:OD1	1:A:973:PHE:N	2.39	0.55
1:B:145:GLU:OE1	1:B:145:GLU:N	2.39	0.55
1:B:1702:PHE:CD2	1:B:2263:LEU:HD21	2.40	0.55
1:A:1714:LYS:NZ	1:A:2254:MET:O	2.33	0.55
1:B:1963:ASP:N	1:B:2030:GLN:OE1	2.36	0.55
1:A:123:THR:HG23	1:A:125:THR:H	1.72	0.55
1:A:2252:ASN:OD1	1:A:2253:ASN:N	2.40	0.55
1:B:189:HIS:ND1	1:B:273:THR:O	2.38	0.55
1:B:653:VAL:HG12	1:B:662:CYS:SG	2.46	0.55
1:B:1714:LYS:NZ	1:B:2254:MET:O	2.33	0.55
1:B:1813:ASP:OD2	1:B:1816:ARG:NE	2.40	0.55
1:B:2252:ASN:OD1	1:B:2253:ASN:N	2.40	0.55
1:A:1813:ASP:OD2	1:A:1816:ARG:NE	2.40	0.55
1:B:1381:LEU:HD13	1:B:1560:ILE:CD1	2.37	0.55
1:B:1942:VAL:HG13	1:B:1974:CYS:HA	1.89	0.55
1:B:2049:MET:HE2	1:B:2049:MET:HA	1.89	0.55
1:B:118:GLN:NE2	1:B:517:VAL:O	2.39	0.54
1:B:1691:PHE:CB	1:B:1723:THR:HG23	2.37	0.54
1:A:974:VAL:HG13	1:A:979:ILE:HD12	1.90	0.54
1:A:1590:LEU:HD13	1:A:1595:PHE:HB2	1.89	0.54
1:A:280:ARG:NH2	1:B:167:PHE:O	2.41	0.54
1:A:1691:PHE:HB2	1:A:1723:THR:HG23	1.88	0.54
1:B:211:ILE:HG23	1:B:217:PHE:HE1	1.71	0.54
1:A:1035:ASP:OD1	1:A:1036:GLU:N	2.39	0.54
1:A:2049:MET:HA	1:A:2049:MET:HE2	1.89	0.54
1:B:974:VAL:HG13	1:B:979:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:559:VAL:HG23	1:B:844:ILE:HG23	1.89	0.54
1:B:1381:LEU:O	1:B:1385:VAL:HG22	2.08	0.54
1:A:1381:LEU:HD13	1:A:1560:ILE:CD1	2.37	0.54
1:B:2319:GLN:NE2	1:B:2400:GLU:OE2	2.41	0.54
1:B:1590:LEU:HD13	1:B:1595:PHE:HB2	1.89	0.54
1:A:1725:TRP:CD2	1:A:1744:LEU:HD13	2.43	0.53
1:B:1865:GLN:OE1	1:B:1919:ARG:NE	2.41	0.53
1:B:2158:THR:OG1	1:B:2234:PRO:O	2.25	0.53
1:A:1691:PHE:CB	1:A:1723:THR:HG23	2.37	0.53
1:A:2319:GLN:NE2	1:A:2400:GLU:OE2	2.41	0.53
1:B:1725:TRP:CD2	1:B:1744:LEU:HD13	2.43	0.53
1:A:1942:VAL:HG13	1:A:1974:CYS:HA	1.89	0.53
1:B:1911:ARG:NH2	1:B:2150:GLU:OE2	2.40	0.53
1:A:1381:LEU:HD12	1:A:1412:PHE:HB2	1.90	0.53
1:A:1515:ILE:HD12	1:A:1538:LEU:HG	1.91	0.53
1:B:1745:ARG:NH1	1:B:2297:ALA:O	2.35	0.53
1:A:1865:GLN:OE1	1:A:1919:ARG:NE	2.41	0.53
1:A:1911:ARG:NH2	1:A:2150:GLU:OE2	2.40	0.53
1:A:2108:VAL:HA	1:A:2128:VAL:HG13	1.91	0.53
1:B:2359:ASP:OD1	1:B:2360:SER:N	2.42	0.53
1:B:133:THR:HG21	1:B:244:ARG:HH12	1.74	0.52
1:B:1381:LEU:HD12	1:B:1412:PHE:HB2	1.90	0.52
1:B:523:ALA:CB	1:B:892:ALA:HB1	2.39	0.52
1:A:167:PHE:O	1:B:280:ARG:NH2	2.41	0.52
1:A:1381:LEU:O	1:A:1385:VAL:HG22	2.08	0.52
1:B:2108:VAL:HA	1:B:2128:VAL:HG13	1.91	0.52
1:A:801:VAL:HG21	1:A:821:ASN:HA	1.92	0.52
1:A:1193:ARG:NH2	1:A:2365:GLU:OE2	2.43	0.52
1:A:2296:VAL:O	1:A:2300:GLY:N	2.38	0.52
1:B:1760:ASP:O	1:B:1800:TRP:N	2.38	0.52
1:A:1222:VAL:HG11	1:A:1250:LEU:HD11	1.92	0.52
1:A:2359:ASP:OD1	1:A:2360:SER:N	2.42	0.52
1:A:1031:VAL:CG1	1:A:1040:VAL:HG11	2.40	0.52
1:A:1235:TYR:CD1	1:A:1257:THR:HG23	2.45	0.52
1:A:1683:GLU:OE1	1:A:1683:GLU:N	2.42	0.52
1:B:1326:GLN:HA	1:B:1330:PHE:HB3	1.92	0.52
1:B:1515:ILE:HD12	1:B:1538:LEU:HG	1.91	0.52
1:B:2359:ASP:N	1:B:2404:GLY:O	2.35	0.52
1:A:51:VAL:HG21	1:A:68:PRO:HA	1.92	0.52
1:A:523:ALA:CB	1:A:892:ALA:HB1	2.39	0.51
1:A:14:VAL:O	1:A:923:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:ASP:HA	1:A:1824:ARG:NH2	2.25	0.51
1:A:1963:ASP:N	1:A:2030:GLN:OE1	2.35	0.51
1:B:1035:ASP:OD1	1:B:1036:GLU:N	2.39	0.51
1:B:1193:ARG:NH2	1:B:2365:GLU:OE2	2.43	0.51
1:A:51:VAL:O	1:A:55:TYR:N	2.44	0.51
1:B:1031:VAL:CG1	1:B:1040:VAL:HG11	2.40	0.51
1:B:1354:TYR:CE1	1:B:1362:THR:HG21	2.46	0.51
1:A:1375:TYR:O	1:A:1379:VAL:HG12	2.11	0.51
1:B:51:VAL:HG21	1:B:68:PRO:HA	1.92	0.51
1:B:75:ASP:OD1	1:B:76:ASP:N	2.44	0.51
1:B:1201:VAL:HG11	1:B:1204:ILE:HD11	1.93	0.51
1:B:129:VAL:HG12	1:B:131:VAL:HG13	1.93	0.51
1:B:1235:TYR:CD1	1:B:1257:THR:HG23	2.45	0.51
1:B:1375:TYR:O	1:B:1379:VAL:HG12	2.11	0.51
1:A:75:ASP:OD1	1:A:76:ASP:N	2.44	0.51
1:A:966:LEU:O	1:A:1048:VAL:HG12	2.11	0.51
1:A:1326:GLN:HA	1:A:1330:PHE:HB3	1.92	0.51
1:A:1354:TYR:CE1	1:A:1362:THR:HG21	2.46	0.51
1:A:2295:ILE:HD13	1:A:2403:THR:O	2.11	0.51
1:B:51:VAL:O	1:B:55:TYR:N	2.44	0.51
1:B:1269:ASP:HA	1:B:1824:ARG:NH2	2.25	0.51
1:B:1971:PRO:O	1:B:1975:GLY:N	2.40	0.51
1:A:133:THR:HG21	1:A:244:ARG:HH12	1.74	0.50
1:A:1124:LEU:HB3	1:A:1129:TYR:HB2	1.92	0.50
1:B:921:VAL:HG22	1:B:921:VAL:O	2.11	0.50
1:B:1222:VAL:HG11	1:B:1250:LEU:HD11	1.92	0.50
1:A:129:VAL:HG12	1:A:131:VAL:HG13	1.93	0.50
1:A:1526:ASP:O	1:A:1530:THR:HG23	2.12	0.50
1:A:1551:HIS:HE2	1:A:1583:PHE:HD2	1.58	0.50
1:B:2295:ILE:HD13	1:B:2403:THR:O	2.11	0.50
1:A:118:GLN:NE2	1:A:517:VAL:O	2.39	0.50
1:B:801:VAL:HG21	1:B:821:ASN:HA	1.92	0.50
1:B:966:LEU:O	1:B:1048:VAL:HG12	2.11	0.50
1:B:1540:PRO:O	1:B:1790:THR:OG1	2.27	0.50
1:A:317:PHE:HB2	1:A:356:LEU:HD21	1.94	0.50
1:A:1201:VAL:HG11	1:A:1204:ILE:HD11	1.93	0.50
1:B:138:THR:HG21	1:B:215:MET:HG3	1.93	0.50
1:A:921:VAL:HG22	1:A:921:VAL:O	2.11	0.50
1:A:1065:ASP:OD2	1:B:964:THR:OG1	2.26	0.50
1:B:1948:LEU:HD13	1:B:1948:LEU:C	2.36	0.50
1:B:1124:LEU:HB3	1:B:1129:TYR:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1201:VAL:HG11	1:B:1204:ILE:HG13	1.94	0.50
1:B:2297:ALA:HB2	1:B:2311:ASN:HB2	1.93	0.50
1:A:1732:VAL:HG22	1:A:2396:MET:HE1	1.94	0.50
1:A:2196:LYS:HZ3	1:A:2197:TRP:N	2.09	0.50
1:A:2297:ALA:HB2	1:A:2311:ASN:HB2	1.93	0.50
1:A:138:THR:HG21	1:A:215:MET:HG3	1.93	0.49
1:A:1499:ARG:NH2	1:A:1523:ALA:O	2.44	0.49
1:A:145:GLU:N	1:A:145:GLU:OE1	2.39	0.49
1:B:802:ASP:OD2	1:B:806:ARG:N	2.43	0.49
1:B:1551:HIS:HE2	1:B:1583:PHE:HD2	1.58	0.49
1:B:1576:CYS:O	1:B:1577:THR:HG22	2.13	0.49
1:B:1725:TRP:CH2	1:B:1744:LEU:HD22	2.48	0.49
1:A:1948:LEU:C	1:A:1948:LEU:HD13	2.36	0.49
1:B:1499:ARG:NH2	1:B:1523:ALA:O	2.44	0.49
1:B:1732:VAL:HG22	1:B:2396:MET:HE1	1.94	0.49
1:A:1201:VAL:HG11	1:A:1204:ILE:HG13	1.94	0.49
1:A:1760:ASP:O	1:A:1800:TRP:N	2.38	0.49
1:A:2241:PHE:CE1	1:A:2270:VAL:HG13	2.46	0.49
1:A:2242:GLY:N	1:A:2243:PRO:CD	2.76	0.49
1:A:555:GLY:N	1:A:901:SER:HG	2.10	0.49
1:A:1725:TRP:CH2	1:A:1744:LEU:HD22	2.48	0.49
1:B:1740:THR:O	1:B:1744:LEU:HG	2.13	0.49
1:B:1526:ASP:O	1:B:1530:THR:HG23	2.12	0.49
1:B:2241:PHE:CE1	1:B:2270:VAL:HG13	2.46	0.49
1:A:77:LEU:HD22	1:A:101:LEU:HD21	1.95	0.49
1:A:2168:LEU:HD23	1:A:2168:LEU:C	2.38	0.49
1:B:317:PHE:HB2	1:B:356:LEU:HD21	1.94	0.49
1:B:1336:ILE:HG22	1:B:1336:ILE:O	2.12	0.49
1:B:1801:CYS:SG	1:B:2392:THR:OG1	2.66	0.49
1:B:1429:LEU:HD21	1:B:1616:SER:HB3	1.95	0.49
1:A:1576:CYS:O	1:A:1577:THR:HG22	2.13	0.49
1:A:1740:THR:O	1:A:1744:LEU:HG	2.13	0.48
1:A:1745:ARG:NH2	1:A:1797:GLU:OE1	2.44	0.48
1:B:1702:PHE:HD2	1:B:2263:LEU:HD21	1.78	0.48
1:B:2147:ILE:HG22	1:B:2368:THR:HG23	1.95	0.48
1:B:77:LEU:HD22	1:B:101:LEU:HD21	1.95	0.48
1:A:1971:PRO:O	1:A:1975:GLY:N	2.40	0.48
1:B:808:MET:SD	1:B:810:ALA:N	2.81	0.48
1:B:1288:ASP:OD1	1:B:1293:TRP:NE1	2.38	0.48
1:B:1308:ILE:HG22	1:B:1353:TRP:O	2.13	0.48
1:A:143:ASP:OD2	1:A:962:TYR:OH	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1336:ILE:O	1:A:1336:ILE:HG22	2.12	0.48
1:B:277:GLN:NE2	1:B:437:GLY:O	2.43	0.48
1:B:594:SER:CB	1:B:672:SER:HG	2.26	0.48
1:B:2168:LEU:C	1:B:2168:LEU:HD23	2.38	0.48
1:A:2147:ILE:HG22	1:A:2368:THR:HG23	1.95	0.48
1:B:211:ILE:HD12	1:B:246:GLU:HG3	1.95	0.48
1:B:1745:ARG:NH2	1:B:1797:GLU:OE1	2.44	0.48
1:A:802:ASP:OD2	1:A:806:ARG:N	2.43	0.48
1:A:1066:SER:N	1:A:1075:SER:O	2.41	0.48
1:A:1409:LEU:HD13	1:A:1560:ILE:HD11	1.96	0.48
1:B:93:GLU:O	1:B:938:VAL:HG23	2.14	0.48
1:B:2242:GLY:N	1:B:2243:PRO:CD	2.76	0.48
1:A:1018:LYS:N	1:A:1085:THR:O	2.46	0.48
1:A:1436:ARG:O	1:A:1809:ARG:NH2	2.43	0.48
1:A:1610:PHE:N	1:A:1611:PRO:CD	2.77	0.48
1:B:555:GLY:N	1:B:901:SER:HG	2.10	0.48
1:A:1308:ILE:HG22	1:A:1353:TRP:O	2.13	0.48
1:A:1657:LEU:HD21	1:A:1726:LEU:HD13	1.96	0.48
1:B:1610:PHE:N	1:B:1611:PRO:CD	2.77	0.48
1:B:1657:LEU:HD21	1:B:1726:LEU:HD13	1.96	0.48
1:A:1646:VAL:HG11	1:A:1658:LEU:HD13	1.96	0.47
1:A:2158:THR:OG1	1:A:2234:PRO:O	2.25	0.47
1:B:1021:GLU:HG2	1:B:1205:THR:HG23	1.95	0.47
1:B:1436:ARG:O	1:B:1809:ARG:NH2	2.43	0.47
1:A:211:ILE:HD12	1:A:246:GLU:HG3	1.95	0.47
1:A:1540:PRO:O	1:A:1790:THR:OG1	2.27	0.47
1:B:1018:LYS:N	1:B:1085:THR:O	2.47	0.47
1:B:1646:VAL:HG11	1:B:1658:LEU:HD13	1.96	0.47
1:A:1731:TRP:HB2	1:A:2393:VAL:HG22	1.97	0.47
1:B:996:ALA:O	1:B:1000:VAL:HG23	2.14	0.47
1:B:1066:SER:N	1:B:1075:SER:O	2.41	0.47
1:B:1409:LEU:HD13	1:B:1560:ILE:HD11	1.96	0.47
1:B:2175:TRP:CZ2	1:B:2371:ALA:HB2	2.50	0.47
1:A:93:GLU:O	1:A:938:VAL:HG23	2.14	0.47
1:A:1021:GLU:HG2	1:A:1205:THR:HG23	1.95	0.47
1:A:1429:LEU:HD21	1:A:1616:SER:HB3	1.95	0.47
1:A:1700:GLU:OE1	1:A:1700:GLU:N	2.45	0.47
1:B:1731:TRP:HB2	1:B:2393:VAL:HG22	1.97	0.47
1:B:14:VAL:O	1:B:923:LYS:NZ	2.43	0.47
1:B:1883:VAL:HG13	1:B:2087:TYR:CZ	2.50	0.47
1:A:1725:TRP:CZ2	1:A:1744:LEU:HD22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1448:GLY:O	1:B:1469:TYR:OH	2.26	0.47
1:B:1524:THR:HG21	1:B:1530:THR:HG21	1.97	0.47
1:B:1683:GLU:OE1	1:B:1683:GLU:N	2.42	0.47
1:B:1725:TRP:CZ2	1:B:1744:LEU:HD22	2.49	0.47
1:A:1444:GLU:OE1	1:A:1453:THR:OG1	2.31	0.47
1:B:247:ALA:HB3	1:B:371:THR:HG21	1.97	0.47
1:B:378:MET:HE2	1:B:378:MET:HA	1.97	0.47
1:A:1457:LEU:HD12	1:A:1462:LEU:HD21	1.97	0.47
1:B:138:THR:HG21	1:B:215:MET:HE2	1.97	0.47
1:A:247:ALA:HB3	1:A:371:THR:HG21	1.97	0.47
1:A:1201:VAL:HG11	1:A:1204:ILE:CD1	2.45	0.47
1:A:1590:LEU:HD11	1:A:1617:THR:HB	1.97	0.47
1:B:1521:LEU:N	1:B:1548:GLU:OE2	2.48	0.46
1:A:234:MET:HE1	1:A:358:VAL:HG12	1.96	0.46
1:A:277:GLN:NE2	1:A:437:GLY:O	2.43	0.46
1:A:378:MET:HE2	1:A:378:MET:HA	1.97	0.46
1:A:1793:THR:HG22	1:A:1794:GLN:H	1.80	0.46
1:A:1856:THR:HG22	1:A:1859:VAL:HG23	1.97	0.46
1:A:2175:TRP:CZ2	1:A:2371:ALA:HB2	2.50	0.46
1:B:272:GLU:OE2	1:B:302:GLN:NE2	2.43	0.46
1:B:1129:TYR:OH	1:B:1196:TYR:O	2.31	0.46
1:B:1487:PHE:O	1:B:1491:MET:N	2.47	0.46
1:A:996:ALA:O	1:A:1000:VAL:HG23	2.14	0.46
1:A:1883:VAL:HG13	1:A:2087:TYR:CZ	2.50	0.46
1:A:2297:ALA:HB2	1:A:2311:ASN:CB	2.45	0.46
1:B:2297:ALA:HB2	1:B:2311:ASN:CB	2.45	0.46
1:B:1590:LEU:HD11	1:B:1617:THR:HB	1.97	0.46
1:B:1793:THR:HG22	1:B:1794:GLN:H	1.80	0.46
1:B:1129:TYR:CE1	1:B:1192:LEU:HD21	2.50	0.46
1:B:1278:TRP:HB3	1:B:2394:LEU:HD22	1.98	0.46
1:A:1331:HIS:HA	1:A:1336:ILE:HB	1.98	0.46
1:A:1877:CYS:SG	1:A:1941:THR:HG21	2.56	0.46
1:B:1201:VAL:HG11	1:B:1204:ILE:CD1	2.45	0.46
1:B:2322:VAL:HG21	1:B:2399:LEU:HD13	1.98	0.46
1:A:1521:LEU:N	1:A:1548:GLU:OE2	2.48	0.46
1:A:1702:PHE:HD2	1:A:2263:LEU:HD21	1.78	0.46
1:B:356:LEU:C	1:B:356:LEU:HD23	2.41	0.46
1:B:1355:ASP:O	1:B:1357:GLY:N	2.42	0.46
1:B:1693:MET:HE2	1:B:1716:LEU:HD22	1.98	0.46
1:B:1102:LEU:HD12	1:B:1207:VAL:HG23	1.98	0.46
1:B:1331:HIS:HA	1:B:1336:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1877:CYS:SG	1:B:1941:THR:HG21	2.56	0.46
1:A:1402:LEU:HD12	1:A:1403:LEU:H	1.81	0.46
1:A:1524:THR:HG21	1:A:1530:THR:HG21	1.97	0.46
1:A:1693:MET:HE2	1:A:1716:LEU:HD22	1.98	0.46
1:B:143:ASP:OD2	1:B:962:TYR:OH	2.21	0.46
1:B:1856:THR:HG22	1:B:1859:VAL:HG23	1.97	0.46
1:A:1007:LEU:HD11	1:A:1167:LEU:HG	1.98	0.46
1:A:1244:ASP:OD1	1:A:1245:ALA:N	2.44	0.46
1:A:1603:THR:HG23	1:A:1603:THR:O	2.16	0.45
1:A:1129:TYR:CE1	1:A:1192:LEU:HD21	2.50	0.45
1:A:1203:ARG:NH2	1:B:2015:ARG:O	2.49	0.45
1:A:2245:VAL:HG11	1:A:2261:MET:HG2	1.98	0.45
1:B:11:ILE:HG22	1:B:12:VAL:N	2.32	0.45
1:B:940:SER:O	1:B:943:THR:N	2.50	0.45
1:A:964:THR:HG21	1:B:1065:ASP:CG	2.41	0.45
1:B:1621:ASP:O	1:B:1623:THR:HG22	2.16	0.45
1:B:1738:ALA:CB	1:B:2316:ALA:HB2	2.47	0.45
1:A:356:LEU:HD23	1:A:356:LEU:C	2.41	0.45
1:A:1416:THR:O	1:A:1420:GLY:N	2.42	0.45
1:B:234:MET:HE1	1:B:358:VAL:HG12	1.96	0.45
1:A:1621:ASP:O	1:A:1623:THR:HG22	2.16	0.45
1:A:2322:VAL:HG21	1:A:2399:LEU:HD13	1.98	0.45
1:B:1744:LEU:HA	1:B:1747:ILE:HD12	1.98	0.45
1:B:2245:VAL:HG11	1:B:2261:MET:HG2	1.98	0.45
1:A:941:ARG:NH2	1:A:961:GLU:O	2.39	0.45
1:A:1278:TRP:HB3	1:A:2394:LEU:HD22	1.98	0.45
1:A:2182:CYS:O	1:A:2207:ARG:N	2.47	0.45
1:B:1457:LEU:HD12	1:B:1462:LEU:HD21	1.97	0.45
1:B:1603:THR:HG23	1:B:1603:THR:O	2.16	0.45
1:B:1700:GLU:OE1	1:B:1700:GLU:N	2.45	0.45
1:A:573:MET:HE2	1:A:573:MET:HA	1.99	0.45
1:A:583:TYR:CE2	1:A:587:ILE:HD11	2.52	0.45
1:B:95:MET:HE3	1:B:163:ARG:HD2	1.98	0.45
1:B:573:MET:HA	1:B:573:MET:HE2	1.98	0.45
1:B:1007:LEU:HD11	1:B:1167:LEU:HG	1.99	0.45
1:B:1402:LEU:HD12	1:B:1403:LEU:H	1.81	0.45
1:A:2154:ALA:H	1:A:2159:TYR:HH	1.64	0.45
1:B:78:GLY:O	1:B:936:TYR:N	2.45	0.45
1:B:319:ALA:HB2	1:B:358:VAL:CG1	2.47	0.45
1:A:1065:ASP:CG	1:B:964:THR:HG21	2.41	0.45
1:A:1288:ASP:OD1	1:A:1293:TRP:NE1	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1738:ALA:CB	1:A:2316:ALA:HB2	2.46	0.45
1:A:1777:LEU:H	1:A:1777:LEU:HD22	1.82	0.45
1:A:11:ILE:HG22	1:A:12:VAL:N	2.32	0.44
1:A:138:THR:HG21	1:A:215:MET:HE2	1.97	0.44
1:A:1102:LEU:HD12	1:A:1207:VAL:HG23	1.98	0.44
1:A:1487:PHE:O	1:A:1491:MET:N	2.47	0.44
1:A:1866:MET:SD	1:A:1866:MET:N	2.90	0.44
1:B:1866:MET:SD	1:B:1866:MET:N	2.90	0.44
1:B:1939:MET:O	1:B:1943:LEU:HD23	2.18	0.44
1:B:2362:GLU:N	1:B:2362:GLU:OE1	2.50	0.44
1:A:95:MET:HE3	1:A:163:ARG:HD2	1.98	0.44
1:A:2096:ARG:HA	1:A:2099:LEU:HG	1.99	0.44
1:A:319:ALA:HB2	1:A:358:VAL:CG1	2.47	0.44
1:A:1744:LEU:HA	1:A:1747:ILE:HD12	1.98	0.44
1:A:2015:ARG:O	1:B:1203:ARG:NH2	2.50	0.44
1:B:1244:ASP:OD1	1:B:1245:ALA:N	2.44	0.44
1:B:2108:VAL:HG22	1:B:2128:VAL:CG1	2.48	0.44
1:A:1040:VAL:HG13	1:A:1068:LEU:HA	2.00	0.44
1:A:1201:VAL:HG11	1:A:1204:ILE:CG1	2.47	0.44
1:A:1302:ILE:O	1:A:1305:ILE:HG22	2.17	0.44
1:A:1939:MET:O	1:A:1943:LEU:HD23	2.18	0.44
1:B:212:LEU:HD22	1:B:937:TRP:HZ2	1.83	0.44
1:B:953:HIS:ND1	1:B:954:LEU:O	2.48	0.44
1:B:1040:VAL:HG13	1:B:1068:LEU:HA	2.00	0.44
1:B:1201:VAL:HG11	1:B:1204:ILE:CG1	2.47	0.44
1:B:1732:VAL:HG22	1:B:2396:MET:CE	2.47	0.44
1:B:1777:LEU:HD22	1:B:1777:LEU:H	1.82	0.44
1:B:2111:CYS:HA	1:B:2129:ILE:HG23	2.00	0.44
1:A:272:GLU:OE2	1:A:302:GLN:NE2	2.43	0.44
1:A:808:MET:SD	1:A:810:ALA:N	2.81	0.44
1:A:940:SER:O	1:A:943:THR:N	2.50	0.44
1:A:1108:GLU:O	1:A:1109:HIS:C	2.61	0.44
1:A:1179:THR:HB	1:A:1226:THR:HG21	1.99	0.44
1:A:1780:GLU:OE1	1:A:1781:GLU:N	2.51	0.44
1:B:1007:LEU:CD2	1:B:1017:VAL:HG21	2.48	0.44
1:B:1302:ILE:O	1:B:1305:ILE:HG22	2.17	0.44
1:A:212:LEU:HD22	1:A:937:TRP:HZ2	1.83	0.44
1:A:1355:ASP:O	1:A:1357:GLY:N	2.42	0.44
1:A:1732:VAL:HG22	1:A:2396:MET:CE	2.47	0.44
1:B:681:ARG:O	1:B:681:ARG:NE	2.46	0.44
1:B:1780:GLU:OE1	1:B:1781:GLU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1816:ARG:HD3	1:B:2372:GLU:HG2	2.00	0.44
1:A:109:ALA:HB1	1:A:252:VAL:HG23	1.99	0.44
1:A:953:HIS:ND1	1:A:954:LEU:O	2.48	0.44
1:A:1309:VAL:O	1:A:1309:VAL:HG22	2.17	0.44
1:A:1381:LEU:HD13	1:A:1560:ILE:HD12	1.99	0.44
1:A:2362:GLU:OE1	1:A:2362:GLU:N	2.50	0.44
1:B:1299:LYS:O	1:B:1303:PRO:HG2	2.18	0.44
1:B:1306:GLU:O	1:B:1310:TYR:N	2.51	0.44
1:B:2034:ASP:O	1:B:2061:ALA:N	2.51	0.44
1:A:1175:VAL:O	1:A:1179:THR:HG23	2.18	0.44
1:A:2108:VAL:HG22	1:A:2128:VAL:CG1	2.48	0.44
1:B:109:ALA:HB1	1:B:252:VAL:HG23	1.99	0.44
1:B:583:TYR:CE2	1:B:587:ILE:HD11	2.52	0.44
1:A:48:ARG:HH21	1:A:212:LEU:HD23	1.83	0.44
1:A:1007:LEU:CD2	1:A:1017:VAL:HG21	2.48	0.44
1:A:1306:GLU:O	1:A:1310:TYR:N	2.51	0.44
1:A:1514:LEU:HD21	1:A:1516:ILE:HG13	2.00	0.44
1:B:12:VAL:HG22	1:B:266:ILE:HG23	2.00	0.44
1:B:511:LEU:HA	1:B:515:ARG:HG3	1.99	0.44
1:B:1309:VAL:HG22	1:B:1309:VAL:O	2.17	0.44
1:B:1514:LEU:HD21	1:B:1516:ILE:HG13	2.00	0.44
1:A:1129:TYR:OH	1:A:1196:TYR:O	2.31	0.43
1:A:1299:LYS:O	1:A:1303:PRO:HG2	2.18	0.43
1:A:2034:ASP:O	1:A:2061:ALA:N	2.51	0.43
1:B:1179:THR:HB	1:B:1226:THR:HG21	1.99	0.43
1:A:277:GLN:HG2	1:B:165:SER:CB	2.48	0.43
1:A:833:GLN:O	1:A:837:VAL:HG12	2.18	0.43
1:B:1006:ALA:HB1	1:B:1084:LEU:HD21	2.00	0.43
1:B:1108:GLU:O	1:B:1109:HIS:C	2.61	0.43
1:B:1641:TYR:N	1:B:1642:PRO:HD2	2.33	0.43
1:B:2096:ARG:HA	1:B:2099:LEU:HG	1.99	0.43
1:A:12:VAL:HG22	1:A:266:ILE:HG23	2.00	0.43
1:A:165:SER:CB	1:B:277:GLN:HG2	2.48	0.43
1:A:681:ARG:O	1:A:681:ARG:NE	2.46	0.43
1:A:1006:ALA:HB1	1:A:1084:LEU:HD21	2.00	0.43
1:B:523:ALA:N	1:B:896:GLU:OE2	2.51	0.43
1:B:833:GLN:O	1:B:837:VAL:HG12	2.18	0.43
1:B:1625:GLU:O	1:B:1626:TYR:C	2.61	0.43
1:A:985:HIS:ND1	1:A:992:VAL:O	2.50	0.43
1:A:1369:LEU:HB2	1:A:1379:VAL:HG11	2.00	0.43
1:A:1816:ARG:HD3	1:A:2372:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:GLN:HA	1:B:865:VAL:HG21	2.01	0.43
1:B:909:MET:HE2	1:B:918:CYS:SG	2.59	0.43
1:B:1948:LEU:O	1:B:1952:VAL:HG22	2.19	0.43
1:B:2175:TRP:CH2	1:B:2371:ALA:HB2	2.54	0.43
1:B:2196:LYS:HZ3	1:B:2197:TRP:N	2.15	0.43
1:B:1296:ALA:O	1:B:1300:GLU:N	2.52	0.43
1:B:1381:LEU:HD13	1:B:1560:ILE:HD12	1.99	0.43
1:A:1031:VAL:HG23	1:A:1077:SER:OG	2.19	0.43
1:A:1535:ARG:HB2	1:A:1595:PHE:CE1	2.53	0.43
1:A:1641:TYR:N	1:A:1642:PRO:HD2	2.33	0.43
1:B:48:ARG:HH21	1:B:212:LEU:HD23	1.83	0.43
1:B:266:ILE:HG21	1:B:448:TYR:HB2	2.01	0.43
1:B:1369:LEU:HB2	1:B:1379:VAL:HG11	2.00	0.43
1:B:1426:ALA:HB2	1:B:1547:LEU:HD21	2.00	0.43
1:B:1590:LEU:HD22	1:B:1595:PHE:CD1	2.53	0.43
1:B:1651:THR:O	1:B:1655:GLN:N	2.44	0.43
1:A:266:ILE:HG21	1:A:448:TYR:HB2	2.00	0.43
1:A:1296:ALA:O	1:A:1300:GLU:N	2.52	0.43
1:A:511:LEU:HA	1:A:515:ARG:HG3	1.99	0.43
1:A:909:MET:HE2	1:A:918:CYS:SG	2.59	0.43
1:A:1590:LEU:HD22	1:A:1595:PHE:CD1	2.53	0.43
1:A:1801:CYS:SG	1:A:2392:THR:OG1	2.66	0.43
1:B:1535:ARG:HB2	1:B:1595:PHE:CE1	2.53	0.43
1:A:151:SER:O	1:A:155:VAL:HG22	2.19	0.43
1:B:974:VAL:HG13	1:B:979:ILE:CD1	2.49	0.43
1:A:1423:LEU:HD23	1:A:1455:TYR:CD1	2.54	0.43
1:A:1625:GLU:O	1:A:1626:TYR:C	2.61	0.43
1:A:1863:VAL:HG23	1:A:1864:GLN:H	1.84	0.43
1:A:1948:LEU:O	1:A:1952:VAL:HG22	2.19	0.43
1:B:559:VAL:HG21	1:B:846:ILE:CD1	2.47	0.43
1:B:2296:VAL:O	1:B:2300:GLY:N	2.38	0.43
1:A:974:VAL:HG13	1:A:979:ILE:CD1	2.49	0.42
1:A:2111:CYS:HA	1:A:2129:ILE:HG23	2.00	0.42
1:B:1109:HIS:CG	1:B:1110:PRO:HD2	2.54	0.42
1:A:1109:HIS:CG	1:A:1110:PRO:HD2	2.54	0.42
1:A:1938:LEU:HD22	1:A:2126:SER:O	2.19	0.42
1:B:600:GLU:OE1	1:B:600:GLU:N	2.44	0.42
1:B:1031:VAL:HG23	1:B:1077:SER:OG	2.19	0.42
1:B:1067:CYS:HB2	1:B:1074:LEU:HD12	2.01	0.42
1:B:1888:PHE:CD2	1:B:2066:THR:HG22	2.54	0.42
1:A:2175:TRP:CH2	1:A:2371:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:PRO:HB3	1:B:175:MET:HE1	2.02	0.42
1:B:476:VAL:HG11	1:B:512:LEU:HD21	2.00	0.42
1:B:1175:VAL:O	1:B:1179:THR:HG23	2.18	0.42
1:B:1797:GLU:OE1	1:B:2423:ARG:NH1	2.53	0.42
1:A:1426:ALA:HB2	1:A:1547:LEU:HD21	2.00	0.42
1:B:151:SER:O	1:B:155:VAL:HG22	2.19	0.42
1:B:1242:VAL:HG21	1:B:1251:PHE:CZ	2.55	0.42
1:B:1863:VAL:HG23	1:B:1864:GLN:H	1.84	0.42
1:B:2182:CYS:O	1:B:2207:ARG:N	2.47	0.42
1:A:476:VAL:HG11	1:A:512:LEU:HD21	2.00	0.42
1:A:832:VAL:O	1:A:836:VAL:HG22	2.20	0.42
1:A:1351:HIS:O	1:A:1355:ASP:N	2.46	0.42
1:A:1888:PHE:CD2	1:A:2066:THR:HG22	2.54	0.42
1:B:1027:ILE:N	1:B:1027:ILE:HD12	2.34	0.42
1:A:157:VAL:O	1:A:176:THR:HG21	2.20	0.42
1:A:523:ALA:N	1:A:896:GLU:OE2	2.51	0.42
1:A:558:SER:OG	1:A:843:ASP:OD2	2.38	0.42
1:A:1702:PHE:HA	1:A:1705:LEU:HG	2.02	0.42
1:B:592:ASP:OD1	1:B:609:LEU:HD12	2.19	0.42
1:B:1031:VAL:HG21	1:B:1042:LEU:HD21	2.01	0.42
1:B:1423:LEU:HD23	1:B:1455:TYR:CD1	2.54	0.42
1:B:2147:ILE:HD11	1:B:2375:VAL:HG21	2.00	0.42
1:A:1067:CYS:HB2	1:A:1074:LEU:HD12	2.01	0.42
1:A:1242:VAL:HG21	1:A:1251:PHE:CZ	2.55	0.42
1:A:1295:THR:HG23	1:A:1298:ASP:H	1.83	0.42
1:A:1385:VAL:HG12	1:A:1402:LEU:HD11	2.02	0.42
1:A:2274:HIS:O	1:A:2278:SER:N	2.52	0.42
1:B:157:VAL:O	1:B:176:THR:HG21	2.20	0.42
1:B:1416:THR:O	1:B:1420:GLY:N	2.42	0.42
1:A:1031:VAL:HG21	1:A:1042:LEU:HD21	2.01	0.42
1:B:253:LEU:HD22	1:B:270:ILE:HD12	2.02	0.42
1:B:1702:PHE:HA	1:B:1705:LEU:HG	2.02	0.42
1:B:2274:HIS:O	1:B:2278:SER:N	2.52	0.42
1:A:173:PRO:HB3	1:A:175:MET:HE1	2.01	0.42
1:A:592:ASP:OD1	1:A:609:LEU:HD12	2.19	0.42
1:A:833:GLN:HA	1:A:865:VAL:HG21	2.01	0.42
1:A:1027:ILE:N	1:A:1027:ILE:HD12	2.34	0.42
1:A:1797:GLU:OE1	1:A:2423:ARG:NH1	2.53	0.42
1:B:12:VAL:HG13	1:B:14:VAL:HG13	2.02	0.42
1:B:1295:THR:HG23	1:B:1298:ASP:H	1.83	0.42
1:A:1624:VAL:HG12	1:A:1625:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1301:ALA:HB1	1:B:1375:TYR:HB3	2.02	0.41
1:B:1891:LEU:HD13	1:B:1891:LEU:C	2.45	0.41
1:A:1744:LEU:HD23	1:A:1747:ILE:HD12	2.02	0.41
1:A:2147:ILE:HD11	1:A:2375:VAL:HG21	2.01	0.41
1:B:649:PHE:O	1:B:795:VAL:HG13	2.20	0.41
1:A:1223:ALA:HB3	1:A:1243:PHE:CE2	2.56	0.41
1:A:1706:THR:HA	1:A:2256:LEU:HD21	2.02	0.41
1:A:78:GLY:O	1:A:936:TYR:N	2.45	0.41
1:A:253:LEU:HD22	1:A:270:ILE:HD12	2.02	0.41
1:A:1891:LEU:C	1:A:1891:LEU:HD13	2.45	0.41
1:A:2267:VAL:O	1:A:2270:VAL:HG22	2.21	0.41
1:B:16:SER:O	1:B:112:ASN:ND2	2.44	0.41
1:B:1744:LEU:HD23	1:B:1747:ILE:HD12	2.02	0.41
1:A:649:PHE:O	1:A:795:VAL:HG13	2.20	0.41
1:B:1385:VAL:HG12	1:B:1402:LEU:HD11	2.02	0.41
1:B:1938:LEU:HD22	1:B:2126:SER:O	2.19	0.41
1:A:12:VAL:HG13	1:A:14:VAL:HG13	2.02	0.41
1:A:202:MET:HE3	1:A:252:VAL:HG13	2.03	0.41
1:A:600:GLU:OE1	1:A:600:GLU:N	2.44	0.41
1:B:832:VAL:O	1:B:836:VAL:HG22	2.20	0.41
1:B:960:SER:N	1:B:969:GLN:O	2.50	0.41
1:B:1624:VAL:HG12	1:B:1625:GLU:N	2.35	0.41
1:A:1201:VAL:HA	1:A:1256:ILE:HA	2.03	0.41
1:B:126:ALA:HB2	1:B:173:PRO:HD2	2.02	0.41
1:B:271:ARG:NH1	1:B:305:LEU:HD21	2.36	0.41
1:B:1223:ALA:HB3	1:B:1243:PHE:CE2	2.56	0.41
1:B:1354:TYR:CD1	1:B:1354:TYR:N	2.87	0.41
1:A:126:ALA:HB2	1:A:173:PRO:HD2	2.02	0.41
1:A:150:TYR:HA	1:B:223:LEU:HD21	2.03	0.41
1:A:1272:MET:HE2	1:A:1820:MET:SD	2.61	0.41
1:A:1610:PHE:N	1:A:1611:PRO:HD3	2.36	0.41
1:B:13:VAL:HG22	1:B:253:LEU:CD2	2.51	0.41
1:B:985:HIS:ND1	1:B:992:VAL:O	2.50	0.41
1:B:996:ALA:HB1	1:B:1173:LEU:HB3	2.03	0.41
1:B:1201:VAL:HA	1:B:1256:ILE:HA	2.03	0.41
1:B:1856:THR:HG22	1:B:1856:THR:O	2.21	0.41
1:A:996:ALA:HB1	1:A:1173:LEU:HB3	2.03	0.41
1:B:1403:LEU:HD13	1:B:1404:ASP:N	2.36	0.41
1:B:1547:LEU:HG	1:B:1614:VAL:HG22	2.03	0.41
1:A:559:VAL:HG21	1:A:846:ILE:CD1	2.47	0.40
1:A:960:SER:N	1:A:969:GLN:O	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1354:TYR:N	1:A:1354:TYR:CD1	2.87	0.40
1:A:1621:ASP:OD1	1:A:1622:ALA:N	2.49	0.40
1:B:1351:HIS:O	1:B:1355:ASP:N	2.46	0.40
1:B:1444:GLU:OE1	1:B:1453:THR:OG1	2.31	0.40
1:B:1542:GLY:HA2	1:B:1791:THR:HG21	2.03	0.40
1:A:594:SER:CB	1:A:672:SER:HG	2.31	0.40
1:A:1301:ALA:HB1	1:A:1375:TYR:HB3	2.03	0.40
1:A:271:ARG:NH1	1:A:305:LEU:HD21	2.36	0.40
1:A:569:GLN:HA	1:A:850:CYS:SG	2.61	0.40
1:A:1203:ARG:NH2	1:A:1254:GLU:OE1	2.54	0.40
1:A:1353:TRP:CD1	1:A:1353:TRP:N	2.89	0.40
1:B:558:SER:OG	1:B:843:ASP:OD2	2.38	0.40
1:B:2174:ARG:HA	1:B:2177:VAL:HG12	2.03	0.40
1:A:175:MET:HE3	1:B:186:VAL:CG1	2.50	0.40
1:A:1403:LEU:HD12	1:A:1407:GLY:HA3	2.04	0.40
1:A:2161:LEU:HD12	1:A:2186:LEU:CD2	2.51	0.40
1:B:569:GLN:HA	1:B:850:CYS:SG	2.61	0.40
1:B:1308:ILE:HD13	1:B:1362:THR:HG23	2.03	0.40
1:B:1318:SER:O	1:B:1321:THR:OG1	2.36	0.40
1:B:1706:THR:HA	1:B:2256:LEU:HD21	2.02	0.40
1:A:1316:PHE:CD2	1:A:1352:LEU:O	2.75	0.40
1:B:1610:PHE:N	1:B:1611:PRO:HD3	2.36	0.40
1:B:2401:LEU:N	1:B:2401:LEU:HD12	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	2236/3046 (73%)	2121 (95%)	113 (5%)	2 (0%)	48 76
1	B	2236/3046 (73%)	2121 (95%)	113 (5%)	2 (0%)	48 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4472/6092 (73%)	4242 (95%)	226 (5%)	4 (0%)	49 76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1623	THR
1	B	1623	THR
1	A	1577	THR
1	B	1577	THR

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	1904/2547 (75%)	1847 (97%)	57 (3%)	36 68
1	B	1904/2547 (75%)	1847 (97%)	57 (3%)	36 68
All	All	3808/5094 (75%)	3694 (97%)	114 (3%)	37 68

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	133	THR
1	A	136	TYR
1	A	142	ARG
1	A	220	GLU
1	A	222	LYS
1	A	276	ASN
1	A	281	THR
1	A	307	ILE
1	A	353	ARG
1	A	378	MET
1	A	384	VAL
1	A	491	GLU
1	A	513	ARG

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Mol	Chain	Res	Type
1	A	573	MET
1	A	619	SER
1	A	884	LEU
1	A	937	TRP
1	A	964	THR
1	A	1019	LEU
1	A	1047	ASP
1	A	1048	VAL
1	A	1070	LYS
1	A	1077	SER
1	A	1162	ASN
1	A	1227	ILE
1	A	1234	ASP
1	A	1375	TYR
1	A	1384	ARG
1	A	1402	LEU
1	A	1403	LEU
1	A	1436	ARG
1	A	1498	ILE
1	A	1524	THR
1	A	1544	MET
1	A	1567	TRP
1	A	1590	LEU
1	A	1605	ARG
1	A	1715	LEU
1	A	1759	LEU
1	A	1790	THR
1	A	1793	THR
1	A	1807	ILE
1	A	1816	ARG
1	A	1827	ILE
1	A	1830	MET
1	A	2088	TRP
1	A	2158	THR
1	A	2187	THR
1	A	2196	LYS
1	A	2320	GLN
1	A	2362	GLU
1	A	2378	ARG
1	A	2387	GLN
1	A	2424	ILE
1	A	2426	ASN

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Mol	Chain	Res	Type
1	A	2431	GLU
1	B	41	GLN
1	B	133	THR
1	B	136	TYR
1	B	142	ARG
1	B	220	GLU
1	B	222	LYS
1	B	276	ASN
1	B	281	THR
1	B	307	ILE
1	B	353	ARG
1	B	378	MET
1	B	384	VAL
1	B	491	GLU
1	B	513	ARG
1	B	573	MET
1	B	619	SER
1	B	884	LEU
1	B	937	TRP
1	B	964	THR
1	B	1019	LEU
1	B	1047	ASP
1	B	1048	VAL
1	B	1070	LYS
1	B	1077	SER
1	B	1162	ASN
1	B	1227	ILE
1	B	1234	ASP
1	B	1375	TYR
1	B	1384	ARG
1	B	1402	LEU
1	B	1403	LEU
1	B	1436	ARG
1	B	1498	ILE
1	B	1524	THR
1	B	1544	MET
1	B	1567	TRP
1	B	1590	LEU
1	B	1605	ARG
1	B	1715	LEU
1	B	1759	LEU
1	B	1790	THR

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Mol	Chain	Res	Type
1	B	1793	THR
1	B	1807	ILE
1	B	1816	ARG
1	B	1827	ILE
1	B	1830	MET
1	B	2088	TRP
1	B	2158	THR
1	B	2187	THR
1	B	2196	LYS
1	B	2320	GLN
1	B	2362	GLU
1	B	2378	ARG
1	B	2387	GLN
1	B	2424	ILE
1	B	2426	ASN
1	B	2431	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	199	GLN
1	A	386	HIS
1	A	527	HIS
1	A	765	HIS
1	A	766	HIS
1	A	946	HIS
1	A	1376	HIS
1	A	1405	HIS
1	A	1415	ASN
1	A	1757	HIS
1	A	1841	GLN
1	A	1988	GLN
1	A	2058	HIS
1	A	2320	GLN
1	A	2387	GLN
1	B	98	GLN
1	B	99	HIS
1	B	199	GLN
1	B	258	GLN
1	B	386	HIS
1	B	765	HIS

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Mol	Chain	Res	Type
1	B	766	HIS
1	B	851	HIS
1	B	946	HIS
1	B	1376	HIS
1	B	1415	ASN
1	B	1757	HIS
1	B	1841	GLN
1	B	1988	GLN
1	B	2058	HIS
1	B	2320	GLN
1	B	2387	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	NAP	A	3500	-	50,52,52	2.95	18 (36%)	71,80,80	2.40	14 (19%)
2	NAP	B	3500	-	50,52,52	2.95	19 (38%)	71,80,80	2.40	14 (19%)

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	NAP	A	3500	-	-	9/35/67/67	0/5/5/5
2	NAP	B	3500	-	-	9/35/67/67	0/5/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3500	NAP	C5A-N7A	7.25	1.52	1.39
2	B	3500	NAP	C5A-N7A	7.22	1.52	1.39
2	B	3500	NAP	C2N-N1N	7.17	1.42	1.35
2	A	3500	NAP	C2N-N1N	7.12	1.42	1.35
2	A	3500	NAP	C7N-N7N	6.82	1.45	1.33
2	B	3500	NAP	C7N-N7N	6.82	1.45	1.33
2	B	3500	NAP	PN-O3	5.16	1.65	1.59
2	A	3500	NAP	PN-O3	5.11	1.65	1.59
2	A	3500	NAP	PA-O3	5.02	1.64	1.59
2	B	3500	NAP	PA-O3	5.02	1.64	1.59
2	A	3500	NAP	C4A-N9A	-4.91	1.27	1.37
2	B	3500	NAP	C4A-N9A	-4.91	1.27	1.37
2	B	3500	NAP	O4B-C1B	4.83	1.53	1.42
2	A	3500	NAP	O4B-C1B	4.83	1.53	1.42
2	B	3500	NAP	C6A-N6A	4.45	1.45	1.34
2	A	3500	NAP	C6A-N6A	4.43	1.45	1.34
2	A	3500	NAP	C8A-N9A	-4.31	1.30	1.37
2	B	3500	NAP	C8A-N9A	-4.31	1.30	1.37
2	A	3500	NAP	C8A-N7A	4.27	1.39	1.31
2	B	3500	NAP	C8A-N7A	4.23	1.39	1.31
2	B	3500	NAP	O4D-C1D	3.79	1.45	1.40
2	B	3500	NAP	O4B-C4B	3.77	1.53	1.45
2	A	3500	NAP	O4D-C1D	3.76	1.45	1.40
2	A	3500	NAP	O4B-C4B	3.75	1.53	1.45
2	B	3500	NAP	C3B-C2B	-3.50	1.45	1.53
2	A	3500	NAP	C3B-C2B	-3.49	1.45	1.53
2	B	3500	NAP	P2B-O2B	3.34	1.65	1.59
2	A	3500	NAP	P2B-O2B	3.32	1.65	1.59
2	B	3500	NAP	C6N-N1N	3.13	1.42	1.35
2	A	3500	NAP	C6N-N1N	3.11	1.42	1.35
2	A	3500	NAP	O7N-C7N	-2.88	1.18	1.24
2	B	3500	NAP	O7N-C7N	-2.85	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3500	NAP	P2B-O2X	-2.27	1.46	1.54
2	A	3500	NAP	P2B-O2X	-2.27	1.46	1.54
2	A	3500	NAP	P2B-O3X	-2.24	1.46	1.54
2	B	3500	NAP	P2B-O3X	-2.24	1.46	1.54
2	B	3500	NAP	C2D-C3D	-2.00	1.47	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3500	NAP	C4A-N9A-C8A	11.78	118.11	105.74
2	B	3500	NAP	C4A-N9A-C8A	11.78	118.11	105.74
2	B	3500	NAP	C6N-N1N-C2N	-6.55	116.30	121.88
2	A	3500	NAP	C6N-N1N-C2N	-6.52	116.33	121.88
2	A	3500	NAP	N3A-C4A-N9A	5.61	136.71	127.17
2	B	3500	NAP	N3A-C4A-N9A	5.61	136.71	127.17
2	B	3500	NAP	C1B-N9A-C8A	-4.89	116.25	127.09
2	A	3500	NAP	C1B-N9A-C8A	-4.88	116.26	127.09
2	A	3500	NAP	C4B-O4B-C1B	-4.85	98.75	109.47
2	B	3500	NAP	C4B-O4B-C1B	-4.84	98.77	109.47
2	A	3500	NAP	C5A-N7A-C8A	-4.16	96.91	103.45
2	B	3500	NAP	C5A-N7A-C8A	-4.14	96.95	103.45
2	A	3500	NAP	C5A-C4A-N3A	-3.93	121.30	126.72
2	B	3500	NAP	C5A-C4A-N3A	-3.92	121.32	126.72
2	B	3500	NAP	C5A-C4A-N9A	-3.52	101.97	105.81
2	A	3500	NAP	C5A-C4A-N9A	-3.50	101.99	105.81
2	A	3500	NAP	O2N-PN-O1N	-2.40	101.30	112.44
2	B	3500	NAP	O2N-PN-O1N	-2.39	101.31	112.44
2	A	3500	NAP	O2A-PA-O1A	-2.37	101.43	112.44
2	B	3500	NAP	O2A-PA-O1A	-2.37	101.44	112.44
2	A	3500	NAP	C2B-C3B-C4B	2.33	107.01	101.99
2	B	3500	NAP	C2B-C3B-C4B	2.33	107.01	101.99
2	A	3500	NAP	C2A-N1A-C6A	-2.21	115.10	118.73
2	B	3500	NAP	C2A-N1A-C6A	-2.20	115.12	118.73
2	A	3500	NAP	O2X-P2B-O2B	2.15	114.23	105.85
2	B	3500	NAP	O2X-P2B-O2B	2.14	114.18	105.85
2	A	3500	NAP	O3X-P2B-O2B	2.11	114.06	105.85
2	B	3500	NAP	O3X-P2B-O2B	2.10	114.04	105.85

There are no chirality outliers.

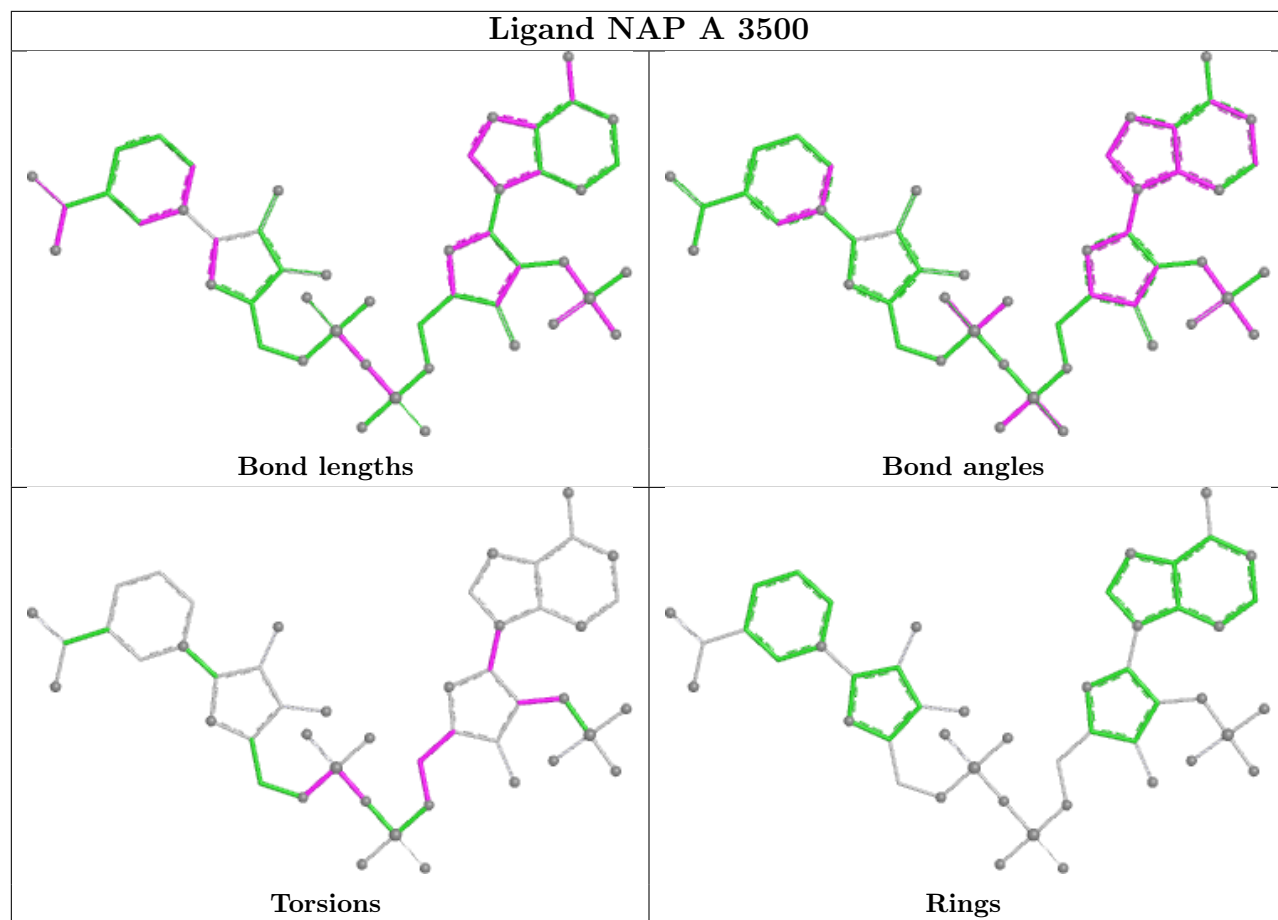
All (18) torsion outliers are listed below:

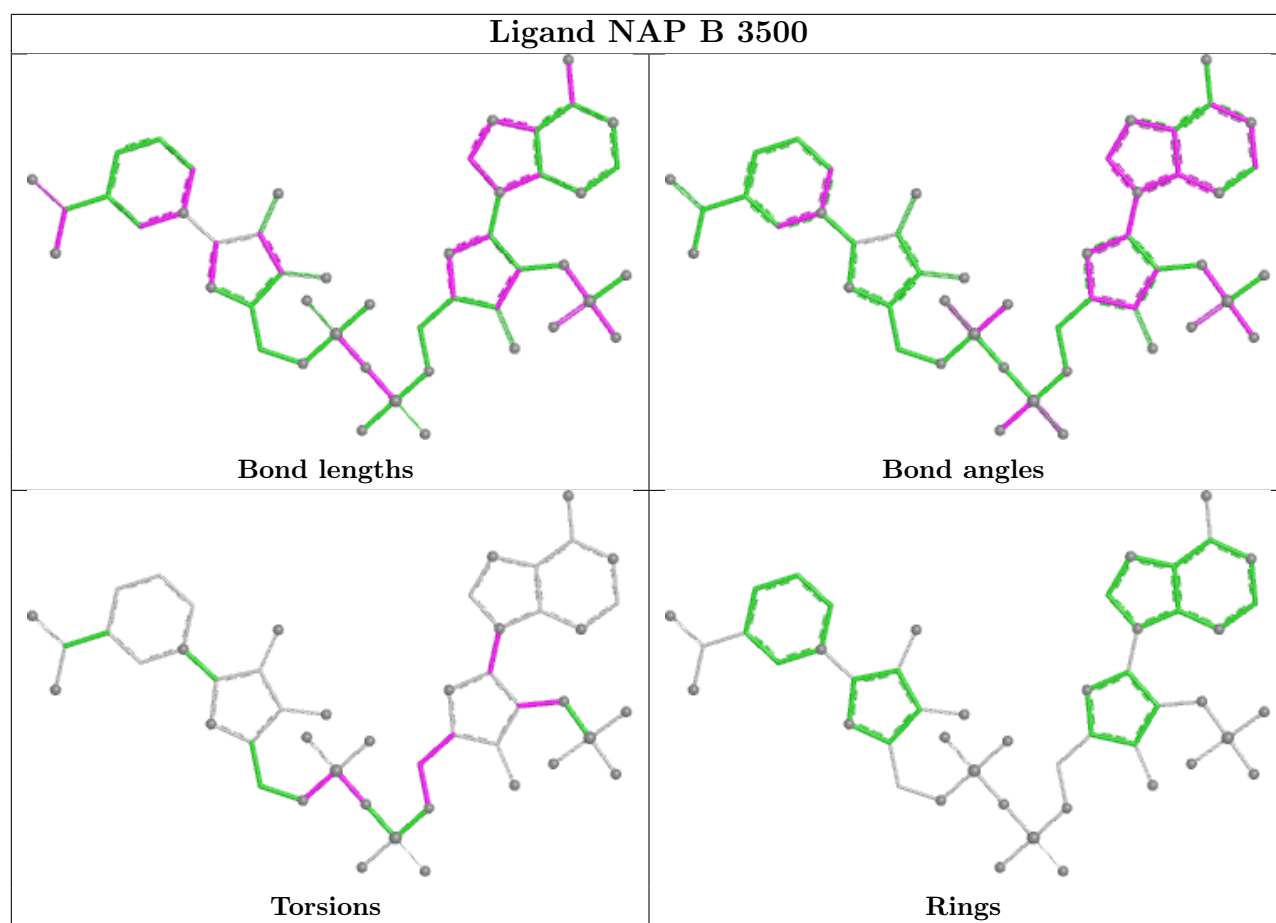
Mol	Chain	Res	Type	Atoms
2	A	3500	NAP	C2B-C1B-N9A-C8A
2	A	3500	NAP	C2B-C1B-N9A-C4A
2	B	3500	NAP	C2B-C1B-N9A-C8A
2	B	3500	NAP	C2B-C1B-N9A-C4A
2	A	3500	NAP	C1B-C2B-O2B-P2B
2	B	3500	NAP	C1B-C2B-O2B-P2B
2	A	3500	NAP	C3B-C2B-O2B-P2B
2	B	3500	NAP	C3B-C2B-O2B-P2B
2	A	3500	NAP	O4B-C4B-C5B-O5B
2	B	3500	NAP	O4B-C4B-C5B-O5B
2	A	3500	NAP	C3B-C4B-C5B-O5B
2	B	3500	NAP	C3B-C4B-C5B-O5B
2	A	3500	NAP	C5D-O5D-PN-O1N
2	B	3500	NAP	C5D-O5D-PN-O1N
2	A	3500	NAP	PA-O3-PN-O2N
2	B	3500	NAP	PA-O3-PN-O2N
2	A	3500	NAP	C4B-C5B-O5B-PA
2	B	3500	NAP	C4B-C5B-O5B-PA

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.

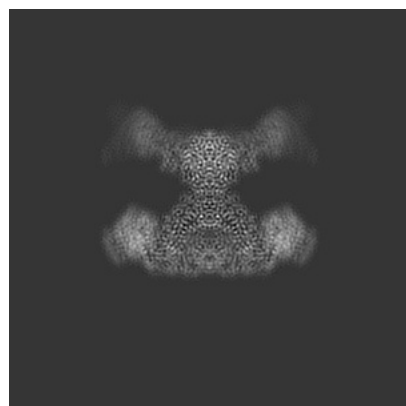
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30434. These allow visual inspection of the internal detail of the map and identification of artifacts.

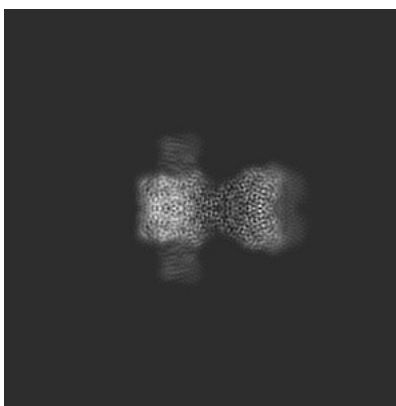
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

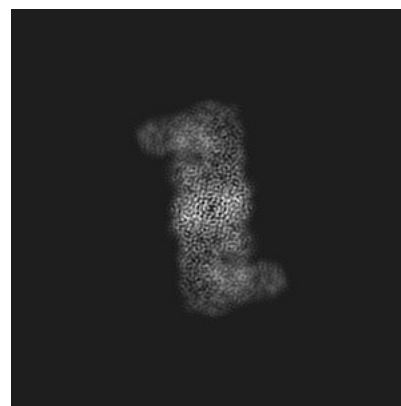
6.1.1 Primary map



X

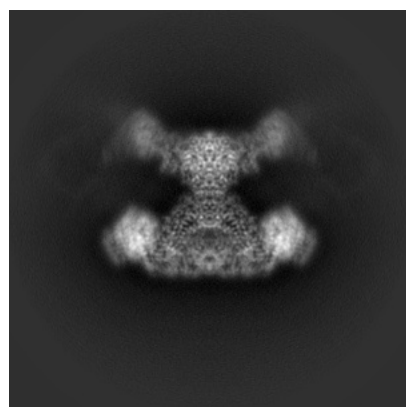


Y

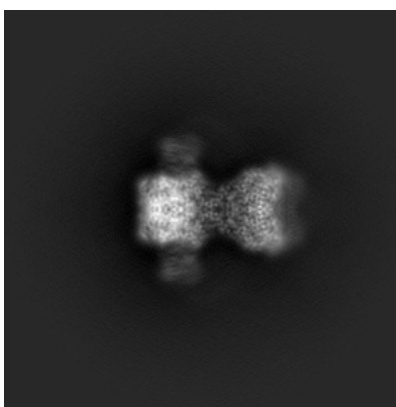


Z

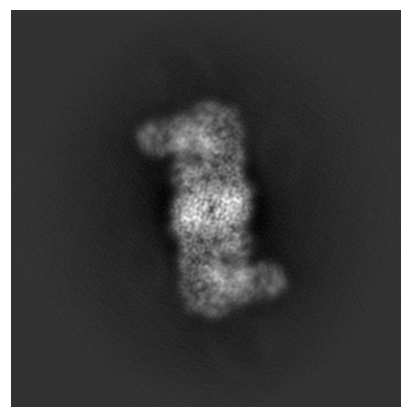
6.1.2 Raw map



X



Y

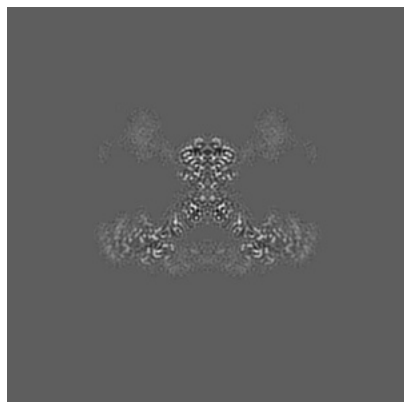


Z

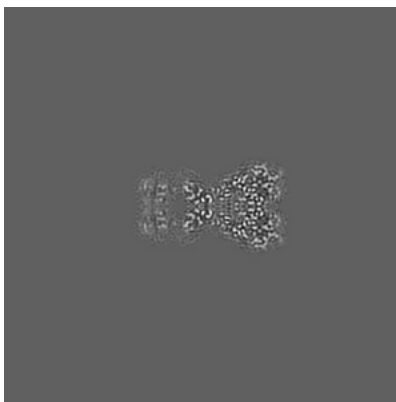
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

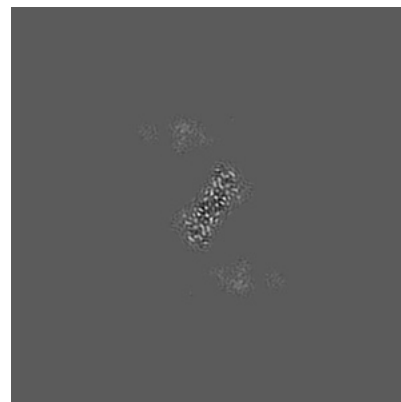
6.2.1 Primary map



X Index: 175

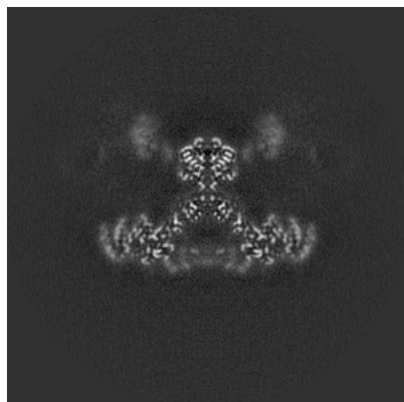


Y Index: 175

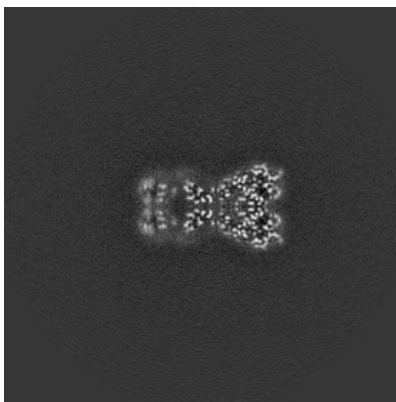


Z Index: 175

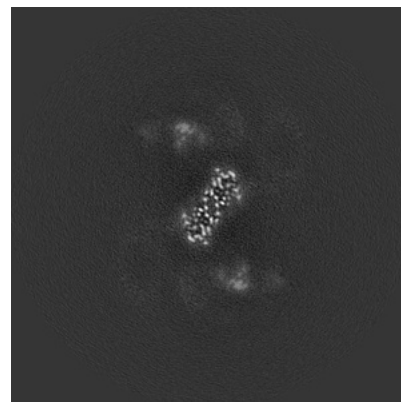
6.2.2 Raw map



X Index: 175



Y Index: 175

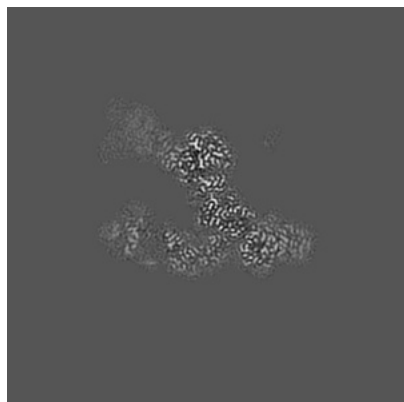


Z Index: 175

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: 185

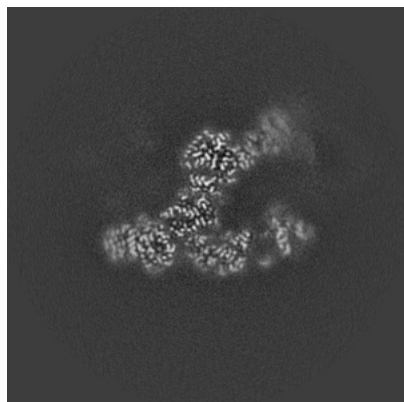


Y Index: 169

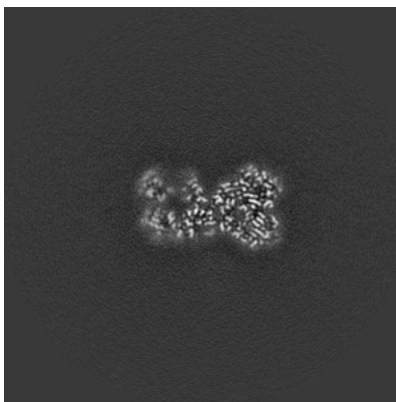


Z Index: 224

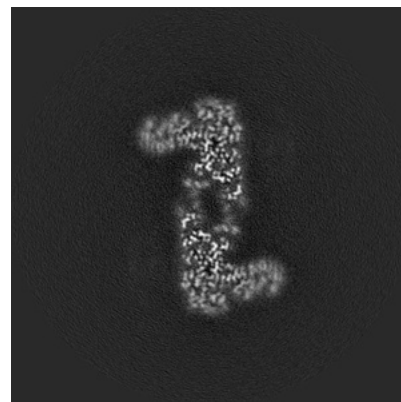
6.3.2 Raw map



X Index: 165



Y Index: 169

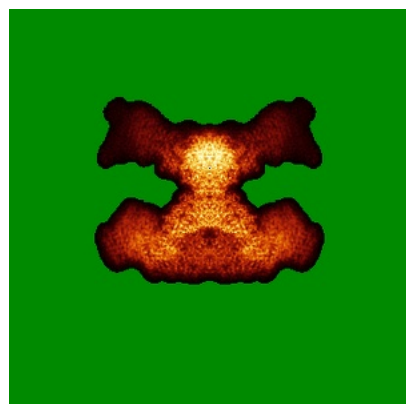


Z Index: 150

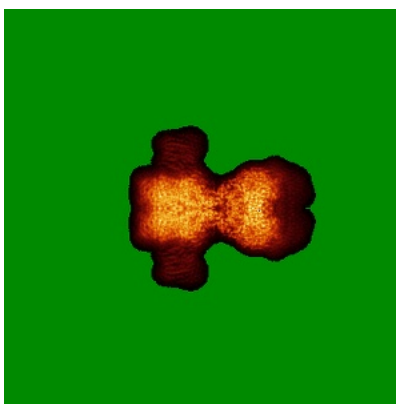
The images above show the largest variance slices of the map in three orthogonal directions.

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

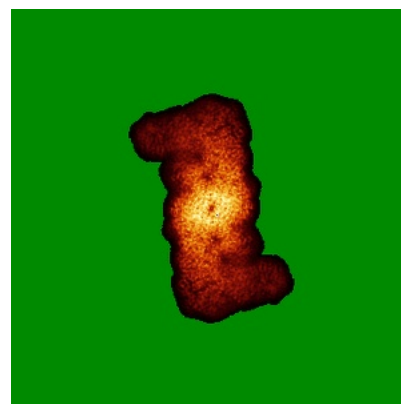
6.4.1 Primary map



X

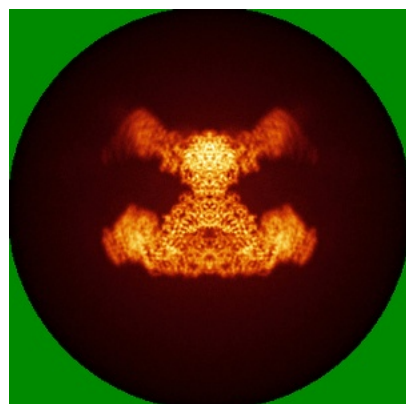


Y

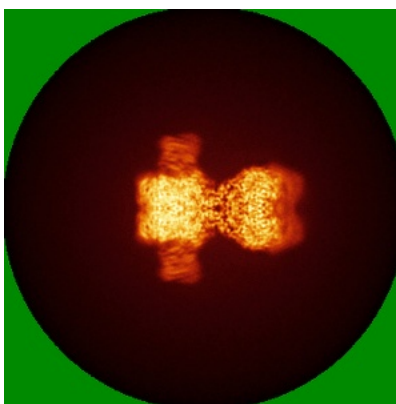


Z

6.4.2 Raw map



X



Y

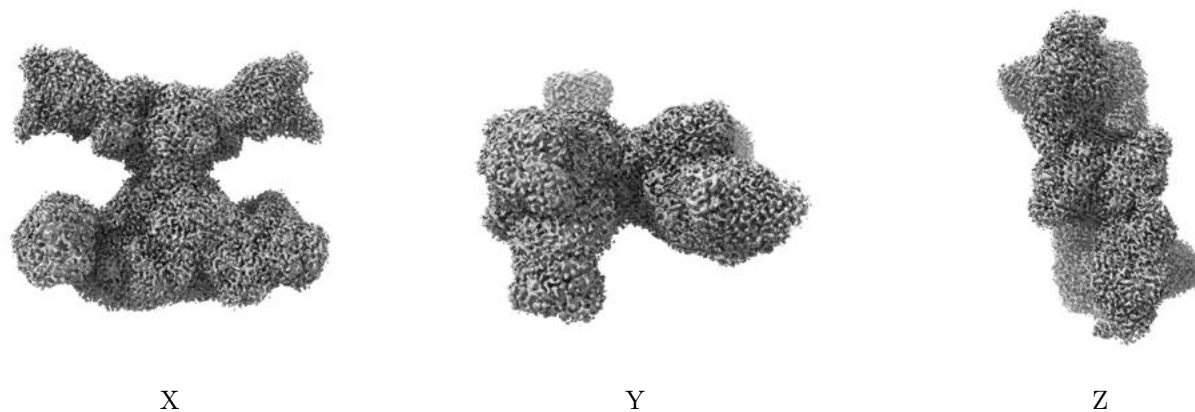


Z

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.

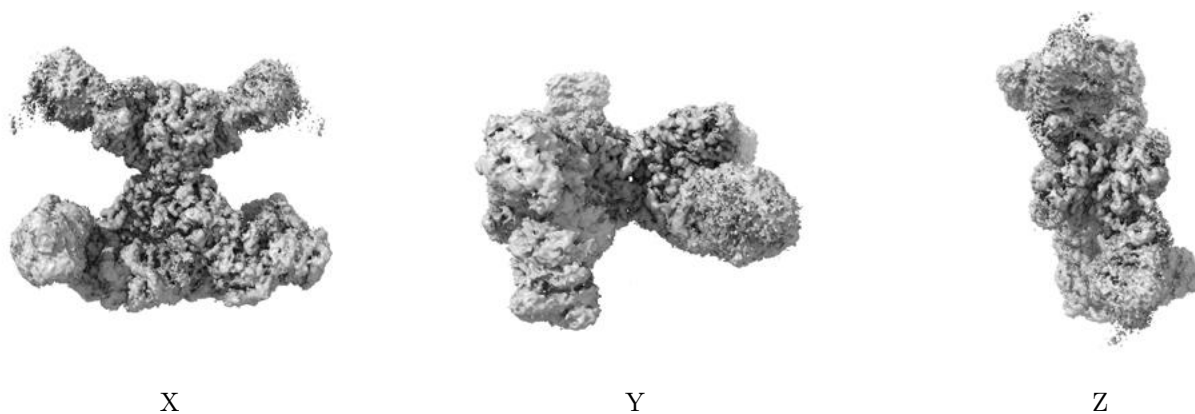
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. 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.

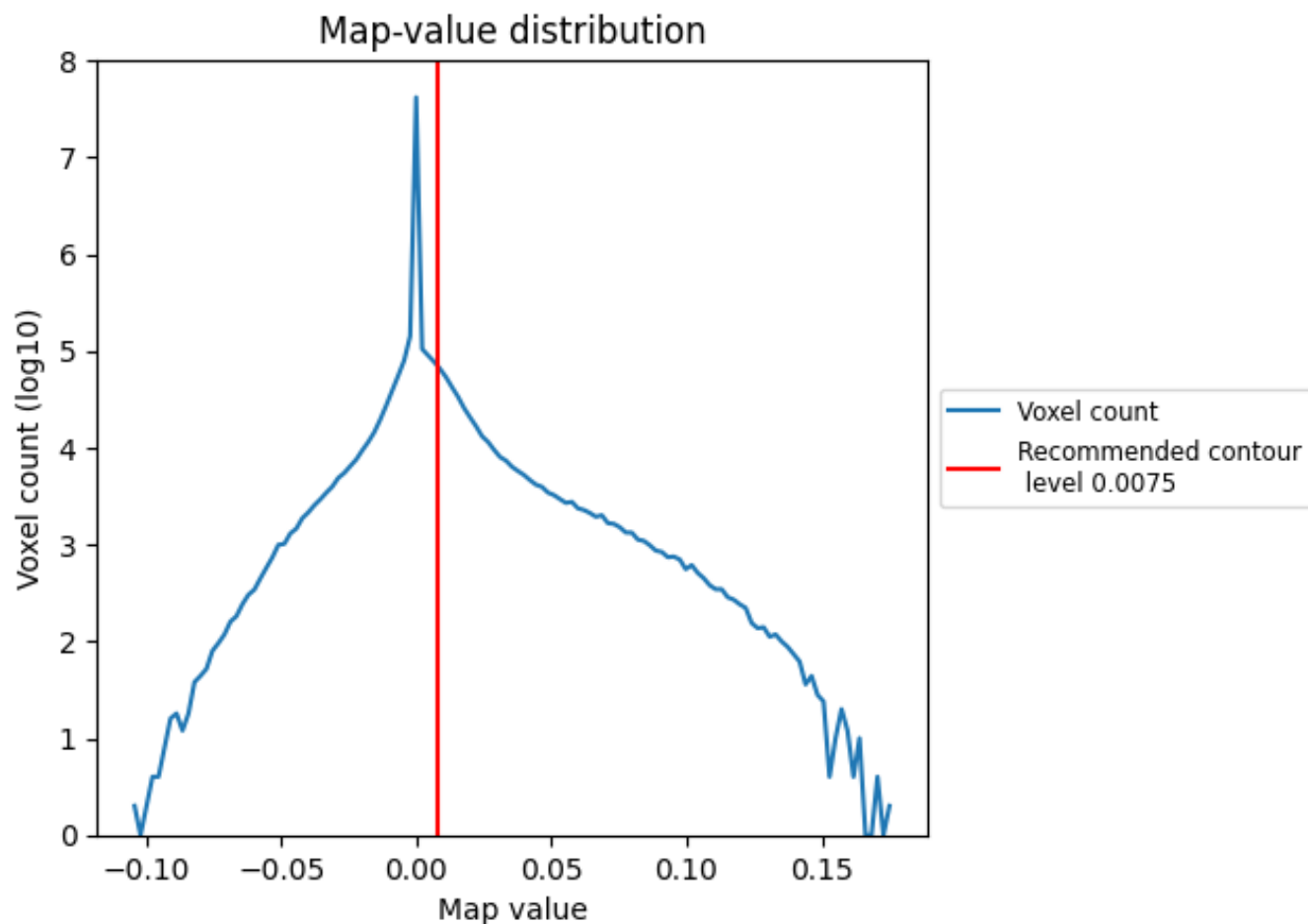
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

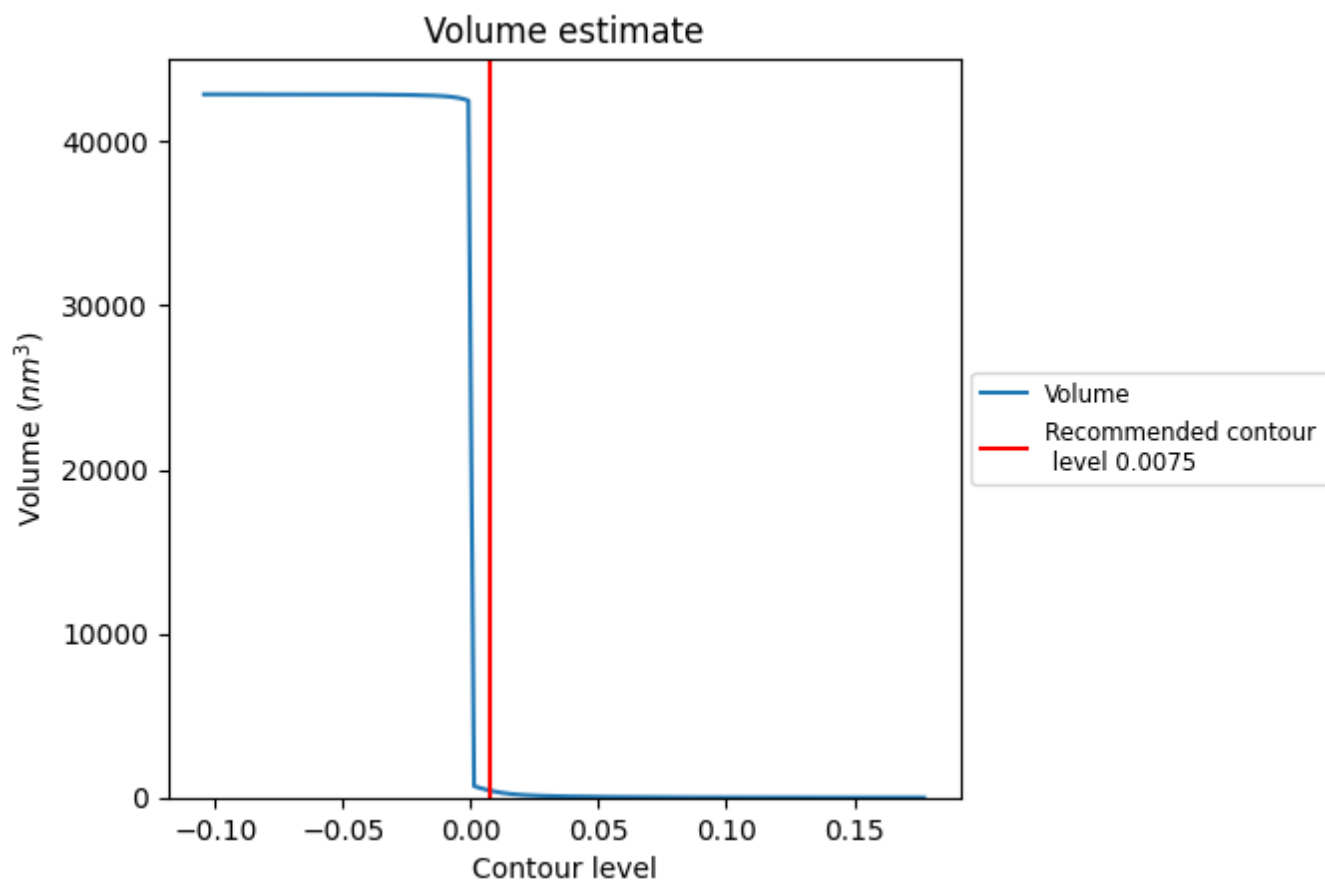
This section contains the results of statistical analysis of the map.

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.

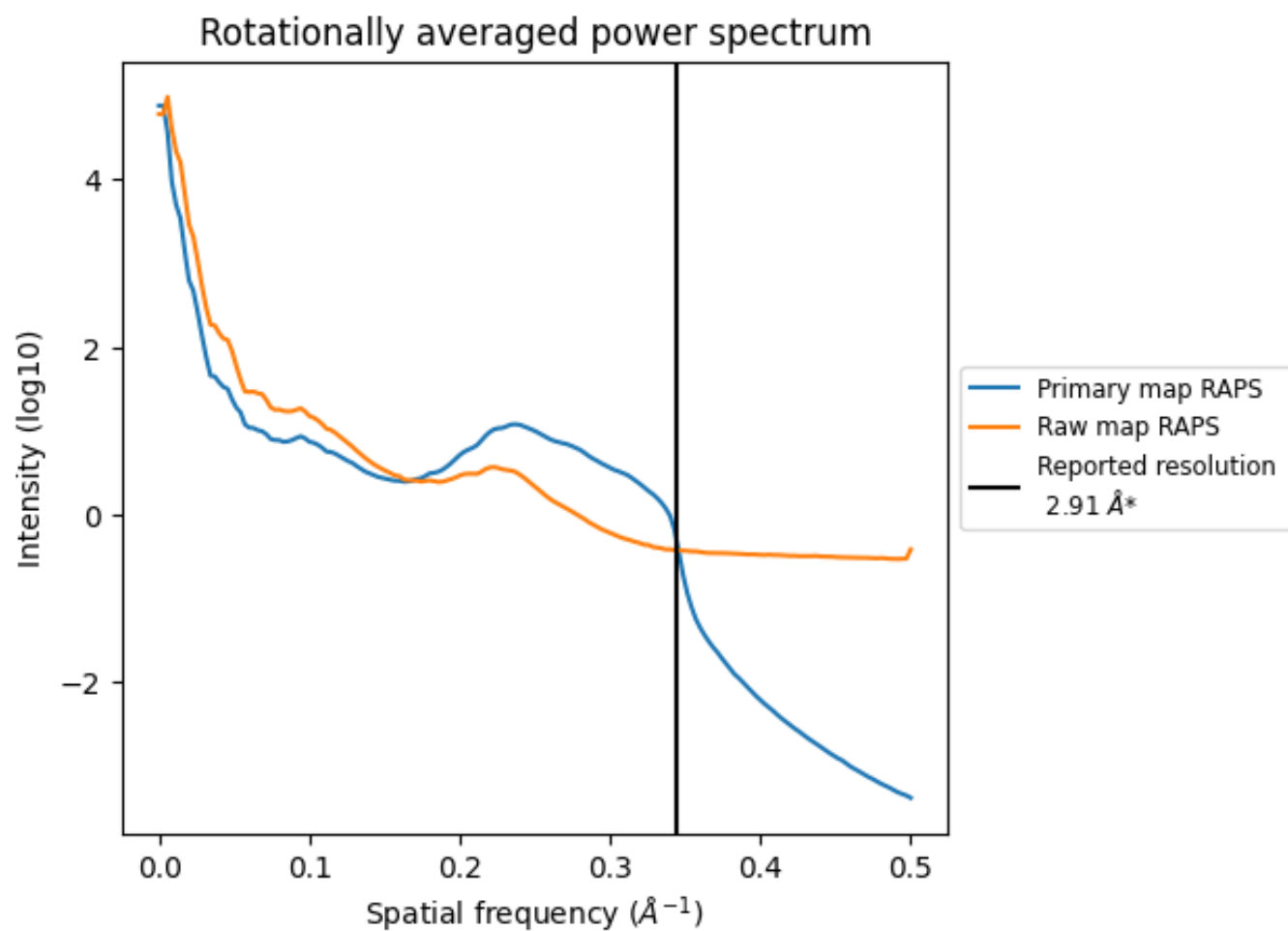
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 428 nm³; this corresponds to an approximate mass of 387 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 ⓘ

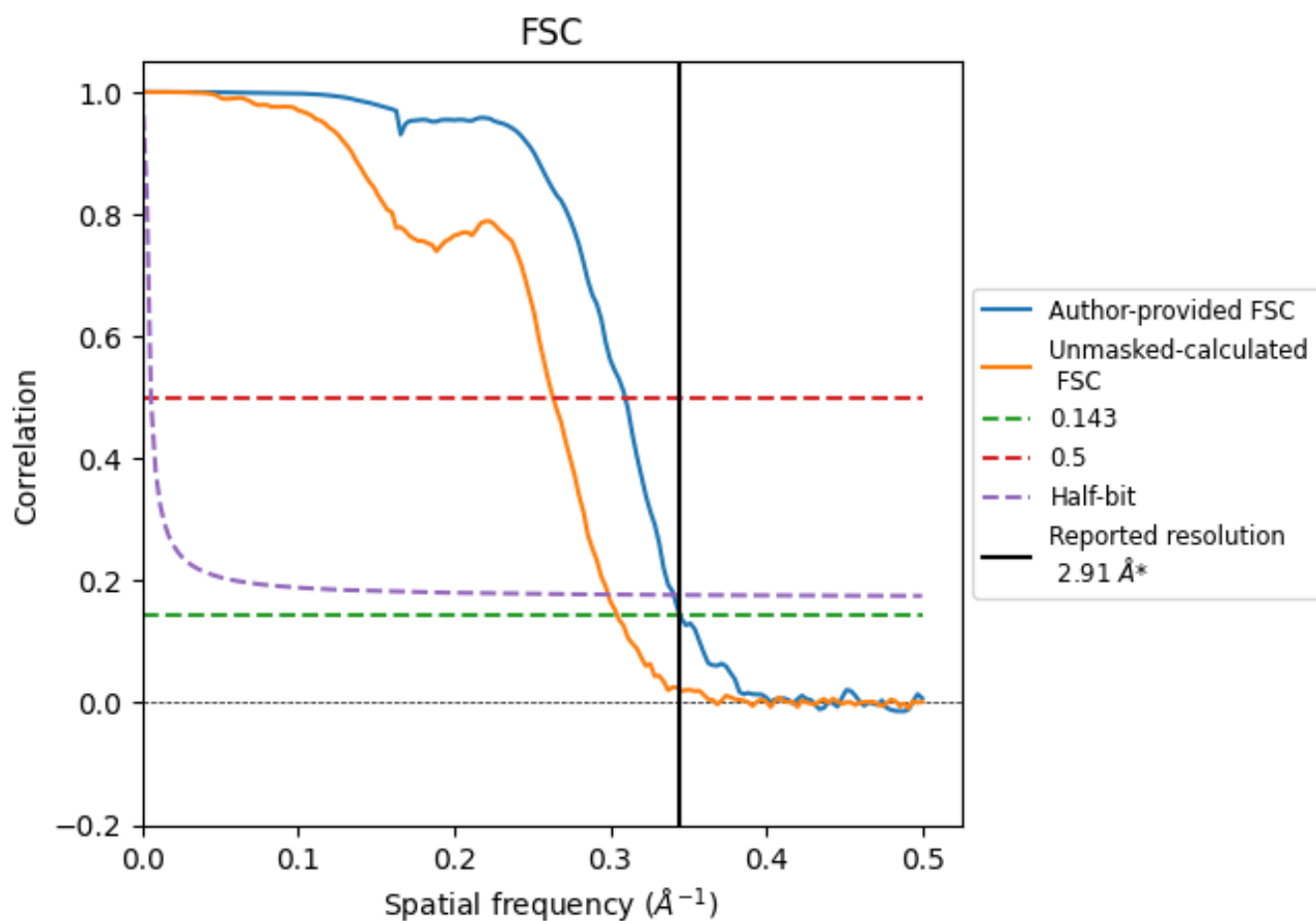


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

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 0.344 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

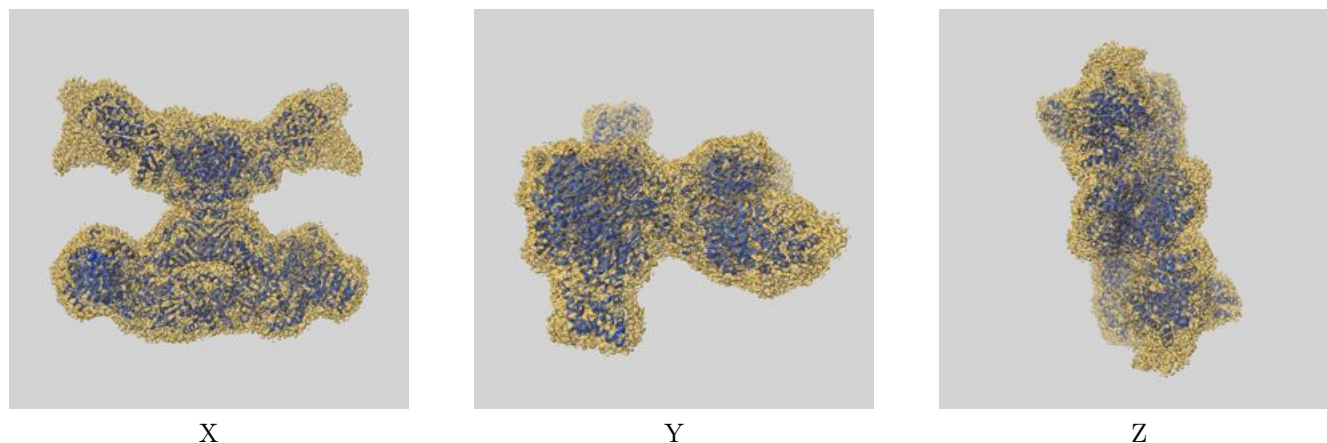
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.90	3.23	2.94
Unmasked-calculated*	3.28	3.80	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.28 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

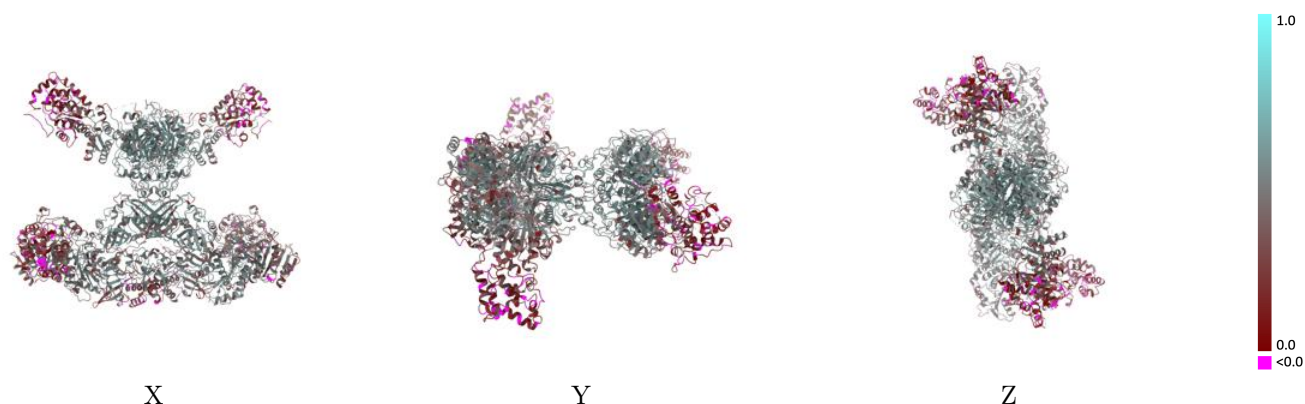
This section contains information regarding the fit between EMDB map EMD-30434 and PDB model 7CPX. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



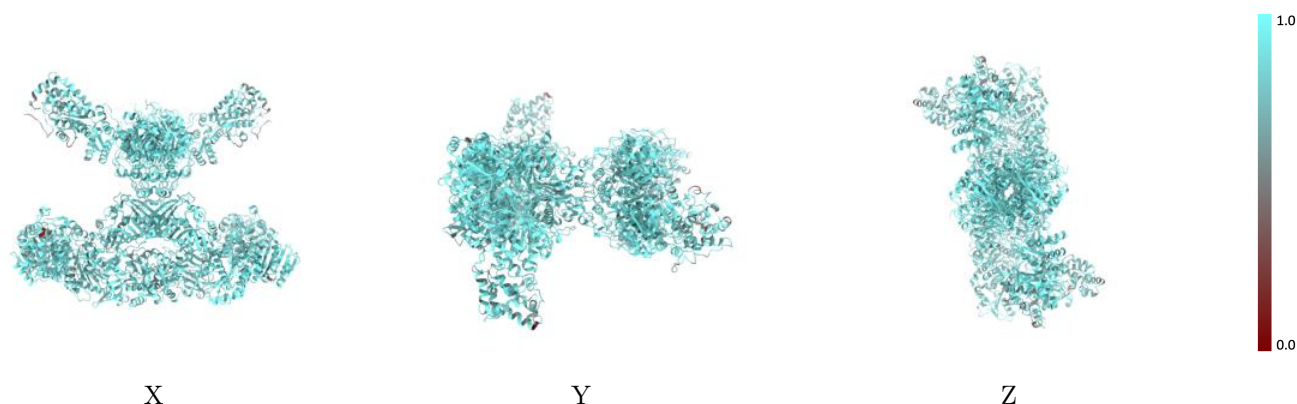
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



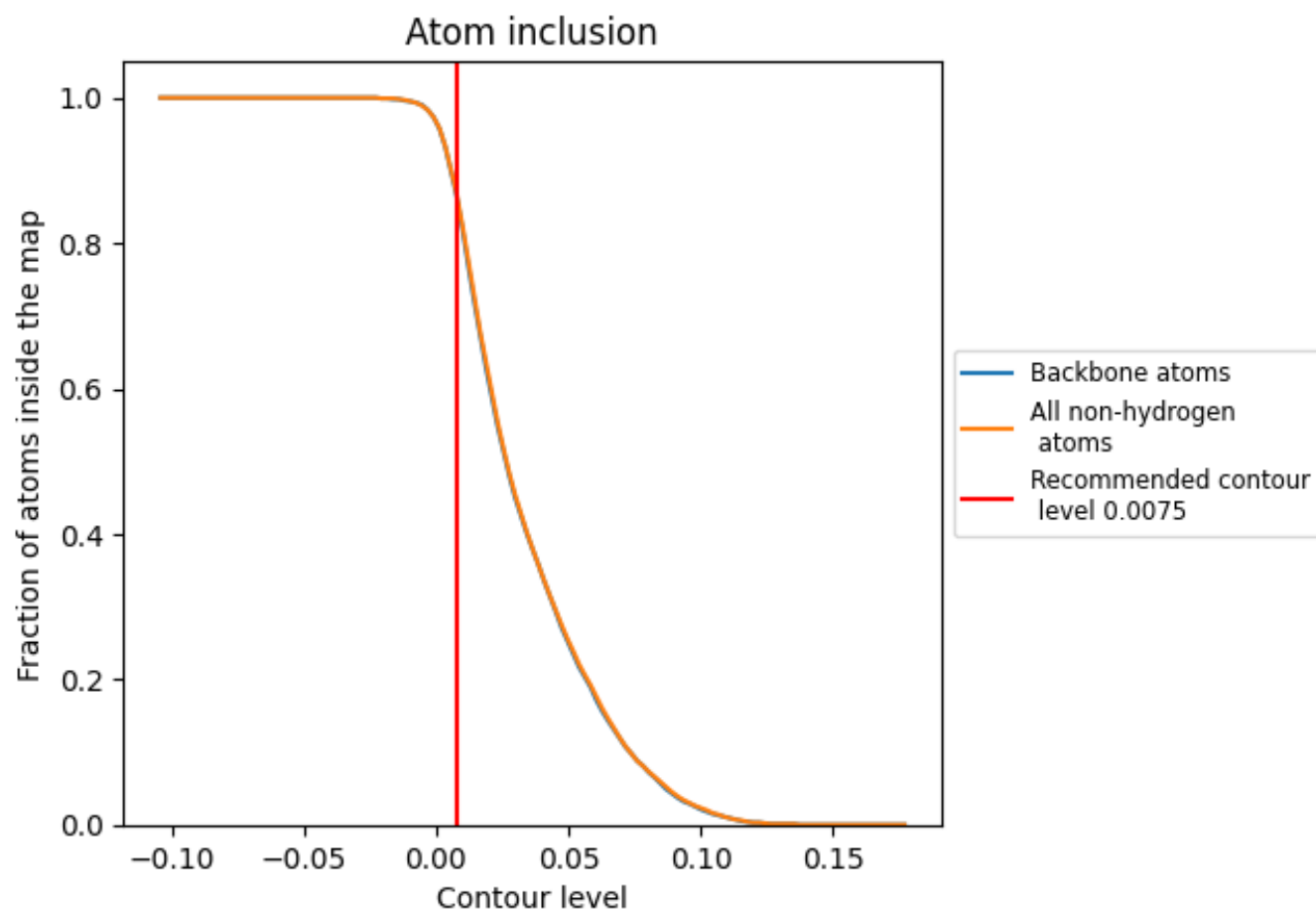
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8730	0.4060
A	0.8770	0.4060
B	0.8770	0.4070

