



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:54 PM UTC

PDB ID : 7XOA / pdb_00007xoax
EMDB ID : EMD-33342
Title : SARS-CoV-2 Omicron BA.2 Variant Spike Trimer with one mouse ACE2 Bound
Authors : Xu, Y.; Wu, C.; Liu, H.; Yin, W.; Xu, H.E.
Deposited on : 2022-05-01
Resolution : 3.20 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:

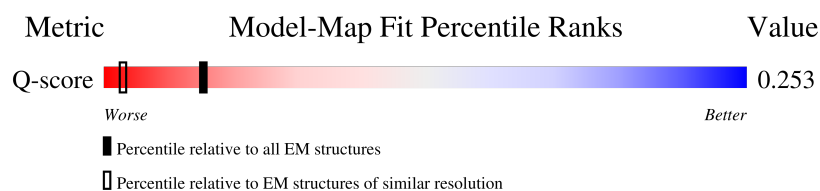
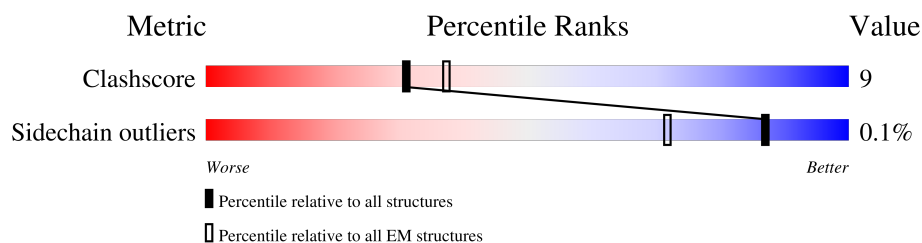
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	1270	
1	B	1270	
1	C	1270	
2	D	805	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1305	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29202 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1026	Total	C	N	O	S	0	0
			8001	5124	1331	1511	35		
1	B	1026	Total	C	N	O	S	0	0
			7950	5099	1319	1497	35		
1	C	1026	Total	C	N	O	S	0	0
			7950	5099	1319	1497	35		

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
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B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
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C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	682	GLY	ARG	engineered mutation	UNP P0DTC2

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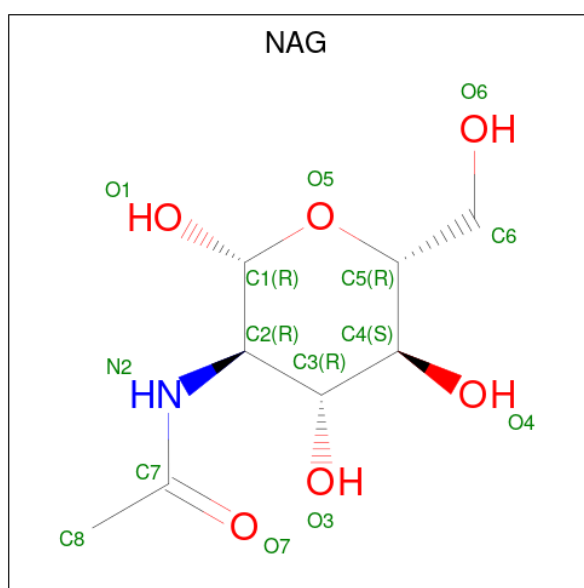
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Chain	Residue	Modelled	Actual	Comment	Reference
C	683	SER	ARG	engineered mutation	UNP P0DTC2
C	685	SER	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	592	Total	C	N	O	S	0	0
			4824	3073	809	913	29		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	A	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	B	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	

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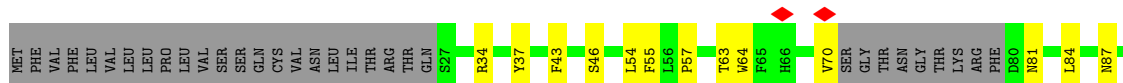
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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	D	1	Total	Zn	0
			1	1	

Chain B: 5% 66% 15% 19%



ILE	GLY	ARG	SER	L584	D509	E433	P346	L248	E181
LYS	MET	SER	SER	L585		T434	T347	M249	E182
GLY	SER	VAL	VAL	N586	F512	E435	T347	D250	E183
LYS	ARG	ALA	ALA	F587	F513	I436	W349	T251	V184
ARG	GLY	TYR	TYR	F588	R514	N437	D350	Y252	V185
LYS	ARG	ALA	ALA		Y515	F438	L361	P253	
LYS	MET	ILE	MET	Q589	Y516	L439	G352	S254	N188
ASN	ASN	ASN	ARG	P590	T517		H353	P258	E189
GLU	ASP	ASP	LYS	L591	R518	Q442	G354	T259	M190
THR	VAL	VAL	TYR	F592	T519	I446		G260	A191
LYS	PHE	GLY	SER	D593	I520		R357		R192
ARG	GLY	LEU	ILE		Y521	L450	I358	G267	A193
GLU	ASN	ASN	ILE	K596	Q522	P451	K359	L267	N194
ASN	ASP	ASN	LYS	E597	F523		M360		A194
PRO	ASN	GLN	ASN	Q598	Q524			R273	N195
TYR	SER	GLN	THR	N599		M455	C361	F274	Y196
LEU	LEU	THR	VAL		A532	L456	T362		N197
ASP	GLU	VAL	VAL	R600	A533	E457	K363	L278	D198
MET	PHE	PHE	PRO	N601	K534	K458	V364	Y279	Y199
ASP	LEU	LEU	PRO	S602	Y535	W459	T365	P280	G200
ILE	GLY	GLY	GLU	F603	N536	R460	M366	L281	
LYS	ILE	GLU	GLU		G537	H461	D367	T282	
GLY	HIS	GLY	ASP	V604	N536	W461	N368		G205
GLY	PRO	PRO	VAL	G605	G537	M462		V283	
GLU	THR	THR	VAL	W606	S538	V463	A372	P284	E208
SER	LEU	ARG	ARG	N607	L539	F464	F285	P284	A209
ASN	GLU	GLU	VAL	T608	H540	R465	E375	F285	E210
ALA	ALA	PRO	SER		K541	G466	Q380	A286	G211
GLY	GLY	PRO	ASP	E609			I379	Q287	A212
PHE	TYR	TYR	LEU	W610	I544	E467	Q380	K288	
GLN	GLN	LYS	LYS		S545	I468		P289	D213
ASN	PRO	PRO	PRO	S611			A386	N290	G214
ASN	PRO	ARG	ARG	P612		P469	R387	D291	Y215
VAL	VAL	VAL	VAL	Y613	Q552	K470	Q388		
ASP	THR	SER	SER		K553	E471	P389	Q300	N216
ALA	ILE	PHE	PHE	A614	L554	Q472		G301	Y217
GLN	TRP	TYR	PHE	D615	L555	W473	L392	Q300	N218
LEU	LEU	LEU	PHE		K556	M474		G301	R219
ILE	ILE	ILE	PHE		M557	K475	G395	W302	N220
ILE	ILE	ILE	THR	SER	LYS			D303	Q221
ILE	ILE	ILE	THR	VAL	VAL	L558	G395	A304	L222
ILE	ILE	ILE	VAL	ARG	PRO		E398	F314	I223
ILE	ILE	ILE	GLN	ILE	ILE	N480	H401		E224
ILE	ILE	ILE	VAL	VAL	SER	K481			
ILE	ILE	ILE	ASN	VAL	SER	L560			
ILE	ILE	ILE	ASN	VAL	LEU				
ILE	ILE	ILE	VAL	VAL	G561	R482			
ILE	ILE	ILE	SER	VAL	LYS	N562			
ILE	ILE	ILE	ASP	VAL	ASP	E483			
ILE	ILE	ILE	VAL	VAL	ALA	I484			
ILE	ILE	ILE	VAL	VAL	E564	V485			
ILE	ILE	ILE	PRO	GLY	P565				
ILE	ILE	ILE	ARG	GLY	W566				
ILE	ILE	ILE	ARG	ALA		E489			
ILE	ILE	ILE	SER	ASN	ASN	P490			
ILE	ILE	ILE	GLU	ALA	A569	L491			
ILE	ILE	ILE	GLU	ALA					
ILE	ILE	ILE	VAL	TYR	N572	P492			
ILE	ILE	ILE	GLU	GLU	W573	H493			
ILE	ILE	ILE	VAL	TRP	V574	D494			
ILE	ILE	ILE	ASP	ALA		E495			
ILE	ILE	ILE	ALA	THR	THR	G575			
ILE	ILE	ILE	ILE	ASN	ASN				
ILE	ILE	ILE	GLU	ASN	A576	T496			
ILE	ILE	ILE	GLU	GLU		Y497			
ILE	ILE	ILE	VAL	NET	R577	C498			
ILE	ILE	ILE	PHE	PHE	N578	D499			
ILE	ILE	ILE	LEU	LEU	W579				
ILE	ILE	ILE	PHE	THR	D580	S502			
ILE	ILE	ILE	ARG	ARG	V581				
ILE	ILE	ILE			K582	H505			
ILE	ILE	ILE			P583				
ILE	ILE	ILE							
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	170078	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.103	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	395.52, 395.52, 395.52	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.824, 0.824, 0.824	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, NAG

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	0.15	0/8192	0.35	4/11154 (0.0%)
1	B	0.16	0/8141	0.36	2/11091 (0.0%)
1	C	0.15	0/8141	0.34	0/11091
2	D	0.09	0/4956	0.25	0/6726
All	All	0.15	0/29430	0.34	6/40062 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	PHE	CA-CB-CG	6.68	120.48	113.80
1	A	371	PHE	CA-C-O	-5.89	114.57	121.46
1	B	520	ALA	CA-C-O	-5.51	112.61	120.16
1	A	287	ASP	O-C-N	-5.48	117.24	123.48
1	B	523	THR	O-C-N	5.21	124.69	120.83
1	A	371	PHE	N-CA-C	-5.14	101.74	109.85

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	8001	0	7796	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7950	0	7718	164	0
1	C	7950	0	7717	150	0
2	D	4824	0	4592	63	0
3	A	154	0	143	14	0
3	B	140	0	130	0	0
3	C	154	0	143	0	0
3	D	28	0	26	1	0
4	D	1	0	0	0	0
All	All	29202	0	28265	504	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 9.

All (504) 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:375:PHE:CZ	1:B:508:TYR:HE2	1.14	1.60
1:B:375:PHE:HZ	1:B:508:TYR:CE2	1.27	1.51
1:C:577:ARG:NH2	1:C:582:LEU:CD1	1.90	1.35
1:B:375:PHE:CZ	1:B:508:TYR:CE2	2.06	1.31
1:B:336:CYS:SG	1:B:363:ALA:HA	1.76	1.25
1:C:577:ARG:NH2	1:C:582:LEU:HD12	1.46	1.24
1:A:187:LYS:HA	1:A:210:ILE:HG12	1.20	1.19
1:B:336:CYS:SG	1:B:362:VAL:O	2.07	1.13
1:C:577:ARG:HH21	1:C:582:LEU:HD12	0.96	1.11
1:B:391:CYS:O	1:B:519:HIS:NE2	1.86	1.07
1:B:363:ALA:HB2	1:B:524:VAL:CG1	1.83	1.06
1:A:657:ASN:HD21	3:A:1305:NAG:H83	1.18	1.05
1:C:577:ARG:NH2	1:C:582:LEU:HD11	1.67	1.02
1:C:577:ARG:HH22	1:C:582:LEU:HD11	1.24	1.02
1:A:657:ASN:ND2	3:A:1305:NAG:C1	2.25	0.99
1:A:657:ASN:HD21	3:A:1305:NAG:C8	1.78	0.97
1:A:657:ASN:ND2	3:A:1305:NAG:H83	1.79	0.96
1:B:375:PHE:CE2	1:B:508:TYR:HE2	1.84	0.96
1:A:657:ASN:ND2	3:A:1305:NAG:C2	2.28	0.96
1:B:176:LEU:HD22	1:B:190:ARG:NH2	1.79	0.95
1:A:119:ILE:HG12	1:A:128:ILE:HG23	1.46	0.93
1:B:336:CYS:HG	1:B:362:VAL:C	1.76	0.93
1:B:391:CYS:C	1:B:519:HIS:HE2	1.75	0.93
1:B:385:THR:HG23	1:C:415:THR:CB	1.98	0.93
1:B:336:CYS:SG	1:B:363:ALA:CA	2.59	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ASN:HD21	3:A:1305:NAG:C2	1.83	0.91
1:A:591:SER:HB2	1:A:619:GLU:OE2	1.72	0.89
1:B:363:ALA:HB2	1:B:524:VAL:HG13	1.54	0.88
1:A:119:ILE:CG1	1:A:128:ILE:HG23	2.03	0.88
1:C:577:ARG:HH22	1:C:582:LEU:CD1	1.71	0.87
1:A:657:ASN:HD21	3:A:1305:NAG:H2	1.39	0.86
1:A:229:LEU:CD1	1:A:231:ILE:HG22	2.07	0.85
2:D:279:TYR:O	2:D:283:VAL:HG23	1.75	0.85
1:A:368:LEU:HD23	1:A:377:PHE:HZ	1.43	0.83
1:A:46:SER:HA	1:A:279:TYR:O	1.78	0.83
1:A:187:LYS:CA	1:A:210:ILE:HG12	2.06	0.82
1:B:129:LYS:HB3	1:B:166:CYS:SG	2.18	0.82
2:D:343:VAL:HG12	2:D:345:HIS:HD2	1.42	0.82
1:B:375:PHE:CE2	1:B:508:TYR:CE2	2.64	0.80
1:A:229:LEU:O	1:A:229:LEU:HD12	1.81	0.80
1:B:201:PHE:CE2	1:B:227:VAL:HG23	2.18	0.78
1:A:119:ILE:HG12	1:A:128:ILE:CG2	2.13	0.78
1:A:971:GLY:H	1:C:755:GLN:HE22	1.31	0.78
2:D:279:TYR:O	2:D:283:VAL:CG2	2.31	0.77
1:B:46:SER:HA	1:B:279:TYR:O	1.84	0.77
1:A:657:ASN:HD22	3:A:1305:NAG:C1	1.98	0.77
1:B:28:TYR:CE1	1:B:63:THR:HG22	2.19	0.77
1:A:324:GLU:HG2	1:A:325:SER:H	1.50	0.76
1:B:480:CYS:HG	1:B:488:CYS:CB	1.99	0.76
1:A:229:LEU:HD12	1:A:231:ILE:HG22	1.66	0.76
1:B:124:THR:O	1:B:124:THR:HG22	1.84	0.76
2:D:343:VAL:CG1	2:D:345:HIS:HD2	1.99	0.75
1:B:63:THR:OG1	1:B:267:VAL:HB	1.88	0.72
1:A:368:LEU:CD2	1:A:377:PHE:HZ	2.03	0.72
1:B:336:CYS:SG	1:B:362:VAL:C	2.67	0.72
2:D:233:ILE:HG22	2:D:233:ILE:O	1.88	0.71
1:A:332:ILE:HG23	1:A:362:VAL:HG11	1.71	0.71
1:A:657:ASN:ND2	3:A:1305:NAG:C7	2.54	0.70
1:A:1088:HIS:HB3	1:A:1120:THR:CG2	2.21	0.70
1:B:171:VAL:HG22	1:B:172:SER:H	1.56	0.70
1:B:171:VAL:HG22	1:B:172:SER:N	2.06	0.70
1:A:368:LEU:CD2	1:A:377:PHE:CZ	2.75	0.70
1:A:189:LEU:HB3	1:A:208:THR:O	1.93	0.69
1:B:363:ALA:CB	1:B:524:VAL:CG1	2.67	0.69
1:A:657:ASN:HD21	3:A:1305:NAG:C7	2.05	0.68
1:C:46:SER:HA	1:C:279:TYR:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLU:HG2	1:A:325:SER:N	2.07	0.68
1:B:902:MET:HB3	1:B:916:LEU:HD11	1.74	0.68
1:A:1093:GLY:HA3	1:A:1105:THR:O	1.93	0.68
1:C:577:ARG:HH21	1:C:582:LEU:CD1	1.70	0.68
1:C:105:ILE:HB	1:C:239:GLN:HB3	1.76	0.68
1:A:657:ASN:ND2	3:A:1305:NAG:N2	2.41	0.67
1:C:127:VAL:HA	1:C:171:VAL:HG12	1.76	0.67
2:D:343:VAL:CG1	2:D:345:HIS:CD2	2.77	0.67
1:C:124:THR:HG22	1:C:124:THR:O	1.94	0.67
1:B:480:CYS:CB	1:B:488:CYS:HG	2.08	0.67
1:B:96:GLU:O	1:B:188:ASN:ND2	2.28	0.66
1:B:1116:THR:HG22	1:B:1117:THR:N	2.11	0.66
1:A:907:ASN:HD22	1:B:1107:ARG:HH22	1.42	0.66
1:C:70:VAL:HG23	1:C:242:LEU:HD12	1.77	0.66
1:B:1076:THR:HB	1:B:1097:SER:HB3	1.78	0.66
1:A:229:LEU:CD1	1:A:231:ILE:CG2	2.74	0.66
1:B:907:ASN:HD22	1:C:1107:ARG:HH22	1.44	0.65
1:A:119:ILE:HG12	1:A:128:ILE:CG1	2.26	0.65
1:C:1116:THR:HG22	1:C:1117:THR:N	2.10	0.65
1:B:403:ARG:HB2	1:B:406:GLU:HB2	1.79	0.65
2:D:343:VAL:HG12	2:D:345:HIS:CD2	2.27	0.65
1:C:81:ASN:HD21	1:C:138:ASP:HB3	1.62	0.64
1:C:475:ALA:HB2	1:C:488:CYS:SG	2.36	0.64
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.78	0.64
1:A:731:MET:HE1	1:A:1014:ARG:HB3	1.80	0.64
1:C:965:GLN:NE2	1:C:1003:SER:OG	2.31	0.64
1:C:403:ARG:HB2	1:C:406:GLU:HB2	1.80	0.64
1:A:969:LYS:HB2	1:C:755:GLN:HE21	1.63	0.64
1:A:699:LEU:HB2	1:C:788:ILE:HD11	1.80	0.63
1:B:480:CYS:CB	1:B:488:CYS:SG	2.86	0.63
1:A:657:ASN:ND2	3:A:1305:NAG:C8	2.49	0.63
1:B:778:THR:HG22	1:B:778:THR:O	1.98	0.63
1:A:1076:THR:HB	1:A:1097:SER:HB3	1.79	0.63
1:C:731:MET:HE1	1:C:1014:ARG:HB3	1.81	0.63
1:B:43:PHE:H	1:C:566:GLY:HA2	1.64	0.63
1:B:105:ILE:HB	1:B:239:GLN:HB3	1.81	0.63
2:D:482:ARG:NH2	2:D:489:GLU:OE2	2.32	0.63
1:C:520:ALA:HA	1:C:565:PHE:HE2	1.64	0.62
1:B:731:MET:HE1	1:B:1014:ARG:HB3	1.80	0.62
1:A:375:PHE:HE2	1:A:508:TYR:CE2	2.18	0.62
1:A:37:TYR:H	1:A:55:PHE:HE1	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:VAL:HG22	1:B:542:ASN:CB	2.30	0.61
1:C:480:CYS:CB	1:C:488:CYS:SG	2.88	0.61
1:C:204:TYR:HB3	1:C:223:LEU:HB3	1.82	0.61
1:C:756:TYR:OH	1:C:994:ASP:OD1	2.17	0.61
1:B:979:ASP:O	1:B:983:ARG:NE	2.34	0.61
1:C:575:ALA:HB1	1:C:584:ILE:HD11	1.81	0.61
1:A:1107:ARG:HH22	1:C:907:ASN:HD22	1.47	0.61
1:A:702:GLU:OE1	1:C:790:LYS:NZ	2.34	0.61
1:B:788:ILE:HD11	1:C:699:LEU:HB2	1.82	0.61
1:B:201:PHE:HE2	1:B:227:VAL:HG23	1.66	0.61
1:B:575:ALA:HB1	1:B:584:ILE:HD11	1.81	0.61
2:D:323:MET:SD	2:D:380:GLN:NE2	2.73	0.61
1:A:983:ARG:HD2	1:B:517:LEU:HD13	1.83	0.60
1:B:28:TYR:CZ	1:B:63:THR:HG22	2.35	0.60
1:B:176:LEU:HD22	1:B:190:ARG:CZ	2.31	0.60
1:C:778:THR:HG22	1:C:778:THR:O	2.01	0.60
1:B:176:LEU:HD22	1:B:190:ARG:HH22	1.62	0.60
1:A:46:SER:CA	1:A:279:TYR:O	2.50	0.60
2:D:332:MET:HE1	2:D:342:VAL:HG11	1.82	0.60
1:A:408:SER:O	1:A:414:GLN:NE2	2.34	0.59
1:C:324:GLU:HB2	1:C:539:VAL:HG12	1.84	0.59
1:A:575:ALA:HB1	1:A:584:ILE:HD11	1.83	0.59
1:B:375:PHE:HZ	1:B:508:TYR:CD2	2.06	0.59
1:C:763:LEU:HG	1:C:1008:VAL:HG21	1.84	0.59
1:A:324:GLU:CG	1:A:325:SER:H	2.15	0.59
1:B:763:LEU:HG	1:B:1008:VAL:HG21	1.84	0.59
1:A:788:ILE:HD11	1:B:699:LEU:HB2	1.83	0.59
1:A:1088:HIS:HB3	1:A:1120:THR:HG22	1.84	0.59
1:B:37:TYR:HB3	1:B:223:LEU:HB2	1.84	0.59
1:C:273:ARG:NH1	1:C:292:ALA:HB3	2.18	0.58
1:A:131:CYS:HA	1:A:166:CYS:HA	1.85	0.58
1:C:46:SER:CA	1:C:279:TYR:O	2.50	0.58
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.36	0.58
1:A:376:ALA:HB3	1:A:435:ALA:HB3	1.85	0.58
1:B:46:SER:CA	1:B:279:TYR:O	2.51	0.58
1:A:657:ASN:ND2	3:A:1305:NAG:H2	2.06	0.58
1:A:726:ILE:HD13	1:A:945:LEU:HD23	1.84	0.58
1:B:1093:GLY:HA3	1:B:1105:THR:O	2.02	0.58
1:B:983:ARG:HD2	1:C:517:LEU:HD13	1.85	0.58
1:C:484:ALA:HB3	1:C:488:CYS:HB2	1.86	0.58
1:A:383:SER:HB3	1:A:386:LYS:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:HD13	1:B:945:LEU:HD23	1.86	0.58
1:C:37:TYR:H	1:C:55:PHE:HE1	1.52	0.58
1:C:34:ARG:NH2	1:C:191:GLU:OE2	2.37	0.58
1:A:201:PHE:HB3	1:A:229:LEU:HD11	1.85	0.57
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.30	0.57
2:D:574:VAL:HG13	2:D:576:ALA:H	1.69	0.57
1:A:319:ARG:HH21	1:C:740:MET:HE2	1.69	0.57
1:B:204:TYR:HB3	1:B:223:LEU:HB3	1.86	0.57
2:D:233:ILE:O	2:D:233:ILE:CG2	2.52	0.57
1:B:480:CYS:HG	1:B:488:CYS:HB3	1.68	0.57
1:C:736:VAL:HG21	1:C:1004:LEU:HD11	1.87	0.57
1:C:1106:GLN:HG3	1:C:1108:ASN:H	1.69	0.57
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.87	0.57
2:D:189:GLU:OE1	2:D:192:ARG:NH1	2.38	0.57
2:D:519:THR:HA	2:D:522:GLN:HE21	1.70	0.57
1:A:560:LEU:H	1:A:563:GLN:HE21	1.53	0.56
1:B:484:ALA:HB3	1:B:488:CYS:HB2	1.86	0.56
1:C:590:CYS:SG	1:C:591:SER:N	2.78	0.56
1:A:319:ARG:NH1	1:C:745:ASP:OD1	2.38	0.56
1:B:176:LEU:CD2	1:B:190:ARG:NH2	2.63	0.56
1:C:822:LEU:HD22	1:C:945:LEU:HD21	1.88	0.56
1:C:773:GLU:OE2	1:C:1019:ARG:NE	2.35	0.56
1:B:591:SER:OG	1:B:619:GLU:OE1	2.20	0.56
1:C:726:ILE:HD13	1:C:945:LEU:HD23	1.86	0.56
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.88	0.56
1:A:204:TYR:HB3	1:A:223:LEU:HB3	1.87	0.56
1:A:983:ARG:HA	1:B:390:LEU:HD11	1.86	0.56
1:B:1106:GLN:HG3	1:B:1108:ASN:H	1.69	0.56
2:D:462:MET:HE3	2:D:468:ILE:HD11	1.87	0.56
1:C:520:ALA:HB3	1:C:521:PRO:HD3	1.88	0.55
1:B:176:LEU:CD2	1:B:190:ARG:CZ	2.84	0.55
2:D:144:LEU:HA	2:D:148:LEU:HD12	1.88	0.55
1:A:368:LEU:HD21	1:A:377:PHE:CZ	2.41	0.55
1:B:84:LEU:HD22	1:B:267:VAL:HG11	1.89	0.55
1:B:171:VAL:CG2	1:B:172:SER:H	2.18	0.55
2:D:47:SER:O	2:D:51:ASN:ND2	2.34	0.55
2:D:287:GLN:NE2	2:D:433:GLU:OE1	2.39	0.55
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.89	0.54
1:C:1093:GLY:HA3	1:C:1105:THR:O	2.08	0.54
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.37	0.54
1:A:1106:GLN:HG3	1:A:1108:ASN:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LYS:NZ	1:A:425:LEU:O	2.39	0.54
1:A:571:ASP:OD1	1:C:964:LYS:NZ	2.39	0.54
2:D:84:SER:OG	2:D:87:GLU:OE1	2.25	0.54
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.35	0.54
1:B:159:VAL:HG13	1:B:159:VAL:O	2.07	0.54
1:A:358:ILE:HB	1:A:395:VAL:HB	1.89	0.54
1:B:1116:THR:H	1:B:1119:ASN:HD21	1.56	0.54
1:B:577:ARG:NH2	1:B:582:LEU:HG	2.23	0.54
1:A:500:THR:OG1	2:D:41:TYR:OH	2.25	0.53
2:D:20:LEU:O	2:D:24:ASN:ND2	2.40	0.53
1:A:90:VAL:HG12	1:A:194:PHE:HB2	1.89	0.53
1:B:350:VAL:HG21	1:B:418:ILE:HD12	1.89	0.53
1:B:986:PRO:O	1:B:990:GLU:HG2	2.08	0.53
1:C:733:LYS:HE3	1:C:771:ALA:HB1	1.90	0.53
1:B:273:ARG:NH1	1:B:292:ALA:HB3	2.24	0.53
1:B:965:GLN:NE2	1:B:1003:SER:OG	2.42	0.53
2:D:457:GLU:OE2	2:D:460:ARG:NH2	2.37	0.53
1:C:273:ARG:HH12	1:C:292:ALA:HB3	1.74	0.53
1:C:778:THR:HG22	1:C:865:LEU:HD12	1.91	0.53
2:D:168:TRP:NE1	2:D:502:SER:OG	2.40	0.53
1:B:778:THR:HG22	1:B:865:LEU:HD12	1.91	0.52
1:B:130:VAL:O	1:B:130:VAL:HG13	2.08	0.52
1:B:822:LEU:HD22	1:B:945:LEU:HD21	1.91	0.52
1:A:99:ASN:OD1	1:A:102:ARG:NH1	2.41	0.52
1:B:363:ALA:CB	1:B:524:VAL:HG12	2.39	0.52
1:B:327:VAL:HG22	1:B:542:ASN:HB3	1.92	0.52
1:A:792:PRO:HG3	1:B:707:TYR:HB3	1.90	0.52
1:B:171:VAL:CG2	1:B:172:SER:N	2.73	0.52
1:C:1116:THR:H	1:C:1119:ASN:HD21	1.56	0.52
1:A:657:ASN:CG	3:A:1305:NAG:H83	2.33	0.52
2:D:29:LEU:HD11	2:D:97:LEU:HG	1.92	0.52
1:A:370:ASN:OD1	1:A:371:PHE:CE1	2.63	0.52
1:A:449:TYR:OH	1:A:498:ARG:NH1	2.41	0.52
1:A:546:LEU:HD21	1:A:573:THR:HG21	1.90	0.52
1:B:327:VAL:HG22	1:B:542:ASN:HB2	1.91	0.52
1:A:324:GLU:CG	1:A:325:SER:N	2.73	0.52
2:D:360:MET:HE1	2:D:372:ALA:HA	1.91	0.52
1:A:756:TYR:OH	1:A:998:THR:OG1	2.27	0.51
2:D:37:GLU:O	2:D:353:HIS:NE2	2.30	0.51
2:D:85:LEU:HB3	2:D:94:LYS:HE3	1.92	0.51
1:A:370:ASN:OD1	1:A:371:PHE:CD1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1104:VAL:HG23	1:C:1115:ILE:HG12	1.92	0.51
1:A:246:ARG:HE	1:A:248:TYR:HE1	1.57	0.51
1:C:708:SER:HB2	1:C:711:SER:HB3	1.92	0.51
2:D:340:ARG:HD3	3:D:903:NAG:H82	1.92	0.51
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	1.93	0.51
2:D:288:LYS:NZ	2:D:431:ASP:OD2	2.37	0.51
1:C:1116:THR:CG2	1:C:1117:THR:N	2.73	0.51
1:B:124:THR:O	1:B:124:THR:CG2	2.55	0.50
1:C:742:ILE:O	1:C:1000:ARG:NH2	2.43	0.50
1:B:1116:THR:CG2	1:B:1117:THR:N	2.74	0.50
1:C:46:SER:N	1:C:279:TYR:O	2.43	0.50
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.94	0.50
1:B:884:SER:OG	1:B:887:THR:OG1	2.29	0.50
2:D:524:GLN:OE1	2:D:580:ASP:N	2.39	0.50
1:C:84:LEU:HD22	1:C:267:VAL:HG11	1.92	0.50
1:A:34:ARG:HH11	1:A:217:PRO:HG2	1.77	0.50
1:C:34:ARG:HH11	1:C:217:PRO:HG2	1.76	0.50
1:C:884:SER:OG	1:C:887:THR:OG1	2.30	0.50
1:A:119:ILE:HG23	1:A:128:ILE:HG13	1.92	0.50
2:D:557:MET:HG2	2:D:569:ALA:HB1	1.94	0.50
1:B:278:LYS:HE2	1:B:287:ASP:HB2	1.94	0.50
1:C:187:LYS:HA	1:C:210:ILE:H	1.77	0.50
1:A:102:ARG:HB3	1:A:141:LEU:HD23	1.94	0.49
1:B:69:HIS:O	1:B:70:VAL:HG12	2.12	0.49
1:A:229:LEU:HD12	1:A:229:LEU:C	2.36	0.49
1:A:453:TYR:OH	2:D:34:GLN:NE2	2.41	0.49
1:C:115:GLN:HB3	1:C:233:ILE:CD1	2.42	0.49
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.94	0.49
1:A:788:ILE:HG23	1:A:876:ALA:HB2	1.95	0.49
1:B:37:TYR:H	1:B:55:PHE:HE1	1.60	0.49
1:C:323:THR:HG23	1:C:324:GLU:HG2	1.95	0.49
1:B:141:LEU:HB2	1:B:160:TYR:HE1	1.78	0.49
1:A:725:GLU:OE2	1:A:1028:LYS:NZ	2.34	0.49
1:B:63:THR:HG1	1:B:267:VAL:HB	1.78	0.49
1:B:733:LYS:HE3	1:B:771:ALA:HB1	1.94	0.49
1:B:108:THR:O	1:B:236:THR:OG1	2.30	0.49
1:B:475:ALA:HB2	1:B:488:CYS:SG	2.52	0.49
1:C:350:VAL:HG21	1:C:418:ILE:HD12	1.94	0.49
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.26	0.48
1:B:675:GLN:HB3	1:B:693:ILE:HD13	1.95	0.48
1:C:37:TYR:OH	1:C:54:LEU:O	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:GLY:HA2	1:C:508:TYR:CG	2.48	0.48
1:A:538:CYS:CB	1:A:590:CYS:SG	3.00	0.48
1:A:375:PHE:HE2	1:A:508:TYR:HE2	1.59	0.48
1:B:126:VAL:HB	1:B:174:PRO:HB3	1.95	0.48
1:B:351:TYR:HE1	1:B:452:LEU:HB2	1.78	0.48
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.95	0.48
1:A:724:THR:HG21	1:A:938:LEU:HD21	1.96	0.48
1:C:124:THR:O	1:C:124:THR:CG2	2.62	0.48
1:C:246:ARG:HB2	1:C:258:TRP:HB2	1.96	0.48
1:C:377:PHE:HE2	1:C:384:PRO:HB3	1.79	0.48
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.94	0.48
1:A:34:ARG:HD2	1:A:216:LEU:HB3	1.96	0.48
1:A:827:THR:OG1	1:A:949:GLN:NE2	2.47	0.48
1:C:87:ASN:OD1	1:C:87:ASN:N	2.46	0.48
2:D:212:ALA:HB3	2:D:215:TYR:HD2	1.78	0.48
2:D:365:THR:OG1	2:D:368:ASN:ND2	2.37	0.48
1:A:366:SER:C	1:A:368:LEU:H	2.21	0.48
1:A:1086:LYS:HD2	1:A:1122:VAL:HG21	1.95	0.48
2:D:392:LEU:HD13	2:D:563:SER:HA	1.95	0.48
1:C:189:LEU:HB3	1:C:208:THR:O	2.13	0.48
1:A:392:PHE:HA	1:A:517:LEU:HD13	1.95	0.48
1:A:368:LEU:HD23	1:A:377:PHE:CZ	2.32	0.47
1:A:187:LYS:HG2	1:A:210:ILE:HB	1.96	0.47
1:C:57:PRO:HG3	1:C:273:ARG:HD2	1.96	0.47
1:C:902:MET:HB2	1:C:916:LEU:HD21	1.96	0.47
1:C:1116:THR:HG22	1:C:1117:THR:H	1.76	0.47
1:A:560:LEU:H	1:A:563:GLN:NE2	2.12	0.47
1:C:520:ALA:HA	1:C:565:PHE:CE2	2.46	0.47
1:C:278:LYS:HE2	1:C:287:ASP:HB2	1.94	0.47
1:A:403:ARG:HB2	1:A:406:GLU:HG3	1.95	0.47
1:B:385:THR:CG2	1:C:415:THR:CB	2.82	0.47
1:B:81:ASN:HD21	1:B:138:ASP:HB3	1.79	0.47
1:A:246:ARG:HD2	1:A:258:TRP:HE3	1.79	0.47
1:A:945:LEU:HD22	1:A:948:LEU:HD12	1.97	0.47
1:B:56:LEU:HD12	1:B:57:PRO:HD2	1.96	0.47
1:B:641:ASN:HD22	1:B:654:GLU:HA	1.80	0.47
1:B:391:CYS:SG	1:B:522:ALA:HB1	2.54	0.47
1:C:1109:PHE:HD1	1:C:1111:GLU:HG3	1.79	0.47
1:B:246:ARG:HB2	1:B:258:TRP:HB2	1.97	0.47
1:B:962:LEU:HD11	1:B:1007:TYR:HB2	1.97	0.47
1:C:70:VAL:CG2	1:C:242:LEU:HD12	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:TRP:HH2	1:B:904:TYR:HB3	1.80	0.47
1:B:1109:PHE:HD2	1:B:1111:GLU:HG3	1.80	0.46
1:B:976:VAL:HG22	1:B:978:ASN:H	1.80	0.46
1:C:109:THR:H	1:C:114:THR:HG21	1.81	0.46
1:C:916:LEU:CD1	1:C:923:ILE:HD12	2.44	0.46
1:C:126:VAL:HB	1:C:174:PRO:HA	1.96	0.46
1:A:201:PHE:HB3	1:A:229:LEU:CD1	2.45	0.46
1:A:563:GLN:HE22	1:C:43:PHE:HD1	1.62	0.46
1:C:663:ASP:OD1	1:C:663:ASP:N	2.48	0.46
1:A:129:LYS:HZ3	1:A:170:TYR:H	1.62	0.46
1:A:895:GLN:HG2	1:B:713:ALA:HB2	1.98	0.46
1:C:675:GLN:HB3	1:C:693:ILE:HD13	1.98	0.46
2:D:431:ASP:OD1	2:D:432:SER:N	2.48	0.46
2:D:509:ASP:OD1	2:D:509:ASP:N	2.47	0.46
1:A:350:VAL:HA	1:A:400:PHE:HB2	1.96	0.46
1:A:405:ASN:ND2	1:A:504:GLY:O	2.49	0.46
1:B:342:PHE:HZ	1:B:513:LEU:HD11	1.81	0.46
1:B:905:ARG:NH2	1:B:1049:LEU:O	2.44	0.46
1:B:1116:THR:HG22	1:B:1117:THR:H	1.77	0.46
1:A:328:ARG:HH11	1:A:580:GLN:HB2	1.80	0.46
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.97	0.46
1:C:192:PHE:HA	1:C:204:TYR:O	2.14	0.46
1:C:250:THR:HG22	1:C:250:THR:O	2.15	0.46
1:A:119:ILE:HG12	1:A:128:ILE:HG12	1.98	0.46
1:A:362:VAL:HG23	1:A:525:CYS:O	2.16	0.46
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.81	0.46
1:C:984:LEU:HB2	1:C:989:ALA:HB2	1.96	0.46
1:C:886:TRP:HH2	1:C:904:TYR:HB3	1.81	0.46
2:D:245:ARG:O	2:D:249:MET:HG3	2.16	0.46
1:A:226:LEU:HG	1:A:227:VAL:HG23	1.98	0.45
1:A:121:ASN:HD22	1:A:176:LEU:HG	1.81	0.45
1:C:119:ILE:HG12	1:C:128:ILE:HG23	1.97	0.45
1:C:641:ASN:HD22	1:C:654:GLU:HA	1.82	0.45
2:D:279:TYR:O	2:D:283:VAL:HG22	2.16	0.45
1:B:99:ASN:OD1	1:B:102:ARG:NH2	2.48	0.45
1:B:65:PHE:HE2	1:B:84:LEU:HD21	1.81	0.45
2:D:604:VAL:HG23	2:D:604:VAL:O	2.17	0.45
1:B:778:THR:O	1:B:778:THR:CG2	2.64	0.45
1:B:709:ASN:OD1	1:B:709:ASN:N	2.50	0.45
1:B:752:LEU:O	1:B:755:GLN:HG2	2.17	0.45
1:C:480:CYS:SG	1:C:488:CYS:CB	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:788:ILE:HG23	1:C:876:ALA:HB2	1.97	0.45
1:C:1116:THR:CG2	1:C:1117:THR:H	2.30	0.45
1:C:412:PRO:HA	1:C:425:LEU:HB2	1.99	0.45
1:C:1096:VAL:HG21	1:C:1110:TYR:HE1	1.82	0.45
2:D:190:MET:O	2:D:194:ASN:ND2	2.39	0.45
1:A:319:ARG:HD2	1:C:740:MET:HE2	1.98	0.45
1:A:375:PHE:CE2	1:A:508:TYR:CE2	3.03	0.45
1:C:317:ASN:HA	1:C:594:GLY:HA2	1.97	0.45
1:C:525:CYS:SG	1:C:526:GLY:N	2.90	0.45
1:C:351:TYR:HE1	1:C:452:LEU:HB2	1.81	0.45
1:B:725:GLU:OE2	1:B:1028:LYS:NZ	2.32	0.44
1:C:138:ASP:OD1	1:C:138:ASP:N	2.50	0.44
1:A:119:ILE:HG13	1:A:128:ILE:HG23	1.94	0.44
1:A:426:PRO:HG3	1:A:463:PRO:HB3	1.99	0.44
1:B:34:ARG:HH11	1:B:217:PRO:HG2	1.81	0.44
1:B:202:LYS:HD3	1:B:202:LYS:HA	1.82	0.44
1:C:115:GLN:HB3	1:C:233:ILE:HD13	2.00	0.44
1:C:480:CYS:SG	1:C:488:CYS:HB3	2.57	0.44
2:D:166:GLU:HG3	2:D:491:LEU:HD12	1.99	0.44
2:D:323:MET:HE1	2:D:379:ILE:HG21	1.99	0.44
1:A:69:HIS:HE1	1:A:244:LEU:HD11	1.83	0.44
1:B:985:ASP:HB2	1:B:988:GLU:HG2	2.00	0.44
2:D:245:ARG:HG2	2:D:249:MET:HE3	1.99	0.44
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	2.00	0.44
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.98	0.44
1:A:142:ASP:H	1:A:157:PHE:HB3	1.82	0.44
1:A:366:SER:C	1:A:368:LEU:N	2.72	0.44
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.50	0.44
1:B:96:GLU:HG3	1:B:101:ILE:HG12	2.00	0.44
1:B:187:LYS:HA	1:B:210:ILE:H	1.83	0.44
1:B:788:ILE:HG23	1:B:876:ALA:HB2	2.00	0.44
1:B:69:HIS:C	1:B:70:VAL:HG12	2.43	0.44
1:C:37:TYR:HB3	1:C:223:LEU:HB2	1.99	0.44
1:A:192:PHE:HA	1:A:204:TYR:O	2.18	0.44
1:B:200:TYR:HE2	1:B:202:LYS:HE2	1.83	0.44
1:B:520:ALA:O	1:B:521:PRO:C	2.59	0.44
1:B:1116:THR:CG2	1:B:1117:THR:H	2.30	0.44
1:A:736:VAL:HG12	1:A:858:LEU:HG	1.99	0.43
1:B:1096:VAL:HG21	1:B:1110:TYR:HE1	1.83	0.43
2:D:184:VAL:O	2:D:188:ASN:ND2	2.40	0.43
2:D:246:ARG:HD3	2:D:602:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:HB2	1:A:176:LEU:HD12	1.99	0.43
1:A:591:SER:CB	1:A:619:GLU:OE2	2.57	0.43
1:C:328:ARG:NH2	1:C:578:ASP:OD1	2.52	0.43
1:A:353:TRP:CD1	1:A:353:TRP:H	2.37	0.43
1:B:336:CYS:SG	1:B:363:ALA:N	2.92	0.43
2:D:25:ALA:HB1	2:D:97:LEU:HD11	2.01	0.43
2:D:450:LEU:HB2	2:D:451:PRO:HD3	2.01	0.43
1:A:199:GLY:O	1:A:231:ILE:N	2.52	0.43
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.53	0.43
1:C:342:PHE:HZ	1:C:513:LEU:HD11	1.82	0.43
1:C:974:SER:H	1:C:980:ILE:HD11	1.83	0.43
1:A:117:LEU:HD11	1:A:128:ILE:HG22	2.00	0.43
1:B:417:ASN:OD1	1:B:417:ASN:N	2.52	0.43
1:C:327:VAL:H	1:C:530:SER:HB3	1.84	0.43
1:A:107:GLY:H	1:A:237:ARG:HB3	1.84	0.43
1:B:138:ASP:OD1	1:B:138:ASP:N	2.50	0.43
1:B:347:PHE:CD2	1:B:399:SER:HB2	2.53	0.43
1:B:1126:CYS:HB2	1:B:1132:ILE:HG21	2.00	0.43
1:C:295:PRO:HB2	1:C:608:VAL:HG21	2.00	0.43
1:C:422:ASN:OD1	1:C:454:ARG:N	2.45	0.43
2:D:346:PRO:HB3	2:D:360:MET:HG3	2.00	0.43
1:A:453:TYR:CZ	1:A:493:ARG:HB2	2.54	0.43
1:B:375:PHE:CE2	1:B:437:ASN:ND2	2.86	0.43
1:C:1126:CYS:HB2	1:C:1132:ILE:HG21	2.01	0.43
1:B:991:VAL:HG12	1:C:995:ARG:HH12	1.84	0.42
1:C:748:GLU:OE1	1:C:748:GLU:N	2.40	0.42
1:A:886:TRP:HH2	1:A:904:TYR:HB3	1.84	0.42
1:B:663:ASP:OD1	1:B:663:ASP:N	2.51	0.42
1:B:992:GLN:OE1	1:B:995:ARG:NH1	2.45	0.42
1:C:63:THR:OG1	1:C:267:VAL:HB	2.19	0.42
2:D:22:GLU:OE2	2:D:90:THR:OG1	2.32	0.42
1:A:1126:CYS:HB3	1:A:1132:ILE:HD13	2.01	0.42
1:B:391:CYS:C	1:B:519:HIS:NE2	2.56	0.42
1:C:175:PHE:CE1	1:C:227:VAL:HG21	2.54	0.42
1:C:501:TYR:HB3	1:C:505:HIS:HB2	2.00	0.42
1:B:898:PHE:N	1:B:899:PRO:HD2	2.35	0.42
2:D:439:LEU:HD21	2:D:540:HIS:CG	2.54	0.42
1:C:985:ASP:O	1:C:989:ALA:N	2.52	0.42
1:A:119:ILE:HG12	1:A:128:ILE:CB	2.50	0.42
1:C:902:MET:CB	1:C:916:LEU:HD21	2.50	0.42
2:D:177:ARG:NH2	2:D:495:GLU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:LEU:HG	1:A:1008:VAL:HG21	2.02	0.42
1:B:1031:GLU:OE2	1:C:1039:ARG:NH1	2.47	0.42
1:C:436:TRP:HZ3	1:C:511:VAL:HG12	1.85	0.42
1:B:28:TYR:CE1	1:B:63:THR:CG2	2.97	0.42
1:B:102:ARG:HE	1:B:141:LEU:HD22	1.85	0.42
1:B:231:ILE:HG13	1:B:233:ILE:HG13	2.01	0.42
1:C:172:SER:OG	1:C:173:GLN:N	2.50	0.42
2:D:343:VAL:HG11	2:D:345:HIS:CD2	2.53	0.42
1:A:117:LEU:HA	1:A:130:VAL:HA	2.01	0.42
1:B:470:THR:O	1:B:470:THR:OG1	2.37	0.42
1:A:63:THR:OG1	1:A:267:VAL:HB	2.20	0.41
1:A:898:PHE:N	1:A:899:PRO:HD2	2.34	0.41
1:A:1019:ARG:NH2	1:B:1017:GLU:OE1	2.53	0.41
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.01	0.41
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.02	0.41
1:B:983:ARG:HG2	1:C:390:LEU:HD11	2.01	0.41
1:C:296:LEU:HG	1:C:300:LYS:HE3	2.02	0.41
2:D:285:PHE:O	2:D:437:ASN:ND2	2.51	0.41
2:D:398:GLU:OE1	2:D:514:ARG:HB3	2.19	0.41
1:A:229:LEU:HD11	1:A:231:ILE:CG2	2.50	0.41
1:A:401:VAL:HG22	1:A:509:ARG:HG2	2.02	0.41
1:A:433:VAL:HG22	1:A:512:VAL:HG22	2.02	0.41
1:B:277:LEU:HD13	1:B:285:ILE:HD13	2.03	0.41
1:C:111:ASP:OD1	1:C:112:SER:N	2.45	0.41
1:C:347:PHE:CE2	1:C:399:SER:HB2	2.55	0.41
1:C:778:THR:O	1:C:778:THR:CG2	2.66	0.41
1:C:977:LEU:HD22	1:C:993:ILE:HD12	2.02	0.41
2:D:209:ALA:HB2	2:D:566:TRP:CD1	2.56	0.41
1:A:985:ASP:OD1	1:A:985:ASP:N	2.52	0.41
1:B:57:PRO:O	1:B:60:SER:OG	2.32	0.41
1:B:559:PHE:CE1	1:B:584:ILE:HG12	2.55	0.41
1:C:102:ARG:HA	1:C:102:ARG:HH21	1.85	0.41
1:C:898:PHE:N	1:C:899:PRO:HD2	2.35	0.41
1:A:277:LEU:HD13	1:A:285:ILE:HD13	2.03	0.41
1:A:359:SER:HB3	1:A:394:ASN:HD22	1.83	0.41
1:B:902:MET:CB	1:B:916:LEU:HD11	2.45	0.41
1:C:277:LEU:HD13	1:C:285:ILE:HD13	2.03	0.41
1:B:1116:THR:HG23	1:B:1140:PRO:HD3	2.03	0.41
1:A:457:ARG:NH1	1:A:459:SER:O	2.48	0.41
1:B:69:HIS:O	1:B:70:VAL:CG1	2.69	0.41
1:C:366:SER:HA	1:C:369:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:ARG:HE	2:D:499:ASP:HB3	1.86	0.41
2:D:303:ASP:N	2:D:303:ASP:OD1	2.51	0.41
2:D:190:MET:SD	2:D:194:ASN:ND2	2.94	0.41
1:B:391:CYS:O	1:B:519:HIS:CE1	2.67	0.41
1:B:557:LYS:HB2	1:B:559:PHE:HE1	1.85	0.41
1:C:557:LYS:HB2	1:C:559:PHE:HE1	1.85	0.41
2:D:359:LYS:HE3	2:D:359:LYS:HB3	1.89	0.41
2:D:429:GLN:OE1	2:D:429:GLN:N	2.53	0.41
1:A:342:PHE:CZ	1:A:368:LEU:CD1	3.04	0.41
1:B:413:GLY:HA3	1:C:987:PRO:HD3	2.02	0.41
1:A:121:ASN:HA	1:A:126:VAL:HG12	2.03	0.40
1:A:598:ILE:HG23	1:A:664:ILE:HG21	2.02	0.40
1:A:709:ASN:OD1	1:A:709:ASN:N	2.52	0.40
1:A:992:GLN:OE1	1:A:995:ARG:NH1	2.48	0.40
1:C:1116:THR:HG23	1:C:1140:PRO:HD3	2.02	0.40
2:D:26:LYS:HE2	2:D:93:ILE:HG13	2.02	0.40
1:A:244:LEU:HD22	1:A:258:TRP:HB3	2.03	0.40
1:B:353:TRP:CD1	1:B:353:TRP:H	2.40	0.40
1:B:363:ALA:HB2	1:B:524:VAL:HG11	1.92	0.40
1:C:102:ARG:NH2	1:C:121:ASN:O	2.41	0.40
1:C:498:ARG:NH2	1:C:501:TYR:OH	2.54	0.40
2:D:119:ILE:HG22	2:D:123:MET:HE2	2.04	0.40
1:A:120:VAL:HG23	1:A:127:VAL:HB	2.04	0.40
1:B:375:PHE:HE2	1:B:437:ASN:ND2	2.20	0.40
1:C:559:PHE:CE1	1:C:584:ILE:HG12	2.56	0.40
1:C:731:MET:HE3	1:C:951:VAL:HG23	2.03	0.40
1:C:804:GLN:NE2	1:C:931:ILE:O	2.55	0.40
1:A:273:ARG:HE	1:A:290:ASP:CG	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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	890/1110 (80%)	888 (100%)	2 (0%)	87	89
1	B	875/1110 (79%)	875 (100%)	0	100	100
1	C	875/1110 (79%)	875 (100%)	0	100	100
2	D	516/707 (73%)	516 (100%)	0	100	100
All	All	3156/4037 (78%)	3154 (100%)	2 (0%)	87	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	371	PHE
1	A	374	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	314	GLN
1	A	317	ASN
1	A	405	ASN
1	A	414	GLN
1	A	450	ASN
1	A	505	HIS
1	A	536	ASN
1	A	563	GLN
1	A	607	GLN
1	A	657	ASN
1	A	703	ASN
1	A	755	GLN
1	A	784	GLN
1	A	787	GLN
1	A	907	ASN
1	A	925	ASN
1	A	926	GLN
1	A	949	GLN
1	A	965	GLN
1	A	1005	GLN

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Mol	Chain	Res	Type
1	A	1048	HIS
1	A	1106	GLN
1	A	1119	ASN
1	B	52	GLN
1	B	81	ASN
1	B	173	GLN
1	B	394	ASN
1	B	544	ASN
1	B	613	GLN
1	B	641	ASN
1	B	644	GLN
1	B	710	ASN
1	B	787	GLN
1	B	804	GLN
1	B	907	ASN
1	B	925	ASN
1	B	935	GLN
1	B	965	GLN
1	B	978	ASN
1	B	1106	GLN
1	B	1119	ASN
1	C	81	ASN
1	C	173	GLN
1	C	207	HIS
1	C	394	ASN
1	C	519	HIS
1	C	542	ASN
1	C	544	ASN
1	C	641	ASN
1	C	644	GLN
1	C	755	GLN
1	C	784	GLN
1	C	895	GLN
1	C	907	ASN
1	C	925	ASN
1	C	935	GLN
1	C	965	GLN
1	C	1106	GLN
1	C	1119	ASN
2	D	42	GLN
2	D	60	GLN
2	D	86	GLN

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Mol	Chain	Res	Type
2	D	96	GLN
2	D	98	GLN
2	D	221	GLN
2	D	325	GLN
2	D	345	HIS
2	D	401	HIS
2	D	442	GLN
2	D	472	GLN
2	D	526	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](#)

Of 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 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	$\# Z > 2$
3	NAG	C	1304	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	A	1307	1	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	B	1304	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	B	1307	1	14,14,15	0.23	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	1306	1	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	C	1309	1	14,14,15	0.45	0	17,19,21	0.45	0
3	NAG	A	1301	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	C	1307	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	D	902	2	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	C	1310	1	14,14,15	0.33	0	17,19,21	0.40	0
3	NAG	B	1302	1	14,14,15	0.22	0	17,19,21	0.43	0
3	NAG	A	1305	-	14,14,15	0.22	0	17,19,21	0.48	0
3	NAG	A	1311	1	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	B	1301	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	A	1303	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	B	1310	1	14,14,15	0.46	0	17,19,21	1.27	1 (5%)
3	NAG	C	1306	1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	B	1305	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	C	1302	1	14,14,15	0.25	0	17,19,21	0.45	0
3	NAG	B	1303	1	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	C	1303	1	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	A	1302	1	14,14,15	0.22	0	17,19,21	0.42	0
3	NAG	C	1311	1	14,14,15	0.35	0	17,19,21	0.83	1 (5%)
3	NAG	D	903	2	14,14,15	0.23	0	17,19,21	0.43	0
3	NAG	A	1304	1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	C	1301	1	14,14,15	0.23	0	17,19,21	0.46	0
3	NAG	A	1310	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	B	1308	1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	B	1309	1	14,14,15	0.26	0	17,19,21	0.46	0
3	NAG	A	1309	1	14,14,15	0.21	0	17,19,21	0.42	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
3	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1307	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1309	1	-	3/6/23/26	0/1/1/1
3	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1306	1	-	0/6/23/26	0/1/1/1
3	NAG	D	902	2	-	0/6/23/26	0/1/1/1
3	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1305	-	-	3/6/23/26	0/1/1/1
3	NAG	A	1311	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1301	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1305	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
3	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
3	NAG	D	903	2	-	2/6/23/26	0/1/1/1
3	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
3	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1308	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1309	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1310	NAG	C1-O5-C5	4.83	118.66	112.19
3	C	1311	NAG	C1-O5-C5	2.13	115.03	112.19

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1311	NAG	C8-C7-N2-C2
3	C	1311	NAG	O7-C7-N2-C2
3	B	1307	NAG	O5-C5-C6-O6
3	A	1308	NAG	O5-C5-C6-O6
3	B	1307	NAG	C4-C5-C6-O6
3	A	1302	NAG	C4-C5-C6-O6
3	C	1310	NAG	C4-C5-C6-O6
3	C	1304	NAG	O5-C5-C6-O6
3	C	1308	NAG	O5-C5-C6-O6
3	A	1308	NAG	C4-C5-C6-O6
3	A	1305	NAG	C8-C7-N2-C2
3	A	1305	NAG	O7-C7-N2-C2
3	C	1305	NAG	C8-C7-N2-C2
3	C	1305	NAG	O7-C7-N2-C2
3	C	1304	NAG	C4-C5-C6-O6
3	C	1308	NAG	C4-C5-C6-O6
3	C	1301	NAG	O5-C5-C6-O6
3	C	1309	NAG	C4-C5-C6-O6
3	A	1302	NAG	O5-C5-C6-O6
3	C	1301	NAG	C4-C5-C6-O6
3	A	1303	NAG	C4-C5-C6-O6
3	A	1303	NAG	O5-C5-C6-O6
3	C	1310	NAG	O5-C5-C6-O6
3	C	1309	NAG	O5-C5-C6-O6
3	D	903	NAG	C4-C5-C6-O6
3	D	903	NAG	O5-C5-C6-O6
3	C	1306	NAG	C4-C5-C6-O6
3	A	1305	NAG	C4-C5-C6-O6
3	C	1309	NAG	C1-C2-N2-C7
3	C	1306	NAG	O5-C5-C6-O6
3	C	1303	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1305	NAG	14	0
3	D	903	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33342. These allow visual inspection of the internal detail of the map and identification of artifacts.

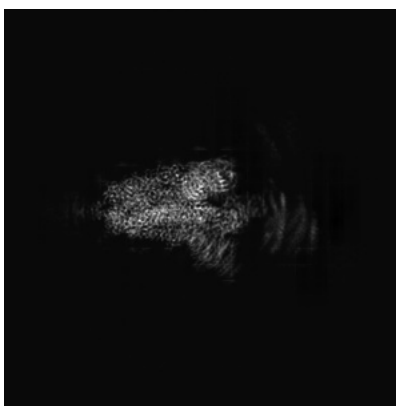
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

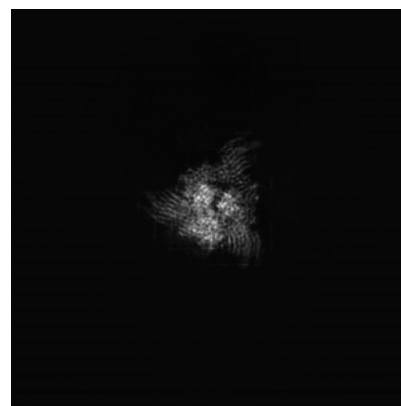
6.1.1 Primary map



X

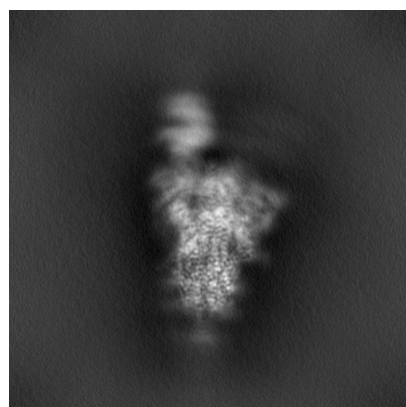


Y

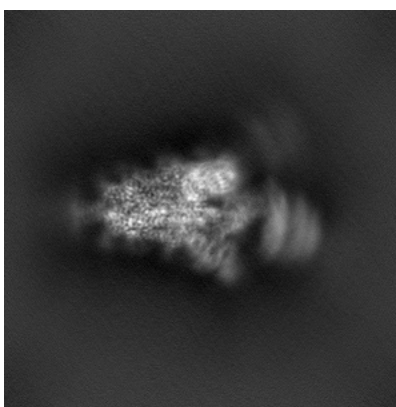


Z

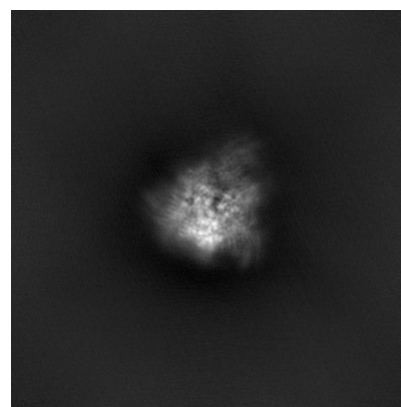
6.1.2 Raw map



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: 240

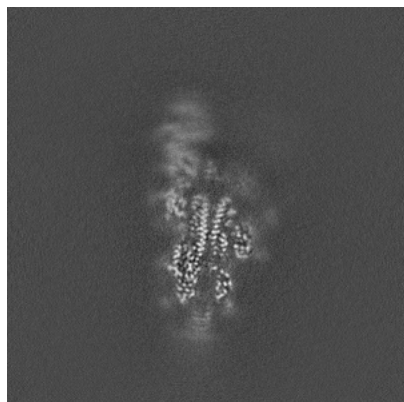


Y Index: 240

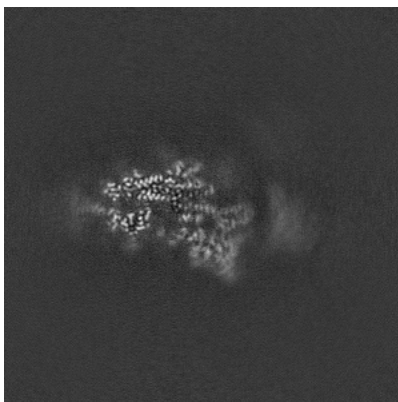


Z Index: 240

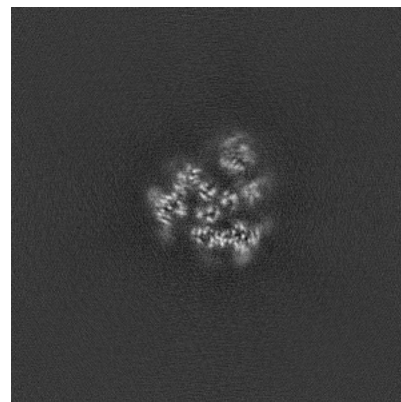
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

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: 229



Y Index: 244

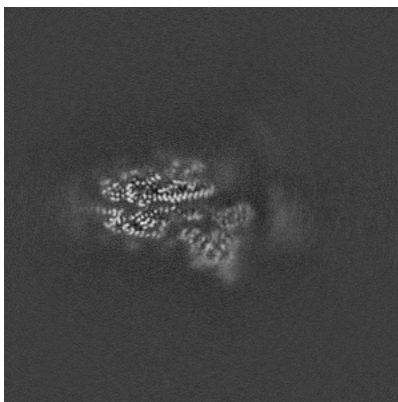


Z Index: 235

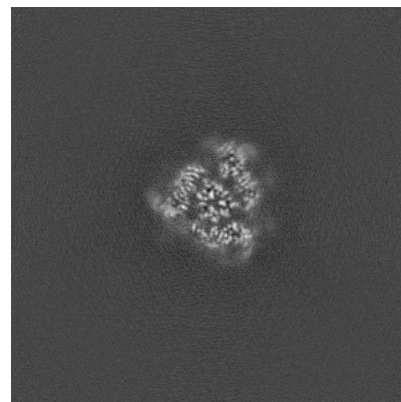
6.3.2 Raw map



X Index: 238



Y Index: 244

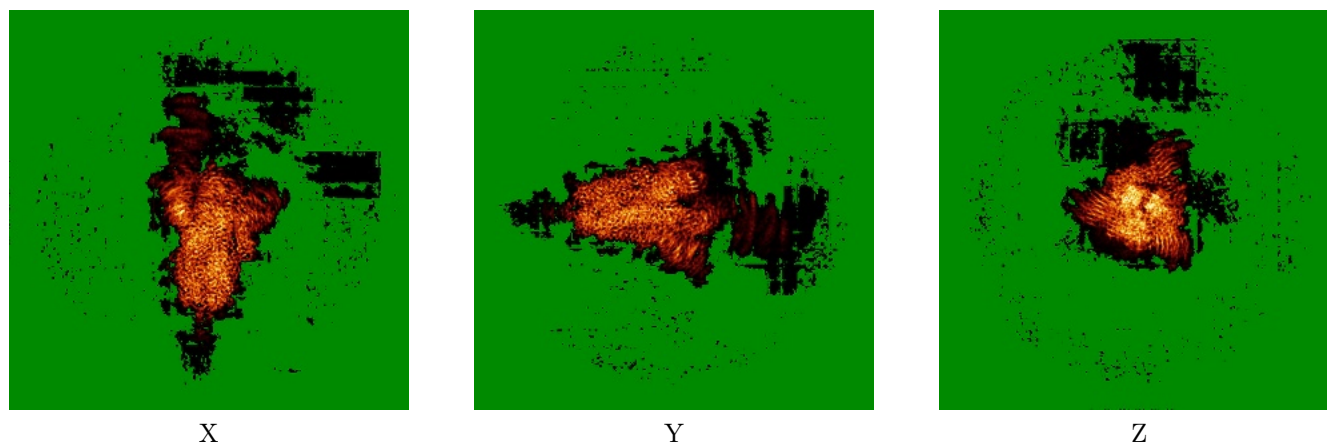


Z Index: 229

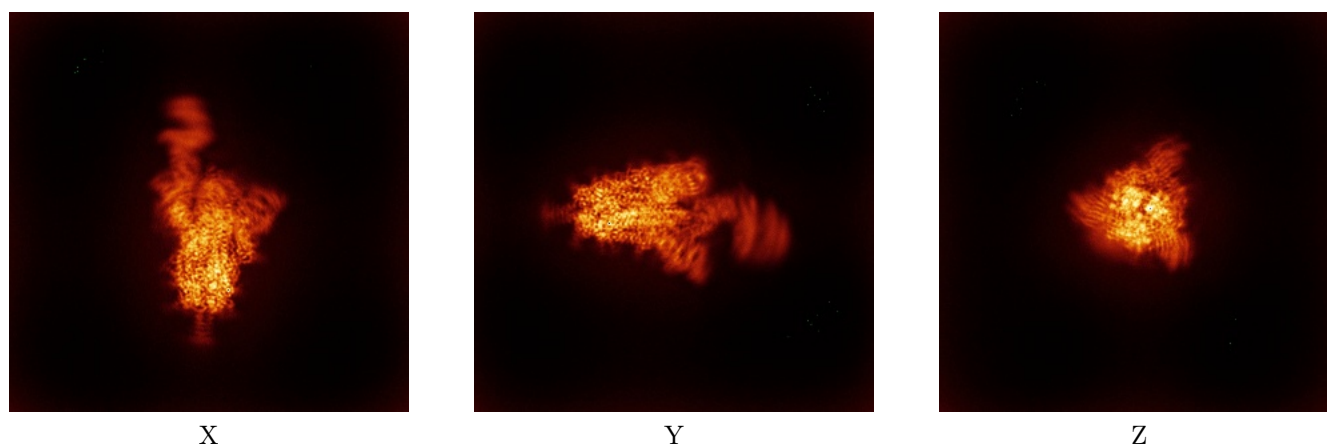
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

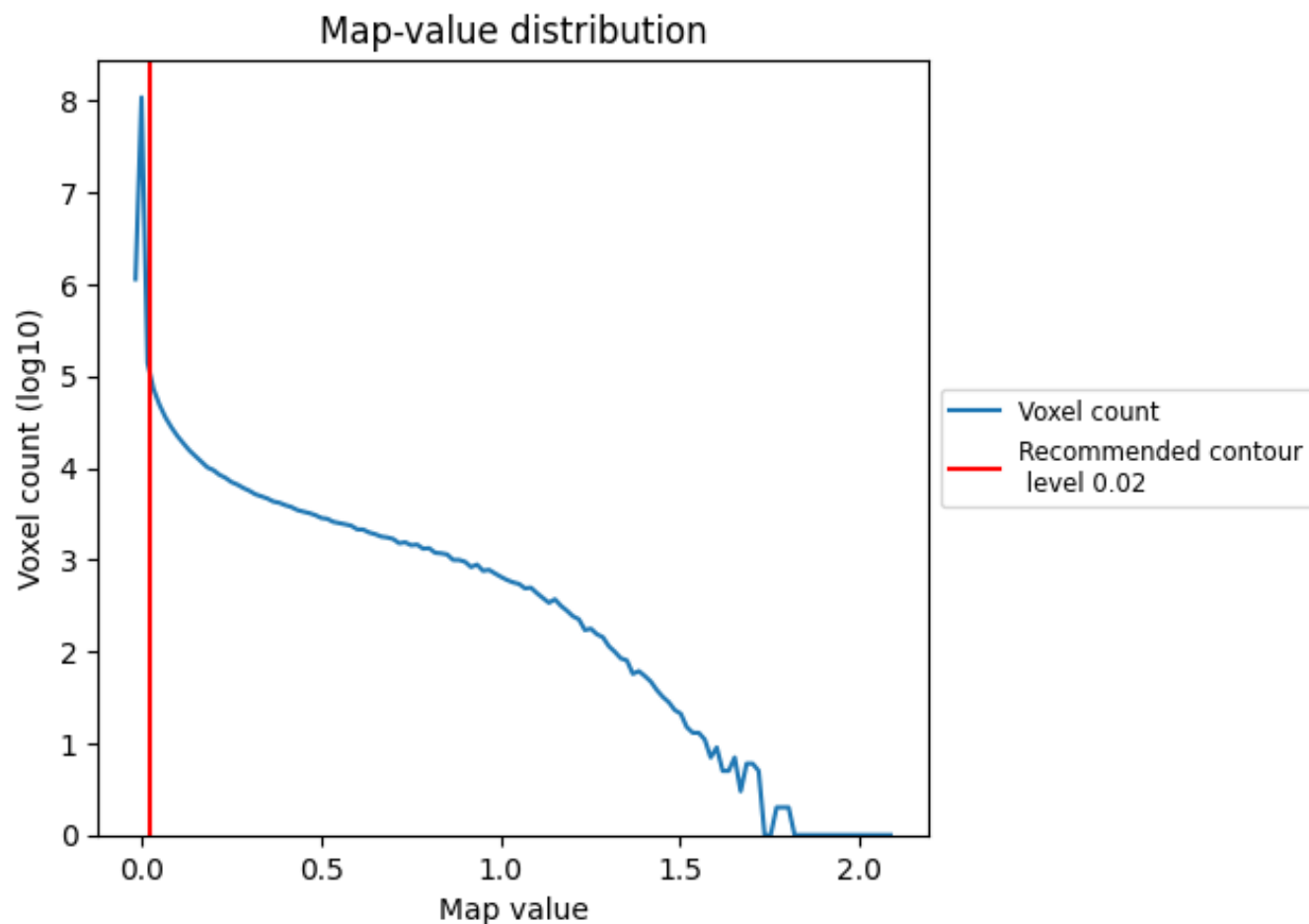
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

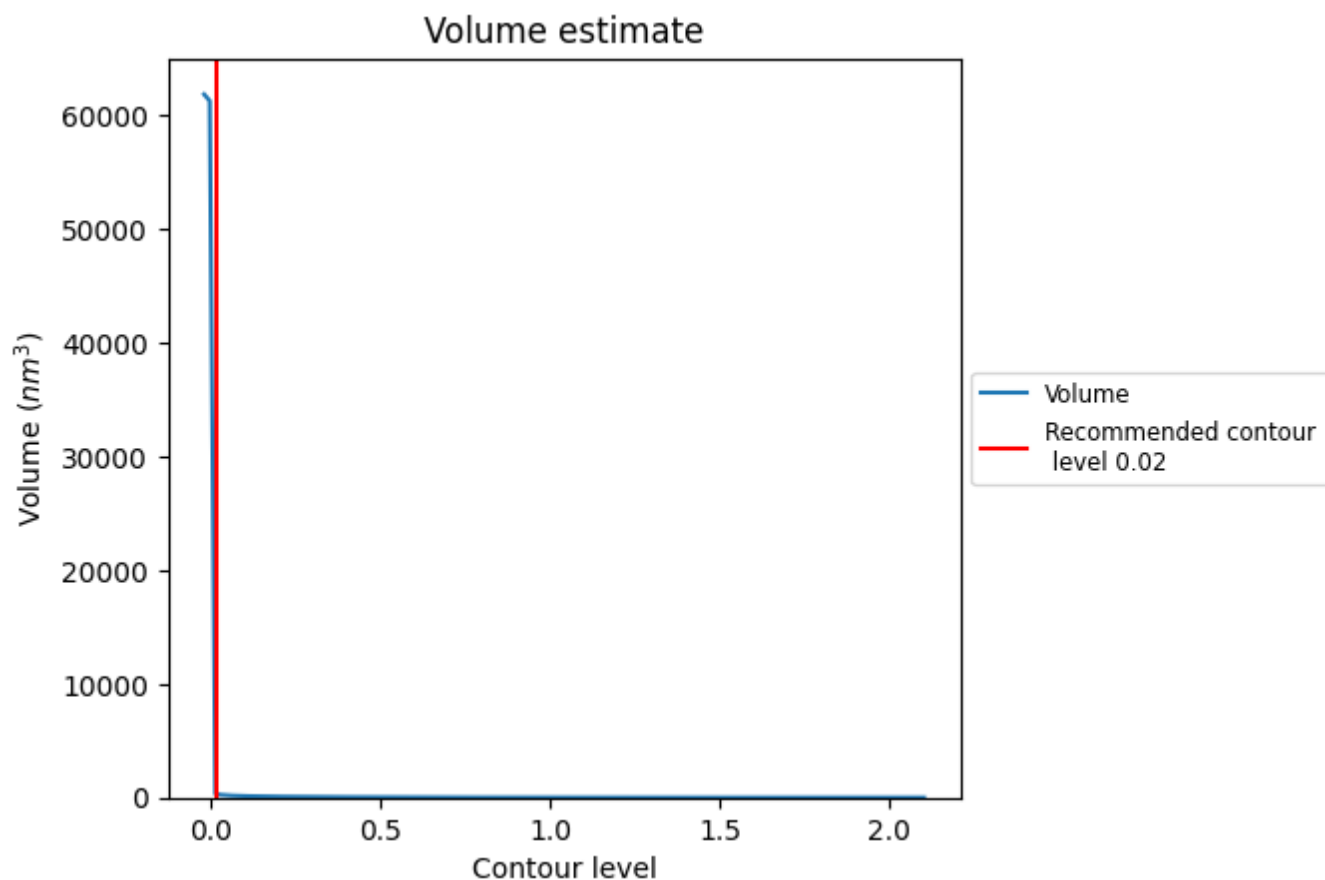
This section contains the results of statistical analysis of the map.

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.

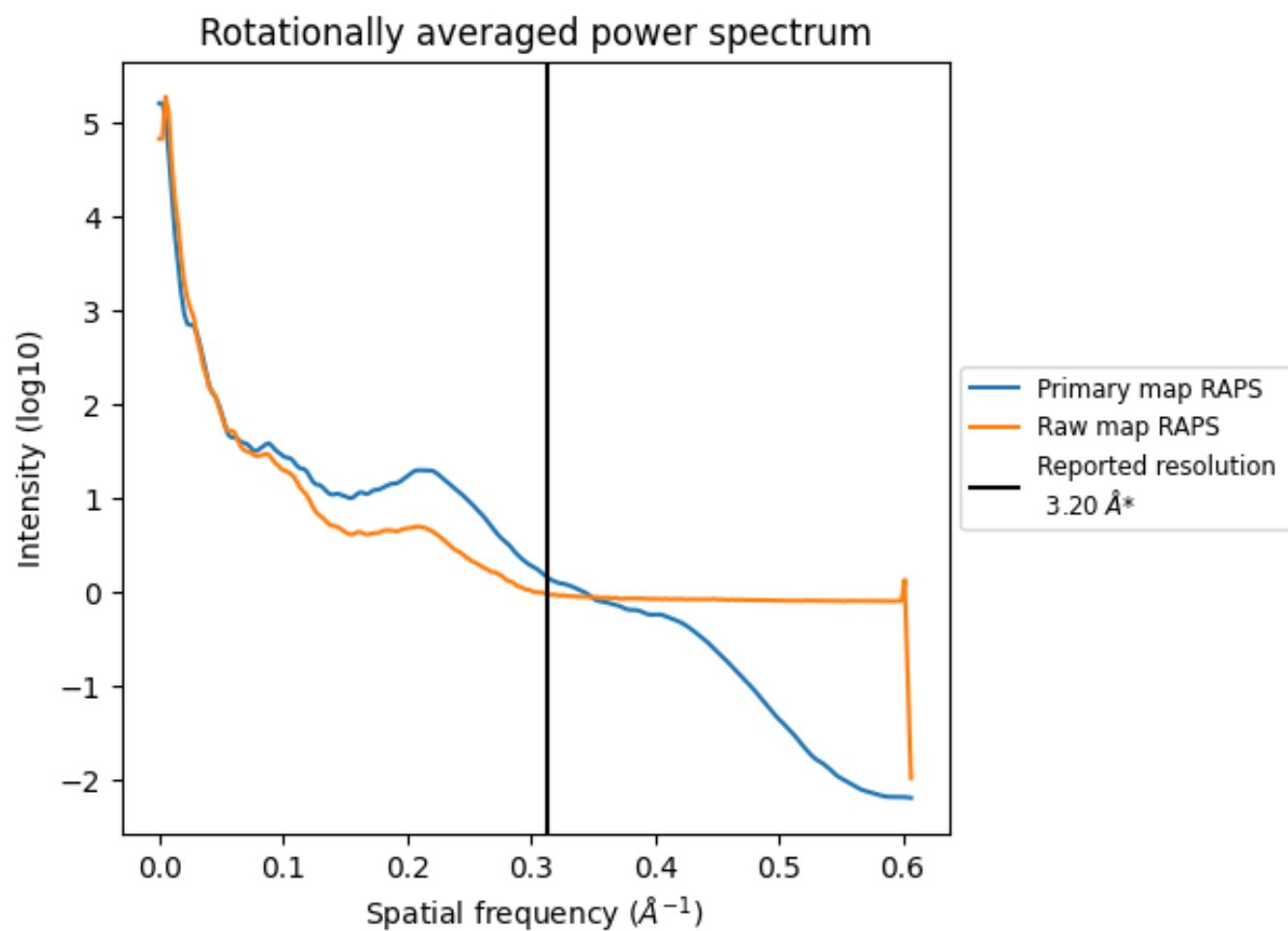
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 292 nm³; this corresponds to an approximate mass of 264 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

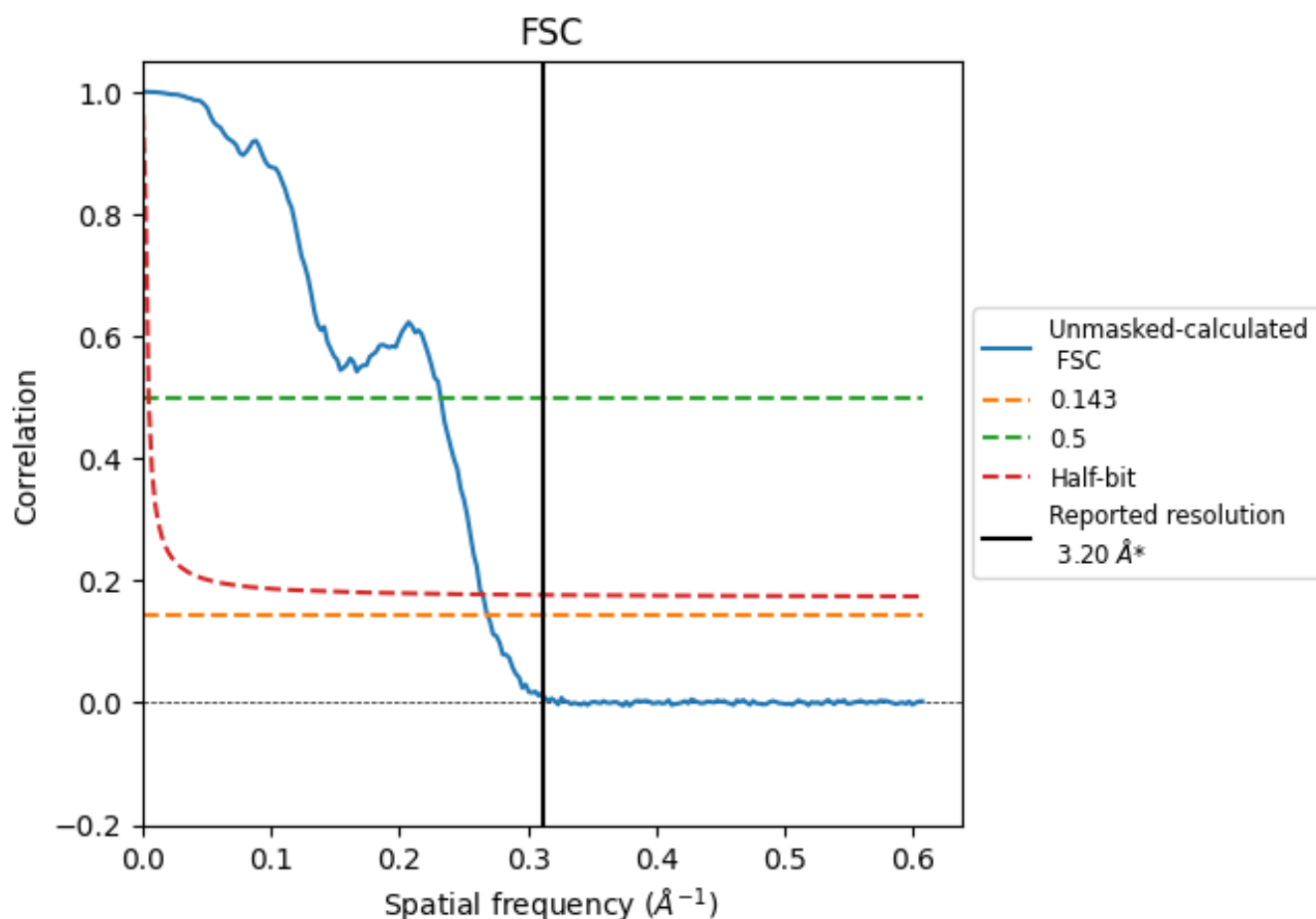


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.72	4.31	3.78

*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 3.72 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

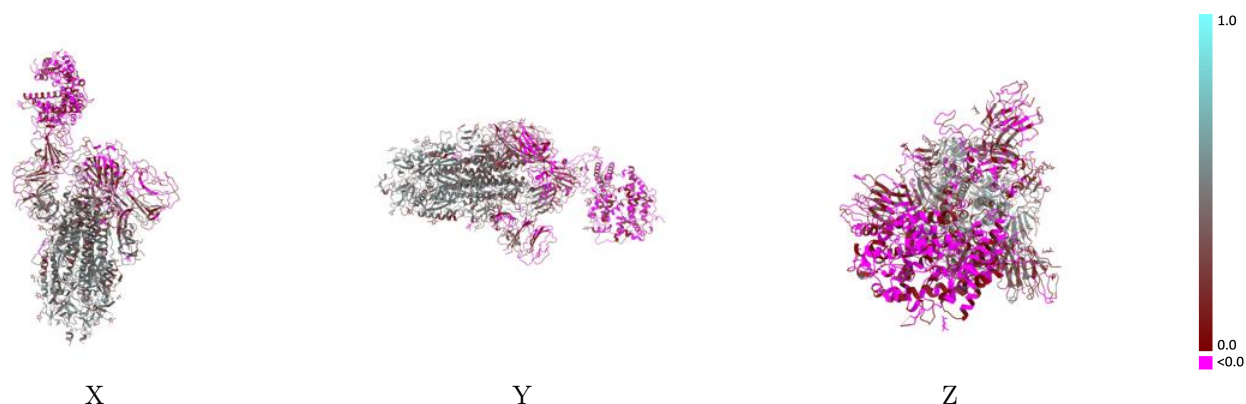
This section contains information regarding the fit between EMDB map EMD-33342 and PDB model 7XOA. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



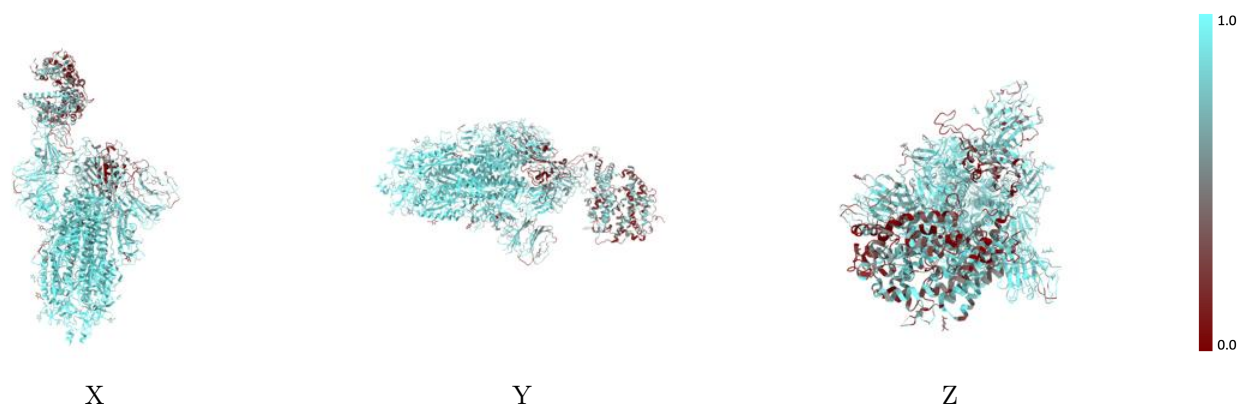
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



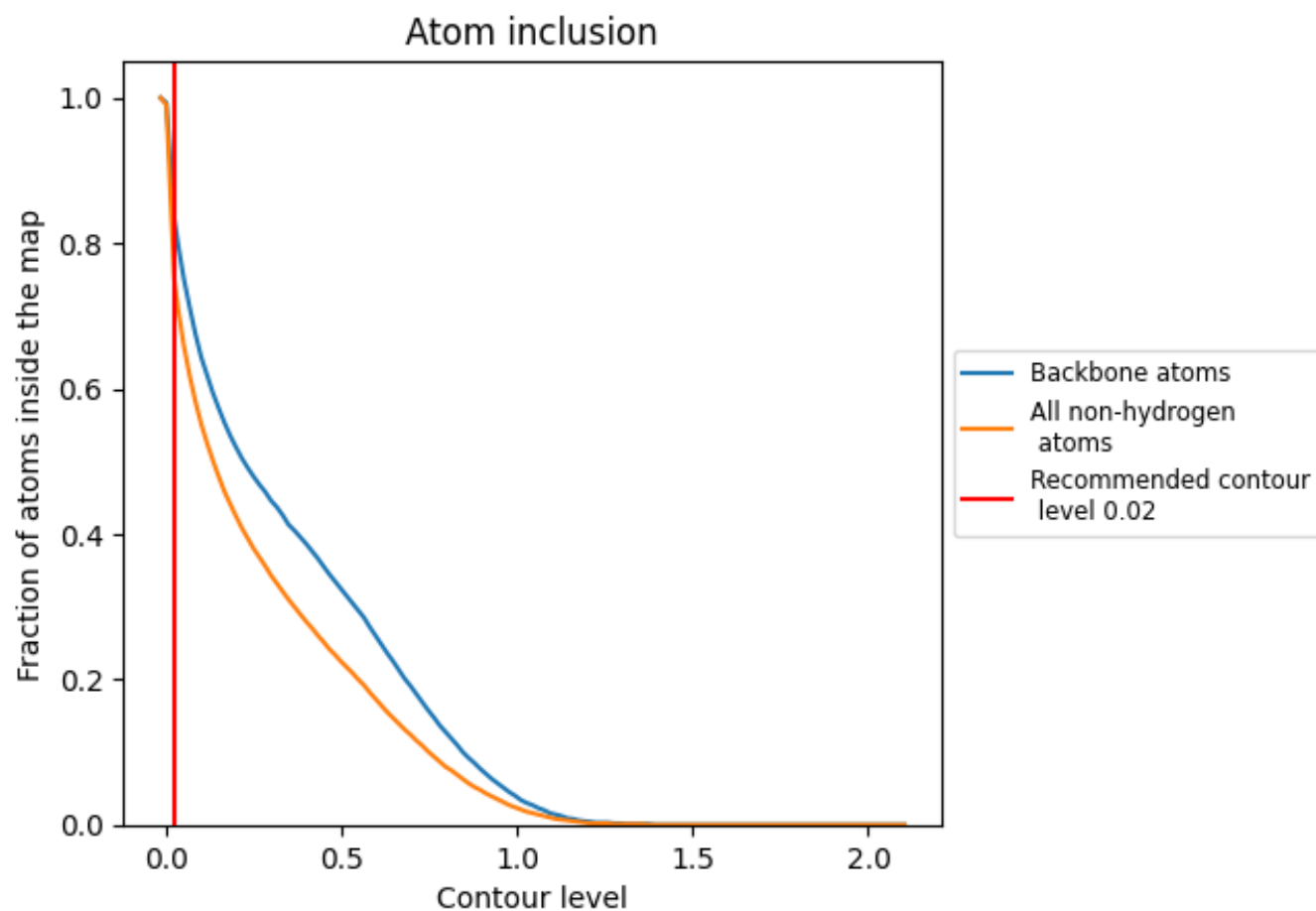
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7520	0.2530
A	0.8140	0.2940
B	0.8310	0.3120
C	0.7730	0.3060
D	0.4810	-0.0030

