



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:43 AM UTC

PDB ID : 6M1D / pdb_00006m1d
EMDB ID : EMD-30041
Title : ACE2-B0AT1 complex, open conformation
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Xia, L.; Zhou, Q.
Deposited on : 2020-02-25
Resolution : 4.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

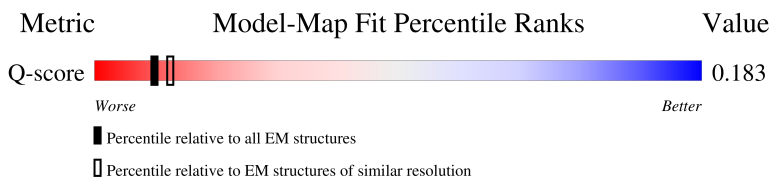
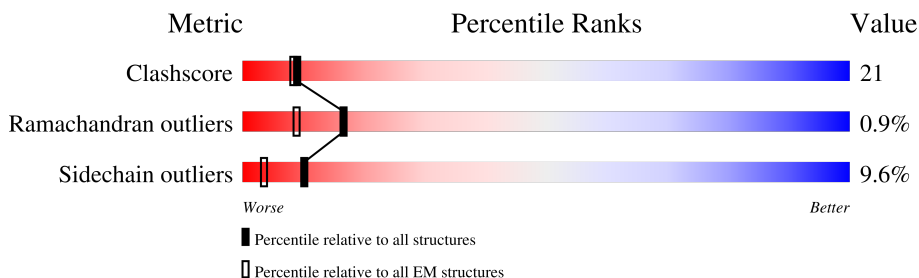
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	654	9% 66% 24% • 7%
1	C	654	15% 65% 25% • 7%
2	B	814	9% 54% 33% • 8%
2	D	814	55% 54% 32% 5% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21776 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 Sodium-dependent neutral amino acid transporter B(0)AT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total	C	N	O	S	0	0
			4799	3171	744	854	30		
1	C	605	Total	C	N	O	S	0	0
			4799	3171	744	854	30		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q695T7
A	-18	ALA	-	expression tag	UNP Q695T7
A	-17	ASP	-	expression tag	UNP Q695T7
A	-16	TYR	-	expression tag	UNP Q695T7
A	-15	LYS	-	expression tag	UNP Q695T7
A	-14	ASP	-	expression tag	UNP Q695T7
A	-13	ASP	-	expression tag	UNP Q695T7
A	-12	ASP	-	expression tag	UNP Q695T7
A	-11	ASP	-	expression tag	UNP Q695T7
A	-10	LYS	-	expression tag	UNP Q695T7
A	-9	SER	-	expression tag	UNP Q695T7
A	-8	GLY	-	expression tag	UNP Q695T7
A	-7	PRO	-	expression tag	UNP Q695T7
A	-6	ASP	-	expression tag	UNP Q695T7
A	-5	GLU	-	expression tag	UNP Q695T7
A	-4	VAL	-	expression tag	UNP Q695T7
A	-3	ASP	-	expression tag	UNP Q695T7
A	-2	ALA	-	expression tag	UNP Q695T7
A	-1	SER	-	expression tag	UNP Q695T7
A	0	GLY	-	expression tag	UNP Q695T7
A	1	ARG	-	expression tag	UNP Q695T7
C	-19	MET	-	initiating methionine	UNP Q695T7
C	-18	ALA	-	expression tag	UNP Q695T7
C	-17	ASP	-	expression tag	UNP Q695T7
C	-16	TYR	-	expression tag	UNP Q695T7
C	-15	LYS	-	expression tag	UNP Q695T7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP Q695T7
C	-13	ASP	-	expression tag	UNP Q695T7
C	-12	ASP	-	expression tag	UNP Q695T7
C	-11	ASP	-	expression tag	UNP Q695T7
C	-10	LYS	-	expression tag	UNP Q695T7
C	-9	SER	-	expression tag	UNP Q695T7
C	-8	GLY	-	expression tag	UNP Q695T7
C	-7	PRO	-	expression tag	UNP Q695T7
C	-6	ASP	-	expression tag	UNP Q695T7
C	-5	GLU	-	expression tag	UNP Q695T7
C	-4	VAL	-	expression tag	UNP Q695T7
C	-3	ASP	-	expression tag	UNP Q695T7
C	-2	ALA	-	expression tag	UNP Q695T7
C	-1	SER	-	expression tag	UNP Q695T7
C	0	GLY	-	expression tag	UNP Q695T7
C	1	ARG	-	expression tag	UNP Q695T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	748	Total	C	N	O	S	0	0
			6089	3906	1018	1131	34		
2	D	748	Total	C	N	O	S	0	0
			6089	3906	1018	1131	34		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	initiating methionine	UNP Q9BYF1
B	-7	ARG	-	expression tag	UNP Q9BYF1
B	10	TRP	-	insertion	UNP Q9BYF1
B	11	SER	-	insertion	UNP Q9BYF1
B	12	HIS	-	insertion	UNP Q9BYF1
B	13	PRO	-	insertion	UNP Q9BYF1
B	14	GLN	-	insertion	UNP Q9BYF1
B	15	PHE	-	insertion	UNP Q9BYF1
B	16	GLU	-	insertion	UNP Q9BYF1
B	17	LYS	-	insertion	UNP Q9BYF1
D	-8	MET	-	initiating methionine	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1

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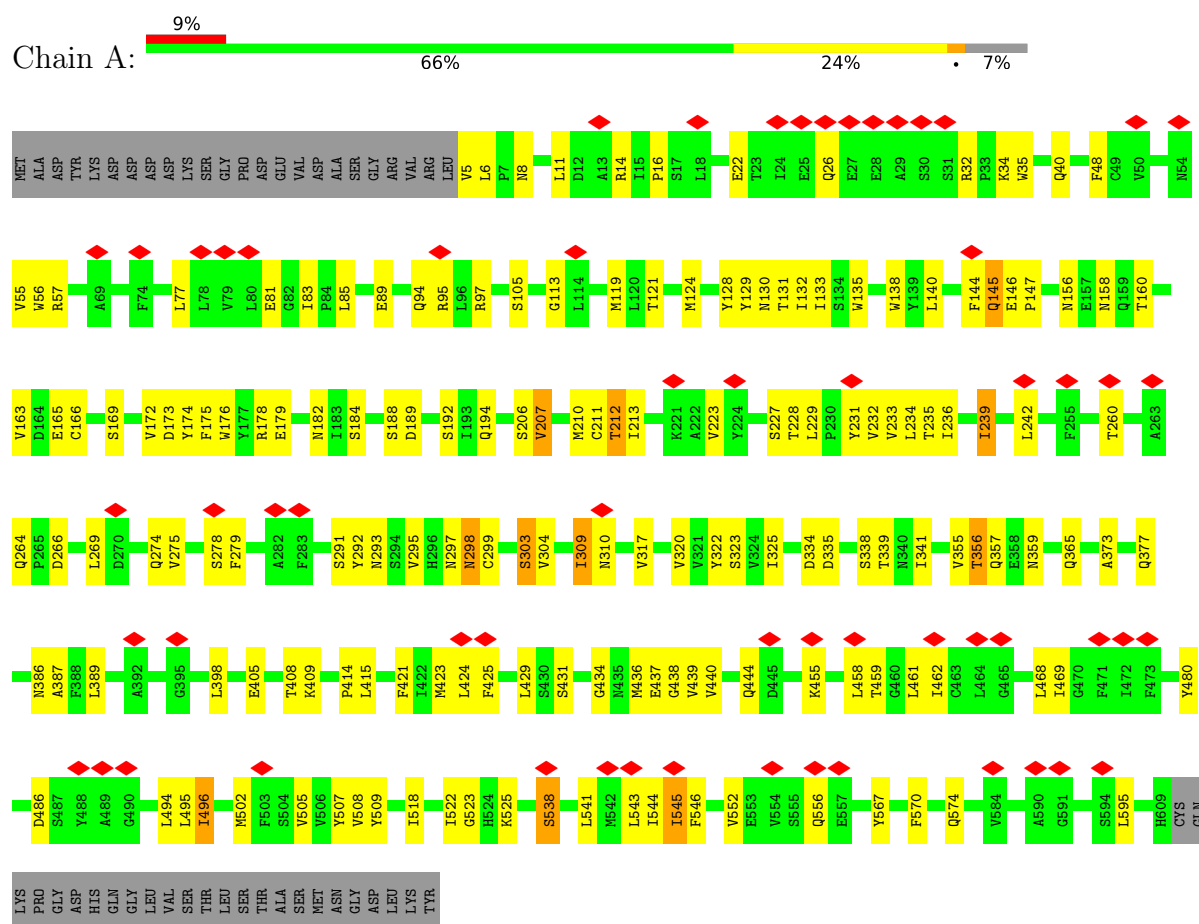
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Chain	Residue	Modelled	Actual	Comment	Reference
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1

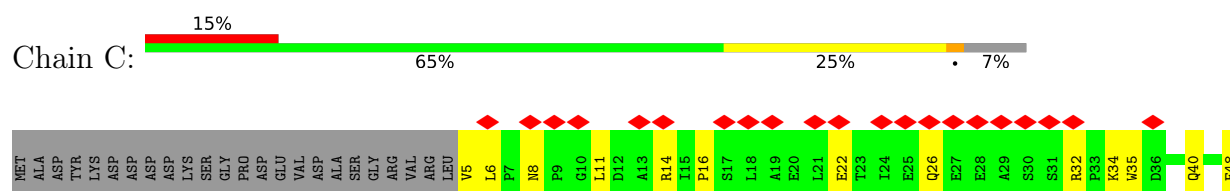
3 Residue-property plots

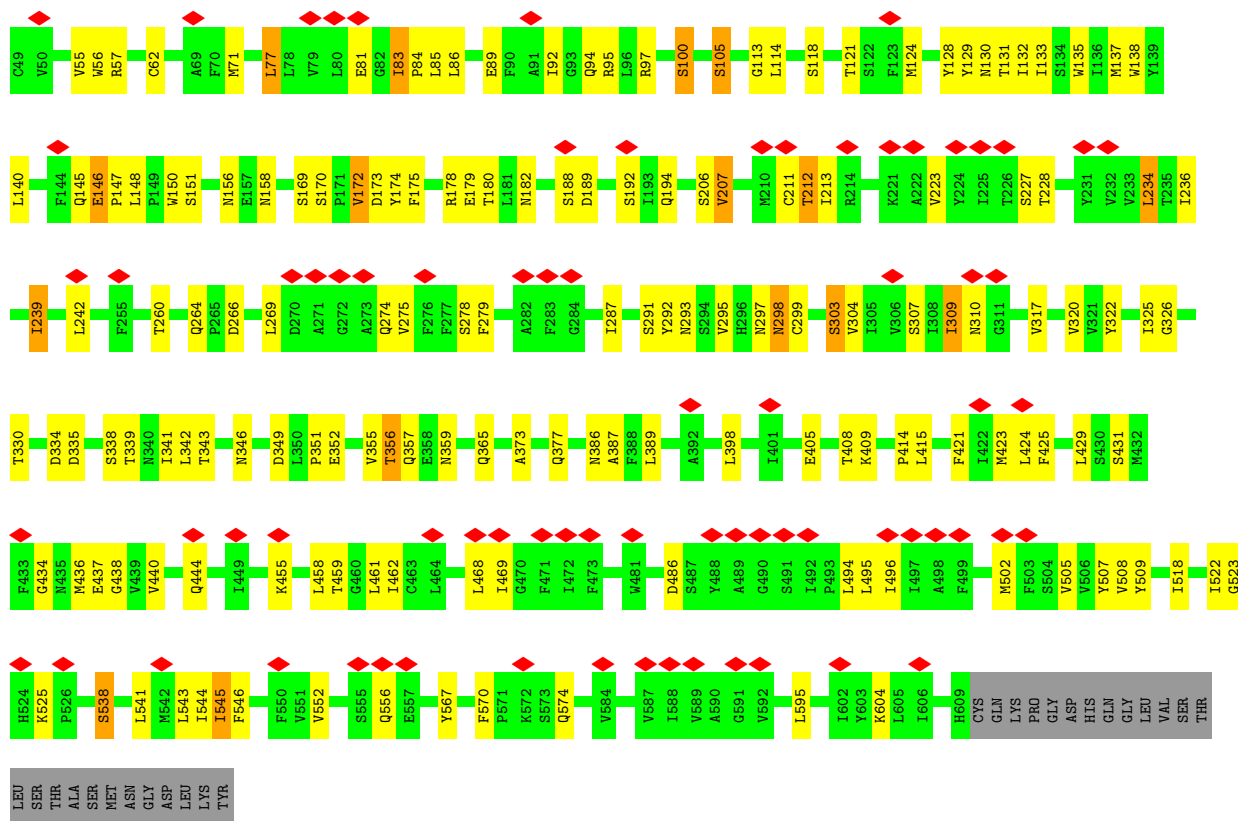
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium-dependent neutral amino acid transporter B(0)AT1

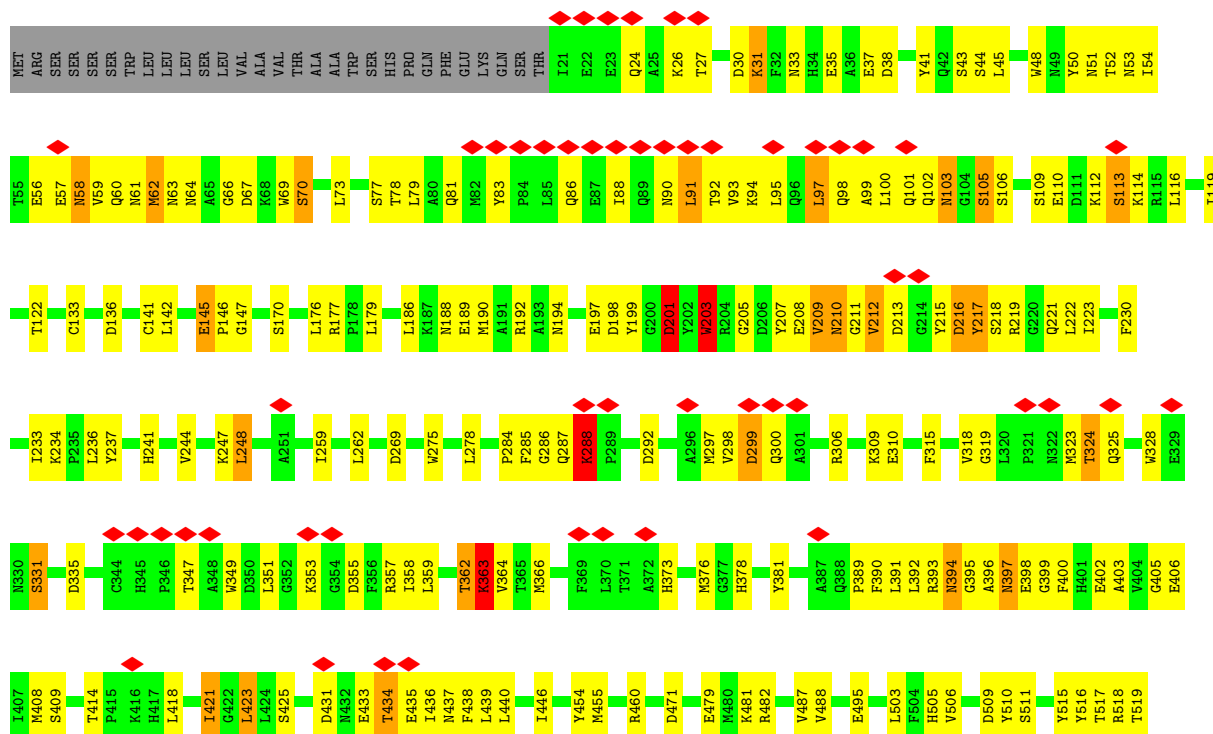


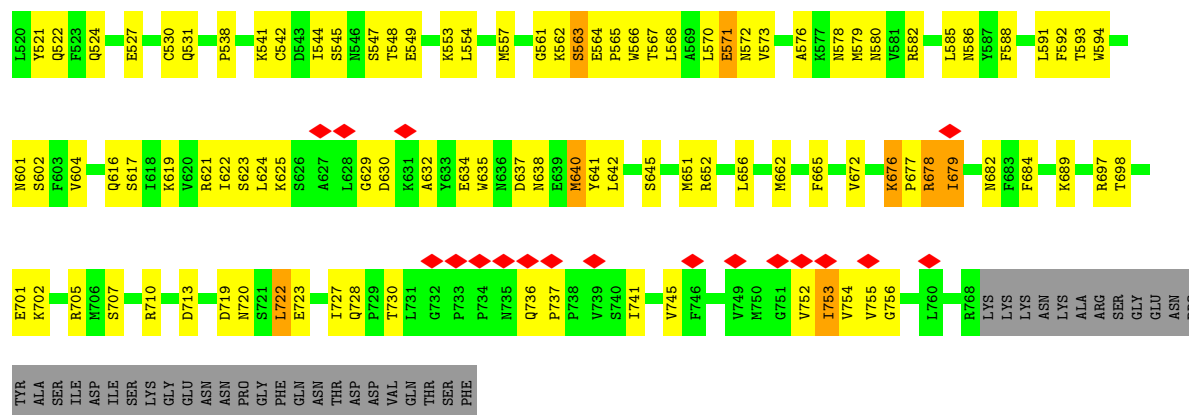
- Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1





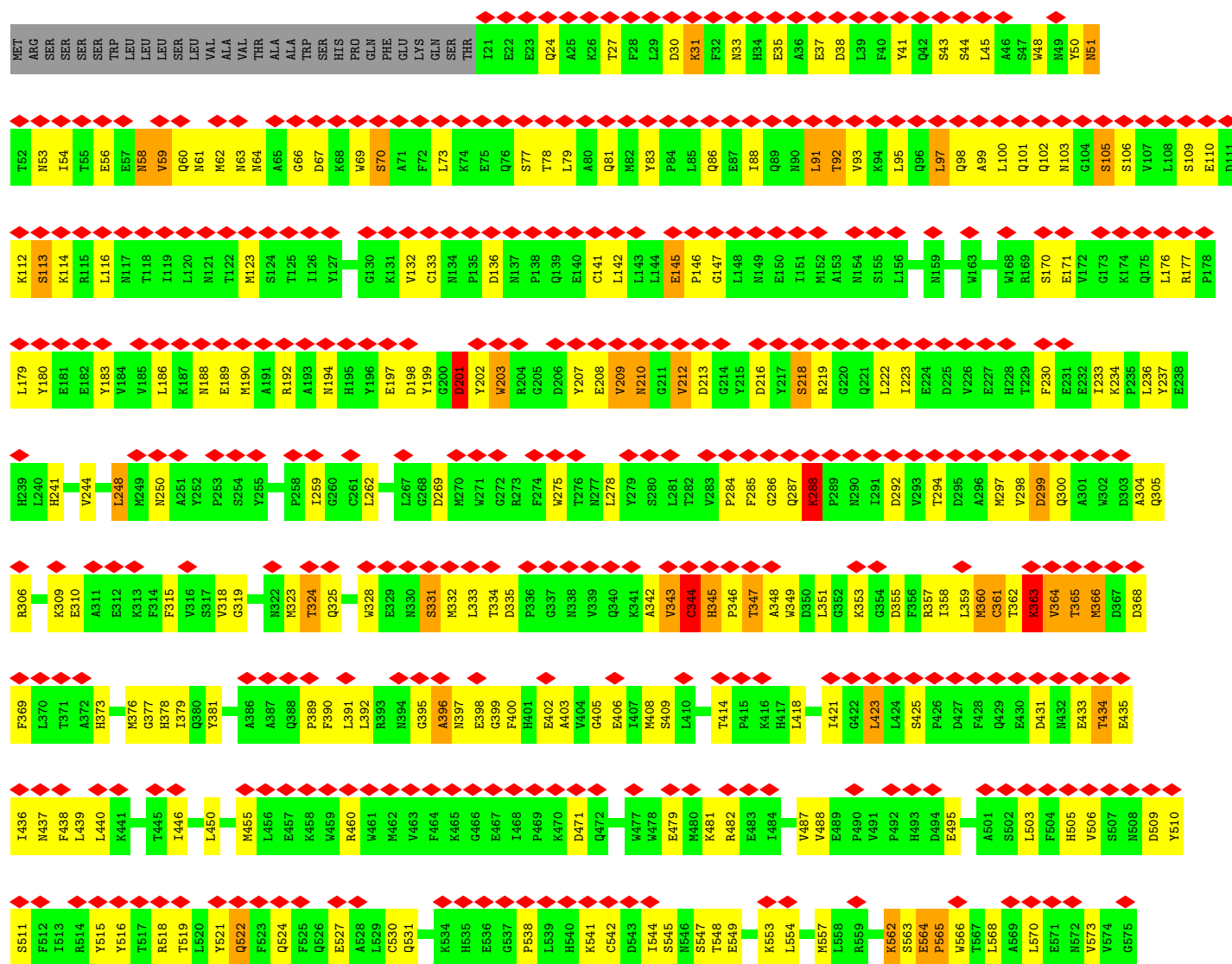
• Molecule 2: Angiotensin-converting enzyme 2

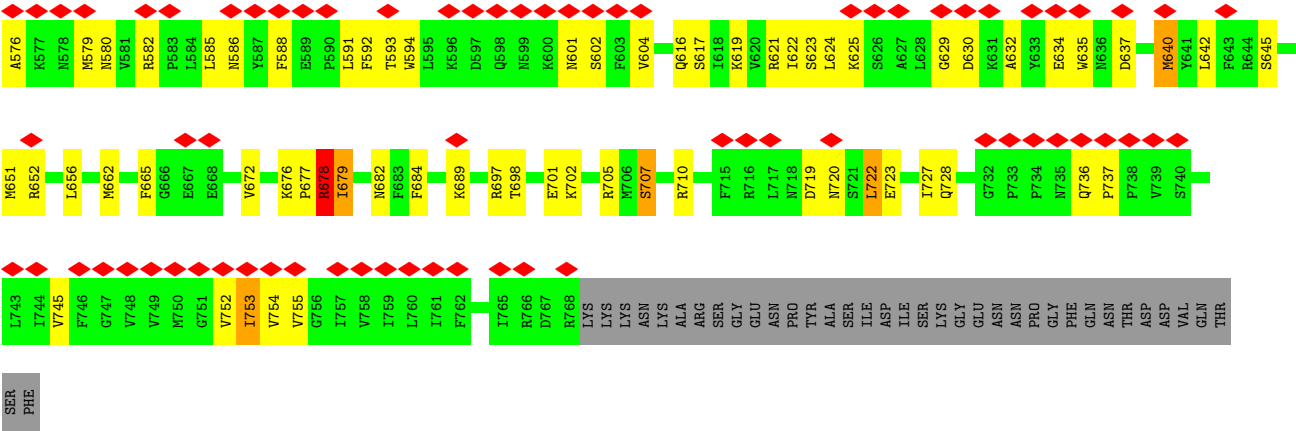




• Molecule 2: Angiotensin-converting enzyme 2

Chain D: 55% 54% 32% 5% 8%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143857	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.111	Depositor
Minimum map value	-0.320	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.26	0/4940	0.69	4/6748 (0.1%)
1	C	0.25	0/4940	0.70	4/6748 (0.1%)
2	B	0.29	1/6252 (0.0%)	0.75	5/8488 (0.1%)
2	D	0.29	1/6252 (0.0%)	0.79	10/8488 (0.1%)
All	All	0.27	2/22384 (0.0%)	0.74	23/30472 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	145	GLU	C-N	5.18	1.38	1.33
2	B	145	GLU	C-N	5.15	1.37	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	51	ASN	N-CA-C	8.17	123.29	113.16
2	B	363	LYS	N-CA-C	-7.75	102.67	113.20
2	B	421	ILE	N-CA-C	-7.24	106.25	113.20
2	D	421	ILE	N-CA-C	-7.24	106.25	113.20
2	D	395	GLY	O-C-N	6.31	127.63	122.71
1	A	387	ALA	N-CA-C	-6.21	105.65	113.72
1	C	387	ALA	N-CA-C	-6.19	105.67	113.72
2	D	365	THR	N-CA-C	6.18	118.10	111.36
2	D	361	CYS	N-CA-C	-5.75	105.09	111.36
2	D	344	CYS	N-CA-C	5.70	122.94	110.80
1	C	113	GLY	N-CA-C	-5.52	107.81	114.66
1	A	113	GLY	N-CA-C	-5.51	107.83	114.66
2	D	201	ASP	N-CA-C	-5.40	104.94	112.45
2	B	201	ASP	N-CA-C	-5.35	105.01	112.45
2	B	203	TRP	N-CA-C	-5.32	105.48	111.28
1	A	523	GLY	CA-C-N	5.32	129.24	121.31
1	A	523	GLY	C-N-CA	5.32	129.24	121.31
1	C	523	GLY	CA-C-N	5.32	129.24	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	523	GLY	C-N-CA	5.32	129.24	121.31
2	D	203	TRP	N-CA-C	-5.28	105.52	111.28
2	D	720	ASN	N-CA-C	-5.22	106.15	112.88
2	B	720	ASN	N-CA-C	-5.21	106.16	112.88
2	D	360	MET	N-CA-C	5.07	117.33	108.76

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	4799	0	4767	111	0
1	C	4799	0	4767	124	0
2	B	6089	0	5907	325	0
2	D	6089	0	5909	351	0
All	All	21776	0	21350	893	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 21.

All (893) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:CD1	1:A:179:GLU:HG2	1.28	1.59
1:A:175:PHE:CE1	1:A:179:GLU:HG2	1.57	1.38
1:A:144:PHE:O	1:A:145:GLN:HG3	1.16	1.33
2:D:358:ILE:CG1	2:D:360:MET:HE2	1.56	1.33
2:D:95:LEU:HD11	2:D:564:GLU:CA	1.58	1.31
2:B:95:LEU:HD12	2:B:563:SER:CA	1.61	1.30
2:D:51:ASN:ND2	2:D:359:LEU:HD22	1.48	1.29
2:D:403:ALA:CA	2:D:518:ARG:HG2	1.66	1.24
1:A:175:PHE:CD1	1:A:179:GLU:CG	2.22	1.23
2:D:403:ALA:CB	2:D:518:ARG:HG2	1.68	1.23
2:B:102:GLN:HG3	2:B:390:PHE:CZ	1.73	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:396:ALA:HB3	2:D:400:PHE:CD2	1.74	1.22
2:D:358:ILE:CD1	2:D:360:MET:HE2	1.74	1.16
2:D:676:LYS:NZ	2:D:677:PRO:HD2	1.58	1.16
1:A:175:PHE:CE1	1:A:179:GLU:CG	2.29	1.16
2:D:95:LEU:CD1	2:D:564:GLU:HA	1.74	1.15
2:B:91:LEU:HD11	2:B:564:GLU:CG	1.78	1.14
2:D:676:LYS:HZ2	2:D:677:PRO:CD	1.60	1.13
2:B:99:ALA:O	2:B:102:GLN:HG2	1.49	1.13
2:D:403:ALA:HB2	2:D:518:ARG:HG2	1.25	1.11
2:B:403:ALA:CA	2:B:518:ARG:HG2	1.82	1.10
2:D:396:ALA:CB	2:D:400:PHE:CD2	2.34	1.09
1:C:234:LEU:HD11	1:C:320:VAL:HG11	1.30	1.09
2:D:363:LYS:O	2:D:364:VAL:HG12	1.51	1.09
1:C:146:GLU:HB3	1:C:147:PRO:CD	1.83	1.07
2:B:91:LEU:HD11	2:B:564:GLU:HG2	1.15	1.07
2:B:515:TYR:O	2:B:519:THR:HG23	1.55	1.06
2:D:95:LEU:CD1	2:D:564:GLU:CA	2.32	1.06
2:D:403:ALA:CA	2:D:518:ARG:CG	2.34	1.06
2:D:358:ILE:HD11	2:D:360:MET:CE	1.86	1.05
2:B:95:LEU:CD1	2:B:563:SER:HA	1.85	1.05
2:B:622:ILE:HB	2:B:679:ILE:CG2	1.85	1.05
2:D:95:LEU:HD11	2:D:564:GLU:HA	1.08	1.05
2:B:217:TYR:OH	2:B:567:THR:HG21	1.57	1.04
2:B:403:ALA:CB	2:B:518:ARG:HG2	1.88	1.04
2:B:91:LEU:CD1	2:B:564:GLU:CG	2.34	1.03
2:D:51:ASN:HD22	2:D:359:LEU:HD22	0.93	1.03
2:D:345:HIS:N	2:D:361:CYS:SG	2.30	1.03
2:D:343:VAL:HG13	2:D:344:CYS:H	1.18	1.03
2:D:298:VAL:HG22	2:D:365:THR:HA	1.40	1.03
1:C:175:PHE:CE1	1:C:179:GLU:HB3	1.93	1.01
2:D:343:VAL:O	2:D:344:CYS:HB2	1.56	1.01
2:D:676:LYS:HZ2	2:D:677:PRO:HD2	0.85	1.01
1:A:144:PHE:O	1:A:145:GLN:CG	2.07	1.01
2:B:207:TYR:HA	2:B:566:TRP:HH2	1.24	1.01
1:C:146:GLU:HB3	1:C:147:PRO:HD3	1.39	1.01
2:D:99:ALA:O	2:D:102:GLN:HG2	1.62	1.00
2:D:363:LYS:HZ2	2:D:363:LYS:HB3	1.26	1.00
2:B:403:ALA:HB2	2:B:518:ARG:HG2	1.40	1.00
2:B:91:LEU:CD1	2:B:564:GLU:HG2	1.90	0.99
2:D:403:ALA:N	2:D:518:ARG:HG3	1.75	0.99
2:D:102:GLN:O	2:D:390:PHE:HZ	1.46	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:LEU:HG	2:B:564:GLU:OE1	1.63	0.99
2:B:298:VAL:HG13	2:B:364:VAL:O	1.61	0.99
2:D:51:ASN:ND2	2:D:359:LEU:CD2	2.26	0.99
2:D:358:ILE:HD11	2:D:360:MET:HE2	1.38	0.99
1:C:175:PHE:CD1	1:C:179:GLU:CB	2.45	0.98
2:B:394:ASN:O	2:B:562:LYS:HB2	1.63	0.96
2:D:345:HIS:CA	2:D:361:CYS:SG	2.54	0.96
2:D:99:ALA:HB1	2:D:102:GLN:NE2	1.80	0.95
2:D:333:LEU:O	2:D:362:THR:HG21	1.66	0.95
2:D:399:GLY:O	2:D:518:ARG:HB2	1.66	0.95
2:D:403:ALA:N	2:D:518:ARG:CG	2.30	0.95
2:B:91:LEU:CD1	2:B:564:GLU:HG3	1.96	0.95
2:B:102:GLN:HG3	2:B:390:PHE:HZ	1.25	0.95
2:B:403:ALA:N	2:B:518:ARG:HG3	1.82	0.95
1:C:148:LEU:HD12	1:C:408:THR:HG22	1.49	0.94
2:D:358:ILE:HG13	2:D:360:MET:HE2	1.48	0.94
2:D:515:TYR:O	2:D:519:THR:HG23	1.67	0.94
2:D:304:ALA:HB2	2:D:362:THR:HG22	1.50	0.93
2:D:343:VAL:HG13	2:D:344:CYS:N	1.83	0.93
1:C:175:PHE:HA	1:C:179:GLU:CD	1.92	0.93
2:D:333:LEU:HD22	2:D:360:MET:HB2	1.49	0.92
2:B:403:ALA:CA	2:B:518:ARG:CG	2.47	0.92
2:D:358:ILE:CG1	2:D:360:MET:CE	2.48	0.91
2:D:622:ILE:HB	2:D:679:ILE:HB	1.51	0.90
2:B:95:LEU:HD12	2:B:563:SER:HA	0.92	0.90
2:B:396:ALA:HB1	2:B:566:TRP:HB3	1.53	0.90
2:D:403:ALA:HA	2:D:518:ARG:CG	1.99	0.90
1:C:148:LEU:HD13	1:C:150:TRP:NE1	1.87	0.89
2:D:95:LEU:HD11	2:D:564:GLU:C	1.97	0.89
1:C:175:PHE:CD1	1:C:179:GLU:HB3	2.05	0.89
1:C:148:LEU:HB2	1:C:151:SER:OG	1.73	0.89
2:B:207:TYR:HA	2:B:566:TRP:CH2	2.07	0.89
2:D:102:GLN:HG3	2:D:390:PHE:CZ	2.07	0.89
2:D:361:CYS:HB2	2:D:363:LYS:NZ	1.88	0.89
2:D:343:VAL:O	2:D:344:CYS:CB	2.17	0.89
2:B:403:ALA:N	2:B:518:ARG:CG	2.36	0.88
2:D:333:LEU:CD2	2:D:360:MET:HB2	2.04	0.88
2:D:676:LYS:CD	2:D:677:PRO:HD2	2.03	0.87
1:C:175:PHE:HA	1:C:179:GLU:OE1	1.73	0.87
1:C:234:LEU:CD1	1:C:320:VAL:HG11	2.04	0.87
2:D:403:ALA:HA	2:D:518:ARG:HG2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ASN:ND2	2:D:349:TRP:HZ2	1.73	0.86
2:B:102:GLN:O	2:B:390:PHE:HZ	1.59	0.86
2:D:347:THR:HG23	2:D:359:LEU:HB3	1.57	0.85
2:D:363:LYS:HZ3	2:D:363:LYS:H	1.24	0.85
2:D:676:LYS:NZ	2:D:677:PRO:CD	2.28	0.85
2:D:363:LYS:CG	2:D:365:THR:HG22	2.05	0.85
2:D:95:LEU:CD1	2:D:564:GLU:N	2.40	0.85
2:B:217:TYR:OH	2:B:578:ASN:HA	1.77	0.84
2:D:102:GLN:O	2:D:390:PHE:CZ	2.29	0.84
2:D:363:LYS:HG2	2:D:365:THR:HG22	1.59	0.84
1:A:175:PHE:O	1:A:179:GLU:HB2	1.77	0.84
2:D:358:ILE:HG12	2:D:360:MET:HE2	1.58	0.84
2:B:209:VAL:HB	2:B:565:PRO:HG3	1.59	0.84
2:D:396:ALA:HB3	2:D:400:PHE:HD2	1.39	0.83
2:B:402:GLU:C	2:B:518:ARG:HG3	2.03	0.83
2:B:217:TYR:CZ	2:B:567:THR:HG21	2.13	0.83
2:B:399:GLY:O	2:B:518:ARG:HB2	1.78	0.82
2:B:403:ALA:HA	2:B:518:ARG:CG	2.09	0.82
2:D:95:LEU:HD12	2:D:564:GLU:N	1.92	0.82
2:D:95:LEU:HD12	2:D:563:SER:C	2.05	0.82
2:B:676:LYS:NZ	2:B:677:PRO:HD2	1.93	0.82
2:D:50:TYR:HB2	2:D:58:ASN:HB2	1.61	0.82
2:D:635:TRP:CE2	2:D:679:ILE:HG23	2.14	0.82
2:B:95:LEU:CD1	2:B:563:SER:CA	2.50	0.82
2:D:363:LYS:O	2:D:364:VAL:CG1	2.27	0.82
2:D:396:ALA:HB3	2:D:400:PHE:CG	2.13	0.82
2:B:91:LEU:HD12	2:B:564:GLU:HG3	1.58	0.81
1:C:175:PHE:O	1:C:179:GLU:HB2	1.80	0.81
2:B:286:GLY:O	2:B:287:GLN:HG3	1.81	0.81
2:B:95:LEU:HD11	2:B:564:GLU:N	1.96	0.81
2:B:566:TRP:O	2:B:570:LEU:HG	1.80	0.81
2:D:635:TRP:CD1	2:D:679:ILE:HD12	2.15	0.80
2:B:56:GLU:O	2:B:59:VAL:HG12	1.80	0.80
2:B:203:TRP:CD1	2:B:511:SER:HB2	2.15	0.80
2:B:102:GLN:CG	2:B:390:PHE:CZ	2.63	0.80
2:B:622:ILE:CB	2:B:679:ILE:CG2	2.60	0.80
2:D:50:TYR:HD2	2:D:51:ASN:OD1	1.64	0.79
2:D:54:ILE:CD1	2:D:342:ALA:O	2.31	0.79
2:D:396:ALA:HB2	2:D:400:PHE:CD2	2.17	0.78
2:B:215:TYR:O	2:B:565:PRO:HG2	1.84	0.78
2:D:33:ASN:HD21	2:D:389:PRO:HB3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:ALA:HA	2:B:518:ARG:HG2	1.65	0.78
2:D:54:ILE:HD11	2:D:342:ALA:O	1.84	0.78
2:D:286:GLY:O	2:D:287:GLN:HG3	1.81	0.78
2:D:676:LYS:CE	2:D:677:PRO:HD2	2.14	0.78
2:D:635:TRP:CG	2:D:679:ILE:HD12	2.19	0.78
2:B:33:ASN:HD21	2:B:389:PRO:HB3	1.47	0.78
2:D:99:ALA:HB1	2:D:102:GLN:CD	2.10	0.77
1:C:148:LEU:HD13	1:C:150:TRP:CE2	2.18	0.77
2:D:676:LYS:HZ3	2:D:677:PRO:HG2	1.50	0.76
2:D:305:GLN:OE1	2:D:333:LEU:HD11	1.86	0.76
2:B:102:GLN:NE2	2:B:390:PHE:CE1	2.53	0.76
2:B:396:ALA:CB	2:B:566:TRP:HB3	2.15	0.76
1:C:148:LEU:HD13	1:C:150:TRP:HE1	1.48	0.76
2:D:676:LYS:CG	2:D:677:PRO:HD2	2.15	0.76
1:C:175:PHE:CA	1:C:179:GLU:OE1	2.34	0.75
2:D:361:CYS:O	2:D:362:THR:OG1	2.04	0.75
2:D:345:HIS:HA	2:D:361:CYS:SG	2.25	0.75
2:B:622:ILE:HB	2:B:679:ILE:CB	2.17	0.74
2:D:676:LYS:HD2	2:D:677:PRO:HD3	1.69	0.74
2:D:635:TRP:CE2	2:D:679:ILE:CG2	2.70	0.74
2:B:363:LYS:NZ	2:B:363:LYS:HB3	2.01	0.74
2:D:288:LYS:HD2	2:D:431:ASP:OD1	1.88	0.74
2:D:676:LYS:HD2	2:D:677:PRO:CD	2.16	0.74
2:B:288:LYS:HD2	2:B:431:ASP:OD1	1.88	0.74
2:D:676:LYS:HG3	2:D:677:PRO:HD2	1.68	0.74
2:D:676:LYS:CD	2:D:677:PRO:CD	2.66	0.74
2:D:361:CYS:HB2	2:D:363:LYS:HZ1	1.49	0.74
2:D:518:ARG:C	2:D:518:ARG:HD2	2.13	0.73
2:B:102:GLN:O	2:B:390:PHE:CZ	2.40	0.73
2:D:396:ALA:CB	2:D:400:PHE:CG	2.71	0.73
2:B:622:ILE:HB	2:B:679:ILE:HG22	1.70	0.73
2:D:399:GLY:C	2:D:518:ARG:HB2	2.13	0.73
2:B:95:LEU:CD1	2:B:564:GLU:N	2.52	0.73
2:B:454:TYR:HB2	2:B:516:TYR:OH	1.89	0.72
2:D:286:GLY:C	2:D:287:GLN:HG3	2.14	0.72
2:B:518:ARG:HD2	2:B:518:ARG:O	1.89	0.72
1:C:145:GLN:O	1:C:414:PRO:HB3	1.88	0.72
2:B:622:ILE:CG1	2:B:679:ILE:HG22	2.20	0.72
2:D:403:ALA:HB2	2:D:518:ARG:CG	2.13	0.72
2:D:402:GLU:C	2:D:518:ARG:HG3	2.14	0.72
2:B:215:TYR:CE1	2:B:567:THR:O	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:286:GLY:C	2:B:287:GLN:HG3	2.14	0.72
2:D:635:TRP:CZ2	2:D:679:ILE:CG2	2.72	0.71
1:C:175:PHE:CD1	1:C:179:GLU:HG2	2.25	0.71
2:D:676:LYS:NZ	2:D:677:PRO:HG2	2.05	0.71
2:B:209:VAL:O	2:B:216:ASP:HA	1.91	0.71
2:B:207:TYR:CA	2:B:566:TRP:HH2	2.01	0.71
2:B:60:GLN:NE2	2:B:64:ASN:OD1	2.24	0.70
2:D:59:VAL:HG13	2:D:60:GLN:HG2	1.73	0.70
2:B:88:ILE:HD11	2:B:93:VAL:HG23	1.74	0.70
2:D:676:LYS:NZ	2:D:677:PRO:CG	2.55	0.70
2:D:677:PRO:O	2:D:679:ILE:HD13	1.91	0.70
2:B:210:ASN:HA	2:B:216:ASP:CG	2.15	0.70
2:B:95:LEU:CD1	2:B:564:GLU:H	2.03	0.70
2:D:298:VAL:HG22	2:D:365:THR:CA	2.18	0.70
2:D:99:ALA:O	2:D:102:GLN:CG	2.39	0.70
1:C:148:LEU:HD12	1:C:408:THR:CG2	2.21	0.70
2:D:363:LYS:N	2:D:363:LYS:HD2	2.06	0.70
2:B:210:ASN:HA	2:B:216:ASP:OD1	1.92	0.70
2:D:363:LYS:HB3	2:D:363:LYS:NZ	2.06	0.70
2:B:622:ILE:HB	2:B:679:ILE:HG21	1.72	0.69
2:D:51:ASN:HB3	2:D:359:LEU:CD1	2.23	0.69
2:B:517:THR:O	2:B:521:TYR:CD2	2.46	0.69
2:D:362:THR:O	2:D:364:VAL:N	2.25	0.69
2:B:102:GLN:HE21	2:B:390:PHE:HE1	1.40	0.69
2:D:304:ALA:HB3	2:D:333:LEU:HD13	1.73	0.69
1:C:175:PHE:CD1	1:C:179:GLU:CG	2.75	0.69
2:D:58:ASN:C	2:D:60:GLN:H	1.98	0.68
2:B:403:ALA:HA	2:B:518:ARG:CD	2.24	0.68
2:B:622:ILE:HB	2:B:679:ILE:HB	1.74	0.68
2:B:676:LYS:HZ2	2:B:677:PRO:HD2	1.56	0.68
2:D:333:LEU:O	2:D:362:THR:CG2	2.41	0.68
2:D:362:THR:O	2:D:363:LYS:C	2.34	0.67
2:D:363:LYS:NZ	2:D:363:LYS:H	1.92	0.67
2:B:515:TYR:O	2:B:519:THR:CG2	2.39	0.67
1:C:148:LEU:HD13	1:C:150:TRP:CZ2	2.30	0.67
1:C:175:PHE:CG	1:C:179:GLU:HB2	2.30	0.67
1:C:293:ASN:HD22	1:C:297:ASN:HD22	1.43	0.67
1:A:175:PHE:CE1	1:A:179:GLU:HG3	2.28	0.67
1:A:293:ASN:HD22	1:A:297:ASN:HD22	1.43	0.67
2:B:399:GLY:O	2:B:518:ARG:CB	2.42	0.67
2:D:363:LYS:HG3	2:D:365:THR:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:635:TRP:CZ2	2:D:679:ILE:HG21	2.29	0.66
1:A:175:PHE:C	1:A:179:GLU:HB2	2.21	0.66
2:D:50:TYR:CD2	2:D:51:ASN:OD1	2.48	0.65
2:B:50:TYR:HA	2:B:58:ASN:HB2	1.79	0.65
2:D:358:ILE:HD11	2:D:360:MET:HE1	1.74	0.65
2:B:145:GLU:HG2	2:B:146:PRO:HD3	1.79	0.65
1:A:145:GLN:CD	2:B:741:ILE:HG21	2.22	0.65
2:B:622:ILE:CB	2:B:679:ILE:HG21	2.26	0.65
1:A:234:LEU:HB2	1:A:423:MET:HE1	1.77	0.65
2:B:99:ALA:HB1	2:B:102:GLN:OE1	1.97	0.65
2:D:361:CYS:HB2	2:D:363:LYS:HZ3	1.62	0.64
2:D:403:ALA:HA	2:D:518:ARG:CD	2.27	0.64
2:B:50:TYR:CE1	2:B:59:VAL:HB	2.33	0.64
2:D:346:PRO:HG3	2:D:363:LYS:HE2	1.80	0.64
2:D:358:ILE:HG12	2:D:360:MET:CE	2.22	0.64
2:D:397:ASN:OD1	2:D:400:PHE:N	2.26	0.64
2:B:217:TYR:OH	2:B:567:THR:CG2	2.41	0.64
2:D:145:GLU:HG2	2:D:146:PRO:HD3	1.79	0.64
2:D:635:TRP:CH2	2:D:679:ILE:HG21	2.33	0.64
2:B:217:TYR:CE2	2:B:567:THR:HG21	2.33	0.63
2:D:58:ASN:C	2:D:60:GLN:N	2.52	0.63
2:D:677:PRO:C	2:D:679:ILE:H	2.07	0.63
2:B:638:ASN:HD21	2:D:656:LEU:HB2	1.63	0.63
2:B:324:THR:OG1	2:B:325:GLN:N	2.33	0.62
2:D:365:THR:O	2:D:366:MET:HB2	1.98	0.62
1:A:144:PHE:C	1:A:145:GLN:HG3	2.17	0.62
2:D:515:TYR:O	2:D:519:THR:CG2	2.46	0.62
2:B:362:THR:C	2:B:364:VAL:H	2.08	0.62
2:B:719:ASP:HA	2:B:722:LEU:HB2	1.82	0.62
2:B:50:TYR:CA	2:B:58:ASN:HB2	2.29	0.61
2:D:505:HIS:HB3	2:D:510:TYR:HB2	1.82	0.61
2:D:298:VAL:CG2	2:D:365:THR:HA	2.24	0.61
2:D:56:GLU:O	2:D:59:VAL:HG12	2.00	0.61
2:B:95:LEU:HD12	2:B:563:SER:N	2.12	0.61
2:B:203:TRP:NE1	2:B:511:SER:HB2	2.15	0.61
2:B:335:ASP:O	2:B:363:LYS:HA	2.00	0.61
2:B:403:ALA:N	2:B:518:ARG:HG2	2.09	0.61
2:D:58:ASN:O	2:D:61:ASN:N	2.32	0.61
2:D:91:LEU:HG	2:D:564:GLU:HB3	1.81	0.61
2:D:635:TRP:CG	2:D:679:ILE:CD1	2.83	0.61
2:B:299:ASP:OD1	2:B:299:ASP:N	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LEU:HB2	1:C:423:MET:HE1	1.82	0.61
2:D:363:LYS:HZ2	2:D:363:LYS:CB	2.09	0.61
1:C:234:LEU:HD11	1:C:320:VAL:CG1	2.20	0.61
2:D:299:ASP:N	2:D:299:ASP:OD1	2.32	0.61
2:B:505:HIS:HB3	2:B:510:TYR:HB2	1.82	0.61
2:D:403:ALA:HA	2:D:518:ARG:HD3	1.82	0.61
2:D:621:ARG:HB3	2:D:723:GLU:HB3	1.83	0.61
2:D:298:VAL:CG2	2:D:365:THR:O	2.49	0.60
2:D:403:ALA:N	2:D:518:ARG:HG2	2.03	0.60
2:B:110:GLU:OE1	2:B:114:LYS:NZ	2.35	0.60
2:D:324:THR:OG1	2:D:325:GLN:N	2.33	0.60
2:D:365:THR:O	2:D:366:MET:CB	2.49	0.60
2:D:110:GLU:OE1	2:D:114:LYS:NZ	2.35	0.60
2:D:396:ALA:HB3	2:D:400:PHE:CB	2.31	0.60
2:B:679:ILE:HD13	2:B:679:ILE:N	2.16	0.60
1:C:352:GLU:OE2	2:D:678:ARG:CG	2.49	0.60
2:B:621:ARG:HB3	2:B:723:GLU:HB3	1.83	0.60
1:C:567:TYR:HB3	1:C:570:PHE:HA	1.84	0.60
2:D:366:MET:O	2:D:366:MET:HG2	2.02	0.60
2:B:217:TYR:CE2	2:B:567:THR:CG2	2.84	0.60
2:B:364:VAL:O	2:B:364:VAL:HG13	2.02	0.60
2:D:177:ARG:NH2	2:D:495:GLU:O	2.35	0.60
2:B:218:SER:HB3	2:B:221:GLN:HG2	1.83	0.60
2:D:439:LEU:HD23	2:D:591:LEU:HD13	1.84	0.60
1:A:567:TYR:HB3	1:A:570:PHE:HA	1.84	0.60
2:D:51:ASN:HB3	2:D:359:LEU:HD11	1.84	0.60
2:D:91:LEU:HG	2:D:564:GLU:CB	2.31	0.60
2:D:102:GLN:HG3	2:D:390:PHE:CE1	2.36	0.60
2:D:719:ASP:HA	2:D:722:LEU:HB2	1.82	0.60
2:D:343:VAL:CG1	2:D:344:CYS:N	2.56	0.60
2:D:635:TRP:HB3	2:D:679:ILE:HD11	1.84	0.60
2:B:177:ARG:NH2	2:B:495:GLU:O	2.35	0.59
2:D:676:LYS:HZ2	2:D:677:PRO:CG	2.10	0.59
1:C:148:LEU:CD1	1:C:150:TRP:HE1	2.15	0.59
2:B:570:LEU:HB3	2:B:576:ALA:HB3	1.84	0.59
1:A:175:PHE:O	1:A:179:GLU:CB	2.48	0.59
2:D:570:LEU:HB3	2:D:576:ALA:HB3	1.84	0.59
2:B:102:GLN:O	2:B:103:ASN:HB2	2.01	0.59
2:B:217:TYR:HE1	2:B:578:ASN:CG	2.10	0.59
2:B:399:GLY:O	2:B:518:ARG:CG	2.50	0.59
1:A:234:LEU:O	1:A:234:LEU:HG	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:363:LYS:O	2:D:364:VAL:CB	2.50	0.59
2:D:51:ASN:ND2	2:D:349:TRP:CZ2	2.63	0.59
2:B:399:GLY:C	2:B:518:ARG:HB2	2.26	0.59
2:D:58:ASN:O	2:D:60:GLN:N	2.37	0.58
2:B:403:ALA:HA	2:B:518:ARG:HD3	1.85	0.58
2:D:102:GLN:CG	2:D:390:PHE:CZ	2.84	0.58
2:B:454:TYR:CB	2:B:516:TYR:OH	2.52	0.58
2:B:517:THR:O	2:B:521:TYR:CE2	2.56	0.58
2:B:527:GLU:O	2:B:531:GLN:NE2	2.37	0.58
1:C:175:PHE:CD1	1:C:179:GLU:HB2	2.31	0.58
2:D:363:LYS:HG2	2:D:365:THR:H	1.69	0.58
2:B:397:ASN:HD21	2:B:400:PHE:HB2	1.69	0.58
2:D:203:TRP:CD1	2:D:511:SER:HB2	2.38	0.58
2:D:564:GLU:OE1	2:D:568:LEU:HD22	2.04	0.58
2:B:51:ASN:HB3	2:B:359:LEU:HD22	1.84	0.58
2:D:656:LEU:HD11	2:D:662:MET:HA	1.85	0.58
2:B:395:GLY:O	2:B:562:LYS:NZ	2.36	0.58
2:D:527:GLU:O	2:D:531:GLN:NE2	2.37	0.58
1:A:175:PHE:HD1	1:A:179:GLU:HG2	1.45	0.57
1:C:434:GLY:HA2	1:C:437:GLU:HB2	1.86	0.57
2:D:218:SER:OG	2:D:219:ARG:N	2.37	0.57
2:D:333:LEU:HB3	2:D:362:THR:HG21	1.85	0.57
2:D:549:GLU:OE2	2:D:553:LYS:NZ	2.37	0.57
1:A:212:THR:O	1:A:455:LYS:NZ	2.38	0.57
2:B:363:LYS:HB3	2:B:363:LYS:HZ3	1.65	0.57
2:B:439:LEU:HD23	2:B:591:LEU:HD13	1.84	0.57
2:B:656:LEU:HD11	2:B:662:MET:HA	1.85	0.57
2:B:90:ASN:HB3	2:B:93:VAL:HG22	1.85	0.57
2:B:549:GLU:OE2	2:B:553:LYS:NZ	2.37	0.57
2:D:518:ARG:O	2:D:522:GLN:HB3	2.04	0.57
1:C:175:PHE:HD1	1:C:179:GLU:HG2	1.67	0.57
1:C:440:VAL:O	1:C:444:GLN:NE2	2.38	0.57
1:A:434:GLY:HA2	1:A:437:GLU:HB2	1.86	0.57
1:A:440:VAL:O	1:A:444:GLN:NE2	2.38	0.57
1:A:146:GLU:HB3	1:A:147:PRO:HD3	1.87	0.57
1:C:212:THR:O	1:C:455:LYS:NZ	2.38	0.57
2:D:344:CYS:SG	2:D:345:HIS:N	2.78	0.57
2:B:95:LEU:HD11	2:B:564:GLU:H	1.65	0.57
2:B:197:GLU:OE2	2:B:201:ASP:OD2	2.22	0.57
2:B:176:LEU:HG	2:B:179:LEU:HD12	1.87	0.56
1:A:232:VAL:O	1:A:235:THR:OG1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:TYR:HB2	2:B:58:ASN:HB2	1.87	0.56
2:B:91:LEU:HG	2:B:564:GLU:CD	2.30	0.56
2:B:215:TYR:OH	2:B:571:GLU:HB3	2.05	0.56
2:B:297:MET:HE3	2:B:366:MET:HA	1.87	0.56
1:A:14:ARG:NH1	1:A:105:SER:O	2.39	0.56
2:B:679:ILE:HD13	2:B:679:ILE:H	1.69	0.56
2:D:455:MET:HE3	2:D:481:LYS:HG3	1.87	0.56
2:B:216:ASP:O	2:B:217:TYR:CG	2.58	0.56
1:C:14:ARG:NH1	1:C:105:SER:O	2.39	0.56
2:D:54:ILE:HG12	2:D:342:ALA:O	2.06	0.56
2:D:679:ILE:HD13	2:D:679:ILE:N	2.20	0.56
1:A:172:VAL:HG21	1:A:405:GLU:OE2	2.06	0.56
2:B:217:TYR:HE2	2:B:567:THR:HG23	1.69	0.56
2:B:455:MET:HE3	2:B:481:LYS:HG3	1.87	0.56
2:B:538:PRO:HB2	2:B:541:LYS:HG3	1.88	0.56
1:C:351:PRO:HA	2:D:677:PRO:HB2	1.88	0.56
1:C:212:THR:O	1:C:212:THR:OG1	2.17	0.56
2:D:698:THR:O	2:D:702:LYS:NZ	2.39	0.56
1:A:175:PHE:CD1	1:A:179:GLU:CB	2.88	0.55
2:B:554:LEU:HG	2:B:557:MET:HE3	1.88	0.55
2:B:617:SER:O	2:B:697:ARG:NH1	2.39	0.55
2:D:617:SER:O	2:D:697:ARG:NH1	2.39	0.55
2:B:591:LEU:HA	2:B:594:TRP:HB3	1.89	0.55
2:B:698:THR:O	2:B:702:LYS:NZ	2.39	0.55
2:D:102:GLN:C	2:D:390:PHE:HZ	2.14	0.55
2:D:176:LEU:HG	2:D:179:LEU:HD12	1.87	0.55
2:D:197:GLU:OE2	2:D:201:ASP:OD2	2.23	0.55
2:D:437:ASN:HA	2:D:440:LEU:HD13	1.89	0.55
2:B:102:GLN:HG3	2:B:390:PHE:CE1	2.37	0.55
2:D:237:TYR:O	2:D:241:HIS:N	2.35	0.55
2:D:538:PRO:HB2	2:D:541:LYS:HG3	1.88	0.55
2:D:50:TYR:CB	2:D:58:ASN:HB2	2.34	0.55
2:D:69:TRP:O	2:D:73:LEU:N	2.39	0.55
2:D:361:CYS:CB	2:D:363:LYS:NZ	2.67	0.55
2:B:516:TYR:HA	2:B:519:THR:OG1	2.06	0.55
2:D:298:VAL:HG23	2:D:365:THR:O	2.06	0.55
2:B:437:ASN:HA	2:B:440:LEU:HD13	1.89	0.55
2:B:571:GLU:HG3	2:B:572:ASN:N	2.21	0.55
2:B:69:TRP:O	2:B:73:LEU:N	2.39	0.55
2:B:397:ASN:HD21	2:B:400:PHE:CB	2.20	0.55
2:D:554:LEU:HG	2:D:557:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:THR:OG1	1:C:357:GLN:N	2.40	0.55
2:D:351:LEU:HB2	2:D:355:ASP:HB3	1.89	0.55
2:D:705:ARG:NH1	2:D:728:GLN:O	2.40	0.55
2:D:99:ALA:HB1	2:D:102:GLN:HE22	1.69	0.55
2:D:591:LEU:HA	2:D:594:TRP:HB3	1.89	0.55
1:A:232:VAL:HG23	1:A:233:VAL:H	1.72	0.54
1:A:172:VAL:HG11	1:A:405:GLU:HG2	1.89	0.54
1:C:175:PHE:C	1:C:179:GLU:OE1	2.50	0.54
1:A:356:THR:OG1	1:A:357:GLN:N	2.40	0.54
2:B:622:ILE:CB	2:B:679:ILE:HG22	2.29	0.54
1:C:486:ASP:N	1:C:486:ASP:OD1	2.41	0.54
2:B:205:GLY:CA	2:B:219:ARG:HH21	2.20	0.54
1:C:94:GLN:NE2	1:C:295:VAL:O	2.41	0.54
2:D:38:ASP:OD1	2:D:38:ASP:N	2.41	0.54
1:C:55:VAL:HG12	1:C:317:VAL:HG11	1.90	0.54
1:A:145:GLN:O	1:A:414:PRO:HB3	2.08	0.54
2:B:98:GLN:HE22	2:B:209:VAL:HA	1.73	0.54
1:A:55:VAL:HG12	1:A:317:VAL:HG11	1.90	0.54
2:B:102:GLN:C	2:B:390:PHE:HZ	2.16	0.54
2:D:305:GLN:OE1	2:D:333:LEU:CD1	2.53	0.54
2:B:207:TYR:CZ	2:B:517:THR:HG21	2.43	0.54
2:B:215:TYR:CE2	2:B:568:LEU:HD12	2.43	0.54
2:B:373:HIS:HA	2:B:376:MET:HB2	1.90	0.54
1:C:567:TYR:OH	1:C:574:GLN:NE2	2.41	0.54
1:A:567:TYR:OH	1:A:574:GLN:NE2	2.41	0.54
1:C:408:THR:OG1	1:C:409:LYS:NZ	2.41	0.54
1:A:408:THR:OG1	1:A:409:LYS:NZ	2.41	0.53
1:A:486:ASP:OD1	1:A:486:ASP:N	2.41	0.53
2:B:91:LEU:CG	2:B:564:GLU:CG	2.86	0.53
2:B:215:TYR:CZ	2:B:568:LEU:HA	2.43	0.53
2:D:396:ALA:HB3	2:D:400:PHE:HB3	1.89	0.53
1:A:94:GLN:NE2	1:A:295:VAL:O	2.41	0.53
2:B:212:VAL:HB	2:B:215:TYR:CD2	2.43	0.53
2:D:346:PRO:HB3	2:D:360:MET:SD	2.48	0.53
2:D:358:ILE:CD1	2:D:360:MET:CE	2.52	0.53
2:B:212:VAL:HB	2:B:215:TYR:HD2	1.73	0.53
2:B:395:GLY:HA2	2:B:561:GLY:O	2.08	0.53
2:B:287:GLN:O	2:B:288:LYS:HB3	2.09	0.53
2:B:622:ILE:HG13	2:B:679:ILE:HG22	1.90	0.53
2:D:98:GLN:HE22	2:D:209:VAL:HA	1.73	0.53
1:A:56:TRP:HB2	1:A:398:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:THR:O	1:A:264:GLN:NE2	2.40	0.53
2:B:351:LEU:HB2	2:B:355:ASP:HB3	1.89	0.53
1:C:175:PHE:O	1:C:179:GLU:CB	2.55	0.53
1:C:260:THR:O	1:C:264:GLN:NE2	2.40	0.53
2:D:349:TRP:HE1	2:D:359:LEU:HB2	1.72	0.53
2:B:38:ASP:OD1	2:B:38:ASP:N	2.41	0.53
1:C:175:PHE:O	1:C:180:THR:N	2.39	0.53
1:C:352:GLU:OE2	2:D:678:ARG:HG2	2.07	0.53
2:D:345:HIS:C	2:D:361:CYS:SG	2.91	0.53
2:D:346:PRO:HD3	2:D:361:CYS:SG	2.49	0.53
2:B:95:LEU:CD1	2:B:563:SER:C	2.82	0.53
2:B:705:ARG:NH1	2:B:728:GLN:O	2.40	0.53
1:C:518:ILE:HD11	1:C:525:LYS:HG2	1.90	0.53
2:D:287:GLN:O	2:D:288:LYS:HB3	2.09	0.53
2:D:297:MET:HA	2:D:300:GLN:HB2	1.91	0.53
1:A:434:GLY:O	1:A:438:GLY:N	2.42	0.53
1:C:56:TRP:HB2	1:C:398:LEU:HD13	1.90	0.53
1:A:274:GLN:O	1:A:278:SER:N	2.41	0.53
1:A:518:ILE:HD11	1:A:525:LYS:HG2	1.90	0.53
2:B:233:ILE:HG23	2:B:236:LEU:HD12	1.91	0.53
2:B:297:MET:HA	2:B:300:GLN:HB2	1.90	0.53
1:A:234:LEU:CD1	1:A:320:VAL:HG11	2.40	0.52
2:B:331:SER:OG	2:B:358:ILE:O	2.27	0.52
2:B:622:ILE:CG2	2:B:679:ILE:HG21	2.39	0.52
1:C:175:PHE:CG	1:C:179:GLU:CB	2.90	0.52
1:C:458:LEU:HA	1:C:461:LEU:HD12	1.91	0.52
2:D:399:GLY:O	2:D:518:ARG:CB	2.49	0.52
1:A:458:LEU:HA	1:A:461:LEU:HD12	1.91	0.52
1:C:83:ILE:HD11	1:C:304:VAL:HA	1.92	0.52
1:C:434:GLY:O	1:C:438:GLY:N	2.42	0.52
2:D:373:HIS:HA	2:D:376:MET:HB2	1.90	0.52
1:A:48:PHE:HA	1:A:431:SER:HA	1.91	0.52
2:B:95:LEU:HD12	2:B:563:SER:C	2.32	0.52
1:C:174:TYR:O	1:C:179:GLU:OE1	2.28	0.52
2:B:318:VAL:HG13	2:B:544:ILE:HB	1.92	0.52
2:D:54:ILE:CG1	2:D:342:ALA:O	2.57	0.52
2:D:361:CYS:CB	2:D:363:LYS:HZ1	2.21	0.52
1:A:83:ILE:HD11	1:A:304:VAL:HA	1.92	0.52
2:D:88:ILE:HD11	2:D:93:VAL:HG23	1.89	0.52
2:D:101:GLN:HG3	2:D:101:GLN:O	2.09	0.52
2:D:210:ASN:HA	2:D:216:ASP:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:ASN:CA	2:B:216:ASP:OD1	2.56	0.52
2:B:392:LEU:HD22	2:B:562:LYS:O	2.09	0.52
2:D:233:ILE:HG23	2:D:236:LEU:HD12	1.91	0.52
2:D:331:SER:OG	2:D:358:ILE:O	2.27	0.52
1:C:140:LEU:HD13	1:C:421:PHE:HB2	1.92	0.52
2:D:363:LYS:N	2:D:363:LYS:CD	2.73	0.52
2:D:564:GLU:HB2	2:D:565:PRO:CD	2.39	0.52
2:D:679:ILE:HD13	2:D:679:ILE:H	1.75	0.52
2:B:710:ARG:O	2:B:710:ARG:NH1	2.43	0.52
1:C:97:ARG:NH1	1:C:291:SER:O	2.43	0.52
1:C:129:TYR:HA	1:C:132:ILE:HD12	1.91	0.52
2:D:66:GLY:O	2:D:70:SER:N	2.43	0.52
2:D:347:THR:CG2	2:D:359:LEU:HD23	2.40	0.52
1:A:97:ARG:NH1	1:A:291:SER:O	2.43	0.52
2:B:91:LEU:C	2:B:93:VAL:H	2.17	0.52
2:B:237:TYR:O	2:B:241:HIS:N	2.35	0.52
1:C:48:PHE:HA	1:C:431:SER:HA	1.90	0.52
2:D:51:ASN:HD22	2:D:349:TRP:HZ2	1.56	0.52
1:A:160:THR:HG22	2:B:730:THR:HB	1.93	0.51
2:D:189:GLU:HA	2:D:192:ARG:HB2	1.92	0.51
2:D:678:ARG:HG2	2:D:678:ARG:O	2.10	0.51
1:A:140:LEU:HD13	1:A:421:PHE:HB2	1.92	0.51
2:B:91:LEU:CG	2:B:564:GLU:HG2	2.39	0.51
2:B:189:GLU:HA	2:B:192:ARG:HB2	1.92	0.51
1:C:156:ASN:ND2	1:C:158:ASN:OD1	2.43	0.51
2:D:60:GLN:NE2	2:D:64:ASN:OD1	2.43	0.51
1:C:148:LEU:CD1	1:C:150:TRP:NE1	2.68	0.51
2:D:318:VAL:HG13	2:D:544:ILE:HB	1.92	0.51
2:D:347:THR:HG21	2:D:359:LEU:HD23	1.91	0.51
2:D:617:SER:HA	2:D:684:PHE:HB3	1.92	0.51
1:A:129:TYR:HA	1:A:132:ILE:HD12	1.91	0.51
1:A:156:ASN:ND2	1:A:158:ASN:OD1	2.43	0.51
1:A:299:CYS:O	1:A:303:SER:OG	2.29	0.51
1:A:334:ASP:HB2	1:A:357:GLN:HE22	1.76	0.51
2:B:102:GLN:HE22	2:B:393:ARG:HG3	1.74	0.51
2:B:625:LYS:HA	2:B:629:GLY:HA2	1.93	0.51
2:B:53:ASN:OD1	2:B:54:ILE:N	2.44	0.51
2:B:86:GLN:NE2	2:B:210:ASN:O	2.44	0.51
2:B:207:TYR:CD1	2:B:566:TRP:CH2	2.99	0.51
2:D:362:THR:C	2:D:364:VAL:N	2.67	0.51
2:D:304:ALA:CB	2:D:333:LEU:HD22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:LYS:HD2	2:B:93:VAL:HG11	1.91	0.51
2:B:92:THR:HG23	2:B:93:VAL:HG13	1.92	0.51
2:B:617:SER:HA	2:B:684:PHE:HB3	1.92	0.51
1:A:145:GLN:NE2	2:B:741:ILE:HG21	2.26	0.51
2:B:217:TYR:OH	2:B:578:ASN:CA	2.56	0.51
1:C:334:ASP:HB2	1:C:357:GLN:HE22	1.76	0.51
2:D:86:GLN:NE2	2:D:210:ASN:O	2.44	0.51
2:D:105:SER:OG	2:D:194:ASN:OD1	2.29	0.51
2:D:363:LYS:NZ	2:D:363:LYS:CB	2.73	0.51
2:B:105:SER:OG	2:B:194:ASN:OD1	2.29	0.51
2:D:710:ARG:O	2:D:710:ARG:NH1	2.43	0.51
1:A:166:CYS:HB2	1:A:174:TYR:CD2	2.46	0.50
1:C:146:GLU:HB3	1:C:147:PRO:HD2	1.88	0.50
2:B:713:ASP:O	2:D:710:ARG:NH2	2.36	0.50
2:D:53:ASN:OD1	2:D:54:ILE:N	2.44	0.50
2:B:90:ASN:O	2:B:91:LEU:HB2	2.11	0.50
2:B:363:LYS:NZ	2:B:363:LYS:CB	2.73	0.50
2:B:479:GLU:HA	2:B:482:ARG:HE	1.77	0.50
2:D:405:GLY:O	2:D:409:SER:N	2.43	0.50
2:D:635:TRP:CE2	2:D:679:ILE:HG21	2.44	0.50
2:B:203:TRP:CE2	2:B:511:SER:HB2	2.46	0.50
1:C:175:PHE:CA	1:C:179:GLU:HB2	2.42	0.50
2:D:99:ALA:HA	2:D:102:GLN:OE1	2.11	0.50
2:B:78:THR:HA	2:B:81:GLN:HB2	1.93	0.50
2:B:440:LEU:HD12	2:B:591:LEU:HD21	1.94	0.50
2:D:625:LYS:HA	2:D:629:GLY:HA2	1.93	0.50
2:D:78:THR:HA	2:D:81:GLN:HB2	1.93	0.50
2:D:518:ARG:HD2	2:D:518:ARG:O	2.10	0.50
2:B:50:TYR:CB	2:B:58:ASN:HB2	2.41	0.50
2:B:323:MET:HG2	2:B:376:MET:HG2	1.94	0.50
1:C:172:VAL:HG11	1:C:405:GLU:HG2	1.93	0.50
1:C:298:ASN:HD22	1:C:522:ILE:HD12	1.77	0.50
2:B:66:GLY:O	2:B:70:SER:N	2.43	0.50
2:B:41:TYR:O	2:B:45:LEU:N	2.36	0.49
1:C:32:ARG:HH22	1:C:291:SER:HB2	1.77	0.49
1:C:322:TYR:HA	1:C:325:ILE:HB	1.93	0.49
2:D:323:MET:HG2	2:D:376:MET:HG2	1.93	0.49
1:A:495:LEU:HD21	1:A:545:ILE:HG22	1.94	0.49
2:D:440:LEU:HD12	2:D:591:LEU:HD21	1.94	0.49
2:B:50:TYR:HA	2:B:58:ASN:CB	2.42	0.49
1:A:322:TYR:HA	1:A:325:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:454:TYR:CA	2:B:516:TYR:OH	2.61	0.49
1:C:495:LEU:HD21	1:C:545:ILE:HG22	1.94	0.49
2:D:373:HIS:NE2	2:D:408:MET:O	2.41	0.49
2:B:60:GLN:O	2:B:64:ASN:N	2.45	0.49
2:B:203:TRP:CG	2:B:511:SER:HB2	2.48	0.49
2:B:244:VAL:O	2:B:248:LEU:N	2.43	0.49
2:D:343:VAL:CG1	2:D:344:CYS:H	1.99	0.49
1:A:266:ASP:HA	1:A:269:LEU:HB3	1.94	0.49
2:B:622:ILE:HG21	2:B:679:ILE:HG21	1.94	0.49
1:C:223:VAL:O	1:C:227:SER:OG	2.31	0.49
2:D:479:GLU:HA	2:D:482:ARG:HE	1.77	0.49
1:A:130:ASN:HA	1:A:133:ILE:HB	1.94	0.49
2:D:564:GLU:HB2	2:D:565:PRO:HD3	1.94	0.49
1:A:298:ASN:HD22	1:A:522:ILE:HD12	1.77	0.49
2:B:67:ASP:HA	2:B:70:SER:HB2	1.95	0.49
2:B:212:VAL:HB	2:B:215:TYR:HB2	1.95	0.49
2:B:286:GLY:C	2:B:287:GLN:CG	2.86	0.49
1:C:175:PHE:C	1:C:179:GLU:HB2	2.37	0.49
1:C:266:ASP:HA	1:C:269:LEU:HB3	1.94	0.49
2:D:298:VAL:HG22	2:D:365:THR:C	2.38	0.49
2:B:27:THR:O	2:B:31:LYS:N	2.46	0.49
2:D:332:MET:O	2:D:333:LEU:HD23	2.13	0.49
1:A:543:LEU:HA	1:A:546:PHE:HB3	1.94	0.48
2:B:217:TYR:HE1	2:B:578:ASN:ND2	2.11	0.48
1:C:299:CYS:O	1:C:303:SER:OG	2.29	0.48
1:A:234:LEU:HB2	1:A:423:MET:CE	2.42	0.48
2:B:60:GLN:C	2:B:62:MET:H	2.19	0.48
2:B:211:GLY:N	2:B:216:ASP:OD1	2.45	0.48
2:B:217:TYR:OH	2:B:578:ASN:O	2.30	0.48
2:D:222:LEU:HD12	2:D:223:ILE:HG23	1.95	0.48
2:B:300:GLN:HE22	2:B:423:LEU:HA	1.78	0.48
2:B:373:HIS:NE2	2:B:408:MET:O	2.41	0.48
2:B:582:ARG:O	2:B:586:ASN:N	2.46	0.48
1:C:543:LEU:HA	1:C:546:PHE:HB3	1.94	0.48
2:D:619:LYS:HA	2:D:682:ASN:HA	1.94	0.48
2:D:286:GLY:C	2:D:287:GLN:CG	2.86	0.48
1:A:32:ARG:HH22	1:A:291:SER:HB2	1.77	0.48
2:B:101:GLN:O	2:B:101:GLN:HG3	2.14	0.48
2:B:102:GLN:O	2:B:103:ASN:CB	2.61	0.48
2:B:215:TYR:O	2:B:565:PRO:CG	2.57	0.48
1:C:148:LEU:HD22	1:C:150:TRP:CZ2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ILE:HA	1:C:459:THR:HG21	1.95	0.48
1:C:130:ASN:HA	1:C:133:ILE:HB	1.95	0.48
1:C:274:GLN:O	1:C:278:SER:N	2.41	0.48
2:B:24:GLN:OE1	2:B:83:TYR:OH	2.32	0.48
2:B:399:GLY:O	2:B:403:ALA:N	2.46	0.48
2:B:619:LYS:HA	2:B:682:ASN:HA	1.94	0.48
2:D:294:THR:HA	2:D:366:MET:SD	2.53	0.48
2:D:300:GLN:HE22	2:D:423:LEU:HA	1.78	0.48
2:D:676:LYS:CE	2:D:677:PRO:CD	2.85	0.48
2:D:136:ASP:OD1	2:D:136:ASP:N	2.46	0.48
1:A:175:PHE:CG	1:A:179:GLU:CB	2.97	0.48
2:B:210:ASN:C	2:B:216:ASP:OD1	2.57	0.48
2:D:677:PRO:O	2:D:679:ILE:N	2.46	0.48
2:B:363:LYS:HB3	2:B:363:LYS:HZ2	1.76	0.47
2:B:588:PHE:O	2:B:592:PHE:N	2.47	0.47
2:D:67:ASP:HA	2:D:70:SER:HB2	1.95	0.47
1:A:386:ASN:HA	1:A:389:LEU:HB2	1.96	0.47
2:B:215:TYR:C	2:B:565:PRO:HG2	2.37	0.47
2:B:222:LEU:HD12	2:B:223:ILE:HG23	1.95	0.47
2:B:362:THR:C	2:B:364:VAL:N	2.73	0.47
2:D:24:GLN:OE1	2:D:83:TYR:OH	2.32	0.47
2:D:27:THR:O	2:D:31:LYS:N	2.46	0.47
2:D:51:ASN:HB3	2:D:359:LEU:HD13	1.95	0.47
1:C:352:GLU:OE2	2:D:678:ARG:HG3	2.14	0.47
2:D:588:PHE:O	2:D:592:PHE:N	2.47	0.47
2:B:208:GLU:OE2	2:B:219:ARG:HG3	2.14	0.47
2:D:244:VAL:O	2:D:248:LEU:N	2.43	0.47
2:B:405:GLY:O	2:B:409:SER:N	2.43	0.47
1:C:121:THR:HA	1:C:124:MET:HE2	1.96	0.47
1:C:178:ARG:NH1	1:C:182:ASN:OD1	2.36	0.47
1:A:173:ASP:O	1:A:176:TRP:HB3	2.15	0.47
1:A:231:TYR:O	1:A:235:THR:HG23	2.15	0.47
2:B:91:LEU:HD13	2:B:91:LEU:HA	1.78	0.47
2:B:635:TRP:CG	2:B:679:ILE:HD12	2.49	0.47
1:C:266:ASP:N	1:C:266:ASP:OD1	2.47	0.47
1:C:386:ASN:HA	1:C:389:LEU:HB2	1.96	0.47
2:D:516:TYR:O	2:D:519:THR:OG1	2.26	0.47
1:A:85:LEU:O	1:A:89:GLU:N	2.44	0.47
1:A:213:ILE:HA	1:A:459:THR:HG21	1.95	0.47
2:B:116:LEU:HD13	2:B:186:LEU:HD22	1.96	0.47
2:B:205:GLY:HA2	2:B:219:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:THR:HA	1:A:124:MET:HE2	1.96	0.47
2:B:557:MET:HE2	2:B:573:VAL:HG21	1.97	0.47
1:C:170:SER:OG	1:C:173:ASP:OD2	2.23	0.47
2:B:736:GLN:HG3	2:B:737:PRO:HD3	1.97	0.47
2:B:622:ILE:CG1	2:B:679:ILE:CG2	2.90	0.46
2:B:91:LEU:C	2:B:93:VAL:N	2.73	0.46
2:B:393:ARG:O	2:B:394:ASN:O	2.33	0.46
2:B:635:TRP:NE1	2:B:640:MET:SD	2.71	0.46
2:D:582:ARG:O	2:D:586:ASN:N	2.46	0.46
2:D:630:ASP:C	2:D:632:ALA:N	2.73	0.46
2:B:630:ASP:C	2:B:632:ALA:N	2.73	0.46
2:D:41:TYR:O	2:D:45:LEU:N	2.36	0.46
2:D:113:SER:HB3	2:D:190:MET:HE2	1.97	0.46
1:C:35:TRP:HE3	1:C:40:GLN:HE21	1.64	0.46
2:D:116:LEU:HD13	2:D:186:LEU:HD22	1.96	0.46
2:D:287:GLN:H	2:D:434:THR:HG23	1.80	0.46
2:D:346:PRO:HA	2:D:360:MET:SD	2.55	0.46
2:B:199:TYR:OH	2:B:509:ASP:OD1	2.34	0.46
1:C:6:LEU:HD12	1:C:508:VAL:HG22	1.98	0.46
1:A:6:LEU:HD12	1:A:508:VAL:HG22	1.98	0.46
2:D:207:TYR:HA	2:D:566:TRP:HH2	1.80	0.46
2:B:230:PHE:O	2:B:234:LYS:N	2.49	0.46
2:D:284:PRO:O	2:D:285:PHE:CG	2.69	0.46
1:A:232:VAL:HG23	1:A:233:VAL:N	2.30	0.46
1:A:505:VAL:HA	1:A:509:TYR:HB3	1.98	0.46
2:B:287:GLN:H	2:B:434:THR:HG23	1.80	0.46
2:B:434:THR:O	2:B:438:PHE:N	2.49	0.46
1:C:338:SER:HA	1:C:341:ILE:HB	1.98	0.46
2:D:95:LEU:HD12	2:D:564:GLU:CA	2.32	0.46
2:D:652:ARG:NH2	2:D:665:PHE:O	2.43	0.46
2:B:136:ASP:OD1	2:B:136:ASP:N	2.46	0.46
2:B:630:ASP:C	2:B:632:ALA:H	2.23	0.46
2:D:450:LEU:O	2:D:516:TYR:OH	2.31	0.46
1:A:22:GLU:O	1:A:26:GLN:NE2	2.49	0.46
1:A:223:VAL:O	1:A:227:SER:OG	2.31	0.46
2:B:309:LYS:HD2	2:B:309:LYS:HA	1.75	0.46
2:D:199:TYR:OH	2:D:509:ASP:OD1	2.34	0.46
1:A:178:ARG:NH1	1:A:182:ASN:OD1	2.36	0.45
2:B:63:ASN:O	2:B:67:ASP:N	2.50	0.45
2:B:77:SER:O	2:B:81:GLN:N	2.49	0.45
2:B:133:CYS:HA	2:B:141:CYS:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ILE:H	1:C:309:ILE:HG12	1.37	0.45
2:D:77:SER:O	2:D:81:GLN:N	2.50	0.45
2:D:99:ALA:O	2:D:102:GLN:CD	2.59	0.45
2:D:333:LEU:C	2:D:362:THR:HG21	2.37	0.45
1:A:234:LEU:HD11	1:A:320:VAL:HG11	1.97	0.45
2:B:676:LYS:HZ3	2:B:677:PRO:HD2	1.77	0.45
2:D:183:TYR:OH	2:D:509:ASP:OD2	2.31	0.45
2:B:50:TYR:CD1	2:B:59:VAL:HB	2.50	0.45
2:B:269:ASP:OD1	2:B:269:ASP:N	2.44	0.45
2:D:230:PHE:O	2:D:234:LYS:N	2.49	0.45
2:D:434:THR:O	2:D:438:PHE:N	2.49	0.45
1:A:35:TRP:HE3	1:A:40:GLN:HE21	1.64	0.45
2:B:113:SER:HB3	2:B:190:MET:HE2	1.97	0.45
2:B:284:PRO:C	2:B:285:PHE:CG	2.95	0.45
2:D:557:MET:HE2	2:D:573:VAL:HG21	1.97	0.45
2:D:736:GLN:HG3	2:D:737:PRO:HD3	1.97	0.45
1:A:77:LEU:HB3	1:A:275:VAL:HG21	1.99	0.45
1:C:175:PHE:O	1:C:179:GLU:N	2.49	0.45
2:B:418:LEU:HD22	2:B:423:LEU:HD22	1.99	0.45
2:B:676:LYS:C	2:B:678:ARG:N	2.73	0.45
1:A:145:GLN:NE2	2:B:741:ILE:CG2	2.80	0.45
2:B:56:GLU:C	2:B:58:ASN:N	2.74	0.45
2:B:91:LEU:HG	2:B:564:GLU:CG	2.47	0.45
1:C:346:ASN:HA	2:D:621:ARG:HH21	1.80	0.45
1:C:505:VAL:HA	1:C:509:TYR:HB3	1.98	0.45
2:D:91:LEU:HD21	2:D:212:VAL:HG22	1.98	0.45
2:D:397:ASN:HD21	2:D:521:TYR:HE2	1.64	0.45
2:D:418:LEU:HD22	2:D:423:LEU:HD22	1.99	0.45
1:A:373:ALA:O	1:A:377:GLN:NE2	2.49	0.45
2:B:94:LYS:HD3	2:B:94:LYS:C	2.42	0.45
2:B:319:GLY:HA3	2:B:548:THR:HG23	1.99	0.45
1:C:85:LEU:O	1:C:89:GLU:N	2.44	0.45
2:D:133:CYS:HA	2:D:141:CYS:HA	1.98	0.45
2:D:284:PRO:C	2:D:285:PHE:CG	2.95	0.45
2:B:284:PRO:O	2:B:285:PHE:CG	2.69	0.45
2:D:202:TYR:CD1	2:D:202:TYR:C	2.94	0.45
1:A:165:GLU:HG3	1:A:174:TYR:CE1	2.52	0.44
1:A:184:SER:O	1:A:480:TYR:OH	2.31	0.44
2:B:324:THR:HA	2:B:328:TRP:HE1	1.82	0.44
2:B:399:GLY:CA	2:B:518:ARG:HB2	2.47	0.44
2:B:678:ARG:HD3	2:B:678:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:HA	1:A:341:ILE:HB	1.98	0.44
2:D:319:GLY:HA3	2:D:548:THR:HG23	1.99	0.44
2:D:753:ILE:HD12	2:D:753:ILE:HA	1.87	0.44
2:B:95:LEU:CG	2:B:564:GLU:H	2.30	0.44
2:B:530:CYS:HB2	2:B:542:CYS:HB3	1.87	0.44
2:D:98:GLN:NE2	2:D:208:GLU:O	2.50	0.44
2:D:635:TRP:NE1	2:D:640:MET:SD	2.71	0.44
2:D:642:LEU:O	2:D:645:SER:OG	2.34	0.44
2:B:98:GLN:NE2	2:B:208:GLU:O	2.50	0.44
2:B:212:VAL:CB	2:B:215:TYR:HD2	2.30	0.44
2:B:454:TYR:N	2:B:516:TYR:OH	2.51	0.44
2:D:63:ASN:O	2:D:67:ASP:N	2.50	0.44
2:D:262:LEU:HB2	2:D:487:VAL:HG23	1.98	0.44
1:A:145:GLN:CG	2:B:741:ILE:HG21	2.47	0.44
2:D:630:ASP:C	2:D:632:ALA:H	2.24	0.44
2:B:58:ASN:O	2:B:61:ASN:N	2.50	0.44
2:B:119:ILE:O	2:B:122:THR:OG1	2.34	0.44
2:B:406:GLU:HA	2:B:409:SER:HB2	2.00	0.44
1:C:77:LEU:HB3	1:C:275:VAL:HG21	1.99	0.44
2:D:544:ILE:HA	2:D:547:SER:HB3	2.00	0.44
2:B:212:VAL:HG23	2:B:565:PRO:HD2	1.99	0.44
2:B:544:ILE:HA	2:B:547:SER:HB3	2.00	0.44
2:D:334:THR:HG23	2:D:334:THR:O	2.16	0.44
1:A:175:PHE:CA	1:A:179:GLU:HB2	2.47	0.44
2:B:351:LEU:HD21	2:B:357:ARG:HB2	2.00	0.44
2:B:395:GLY:O	2:B:562:LYS:CE	2.65	0.44
1:C:239:ILE:H	1:C:239:ILE:HG12	1.31	0.44
2:B:753:ILE:HD12	2:B:753:ILE:HA	1.87	0.44
1:C:373:ALA:O	1:C:377:GLN:NE2	2.49	0.44
2:D:324:THR:HA	2:D:328:TRP:HE1	1.82	0.44
1:A:81:GLU:HG3	1:A:541:LEU:HD12	2.00	0.43
1:A:309:ILE:H	1:A:309:ILE:HG12	1.37	0.43
2:D:389:PRO:HD2	2:D:392:LEU:HD12	2.00	0.43
2:D:397:ASN:H	2:D:400:PHE:HB3	1.83	0.43
2:B:521:TYR:OH	2:B:566:TRP:NE1	2.52	0.43
2:B:568:LEU:O	2:B:571:GLU:HG3	2.19	0.43
2:D:349:TRP:HB2	2:D:357:ARG:H	1.83	0.43
2:D:564:GLU:CB	2:D:565:PRO:CD	2.97	0.43
2:B:642:LEU:O	2:B:645:SER:OG	2.34	0.43
2:D:59:VAL:CG1	2:D:60:GLN:HG2	2.46	0.43
2:B:48:TRP:HZ3	2:B:359:LEU:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:LEU:HB2	2:B:487:VAL:HG23	1.98	0.43
2:B:563:SER:O	2:B:564:GLU:HB2	2.19	0.43
2:B:637:ASP:OD1	2:B:637:ASP:N	2.51	0.43
2:B:652:ARG:NH2	2:B:665:PHE:O	2.43	0.43
1:A:229:LEU:HA	1:A:232:VAL:HG22	1.99	0.43
2:B:349:TRP:HB2	2:B:357:ARG:H	1.83	0.43
1:A:5:VAL:N	1:A:507:TYR:O	2.52	0.43
2:D:92:THR:HG22	2:D:93:VAL:HG13	2.00	0.43
2:D:637:ASP:OD1	2:D:637:ASP:N	2.51	0.43
2:B:215:TYR:CE1	2:B:567:THR:C	2.96	0.43
2:D:306:ARG:NH1	2:D:310:GLU:OE1	2.51	0.43
1:A:163:VAL:HG21	1:A:174:TYR:CE2	2.54	0.43
2:D:91:LEU:O	2:D:563:SER:O	2.36	0.43
1:A:145:GLN:HG2	2:B:741:ILE:HD13	2.01	0.43
2:B:218:SER:HB3	2:B:221:GLN:CG	2.49	0.43
1:C:279:PHE:HE1	1:C:310:ASN:HB2	1.84	0.43
2:D:351:LEU:HD21	2:D:357:ARG:HB2	2.00	0.43
1:A:541:LEU:HA	1:A:544:ILE:HD12	2.01	0.43
1:A:210:MET:HE3	2:B:756:GLY:HA3	2.00	0.42
2:B:389:PRO:HD2	2:B:392:LEU:HD12	2.00	0.42
1:C:56:TRP:HD1	1:C:57:ARG:HG3	1.84	0.42
1:C:81:GLU:HG3	1:C:541:LEU:HD12	2.00	0.42
2:D:406:GLU:HA	2:D:409:SER:HB2	2.00	0.42
1:A:34:LYS:HA	1:A:292:TYR:HB3	2.02	0.42
1:A:239:ILE:H	1:A:239:ILE:HG12	1.31	0.42
2:B:188:ASN:HB3	2:B:192:ARG:HH11	1.85	0.42
2:B:363:LYS:C	2:B:364:VAL:HG12	2.44	0.42
1:C:541:LEU:HA	1:C:544:ILE:HD12	2.01	0.42
2:D:269:ASP:OD1	2:D:269:ASP:N	2.44	0.42
1:A:279:PHE:HE1	1:A:310:ASN:HB2	1.84	0.42
2:B:60:GLN:C	2:B:62:MET:N	2.78	0.42
1:C:5:VAL:N	1:C:507:TYR:O	2.52	0.42
2:D:250:ASN:OD1	2:D:250:ASN:N	2.53	0.42
2:D:309:LYS:HD2	2:D:309:LYS:HA	1.75	0.42
1:A:56:TRP:HD1	1:A:57:ARG:HG3	1.84	0.42
1:A:266:ASP:OD1	1:A:266:ASP:N	2.47	0.42
2:B:287:GLN:H	2:B:434:THR:CG2	2.33	0.42
2:B:306:ARG:NH1	2:B:310:GLU:OE1	2.51	0.42
1:A:189:ASP:OD1	1:A:189:ASP:N	2.50	0.42
2:B:568:LEU:HA	2:B:571:GLU:HG2	2.00	0.42
1:C:335:ASP:O	1:C:339:THR:OG1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:LEU:HG	2:D:564:GLU:HB2	2.01	0.42
2:D:378:HIS:HA	2:D:381:TYR:HD2	1.84	0.42
1:A:128:TYR:O	1:A:131:THR:OG1	2.31	0.42
1:A:496:ILE:H	1:A:496:ILE:HG12	1.33	0.42
1:C:8:ASN:HB3	1:C:11:LEU:HB2	2.02	0.42
1:C:192:SER:OG	1:C:194:GLN:OE1	2.38	0.42
1:C:342:LEU:HG	2:D:678:ARG:HH12	1.85	0.42
1:C:604:LYS:HD2	1:C:604:LYS:HA	1.88	0.42
1:A:192:SER:OG	1:A:194:GLN:OE1	2.38	0.42
2:B:97:LEU:HA	2:B:100:LEU:HB2	2.02	0.42
2:B:142:LEU:HB3	2:B:147:GLY:HA3	2.00	0.42
2:B:198:ASP:O	2:B:201:ASP:HB2	2.20	0.42
2:B:616:GLN:NE2	2:B:697:ARG:H	2.18	0.42
2:B:676:LYS:HA	2:B:676:LYS:HD2	1.60	0.42
1:C:502:MET:HE2	1:C:538:SER:HB2	2.02	0.42
2:D:188:ASN:HB3	2:D:192:ARG:HH11	1.85	0.42
2:D:524:GLN:OE1	2:D:580:ASN:N	2.53	0.42
2:D:676:LYS:HZ3	2:D:677:PRO:CG	2.21	0.42
1:A:207:VAL:HG21	1:A:425:PHE:HZ	1.85	0.42
2:B:215:TYR:HE2	2:B:568:LEU:HD12	1.84	0.42
1:C:326:GLY:O	1:C:330:THR:OG1	2.28	0.42
1:A:8:ASN:HB3	1:A:11:LEU:HB2	2.01	0.42
1:A:212:THR:O	1:A:212:THR:OG1	2.16	0.42
2:B:275:TRP:HB3	2:B:278:LEU:HD12	2.02	0.42
2:D:198:ASP:O	2:D:201:ASP:HB2	2.19	0.42
2:D:335:ASP:HB3	2:D:361:CYS:O	2.19	0.42
2:B:363:LYS:O	2:B:364:VAL:HG12	2.20	0.42
2:B:435:GLU:HA	2:B:438:PHE:HB3	2.02	0.42
1:C:189:ASP:OD1	1:C:189:ASP:N	2.50	0.42
2:D:142:LEU:HB3	2:D:147:GLY:HA3	2.00	0.42
2:D:343:VAL:HG22	2:D:344:CYS:N	2.35	0.42
2:D:435:GLU:HA	2:D:438:PHE:HB3	2.02	0.42
2:D:530:CYS:HB2	2:D:542:CYS:HB3	1.87	0.42
2:D:676:LYS:CG	2:D:677:PRO:CD	2.91	0.42
1:A:552:VAL:HB	1:A:556:GLN:HE22	1.85	0.41
1:C:34:LYS:HA	1:C:292:TYR:HB3	2.02	0.41
2:D:54:ILE:HG12	2:D:342:ALA:N	2.35	0.41
2:D:676:LYS:HD2	2:D:676:LYS:HA	1.63	0.41
2:B:57:GLU:CD	2:B:57:GLU:C	2.88	0.41
2:B:701:GLU:HA	2:B:727:ILE:HD11	2.02	0.41
2:D:287:GLN:H	2:D:434:THR:CG2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:HG3	1:A:439:VAL:HA	2.02	0.41
1:A:502:MET:HE2	1:A:538:SER:HB2	2.01	0.41
2:B:216:ASP:O	2:B:217:TYR:CD1	2.73	0.41
2:D:389:PRO:HB2	2:D:391:LEU:H	1.86	0.41
1:A:16:PRO:O	1:A:95:ARG:NH1	2.53	0.41
2:B:378:HIS:HA	2:B:381:TYR:HD2	1.84	0.41
1:C:135:TRP:HA	1:C:138:TRP:HB3	2.01	0.41
1:C:128:TYR:O	1:C:131:THR:OG1	2.31	0.41
1:C:207:VAL:HG21	1:C:425:PHE:HZ	1.85	0.41
1:A:135:TRP:HA	1:A:138:TRP:HB3	2.01	0.41
2:B:315:PHE:O	2:B:319:GLY:N	2.54	0.41
1:C:175:PHE:CE1	1:C:179:GLU:CB	2.76	0.41
2:B:48:TRP:CD2	2:B:357:ARG:HD3	2.56	0.41
2:B:95:LEU:HG	2:B:564:GLU:H	1.84	0.41
1:C:16:PRO:O	1:C:95:ARG:NH1	2.53	0.41
1:C:22:GLU:O	1:C:26:GLN:NE2	2.49	0.41
1:C:175:PHE:HA	1:C:179:GLU:CG	2.49	0.41
2:B:48:TRP:CZ2	2:B:331:SER:HA	2.56	0.41
1:C:175:PHE:HA	1:C:179:GLU:HB2	2.03	0.41
2:D:275:TRP:HB3	2:D:278:LEU:HD12	2.02	0.41
2:D:315:PHE:O	2:D:319:GLY:N	2.54	0.41
2:D:562:LYS:HD3	2:D:562:LYS:HA	1.66	0.41
2:D:656:LEU:HD21	2:D:662:MET:HB2	2.03	0.41
1:A:146:GLU:HB3	1:A:147:PRO:CD	2.51	0.41
2:B:208:GLU:HG2	2:B:219:ARG:HG3	2.03	0.41
2:B:247:LYS:HA	2:B:247:LYS:HD3	1.90	0.41
2:B:284:PRO:HB2	2:B:285:PHE:CD2	2.56	0.41
2:B:524:GLN:OE1	2:B:580:ASN:N	2.53	0.41
2:B:641:TYR:OH	2:D:665:PHE:N	2.46	0.41
1:C:339:THR:O	1:C:343:THR:OG1	2.31	0.41
1:C:349:ASP:HB3	2:D:676:LYS:HG2	2.02	0.41
2:D:48:TRP:CD2	2:D:357:ARG:HD3	2.56	0.41
2:D:460:ARG:NH2	2:D:510:TYR:O	2.47	0.41
2:D:616:GLN:NE2	2:D:697:ARG:H	2.18	0.41
2:D:701:GLU:HA	2:D:727:ILE:HD11	2.02	0.41
2:B:215:TYR:CE2	2:B:568:LEU:CB	3.03	0.41
2:D:123:MET:HE3	2:D:180:TYR:HE1	1.86	0.41
2:D:284:PRO:HB2	2:D:285:PHE:CD2	2.56	0.41
2:D:132:VAL:HG22	2:D:171:GLU:HG3	2.04	0.40
1:A:320:VAL:O	1:A:323:SER:OG	2.39	0.40
1:A:335:ASP:O	1:A:339:THR:OG1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:TYR:CB	2:B:566:TRP:HH2	2.35	0.40
2:B:215:TYR:OH	2:B:571:GLU:CB	2.69	0.40
2:B:460:ARG:NH2	2:B:510:TYR:O	2.47	0.40
1:C:303:SER:O	1:C:307:SER:OG	2.27	0.40
2:D:97:LEU:HA	2:D:100:LEU:HB2	2.02	0.40
2:D:377:GLY:HA3	2:D:408:MET:HE1	2.03	0.40
2:D:521:TYR:OH	2:D:566:TRP:NE1	2.54	0.40
1:C:502:MET:N	1:C:502:MET:SD	2.95	0.40
2:D:347:THR:HG23	2:D:359:LEU:CB	2.41	0.40
2:D:348:ALA:HB1	2:D:379:ILE:HD11	2.02	0.40
2:D:707:SER:O	2:D:707:SER:OG	2.35	0.40
2:B:638:ASN:O	2:B:642:LEU:HG	2.22	0.40
1:C:552:VAL:HB	1:C:556:GLN:HE22	1.85	0.40
2:D:298:VAL:HG22	2:D:365:THR:O	2.20	0.40
2:D:368:ASP:OD1	2:D:369:PHE:N	2.55	0.40
2:B:114:LYS:HA	2:B:114:LYS:HD3	1.89	0.40
2:B:389:PRO:HB2	2:B:391:LEU:H	1.86	0.40
2:B:421:ILE:HD12	2:B:421:ILE:HA	2.01	0.40
1:C:81:GLU:C	1:C:84:PRO:HD2	2.47	0.40
1:C:100:SER:HB3	1:C:287:ILE:HD12	2.03	0.40
1:C:342:LEU:HG	2:D:678:ARG:NH1	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	603/654 (92%)	546 (90%)	55 (9%)	2 (0%)	36	71
1	C	603/654 (92%)	547 (91%)	54 (9%)	2 (0%)	36	71
2	B	746/814 (92%)	664 (89%)	76 (10%)	6 (1%)	16	53
2	D	746/814 (92%)	667 (89%)	66 (9%)	13 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2698/2936 (92%)	2424 (90%)	251 (9%)	23 (1%)	16	49

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	103	ASN
2	B	394	ASN
2	D	103	ASN
2	D	344	CYS
2	D	345	HIS
2	D	364	VAL
2	D	366	MET
2	B	216	ASP
2	D	343	VAL
2	D	363	LYS
2	D	396	ALA
1	A	359	ASN
2	B	397	ASN
1	C	146	GLU
1	C	359	ASN
2	D	678	ARG
2	B	217	TYR
2	B	288	LYS
2	D	288	LYS
2	D	565	PRO
2	D	59	VAL
1	A	145	GLN
2	D	564	GLU

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	417/572 (73%)	389 (93%)	28 (7%)	15	37
1	C	531/572 (93%)	490 (92%)	41 (8%)	12	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	645/720 (90%)	570 (88%)	75 (12%)	5	19
2	D	662/720 (92%)	590 (89%)	72 (11%)	6	21
All	All	2255/2584 (87%)	2039 (90%)	216 (10%)	10	25

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	SER
1	A	188	SER
1	A	206	SER
1	A	207	VAL
1	A	211	CYS
1	A	212	THR
1	A	228	THR
1	A	236	ILE
1	A	239	ILE
1	A	242	LEU
1	A	298	ASN
1	A	303	SER
1	A	309	ILE
1	A	355	VAL
1	A	356	THR
1	A	365	GLN
1	A	415	LEU
1	A	424	LEU
1	A	429	LEU
1	A	436	MET
1	A	462	ILE
1	A	468	LEU
1	A	469	ILE
1	A	494	LEU
1	A	496	ILE
1	A	538	SER
1	A	545	ILE
1	A	595	LEU
2	B	30	ASP
2	B	31	LYS
2	B	35	GLU
2	B	37	GLU
2	B	43	SER
2	B	44	SER

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Mol	Chain	Res	Type
2	B	52	THR
2	B	58	ASN
2	B	62	MET
2	B	70	SER
2	B	79	LEU
2	B	91	LEU
2	B	97	LEU
2	B	105	SER
2	B	106	SER
2	B	109	SER
2	B	112	LYS
2	B	113	SER
2	B	170	SER
2	B	201	ASP
2	B	203	TRP
2	B	209	VAL
2	B	210	ASN
2	B	212	VAL
2	B	213	ASP
2	B	248	LEU
2	B	259	ILE
2	B	288	LYS
2	B	292	ASP
2	B	299	ASP
2	B	324	THR
2	B	331	SER
2	B	347	THR
2	B	353	LYS
2	B	362	THR
2	B	363	LYS
2	B	398	GLU
2	B	414	THR
2	B	423	LEU
2	B	425	SER
2	B	433	GLU
2	B	434	THR
2	B	436	ILE
2	B	446	ILE
2	B	471	ASP
2	B	488	VAL
2	B	503	LEU
2	B	506	VAL

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Mol	Chain	Res	Type
2	B	522	GLN
2	B	545	SER
2	B	563	SER
2	B	571	GLU
2	B	579	MET
2	B	585	LEU
2	B	593	THR
2	B	601	ASN
2	B	602	SER
2	B	604	VAL
2	B	623	SER
2	B	624	LEU
2	B	634	GLU
2	B	640	MET
2	B	651	MET
2	B	672	VAL
2	B	676	LYS
2	B	678	ARG
2	B	679	ILE
2	B	689	LYS
2	B	707	SER
2	B	722	LEU
2	B	745	VAL
2	B	752	VAL
2	B	753	ILE
2	B	754	VAL
2	B	755	VAL
1	C	62	CYS
1	C	71	MET
1	C	77	LEU
1	C	83	ILE
1	C	86	LEU
1	C	92	ILE
1	C	100	SER
1	C	105	SER
1	C	114	LEU
1	C	118	SER
1	C	137	MET
1	C	169	SER
1	C	172	VAL
1	C	188	SER
1	C	206	SER

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Mol	Chain	Res	Type
1	C	207	VAL
1	C	211	CYS
1	C	212	THR
1	C	228	THR
1	C	234	LEU
1	C	236	ILE
1	C	239	ILE
1	C	242	LEU
1	C	298	ASN
1	C	303	SER
1	C	309	ILE
1	C	355	VAL
1	C	356	THR
1	C	365	GLN
1	C	415	LEU
1	C	424	LEU
1	C	429	LEU
1	C	436	MET
1	C	462	ILE
1	C	468	LEU
1	C	469	ILE
1	C	494	LEU
1	C	496	ILE
1	C	538	SER
1	C	545	ILE
1	C	595	LEU
2	D	30	ASP
2	D	31	LYS
2	D	35	GLU
2	D	37	GLU
2	D	43	SER
2	D	44	SER
2	D	58	ASN
2	D	62	MET
2	D	70	SER
2	D	79	LEU
2	D	91	LEU
2	D	92	THR
2	D	97	LEU
2	D	105	SER
2	D	106	SER
2	D	109	SER

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Mol	Chain	Res	Type
2	D	112	LYS
2	D	113	SER
2	D	170	SER
2	D	201	ASP
2	D	209	VAL
2	D	210	ASN
2	D	212	VAL
2	D	213	ASP
2	D	218	SER
2	D	248	LEU
2	D	259	ILE
2	D	288	LYS
2	D	292	ASP
2	D	299	ASP
2	D	324	THR
2	D	331	SER
2	D	347	THR
2	D	353	LYS
2	D	363	LYS
2	D	398	GLU
2	D	414	THR
2	D	423	LEU
2	D	425	SER
2	D	433	GLU
2	D	434	THR
2	D	436	ILE
2	D	446	ILE
2	D	471	ASP
2	D	488	VAL
2	D	503	LEU
2	D	506	VAL
2	D	522	GLN
2	D	545	SER
2	D	562	LYS
2	D	579	MET
2	D	585	LEU
2	D	593	THR
2	D	601	ASN
2	D	602	SER
2	D	604	VAL
2	D	623	SER
2	D	624	LEU

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Mol	Chain	Res	Type
2	D	634	GLU
2	D	640	MET
2	D	651	MET
2	D	672	VAL
2	D	678	ARG
2	D	679	ILE
2	D	689	LYS
2	D	707	SER
2	D	722	LEU
2	D	745	VAL
2	D	752	VAL
2	D	753	ILE
2	D	754	VAL
2	D	755	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	249	ASN
1	A	274	GLN
1	A	297	ASN
1	A	298	ASN
1	A	354	ASN
1	A	357	GLN
1	A	365	GLN
1	A	377	GLN
1	A	444	GLN
1	A	479	GLN
1	A	574	GLN
2	B	33	ASN
2	B	51	ASN
2	B	60	GLN
2	B	86	GLN
2	B	89	GLN
2	B	121	ASN
2	B	210	ASN
2	B	300	GLN
2	B	305	GLN
2	B	322	ASN
2	B	556	ASN
2	B	616	GLN

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Mol	Chain	Res	Type
2	B	660	ASN
2	B	661	GLN
2	B	690	ASN
2	B	735	ASN
1	C	40	GLN
1	C	108	HIS
1	C	130	ASN
1	C	194	GLN
1	C	249	ASN
1	C	274	GLN
1	C	297	ASN
1	C	298	ASN
1	C	354	ASN
1	C	357	GLN
1	C	365	GLN
1	C	377	GLN
1	C	444	GLN
1	C	479	GLN
1	C	574	GLN
2	D	33	ASN
2	D	42	GLN
2	D	51	ASN
2	D	60	GLN
2	D	86	GLN
2	D	89	GLN
2	D	121	ASN
2	D	159	ASN
2	D	210	ASN
2	D	300	GLN
2	D	322	ASN
2	D	556	ASN
2	D	616	GLN
2	D	660	ASN
2	D	690	ASN
2	D	735	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

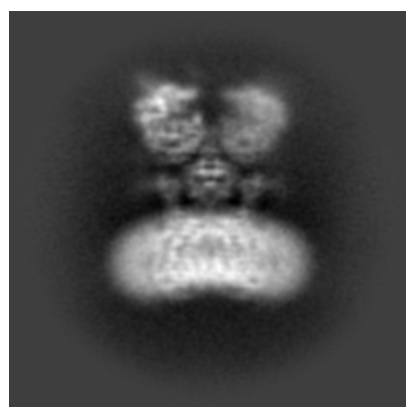
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30041. These allow visual inspection of the internal detail of the map and identification of artifacts.

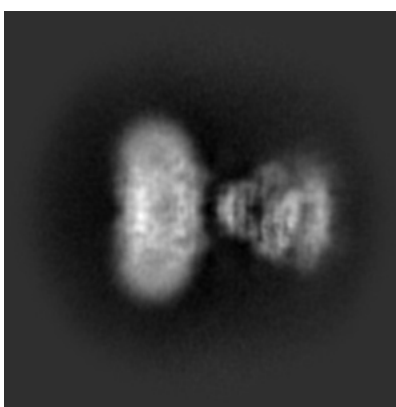
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

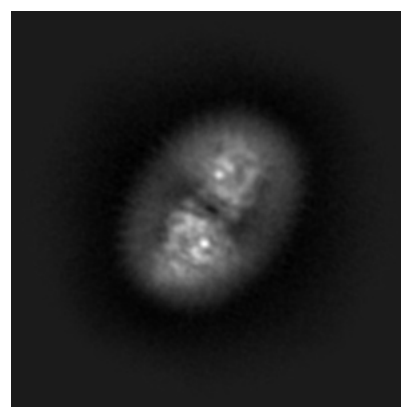
6.1.1 Primary map



X



Y

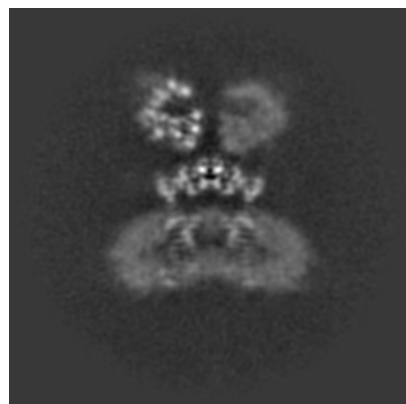


Z

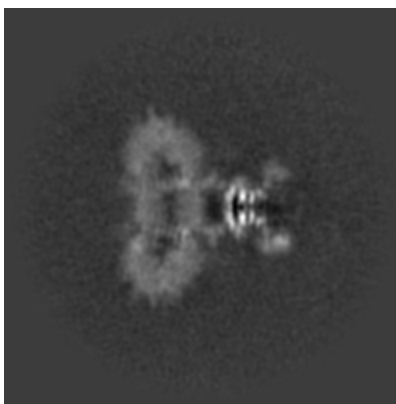
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

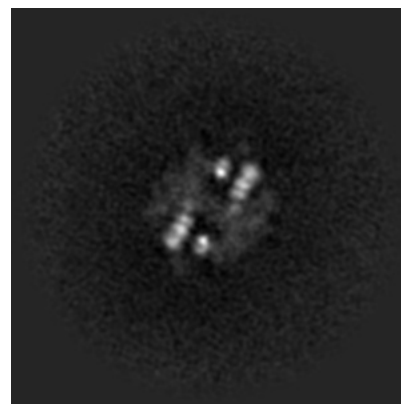
6.2.1 Primary map



X Index: 144



Y Index: 144

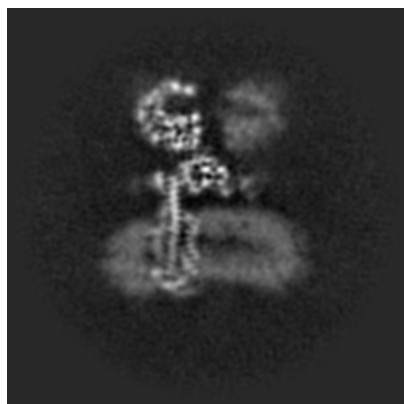


Z Index: 144

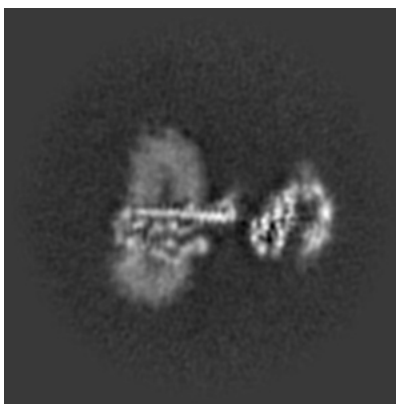
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

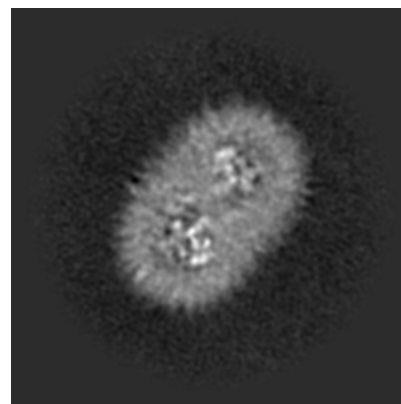
6.3.1 Primary map



X Index: 138



Y Index: 119

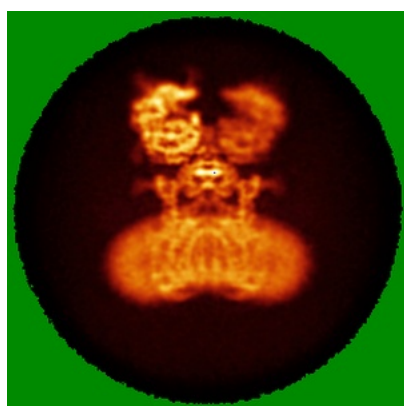


Z Index: 98

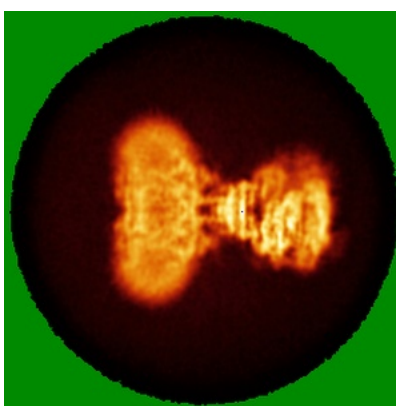
The images above show the largest variance slices of the map in three orthogonal directions.

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

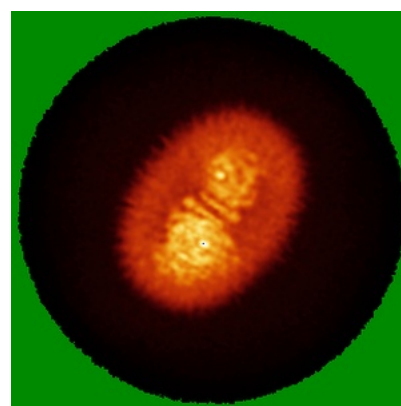
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

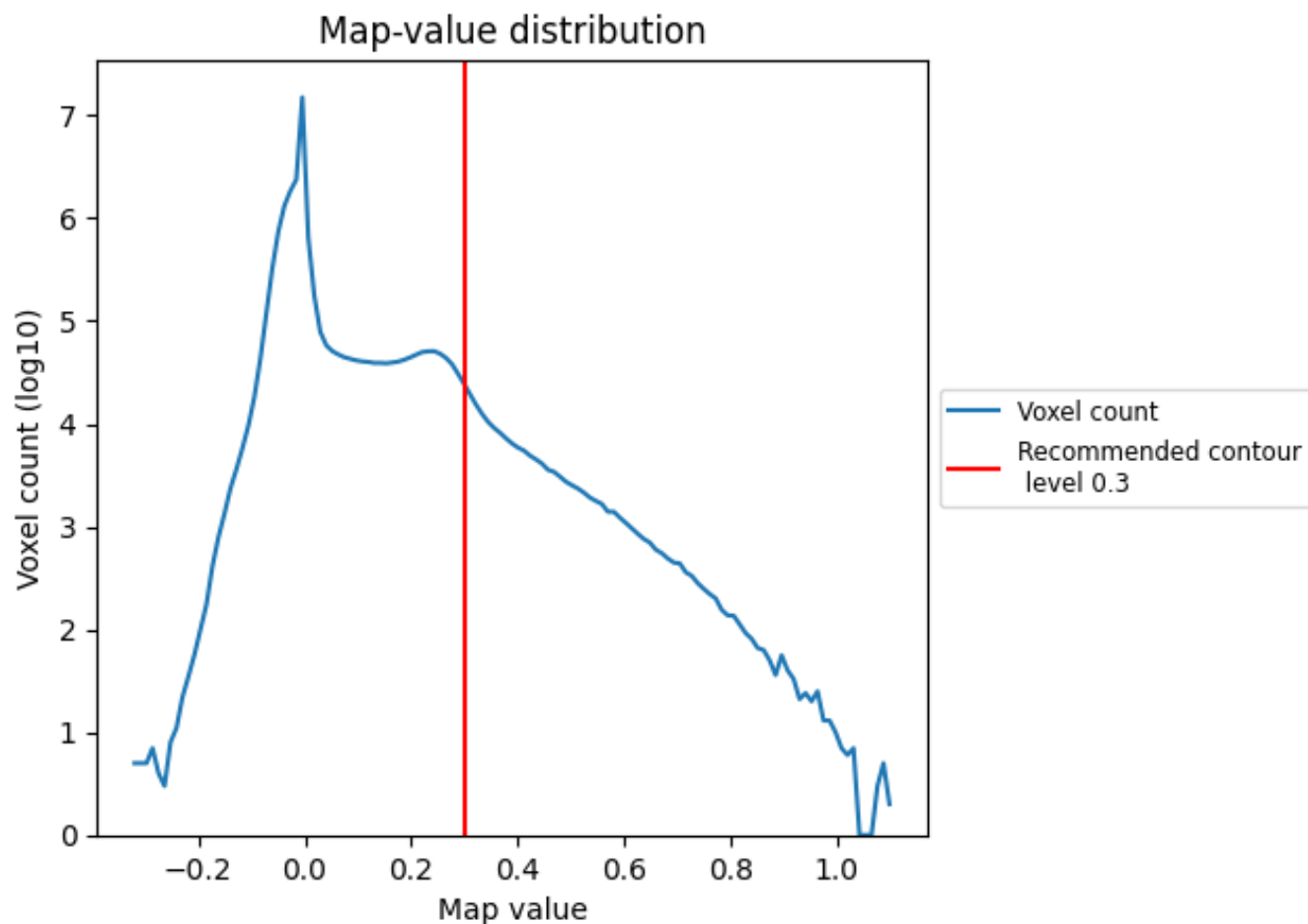
6.6 Mask visualisation

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

7 Map analysis [i](#)

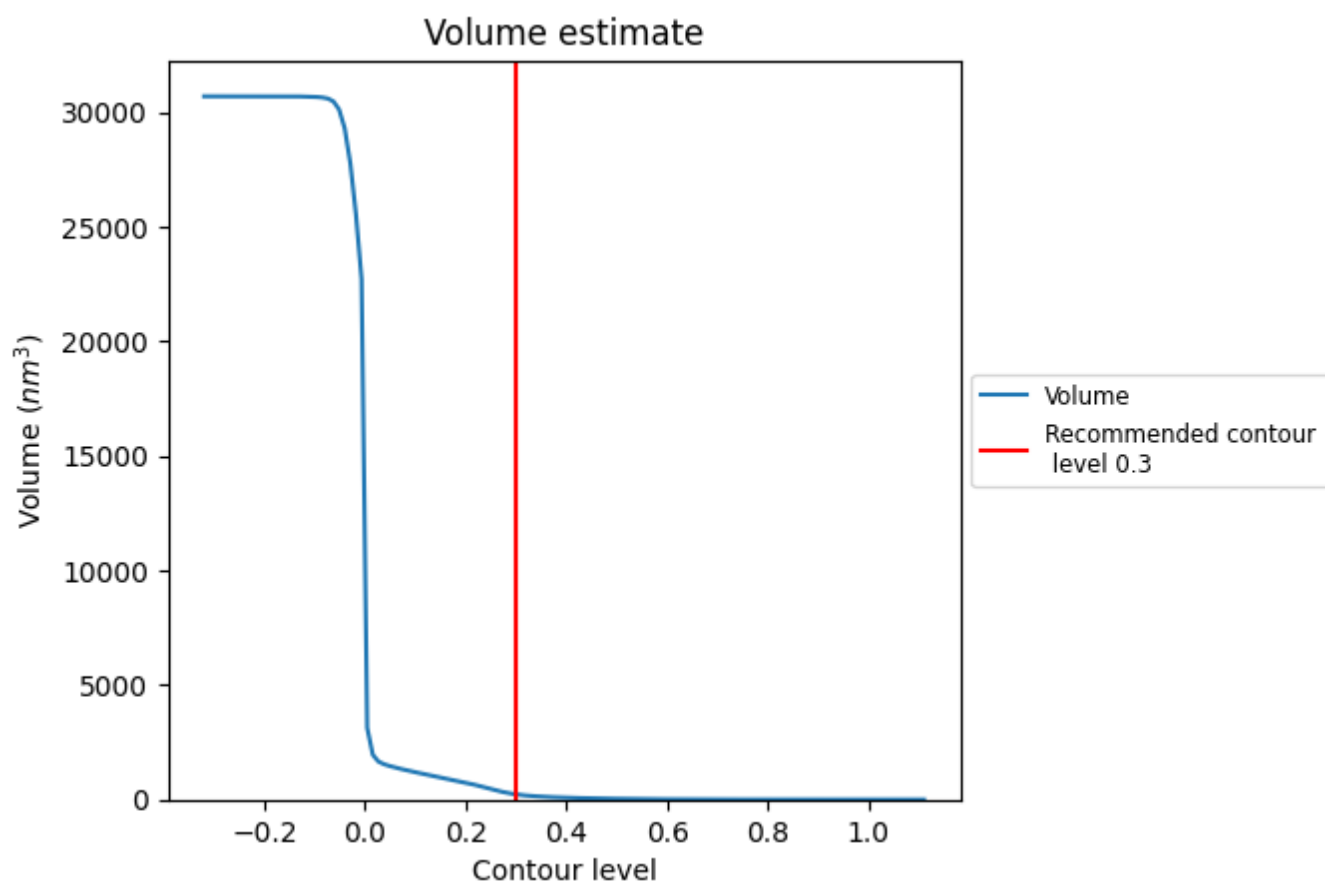
This section contains the results of statistical analysis of the map.

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.

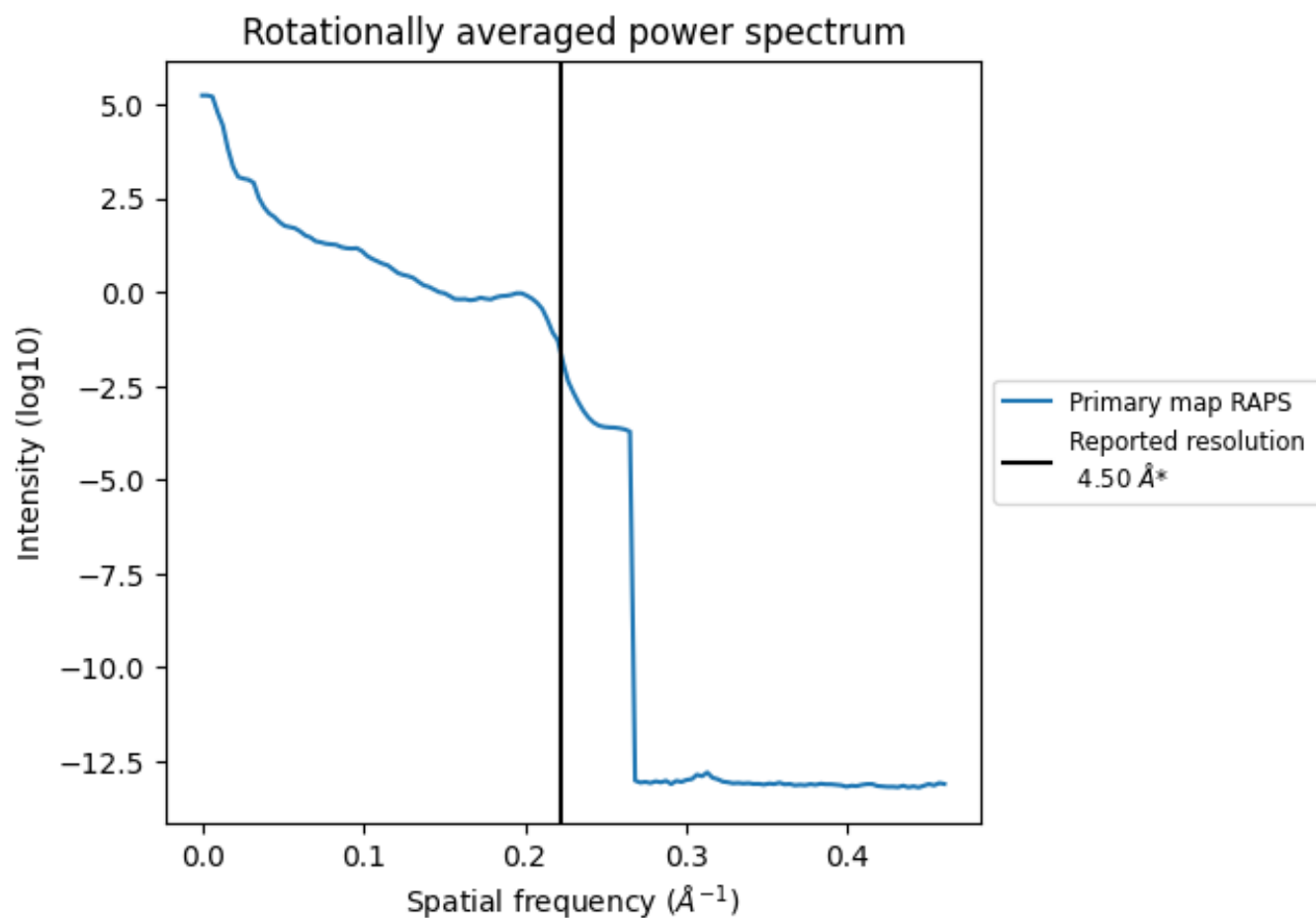
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm³; this corresponds to an approximate mass of 205 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 0.222 $\text{\AA}^{-1}$

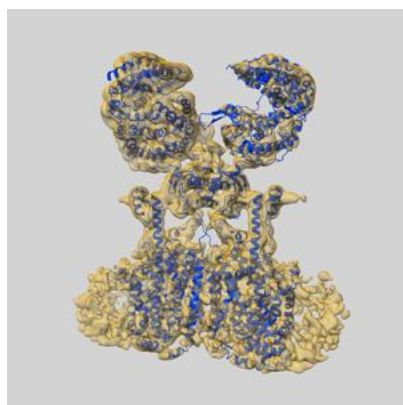
8 Fourier-Shell correlation ⓘ

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

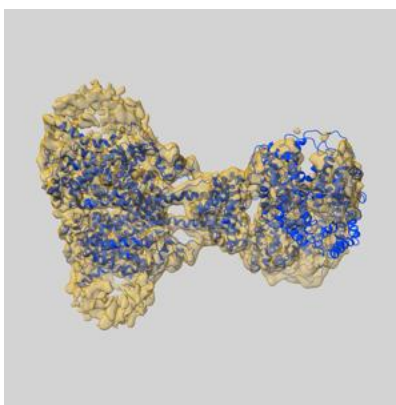
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30041 and PDB model 6M1D. Per-residue inclusion information can be found in section 3 on page 6.

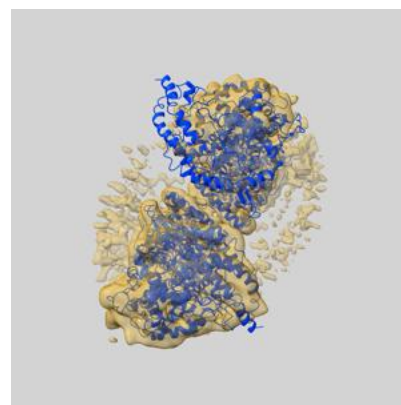
9.1 Map-model overlay [i](#)



X



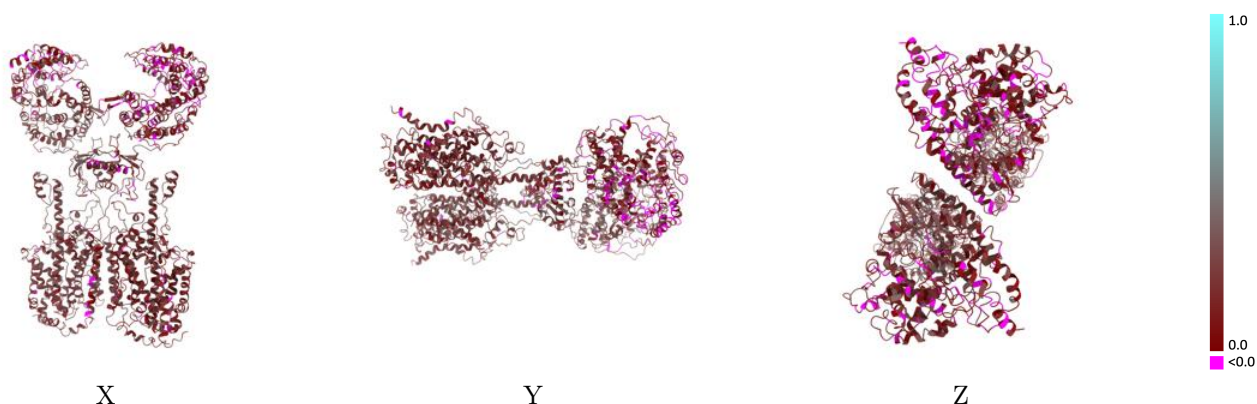
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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](#)

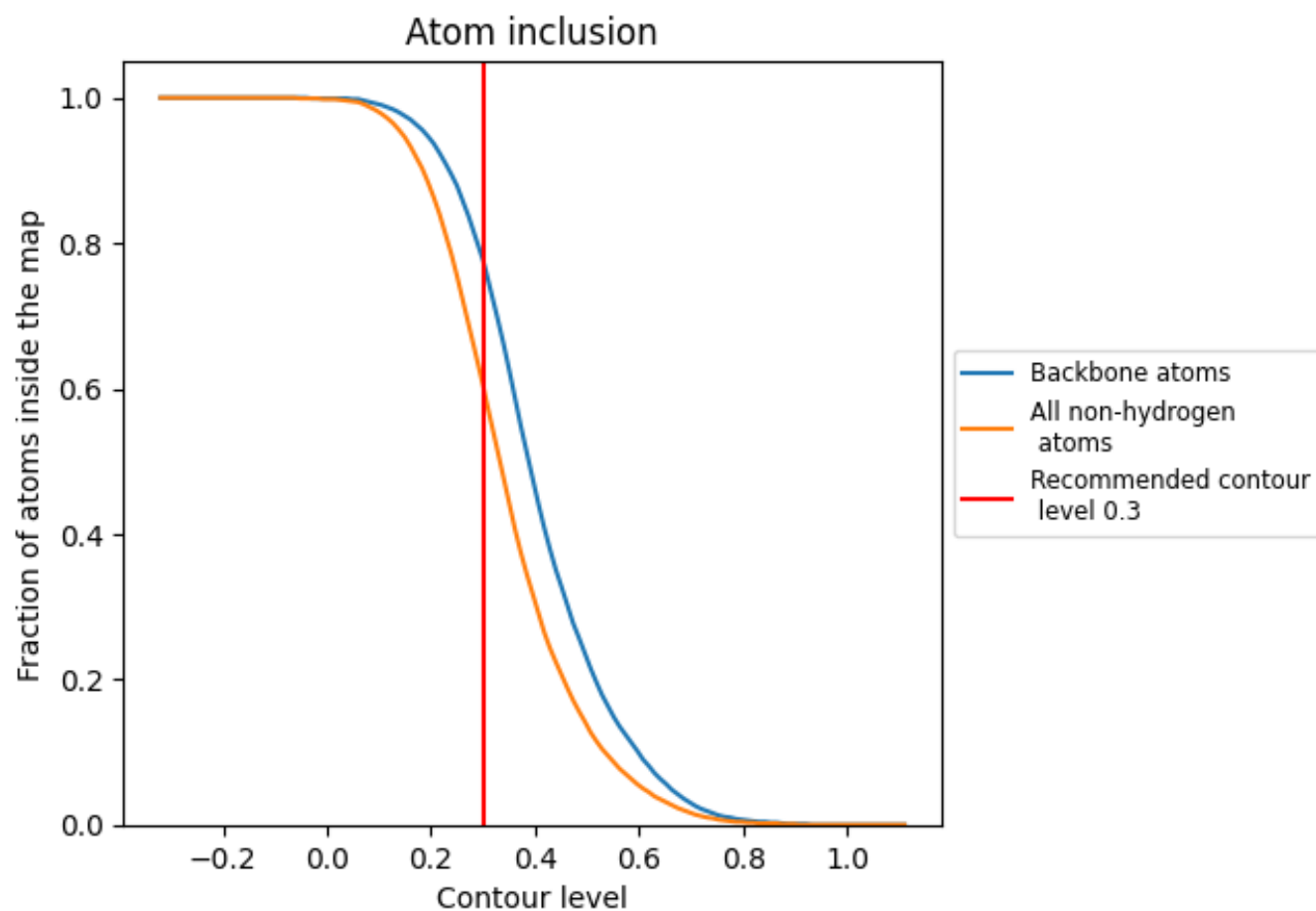


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 60% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6050	0.1830
A	0.6840	0.2170
B	0.7740	0.2030
C	0.6300	0.2050
D	0.3520	0.1180

