



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:00 AM UTC

PDB ID : 8STA / pdb_00008sta
EMDB ID : EMD-40758
Title : Isobutyryl-CoA mutase fused in the presence of GMPPCP
Authors : Vaccaro, F.A.; Drennan, C.L.
Deposited on : 2023-05-09
Resolution : 7.30 Å(reported)
Based on initial model : 4XC6

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

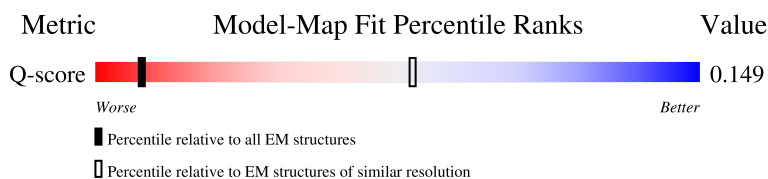
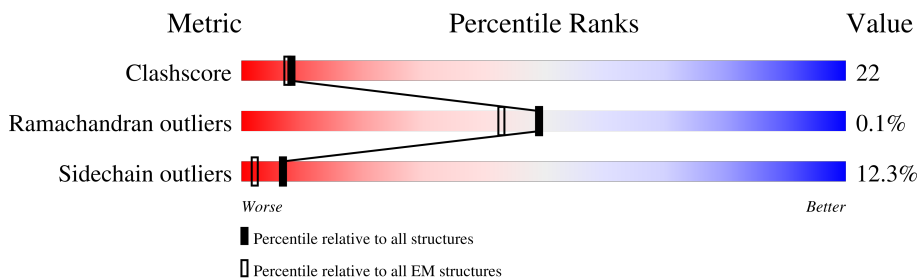
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.30 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	436 (6.80 - 7.80)

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	1113	
1	B	1113	
1	C	1113	
1	D	1113	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 32458 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 Isobutyryl-CoA mutase fused.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1061	Total	C	N	O	S	0	0
			8116	5061	1469	1549	37		
1	B	1061	Total	C	N	O	S	0	0
			8116	5061	1469	1549	37		
1	C	1061	Total	C	N	O	S	0	0
			8116	5061	1469	1549	37		
1	D	1061	Total	C	N	O	S	0	0
			8110	5059	1468	1546	37		

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression tag	UNP Q1LRY0
A	-12	HIS	-	expression tag	UNP Q1LRY0
A	-11	HIS	-	expression tag	UNP Q1LRY0
A	-10	HIS	-	expression tag	UNP Q1LRY0
A	-9	SER	-	expression tag	UNP Q1LRY0
A	-8	SER	-	expression tag	UNP Q1LRY0
A	-7	GLY	-	expression tag	UNP Q1LRY0
A	-6	LEU	-	expression tag	UNP Q1LRY0
A	-5	VAL	-	expression tag	UNP Q1LRY0
A	-4	PRO	-	expression tag	UNP Q1LRY0
A	-3	ARG	-	expression tag	UNP Q1LRY0
A	-2	GLY	-	expression tag	UNP Q1LRY0
A	-1	SER	-	expression tag	UNP Q1LRY0
A	0	HIS	-	expression tag	UNP Q1LRY0
B	-19	MET	-	initiating methionine	UNP Q1LRY0
B	-18	GLY	-	expression tag	UNP Q1LRY0

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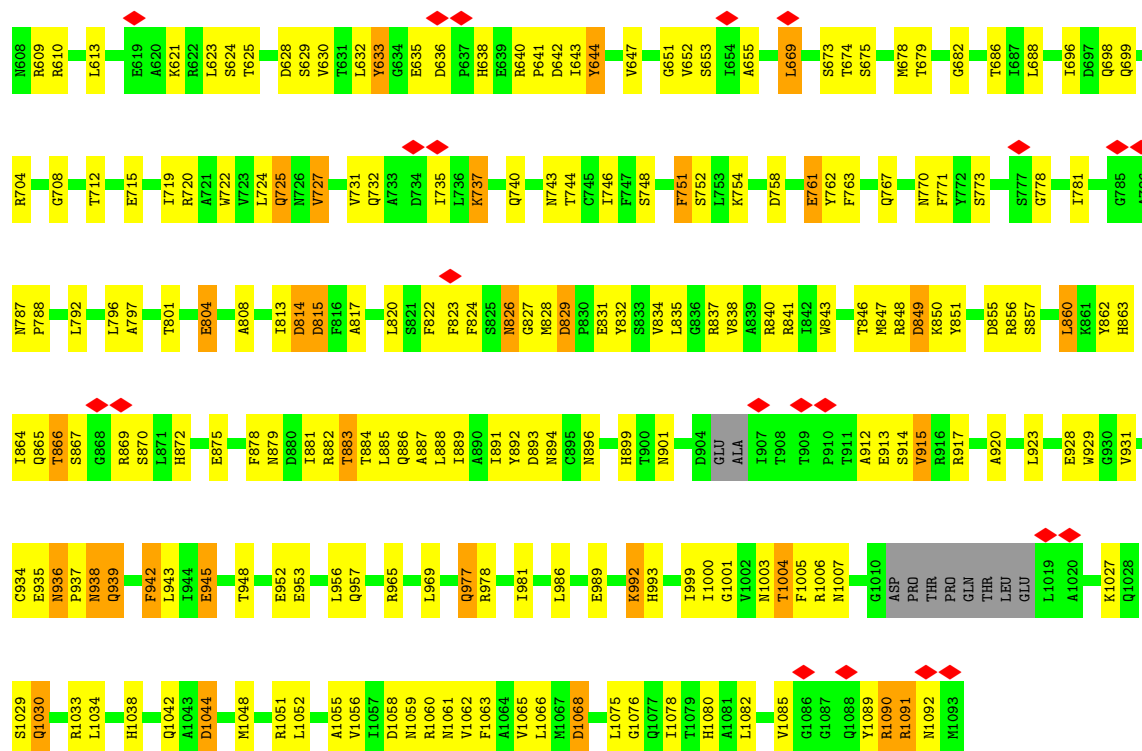
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP Q1LRY0
B	-16	SER	-	expression tag	UNP Q1LRY0
B	-15	HIS	-	expression tag	UNP Q1LRY0
B	-14	HIS	-	expression tag	UNP Q1LRY0
B	-13	HIS	-	expression tag	UNP Q1LRY0
B	-12	HIS	-	expression tag	UNP Q1LRY0
B	-11	HIS	-	expression tag	UNP Q1LRY0
B	-10	HIS	-	expression tag	UNP Q1LRY0
B	-9	SER	-	expression tag	UNP Q1LRY0
B	-8	SER	-	expression tag	UNP Q1LRY0
B	-7	GLY	-	expression tag	UNP Q1LRY0
B	-6	LEU	-	expression tag	UNP Q1LRY0
B	-5	VAL	-	expression tag	UNP Q1LRY0
B	-4	PRO	-	expression tag	UNP Q1LRY0
B	-3	ARG	-	expression tag	UNP Q1LRY0
B	-2	GLY	-	expression tag	UNP Q1LRY0
B	-1	SER	-	expression tag	UNP Q1LRY0
B	0	HIS	-	expression tag	UNP Q1LRY0
C	-19	MET	-	initiating methionine	UNP Q1LRY0
C	-18	GLY	-	expression tag	UNP Q1LRY0
C	-17	SER	-	expression tag	UNP Q1LRY0
C	-16	SER	-	expression tag	UNP Q1LRY0
C	-15	HIS	-	expression tag	UNP Q1LRY0
C	-14	HIS	-	expression tag	UNP Q1LRY0
C	-13	HIS	-	expression tag	UNP Q1LRY0
C	-12	HIS	-	expression tag	UNP Q1LRY0
C	-11	HIS	-	expression tag	UNP Q1LRY0
C	-10	HIS	-	expression tag	UNP Q1LRY0
C	-9	SER	-	expression tag	UNP Q1LRY0
C	-8	SER	-	expression tag	UNP Q1LRY0
C	-7	GLY	-	expression tag	UNP Q1LRY0
C	-6	LEU	-	expression tag	UNP Q1LRY0
C	-5	VAL	-	expression tag	UNP Q1LRY0
C	-4	PRO	-	expression tag	UNP Q1LRY0
C	-3	ARG	-	expression tag	UNP Q1LRY0
C	-2	GLY	-	expression tag	UNP Q1LRY0
C	-1	SER	-	expression tag	UNP Q1LRY0
C	0	HIS	-	expression tag	UNP Q1LRY0
D	-19	MET	-	initiating methionine	UNP Q1LRY0
D	-18	GLY	-	expression tag	UNP Q1LRY0
D	-17	SER	-	expression tag	UNP Q1LRY0
D	-16	SER	-	expression tag	UNP Q1LRY0

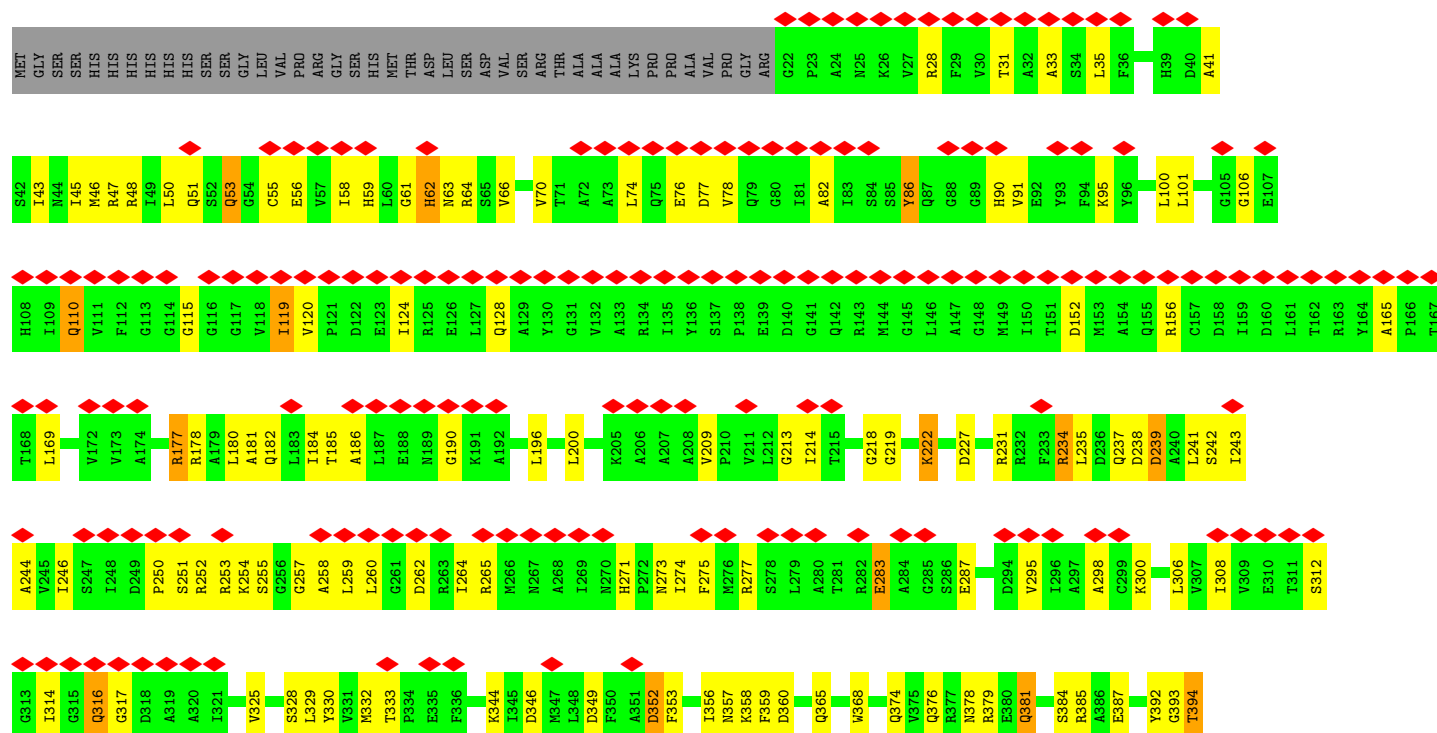
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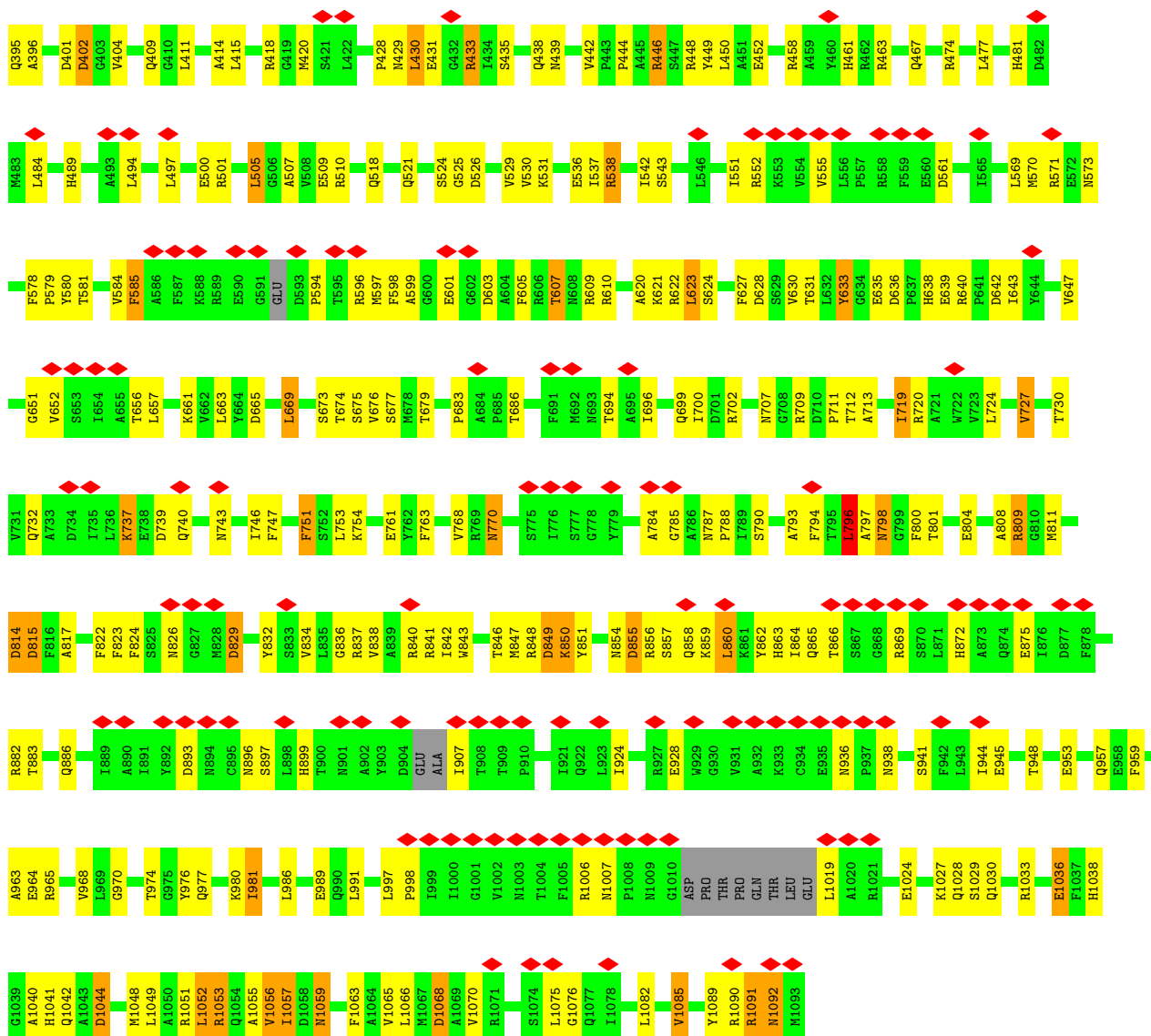
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	expression tag	UNP Q1LRY0
D	-14	HIS	-	expression tag	UNP Q1LRY0
D	-13	HIS	-	expression tag	UNP Q1LRY0
D	-12	HIS	-	expression tag	UNP Q1LRY0
D	-11	HIS	-	expression tag	UNP Q1LRY0
D	-10	HIS	-	expression tag	UNP Q1LRY0
D	-9	SER	-	expression tag	UNP Q1LRY0
D	-8	SER	-	expression tag	UNP Q1LRY0
D	-7	GLY	-	expression tag	UNP Q1LRY0
D	-6	LEU	-	expression tag	UNP Q1LRY0
D	-5	VAL	-	expression tag	UNP Q1LRY0
D	-4	PRO	-	expression tag	UNP Q1LRY0
D	-3	ARG	-	expression tag	UNP Q1LRY0
D	-2	GLY	-	expression tag	UNP Q1LRY0
D	-1	SER	-	expression tag	UNP Q1LRY0
D	0	HIS	-	expression tag	UNP Q1LRY0

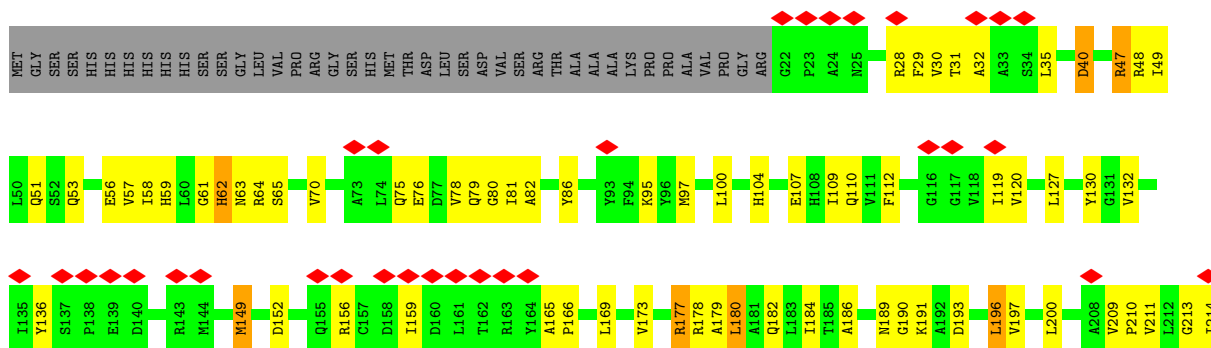


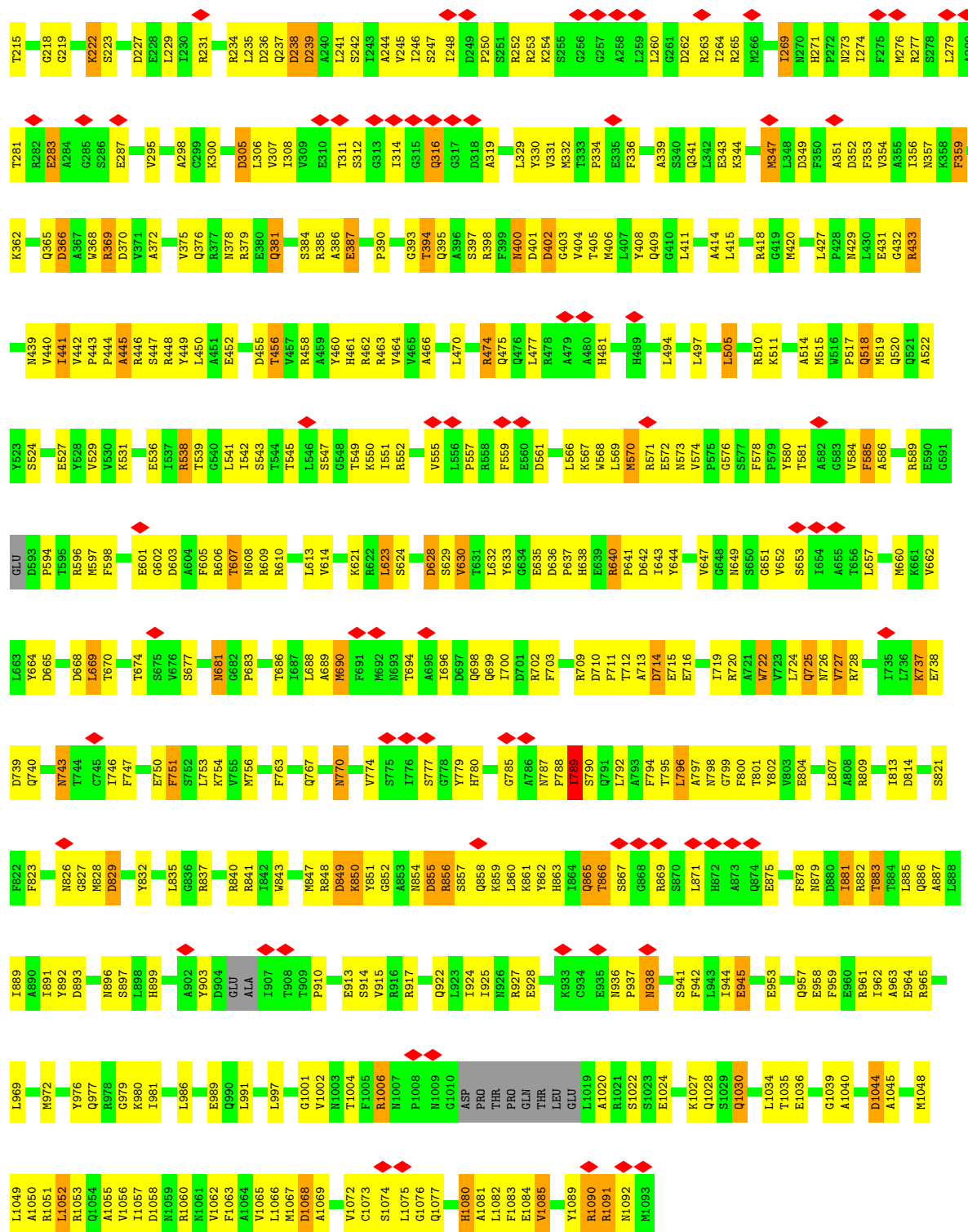
● Molecule 1: Isobutyryl-CoA mutase fused





• Molecule 1: Isobutyryl-CoA mutase fused





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138956	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.81	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	11.211	Depositor
Minimum map value	0.000	Depositor
Average map value	0.273	Depositor
Map value standard deviation	0.956	Depositor
Recommended contour level	2.36	Depositor
Map size (Å)	257.8304, 257.8304, 257.8304	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0143, 2.0143, 2.0143	Depositor

5 Model quality

5.1 Standard geometry

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	0.18	0/8254	0.37	1/11168 (0.0%)
1	B	0.16	0/8254	0.35	3/11168 (0.0%)
1	C	0.16	0/8254	0.34	2/11168 (0.0%)
1	D	0.24	0/8248	0.41	2/11160 (0.0%)
All	All	0.19	0/33010	0.37	8/44664 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	796	LEU	N-CA-C	-7.12	103.45	111.07
1	D	789	ILE	CB-CA-C	-6.88	103.17	111.97
1	B	443	PRO	N-CA-C	-6.70	102.53	110.70
1	D	789	ILE	N-CA-C	-6.53	104.15	110.42
1	B	447	SER	N-CA-C	5.89	123.35	110.80
1	A	447	SER	N-CA-C	5.68	122.89	110.80
1	B	442	VAL	N-CA-C	5.14	113.06	108.63
1	C	796	LEU	CB-CA-C	-5.07	102.91	110.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8116	0	7885	399	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8116	0	7885	327	0
1	C	8116	0	7885	303	0
1	D	8110	0	7879	426	0
All	All	32458	0	31534	1392	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 22.

All (1392) 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:C:796:LEU:HD12	1:C:800:PHE:CZ	1.44	1.51
1:C:796:LEU:HD12	1:C:800:PHE:CE1	1.57	1.39
1:B:344:LYS:NZ	1:C:258:ALA:HB1	1.38	1.38
1:A:441:ILE:HD11	1:A:750:GLU:CB	1.53	1.38
1:D:442:VAL:HG22	1:D:443:PRO:CD	1.57	1.31
1:D:800:PHE:HZ	1:D:843:TRP:CE3	1.47	1.31
1:D:442:VAL:CG2	1:D:443:PRO:HD2	1.60	1.31
1:D:800:PHE:CZ	1:D:843:TRP:CZ3	2.20	1.30
1:D:800:PHE:CZ	1:D:843:TRP:CE3	2.32	1.17
1:A:442:VAL:HG22	1:A:443:PRO:CD	1.75	1.16
1:A:441:ILE:HD11	1:A:750:GLU:CA	1.73	1.15
1:C:796:LEU:HG	1:C:959:PHE:HZ	1.11	1.15
1:A:442:VAL:HG22	1:A:443:PRO:HD2	1.22	1.11
1:A:445:ALA:HA	1:D:448:ARG:NH1	1.66	1.11
1:C:796:LEU:CD1	1:C:800:PHE:CZ	2.35	1.09
1:A:441:ILE:HG21	1:A:969:LEU:HD21	1.34	1.08
1:B:443:PRO:HG2	1:B:446:ARG:HE	1.09	1.08
1:C:796:LEU:HG	1:C:959:PHE:CZ	1.88	1.07
1:D:798:ASN:O	1:D:801:THR:HG22	1.54	1.07
1:A:441:ILE:HD11	1:A:750:GLU:HB3	1.35	1.06
1:D:797:ALA:HB2	1:D:959:PHE:HE1	1.20	1.05
1:C:796:LEU:CD1	1:C:800:PHE:CE1	2.40	1.05
1:D:800:PHE:HZ	1:D:843:TRP:CZ3	1.67	1.04
1:C:796:LEU:CG	1:C:959:PHE:HZ	1.70	1.04
1:A:441:ILE:HD11	1:A:750:GLU:HA	1.41	1.00
1:D:449:TYR:OH	1:D:801:THR:HB	1.61	0.99
1:A:441:ILE:CD1	1:A:750:GLU:CB	2.44	0.96
1:D:800:PHE:CZ	1:D:843:TRP:HZ3	1.84	0.95
1:B:344:LYS:HZ3	1:C:258:ALA:HB1	1.20	0.94
1:A:446:ARG:HA	1:A:446:ARG:NH1	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:792:LEU:HD23	1:D:835:LEU:HD21	1.46	0.93
1:B:447:SER:O	1:B:449:TYR:HD1	1.50	0.93
1:B:440:VAL:HG13	1:B:440:VAL:O	1.67	0.93
1:A:441:ILE:CD1	1:A:750:GLU:HA	1.99	0.92
1:D:603:ASP:OD2	1:D:605:PHE:HB2	1.69	0.92
1:D:797:ALA:HB2	1:D:959:PHE:CE1	2.05	0.91
1:A:441:ILE:CD1	1:A:750:GLU:HB3	1.99	0.91
1:A:446:ARG:HG3	1:A:446:ARG:HH11	1.34	0.90
1:A:445:ALA:HA	1:D:448:ARG:HH12	1.36	0.90
1:C:801:THR:HG21	1:C:968:VAL:HG21	1.54	0.90
1:B:443:PRO:HG2	1:B:446:ARG:NE	1.88	0.89
1:D:555:VAL:H	1:D:936:ASN:HD21	1.23	0.87
1:D:787:ASN:CB	1:D:789:ILE:CD1	2.52	0.87
1:B:447:SER:O	1:B:449:TYR:CD1	2.26	0.87
1:C:801:THR:CG2	1:C:968:VAL:HG21	2.06	0.85
1:D:630:VAL:HG13	1:D:635:GLU:HB2	1.59	0.85
1:C:449:TYR:OH	1:C:801:THR:CG2	2.25	0.84
1:A:242:SER:HB2	1:A:305:ASP:H	1.43	0.83
1:D:444:PRO:O	1:D:447:SER:HB3	1.79	0.82
1:B:344:LYS:HZ2	1:C:258:ALA:HB1	1.39	0.81
1:C:449:TYR:HE2	1:C:800:PHE:CB	1.93	0.81
1:C:449:TYR:OH	1:C:801:THR:HG23	1.80	0.81
1:A:35:LEU:HA	1:A:63:ASN:HA	1.63	0.81
1:D:603:ASP:OD2	1:D:605:PHE:CB	2.29	0.81
1:D:792:LEU:CD2	1:D:835:LEU:HD11	2.12	0.80
1:D:35:LEU:HA	1:D:63:ASN:HA	1.64	0.80
1:D:61:GLY:HA3	1:D:1091:ARG:HE	1.46	0.80
1:A:476:GLN:HG3	1:B:476:GLN:HG3	1.63	0.79
1:A:543:SER:HB2	1:A:551:ILE:HB	1.62	0.79
1:A:441:ILE:CG1	1:A:750:GLU:HB3	2.13	0.78
1:A:477:LEU:HD11	1:A:497:LEU:HB3	1.64	0.78
1:A:402:ASP:OD1	1:A:402:ASP:N	2.17	0.78
1:A:441:ILE:CG2	1:A:969:LEU:HD21	2.13	0.78
1:B:242:SER:HB2	1:B:305:ASP:H	1.46	0.78
1:B:250:PRO:HD3	1:B:312:SER:HB2	1.65	0.77
1:D:792:LEU:HD21	1:D:835:LEU:HD11	1.64	0.77
1:A:445:ALA:CA	1:D:448:ARG:NH1	2.46	0.77
1:B:446:ARG:HD3	1:B:804:GLU:HB2	1.66	0.77
1:D:636:ASP:HB2	1:D:1076:GLY:HA3	1.64	0.77
1:A:442:VAL:CG2	1:A:443:PRO:CD	2.60	0.77
1:C:251:SER:HA	1:C:258:ALA:HB2	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:817:ALA:HB3	1:B:857:SER:HB3	1.66	0.77
1:A:446:ARG:HA	1:A:446:ARG:CZ	2.15	0.76
1:A:61:GLY:HA3	1:A:1091:ARG:HE	1.50	0.75
1:B:35:LEU:HA	1:B:63:ASN:HA	1.67	0.75
1:C:449:TYR:CE2	1:C:800:PHE:CB	2.69	0.75
1:D:366:ASP:OD1	1:D:366:ASP:N	2.18	0.74
1:B:477:LEU:HD11	1:B:497:LEU:HB3	1.69	0.74
1:C:329:LEU:HD23	1:C:353:PHE:HB3	1.70	0.74
1:C:794:PHE:O	1:C:797:ALA:HB3	1.88	0.74
1:D:629:SER:HB2	1:D:633:TYR:CE2	2.22	0.74
1:D:991:LEU:HB3	1:D:997:LEU:HB2	1.70	0.74
1:A:564:GLU:O	1:A:567:LYS:NZ	2.21	0.74
1:B:440:VAL:O	1:B:440:VAL:CG1	2.36	0.73
1:C:597:MET:HB2	1:C:623:LEU:HA	1.70	0.73
1:C:633:TYR:HB3	1:C:635:GLU:HG2	1.71	0.73
1:D:200:LEU:HD11	1:D:298:ALA:HA	1.71	0.73
1:A:442:VAL:HG22	1:A:443:PRO:HD3	1.68	0.73
1:C:991:LEU:HB3	1:C:997:LEU:HB2	1.71	0.73
1:A:1090:ARG:O	1:A:1092:ASN:ND2	2.21	0.73
1:D:398:ARG:HH22	1:D:441:ILE:HG12	1.54	0.73
1:D:566:LEU:HG	1:D:570:MET:HE2	1.70	0.73
1:A:441:ILE:HD11	1:A:750:GLU:HB2	1.64	0.73
1:B:448:ARG:NH1	1:C:444:PRO:O	2.21	0.73
1:C:837:ARG:HH11	1:C:938:ASN:HD22	1.36	0.72
1:D:792:LEU:CD2	1:D:835:LEU:HD21	2.18	0.72
1:C:796:LEU:CB	1:C:959:PHE:HZ	2.01	0.72
1:C:699:GLN:HE21	1:C:719:ILE:HG13	1.54	0.72
1:D:720:ARG:HH12	1:D:724:LEU:HG	1.54	0.72
1:A:598:PHE:HA	1:A:624:SER:HB2	1.70	0.72
1:A:398:ARG:NH2	1:A:441:ILE:H	1.87	0.72
1:C:449:TYR:HE2	1:C:800:PHE:HB2	1.54	0.72
1:A:633:TYR:HB3	1:A:635:GLU:HG2	1.70	0.72
1:C:824:PHE:N	1:C:863:HIS:O	2.23	0.72
1:D:794:PHE:HZ	1:D:980:LYS:HE2	1.55	0.72
1:A:746:ILE:O	1:A:1089:TYR:N	2.23	0.71
1:B:555:VAL:H	1:B:936:ASN:HD21	1.36	0.71
1:B:581:THR:O	1:B:840:ARG:NH2	2.23	0.71
1:B:621:LYS:HB2	1:B:674:THR:HA	1.72	0.71
1:C:449:TYR:CE2	1:C:800:PHE:HB2	2.25	0.71
1:D:263:ARG:HH12	1:D:269:ILE:HG21	1.54	0.71
1:D:441:ILE:N	1:D:441:ILE:HD13	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLN:HB3	1:D:965:ARG:HH22	1.55	0.71
1:A:824:PHE:N	1:A:863:HIS:O	2.23	0.71
1:D:62:HIS:O	1:D:1091:ARG:NH2	2.24	0.71
1:C:450:LEU:HB2	1:C:963:ALA:HB2	1.72	0.71
1:C:796:LEU:HD12	1:C:800:PHE:HZ	1.43	0.70
1:D:444:PRO:O	1:D:447:SER:CB	2.40	0.70
1:A:62:HIS:O	1:A:1091:ARG:NH2	2.24	0.70
1:A:872:HIS:O	1:A:879:ASN:ND2	2.24	0.70
1:A:398:ARG:HH22	1:A:441:ILE:HG12	1.56	0.70
1:B:365:GLN:HB3	1:C:965:ARG:HH22	1.57	0.70
1:D:863:HIS:HA	1:D:897:SER:HB2	1.74	0.70
1:C:246:ILE:HG22	1:C:277:ARG:HB3	1.73	0.69
1:D:637:PRO:HG2	1:D:1034:LEU:HD22	1.74	0.69
1:D:543:SER:HB2	1:D:551:ILE:HB	1.75	0.69
1:B:53:GLN:NE2	1:B:55:CYS:SG	2.66	0.69
1:B:376:GLN:NE2	1:B:381:GLN:O	2.25	0.69
1:B:1006:ARG:NH1	1:B:1007:ASN:OD1	2.25	0.69
1:D:629:SER:HB2	1:D:633:TYR:HE2	1.56	0.69
1:C:449:TYR:OH	1:C:801:THR:HG22	1.93	0.69
1:D:570:MET:SD	1:D:570:MET:N	2.66	0.69
1:B:104:HIS:HB3	1:B:178:ARG:HH22	1.58	0.68
1:A:686:THR:HG21	1:A:1075:LEU:HD13	1.75	0.68
1:B:1044:ASP:HB2	1:B:1048:MET:HE2	1.74	0.68
1:A:505:LEU:O	1:A:510:ARG:NH2	2.26	0.68
1:C:61:GLY:HA3	1:C:1091:ARG:HE	1.58	0.68
1:D:628:ASP:OD1	1:D:628:ASP:N	2.18	0.68
1:D:785:GLY:HA2	1:D:869:ARG:HD3	1.74	0.68
1:B:344:LYS:HZ1	1:C:258:ALA:HB1	1.53	0.68
1:A:630:VAL:HG13	1:A:635:GLU:HB2	1.76	0.68
1:D:402:ASP:OD1	1:D:402:ASP:N	2.25	0.68
1:D:709:ARG:NH2	1:D:715:GLU:OE2	2.27	0.68
1:D:787:ASN:CB	1:D:789:ILE:HD13	2.24	0.68
1:D:1049:LEU:HA	1:D:1052:LEU:HD23	1.76	0.68
1:A:234:ARG:HH21	1:A:271:HIS:HB2	1.59	0.67
1:B:505:LEU:O	1:B:510:ARG:NH2	2.27	0.67
1:B:344:LYS:NZ	1:C:258:ALA:CB	2.35	0.67
1:C:446:ARG:NH2	1:C:452:GLU:OE1	2.26	0.67
1:D:789:ILE:HD12	1:D:789:ILE:H	1.59	0.67
1:A:709:ARG:NH2	1:A:715:GLU:OE2	2.27	0.67
1:B:62:HIS:O	1:B:1091:ARG:NH2	2.27	0.67
1:A:177:ARG:HA	1:A:180:LEU:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:903:TYR:H	1:D:910:PRO:HB3	1.59	0.67
1:C:796:LEU:CG	1:C:959:PHE:CZ	2.60	0.67
1:A:443:PRO:HB2	1:A:446:ARG:HB2	1.75	0.67
1:A:264:ILE:HG23	1:A:265:ARG:HD3	1.77	0.67
1:A:445:ALA:O	1:D:448:ARG:NH1	2.28	0.67
1:A:862:TYR:O	1:A:896:ASN:ND2	2.26	0.66
1:C:379:ARG:O	1:C:381:GLN:NE2	2.28	0.66
1:A:463:ARG:NH1	1:A:509:GLU:OE2	2.26	0.66
1:B:209:VAL:HG22	1:B:300:LYS:HG2	1.77	0.66
1:B:252:ARG:HH21	1:C:349:ASP:HB2	1.59	0.66
1:A:376:GLN:NE2	1:A:384:SER:O	2.28	0.66
1:A:445:ALA:HA	1:D:448:ARG:HH11	1.58	0.66
1:C:801:THR:HG21	1:C:968:VAL:CG2	2.24	0.66
1:A:445:ALA:CA	1:D:448:ARG:HH12	2.06	0.66
1:B:543:SER:O	1:B:551:ILE:N	2.22	0.66
1:B:838:VAL:HG22	1:B:948:THR:HG23	1.77	0.66
1:A:570:MET:SD	1:A:570:MET:N	2.68	0.66
1:D:529:VAL:HA	1:D:538:ARG:HA	1.77	0.66
1:A:458:ARG:HH12	1:A:462:ARG:HH11	1.42	0.66
1:D:1058:ASP:O	1:D:1060:ARG:NH1	2.29	0.66
1:C:169:LEU:HD21	1:C:196:LEU:HD11	1.78	0.66
1:C:543:SER:HB2	1:C:551:ILE:HB	1.77	0.66
1:D:747:PHE:HB3	1:D:751:PHE:HE1	1.60	0.66
1:C:356:ILE:HB	1:C:393:GLY:HA2	1.77	0.65
1:D:330:TYR:HB3	1:D:354:VAL:HG22	1.78	0.65
1:D:746:ILE:O	1:D:1089:TYR:N	2.28	0.65
1:C:450:LEU:CD2	1:C:800:PHE:CD2	2.79	0.65
1:D:213:GLY:O	1:D:329:LEU:N	2.29	0.65
1:D:242:SER:OG	1:D:273:ASN:ND2	2.30	0.65
1:D:356:ILE:HB	1:D:393:GLY:HA2	1.77	0.65
1:D:1036:GLU:O	1:D:1040:ALA:N	2.29	0.65
1:A:186:ALA:O	1:A:190:GLY:N	2.29	0.65
1:A:372:ALA:HB1	1:A:386:ALA:HB1	1.79	0.65
1:B:1058:ASP:O	1:B:1060:ARG:NH1	2.30	0.65
1:D:1001:GLY:O	1:D:1006:ARG:NH2	2.30	0.65
1:A:555:VAL:H	1:A:936:ASN:HD21	1.44	0.65
1:B:329:LEU:HD23	1:B:353:PHE:HB3	1.79	0.65
1:B:647:VAL:O	1:B:1027:LYS:NZ	2.29	0.65
1:C:647:VAL:O	1:C:1027:LYS:NZ	2.30	0.65
1:B:378:ASN:OD1	1:C:48:ARG:NH2	2.30	0.65
1:B:554:VAL:HG22	1:B:935:GLU:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:SER:HB3	1:C:352:ASP:H	1.62	0.65
1:A:545:THR:HG22	1:A:549:THR:H	1.63	0.64
1:A:1024:GLU:OE2	1:A:1028:GLN:NE2	2.30	0.64
1:A:378:ASN:OD1	1:D:48:ARG:NH2	2.30	0.64
1:A:649:ASN:ND2	1:A:1020:ALA:O	2.30	0.64
1:C:449:TYR:CE2	1:C:800:PHE:HB3	2.31	0.64
1:D:305:ASP:N	1:D:305:ASP:OD1	2.29	0.64
1:B:33:ALA:HB3	1:B:62:HIS:HA	1.78	0.64
1:D:31:THR:HG22	1:D:82:ALA:HB3	1.78	0.64
1:A:263:ARG:HD2	1:A:276:MET:HG3	1.80	0.64
1:B:264:ILE:HG23	1:B:265:ARG:HD3	1.78	0.64
1:B:530:VAL:O	1:B:537:ILE:N	2.30	0.64
1:C:376:GLN:NE2	1:C:384:SER:O	2.29	0.64
1:D:794:PHE:CZ	1:D:980:LYS:HE2	2.31	0.64
1:C:838:VAL:HG22	1:C:948:THR:HG23	1.80	0.64
1:C:869:ARG:O	1:C:872:HIS:NE2	2.30	0.64
1:D:914:SER:HA	1:D:917:ARG:HD2	1.78	0.64
1:C:1044:ASP:HB2	1:C:1048:MET:HE2	1.80	0.64
1:D:40:ASP:OD1	1:D:40:ASP:N	2.31	0.64
1:A:252:ARG:NH1	1:D:343:GLU:O	2.30	0.64
1:B:633:TYR:HB3	1:B:635:GLU:HG2	1.79	0.64
1:B:862:TYR:O	1:B:896:ASN:ND2	2.25	0.64
1:A:720:ARG:HH22	1:A:724:LEU:HD21	1.62	0.63
1:B:936:ASN:OD1	1:B:936:ASN:N	2.30	0.63
1:C:579:PRO:HG2	1:C:581:THR:HG23	1.80	0.63
1:D:722:TRP:O	1:D:725:GLN:NE2	2.31	0.63
1:D:826:ASN:HD22	1:D:832:TYR:HB3	1.63	0.63
1:A:344:LYS:HD3	1:D:250:PRO:HD2	1.79	0.63
1:A:398:ARG:NH2	1:A:441:ILE:HG12	2.13	0.63
1:B:344:LYS:HZ3	1:C:258:ALA:CB	2.03	0.63
1:B:579:PRO:HG2	1:B:581:THR:HG23	1.80	0.63
1:A:450:LEU:HB2	1:A:963:ALA:HB2	1.80	0.63
1:A:543:SER:O	1:A:551:ILE:N	2.29	0.63
1:D:699:GLN:HE21	1:D:719:ILE:HG13	1.63	0.63
1:D:827:GLY:HA2	1:D:867:SER:HB2	1.81	0.63
1:A:398:ARG:HH22	1:A:441:ILE:N	1.96	0.63
1:B:814:ASP:OD1	1:B:814:ASP:N	2.30	0.63
1:C:48:ARG:HG2	1:C:51:GLN:HE21	1.64	0.63
1:D:640:ARG:HA	1:D:640:ARG:HH11	1.63	0.63
1:D:826:ASN:HB3	1:D:889:ILE:HD11	1.79	0.63
1:A:497:LEU:HD21	1:B:484:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:814:ASP:OD1	1:C:814:ASP:N	2.31	0.62
1:D:319:ALA:HA	1:D:347:MET:HE2	1.81	0.62
1:A:786:ALA:O	1:A:869:ARG:NH2	2.32	0.62
1:C:863:HIS:HA	1:C:897:SER:HB2	1.80	0.62
1:D:800:PHE:CZ	1:D:843:TRP:HE3	2.09	0.62
1:A:1090:ARG:HG2	1:A:1092:ASN:HD22	1.65	0.62
1:B:242:SER:OG	1:B:273:ASN:ND2	2.32	0.62
1:B:328:SER:HB3	1:B:352:ASP:H	1.63	0.62
1:D:186:ALA:O	1:D:190:GLY:N	2.32	0.62
1:D:379:ARG:O	1:D:381:GLN:NE2	2.33	0.62
1:D:649:ASN:ND2	1:D:1020:ALA:O	2.27	0.62
1:B:484:LEU:HD23	1:B:494:LEU:HD11	1.80	0.62
1:A:446:ARG:HB3	1:A:804:GLU:OE2	2.00	0.62
1:C:530:VAL:O	1:C:537:ILE:N	2.29	0.62
1:D:58:ILE:HG12	1:D:260:LEU:HB2	1.81	0.62
1:D:398:ARG:NH1	1:D:439:ASN:O	2.33	0.62
1:A:104:HIS:HB3	1:A:178:ARG:HH22	1.64	0.62
1:D:598:PHE:HA	1:D:624:SER:HB2	1.81	0.62
1:D:789:ILE:HD12	1:D:789:ILE:N	2.15	0.62
1:D:264:ILE:HD11	1:D:1091:ARG:HG2	1.82	0.62
1:B:869:ARG:O	1:B:872:HIS:NE2	2.33	0.62
1:C:62:HIS:O	1:C:1091:ARG:NH2	2.32	0.62
1:D:542:ILE:HD11	1:D:550:LYS:HG2	1.81	0.62
1:C:529:VAL:HA	1:C:538:ARG:HA	1.82	0.61
1:C:953:GLU:OE2	1:C:957:GLN:NE2	2.33	0.61
1:D:1055:ALA:HB2	1:D:1065:VAL:HG21	1.81	0.61
1:B:953:GLU:OE2	1:B:957:GLN:NE2	2.33	0.61
1:C:531:LYS:HA	1:C:536:GLU:HA	1.82	0.61
1:C:569:LEU:O	1:C:573:ASN:ND2	2.32	0.61
1:D:442:VAL:CG2	1:D:443:PRO:CD	2.44	0.61
1:D:219:GLY:HA2	1:D:265:ARG:HH22	1.66	0.61
1:A:814:ASP:N	1:A:814:ASP:OD1	2.29	0.61
1:A:722:TRP:O	1:A:725:GLN:NE2	2.33	0.61
1:C:63:ASN:ND2	1:C:633:TYR:OH	2.32	0.61
1:A:356:ILE:HB	1:A:393:GLY:HA2	1.82	0.61
1:A:401:ASP:OD2	1:A:404:VAL:N	2.33	0.61
1:A:1068:ASP:OD1	1:A:1068:ASP:N	2.32	0.61
1:B:31:THR:HG22	1:B:82:ALA:HB3	1.83	0.61
1:B:81:ILE:HG21	1:B:97:MET:HE1	1.83	0.61
1:B:464:VAL:HG21	1:B:571:ARG:HH12	1.66	0.61
1:B:567:LYS:HZ3	1:B:567:LYS:HB3	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:GLN:HE22	1:D:397:SER:HB3	1.66	0.61
1:D:862:TYR:O	1:D:896:ASN:ND2	2.32	0.61
1:A:209:VAL:HG22	1:A:300:LYS:HG2	1.82	0.61
1:B:447:SER:O	1:B:449:TYR:N	2.33	0.61
1:D:193:ASP:HB3	1:D:196:LEU:HB3	1.83	0.61
1:A:215:THR:HG22	1:A:311:THR:HG21	1.82	0.61
1:C:526:ASP:HB2	1:C:542:ILE:HB	1.82	0.61
1:A:65:SER:HB3	1:A:68:GLU:HB2	1.83	0.60
1:C:796:LEU:CB	1:C:959:PHE:CZ	2.83	0.60
1:D:962:ILE:CD1	1:D:976:TYR:CE2	2.84	0.60
1:B:529:VAL:HA	1:B:538:ARG:HA	1.82	0.60
1:A:62:HIS:NE2	1:A:743:ASN:O	2.35	0.60
1:A:242:SER:OG	1:A:273:ASN:ND2	2.34	0.60
1:D:1082:LEU:O	1:D:1085:VAL:HG12	2.02	0.60
1:A:369:ARG:HH22	1:D:979:GLY:HA3	1.66	0.60
1:B:211:VAL:HG22	1:B:307:VAL:HB	1.83	0.60
1:C:358:LYS:HE3	1:C:396:ALA:HB3	1.82	0.60
1:B:746:ILE:O	1:B:1089:TYR:N	2.34	0.60
1:D:359:PHE:N	1:D:394:THR:O	2.34	0.60
1:D:477:LEU:HD11	1:D:497:LEU:HB3	1.83	0.60
1:A:329:LEU:HD23	1:A:353:PHE:HB3	1.84	0.60
1:A:647:VAL:O	1:A:1027:LYS:NZ	2.34	0.60
1:B:81:ILE:HB	1:B:111:VAL:HA	1.82	0.60
1:C:638:HIS:H	1:C:643:ILE:HD11	1.66	0.60
1:D:647:VAL:O	1:D:1027:LYS:NZ	2.34	0.60
1:A:603:ASP:O	1:A:607:THR:OG1	2.20	0.60
1:C:450:LEU:HD21	1:C:800:PHE:CD2	2.37	0.60
1:D:1044:ASP:OD1	1:D:1044:ASP:N	2.35	0.60
1:A:53:GLN:NE2	1:A:55:CYS:SG	2.75	0.60
1:A:464:VAL:HG21	1:A:571:ARG:HH12	1.66	0.60
1:A:602:GLY:HA3	1:A:606:ARG:HD3	1.82	0.60
1:D:211:VAL:HG22	1:D:307:VAL:HB	1.84	0.60
1:D:442:VAL:CB	1:D:443:PRO:HD2	2.31	0.60
1:A:640:ARG:HA	1:A:640:ARG:HH11	1.65	0.60
1:B:564:GLU:O	1:B:567:LYS:NZ	2.35	0.60
1:B:679:THR:HA	1:B:732:GLN:HB2	1.82	0.60
1:C:250:PRO:HD3	1:C:312:SER:HB2	1.82	0.60
1:D:62:HIS:NE2	1:D:743:ASN:O	2.30	0.60
1:A:452:GLU:O	1:A:456:THR:OG1	2.20	0.59
1:A:229:LEU:HD22	1:A:408:TYR:HB2	1.83	0.59
1:D:569:LEU:O	1:D:573:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:SER:O	1:B:552:ARG:NH2	2.35	0.59
1:C:186:ALA:O	1:C:190:GLY:N	2.29	0.59
1:B:712:THR:HG22	1:B:715:GLU:HG3	1.83	0.59
1:C:796:LEU:CD1	1:C:800:PHE:HE1	2.14	0.59
1:D:642:ASP:OD1	1:D:643:ILE:N	2.34	0.59
1:A:200:LEU:HD11	1:A:298:ALA:HA	1.83	0.59
1:C:262:ASP:OD1	1:C:265:ARG:NH2	2.36	0.59
1:C:598:PHE:HA	1:C:624:SER:HB2	1.84	0.59
1:D:681:ASN:ND2	1:D:738:GLU:OE2	2.35	0.59
1:A:567:LYS:HZ2	1:A:567:LYS:HB3	1.67	0.59
1:A:1044:ASP:OD1	1:A:1044:ASP:N	2.33	0.59
1:B:822:PHE:HD2	1:B:860:LEU:HD21	1.66	0.59
1:C:209:VAL:HG22	1:C:300:LYS:HG2	1.84	0.59
1:D:244:ALA:O	1:D:308:ILE:N	2.32	0.59
1:B:250:PRO:HG2	1:C:344:LYS:HG3	1.83	0.59
1:C:101:LEU:O	1:C:106:GLY:N	2.25	0.59
1:D:795:THR:HG23	1:D:796:LEU:HD13	1.84	0.59
1:A:70:VAL:HG13	1:A:101:LEU:HD21	1.85	0.59
1:A:1044:ASP:HB2	1:A:1048:MET:HE2	1.84	0.59
1:D:696:ILE:HG23	1:D:719:ILE:HG21	1.84	0.59
1:B:737:LYS:HA	1:B:740:GLN:HG2	1.85	0.59
1:B:804:GLU:O	1:B:808:ALA:N	2.27	0.59
1:D:329:LEU:HD23	1:D:353:PHE:HB3	1.84	0.59
1:D:962:ILE:HD11	1:D:976:TYR:CE2	2.37	0.59
1:A:797:ALA:O	1:A:801:THR:OG1	2.20	0.58
1:B:447:SER:C	1:B:449:TYR:H	2.11	0.58
1:C:31:THR:HG22	1:C:82:ALA:HB3	1.85	0.58
1:A:56:GLU:OE1	1:A:56:GLU:N	2.36	0.58
1:B:929:TRP:NE1	1:B:931:VAL:HB	2.18	0.58
1:C:242:SER:OG	1:C:273:ASN:ND2	2.35	0.58
1:C:253:ARG:NH1	1:C:283:GLU:O	2.36	0.58
1:A:288:ILE:HD12	1:A:321:ILE:HD11	1.85	0.58
1:B:792:LEU:HD22	1:B:835:LEU:HD11	1.83	0.58
1:A:31:THR:O	1:A:59:HIS:ND1	2.34	0.58
1:C:376:GLN:NE2	1:C:381:GLN:O	2.35	0.58
1:D:245:VAL:HG22	1:D:308:ILE:HB	1.84	0.58
1:C:832:TYR:OH	1:C:869:ARG:NH2	2.35	0.58
1:A:81:ILE:O	1:A:112:PHE:N	2.34	0.58
1:A:838:VAL:HG22	1:A:948:THR:HG23	1.86	0.58
1:A:1055:ALA:HB2	1:A:1065:VAL:HG21	1.85	0.58
1:A:476:GLN:HE21	1:B:476:GLN:HA	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:VAL:HG21	1:B:969:LEU:HD21	1.84	0.58
1:B:870:SER:O	1:B:882:ARG:NH2	2.36	0.58
1:C:543:SER:O	1:C:551:ILE:N	2.32	0.58
1:C:924:ILE:HG23	1:C:928:GLU:HB2	1.85	0.58
1:A:175:GLY:O	1:A:177:ARG:NE	2.37	0.58
1:B:636:ASP:HB2	1:B:1076:GLY:HA3	1.86	0.58
1:A:346:ASP:OD2	1:D:253:ARG:N	2.36	0.58
1:C:543:SER:N	1:C:551:ILE:O	2.37	0.58
1:D:234:ARG:HH21	1:D:271:HIS:HB2	1.68	0.58
1:D:821:SER:HA	1:D:861:LYS:HG3	1.85	0.58
1:A:252:ARG:HH21	1:D:349:ASP:HB2	1.68	0.57
1:A:879:ASN:O	1:A:883:THR:OG1	2.22	0.57
1:C:770:ASN:O	1:C:770:ASN:ND2	2.36	0.57
1:A:398:ARG:HH22	1:A:441:ILE:H	1.52	0.57
1:B:200:LEU:HD11	1:B:298:ALA:HA	1.85	0.57
1:D:629:SER:O	1:D:633:TYR:HD2	1.87	0.57
1:A:568:TRP:O	1:A:572:GLU:N	2.23	0.57
1:A:929:TRP:NE1	1:A:931:VAL:HB	2.19	0.57
1:C:1053:ARG:HA	1:C:1056:VAL:HB	1.87	0.57
1:D:444:PRO:O	1:D:447:SER:N	2.37	0.57
1:A:218:GLY:HA2	1:A:222:LYS:NZ	2.20	0.57
1:A:442:VAL:CG2	1:A:443:PRO:HD3	2.30	0.57
1:B:832:TYR:OH	1:B:869:ARG:NH2	2.38	0.57
1:B:1044:ASP:OD1	1:B:1044:ASP:N	2.38	0.57
1:A:817:ALA:HB3	1:A:857:SER:HB3	1.86	0.57
1:A:953:GLU:OE2	1:A:957:GLN:NE2	2.38	0.57
1:C:200:LEU:HD11	1:C:298:ALA:HA	1.87	0.57
1:D:481:HIS:HA	1:D:494:LEU:HD13	1.87	0.57
1:A:398:ARG:NH2	1:A:441:ILE:N	2.52	0.57
1:A:638:HIS:H	1:A:643:ILE:HD11	1.69	0.57
1:B:682:GLY:HA2	1:B:735:ILE:HD11	1.86	0.57
1:C:1063:PHE:HA	1:C:1066:LEU:HB2	1.85	0.57
1:A:543:SER:N	1:A:551:ILE:O	2.35	0.57
1:B:914:SER:HA	1:B:917:ARG:HD2	1.86	0.57
1:C:77:ASP:OD2	1:C:182:GLN:NE2	2.38	0.57
1:D:442:VAL:HG22	1:D:443:PRO:HD2	0.70	0.57
1:A:224:SER:HB3	1:A:396:ALA:HB1	1.87	0.56
1:A:414:ALA:O	1:A:418:ARG:N	2.36	0.56
1:A:884:THR:O	1:A:888:LEU:HG	2.04	0.56
1:C:450:LEU:HD21	1:C:800:PHE:HD2	1.69	0.56
1:D:477:LEU:HD21	1:D:497:LEU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLY:HA2	1:C:265:ARG:HH22	1.70	0.56
1:D:1044:ASP:HB2	1:D:1048:MET:HE2	1.85	0.56
1:B:224:SER:OG	1:B:1090:ARG:NH1	2.39	0.56
1:C:477:LEU:HD21	1:C:497:LEU:HB3	1.88	0.56
1:D:814:ASP:N	1:D:814:ASP:OD1	2.38	0.56
1:A:788:PRO:HB3	1:A:832:TYR:CE1	2.40	0.56
1:B:28:ARG:H	1:B:79:GLN:HG2	1.71	0.56
1:C:165:ALA:HA	1:C:182:GLN:HB3	1.88	0.56
1:D:603:ASP:OD1	1:D:606:ARG:N	2.24	0.56
1:B:120:VAL:HG12	1:B:122:ASP:H	1.70	0.56
1:C:941:SER:HB3	1:C:944:ILE:HG12	1.86	0.56
1:D:1002:VAL:HA	1:D:1006:ARG:HH21	1.70	0.56
1:A:262:ASP:OD1	1:A:265:ARG:NH2	2.39	0.56
1:B:219:GLY:HA2	1:B:265:ARG:HH22	1.70	0.56
1:C:700:ILE:HG23	1:C:711:PRO:HG2	1.87	0.56
1:A:526:ASP:HB2	1:A:542:ILE:HB	1.88	0.56
1:C:801:THR:CG2	1:C:968:VAL:CG2	2.82	0.56
1:D:763:PHE:O	1:D:767:GLN:N	2.39	0.56
1:D:800:PHE:CE1	1:D:843:TRP:CZ3	2.89	0.56
1:B:432:GLY:HA2	1:B:433:ARG:HH21	1.71	0.56
1:B:568:TRP:O	1:B:572:GLU:N	2.28	0.56
1:D:214:ILE:HG23	1:D:329:LEU:HD12	1.87	0.56
1:D:660:MET:HB3	1:D:664:TYR:CE2	2.41	0.56
1:D:219:GLY:HA2	1:D:265:ARG:NH2	2.20	0.56
1:D:603:ASP:OD2	1:D:605:PHE:CG	2.59	0.56
1:A:864:ILE:O	1:A:899:HIS:N	2.37	0.55
1:B:621:LYS:O	1:B:675:SER:N	2.28	0.55
1:D:962:ILE:HD11	1:D:976:TYR:HE2	1.71	0.55
1:C:524:SER:O	1:C:552:ARG:NH2	2.40	0.55
1:D:215:THR:HG22	1:D:311:THR:HG21	1.88	0.55
1:A:1001:GLY:N	1:A:1004:THR:O	2.37	0.55
1:B:177:ARG:CZ	1:B:177:ARG:H	2.19	0.55
1:B:376:GLN:NE2	1:B:384:SER:O	2.39	0.55
1:B:556:LEU:HD23	1:B:556:LEU:H	1.70	0.55
1:A:330:TYR:HD2	1:A:354:VAL:HG13	1.70	0.55
1:B:641:PRO:HA	1:B:644:TYR:HB2	1.88	0.55
1:C:679:THR:HA	1:C:732:GLN:HB2	1.89	0.55
1:D:1063:PHE:O	1:D:1067:MET:N	2.33	0.55
1:B:227:ASP:OD1	1:B:267:ASN:ND2	2.40	0.55
1:D:70:VAL:HG11	1:D:100:LEU:HD23	1.87	0.55
1:B:75:GLN:NE2	1:B:276:MET:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ILE:HG23	1:D:265:ARG:HD3	1.87	0.55
1:D:737:LYS:HZ1	1:D:780:HIS:H	1.53	0.55
1:B:287:GLU:HB3	1:C:316:GLN:HE22	1.71	0.55
1:B:372:ALA:HB1	1:B:386:ALA:HB1	1.89	0.55
1:B:433:ARG:H	1:B:433:ARG:HE	1.55	0.55
1:B:629:SER:HA	1:B:632:LEU:HB2	1.88	0.55
1:C:720:ARG:HH22	1:C:724:LEU:HD21	1.72	0.55
1:D:79:GLN:HA	1:D:109:ILE:HD12	1.88	0.55
1:D:177:ARG:CZ	1:D:177:ARG:H	2.20	0.55
1:A:409:GLN:HE22	1:A:429:ASN:HA	1.72	0.55
1:B:727:VAL:HG22	1:B:771:PHE:HB2	1.89	0.55
1:C:177:ARG:H	1:C:177:ARG:CZ	2.20	0.55
1:C:317:GLY:HA2	1:C:346:ASP:HB3	1.89	0.55
1:C:800:PHE:HZ	1:C:959:PHE:CZ	2.25	0.55
1:A:936:ASN:N	1:A:936:ASN:OD1	2.40	0.54
1:A:965:ARG:HH22	1:D:365:GLN:HB3	1.72	0.54
1:A:1048:MET:SD	1:A:1048:MET:N	2.80	0.54
1:B:505:LEU:HD22	1:B:510:ARG:HB2	1.88	0.54
1:B:638:HIS:H	1:B:643:ILE:HD11	1.71	0.54
1:B:999:ILE:H	1:B:1003:ASN:HB2	1.72	0.54
1:D:712:THR:HG22	1:D:715:GLU:HG3	1.89	0.54
1:A:28:ARG:HB2	1:A:78:VAL:HA	1.89	0.54
1:A:346:ASP:HA	1:D:252:ARG:HE	1.72	0.54
1:C:555:VAL:HB	1:C:936:ASN:HD21	1.73	0.54
1:D:169:LEU:O	1:D:173:VAL:N	2.29	0.54
1:D:800:PHE:HE2	1:D:847:MET:SD	2.30	0.54
1:D:871:LEU:HA	1:D:882:ARG:HH22	1.71	0.54
1:A:374:GLN:OE1	1:D:48:ARG:NH2	2.41	0.54
1:B:36:PHE:HZ	1:B:635:GLU:HG3	1.71	0.54
1:C:683:PRO:HB3	1:C:1075:LEU:HD11	1.90	0.54
1:C:796:LEU:HB3	1:C:959:PHE:CZ	2.42	0.54
1:D:787:ASN:C	1:D:789:ILE:HD12	2.32	0.54
1:A:597:MET:HE1	1:A:618:MET:HG3	1.89	0.54
1:B:181:ALA:HA	1:B:277:ARG:HH12	1.72	0.54
1:C:28:ARG:HH22	1:C:185:THR:HG22	1.71	0.54
1:C:374:GLN:NE2	1:C:378:ASN:OD1	2.39	0.54
1:D:372:ALA:HB1	1:D:386:ALA:HB1	1.89	0.54
1:A:446:ARG:NH1	1:A:446:ARG:HG3	2.13	0.54
1:A:1006:ARG:NH1	1:A:1007:ASN:OD1	2.40	0.54
1:A:878:PHE:O	1:A:882:ARG:HG3	2.07	0.54
1:B:477:LEU:HD22	1:B:498:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:ASP:OD1	1:C:643:ILE:N	2.41	0.54
1:B:356:ILE:HB	1:B:393:GLY:HA2	1.90	0.54
1:A:234:ARG:NH1	1:A:239:ASP:OD2	2.41	0.54
1:B:452:GLU:O	1:B:456:THR:OG1	2.26	0.54
1:C:115:GLY:H	1:C:119:ILE:HD11	1.72	0.54
1:C:264:ILE:HG23	1:C:265:ARG:HD3	1.89	0.54
1:C:603:ASP:O	1:C:607:THR:OG1	2.26	0.54
1:A:389:MET:HE3	1:A:390:PRO:HD2	1.90	0.54
1:C:1082:LEU:O	1:C:1085:VAL:HG12	2.08	0.54
1:A:28:ARG:H	1:A:79:GLN:HG2	1.73	0.53
1:A:834:VAL:HG11	1:A:944:ILE:HG23	1.89	0.53
1:B:531:LYS:HA	1:B:536:GLU:HA	1.90	0.53
1:C:332:MET:O	1:C:357:ASN:N	2.41	0.53
1:C:1051:ARG:HE	1:C:1065:VAL:HG13	1.73	0.53
1:A:379:ARG:O	1:A:381:GLN:NE2	2.40	0.53
1:A:621:LYS:O	1:A:675:SER:N	2.32	0.53
1:A:997:LEU:HD12	1:A:998:PRO:HD2	1.90	0.53
1:B:570:MET:SD	1:B:570:MET:N	2.81	0.53
1:C:56:GLU:OE1	1:C:56:GLU:N	2.41	0.53
1:C:796:LEU:CD1	1:C:800:PHE:HZ	2.05	0.53
1:D:621:LYS:HB2	1:D:674:THR:HG23	1.91	0.53
1:C:213:GLY:HA3	1:C:325:VAL:HG21	1.90	0.53
1:C:578:PHE:CZ	1:C:848:ARG:HD2	2.42	0.53
1:D:961:ARG:HH21	1:D:965:ARG:HE	1.55	0.53
1:B:598:PHE:HA	1:B:624:SER:HB2	1.89	0.53
1:C:213:GLY:O	1:C:329:LEU:N	2.40	0.53
1:A:46:MET:O	1:A:50:LEU:HG	2.08	0.53
1:A:446:ARG:CZ	1:A:446:ARG:CA	2.84	0.53
1:A:448:ARG:CZ	1:D:448:ARG:HE	2.22	0.53
1:B:448:ARG:HE	1:C:448:ARG:HH21	1.57	0.53
1:D:433:ARG:H	1:D:433:ARG:HE	1.56	0.53
1:A:177:ARG:CZ	1:A:177:ARG:H	2.22	0.53
1:C:1041:HIS:ND1	1:C:1044:ASP:OD2	2.42	0.53
1:D:524:SER:O	1:D:552:ARG:NH2	2.42	0.53
1:B:521:GLN:O	1:B:524:SER:OG	2.25	0.53
1:C:676:VAL:O	1:C:730:THR:N	2.37	0.53
1:D:608:ASN:ND2	1:D:662:VAL:O	2.37	0.53
1:D:64:ARG:HA	1:D:64:ARG:NH1	2.23	0.53
1:C:401:ASP:OD1	1:C:435:SER:OG	2.25	0.53
1:D:239:ASP:OD1	1:D:239:ASP:N	2.41	0.53
1:A:62:HIS:HE2	1:A:744:THR:HA	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:886:GLN:O	1:D:889:ILE:HG12	2.09	0.52
1:B:332:MET:HG3	1:B:356:ILE:HA	1.91	0.52
1:D:193:ASP:OD2	1:D:196:LEU:N	2.39	0.52
1:D:505:LEU:O	1:D:510:ARG:NH2	2.42	0.52
1:D:1027:LYS:O	1:D:1030:GLN:NE2	2.42	0.52
1:A:177:ARG:HG2	1:A:275:PHE:CG	2.43	0.52
1:B:218:GLY:HA2	1:B:222:LYS:NZ	2.25	0.52
1:B:243:ILE:HB	1:B:274:ILE:HG23	1.91	0.52
1:B:345:ILE:HG22	1:B:348:LEU:H	1.74	0.52
1:C:359:PHE:N	1:C:394:THR:O	2.42	0.52
1:C:360:ASP:OD2	1:C:395:GLN:NE2	2.42	0.52
1:C:1055:ALA:HB2	1:C:1065:VAL:HG21	1.91	0.52
1:C:1068:ASP:OD1	1:C:1068:ASP:N	2.41	0.52
1:D:770:ASN:O	1:D:770:ASN:ND2	2.32	0.52
1:D:849:ASP:OD1	1:D:849:ASP:N	2.42	0.52
1:A:234:ARG:NH2	1:A:270:ASN:O	2.42	0.52
1:B:414:ALA:O	1:B:418:ARG:N	2.42	0.52
1:B:1082:LEU:O	1:B:1085:VAL:HG12	2.09	0.52
1:C:607:THR:HB	1:C:663:LEU:HD11	1.90	0.52
1:C:737:LYS:HA	1:C:740:GLN:HG2	1.91	0.52
1:A:75:GLN:HB3	1:A:275:PHE:CE1	2.45	0.52
1:A:671:ASN:HD21	1:A:673:SER:HB2	1.75	0.52
1:A:1001:GLY:O	1:A:1006:ARG:NH2	2.31	0.52
1:B:220:ALA:O	1:B:357:ASN:ND2	2.43	0.52
1:C:70:VAL:HG11	1:C:100:LEU:HD23	1.90	0.52
1:D:330:TYR:N	1:D:353:PHE:O	2.32	0.52
1:A:250:PRO:HD2	1:D:344:LYS:HZ1	1.75	0.52
1:B:647:VAL:HB	1:B:1027:LYS:HD3	1.92	0.52
1:C:620:ALA:HA	1:C:673:SER:HB3	1.91	0.52
1:C:1044:ASP:OD1	1:C:1044:ASP:N	2.41	0.52
1:D:801:THR:O	1:D:804:GLU:HB3	2.10	0.52
1:A:112:PHE:HB3	1:A:136:TYR:HE2	1.74	0.52
1:A:601:GLU:OE1	1:A:651:GLY:N	2.43	0.52
1:A:823:PHE:CD2	1:A:863:HIS:HB3	2.45	0.52
1:B:843:TRP:O	1:B:846:THR:OG1	2.26	0.52
1:B:938:ASN:OD1	1:B:938:ASN:N	2.42	0.52
1:B:1055:ALA:HB2	1:B:1065:VAL:HG21	1.90	0.52
1:C:414:ALA:O	1:C:418:ARG:N	2.42	0.52
1:D:177:ARG:H	1:D:177:ARG:NE	2.08	0.52
1:D:941:SER:HB3	1:D:944:ILE:HG12	1.92	0.52
1:A:147:ALA:HA	1:A:150:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:TRP:O	1:D:572:GLU:N	2.36	0.52
1:D:823:PHE:CD2	1:D:863:HIS:HB3	2.45	0.52
1:A:35:LEU:HD11	1:A:65:SER:HA	1.90	0.52
1:A:1036:GLU:O	1:A:1040:ALA:N	2.40	0.52
1:B:28:ARG:HB2	1:B:78:VAL:HA	1.91	0.52
1:D:414:ALA:O	1:D:418:ARG:N	2.43	0.52
1:D:460:TYR:O	1:D:464:VAL:HG23	2.10	0.52
1:B:884:THR:O	1:B:888:LEU:HG	2.10	0.51
1:C:505:LEU:O	1:C:510:ARG:NH2	2.34	0.51
1:D:686:THR:HG21	1:D:1075:LEU:HD13	1.91	0.51
1:B:101:LEU:HD22	1:B:106:GLY:HA3	1.92	0.51
1:B:443:PRO:CG	1:B:446:ARG:HE	2.00	0.51
1:B:538:ARG:CZ	1:B:538:ARG:H	2.23	0.51
1:B:824:PHE:O	1:B:865:GLN:N	2.41	0.51
1:B:90:HIS:HA	1:B:93:TYR:CD2	2.45	0.51
1:A:392:TYR:CE1	1:A:433:ARG:HB2	2.45	0.51
1:B:70:VAL:HG11	1:B:100:LEU:HD23	1.92	0.51
1:B:581:THR:HB	1:B:837:ARG:HE	1.75	0.51
1:C:450:LEU:CD2	1:C:800:PHE:CE2	2.93	0.51
1:D:152:ASP:O	1:D:156:ARG:HB2	2.11	0.51
1:D:481:HIS:HB2	1:D:494:LEU:HB3	1.93	0.51
1:D:756:MET:HE3	1:D:774:VAL:HG22	1.91	0.51
1:D:837:ARG:NH1	1:D:938:ASN:HD22	2.09	0.51
1:A:222:LYS:NZ	1:A:310:GLU:OE2	2.43	0.51
1:B:56:GLU:OE2	1:B:282:ARG:NH2	2.43	0.51
1:D:347:MET:O	1:D:351:ALA:N	2.43	0.51
1:B:222:LYS:HD2	1:B:223:SER:N	2.25	0.51
1:B:330:TYR:CE2	1:B:332:MET:HB3	2.45	0.51
1:B:827:GLY:O	1:B:886:GLN:NE2	2.43	0.51
1:B:866:THR:OG1	1:B:867:SER:N	2.42	0.51
1:C:119:ILE:HD12	1:C:124:ILE:HD11	1.91	0.51
1:D:215:THR:O	1:D:331:VAL:N	2.43	0.51
1:D:398:ARG:HH22	1:D:441:ILE:CG1	2.21	0.51
1:D:829:ASP:OD1	1:D:829:ASP:N	2.42	0.51
1:D:1024:GLU:OE2	1:D:1028:GLN:NE2	2.43	0.51
1:A:445:ALA:C	1:D:448:ARG:NH1	2.69	0.51
1:B:731:VAL:HB	1:B:773:SER:HA	1.92	0.51
1:C:796:LEU:HG	1:C:959:PHE:CE2	2.42	0.51
1:C:849:ASP:OD1	1:C:849:ASP:N	2.42	0.51
1:B:849:ASP:N	1:B:849:ASP:OD1	2.42	0.51
1:B:887:ALA:O	1:B:891:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ARG:HB2	1:C:78:VAL:HA	1.93	0.51
1:C:621:LYS:O	1:C:675:SER:N	2.35	0.51
1:D:628:ASP:OD2	1:D:653:SER:OG	2.28	0.51
1:D:683:PRO:HB3	1:D:1075:LEU:HD11	1.92	0.51
1:D:714:ASP:OD1	1:D:714:ASP:N	2.42	0.51
1:D:1048:MET:SD	1:D:1048:MET:N	2.83	0.51
1:A:92:GLU:O	1:A:96:TYR:HB3	2.11	0.51
1:B:314:ILE:HD13	1:B:314:ILE:H	1.76	0.51
1:C:1049:LEU:HA	1:C:1052:LEU:HD23	1.92	0.51
1:A:556:LEU:HD23	1:A:556:LEU:H	1.76	0.51
1:B:889:ILE:O	1:B:893:ASP:N	2.31	0.51
1:D:703:PHE:CE2	1:D:719:ILE:HD11	2.45	0.51
1:D:799:GLY:O	1:D:802:TYR:HB2	2.10	0.51
1:A:521:GLN:O	1:A:524:SER:OG	2.25	0.50
1:B:400:ASN:HD22	1:B:1059:ASN:HD21	1.58	0.50
1:B:686:THR:HG21	1:B:1075:LEU:HD13	1.92	0.50
1:C:359:PHE:HB3	1:C:395:GLN:HB2	1.93	0.50
1:C:402:ASP:N	1:C:402:ASP:OD1	2.41	0.50
1:A:197:VAL:HG12	1:A:201:HIS:CE1	2.46	0.50
1:B:461:HIS:CE1	1:B:841:ARG:HH22	2.29	0.50
1:B:1048:MET:SD	1:B:1048:MET:N	2.84	0.50
1:C:31:THR:O	1:C:59:HIS:ND1	2.36	0.50
1:C:58:ILE:HG12	1:C:260:LEU:HB2	1.93	0.50
1:C:463:ARG:O	1:C:467:GLN:HG2	2.11	0.50
1:A:387:GLU:CD	1:A:387:GLU:H	2.18	0.50
1:A:792:LEU:O	1:A:796:LEU:HG	2.12	0.50
1:A:923:LEU:HD23	1:B:1005:PHE:HB2	1.93	0.50
1:B:215:THR:HG22	1:B:311:THR:HG21	1.92	0.50
1:C:461:HIS:CE1	1:C:841:ARG:HH22	2.30	0.50
1:D:578:PHE:CZ	1:D:848:ARG:HD2	2.47	0.50
1:C:788:PRO:HB3	1:C:832:TYR:CE1	2.46	0.50
1:C:793:ALA:O	1:C:796:LEU:HB2	2.11	0.50
1:C:1092:ASN:H	1:C:1092:ASN:HD22	1.60	0.50
1:D:601:GLU:OE1	1:D:651:GLY:N	2.45	0.50
1:A:446:ARG:HH11	1:A:446:ARG:CG	2.09	0.50
1:A:1024:GLU:HA	1:A:1027:LYS:HD2	1.94	0.50
1:B:508:VAL:O	1:B:512:LEU:HG	2.12	0.50
1:C:661:LYS:HG2	1:C:694:THR:HG23	1.94	0.50
1:C:797:ALA:HA	1:C:800:PHE:CD2	2.47	0.50
1:C:800:PHE:CZ	1:C:959:PHE:CZ	2.99	0.50
1:D:629:SER:HA	1:D:632:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:THR:O	1:D:716:GLU:N	2.41	0.50
1:A:81:ILE:HB	1:A:111:VAL:HA	1.93	0.50
1:A:213:GLY:O	1:A:329:LEU:N	2.37	0.50
1:A:441:ILE:HD12	1:A:750:GLU:HA	1.91	0.50
1:B:239:ASP:OD1	1:B:239:ASP:N	2.45	0.50
1:B:699:GLN:HE21	1:B:719:ILE:HG13	1.77	0.50
1:B:763:PHE:O	1:B:767:GLN:N	2.44	0.50
1:B:1001:GLY:O	1:B:1006:ARG:NH2	2.36	0.50
1:C:746:ILE:HA	1:C:1089:TYR:HB3	1.94	0.50
1:D:166:PRO:HG2	1:D:179:ALA:HB2	1.93	0.50
1:D:798:ASN:O	1:D:801:THR:CG2	2.44	0.50
1:D:863:HIS:NE2	1:D:899:HIS:HB2	2.27	0.50
1:A:314:ILE:HD13	1:A:314:ILE:H	1.77	0.50
1:A:609:ARG:O	1:A:613:LEU:HG	2.12	0.50
1:B:569:LEU:O	1:B:573:ASN:ND2	2.45	0.50
1:B:892:TYR:HA	1:B:937:PRO:HG2	1.93	0.50
1:C:415:LEU:HB3	1:C:420:MET:HB3	1.93	0.50
1:D:601:GLU:H	1:D:607:THR:HG23	1.77	0.50
1:D:823:PHE:HD2	1:D:863:HIS:HB3	1.75	0.50
1:C:622:ARG:HA	1:C:675:SER:HB2	1.93	0.50
1:D:334:PRO:HD3	1:D:357:ASN:O	2.12	0.50
1:B:31:THR:O	1:B:59:HIS:ND1	2.29	0.50
1:B:170:ASP:N	1:B:170:ASP:OD1	2.41	0.50
1:A:529:VAL:HA	1:A:538:ARG:HA	1.94	0.49
1:A:628:ASP:OD1	1:A:628:ASP:N	2.27	0.49
1:B:642:ASP:OD1	1:B:643:ILE:N	2.44	0.49
1:D:376:GLN:OE1	1:D:384:SER:OG	2.30	0.49
1:D:576:GLY:HA3	1:D:586:ALA:HB2	1.93	0.49
1:D:969:LEU:HA	1:D:972:MET:HE2	1.94	0.49
1:A:446:ARG:NH1	1:A:446:ARG:CG	2.72	0.49
1:A:557:PRO:HB3	1:B:942:PHE:CE1	2.47	0.49
1:B:219:GLY:H	1:B:222:LYS:HE2	1.76	0.49
1:C:747:PHE:HB3	1:C:751:PHE:HE2	1.76	0.49
1:D:210:PRO:HG2	1:D:306:LEU:HA	1.92	0.49
1:D:332:MET:HG3	1:D:356:ILE:HA	1.94	0.49
1:B:826:ASN:N	1:B:865:GLN:O	2.37	0.49
1:B:834:VAL:O	1:B:838:VAL:HG23	2.12	0.49
1:C:484:LEU:HG	1:C:489:HIS:HB2	1.94	0.49
1:C:784:ALA:HB1	1:C:981:ILE:HD11	1.94	0.49
1:C:815:ASP:N	1:C:815:ASP:OD1	2.44	0.49
1:C:1006:ARG:NH1	1:C:1007:ASN:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:ASP:OD1	1:D:606:ARG:HB3	2.12	0.49
1:A:242:SER:HB3	1:A:304:PHE:HD1	1.77	0.49
1:A:376:GLN:NE2	1:A:381:GLN:O	2.45	0.49
1:B:655:ALA:HB1	1:B:1034:LEU:HD13	1.94	0.49
1:D:801:THR:O	1:D:804:GLU:N	2.45	0.49
1:A:60:LEU:HD22	1:A:264:ILE:HA	1.94	0.49
1:A:181:ALA:HA	1:A:277:ARG:NH1	2.27	0.49
1:A:354:VAL:HB	1:A:391:VAL:HG22	1.93	0.49
1:A:474:ARG:HH11	1:A:474:ARG:HB3	1.77	0.49
1:A:571:ARG:HA	1:A:571:ARG:HH11	1.78	0.49
1:A:599:ALA:HB1	1:A:610:ARG:HD3	1.95	0.49
1:A:714:ASP:N	1:A:714:ASP:OD1	2.45	0.49
1:B:1051:ARG:HG3	1:B:1065:VAL:HG13	1.95	0.49
1:C:35:LEU:HA	1:C:63:ASN:HA	1.95	0.49
1:C:178:ARG:O	1:C:182:GLN:HG2	2.13	0.49
1:C:793:ALA:O	1:C:796:LEU:CB	2.61	0.49
1:C:863:HIS:NE2	1:C:899:HIS:HB2	2.27	0.49
1:C:1024:GLU:OE2	1:C:1028:GLN:NE2	2.45	0.49
1:D:603:ASP:OD2	1:D:605:PHE:N	2.44	0.49
1:A:345:ILE:O	1:D:252:ARG:NH2	2.45	0.49
1:A:864:ILE:HD12	1:A:895:CYS:HB3	1.94	0.49
1:B:449:TYR:O	1:B:453:LEU:HG	2.13	0.49
1:B:829:ASP:OD1	1:B:829:ASP:N	2.44	0.49
1:B:1038:HIS:O	1:B:1042:GLN:N	2.46	0.49
1:C:76:GLU:OE1	1:C:277:ARG:HA	2.13	0.49
1:C:219:GLY:HA2	1:C:265:ARG:HH12	1.77	0.49
1:D:56:GLU:N	1:D:56:GLU:OE1	2.46	0.49
1:D:657:LEU:HD11	1:D:694:THR:OG1	2.12	0.49
1:D:1063:PHE:HA	1:D:1066:LEU:HB2	1.94	0.49
1:A:193:ASP:O	1:A:197:VAL:HG23	2.13	0.49
1:A:334:PRO:HD3	1:A:357:ASN:O	2.12	0.49
1:A:509:GLU:H	1:A:509:GLU:CD	2.19	0.49
1:B:169:LEU:HD11	1:B:196:LEU:HD11	1.95	0.49
1:B:222:LYS:HA	1:B:225:LEU:HD12	1.95	0.49
1:D:466:ALA:O	1:D:470:LEU:HG	2.12	0.49
1:D:668:ASP:OD1	1:D:670:THR:OG1	2.31	0.49
1:D:698:GLN:HG2	1:D:702:ARG:HH21	1.78	0.49
1:B:628:ASP:N	1:B:651:GLY:HA3	2.27	0.49
1:B:679:THR:HG22	1:B:732:GLN:HG3	1.94	0.49
1:D:505:LEU:HD22	1:D:510:ARG:HB2	1.95	0.49
1:A:824:PHE:O	1:A:865:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:LEU:O	1:B:796:LEU:HG	2.13	0.49
1:C:74:LEU:HD13	1:C:178:ARG:NH2	2.28	0.49
1:D:219:GLY:H	1:D:222:LYS:HE2	1.77	0.49
1:D:545:THR:HG23	1:D:547:SER:H	1.78	0.49
1:A:28:ARG:HH22	1:A:185:THR:HG22	1.77	0.48
1:A:44:ASN:O	1:A:48:ARG:HG3	2.13	0.48
1:A:679:THR:HA	1:A:732:GLN:HB2	1.95	0.48
1:B:58:ILE:HG12	1:B:260:LEU:HB2	1.95	0.48
1:B:168:THR:HG1	1:B:170:ASP:CG	2.20	0.48
1:B:507:ALA:HA	1:B:510:ARG:NH1	2.28	0.48
1:B:813:ILE:HG21	1:B:851:TYR:HB3	1.94	0.48
1:D:398:ARG:CZ	1:D:440:VAL:HA	2.42	0.48
1:D:402:ASP:O	1:D:405:THR:OG1	2.27	0.48
1:D:703:PHE:HE2	1:D:719:ILE:HD11	1.77	0.48
1:D:854:ASN:OD1	1:D:857:SER:N	2.41	0.48
1:A:210:PRO:HB3	1:A:420:MET:HE3	1.94	0.48
1:B:550:LYS:HB2	1:B:550:LYS:HE2	1.61	0.48
1:D:879:ASN:O	1:D:883:THR:OG1	2.30	0.48
1:B:827:GLY:HA2	1:B:867:SER:HB2	1.95	0.48
1:B:865:GLN:HG3	1:B:866:THR:O	2.13	0.48
1:C:446:ARG:C	1:C:446:ARG:HH11	2.21	0.48
1:A:969:LEU:HA	1:A:972:MET:HE2	1.94	0.48
1:C:53:GLN:NE2	1:C:55:CYS:SG	2.86	0.48
1:A:484:LEU:HD23	1:A:494:LEU:HD11	1.95	0.48
1:D:629:SER:O	1:D:633:TYR:CD2	2.66	0.48
1:A:359:PHE:HB2	1:A:394:THR:C	2.38	0.48
1:A:538:ARG:CZ	1:A:538:ARG:H	2.26	0.48
1:B:36:PHE:CZ	1:B:635:GLU:HG3	2.49	0.48
1:C:739:ASP:O	1:C:743:ASN:ND2	2.45	0.48
1:C:824:PHE:HB2	1:C:864:ILE:HG12	1.95	0.48
1:D:855:ASP:OD1	1:D:855:ASP:N	2.43	0.48
1:A:74:LEU:HD21	1:A:101:LEU:HD22	1.95	0.48
1:A:466:ALA:O	1:A:470:LEU:HG	2.14	0.48
1:B:482:ASP:O	1:B:486:GLY:N	2.42	0.48
1:D:807:LEU:HD21	1:D:813:ILE:HB	1.96	0.48
1:A:891:ILE:HG13	1:A:925:ILE:HG21	1.95	0.48
1:B:599:ALA:HB1	1:B:610:ARG:HD2	1.94	0.48
1:B:939:GLN:HE21	1:B:939:GLN:HB3	1.48	0.48
1:B:1051:ARG:CZ	1:B:1065:VAL:HG22	2.44	0.48
1:C:863:HIS:HD2	1:C:864:ILE:H	1.62	0.48
1:C:986:LEU:O	1:C:989:GLU:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1035:THR:O	1:D:1039:GLY:N	2.38	0.48
1:C:826:ASN:HD22	1:C:832:TYR:HB3	1.78	0.48
1:C:854:ASN:O	1:C:858:GLN:HG3	2.14	0.48
1:D:376:GLN:NE2	1:D:381:GLN:O	2.47	0.48
1:D:795:THR:HA	1:D:798:ASN:ND2	2.29	0.48
1:A:377:ARG:HG2	1:D:48:ARG:CZ	2.44	0.48
1:A:776:ILE:O	1:A:823:PHE:N	2.46	0.48
1:A:834:VAL:O	1:A:838:VAL:HG23	2.14	0.48
1:A:924:ILE:HG12	1:B:1000:ILE:HG13	1.95	0.48
1:B:330:TYR:HD2	1:B:354:VAL:HG13	1.78	0.48
1:B:878:PHE:O	1:B:882:ARG:HG3	2.14	0.48
1:D:800:PHE:CE1	1:D:843:TRP:HZ3	2.27	0.48
1:A:222:LYS:HD2	1:A:223:SER:N	2.29	0.47
1:A:1034:LEU:HG	1:A:1038:HIS:CE1	2.48	0.47
1:B:120:VAL:HB	1:B:123:GLU:HG3	1.95	0.47
1:B:402:ASP:OD1	1:B:402:ASP:N	2.47	0.47
1:B:609:ARG:O	1:B:613:LEU:HG	2.14	0.47
1:B:823:PHE:CD2	1:B:863:HIS:HB3	2.49	0.47
1:B:1068:ASP:OD1	1:B:1068:ASP:N	2.45	0.47
1:C:798:ASN:N	1:C:798:ASN:ND2	2.59	0.47
1:C:809:ARG:HB2	1:C:811:MET:HG2	1.95	0.47
1:D:843:TRP:O	1:D:847:MET:HG2	2.14	0.47
1:A:74:LEU:HD13	1:A:178:ARG:HH21	1.79	0.47
1:A:770:ASN:O	1:A:770:ASN:ND2	2.37	0.47
1:B:864:ILE:O	1:B:899:HIS:N	2.45	0.47
1:C:184:ILE:HD11	1:C:295:VAL:HG13	1.95	0.47
1:C:639:GLU:OE2	1:C:640:ARG:NH1	2.47	0.47
1:C:953:GLU:O	1:C:957:GLN:HG2	2.15	0.47
1:D:800:PHE:CE1	1:D:843:TRP:CE3	2.96	0.47
1:A:843:TRP:O	1:A:847:MET:HG2	2.14	0.47
1:B:590:GLU:OE1	1:B:591:GLY:N	2.46	0.47
1:B:600:GLY:HA2	1:B:607:THR:HG22	1.95	0.47
1:C:376:GLN:HE22	1:C:384:SER:C	2.21	0.47
1:D:184:ILE:HD11	1:D:295:VAL:HG13	1.96	0.47
1:A:657:LEU:HD13	1:A:690:MET:HB3	1.96	0.47
1:A:970:GLY:O	1:A:974:THR:OG1	2.26	0.47
1:A:1038:HIS:O	1:A:1042:GLN:N	2.47	0.47
1:C:252:ARG:HB3	1:C:255:SER:HB3	1.97	0.47
1:D:165:ALA:HA	1:D:182:GLN:HB3	1.96	0.47
1:D:461:HIS:CE1	1:D:841:ARG:HH12	2.32	0.47
1:D:866:THR:OG1	1:D:867:SER:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:LEU:O	1:A:1085:VAL:HG12	2.13	0.47
1:C:1036:GLU:O	1:C:1040:ALA:N	2.44	0.47
1:D:248:ILE:HG22	1:D:312:SER:HB3	1.95	0.47
1:D:368:TRP:CD1	1:D:368:TRP:C	2.93	0.47
1:A:40:ASP:OD1	1:A:40:ASP:N	2.48	0.47
1:A:458:ARG:NH1	1:A:462:ARG:HH11	2.11	0.47
1:B:481:HIS:HA	1:B:494:LEU:HD13	1.97	0.47
1:C:712:THR:OG1	1:C:713:ALA:N	2.47	0.47
1:C:970:GLY:O	1:C:974:THR:OG1	2.28	0.47
1:D:32:ALA:HA	1:D:59:HIS:CE1	2.49	0.47
1:D:543:SER:O	1:D:551:ILE:N	2.23	0.47
1:D:557:PRO:HB3	1:D:559:PHE:CZ	2.50	0.47
1:A:647:VAL:HG11	1:A:1027:LYS:HB3	1.95	0.47
1:A:712:THR:OG1	1:A:713:ALA:N	2.48	0.47
1:A:723:VAL:O	1:A:727:VAL:N	2.48	0.47
1:B:328:SER:O	1:B:353:PHE:N	2.48	0.47
1:C:746:ILE:O	1:C:1089:TYR:N	2.45	0.47
1:D:785:GLY:O	1:D:869:ARG:NH1	2.46	0.47
1:D:787:ASN:CB	1:D:789:ILE:HD12	2.42	0.47
1:D:863:HIS:HE2	1:D:899:HIS:HB2	1.80	0.47
1:D:913:GLU:HB3	1:D:917:ARG:CZ	2.45	0.47
1:A:79:GLN:O	1:A:110:GLN:N	2.48	0.47
1:A:169:LEU:HD11	1:A:196:LEU:HD11	1.97	0.47
1:A:359:PHE:N	1:A:394:THR:O	2.47	0.47
1:A:647:VAL:HB	1:A:1027:LYS:HD3	1.97	0.47
1:B:1089:TYR:HE2	1:B:1091:ARG:HH11	1.63	0.47
1:C:46:MET:HE2	1:C:50:LEU:HD11	1.97	0.47
1:C:656:THR:OG1	1:C:657:LEU:N	2.48	0.47
1:C:997:LEU:HD12	1:C:998:PRO:HD2	1.96	0.47
1:D:602:GLY:HA3	1:D:606:ARG:HD3	1.97	0.47
1:D:629:SER:HB2	1:D:633:TYR:CD2	2.50	0.47
1:A:704:ARG:O	1:A:708:GLY:N	2.48	0.47
1:A:887:ALA:O	1:A:891:ILE:HG12	2.14	0.47
1:A:923:LEU:HD11	1:A:927:ARG:HE	1.80	0.47
1:B:64:ARG:HA	1:B:64:ARG:HH11	1.80	0.47
1:B:999:ILE:O	1:B:1004:THR:N	2.48	0.47
1:D:794:PHE:CZ	1:D:958:GLU:OE2	2.68	0.47
1:D:1051:ARG:CZ	1:D:1065:VAL:HG22	2.45	0.47
1:A:75:GLN:HB3	1:A:275:PHE:HE1	1.80	0.47
1:C:597:MET:O	1:C:624:SER:N	2.44	0.47
1:D:887:ALA:O	1:D:891:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:HD2	1:B:274:ILE:HG13	1.80	0.46
1:B:788:PRO:HG2	1:B:831:GLU:OE1	2.16	0.46
1:B:817:ALA:HA	1:B:820:LEU:HG	1.95	0.46
1:C:152:ASP:O	1:C:156:ARG:HB2	2.16	0.46
1:C:181:ALA:HA	1:C:277:ARG:NH1	2.30	0.46
1:C:843:TRP:O	1:C:846:THR:OG1	2.28	0.46
1:D:177:ARG:HA	1:D:180:LEU:HB2	1.96	0.46
1:D:398:ARG:NH2	1:D:441:ILE:HG12	2.26	0.46
1:D:720:ARG:HH22	1:D:724:LEU:HD11	1.79	0.46
1:D:792:LEU:CD2	1:D:835:LEU:CD1	2.91	0.46
1:A:58:ILE:HG12	1:A:260:LEU:HD12	1.97	0.46
1:A:237:GLN:O	1:A:237:GLN:NE2	2.47	0.46
1:A:330:TYR:CE2	1:A:332:MET:HB3	2.50	0.46
1:A:712:THR:HG22	1:A:715:GLU:HG3	1.97	0.46
1:B:746:ILE:HD12	1:B:1089:TYR:H	1.80	0.46
1:B:797:ALA:O	1:B:801:THR:OG1	2.34	0.46
1:B:989:GLU:HA	1:B:992:LYS:HE2	1.98	0.46
1:B:1055:ALA:HB1	1:B:1062:VAL:HG13	1.95	0.46
1:C:244:ALA:O	1:C:308:ILE:N	2.36	0.46
1:C:1053:ARG:O	1:C:1057:ILE:HG22	2.15	0.46
1:D:253:ARG:NH1	1:D:283:GLU:O	2.47	0.46
1:D:1069:ALA:O	1:D:1073:CYS:N	2.48	0.46
1:A:218:GLY:O	1:D:341:GLN:NE2	2.48	0.46
1:A:515:MET:O	1:A:519:MET:HG2	2.16	0.46
1:B:81:ILE:O	1:B:112:PHE:N	2.36	0.46
1:B:222:LYS:NZ	1:B:310:GLU:OE2	2.48	0.46
1:B:965:ARG:HH22	1:C:365:GLN:HB3	1.81	0.46
1:B:986:LEU:O	1:B:989:GLU:HG2	2.16	0.46
1:C:801:THR:HG23	1:C:968:VAL:HG21	1.92	0.46
1:D:442:VAL:HG21	1:D:804:GLU:HG2	1.96	0.46
1:A:463:ARG:NH1	1:A:467:GLN:HG3	2.30	0.46
1:A:818:PRO:HG3	1:A:857:SER:HA	1.97	0.46
1:A:986:LEU:O	1:A:989:GLU:HG2	2.15	0.46
1:D:581:THR:HG22	1:D:841:ARG:HG3	1.98	0.46
1:A:238:ASP:OD1	1:A:238:ASP:N	2.49	0.46
1:C:120:VAL:O	1:C:124:ILE:N	2.43	0.46
1:D:247:SER:HB2	1:D:276:MET:HE1	1.97	0.46
1:A:120:VAL:HG12	1:A:122:ASP:H	1.79	0.46
1:A:246:ILE:HG13	1:A:309:VAL:HG13	1.98	0.46
1:B:218:GLY:HA2	1:B:222:LYS:HZ1	1.80	0.46
1:B:485:GLN:HE22	1:B:491:SER:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:VAL:HG13	1:B:635:GLU:HB2	1.97	0.46
1:B:720:ARG:HH22	1:B:724:LEU:HD21	1.81	0.46
1:C:110:GLN:CD	1:C:156:ARG:HH12	2.23	0.46
1:D:398:ARG:HH22	1:D:441:ILE:CD1	2.28	0.46
1:D:403:GLY:HA2	1:D:406:MET:SD	2.55	0.46
1:D:518:GLN:HE21	1:D:518:GLN:HB3	1.50	0.46
1:A:246:ILE:HD11	1:A:309:VAL:HG22	1.98	0.46
1:A:554:VAL:HG23	1:A:935:GLU:HB2	1.98	0.46
1:C:696:ILE:HG23	1:C:719:ILE:HG21	1.97	0.46
1:A:605:PHE:HE1	1:A:662:VAL:HG11	1.80	0.46
1:A:628:ASP:O	1:A:631:THR:OG1	2.34	0.46
1:A:730:THR:HA	1:A:772:TYR:O	2.16	0.46
1:B:44:ASN:OD1	1:B:48:ARG:NE	2.49	0.46
1:B:359:PHE:HB2	1:B:394:THR:C	2.41	0.46
1:B:433:ARG:HE	1:B:433:ARG:N	2.13	0.46
1:D:189:ASN:OD1	1:D:191:LYS:NZ	2.46	0.46
1:D:727:VAL:O	1:D:770:ASN:HB3	2.16	0.46
1:A:467:GLN:HE22	1:A:506:GLY:H	1.63	0.46
1:A:559:PHE:HB2	1:A:565:ILE:HD11	1.98	0.46
1:A:627:PHE:HD1	1:A:627:PHE:HA	1.66	0.46
1:A:1034:LEU:HD11	1:A:1074:SER:HB2	1.98	0.46
1:B:181:ALA:HA	1:B:277:ARG:NH1	2.31	0.46
1:C:796:LEU:CG	1:C:800:PHE:CZ	2.98	0.46
1:D:409:GLN:NE2	1:D:429:ASN:OD1	2.49	0.46
1:D:463:ARG:NH2	1:D:464:VAL:HG22	2.31	0.46
1:A:29:PHE:HB2	1:A:57:VAL:HG22	1.98	0.46
1:A:518:GLN:H	1:A:518:GLN:HG2	1.55	0.46
1:B:545:THR:HG23	1:B:547:SER:H	1.80	0.46
1:C:368:TRP:C	1:C:368:TRP:CD1	2.94	0.46
1:A:647:VAL:HB	1:A:1027:LYS:HZ2	1.80	0.45
1:B:847:MET:N	1:B:847:MET:SD	2.89	0.45
1:C:628:ASP:N	1:C:651:GLY:HA3	2.31	0.45
1:A:91:VAL:O	1:A:95:LYS:HE2	2.15	0.45
1:A:550:LYS:HE2	1:A:550:LYS:HB2	1.73	0.45
1:B:704:ARG:O	1:B:708:GLY:N	2.47	0.45
1:B:1034:LEU:HG	1:B:1038:HIS:CE1	2.50	0.45
1:C:381:GLN:HB3	1:C:384:SER:HG	1.81	0.45
1:D:253:ARG:HH22	1:D:281:THR:HG21	1.80	0.45
1:D:401:ASP:OD2	1:D:404:VAL:N	2.48	0.45
1:D:628:ASP:HB3	1:D:649:ASN:O	2.15	0.45
1:D:669:LEU:H	1:D:669:LEU:HG	1.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:779:TYR:HB2	1:D:823:PHE:CE1	2.51	0.45
1:D:828:MET:HE3	1:D:828:MET:HB3	1.88	0.45
1:A:501:ARG:O	1:A:505:LEU:N	2.47	0.45
1:A:964:GLU:O	1:D:362:LYS:NZ	2.46	0.45
1:B:56:GLU:N	1:B:56:GLU:OE1	2.49	0.45
1:B:848:ARG:HD3	1:B:849:ASP:OD1	2.16	0.45
1:C:1038:HIS:O	1:C:1042:GLN:N	2.49	0.45
1:D:107:GLU:H	1:D:107:GLU:CD	2.24	0.45
1:D:458:ARG:NH1	1:D:462:ARG:HB2	2.31	0.45
1:D:511:LYS:O	1:D:515:MET:HG2	2.16	0.45
1:D:843:TRP:CD1	1:D:860:LEU:HB2	2.52	0.45
1:B:748:SER:OG	1:B:751:PHE:HB3	2.15	0.45
1:B:879:ASN:O	1:B:883:THR:OG1	2.35	0.45
1:C:409:GLN:NE2	1:C:429:ASN:OD1	2.49	0.45
1:C:763:PHE:HB3	1:C:768:VAL:HB	1.97	0.45
1:D:231:ARG:O	1:D:235:LEU:HG	2.17	0.45
1:D:531:LYS:HA	1:D:536:GLU:HA	1.97	0.45
1:D:580:TYR:CD1	1:D:584:VAL:HA	2.51	0.45
1:D:641:PRO:HA	1:D:644:TYR:CD2	2.52	0.45
1:D:670:THR:HB	1:D:726:ASN:ND2	2.31	0.45
1:D:788:PRO:HB3	1:D:832:TYR:CZ	2.51	0.45
1:A:555:VAL:HB	1:B:943:LEU:HD23	1.98	0.45
1:A:759:ILE:HG12	1:A:763:PHE:CZ	2.52	0.45
1:B:392:TYR:CE1	1:B:433:ARG:HB2	2.52	0.45
1:B:443:PRO:HB2	1:B:446:ARG:HB2	1.99	0.45
1:C:47:ARG:HE	1:C:259:LEU:HD21	1.80	0.45
1:C:252:ARG:N	1:C:257:GLY:O	2.37	0.45
1:C:438:GLN:HG2	1:C:439:ASN:H	1.82	0.45
1:A:338:ALA:O	1:A:341:GLN:HG2	2.17	0.45
1:A:448:ARG:NH1	1:D:447:SER:OG	2.36	0.45
1:A:827:GLY:C	1:A:886:GLN:HE22	2.25	0.45
1:B:330:TYR:HE2	1:B:332:MET:HB3	1.82	0.45
1:C:214:ILE:HG23	1:C:329:LEU:HD12	1.99	0.45
1:C:883:THR:HA	1:C:886:GLN:HG2	1.98	0.45
1:C:907:ILE:O	1:C:1019:LEU:N	2.49	0.45
1:D:594:PRO:HB2	1:D:596:ARG:HE	1.81	0.45
1:D:843:TRP:CD2	1:D:860:LEU:HD12	2.52	0.45
1:D:1068:ASP:OD1	1:D:1068:ASP:N	2.49	0.45
1:A:30:VAL:HG23	1:A:78:VAL:HG21	1.98	0.45
1:A:725:GLN:HE21	1:A:725:GLN:HB3	1.62	0.45
1:B:578:PHE:CZ	1:B:848:ARG:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:ASN:ND2	1:C:790:SER:H	2.15	0.45
1:D:443:PRO:HG2	1:D:443:PRO:O	2.17	0.45
1:D:1080:HIS:HA	1:D:1083:PHE:CD2	2.51	0.45
1:A:119:ILE:HD12	1:A:124:ILE:HD11	1.99	0.45
1:B:29:PHE:HB2	1:B:57:VAL:HG22	1.98	0.45
1:C:239:ASP:N	1:C:239:ASP:OD1	2.50	0.45
1:C:727:VAL:HG11	1:C:768:VAL:HG13	1.99	0.45
1:C:840:ARG:HH12	1:C:893:ASP:HB3	1.82	0.45
1:A:165:ALA:HA	1:A:182:GLN:HB3	1.98	0.45
1:A:472:ARG:HH21	1:B:561:ASP:HA	1.82	0.45
1:A:785:GLY:HA2	1:A:869:ARG:HD3	1.98	0.45
1:B:44:ASN:O	1:B:48:ARG:HG3	2.17	0.45
1:B:168:THR:OG1	1:B:169:LEU:N	2.49	0.45
1:C:64:ARG:HA	1:C:64:ARG:NH1	2.32	0.45
1:C:580:TYR:CD2	1:C:584:VAL:HA	2.52	0.45
1:C:865:GLN:HG3	1:C:866:THR:O	2.17	0.45
1:D:892:TYR:CD1	1:D:937:PRO:HG2	2.52	0.45
1:D:1052:LEU:HD13	1:D:1081:ALA:HB1	1.99	0.45
1:A:354:VAL:HB	1:A:391:VAL:HG13	2.00	0.44
1:A:448:ARG:HE	1:D:448:ARG:HH21	1.64	0.44
1:A:507:ALA:HA	1:A:510:ARG:NH1	2.31	0.44
1:A:879:ASN:HA	1:A:882:ARG:NE	2.31	0.44
1:A:943:LEU:HD22	1:B:555:VAL:HB	1.99	0.44
1:B:601:GLU:OE1	1:B:651:GLY:N	2.50	0.44
1:B:977:GLN:HE22	1:B:978:ARG:HG3	1.82	0.44
1:B:1063:PHE:HA	1:B:1066:LEU:HB2	1.99	0.44
1:D:136:TYR:CE1	1:D:149:MET:HG3	2.53	0.44
1:D:229:LEU:HD22	1:D:408:TYR:HD2	1.81	0.44
1:D:375:VAL:HA	1:D:378:ASN:ND2	2.32	0.44
1:D:514:ALA:O	1:D:517:PRO:HD2	2.16	0.44
1:D:628:ASP:N	1:D:651:GLY:HA3	2.33	0.44
1:D:643:ILE:O	1:D:647:VAL:HG23	2.16	0.44
1:D:878:PHE:O	1:D:882:ARG:HG3	2.17	0.44
1:B:901:ASN:OD1	1:B:901:ASN:N	2.50	0.44
1:B:929:TRP:HA	1:B:929:TRP:CE3	2.51	0.44
1:B:945:GLU:H	1:B:945:GLU:HG2	1.51	0.44
1:B:1029:SER:O	1:B:1033:ARG:HG3	2.16	0.44
1:C:477:LEU:HD11	1:C:497:LEU:HB3	1.99	0.44
1:C:699:GLN:HG2	1:C:702:ARG:HH21	1.82	0.44
1:A:953:GLU:O	1:A:957:GLN:HG2	2.18	0.44
1:B:248:ILE:HD11	1:B:292:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ILE:HG21	1:B:321:ILE:HD11	1.99	0.44
1:B:415:LEU:HB3	1:B:420:MET:HB3	1.99	0.44
1:C:707:ASN:HB3	1:C:709:ARG:NH1	2.32	0.44
1:D:193:ASP:H	1:D:196:LEU:HD23	1.82	0.44
1:D:432:GLY:HA2	1:D:433:ARG:HH21	1.82	0.44
1:A:989:GLU:HA	1:A:992:LYS:HE2	1.98	0.44
1:B:389:MET:HE3	1:B:390:PRO:HD2	1.98	0.44
1:C:177:ARG:HG2	1:C:275:PHE:CG	2.52	0.44
1:C:446:ARG:HH21	1:C:452:GLU:CD	2.25	0.44
1:D:48:ARG:HG3	1:D:51:GLN:HE21	1.81	0.44
1:D:75:GLN:NE2	1:D:276:MET:O	2.50	0.44
1:D:209:VAL:HG22	1:D:300:LYS:HG2	1.99	0.44
1:D:938:ASN:OD1	1:D:938:ASN:N	2.51	0.44
1:A:267:ASN:HB2	1:A:1088:GLN:HE22	1.83	0.44
1:A:627:PHE:HB3	1:A:632:LEU:HG	2.00	0.44
1:B:237:GLN:O	1:B:237:GLN:NE2	2.50	0.44
1:B:269:ILE:H	1:B:269:ILE:HG13	1.61	0.44
1:C:218:GLY:HA2	1:C:222:LYS:HZ3	1.83	0.44
1:C:824:PHE:O	1:C:865:GLN:N	2.50	0.44
1:B:633:TYR:OH	1:B:744:THR:O	2.23	0.44
1:B:969:LEU:HD12	1:B:969:LEU:H	1.82	0.44
1:C:41:ALA:O	1:C:45:ILE:HG12	2.18	0.44
1:A:843:TRP:NE1	1:A:858:GLN:O	2.51	0.44
1:A:1005:PHE:HB2	1:B:923:LEU:HD23	1.99	0.44
1:A:1051:ARG:CZ	1:A:1065:VAL:HG22	2.47	0.44
1:B:801:THR:HA	1:B:804:GLU:CD	2.43	0.44
1:B:965:ARG:NH2	1:C:365:GLN:HB3	2.32	0.44
1:C:581:THR:HG22	1:C:841:ARG:HB2	2.00	0.44
1:C:599:ALA:HB1	1:C:610:ARG:HD2	1.99	0.44
1:C:785:GLY:HA2	1:C:869:ARG:HD3	1.99	0.44
1:D:609:ARG:O	1:D:613:LEU:HG	2.17	0.44
1:B:246:ILE:HG13	1:B:309:VAL:HG13	2.00	0.44
1:B:643:ILE:O	1:B:647:VAL:HG23	2.18	0.44
1:C:796:LEU:HA	1:C:796:LEU:HD13	1.62	0.44
1:D:369:ARG:NE	1:D:370:ASP:OD1	2.51	0.44
1:D:557:PRO:HB3	1:D:559:PHE:CE2	2.52	0.44
1:A:64:ARG:HH22	1:A:68:GLU:HB3	1.82	0.44
1:A:777:SER:HB3	1:A:823:PHE:HB3	1.99	0.44
1:B:573:ASN:ND2	1:B:578:PHE:O	2.51	0.44
1:B:1030:GLN:HE21	1:B:1030:GLN:HB3	1.57	0.44
1:B:1075:LEU:HA	1:B:1078:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:THR:HG23	1:C:1070:VAL:HG12	2.00	0.44
1:D:353:PHE:CE2	1:D:390:PRO:HB2	2.52	0.44
1:D:856:ARG:HA	1:D:859:LYS:HE3	1.99	0.44
1:A:34:SER:OG	1:A:35:LEU:N	2.51	0.43
1:A:518:GLN:O	1:A:522:ALA:N	2.33	0.43
1:A:629:SER:HA	1:A:632:LEU:HB2	2.00	0.43
1:A:828:MET:HA	1:A:886:GLN:OE1	2.18	0.43
1:B:778:GLY:HA2	1:B:781:ILE:HD12	2.00	0.43
1:B:912:ALA:O	1:B:915:VAL:HG22	2.18	0.43
1:D:193:ASP:O	1:D:197:VAL:HG23	2.18	0.43
1:D:515:MET:O	1:D:519:MET:HG2	2.18	0.43
1:A:642:ASP:OD1	1:A:643:ILE:N	2.48	0.43
1:B:374:GLN:OE1	1:B:378:ASN:ND2	2.47	0.43
1:D:1050:ALA:HA	1:D:1053:ARG:NH1	2.33	0.43
1:A:219:GLY:HA2	1:A:265:ARG:HH22	1.83	0.43
1:A:354:VAL:O	1:A:391:VAL:HA	2.17	0.43
1:A:360:ASP:OD1	1:A:360:ASP:N	2.51	0.43
1:A:431:GLU:N	1:A:431:GLU:OE1	2.51	0.43
1:A:443:PRO:HG2	1:A:446:ARG:HD2	2.00	0.43
1:A:501:ARG:HA	1:A:504:SER:HB2	2.00	0.43
1:A:815:ASP:OD1	1:A:815:ASP:N	2.51	0.43
1:B:815:ASP:OD1	1:B:815:ASP:N	2.51	0.43
1:D:30:VAL:HG23	1:D:78:VAL:HG21	1.99	0.43
1:A:849:ASP:OD1	1:A:849:ASP:N	2.50	0.43
1:B:60:LEU:HD12	1:B:69:VAL:HG22	2.01	0.43
1:C:500:GLU:OE1	1:C:501:ARG:NH1	2.51	0.43
1:C:817:ALA:HB3	1:C:857:SER:HB3	1.99	0.43
1:C:829:ASP:OD1	1:C:829:ASP:N	2.51	0.43
1:C:836:GLY:O	1:C:840:ARG:HG3	2.18	0.43
1:D:458:ARG:HH12	1:D:462:ARG:HH11	1.67	0.43
1:A:107:GLU:CD	1:A:107:GLU:H	2.26	0.43
1:A:211:VAL:HG22	1:A:307:VAL:HB	1.99	0.43
1:A:349:ASP:HB2	1:D:252:ARG:NH2	2.33	0.43
1:A:516:TRP:CH2	1:A:520:GLN:HB2	2.53	0.43
1:A:976:TYR:O	1:A:980:LYS:HG2	2.18	0.43
1:B:823:PHE:HD2	1:B:863:HIS:HB3	1.83	0.43
1:C:570:MET:SD	1:C:570:MET:N	2.92	0.43
1:C:804:GLU:O	1:C:808:ALA:N	2.44	0.43
1:D:381:GLN:HB3	1:D:384:SER:OG	2.18	0.43
1:A:31:THR:HG22	1:A:82:ALA:HB3	2.00	0.43
1:A:882:ARG:O	1:A:886:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:834:VAL:O	1:C:838:VAL:HG23	2.18	0.43
1:C:862:TYR:O	1:C:896:ASN:ND2	2.49	0.43
1:D:402:ASP:HB2	1:D:406:MET:HE3	2.00	0.43
1:D:747:PHE:HB3	1:D:751:PHE:CE1	2.48	0.43
1:D:1081:ALA:O	1:D:1084:GLU:HB3	2.18	0.43
1:A:78:VAL:O	1:A:109:ILE:HD12	2.19	0.43
1:A:83:ILE:HB	1:A:113:GLY:HA2	1.99	0.43
1:A:990:GLN:O	1:A:994:ASP:HB2	2.18	0.43
1:B:621:LYS:N	1:B:673:SER:O	2.48	0.43
1:B:758:ASP:HB3	1:B:1061:ASN:CG	2.44	0.43
1:C:241:LEU:HD21	1:C:306:LEU:HD23	2.00	0.43
1:C:628:ASP:N	1:C:628:ASP:OD1	2.52	0.43
1:C:822:PHE:CE2	1:C:860:LEU:HD11	2.53	0.43
1:D:81:ILE:HG21	1:D:97:MET:HE1	2.00	0.43
1:D:474:ARG:NH2	1:D:475:GLN:HA	2.34	0.43
1:D:881:ILE:H	1:D:881:ILE:HG13	1.58	0.43
1:D:976:TYR:CZ	1:D:980:LYS:HD3	2.53	0.43
1:D:1022:SER:HB3	1:D:1027:LYS:NZ	2.34	0.43
1:A:244:ALA:N	1:A:306:LEU:O	2.42	0.43
1:A:411:LEU:O	1:A:415:LEU:HG	2.18	0.43
1:A:449:TYR:O	1:A:453:LEU:HG	2.19	0.43
1:B:177:ARG:HG2	1:B:275:PHE:CG	2.54	0.43
1:B:215:THR:O	1:B:331:VAL:N	2.37	0.43
1:B:447:SER:C	1:B:449:TYR:N	2.75	0.43
1:B:827:GLY:C	1:B:886:GLN:HE22	2.27	0.43
1:C:385:ARG:HA	1:C:385:ARG:HD2	1.76	0.43
1:C:418:ARG:HD2	1:C:418:ARG:HA	1.80	0.43
1:D:35:LEU:HD11	1:D:65:SER:HA	2.01	0.43
1:D:241:LEU:HD12	1:D:305:ASP:HB2	2.01	0.43
1:D:464:VAL:HG21	1:D:571:ARG:HH12	1.84	0.43
1:D:609:ARG:HA	1:D:609:ARG:HH11	1.84	0.43
1:D:942:PHE:O	1:D:945:GLU:HG2	2.19	0.43
1:A:178:ARG:O	1:A:182:GLN:HG2	2.19	0.43
1:A:218:GLY:HA2	1:A:222:LYS:HZ3	1.84	0.43
1:A:540:GLY:O	1:A:553:LYS:NZ	2.38	0.43
1:D:100:LEU:O	1:D:104:HIS:N	2.52	0.43
1:D:359:PHE:HD1	1:D:359:PHE:HA	1.73	0.43
1:A:282:ARG:HA	1:A:282:ARG:HD3	1.66	0.43
1:A:381:GLN:HB3	1:A:384:SER:OG	2.19	0.43
1:A:385:ARG:HA	1:A:385:ARG:HD2	1.81	0.43
1:A:468:SER:HA	1:A:566:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ARG:O	1:B:51:GLN:NE2	2.52	0.43
1:B:555:VAL:H	1:B:936:ASN:ND2	2.12	0.43
1:B:826:ASN:ND2	1:B:832:TYR:HB3	2.33	0.43
1:C:605:PHE:O	1:C:609:ARG:HG2	2.19	0.43
1:C:636:ASP:HB2	1:C:1076:GLY:HA3	2.00	0.43
1:D:29:PHE:HB2	1:D:57:VAL:HG22	2.01	0.43
1:D:210:PRO:HB3	1:D:420:MET:HE3	2.00	0.43
1:D:418:ARG:HD2	1:D:418:ARG:HA	1.66	0.43
1:A:44:ASN:OD1	1:A:48:ARG:NE	2.49	0.42
1:A:433:ARG:H	1:A:433:ARG:HE	1.65	0.42
1:A:476:GLN:NE2	1:B:479:ALA:HB3	2.34	0.42
1:A:777:SER:HA	1:A:823:PHE:O	2.19	0.42
1:D:59:HIS:CE1	1:D:61:GLY:H	2.37	0.42
1:D:75:GLN:HE22	1:D:276:MET:HB3	1.83	0.42
1:D:262:ASP:HA	1:D:265:ARG:HE	1.84	0.42
1:D:441:ILE:HD11	1:D:750:GLU:HB2	2.01	0.42
1:D:713:ALA:HA	1:D:716:GLU:HB3	2.00	0.42
1:D:728:ARG:HG2	1:D:770:ASN:ND2	2.34	0.42
1:D:843:TRP:NE1	1:D:858:GLN:O	2.43	0.42
1:A:239:ASP:OD1	1:A:239:ASP:N	2.52	0.42
1:B:449:TYR:OH	1:B:801:THR:OG1	2.23	0.42
1:C:368:TRP:CZ2	1:C:433:ARG:HG3	2.54	0.42
1:C:585:PHE:HD1	1:C:585:PHE:HA	1.72	0.42
1:C:823:PHE:CD2	1:C:863:HIS:HB3	2.53	0.42
1:D:47:ARG:HH11	1:D:59:HIS:HD2	1.67	0.42
1:D:127:LEU:HB3	1:D:132:VAL:HG11	2.01	0.42
1:D:400:ASN:OD1	1:D:400:ASN:N	2.53	0.42
1:D:657:LEU:HD13	1:D:690:MET:HB3	2.01	0.42
1:D:777:SER:HA	1:D:823:PHE:HB3	2.01	0.42
1:A:91:VAL:HG22	1:A:127:LEU:HD21	2.01	0.42
1:A:377:ARG:NH2	1:D:49:ILE:HG13	2.35	0.42
1:A:923:LEU:HD12	1:A:923:LEU:HA	1.92	0.42
1:A:1081:ALA:HA	1:A:1084:GLU:HB3	2.00	0.42
1:B:596:ARG:HA	1:B:596:ARG:HD3	1.80	0.42
1:D:848:ARG:O	1:D:852:GLY:N	2.44	0.42
1:D:882:ARG:O	1:D:886:GLN:HG2	2.18	0.42
1:D:1045:ALA:HA	1:D:1048:MET:HG2	2.01	0.42
1:A:1078:ILE:O	1:A:1082:LEU:HG	2.18	0.42
1:B:282:ARG:HD3	1:B:282:ARG:HA	1.78	0.42
1:B:379:ARG:HA	1:B:379:ARG:NH1	2.34	0.42
1:B:411:LEU:HD22	1:B:411:LEU:HA	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:TYR:CE2	1:B:804:GLU:OE1	2.72	0.42
1:B:1001:GLY:N	1:B:1004:THR:O	2.43	0.42
1:C:446:ARG:O	1:C:446:ARG:HD3	2.19	0.42
1:C:571:ARG:HA	1:C:571:ARG:HH11	1.85	0.42
1:D:385:ARG:HB3	1:D:387:GLU:OE1	2.19	0.42
1:D:927:ARG:NE	1:D:928:GLU:OE2	2.53	0.42
1:A:362:LYS:NZ	1:D:964:GLU:O	2.51	0.42
1:A:415:LEU:HB3	1:A:420:MET:HB3	2.01	0.42
1:A:774:VAL:HG21	1:A:820:LEU:HD23	2.01	0.42
1:C:677:SER:HA	1:C:730:THR:HB	2.02	0.42
1:D:527:GLU:HG3	1:D:539:THR:C	2.45	0.42
1:D:787:ASN:O	1:D:790:SER:HB2	2.19	0.42
1:A:219:GLY:HA2	1:A:265:ARG:NH2	2.35	0.42
1:A:608:ASN:ND2	1:A:662:VAL:O	2.50	0.42
1:A:813:ILE:HG21	1:A:851:TYR:HB3	2.02	0.42
1:B:186:ALA:O	1:B:190:GLY:N	2.52	0.42
1:B:510:ARG:HA	1:B:513:LEU:HB3	2.01	0.42
1:C:976:TYR:O	1:C:980:LYS:HG2	2.20	0.42
1:D:238:ASP:N	1:D:238:ASP:OD1	2.49	0.42
1:D:336:PHE:HE2	1:D:339:ALA:HA	1.83	0.42
1:D:883:THR:HA	1:D:886:GLN:HG2	2.01	0.42
1:A:215:THR:HA	1:A:311:THR:OG1	2.19	0.42
1:A:441:ILE:HG13	1:A:750:GLU:HB3	1.96	0.42
1:A:836:GLY:O	1:A:840:ARG:HG3	2.19	0.42
1:B:360:ASP:OD1	1:B:360:ASP:N	2.51	0.42
1:C:231:ARG:O	1:C:235:LEU:HG	2.19	0.42
1:C:234:ARG:HH21	1:C:271:HIS:HB2	1.85	0.42
1:D:865:GLN:HB2	1:D:899:HIS:HB3	2.00	0.42
1:A:63:ASN:HD21	1:A:744:THR:HG22	1.85	0.42
1:A:395:GLN:OE1	1:A:397:SER:N	2.52	0.42
1:A:866:THR:OG1	1:A:867:SER:N	2.53	0.42
1:B:559:PHE:HB2	1:B:565:ILE:HD11	2.02	0.42
1:C:330:TYR:HE2	1:C:332:MET:HB3	1.84	0.42
1:C:842:ILE:O	1:C:846:THR:HG23	2.20	0.42
1:C:1059:ASN:OD1	1:C:1059:ASN:N	2.52	0.42
1:D:218:GLY:HA2	1:D:222:LYS:NZ	2.34	0.42
1:A:1048:MET:HB3	1:A:1073:CYS:SG	2.60	0.42
1:A:1053:ARG:O	1:A:1057:ILE:HG22	2.20	0.42
1:B:97:MET:HE2	1:B:101:LEU:HD11	2.02	0.42
1:B:725:GLN:HE21	1:B:725:GLN:HB3	1.64	0.42
1:B:952:GLU:O	1:B:956:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1090:ARG:H	1:B:1090:ARG:HD3	1.84	0.42
1:B:1090:ARG:HG2	1:B:1092:ASN:HD22	1.85	0.42
1:C:481:HIS:HA	1:C:494:LEU:HD13	2.01	0.42
1:C:601:GLU:OE1	1:C:651:GLY:N	2.52	0.42
1:D:76:GLU:OE1	1:D:277:ARG:HA	2.20	0.42
1:D:112:PHE:HB3	1:D:136:TYR:HE2	1.85	0.42
1:D:245:VAL:HA	1:D:308:ILE:O	2.20	0.42
1:A:152:ASP:O	1:A:156:ARG:HB2	2.19	0.42
1:A:160:ASP:OD1	1:A:163:ARG:NE	2.36	0.42
1:A:313:GLY:O	1:D:316:GLN:NE2	2.48	0.42
1:A:377:ARG:HH21	1:D:49:ILE:HG13	1.85	0.42
1:A:457:VAL:HG13	1:A:461:HIS:CE1	2.55	0.42
1:A:561:ASP:HA	1:B:472:ARG:HH21	1.85	0.42
1:A:850:LYS:HB3	1:A:851:TYR:CD2	2.54	0.42
1:A:850:LYS:HD2	1:A:851:TYR:CE1	2.55	0.42
1:B:515:MET:HA	1:B:518:GLN:OE1	2.20	0.42
1:B:625:THR:HB	1:B:678:MET:HA	2.02	0.42
1:C:669:LEU:H	1:C:669:LEU:HG	1.59	0.42
1:D:234:ARG:NH1	1:D:239:ASP:OD2	2.53	0.42
1:D:571:ARG:HA	1:D:571:ARG:HH11	1.85	0.42
1:D:601:GLU:O	1:D:607:THR:HG23	2.20	0.42
1:D:638:HIS:CE1	1:D:640:ARG:HG2	2.54	0.42
1:D:840:ARG:NH1	1:D:893:ASP:O	2.38	0.42
1:A:298:ALA:O	1:A:302:ALA:N	2.53	0.41
1:A:474:ARG:HB3	1:A:474:ARG:NH1	2.35	0.41
1:A:476:GLN:HA	1:B:476:GLN:HE21	1.85	0.41
1:A:627:PHE:CE1	1:A:652:VAL:HG13	2.55	0.41
1:A:1029:SER:O	1:A:1033:ARG:HG3	2.19	0.41
1:B:577:SER:O	1:B:580:TYR:N	2.41	0.41
1:B:824:PHE:N	1:B:863:HIS:O	2.46	0.41
1:C:854:ASN:OD1	1:C:857:SER:N	2.48	0.41
1:C:882:ARG:O	1:C:886:GLN:HG2	2.19	0.41
1:D:28:ARG:HB2	1:D:78:VAL:HA	2.02	0.41
1:D:792:LEU:HD22	1:D:835:LEU:CG	2.50	0.41
1:D:850:LYS:HB3	1:D:851:TYR:CE2	2.54	0.41
1:D:879:ASN:HA	1:D:882:ARG:NE	2.34	0.41
1:A:432:GLY:HA2	1:A:433:ARG:NH2	2.35	0.41
1:A:475:GLN:NE2	1:A:562:GLU:H	2.17	0.41
1:A:727:VAL:O	1:A:770:ASN:HB3	2.21	0.41
1:B:628:ASP:OD2	1:B:653:SER:OG	2.36	0.41
1:C:328:SER:H	1:C:352:ASP:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:VAL:HG13	1:C:635:GLU:HB2	2.01	0.41
1:C:850:LYS:HB3	1:C:851:TYR:CD2	2.55	0.41
1:D:222:LYS:HD2	1:D:223:SER:N	2.35	0.41
1:D:445:ALA:C	1:D:447:SER:H	2.27	0.41
1:A:64:ARG:NH1	1:A:64:ARG:HA	2.36	0.41
1:A:1005:PHE:CE2	1:B:920:ALA:HB2	2.54	0.41
1:B:211:VAL:HA	1:B:307:VAL:O	2.21	0.41
1:C:525:GLY:C	1:C:552:ARG:HH21	2.29	0.41
1:D:95:LYS:HG2	1:D:130:TYR:CZ	2.55	0.41
1:D:236:ASP:HB2	1:D:427:LEU:HD11	2.02	0.41
1:D:329:LEU:HD22	1:D:330:TYR:N	2.36	0.41
1:D:511:LYS:HB3	1:D:511:LYS:HE3	1.86	0.41
1:D:518:GLN:O	1:D:522:ALA:N	2.48	0.41
1:D:545:THR:HG22	1:D:549:THR:H	1.86	0.41
1:D:924:ILE:HG23	1:D:928:GLU:HB2	2.02	0.41
1:D:991:LEU:HD13	1:D:997:LEU:HD13	2.02	0.41
1:D:1048:MET:HE3	1:D:1072:VAL:HB	2.02	0.41
1:A:449:TYR:OH	1:A:801:THR:OG1	2.39	0.41
1:D:29:PHE:HD1	1:D:80:GLY:HA3	1.85	0.41
1:D:737:LYS:HA	1:D:740:GLN:HG2	2.02	0.41
1:D:885:LEU:O	1:D:889:ILE:HG23	2.21	0.41
1:D:953:GLU:O	1:D:957:GLN:HG2	2.20	0.41
1:A:517:PRO:HA	1:A:520:GLN:OE1	2.21	0.41
1:B:354:VAL:HB	1:B:391:VAL:HG22	2.02	0.41
1:B:696:ILE:HG23	1:B:719:ILE:HG21	2.03	0.41
1:C:458:ARG:HE	1:C:458:ARG:HB3	1.72	0.41
1:D:597:MET:HB2	1:D:623:LEU:HA	2.02	0.41
1:D:1045:ALA:O	1:D:1049:LEU:HG	2.21	0.41
1:A:76:GLU:OE1	1:A:277:ARG:HD2	2.21	0.41
1:A:445:ALA:C	1:D:448:ARG:HH12	2.29	0.41
1:A:646:LYS:HB3	1:A:646:LYS:HE2	1.87	0.41
1:B:376:GLN:HE22	1:B:384:SER:C	2.29	0.41
1:D:700:ILE:HG23	1:D:711:PRO:HG2	2.02	0.41
1:D:788:PRO:N	1:D:789:ILE:HD12	2.36	0.41
1:D:986:LEU:O	1:D:989:GLU:HG2	2.21	0.41
1:A:245:VAL:O	1:A:276:MET:HA	2.21	0.41
1:A:756:MET:O	1:A:759:ILE:HG22	2.20	0.41
1:A:987:TYR:O	1:A:991:LEU:HG	2.21	0.41
1:B:313:GLY:O	1:C:316:GLN:NE2	2.53	0.41
1:B:368:TRP:CZ2	1:B:392:TYR:HA	2.56	0.41
1:B:418:ARG:HA	1:B:418:ARG:HD2	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LEU:H	1:B:546:LEU:HD22	1.86	0.41
1:B:581:THR:HG22	1:B:841:ARG:HB2	2.03	0.41
1:D:234:ARG:HG2	1:D:239:ASP:HA	2.02	0.41
1:D:271:HIS:CD2	1:D:274:ILE:HG13	2.55	0.41
1:D:431:GLU:N	1:D:431:GLU:OE1	2.54	0.41
1:A:742:GLN:O	1:A:744:THR:HG23	2.20	0.41
1:A:1030:GLN:HE21	1:A:1030:GLN:HB3	1.57	0.41
1:B:669:LEU:H	1:B:669:LEU:HG	1.59	0.41
1:D:415:LEU:HB3	1:D:420:MET:HB3	2.02	0.41
1:D:452:GLU:O	1:D:456:THR:OG1	2.30	0.41
1:A:181:ALA:HA	1:A:277:ARG:HH12	1.85	0.41
1:A:275:PHE:CE2	1:A:277:ARG:HB2	2.56	0.41
1:A:406:MET:HE2	1:A:431:GLU:O	2.20	0.41
1:A:621:LYS:HB2	1:A:674:THR:HA	2.02	0.41
1:A:778:GLY:O	1:A:782:ALA:N	2.37	0.41
1:A:828:MET:HE3	1:A:828:MET:HB3	1.95	0.41
1:A:881:ILE:H	1:A:881:ILE:HG13	1.55	0.41
1:A:1000:ILE:HG12	1:B:928:GLU:HG2	2.02	0.41
1:A:1045:ALA:HA	1:A:1048:MET:HG2	2.03	0.41
1:B:98:ILE:HD12	1:B:130:TYR:HE2	1.86	0.41
1:B:879:ASN:HA	1:B:882:ARG:NE	2.35	0.41
1:B:913:GLU:HB3	1:B:917:ARG:CZ	2.51	0.41
1:C:33:ALA:HB2	1:C:43:ILE:HD13	2.02	0.41
1:C:86:TYR:HD1	1:C:86:TYR:HA	1.69	0.41
1:C:264:ILE:HD11	1:C:1091:ARG:HG2	2.02	0.41
1:C:433:ARG:H	1:C:433:ARG:HE	1.69	0.41
1:C:627:PHE:HB3	1:C:631:THR:OG1	2.21	0.41
1:C:965:ARG:HA	1:C:965:ARG:HD3	1.79	0.41
1:C:1029:SER:O	1:C:1033:ARG:HG3	2.21	0.41
1:D:234:ARG:O	1:D:238:ASP:N	2.54	0.41
1:D:306:LEU:HD21	1:D:308:ILE:HD11	2.01	0.41
1:D:576:GLY:HA2	1:D:584:VAL:O	2.20	0.41
1:D:796:LEU:N	1:D:796:LEU:CD1	2.81	0.41
1:A:153:MET:HE2	1:A:153:MET:HB3	1.86	0.41
1:A:817:ALA:HA	1:A:820:LEU:HG	2.03	0.41
1:A:843:TRP:O	1:A:846:THR:OG1	2.31	0.41
1:B:788:PRO:HD3	1:B:869:ARG:HH22	1.86	0.41
1:B:1062:VAL:O	1:B:1066:LEU:HG	2.21	0.41
1:C:91:VAL:HG12	1:C:95:LYS:HE2	2.03	0.41
1:C:262:ASP:HA	1:C:265:ARG:HE	1.86	0.41
1:C:420:MET:HE2	1:C:420:MET:HB2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:PRO:HB2	1:C:596:ARG:HH21	1.86	0.41
1:C:843:TRP:O	1:C:847:MET:HG2	2.21	0.41
1:D:248:ILE:HA	1:D:279:LEU:O	2.20	0.41
1:D:581:THR:O	1:D:837:ARG:HG3	2.21	0.41
1:D:589:ARG:HA	1:D:589:ARG:HD2	1.94	0.41
1:D:922:GLN:HA	1:D:925:ILE:HD12	2.02	0.41
1:A:792:LEU:O	1:A:795:THR:OG1	2.33	0.40
1:B:245:VAL:HA	1:B:308:ILE:O	2.21	0.40
1:B:828:MET:HE3	1:B:828:MET:HB3	1.97	0.40
1:C:368:TRP:CZ3	1:C:392:TYR:HA	2.56	0.40
1:D:433:ARG:HE	1:D:433:ARG:N	2.19	0.40
1:D:585:PHE:HD1	1:D:585:PHE:HA	1.79	0.40
1:D:739:ASP:O	1:D:743:ASN:ND2	2.52	0.40
1:D:789:ILE:CD1	1:D:789:ILE:H	2.13	0.40
1:A:971:ALA:O	1:A:975:GLY:N	2.44	0.40
1:A:1062:VAL:O	1:A:1066:LEU:HG	2.21	0.40
1:C:243:ILE:HB	1:C:274:ILE:HG12	2.02	0.40
1:D:610:ARG:O	1:D:614:VAL:HG23	2.21	0.40
1:D:1062:VAL:O	1:D:1066:LEU:HG	2.21	0.40
1:A:696:ILE:HG23	1:A:719:ILE:HG21	2.02	0.40
1:A:938:ASN:OD1	1:A:938:ASN:N	2.52	0.40
1:B:219:GLY:HA2	1:B:265:ARG:HH12	1.87	0.40
1:B:263:ARG:HD2	1:B:276:MET:HG3	2.02	0.40
1:B:640:ARG:HD3	1:B:640:ARG:HA	1.89	0.40
1:C:431:GLU:OE1	1:C:431:GLU:N	2.53	0.40
1:C:507:ALA:HA	1:C:510:ARG:NH1	2.36	0.40
1:C:661:LYS:O	1:C:665:ASP:N	2.53	0.40
1:D:387:GLU:CD	1:D:387:GLU:H	2.28	0.40
1:D:450:LEU:HB2	1:D:963:ALA:HB2	2.03	0.40
1:D:460:TYR:HE2	1:D:841:ARG:NH2	2.19	0.40
1:A:342:LEU:HD11	1:A:371:VAL:HG22	2.02	0.40
1:A:629:SER:O	1:A:633:TYR:N	2.32	0.40
1:C:428:PRO:O	1:C:430:LEU:HD22	2.22	0.40
1:C:621:LYS:HB2	1:C:674:THR:HA	2.02	0.40
1:C:855:ASP:O	1:C:859:LYS:HG3	2.22	0.40
1:D:178:ARG:O	1:D:182:GLN:HG2	2.21	0.40
1:D:1090:ARG:HG2	1:D:1092:ASN:HD22	1.86	0.40
1:A:184:ILE:HB	1:A:277:ARG:HH12	1.86	0.40
1:A:441:ILE:HD13	1:A:441:ILE:HA	1.94	0.40
1:A:545:THR:HG23	1:A:547:SER:H	1.86	0.40
1:B:29:PHE:O	1:B:57:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ARG:HG2	1:C:48:ARG:NH1	2.36	0.40
1:B:746:ILE:HA	1:B:1089:TYR:HB3	2.04	0.40
1:B:761:GLU:OE1	1:B:1061:ASN:ND2	2.51	0.40
1:C:90:HIS:CE1	1:C:119:ILE:HG23	2.56	0.40
1:C:463:ARG:NH1	1:C:509:GLU:OE2	2.54	0.40
1:C:573:ASN:HB2	1:C:579:PRO:HD2	2.01	0.40
1:C:597:MET:O	1:C:623:LEU:HD23	2.22	0.40
1:D:689:ALA:HB2	1:D:1063:PHE:HE1	1.86	0.40
1:D:1002:VAL:O	1:D:1006:ARG:NE	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1053/1113 (95%)	1018 (97%)	34 (3%)	1 (0%)	48	83
1	B	1053/1113 (95%)	1026 (97%)	25 (2%)	2 (0%)	43	78
1	C	1053/1113 (95%)	1033 (98%)	20 (2%)	0	100	100
1	D	1053/1113 (95%)	1028 (98%)	23 (2%)	2 (0%)	43	78
All	All	4212/4452 (95%)	4105 (98%)	102 (2%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	SER
1	B	447	SER
1	B	448	ARG
1	D	446	ARG
1	D	445	ALA

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	826/906 (91%)	709 (86%)	117 (14%)	3	13
1	B	826/906 (91%)	724 (88%)	102 (12%)	4	17
1	C	826/906 (91%)	745 (90%)	81 (10%)	7	24
1	D	824/906 (91%)	717 (87%)	107 (13%)	4	15
All	All	3302/3624 (91%)	2895 (88%)	407 (12%)	7	17

All (407) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	44	ASN
1	A	53	GLN
1	A	62	HIS
1	A	63	ASN
1	A	66	VAL
1	A	86	TYR
1	A	110	GLN
1	A	119	ILE
1	A	149	MET
1	A	160	ASP
1	A	177	ARG
1	A	184	ILE
1	A	209	VAL
1	A	222	LYS
1	A	227	ASP
1	A	232	ARG
1	A	237	GLN
1	A	238	ASP
1	A	239	ASP
1	A	246	ILE
1	A	254	LYS
1	A	264	ILE
1	A	267	ASN

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Mol	Chain	Res	Type
1	A	269	ILE
1	A	281	THR
1	A	283	GLU
1	A	287	GLU
1	A	288	ILE
1	A	314	ILE
1	A	318	ASP
1	A	329	LEU
1	A	333	THR
1	A	344	LYS
1	A	352	ASP
1	A	359	PHE
1	A	366	ASP
1	A	374	GLN
1	A	381	GLN
1	A	394	THR
1	A	402	ASP
1	A	404	VAL
1	A	411	LEU
1	A	422	LEU
1	A	430	LEU
1	A	433	ARG
1	A	446	ARG
1	A	475	GLN
1	A	497	LEU
1	A	518	GLN
1	A	520	GLN
1	A	538	ARG
1	A	541	LEU
1	A	561	ASP
1	A	567	LYS
1	A	570	MET
1	A	607	THR
1	A	623	LEU
1	A	627	PHE
1	A	628	ASP
1	A	633	TYR
1	A	640	ARG
1	A	652	VAL
1	A	665	ASP
1	A	669	LEU
1	A	688	LEU

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Mol	Chain	Res	Type
1	A	709	ARG
1	A	710	ASP
1	A	714	ASP
1	A	716	GLU
1	A	722	TRP
1	A	725	GLN
1	A	727	VAL
1	A	737	LYS
1	A	743	ASN
1	A	751	PHE
1	A	752	SER
1	A	753	LEU
1	A	761	GLU
1	A	770	ASN
1	A	787	ASN
1	A	801	THR
1	A	813	ILE
1	A	814	ASP
1	A	815	ASP
1	A	822	PHE
1	A	849	ASP
1	A	850	LYS
1	A	855	ASP
1	A	856	ARG
1	A	860	LEU
1	A	865	GLN
1	A	875	GLU
1	A	881	ILE
1	A	883	THR
1	A	885	LEU
1	A	894	ASN
1	A	934	CYS
1	A	938	ASN
1	A	942	PHE
1	A	943	LEU
1	A	974	THR
1	A	977	GLN
1	A	981	ILE
1	A	992	LYS
1	A	993	HIS
1	A	1004	THR
1	A	1030	GLN

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Mol	Chain	Res	Type
1	A	1044	ASP
1	A	1052	LEU
1	A	1056	VAL
1	A	1059	ASN
1	A	1068	ASP
1	A	1077	GLN
1	A	1080	HIS
1	A	1090	ARG
1	A	1091	ARG
1	B	43	ILE
1	B	44	ASN
1	B	53	GLN
1	B	62	HIS
1	B	66	VAL
1	B	86	TYR
1	B	110	GLN
1	B	119	ILE
1	B	160	ASP
1	B	170	ASP
1	B	177	ARG
1	B	184	ILE
1	B	222	LYS
1	B	237	GLN
1	B	239	ASP
1	B	267	ASN
1	B	269	ILE
1	B	283	GLU
1	B	287	GLU
1	B	314	ILE
1	B	318	ASP
1	B	329	LEU
1	B	333	THR
1	B	387	GLU
1	B	402	ASP
1	B	409	GLN
1	B	411	LEU
1	B	422	LEU
1	B	433	ARG
1	B	434	ILE
1	B	450	LEU
1	B	455	ASP
1	B	456	THR

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Mol	Chain	Res	Type
1	B	474	ARG
1	B	475	GLN
1	B	485	GLN
1	B	491	SER
1	B	518	GLN
1	B	520	GLN
1	B	538	ARG
1	B	542	ILE
1	B	543	SER
1	B	561	ASP
1	B	567	LYS
1	B	570	MET
1	B	585	PHE
1	B	607	THR
1	B	623	LEU
1	B	633	TYR
1	B	644	TYR
1	B	652	VAL
1	B	669	LEU
1	B	688	LEU
1	B	698	GLN
1	B	722	TRP
1	B	725	GLN
1	B	727	VAL
1	B	737	LYS
1	B	743	ASN
1	B	751	PHE
1	B	752	SER
1	B	754	LYS
1	B	761	GLU
1	B	762	TYR
1	B	770	ASN
1	B	787	ASN
1	B	804	GLU
1	B	814	ASP
1	B	815	ASP
1	B	826	ASN
1	B	829	ASP
1	B	849	ASP
1	B	850	LYS
1	B	855	ASP
1	B	856	ARG

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Mol	Chain	Res	Type
1	B	860	LEU
1	B	866	THR
1	B	875	GLU
1	B	881	ILE
1	B	883	THR
1	B	885	LEU
1	B	894	ASN
1	B	915	VAL
1	B	934	CYS
1	B	936	ASN
1	B	938	ASN
1	B	939	GLN
1	B	942	PHE
1	B	945	GLU
1	B	977	GLN
1	B	981	ILE
1	B	992	LYS
1	B	993	HIS
1	B	1004	THR
1	B	1030	GLN
1	B	1044	ASP
1	B	1052	LEU
1	B	1056	VAL
1	B	1068	ASP
1	B	1080	HIS
1	B	1090	ARG
1	B	1091	ARG
1	C	53	GLN
1	C	62	HIS
1	C	66	VAL
1	C	86	TYR
1	C	110	GLN
1	C	119	ILE
1	C	128	GLN
1	C	177	ARG
1	C	180	LEU
1	C	222	LYS
1	C	227	ASP
1	C	234	ARG
1	C	237	GLN
1	C	238	ASP
1	C	239	ASP

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Mol	Chain	Res	Type
1	C	254	LYS
1	C	283	GLU
1	C	287	GLU
1	C	314	ILE
1	C	316	GLN
1	C	333	THR
1	C	352	ASP
1	C	381	GLN
1	C	387	GLU
1	C	394	THR
1	C	402	ASP
1	C	404	VAL
1	C	411	LEU
1	C	430	LEU
1	C	433	ARG
1	C	442	VAL
1	C	446	ARG
1	C	474	ARG
1	C	505	LEU
1	C	518	GLN
1	C	521	GLN
1	C	538	ARG
1	C	561	ASP
1	C	585	PHE
1	C	607	THR
1	C	623	LEU
1	C	633	TYR
1	C	652	VAL
1	C	669	LEU
1	C	719	ILE
1	C	727	VAL
1	C	737	LYS
1	C	751	PHE
1	C	753	LEU
1	C	754	LYS
1	C	761	GLU
1	C	770	ASN
1	C	796	LEU
1	C	798	ASN
1	C	809	ARG
1	C	814	ASP
1	C	815	ASP

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Mol	Chain	Res	Type
1	C	829	ASP
1	C	849	ASP
1	C	850	LYS
1	C	855	ASP
1	C	856	ARG
1	C	860	LEU
1	C	875	GLU
1	C	945	GLU
1	C	964	GLU
1	C	977	GLN
1	C	981	ILE
1	C	1030	GLN
1	C	1036	GLU
1	C	1044	ASP
1	C	1052	LEU
1	C	1053	ARG
1	C	1056	VAL
1	C	1057	ILE
1	C	1059	ASN
1	C	1068	ASP
1	C	1085	VAL
1	C	1090	ARG
1	C	1091	ARG
1	C	1092	ASN
1	D	40	ASP
1	D	47	ARG
1	D	53	GLN
1	D	62	HIS
1	D	86	TYR
1	D	110	GLN
1	D	119	ILE
1	D	120	VAL
1	D	149	MET
1	D	159	ILE
1	D	177	ARG
1	D	180	LEU
1	D	196	LEU
1	D	222	LYS
1	D	227	ASP
1	D	237	GLN
1	D	238	ASP
1	D	239	ASP

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Mol	Chain	Res	Type
1	D	246	ILE
1	D	254	LYS
1	D	269	ILE
1	D	283	GLU
1	D	287	GLU
1	D	305	ASP
1	D	314	ILE
1	D	316	GLN
1	D	347	MET
1	D	352	ASP
1	D	359	PHE
1	D	366	ASP
1	D	369	ARG
1	D	381	GLN
1	D	387	GLU
1	D	394	THR
1	D	400	ASN
1	D	402	ASP
1	D	411	LEU
1	D	433	ARG
1	D	441	ILE
1	D	455	ASP
1	D	456	THR
1	D	474	ARG
1	D	505	LEU
1	D	518	GLN
1	D	520	GLN
1	D	538	ARG
1	D	541	LEU
1	D	561	ASP
1	D	567	LYS
1	D	570	MET
1	D	574	VAL
1	D	585	PHE
1	D	607	THR
1	D	623	LEU
1	D	628	ASP
1	D	630	VAL
1	D	640	ARG
1	D	652	VAL
1	D	665	ASP
1	D	669	LEU

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Mol	Chain	Res	Type
1	D	677	SER
1	D	681	ASN
1	D	688	LEU
1	D	690	MET
1	D	710	ASP
1	D	714	ASP
1	D	722	TRP
1	D	725	GLN
1	D	727	VAL
1	D	737	LYS
1	D	743	ASN
1	D	751	PHE
1	D	753	LEU
1	D	754	LYS
1	D	770	ASN
1	D	789	ILE
1	D	796	LEU
1	D	809	ARG
1	D	829	ASP
1	D	849	ASP
1	D	850	LYS
1	D	855	ASP
1	D	856	ARG
1	D	865	GLN
1	D	866	THR
1	D	875	GLU
1	D	881	ILE
1	D	883	THR
1	D	915	VAL
1	D	938	ASN
1	D	945	GLU
1	D	977	GLN
1	D	981	ILE
1	D	1004	THR
1	D	1006	ARG
1	D	1030	GLN
1	D	1044	ASP
1	D	1052	LEU
1	D	1056	VAL
1	D	1057	ILE
1	D	1068	ASP
1	D	1074	SER

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Mol	Chain	Res	Type
1	D	1077	GLN
1	D	1080	HIS
1	D	1085	VAL
1	D	1090	ARG
1	D	1091	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	87	GLN
1	A	203	GLN
1	A	237	GLN
1	A	273	ASN
1	A	409	GLN
1	A	467	GLN
1	A	476	GLN
1	A	573	ASN
1	A	693	ASN
1	A	699	GLN
1	A	725	GLN
1	A	726	ASN
1	A	742	GLN
1	A	743	ASN
1	A	765	HIS
1	A	770	ASN
1	A	780	HIS
1	A	858	GLN
1	A	894	ASN
1	A	939	GLN
1	A	1003	ASN
1	A	1038	HIS
1	A	1041	HIS
1	A	1092	ASN
1	B	39	HIS
1	B	53	GLN
1	B	75	GLN
1	B	267	ASN
1	B	270	ASN
1	B	271	HIS
1	B	273	ASN
1	B	376	GLN

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Mol	Chain	Res	Type
1	B	381	GLN
1	B	400	ASN
1	B	409	GLN
1	B	467	GLN
1	B	476	GLN
1	B	573	ASN
1	B	671	ASN
1	B	681	ASN
1	B	699	GLN
1	B	725	GLN
1	B	726	ASN
1	B	732	GLN
1	B	765	HIS
1	B	766	HIS
1	B	767	GLN
1	B	791	GLN
1	B	819	ASN
1	B	858	GLN
1	B	886	GLN
1	B	939	GLN
1	B	977	GLN
1	B	990	GLN
1	B	1003	ASN
1	B	1092	ASN
1	C	53	GLN
1	C	75	GLN
1	C	90	HIS
1	C	108	HIS
1	C	203	GLN
1	C	267	ASN
1	C	273	ASN
1	C	316	GLN
1	C	374	GLN
1	C	378	ASN
1	C	409	GLN
1	C	671	ASN
1	C	699	GLN
1	C	725	GLN
1	C	732	GLN
1	C	740	GLN
1	C	760	GLN
1	C	767	GLN

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Mol	Chain	Res	Type
1	C	787	ASN
1	C	798	ASN
1	C	858	GLN
1	C	865	GLN
1	C	922	GLN
1	C	938	ASN
1	C	977	GLN
1	C	1003	ASN
1	C	1038	HIS
1	C	1092	ASN
1	D	53	GLN
1	D	75	GLN
1	D	203	GLN
1	D	273	ASN
1	D	376	GLN
1	D	409	GLN
1	D	467	GLN
1	D	671	ASN
1	D	693	ASN
1	D	699	GLN
1	D	707	ASN
1	D	725	GLN
1	D	740	GLN
1	D	765	HIS
1	D	767	GLN
1	D	826	ASN
1	D	858	GLN
1	D	865	GLN
1	D	886	GLN
1	D	896	ASN
1	D	922	GLN
1	D	938	ASN
1	D	957	GLN
1	D	977	GLN
1	D	1003	ASN
1	D	1032	HIS
1	D	1077	GLN
1	D	1092	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.

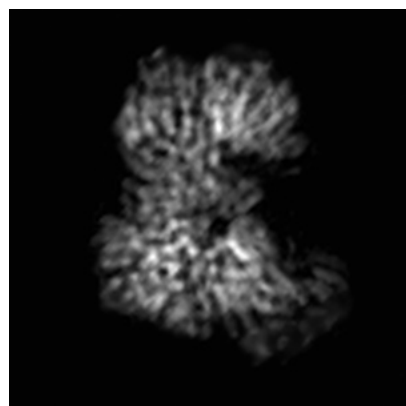
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40758. These allow visual inspection of the internal detail of the map and identification of artifacts.

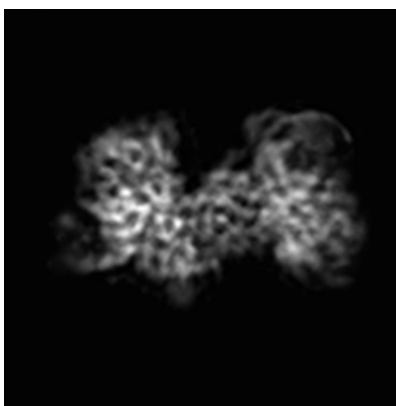
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

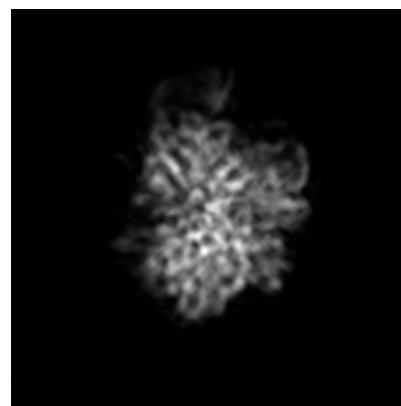
6.1.1 Primary map



X

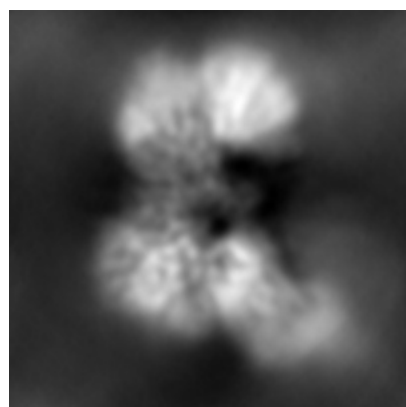


Y

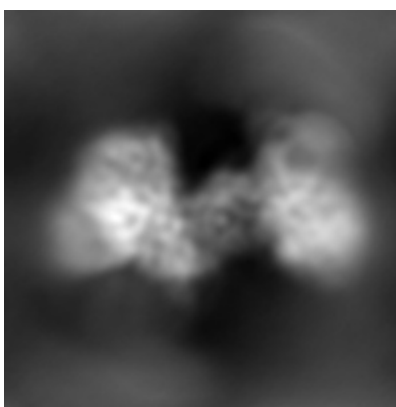


Z

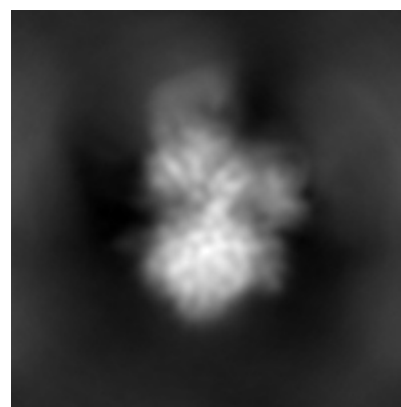
6.1.2 Raw map



X



Y

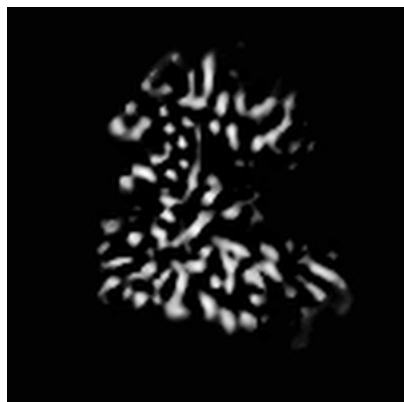


Z

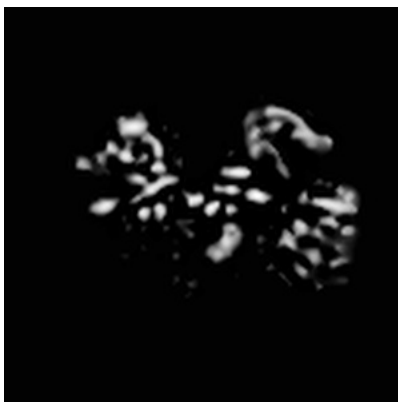
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 64

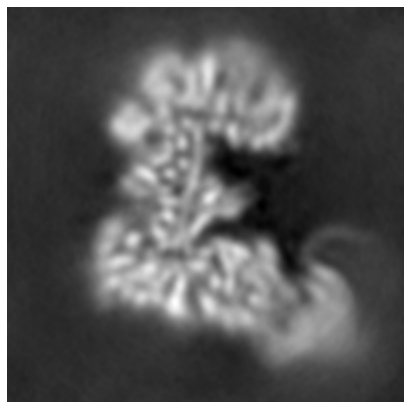


Y Index: 64

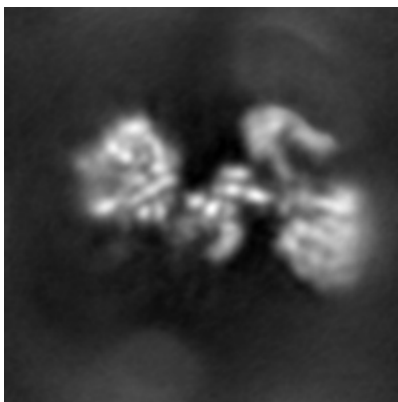


Z Index: 64

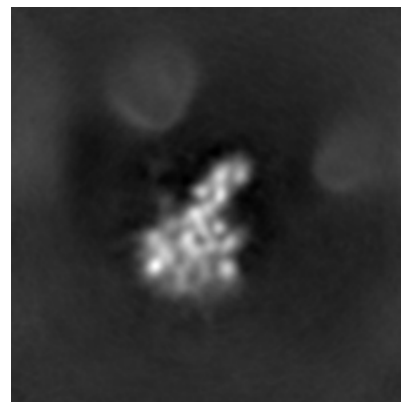
6.2.2 Raw map



X Index: 64



Y Index: 64

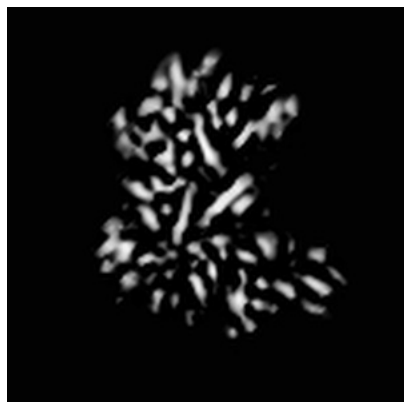


Z Index: 64

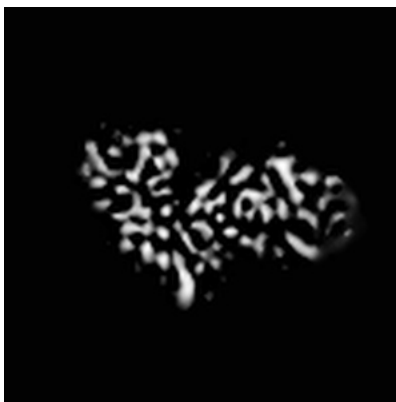
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 67

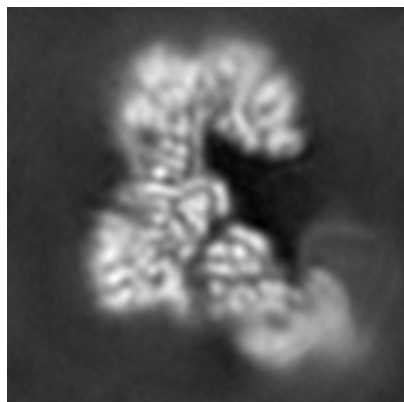


Y Index: 51

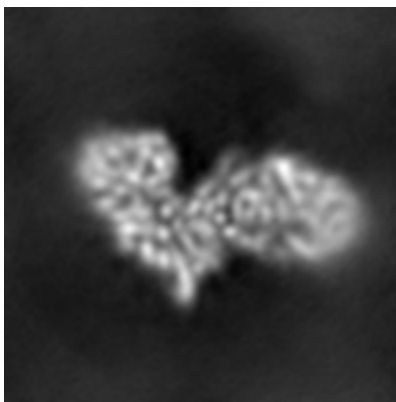


Z Index: 50

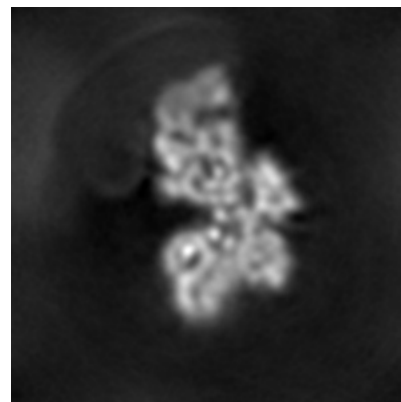
6.3.2 Raw map



X Index: 60



Y Index: 51

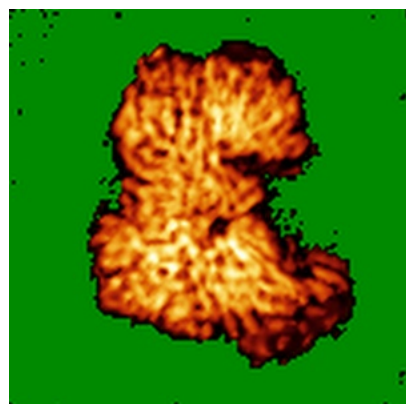


Z Index: 38

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

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

6.4.1 Primary map



X

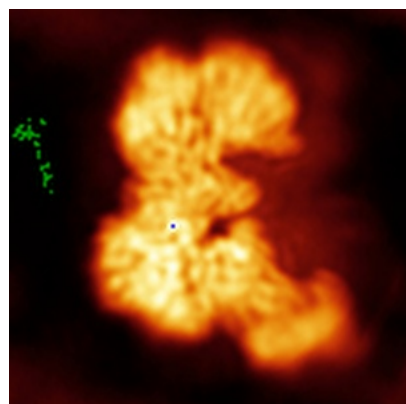


Y

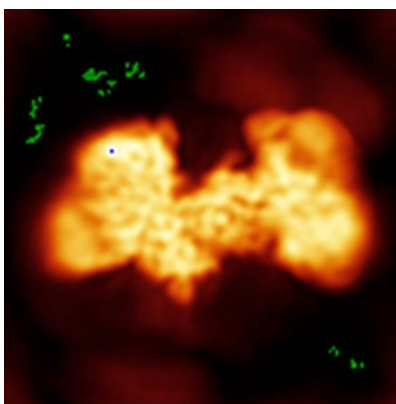


Z

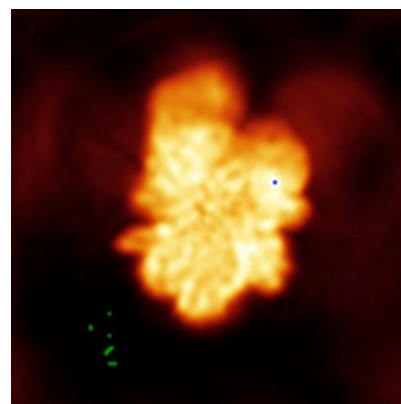
6.4.2 Raw map



X



Y

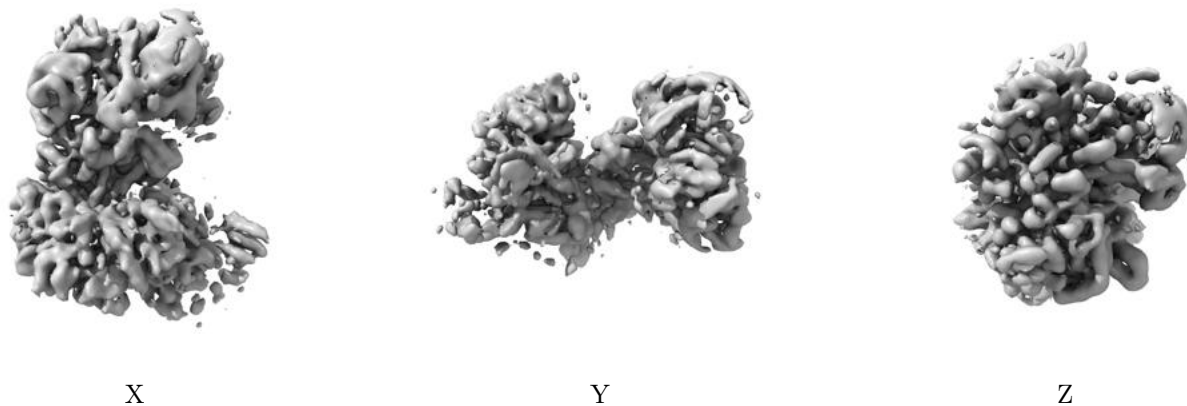


Z

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

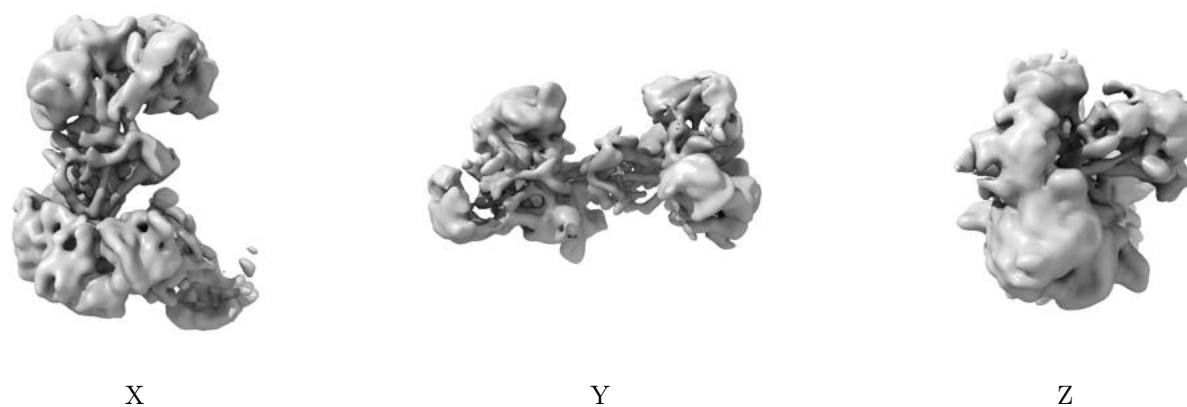
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

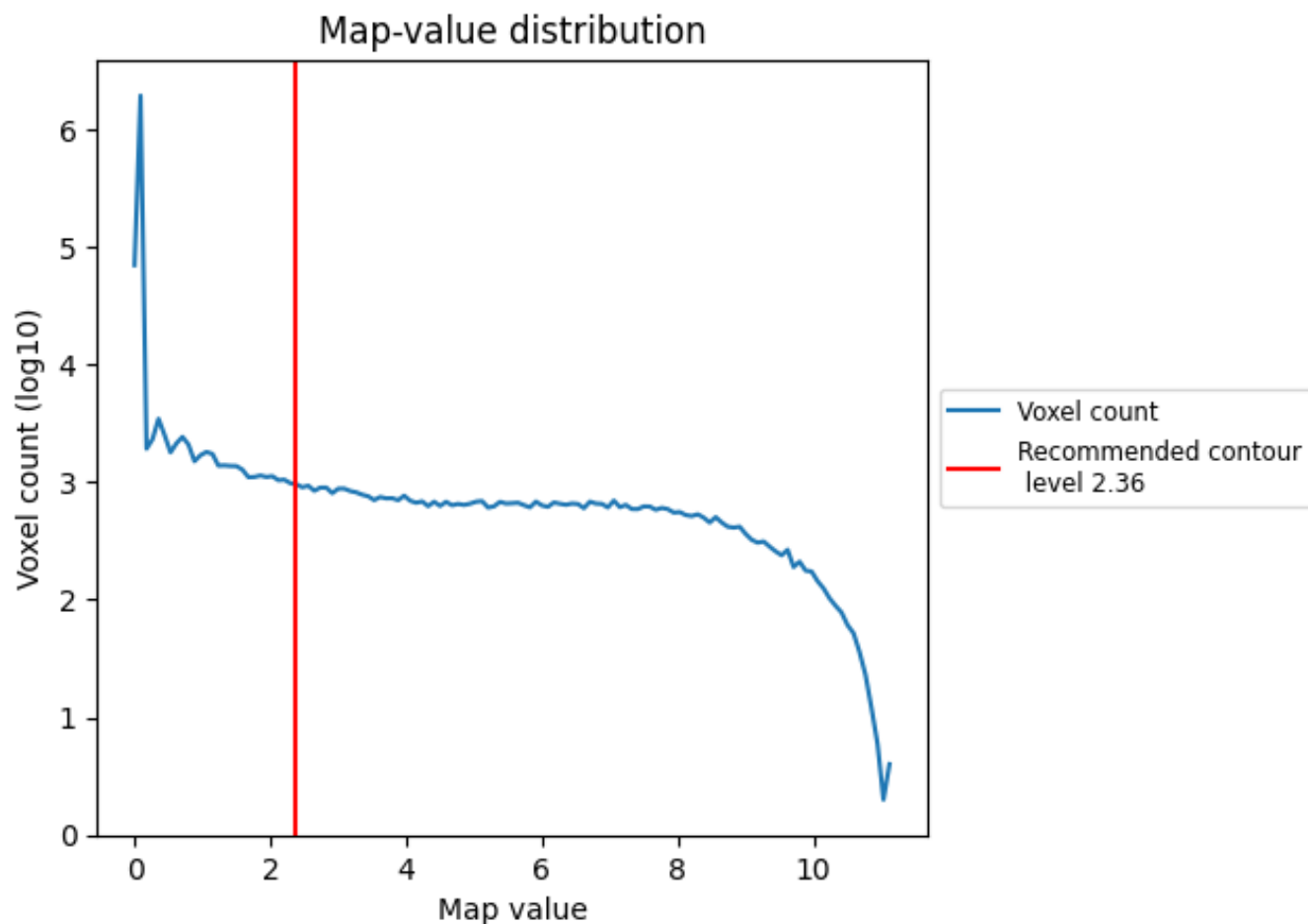
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

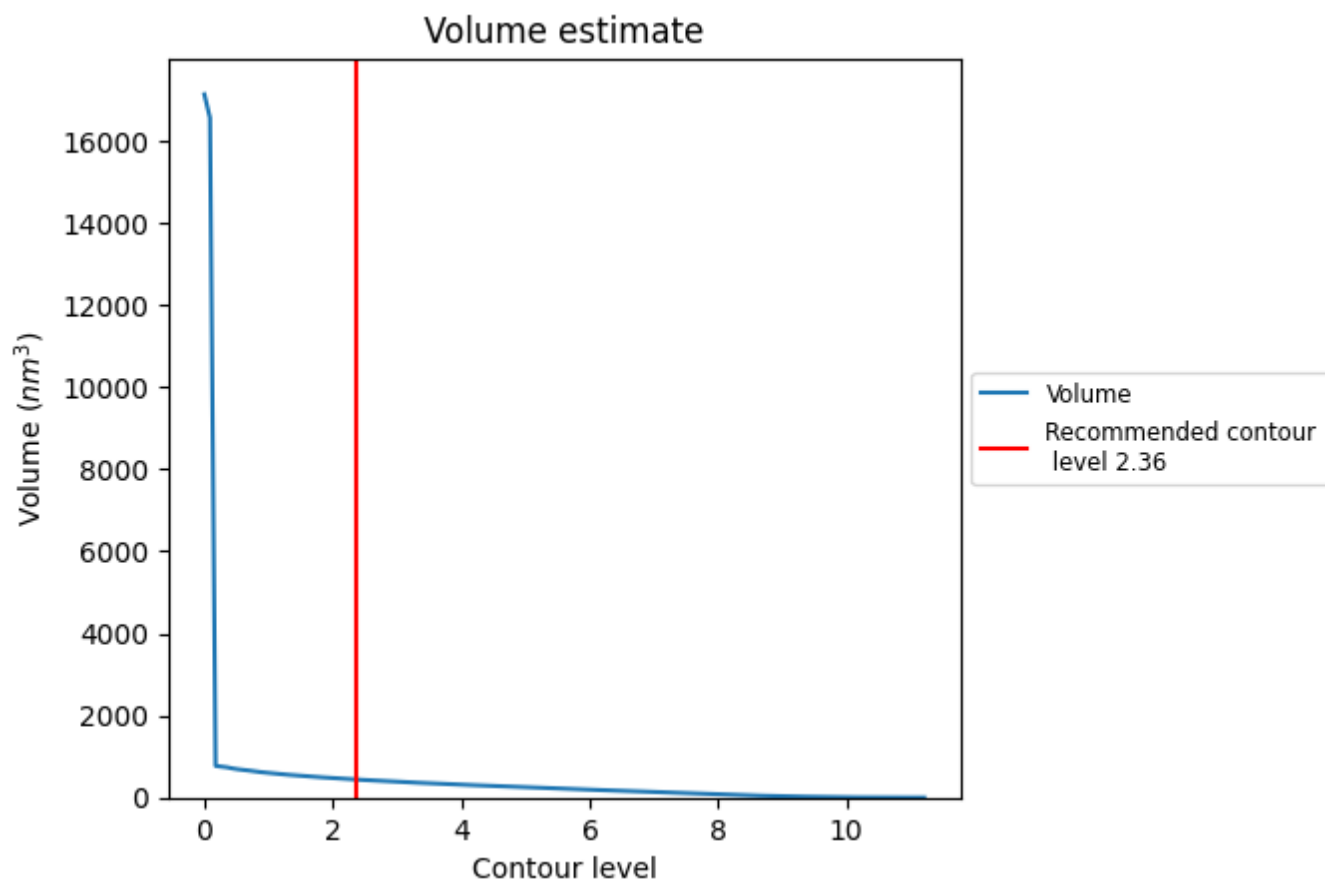
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

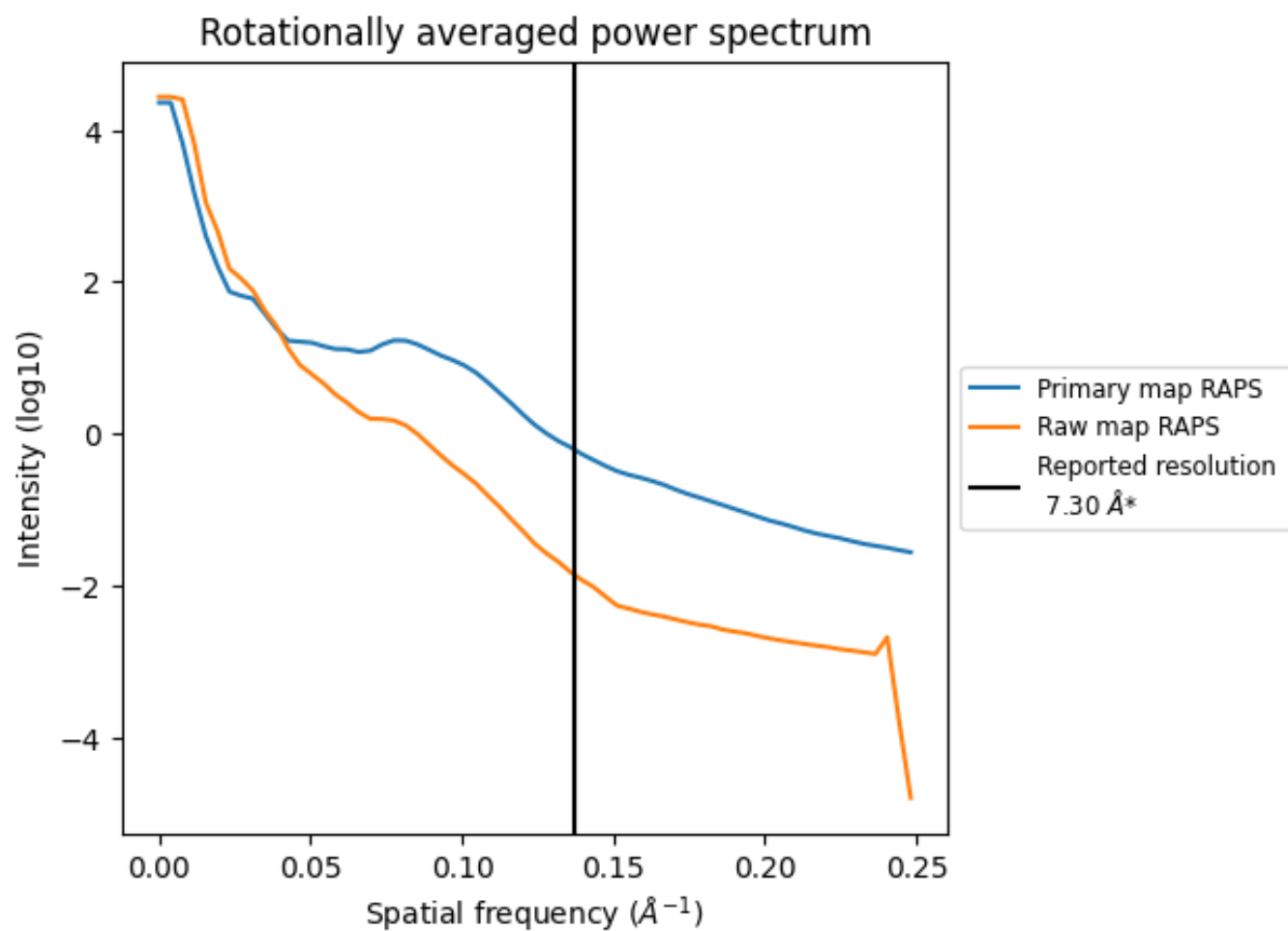
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 440 nm³; this corresponds to an approximate mass of 398 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 ⓘ

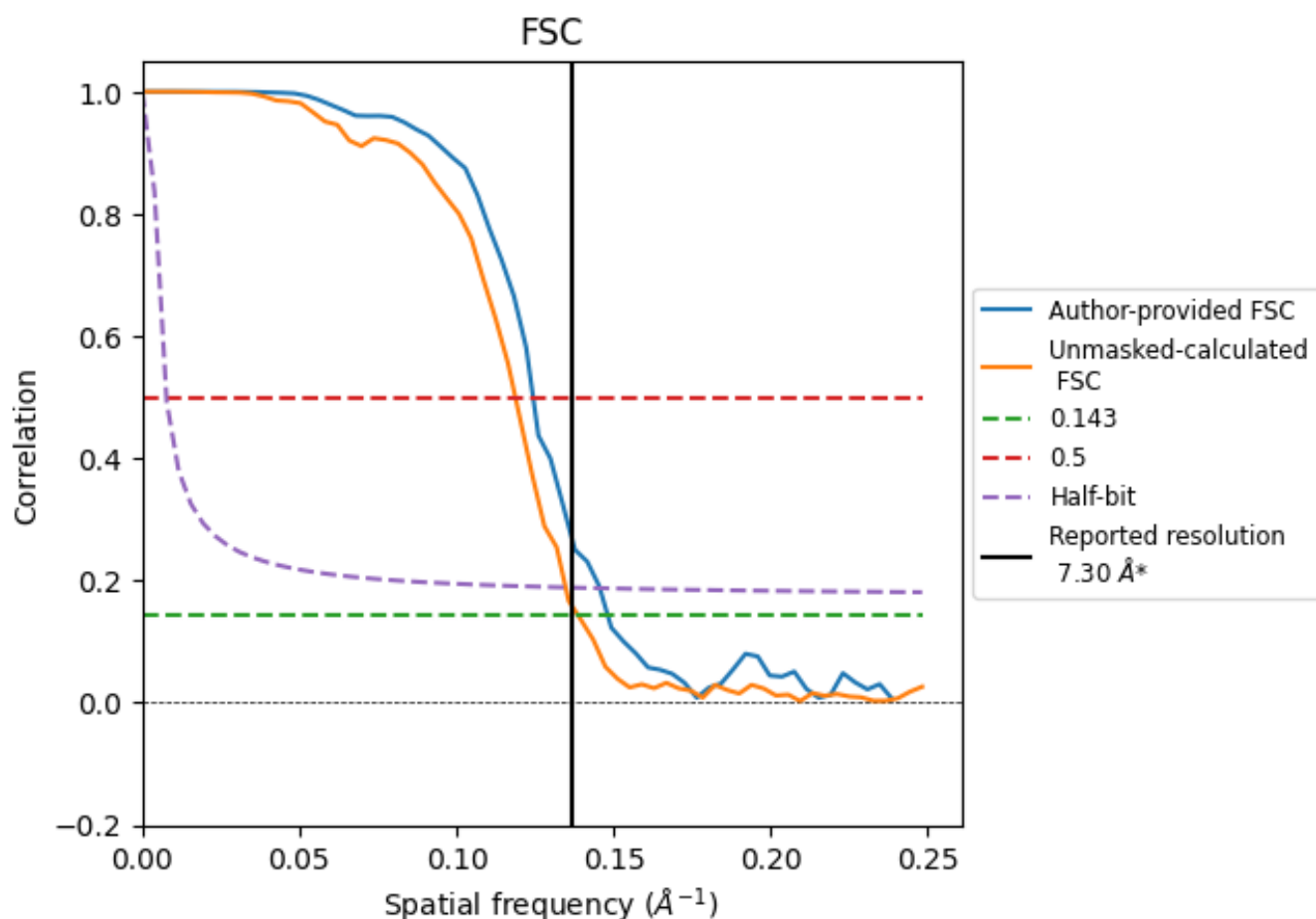


*Reported resolution corresponds to spatial frequency of $0.137 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.137 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

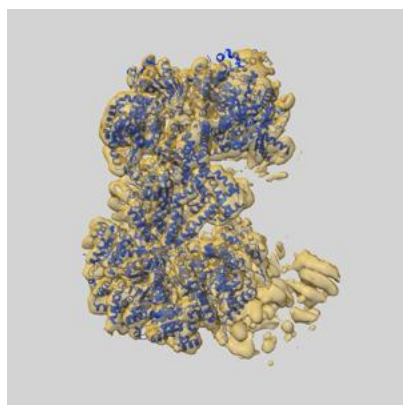
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.30	-	-
Author-provided FSC curve	6.75	8.04	6.86
Unmasked-calculated*	7.21	8.42	7.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

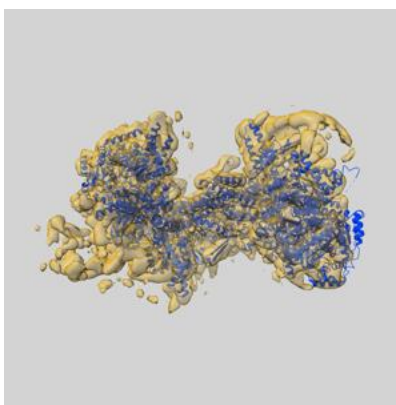
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40758 and PDB model 8STA. Per-residue inclusion information can be found in section [3](#) on page [6](#).

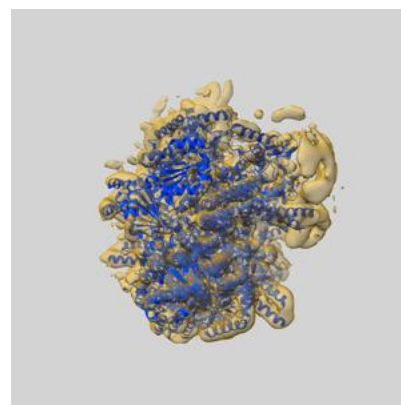
9.1 Map-model overlay [i](#)



X



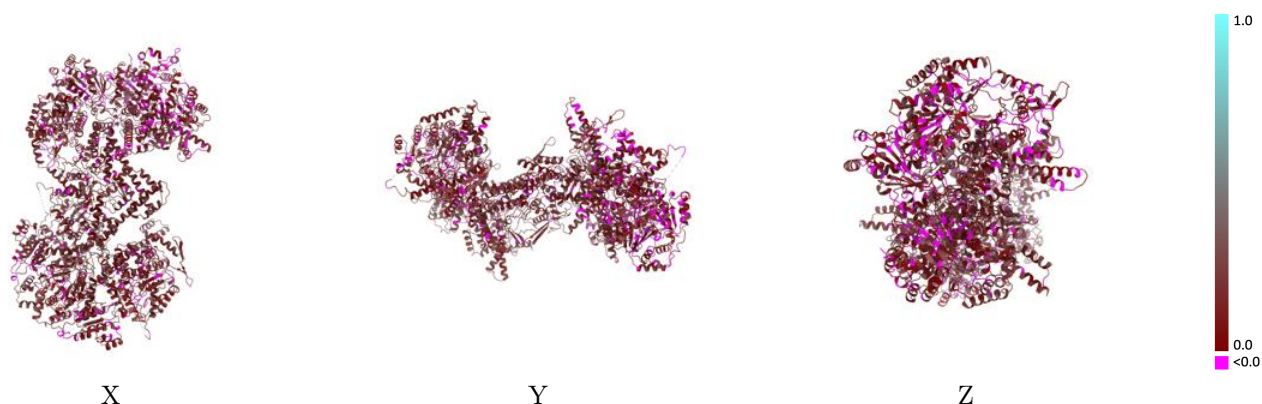
Y



Z

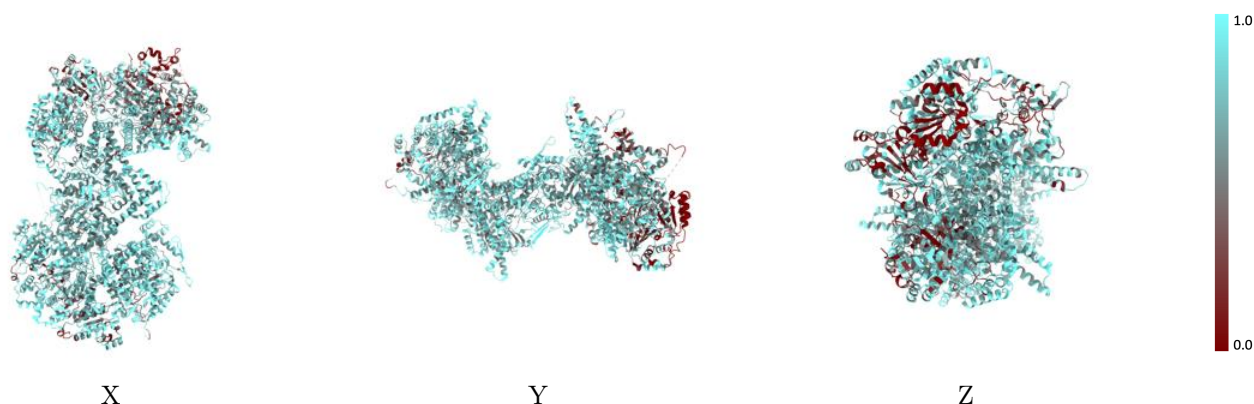
The images above show the 3D surface view of the map at the recommended contour level 2.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



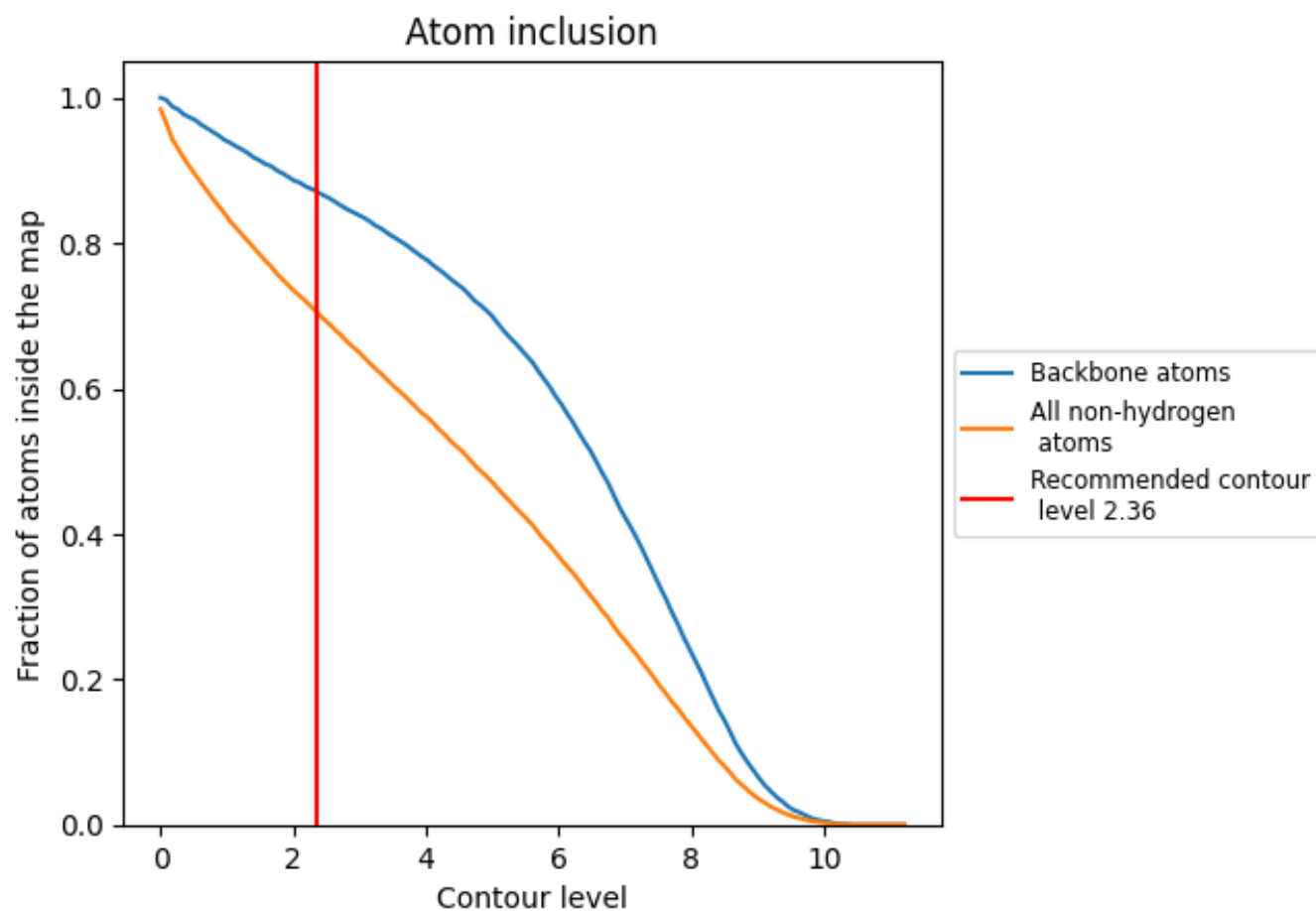
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.36).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 70% 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 (2.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7040	0.1490
A	0.7720	0.1720
B	0.7030	0.1500
C	0.5940	0.1150
D	0.7480	0.1600

