



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:47 AM UTC

PDB ID : 6Z9M / pdb_00006z9m
EMDB ID : EMD-11123
Title : Pseudoatomic model of the pre-fusion conformation of glycoprotein B of Herpes simplex virus 1
Authors : Vollmer, B.; Prazak, V.; Vasishtan, D.; Jefferys, E.E.; Hernandez-Duran, A.; Vallbracht, M.; Klupp, B.; Mettenleiter, T.C.; Backovic, M.; Rey, F.A.; Topf, M.; Gruenewald, K.
Deposited on : 2020-06-04
Resolution : 9.10 Å(reported)
Based on initial model : 5V2S

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

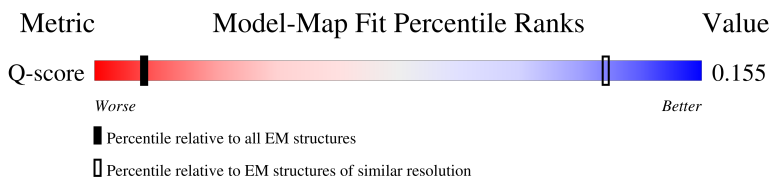
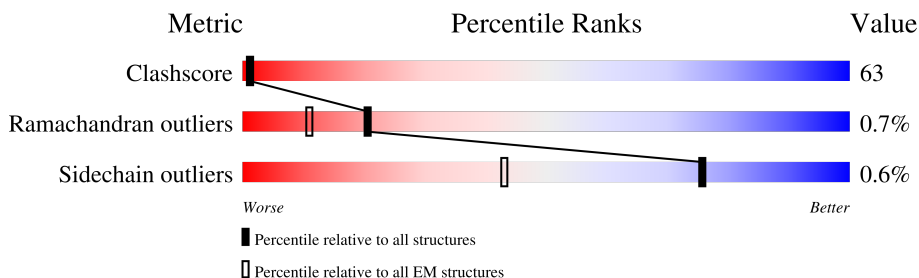
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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	244 (8.60 - 9.60)

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	904	20% 15% 50% 33%
1	B	904	20% 15% 51% 33%
1	C	904	22% 15% 50% 33%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14694 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 Envelope glycoprotein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	606	Total	C	N	O	S	0	0
			4898	3089	863	924	22		
1	B	606	Total	C	N	O	S	0	0
			4898	3089	863	924	22		
1	C	606	Total	C	N	O	S	0	0
			4898	3089	863	924	22		

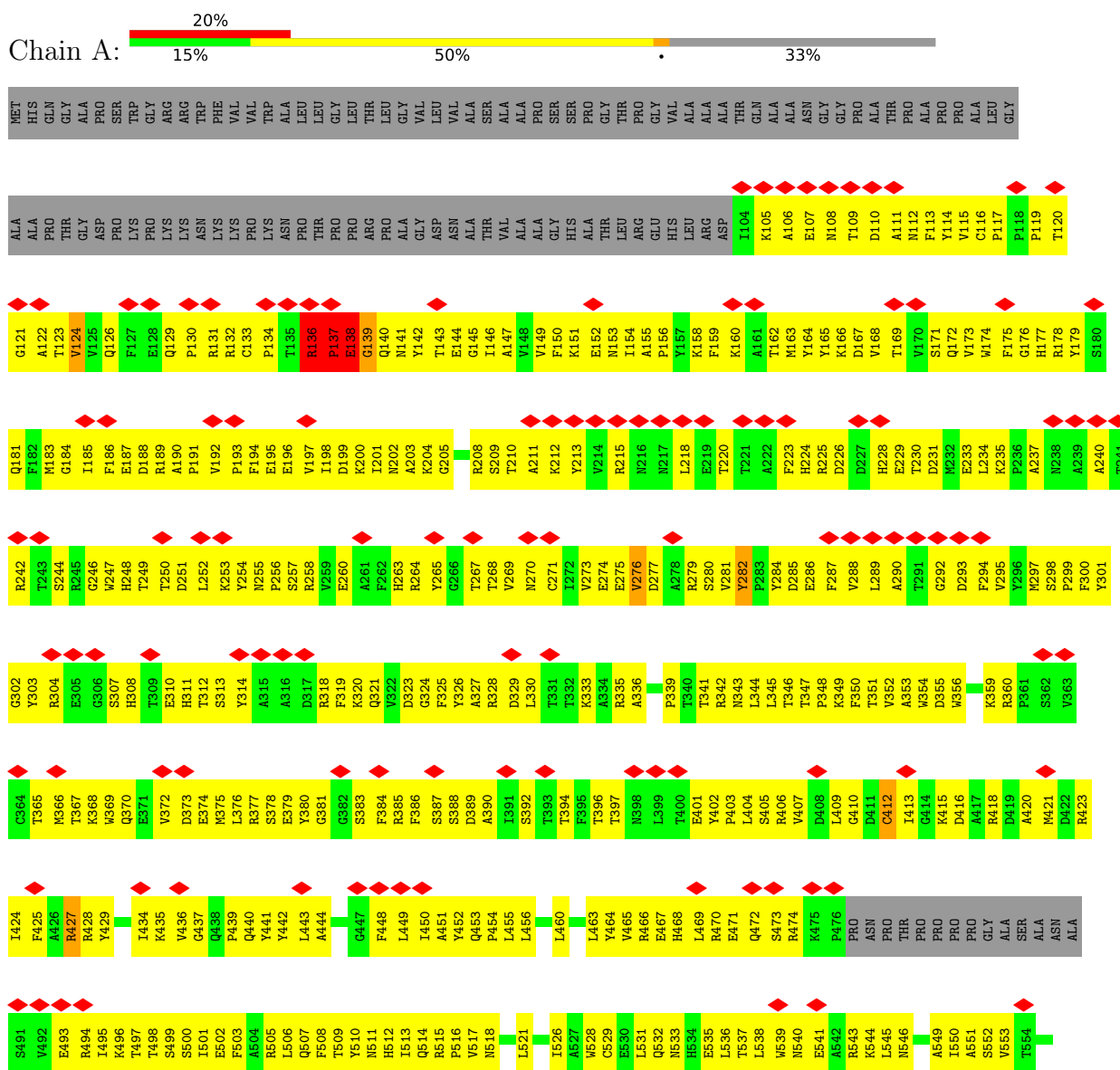
There are 3 discrepancies between the modelled and reference sequences:

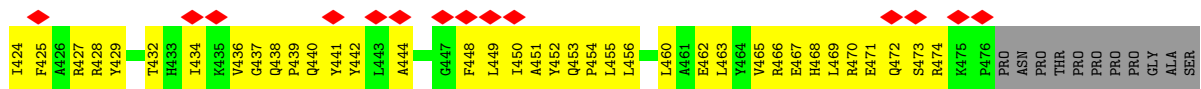
Chain	Residue	Modelled	Actual	Comment	Reference
A	516	PRO	HIS	engineered mutation	UNP A1Z0P7
B	516	PRO	HIS	engineered mutation	UNP A1Z0P7
C	516	PRO	HIS	engineered mutation	UNP A1Z0P7

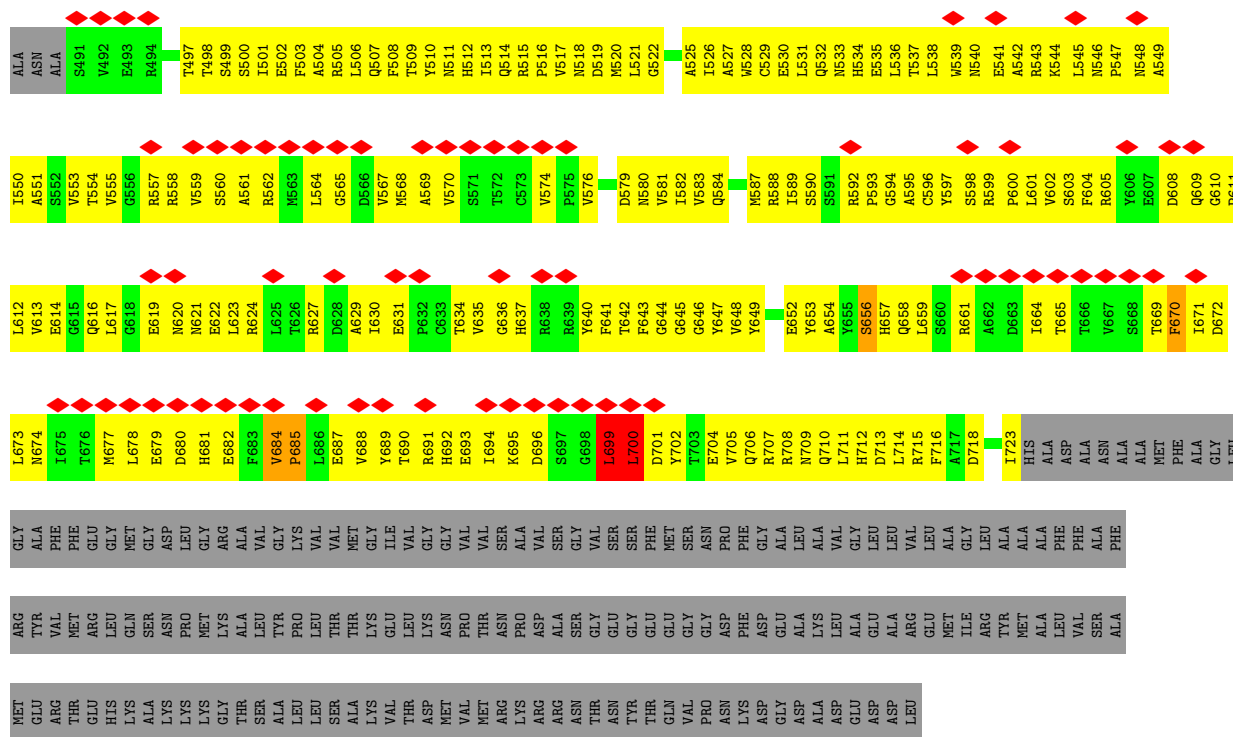
3 Residue-property plots

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

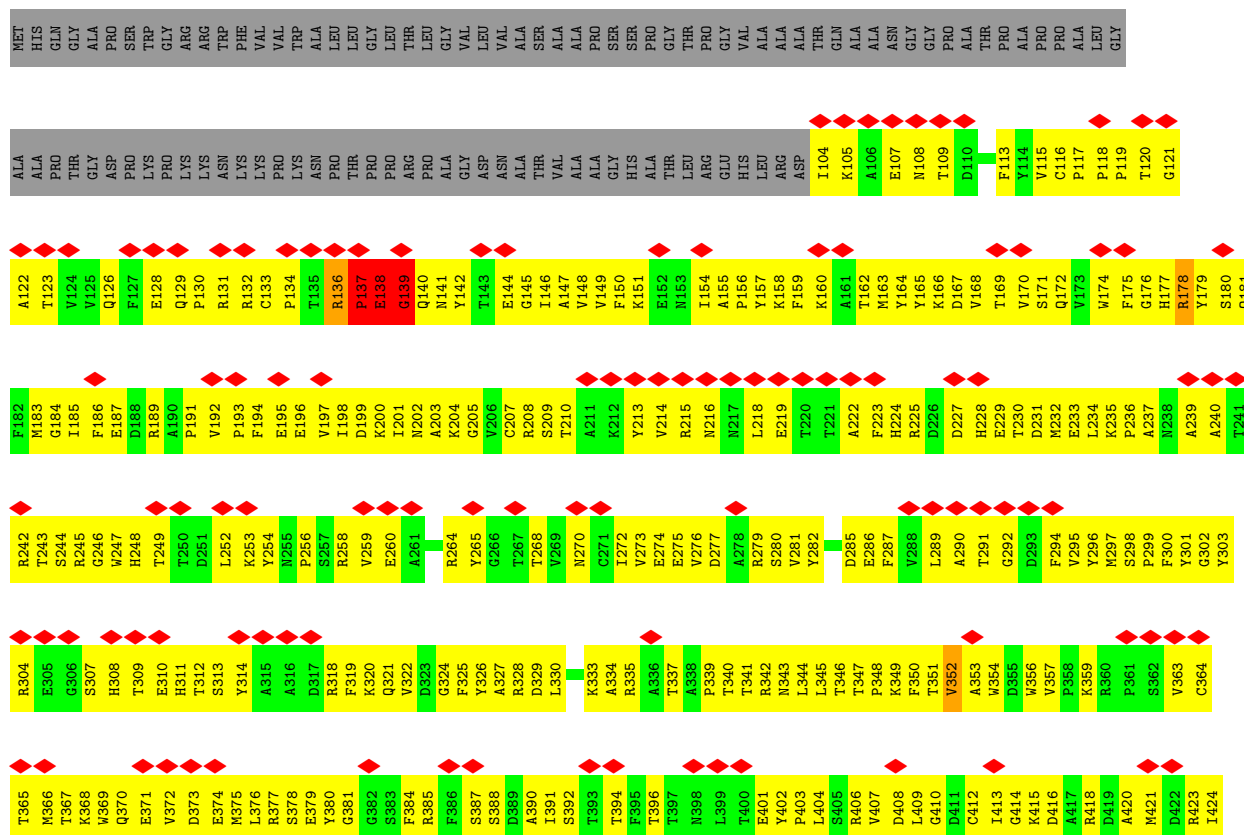
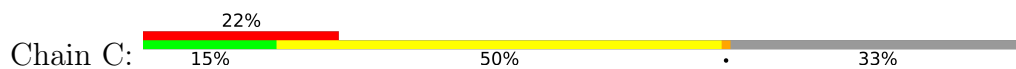
• Molecule 1: Envelope glycoprotein B







• Molecule 1: Envelope glycoprotein B



ALA	LYS	ASN	GLY	D680	N620	R657	E493	F425
LYS	PRO	ASP	LEU	H681	N621	R558	R494	A426
GLY	LYS	MET	GLY	E682	E622	R559	L495	R427
THR	ALA	ALA	ARG	F683	R624	S660	S500	R428
LEU	ALA	VAL	VAL	V684	R625	A561	I501	Y429
LEU	LEU	GLY	GLY	P685	T626	R562	E502	T434
LEU	LEU	VAL	VAL	L686	R627	R563	F503	T435
SER	THR	VAL	VAL	E687	D628	L564	A504	V436
THR	THR	VAL	VAL	V688	T630	G565	R505	Q437
ALA	ALA	MET	MET	V689	E631	D566	L506	Q438
LYS	LYS	GLY	GLY	T690	P632	V567	Q507	P439
VAL	GLY	ILE	VAL	R691	C633	R568	T509	Q440
THR	THR	VAL	VAL	H692	T634	A569	Y441	Y441
ASP	ASP	GLY	GLY	E693	V635	V570	N511	Y442
MET	MET	ASN	GLY	T694	C636	S571	H512	L443
VAL	VAL	THR	VAL	K695	H637	T572	L513	A444
THR	THR	VAL	VAL	D696	R638	C573	Q514	N445
GLY	GLY	SER	SER	P697	T639	V581	R515	G446
ARG	ARG	VAL	VAL	S697	R639	V574	P516	G447
ARG	ARG	ALA	SER	G698	V640	P575	N517	F448
ASN	ASN	SER	GLY	L699	F641	V576	N518	L449
THR	THR	GLY	VAL	GLY	T642	A577	D519	L450
ASN	ASN	GLY	SER	L700	F643	A578	N520	A451
TYR	GLY	SER	GLY	D701	G644	D579	L521	Y452
THR	THR	PHE	PHE	Y702	C645	N580	G522	Q453
GLY	GLY	GLY	MET	T703	G646	V582	R523	P454
VAL	VAL	SER	SER	E704	V647	V583	V524	L455
PRO	PRO	GLY	ASN	V705	V648	Q584	A525	L456
ASN	ASN	ASP	PRO	Q706	V649	R585	I526	
LYS	LYS	PHE	PHE	R707	F650	N588	A527	L463
ASP	ASP	GLY	GLY	R708	E652	R589	N528	Y464
GLY	GLY	ALA	ALA	N709	V653		C529	V465
ASP	ASP	ALA	LEU	O710	A654		E530	R466
ALA	LYS	ALA	ALA	L711	V655	P693	L531	E467
ASP	ASP	VAL	VAL	H712	H656	G594	Q532	H468
GLY	ALA	GLY	GLY	D713	S657	A595	N533	R470
ASP	GLY	LEU	LEU	L714	H657	C596	H534	E471
ASP	ALA	LEU	LEU	R715	Q658	V597	L536	Q472
LEU	ARG	VAL	VAL	F716	L659	R598	T537	S473
GLY	GLY	LEU	LEU	A717	S660	S598	L538	R474
MET	MET	ALA	ALA	D718	R661	R599	N539	K475
ILE	ILE	GLY	GLY		A662	P600	N540	R476
ARG	ARG	LEU	LEU	L723	D663	L601	E541	
TYR	TYR	ALA	ALA	HIS	T664	S603	A542	PRO
MET	MET	ALA	ALA	ALA	T665	F604	R543	ASN
LEU	LEU	ALA	PHE	ASP	V666	R605	K544	PRO
VAL	VAL	PHE	PHE	ALA	V666	V606	L545	THR
SER	SER	ALA	ALA	ASN	V667	E607	N546	PRO
VAL	VAL	PHE	PHE	ALA	S668	D608	P547	PRO
MET	MET	ARG	ARG	MET	T669	Q609	N548	PRO
THR	THR	TYR	TYR	PHE	F670	G610	A549	PRO
ARG	ARG	VAL	VAL	ALA			I550	GLY
GLY	GLY	VAL	MET	GLY	D671	P611	AL51	ALA
THR	THR	GLY	GLY	GLY	O672	L612	S552	SER
GLY	GLY	LEU	LEU	LEU	L673	V613		ALA
HIS	HIS	LEU	LEU	ALA	N674	E614		ALA
LYS	LYS	PHE	PHE	PHE	L675	Q615	V555	ASN
		PHE	PHE	PHE	T676	Q616	G556	ALA
		GLY	GLY	GLY	L677	L617		
		GLY	GLY	GLY	N677	G618		
		MET	MET	MET	E679	E619		

4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of subtomograms used	46067	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.3	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.311	Depositor
Minimum map value	-0.336	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.056	Depositor
Map size ($\text{\AA}$)	160.0, 160.0, 160.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.6, 1.6, 1.6	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/5018	0.71	6/6817 (0.1%)
1	B	0.30	0/5018	0.71	7/6817 (0.1%)
1	C	0.31	0/5018	0.71	7/6817 (0.1%)
All	All	0.31	0/15054	0.71	20/20451 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10
1	B	0	6
1	C	0	8
All	All	0	24

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	ILE	N-CA-C	-8.39	102.98	111.88
1	C	137	PRO	CA-C-N	7.76	136.36	121.54
1	C	137	PRO	C-N-CA	7.76	136.36	121.54
1	B	699	LEU	CA-C-N	6.78	134.48	121.54
1	B	699	LEU	C-N-CA	6.78	134.48	121.54
1	B	178	ARG	N-CA-C	-6.40	106.68	114.75
1	A	124	VAL	N-CA-C	-6.04	106.85	112.83
1	A	427	ARG	CA-C-N	-6.00	112.28	122.11
1	A	427	ARG	C-N-CA	-6.00	112.28	122.11
1	B	700	LEU	CA-C-N	5.99	132.49	121.70
1	B	700	LEU	C-N-CA	5.99	132.49	121.70
1	C	178	ARG	N-CA-C	-5.78	105.13	114.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	GLY	N-CA-C	5.61	126.47	113.18
1	C	137	PRO	N-CA-C	5.54	123.89	112.47
1	C	672	ASP	N-CA-C	-5.54	104.09	111.02
1	A	672	ASP	CA-C-N	5.54	131.67	121.70
1	A	672	ASP	C-N-CA	5.54	131.67	121.70
1	B	718	ASP	CA-C-N	-5.25	117.56	122.66
1	B	718	ASP	C-N-CA	-5.25	117.56	122.66
1	C	391	ILE	N-CA-C	-5.22	107.62	112.43

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ARG	Peptide
1	A	137	PRO	Peptide
1	A	138	GLU	Peptide
1	A	139	GLY	Peptide
1	A	670	PHE	Peptide
1	A	671	ILE	Peptide
1	A	683	PHE	Peptide
1	A	684	VAL	Peptide
1	A	686	LEU	Peptide
1	A	700	LEU	Peptide
1	B	138	GLU	Peptide
1	B	140	GLN	Peptide
1	B	670	PHE	Peptide
1	B	684	VAL	Peptide
1	B	699	LEU	Peptide
1	B	716	PHE	Peptide
1	C	136	ARG	Peptide
1	C	138	GLU	Peptide
1	C	363	VAL	Peptide
1	C	671	ILE	Peptide
1	C	673	LEU	Peptide
1	C	684	VAL	Peptide
1	C	687	GLU	Peptide
1	C	688	VAL	Peptide

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	4898	0	4726	671	0
1	B	4898	0	4726	653	0
1	C	4898	0	4726	602	0
All	All	14694	0	14178	1822	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 63.

All (1822) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:PRO:HA	1:B:452:TYR:O	1.36	1.20
1:B:604:PHE:O	1:B:612:LEU:HA	1.42	1.15
1:C:604:PHE:O	1:C:612:LEU:HA	1.48	1.13
1:C:149:VAL:HA	1:C:449:LEU:O	1.56	1.06
1:B:174:TRP:HB2	1:B:183:MET:HG2	1.40	1.02
1:A:142:TYR:HA	1:A:377:ARG:O	1.61	0.99
1:A:145:GLY:O	1:A:375:MET:HB2	1.63	0.98
1:A:441:TYR:HA	1:A:450:ILE:O	1.64	0.97
1:A:343:ASN:O	1:A:353:ALA:HA	1.64	0.96
1:A:156:PRO:HA	1:A:280:SER:O	1.66	0.96
1:A:604:PHE:O	1:A:612:LEU:HA	1.66	0.95
1:B:672:ASP:HA	1:B:673:LEU:HB3	1.48	0.95
1:C:145:GLY:O	1:C:375:MET:HB3	1.67	0.94
1:C:692:HIS:HA	1:C:695:LYS:HE2	1.50	0.92
1:B:169:THR:HA	1:B:186:PHE:O	1.69	0.92
1:A:381:GLY:HA3	1:A:385:ARG:HH21	1.34	0.92
1:B:106:ALA:HB2	1:B:581:VAL:HB	1.52	0.89
1:A:617:LEU:O	1:A:624:ARG:NH1	2.06	0.89
1:A:149:VAL:HG13	1:A:369:TRP:HB2	1.53	0.88
1:B:589:ILE:HG22	1:B:595:ALA:HB3	1.53	0.88
1:B:699:LEU:H	1:B:700:LEU:HB2	1.38	0.88
1:A:386:PHE:O	1:A:394:THR:HA	1.72	0.88
1:C:589:ILE:HG22	1:C:595:ALA:HB3	1.55	0.88
1:B:154:ILE:HB	1:B:282:TYR:HB3	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG12	1:A:117:PRO:HD3	1.55	0.87
1:C:440:GLN:HB3	1:C:442:TYR:HE1	1.38	0.86
1:A:588:ARG:HA	1:A:596:CYS:HA	1.58	0.86
1:B:502:GLU:HA	1:B:505:ARG:HB2	1.59	0.85
1:C:682:GLU:HA	1:C:689:TYR:HD1	1.42	0.85
1:A:242:ARG:NH1	1:A:623:LEU:O	2.08	0.85
1:B:600:PRO:HB2	1:B:617:LEU:HB3	1.57	0.85
1:A:707:ARG:O	1:A:710:GLN:NE2	2.10	0.84
1:A:388:SER:O	1:A:392:SER:HA	1.77	0.84
1:B:136:ARG:HB2	1:B:526:ILE:HD11	1.58	0.83
1:B:149:VAL:HA	1:B:449:LEU:O	1.79	0.83
1:C:423:ARG:HB3	1:C:427:ARG:HH21	1.42	0.83
1:C:529:CYS:SG	1:C:533:ASN:ND2	2.50	0.83
1:B:640:TYR:HA	1:B:648:VAL:O	1.78	0.83
1:B:344:LEU:HA	1:B:352:VAL:O	1.78	0.82
1:A:558:ARG:HH22	1:A:576:VAL:HG12	1.44	0.82
1:B:113:PHE:HA	1:B:621:ASN:HB3	1.60	0.82
1:A:149:VAL:HA	1:A:449:LEU:O	1.78	0.82
1:B:466:ARG:NH2	1:B:507:GLN:OE1	2.12	0.82
1:B:637:HIS:HB3	1:B:652:GLU:HA	1.61	0.81
1:B:710:GLN:HE22	1:B:713:ASP:HB3	1.45	0.81
1:C:597:TYR:HA	1:C:630:ILE:HA	1.60	0.81
1:B:561:ALA:HA	1:B:569:ALA:O	1.81	0.81
1:B:470:ARG:NH1	1:B:471:GLU:OE2	2.12	0.81
1:C:638:ARG:HH11	1:C:651:GLU:HB2	1.44	0.81
1:A:163:MET:O	1:A:273:VAL:HA	1.82	0.80
1:A:712:HIS:HB3	1:A:715:ARG:HH21	1.46	0.80
1:C:599:ARG:NE	1:C:617:LEU:O	2.13	0.80
1:B:423:ARG:HB3	1:B:427:ARG:HH21	1.46	0.80
1:B:164:TYR:HB3	1:B:192:VAL:HB	1.63	0.80
1:A:701:ASP:HB3	1:A:704:GLU:HB2	1.64	0.80
1:A:470:ARG:O	1:A:474:ARG:NH1	2.15	0.80
1:A:616:GLN:OE1	1:A:624:ARG:NH2	2.14	0.80
1:B:151:LYS:HZ2	1:B:369:TRP:HA	1.45	0.80
1:B:300:PHE:HB2	1:B:310:GLU:HG2	1.64	0.80
1:C:318:ARG:HH21	1:C:347:THR:HA	1.47	0.80
1:C:470:ARG:HH22	1:C:474:ARG:HH21	1.24	0.80
1:A:464:TYR:O	1:A:468:HIS:HB2	1.81	0.79
1:B:597:TYR:HA	1:B:630:ILE:HA	1.61	0.79
1:A:440:GLN:H	1:A:452:TYR:H	1.29	0.79
1:C:707:ARG:O	1:C:710:GLN:NE2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:SER:HA	1:A:184:GLY:O	1.83	0.78
1:A:545:LEU:HD22	1:C:541:GLU:HB2	1.63	0.78
1:A:558:ARG:NH2	1:A:574:VAL:O	2.16	0.78
1:C:514:GLN:HG2	1:C:518:ASN:HD21	1.47	0.78
1:C:147:ALA:HB2	1:C:375:MET:HG2	1.66	0.78
1:C:444:ALA:HB3	1:C:448:PHE:HB2	1.66	0.77
1:B:466:ARG:NH2	1:B:467:GLU:OE2	2.16	0.77
1:B:699:LEU:HB3	1:B:700:LEU:HG	1.66	0.77
1:C:708:ARG:O	1:C:715:ARG:NH2	2.17	0.77
1:A:425:PHE:HA	1:A:429:TYR:HD1	1.49	0.77
1:C:541:GLU:HA	1:C:544:LYS:HD2	1.67	0.77
1:C:588:ARG:HA	1:C:596:CYS:HA	1.65	0.77
1:C:233:GLU:O	1:C:235:LYS:NZ	2.17	0.77
1:A:113:PHE:O	1:A:558:ARG:NH1	2.19	0.76
1:A:444:ALA:HB3	1:A:448:PHE:HB2	1.67	0.76
1:B:285:ASP:HA	1:B:298:SER:HB2	1.67	0.76
1:B:210:THR:HG22	1:B:223:PHE:HA	1.68	0.76
1:B:329:ASP:N	1:B:334:ALA:O	2.19	0.76
1:B:581:VAL:HG13	1:B:602:VAL:HG11	1.66	0.76
1:A:470:ARG:NH1	1:A:471:GLU:OE1	2.19	0.76
1:A:631:GLU:OE2	1:B:707:ARG:NH1	2.19	0.76
1:A:150:PHE:HA	1:A:368:LYS:HA	1.67	0.76
1:A:466:ARG:NH2	1:A:507:GLN:OE1	2.19	0.76
1:C:121:GLY:HA3	1:C:292:GLY:HA2	1.68	0.75
1:C:160:LYS:NZ	1:C:277:ASP:OD1	2.17	0.75
1:C:133:CYS:SG	1:C:533:ASN:ND2	2.60	0.75
1:B:142:TYR:HB3	1:B:376:LEU:HD22	1.68	0.75
1:B:279:ARG:HH21	1:C:678:LEU:HD13	1.50	0.75
1:C:466:ARG:NH2	1:C:467:GLU:OE2	2.20	0.75
1:B:444:ALA:HB3	1:B:448:PHE:HB2	1.69	0.75
1:A:378:SER:HB3	1:A:385:ARG:HB2	1.69	0.74
1:C:439:PRO:HA	1:C:452:TYR:O	1.86	0.74
1:B:712:HIS:O	1:B:715:ARG:NH1	2.20	0.74
1:A:686:LEU:HD12	1:C:187:GLU:HG2	1.68	0.74
1:C:296:TYR:O	1:C:313:SER:OG	2.05	0.74
1:C:169:THR:HA	1:C:186:PHE:O	1.85	0.74
1:B:582:ILE:O	1:B:602:VAL:HA	1.87	0.74
1:A:105:LYS:HA	1:A:582:ILE:HG13	1.69	0.74
1:A:377:ARG:NH1	1:A:379:GLU:OE1	2.21	0.74
1:C:379:GLU:HG3	1:C:384:PHE:HE1	1.51	0.74
1:C:377:ARG:NH2	1:C:471:GLU:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:NH2	1:C:394:THR:O	2.20	0.73
1:C:376:LEU:HG	1:C:387:SER:HB2	1.71	0.73
1:A:598:SER:OG	1:A:624:ARG:NH2	2.21	0.73
1:B:551:ALA:O	1:B:555:VAL:HB	1.87	0.73
1:C:207:CYS:O	1:C:232:MET:N	2.21	0.73
1:C:328:ARG:HA	1:C:335:ARG:HA	1.69	0.73
1:C:644:GLY:O	1:C:661:ARG:NH2	2.21	0.73
1:C:163:MET:HA	1:C:351:THR:O	1.88	0.73
1:A:436:VAL:O	1:A:453:GLN:NE2	2.21	0.73
1:B:530:GLU:O	1:B:534:HIS:N	2.21	0.73
1:B:644:GLY:O	1:B:661:ARG:NH1	2.16	0.73
1:C:142:TYR:N	1:C:377:ARG:O	2.22	0.73
1:C:156:PRO:HA	1:C:281:VAL:HA	1.68	0.73
1:A:235:LYS:O	1:A:248:HIS:N	2.19	0.72
1:A:605:ARG:HE	1:A:612:LEU:HD13	1.51	0.72
1:A:502:GLU:HA	1:A:505:ARG:HB2	1.70	0.72
1:B:210:THR:OG1	1:B:229:GLU:OE2	2.06	0.72
1:A:169:THR:HA	1:A:186:PHE:O	1.89	0.72
1:B:226:ASP:OD2	1:B:264:ARG:NH2	2.23	0.72
1:C:439:PRO:HG3	1:C:453:GLN:HB2	1.70	0.72
1:B:236:PRO:HA	1:B:247:TRP:HA	1.70	0.72
1:B:588:ARG:HA	1:B:596:CYS:HA	1.71	0.72
1:C:132:ARG:NH1	1:C:133:CYS:O	2.23	0.72
1:A:151:LYS:HG3	1:A:369:TRP:NE1	2.04	0.72
1:A:318:ARG:O	1:A:320:LYS:NZ	2.23	0.72
1:B:163:MET:HE1	1:B:352:VAL:HG13	1.71	0.72
1:A:117:PRO:O	1:A:560:SER:OG	2.06	0.72
1:A:149:VAL:O	1:A:369:TRP:N	2.22	0.72
1:A:178:ARG:HA	1:A:258:ARG:HH22	1.53	0.72
1:A:275:GLU:HG3	1:A:330:LEU:HD12	1.72	0.72
1:C:142:TYR:CA	1:C:377:ARG:O	2.38	0.72
1:C:404:LEU:HB2	1:C:410:GLY:HA3	1.71	0.72
1:C:344:LEU:HA	1:C:352:VAL:O	1.90	0.72
1:A:210:THR:OG1	1:A:229:GLU:OE2	2.08	0.71
1:A:703:THR:O	1:C:702:TYR:OH	2.07	0.71
1:C:225:ARG:HD3	1:C:254:TYR:HB2	1.72	0.71
1:A:703:THR:OG1	1:A:707:ARG:NH2	2.23	0.71
1:B:602:VAL:HB	1:B:623:LEU:HD11	1.73	0.71
1:B:167:ASP:HA	1:B:188:ASP:O	1.91	0.71
1:A:209:SER:N	1:A:230:THR:O	2.23	0.71
1:A:463:LEU:HD22	1:A:466:ARG:HE	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:LEU:HD13	1:B:466:ARG:HH11	1.54	0.71
1:C:210:THR:OG1	1:C:229:GLU:OE1	2.08	0.71
1:A:402:TYR:HE2	1:A:407:VAL:HG13	1.56	0.71
1:C:235:LYS:N	1:C:248:HIS:O	2.23	0.71
1:B:535:GLU:HA	1:B:538:LEU:HD13	1.72	0.71
1:B:162:THR:HA	1:B:275:GLU:HA	1.73	0.71
1:A:624:ARG:NH1	1:B:701:ASP:OD1	2.23	0.71
1:C:435:LYS:NZ	1:C:437:GLY:O	2.24	0.71
1:B:132:ARG:NH1	1:B:133:CYS:O	2.24	0.71
1:C:704:GLU:OE1	1:C:707:ARG:NE	2.23	0.71
1:B:200:LYS:O	1:B:206:VAL:N	2.22	0.70
1:B:408:ASP:HB2	1:B:409:LEU:HD12	1.72	0.70
1:B:649:TYR:HB3	1:B:657:HIS:O	1.91	0.70
1:C:378:SER:OG	1:C:385:ARG:HB2	1.91	0.70
1:A:120:THR:OG1	1:B:680:ASP:OD1	2.06	0.70
1:A:123:THR:O	1:A:126:GLN:NE2	2.23	0.70
1:A:713:ASP:OD1	1:A:713:ASP:N	2.22	0.70
1:C:159:PHE:CE2	1:C:354:TRP:HB2	2.26	0.70
1:C:322:VAL:HG22	1:C:325:PHE:HB2	1.73	0.70
1:A:388:SER:O	1:A:392:SER:CA	2.40	0.70
1:B:320:LYS:HZ1	1:B:346:THR:HG23	1.57	0.70
1:B:596:CYS:O	1:B:631:GLU:N	2.25	0.70
1:B:164:TYR:HD1	1:B:273:VAL:HG22	1.57	0.70
1:C:647:TYR:O	1:C:658:GLN:HA	1.91	0.70
1:A:142:TYR:HB3	1:A:376:LEU:HD11	1.73	0.70
1:A:234:LEU:HB2	1:A:333:LYS:HE2	1.74	0.69
1:A:601:LEU:HD12	1:A:616:GLN:HG2	1.73	0.69
1:B:501:ILE:HD12	1:B:504:ALA:HB3	1.74	0.69
1:C:466:ARG:O	1:C:469:LEU:HB3	1.91	0.69
1:B:501:ILE:HG13	1:B:505:ARG:HD2	1.74	0.69
1:A:175:PHE:HB3	1:A:260:GLU:HG2	1.73	0.69
1:C:471:GLU:OE2	1:C:510:TYR:OH	2.10	0.69
1:C:598:SER:N	1:C:629:ALA:O	2.18	0.69
1:A:692:HIS:HA	1:A:695:LYS:HD2	1.74	0.69
1:C:620:ASN:HA	1:C:642:THR:HB	1.74	0.69
1:A:644:GLY:O	1:A:661:ARG:NH2	2.25	0.69
1:A:160:LYS:NZ	1:A:277:ASP:OD1	2.20	0.69
1:B:620:ASN:H	1:B:642:THR:HB	1.58	0.69
1:B:138:GLU:O	1:B:140:GLN:NE2	2.26	0.69
1:B:498:THR:HG21	1:B:504:ALA:H	1.56	0.69
1:B:723:ILE:HA	1:C:181:GLN:HE21	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:TYR:HA	1:C:377:ARG:O	1.93	0.69
1:C:209:SER:H	1:C:230:THR:H	1.39	0.69
1:A:587:MET:HE1	1:A:601:LEU:HB2	1.73	0.69
1:A:672:ASP:HB2	1:A:674:ASN:HD21	1.58	0.69
1:A:187:GLU:OE2	1:A:188:ASP:N	2.25	0.68
1:A:665:THR:OG1	1:C:126:GLN:NE2	2.26	0.68
1:B:209:SER:N	1:B:230:THR:O	2.23	0.68
1:B:637:HIS:N	1:B:652:GLU:OE1	2.24	0.68
1:C:298:SER:HB2	1:C:311:HIS:HB3	1.74	0.68
1:C:465:VAL:HA	1:C:468:HIS:HE1	1.58	0.68
1:A:303:TYR:N	1:A:321:GLN:OE1	2.26	0.68
1:B:114:TYR:HA	1:B:576:VAL:HG21	1.75	0.68
1:A:576:VAL:HG11	1:A:623:LEU:HD22	1.75	0.68
1:C:151:LYS:O	1:C:367:THR:N	2.25	0.68
1:C:196:GLU:HG3	1:C:200:LYS:HB2	1.75	0.68
1:A:247:TRP:HZ3	1:A:275:GLU:H	1.40	0.68
1:A:301:TYR:O	1:A:308:HIS:ND1	2.26	0.68
1:B:235:LYS:O	1:B:248:HIS:ND1	2.27	0.68
1:C:298:SER:HB3	1:C:301:TYR:HB2	1.75	0.68
1:C:637:HIS:O	1:C:652:GLU:N	2.17	0.68
1:C:237:ALA:H	1:C:247:TRP:HA	1.59	0.68
1:A:122:ALA:HB3	1:A:123:THR:HA	1.74	0.68
1:A:712:HIS:HA	1:A:715:ARG:HE	1.59	0.68
1:C:372:VAL:HG22	1:C:390:ALA:HB3	1.75	0.68
1:A:708:ARG:NH2	1:C:631:GLU:OE1	2.26	0.68
1:B:143:THR:O	1:B:452:TYR:OH	2.12	0.68
1:B:208:ARG:HA	1:B:231:ASP:HA	1.76	0.68
1:B:106:ALA:H	1:B:581:VAL:H	1.42	0.68
1:A:558:ARG:HH12	1:A:576:VAL:H	1.40	0.67
1:B:526:ILE:O	1:B:529:CYS:HB3	1.93	0.67
1:B:634:THR:OG1	1:B:692:HIS:O	2.09	0.67
1:A:700:LEU:HD11	1:A:708:ARG:HG3	1.74	0.67
1:B:634:THR:N	1:B:653:TYR:OH	2.28	0.67
1:A:142:TYR:HD1	1:A:376:LEU:HD21	1.59	0.67
1:B:130:PRO:HG3	1:B:536:LEU:HB2	1.76	0.67
1:A:147:ALA:HB3	1:A:375:MET:HG3	1.77	0.67
1:A:551:ALA:HB3	1:A:559:VAL:HG11	1.76	0.67
1:A:466:ARG:NH1	1:A:467:GLU:HG2	2.09	0.67
1:A:303:TYR:HA	1:A:308:HIS:HB2	1.76	0.67
1:B:178:ARG:O	1:B:258:ARG:NH2	2.27	0.67
1:B:297:MET:H	1:B:311:HIS:CE1	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:MET:HE1	1:A:352:VAL:HG13	1.76	0.67
1:A:703:THR:HG21	1:C:545:LEU:HD13	1.75	0.67
1:B:463:LEU:HD21	1:B:506:LEU:HB2	1.76	0.67
1:B:159:PHE:HE2	1:B:354:TRP:HB2	1.59	0.67
1:C:208:ARG:HB3	1:C:229:GLU:HG3	1.77	0.67
1:B:303:TYR:N	1:B:321:GLN:OE1	2.25	0.66
1:C:682:GLU:HA	1:C:689:TYR:CD1	2.27	0.66
1:A:369:TRP:O	1:B:669:THR:OG1	2.09	0.66
1:A:405:SER:OG	1:A:406:ARG:NH1	2.28	0.66
1:B:637:HIS:O	1:B:652:GLU:N	2.15	0.66
1:C:470:ARG:HH21	1:C:471:GLU:CD	2.02	0.66
1:A:276:VAL:HB	1:A:290:ALA:HB3	1.75	0.66
1:A:328:ARG:HA	1:A:335:ARG:HA	1.76	0.66
1:B:509:THR:O	1:B:513:ILE:N	2.27	0.66
1:C:234:LEU:HB3	1:C:247:TRP:HB2	1.77	0.66
1:C:296:TYR:O	1:C:311:HIS:HE1	1.79	0.66
1:A:571:SER:HA	1:B:677:MET:H	1.59	0.66
1:B:117:PRO:HD2	1:B:560:SER:HB2	1.77	0.66
1:B:118:PRO:HB2	1:C:680:ASP:HB3	1.77	0.66
1:B:152:GLU:HA	1:B:366:MET:HA	1.78	0.66
1:C:240:ALA:H	1:C:245:ARG:HD3	1.61	0.66
1:C:343:ASN:O	1:C:353:ALA:HA	1.95	0.66
1:A:435:LYS:NZ	1:A:437:GLY:O	2.20	0.66
1:A:210:THR:HG22	1:A:223:PHE:HA	1.78	0.66
1:A:466:ARG:NH2	1:A:467:GLU:OE2	2.27	0.66
1:A:618:GLY:N	1:A:622:GLU:O	2.20	0.66
1:B:240:ALA:HA	1:B:246:GLY:H	1.60	0.66
1:C:242:ARG:NH1	1:C:572:THR:O	2.29	0.66
1:A:558:ARG:NH1	1:A:576:VAL:H	1.94	0.66
1:B:196:GLU:HG3	1:B:200:LYS:HB2	1.76	0.66
1:B:547:PRO:HB2	1:B:561:ALA:H	1.59	0.66
1:C:421:MET:HE1	1:C:439:PRO:HB3	1.78	0.66
1:C:444:ALA:HB2	1:C:450:ILE:HD11	1.77	0.66
1:C:543:ARG:HD3	1:C:568:MET:HE3	1.78	0.66
1:A:121:GLY:HA3	1:A:569:ALA:HA	1.77	0.66
1:B:590:SER:HA	1:B:594:GLY:H	1.61	0.66
1:A:196:GLU:HA	1:A:200:LYS:HG2	1.78	0.66
1:A:281:VAL:N	1:A:286:GLU:OE2	2.23	0.66
1:B:122:ALA:H	1:B:123:THR:HA	1.59	0.66
1:B:194:PHE:HB2	1:B:320:LYS:HE3	1.78	0.66
1:C:463:LEU:HD13	1:C:467:GLU:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:O	1:C:455:LEU:N	2.26	0.65
1:C:158:LYS:HD2	1:C:279:ARG:HG3	1.76	0.65
1:A:369:TRP:HA	1:B:670:PHE:HD1	1.62	0.65
1:C:245:ARG:NH1	1:C:246:GLY:O	2.28	0.65
1:A:597:TYR:HA	1:A:630:ILE:HA	1.76	0.65
1:C:194:PHE:HD1	1:C:344:LEU:HD22	1.61	0.65
1:C:605:ARG:HE	1:C:612:LEU:HG	1.60	0.65
1:C:589:ILE:HB	1:C:630:ILE:HG21	1.77	0.65
1:C:672:ASP:N	1:C:673:LEU:O	2.29	0.65
1:A:215:ARG:HE	1:A:218:LEU:HD23	1.61	0.65
1:B:152:GLU:HG3	1:B:365:THR:HB	1.79	0.65
1:C:602:VAL:N	1:C:627:ARG:HH21	1.95	0.65
1:B:140:GLN:HG3	1:B:518:ASN:HB3	1.79	0.65
1:B:171:SER:HA	1:B:184:GLY:O	1.97	0.65
1:A:208:ARG:HH22	1:A:212:LYS:H	1.45	0.65
1:B:582:ILE:H	1:B:602:VAL:HG13	1.61	0.65
1:A:156:PRO:CA	1:A:280:SER:O	2.42	0.65
1:B:150:PHE:HA	1:B:368:LYS:HA	1.79	0.65
1:B:288:VAL:HG12	1:B:294:PHE:HD1	1.62	0.65
1:C:530:GLU:OE1	1:C:534:HIS:NE2	2.29	0.65
1:C:508:PHE:O	1:C:512:HIS:ND1	2.30	0.64
1:A:320:LYS:NZ	1:A:344:LEU:O	2.29	0.64
1:C:166:LYS:NZ	1:C:210:THR:O	2.29	0.64
1:C:402:TYR:N	1:C:441:TYR:O	2.31	0.64
1:A:132:ARG:HB2	1:B:557:ARG:HH22	1.61	0.64
1:A:174:TRP:HB3	1:A:181:GLN:HB2	1.78	0.64
1:A:223:PHE:CD1	1:A:228:HIS:HA	2.33	0.64
1:B:392:SER:HA	1:B:528:TRP:HE1	1.62	0.64
1:B:531:LEU:O	1:B:534:HIS:HB3	1.98	0.64
1:C:109:THR:HA	1:C:645:GLY:H	1.61	0.64
1:B:462:GLU:HG3	1:B:506:LEU:HD13	1.78	0.64
1:A:605:ARG:NH1	1:A:610:GLY:O	2.29	0.64
1:B:157:TYR:O	1:B:158:LYS:NZ	2.30	0.64
1:B:462:GLU:HG2	1:B:463:LEU:HG	1.79	0.64
1:C:224:HIS:CE1	1:C:268:THR:HG23	2.32	0.64
1:A:234:LEU:HB3	1:A:247:TRP:HB3	1.79	0.64
1:B:463:LEU:HD22	1:B:466:ARG:HE	1.62	0.64
1:A:197:VAL:O	1:A:202:ASN:N	2.20	0.64
1:A:540:ASN:HB3	1:A:543:ARG:HH21	1.61	0.64
1:A:557:ARG:NH1	1:A:558:ARG:O	2.29	0.64
1:B:149:VAL:O	1:B:369:TRP:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLU:OE1	1:B:390:ALA:N	2.31	0.64
1:A:700:LEU:HG	1:A:705:VAL:HA	1.79	0.64
1:B:378:SER:OG	1:B:385:ARG:HB2	1.97	0.64
1:B:677:MET:HA	1:B:677:MET:HE3	1.79	0.64
1:B:257:SER:H	1:B:264:ARG:HH21	1.45	0.63
1:B:616:GLN:HE22	1:B:629:ALA:HB3	1.63	0.63
1:B:589:ILE:O	1:B:595:ALA:N	2.21	0.63
1:B:709:ASN:HA	1:B:712:HIS:HE1	1.64	0.63
1:C:148:VAL:HG22	1:C:371:GLU:HG2	1.80	0.63
1:C:197:VAL:HA	1:C:201:ILE:HB	1.78	0.63
1:C:522:GLY:O	1:C:526:ILE:HG13	1.97	0.63
1:A:113:PHE:HA	1:A:621:ASN:HB3	1.79	0.63
1:A:599:ARG:HE	1:A:617:LEU:HG	1.62	0.63
1:B:584:GLN:OE1	1:B:603:SER:N	2.32	0.63
1:B:505:ARG:O	1:B:508:PHE:HB3	1.98	0.63
1:C:403:PRO:HG2	1:C:406:ARG:HG3	1.80	0.63
1:B:153:ASN:N	1:B:365:THR:O	2.32	0.63
1:B:193:PRO:HB2	1:B:195:GLU:HG3	1.79	0.63
1:B:282:TYR:HA	1:B:284:TYR:N	2.13	0.63
1:B:438:GLN:O	1:B:440:GLN:NE2	2.31	0.63
1:A:639:ARG:NH1	1:C:563:MET:SD	2.72	0.63
1:C:166:LYS:HZ1	1:C:208:ARG:HB2	1.64	0.63
1:A:224:HIS:CE1	1:A:268:THR:HG23	2.33	0.63
1:B:140:GLN:HE22	1:B:378:SER:HB2	1.64	0.63
1:B:194:PHE:HD1	1:B:344:LEU:HD22	1.63	0.63
1:B:324:GLY:HA2	1:B:339:PRO:HB2	1.80	0.63
1:C:279:ARG:NH2	1:C:289:LEU:O	2.31	0.63
1:A:178:ARG:HE	1:A:258:ARG:HH22	1.47	0.63
1:A:210:THR:HG23	1:A:229:GLU:HA	1.81	0.63
1:C:258:ARG:NE	1:C:260:GLU:OE1	2.25	0.63
1:A:288:VAL:HG11	1:B:677:MET:HE2	1.80	0.62
1:B:123:THR:N	1:B:126:GLN:OE1	2.29	0.62
1:B:164:TYR:HB2	1:B:351:THR:HB	1.80	0.62
1:A:114:TYR:O	1:A:623:LEU:N	2.32	0.62
1:A:201:ILE:O	1:A:328:ARG:NH1	2.24	0.62
1:A:436:VAL:HG22	1:A:456:LEU:HD23	1.81	0.62
1:C:691:ARG:HG2	1:C:695:LYS:HZ3	1.64	0.62
1:B:198:ILE:HD13	1:B:325:PHE:CZ	2.34	0.62
1:A:330:LEU:HA	1:A:333:LYS:HD3	1.81	0.62
1:A:605:ARG:HH21	1:A:612:LEU:HB2	1.64	0.62
1:A:664:ILE:HB	1:C:126:GLN:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ALA:HB1	1:C:611:PRO:HG2	1.81	0.62
1:C:369:TRP:CD2	1:C:370:GLN:HG2	2.35	0.62
1:A:424:ILE:HD12	1:A:427:ARG:HH22	1.65	0.62
1:A:599:ARG:NH1	1:A:619:GLU:OE2	2.32	0.62
1:C:585:ASN:OD1	1:C:655:TYR:N	2.31	0.62
1:C:704:GLU:O	1:C:708:ARG:HG2	1.98	0.62
1:C:280:SER:HA	1:C:287:PHE:HB3	1.82	0.62
1:A:670:PHE:HB3	1:C:369:TRP:NE1	2.14	0.62
1:C:640:TYR:HA	1:C:648:VAL:O	1.99	0.62
1:B:256:PRO:HB2	1:B:264:ARG:HG3	1.82	0.62
1:C:151:LYS:HG3	1:C:367:THR:HB	1.81	0.62
1:C:517:VAL:O	1:C:521:LEU:HG	2.00	0.62
1:C:381:GLY:HA3	1:C:385:ARG:NH2	2.14	0.62
1:A:151:LYS:O	1:A:367:THR:N	2.22	0.61
1:A:463:LEU:HD13	1:A:466:ARG:HH11	1.65	0.61
1:A:709:ASN:HA	1:A:712:HIS:CE1	2.35	0.61
1:A:110:ASP:HB2	1:A:645:GLY:HA3	1.82	0.61
1:A:290:ALA:HB1	1:B:679:GLU:CD	2.24	0.61
1:B:164:TYR:HD2	1:B:351:THR:HB	1.65	0.61
1:B:174:TRP:HE3	1:B:181:GLN:HB2	1.64	0.61
1:A:343:ASN:HD21	1:A:356:TRP:HB2	1.65	0.61
1:A:558:ARG:NH2	1:A:576:VAL:HG12	2.16	0.61
1:B:235:LYS:N	1:B:248:HIS:O	2.33	0.61
1:C:164:TYR:HB2	1:C:351:THR:HB	1.82	0.61
1:C:303:TYR:N	1:C:321:GLN:OE1	2.32	0.61
1:A:162:THR:HA	1:A:274:GLU:O	2.01	0.61
1:C:150:PHE:HZ	1:C:416:ASP:HB2	1.64	0.61
1:C:168:VAL:O	1:C:187:GLU:HA	2.01	0.61
1:C:440:GLN:HB3	1:C:442:TYR:CE1	2.30	0.61
1:B:463:LEU:HD11	1:B:506:LEU:HB3	1.83	0.61
1:B:687:GLU:HG2	1:B:688:VAL:H	1.65	0.61
1:C:174:TRP:HE3	1:C:181:GLN:HB2	1.64	0.61
1:B:515:ARG:O	1:B:519:ASP:N	2.28	0.61
1:C:240:ALA:HB3	1:C:245:ARG:HB3	1.82	0.61
1:C:640:TYR:HB3	1:C:647:TYR:CD2	2.36	0.61
1:A:678:LEU:HD13	1:C:276:VAL:HG12	1.83	0.61
1:B:105:LYS:HD2	1:B:582:ILE:HD11	1.82	0.61
1:B:142:TYR:HA	1:B:377:ARG:O	2.01	0.61
1:C:470:ARG:NH2	1:C:474:ARG:HH21	1.96	0.61
1:C:600:PRO:HG2	1:C:617:LEU:HD23	1.83	0.61
1:A:420:ALA:HA	1:A:423:ARG:HE	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASN:C	1:B:328:ARG:HE	2.07	0.60
1:C:117:PRO:O	1:C:560:SER:OG	2.15	0.60
1:C:164:TYR:HB3	1:C:192:VAL:HB	1.83	0.60
1:C:225:ARG:NH1	1:C:268:THR:OG1	2.34	0.60
1:C:259:VAL:HB	1:C:264:ARG:HD2	1.82	0.60
1:A:154:ILE:HA	1:A:282:TYR:HD2	1.66	0.60
1:B:555:VAL:HG12	1:C:674:ASN:HD21	1.65	0.60
1:A:149:VAL:HG22	1:A:369:TRP:CD1	2.35	0.60
1:B:562:ARG:HG2	1:B:569:ALA:HB3	1.83	0.60
1:C:616:GLN:HB2	1:C:624:ARG:HG3	1.83	0.60
1:A:173:VAL:HG21	1:A:255:ASN:HD22	1.66	0.60
1:A:637:HIS:HB3	1:A:652:GLU:HA	1.83	0.60
1:B:199:ASP:OD2	1:B:200:LYS:N	2.34	0.60
1:B:366:MET:HB3	1:B:413:ILE:HD11	1.81	0.60
1:B:439:PRO:CA	1:B:452:TYR:O	2.31	0.60
1:C:177:HIS:CD2	1:C:178:ARG:H	2.19	0.60
1:A:153:ASN:N	1:A:365:THR:O	2.35	0.60
1:A:191:PRO:HA	1:A:350:PHE:HA	1.84	0.60
1:A:639:ARG:HH11	1:C:565:GLY:N	1.99	0.60
1:A:681:HIS:CE1	1:C:291:THR:HB	2.37	0.60
1:B:170:VAL:HG22	1:B:186:PHE:HB3	1.83	0.60
1:B:379:GLU:OE2	1:B:474:ARG:NH1	2.35	0.60
1:C:379:GLU:OE2	1:C:474:ARG:NH1	2.35	0.60
1:A:196:GLU:O	1:A:201:ILE:N	2.35	0.60
1:A:247:TRP:CG	1:A:333:LYS:HZ1	2.20	0.60
1:A:329:ASP:O	1:A:333:LYS:N	2.34	0.60
1:A:389:ASP:HB3	1:A:528:TRP:CE2	2.35	0.60
1:C:425:PHE:HA	1:C:429:TYR:HD1	1.66	0.60
1:A:112:ASN:HB3	1:A:577:ALA:HA	1.83	0.60
1:B:159:PHE:CE2	1:B:354:TRP:HB2	2.36	0.60
1:B:428:ARG:HB3	1:B:429:TYR:CE1	2.37	0.60
1:B:465:VAL:HA	1:B:468:HIS:CD2	2.36	0.60
1:C:634:THR:O	1:C:637:HIS:N	2.34	0.60
1:A:535:GLU:HB3	1:A:539:TRP:CZ2	2.37	0.60
1:B:111:ALA:O	1:B:621:ASN:ND2	2.34	0.60
1:A:156:PRO:HB3	1:A:281:VAL:HG12	1.83	0.60
1:A:158:LYS:HD2	1:A:279:ARG:HG3	1.84	0.60
1:A:297:MET:HB2	1:A:314:TYR:HE2	1.66	0.60
1:A:355:ASP:N	1:A:355:ASP:OD1	2.33	0.60
1:A:607:GLU:HG2	1:A:609:GLN:H	1.67	0.60
1:B:440:GLN:H	1:B:452:TYR:H	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ASP:OD2	1:A:704:GLU:N	2.32	0.60
1:B:177:HIS:HB3	1:B:179:TYR:CE1	2.37	0.60
1:B:602:VAL:HG12	1:B:604:PHE:HD1	1.66	0.60
1:C:373:ASP:OD1	1:C:428:ARG:NH1	2.35	0.60
1:B:126:GLN:HE22	1:B:567:VAL:HG23	1.67	0.59
1:B:202:ASN:O	1:B:328:ARG:NE	2.23	0.59
1:B:210:THR:HA	1:B:222:ALA:O	2.02	0.59
1:C:150:PHE:HB2	1:C:449:LEU:HB3	1.83	0.59
1:C:155:ALA:H	1:C:282:TYR:HB3	1.66	0.59
1:C:210:THR:HA	1:C:222:ALA:O	2.01	0.59
1:A:113:PHE:HB2	1:A:576:VAL:HG13	1.83	0.59
1:A:376:LEU:HB3	1:A:387:SER:OG	2.02	0.59
1:A:452:TYR:O	1:A:454:PRO:HD3	2.02	0.59
1:B:150:PHE:HZ	1:B:416:ASP:HB2	1.66	0.59
1:B:235:LYS:HE3	1:B:248:HIS:CE1	2.37	0.59
1:B:374:GLU:HB3	1:B:390:ALA:HB2	1.83	0.59
1:A:318:ARG:HE	1:A:345:LEU:HD11	1.66	0.59
1:A:428:ARG:HB3	1:A:429:TYR:CE1	2.38	0.59
1:A:558:ARG:NE	1:A:573:CYS:SG	2.64	0.59
1:B:127:PHE:HZ	1:B:567:VAL:HA	1.66	0.59
1:B:327:ALA:H	1:B:337:THR:HG1	1.50	0.59
1:B:377:ARG:NH2	1:B:474:ARG:HD2	2.17	0.59
1:B:600:PRO:O	1:B:617:LEU:N	2.22	0.59
1:C:343:ASN:HB2	1:C:354:TRP:CE2	2.36	0.59
1:C:561:ALA:HA	1:C:569:ALA:O	2.03	0.59
1:A:108:ASN:O	1:A:645:GLY:N	2.26	0.59
1:A:141:ASN:OD1	1:A:474:ARG:NH2	2.36	0.59
1:A:518:ASN:HA	1:A:521:LEU:HD12	1.85	0.59
1:B:156:PRO:HB2	1:B:158:LYS:NZ	2.17	0.59
1:C:175:PHE:HB3	1:C:260:GLU:HG2	1.83	0.59
1:C:640:TYR:HB3	1:C:647:TYR:HD2	1.67	0.59
1:A:439:PRO:HA	1:A:452:TYR:C	2.27	0.59
1:A:640:TYR:CD1	1:A:649:TYR:HB2	2.37	0.59
1:B:125:VAL:HG13	1:C:667:VAL:HA	1.84	0.59
1:B:256:PRO:HB3	1:B:265:TYR:C	2.28	0.59
1:C:159:PHE:HE2	1:C:354:TRP:HB2	1.64	0.59
1:C:650:PHE:CZ	1:C:655:TYR:HB2	2.37	0.59
1:A:303:TYR:HB2	1:A:304:ARG:CZ	2.32	0.59
1:C:297:MET:HE2	1:C:314:TYR:HD2	1.67	0.59
1:A:141:ASN:HB3	1:A:377:ARG:NH2	2.17	0.59
1:B:329:ASP:O	1:B:333:LYS:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:TYR:O	1:B:514:GLN:HG3	2.03	0.59
1:A:620:ASN:HA	1:A:642:THR:HG21	1.84	0.59
1:A:667:VAL:HG23	1:A:670:PHE:CE1	2.38	0.59
1:B:375:MET:O	1:B:452:TYR:OH	2.21	0.59
1:A:176:GLY:HA3	1:A:179:TYR:CE2	2.38	0.58
1:A:599:ARG:HG2	1:A:600:PRO:HD2	1.85	0.58
1:B:318:ARG:O	1:B:320:LYS:NZ	2.34	0.58
1:B:516:PRO:O	1:B:519:ASP:HB2	2.03	0.58
1:B:646:GLY:HA2	1:B:661:ARG:HG3	1.85	0.58
1:A:124:VAL:HG22	1:B:665:THR:H	1.68	0.58
1:A:473:SER:OG	1:A:474:ARG:NH1	2.36	0.58
1:A:108:ASN:HB3	1:A:645:GLY:N	2.17	0.58
1:A:537:THR:HA	1:A:540:ASN:ND2	2.17	0.58
1:B:276:VAL:HB	1:B:290:ALA:HB3	1.85	0.58
1:C:465:VAL:HA	1:C:468:HIS:CE1	2.36	0.58
1:C:598:SER:OG	1:C:631:GLU:HG2	2.03	0.58
1:A:682:GLU:HA	1:A:684:VAL:HG13	1.84	0.58
1:C:194:PHE:O	1:C:198:ILE:HG12	2.02	0.58
1:A:143:THR:HB	1:A:377:ARG:HB3	1.84	0.58
1:B:129:GLN:H	1:B:131:ARG:NH2	2.00	0.58
1:B:200:LYS:HA	1:B:204:LYS:HD2	1.86	0.58
1:A:129:GLN:OE1	1:B:661:ARG:NH1	2.36	0.58
1:A:168:VAL:HG12	1:A:269:VAL:HG22	1.86	0.58
1:A:634:THR:O	1:A:653:TYR:OH	2.21	0.58
1:C:116:CYS:HB2	1:C:623:LEU:O	2.03	0.58
1:C:649:TYR:CD1	1:C:656:SER:HB3	2.39	0.58
1:A:178:ARG:HA	1:A:258:ARG:NH2	2.18	0.58
1:B:213:TYR:OH	1:B:348:PRO:O	2.17	0.58
1:B:711:LEU:HD12	1:B:714:LEU:HB2	1.84	0.58
1:C:502:GLU:HA	1:C:505:ARG:HD2	1.85	0.58
1:C:661:ARG:HA	1:C:664:ILE:HG12	1.85	0.58
1:A:347:THR:N	1:A:350:PHE:O	2.37	0.58
1:B:589:ILE:N	1:B:595:ALA:O	2.31	0.58
1:B:681:HIS:CG	1:B:682:GLU:H	2.21	0.58
1:C:200:LYS:HA	1:C:204:LYS:HB2	1.85	0.58
1:C:209:SER:N	1:C:230:THR:O	2.36	0.58
1:C:298:SER:OG	1:C:310:GLU:OE1	2.14	0.58
1:C:377:ARG:NH2	1:C:474:ARG:HG3	2.19	0.58
1:C:600:PRO:HB2	1:C:617:LEU:HB3	1.86	0.58
1:A:369:TRP:CD2	1:B:670:PHE:HE1	2.22	0.58
1:B:542:ALA:O	1:B:546:ASN:ND2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ARG:NE	1:B:610:GLY:O	2.37	0.58
1:B:705:VAL:HA	1:B:708:ARG:NE	2.19	0.58
1:C:116:CYS:SG	1:C:622:GLU:HB3	2.44	0.58
1:C:138:GLU:OE2	1:C:518:ASN:HB2	2.04	0.58
1:C:439:PRO:HB2	1:C:441:TYR:CE2	2.38	0.58
1:A:156:PRO:HA	1:A:281:VAL:HA	1.86	0.57
1:A:257:SER:O	1:A:264:ARG:NH1	2.37	0.57
1:A:642:THR:HG23	1:A:661:ARG:NH2	2.19	0.57
1:B:151:LYS:HD3	1:B:369:TRP:CG	2.39	0.57
1:B:320:LYS:NZ	1:B:346:THR:H	2.01	0.57
1:B:555:VAL:O	1:C:674:ASN:ND2	2.37	0.57
1:C:141:ASN:H	1:C:379:GLU:HB3	1.68	0.57
1:A:436:VAL:HB	1:A:454:PRO:HB2	1.85	0.57
1:A:585:ASN:OD1	1:A:655:TYR:N	2.36	0.57
1:A:605:ARG:NH2	1:A:612:LEU:HB2	2.19	0.57
1:B:244:SER:HB2	1:B:275:GLU:C	2.28	0.57
1:B:402:TYR:HA	1:B:406:ARG:HH21	1.69	0.57
1:B:599:ARG:HB3	1:B:616:GLN:HG2	1.86	0.57
1:C:319:PHE:CE1	1:C:343:ASN:HB3	2.40	0.57
1:C:326:TYR:HB3	1:C:335:ARG:HG2	1.86	0.57
1:A:154:ILE:O	1:A:282:TYR:N	2.37	0.57
1:A:307:SER:HB2	1:A:356:TRP:HZ2	1.69	0.57
1:B:441:TYR:HD1	1:B:449:LEU:HD11	1.69	0.57
1:B:507:GLN:HE21	1:B:511:ASN:HD21	1.52	0.57
1:C:156:PRO:HA	1:C:280:SER:O	2.05	0.57
1:C:289:LEU:HD13	1:C:294:PHE:HA	1.87	0.57
1:A:174:TRP:HB2	1:A:183:MET:HG2	1.87	0.57
1:A:634:THR:N	1:A:653:TYR:OH	2.37	0.57
1:B:161:ALA:HA	1:B:353:ALA:O	2.04	0.57
1:B:532:GLN:NE2	1:B:533:ASN:OD1	2.37	0.57
1:C:632:PRO:HB3	1:C:695:LYS:HG3	1.87	0.57
1:A:116:CYS:SG	1:A:622:GLU:HB3	2.45	0.57
1:A:682:GLU:HB3	1:C:189:ARG:HD2	1.86	0.57
1:C:614:GLU:HB2	1:C:627:ARG:HD2	1.86	0.57
1:C:700:LEU:HD22	1:C:705:VAL:HA	1.85	0.57
1:A:557:ARG:NE	1:B:674:ASN:O	2.31	0.57
1:A:701:ASP:OD2	1:A:703:THR:OG1	2.19	0.57
1:B:320:LYS:HZ1	1:B:346:THR:H	1.51	0.57
1:B:343:ASN:HB2	1:B:354:TRP:CE2	2.40	0.57
1:B:401:GLU:HA	1:B:441:TYR:O	2.04	0.57
1:C:428:ARG:HB3	1:C:429:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:ASP:OD1	1:C:713:ASP:N	2.34	0.57
1:A:388:SER:O	1:A:392:SER:N	2.38	0.57
1:B:329:ASP:HB2	1:B:336:ALA:HB2	1.87	0.57
1:C:708:ARG:C	1:C:715:ARG:HH22	2.13	0.57
1:A:434:ILE:HB	1:A:456:LEU:HG	1.86	0.57
1:B:155:ALA:O	1:B:284:TYR:OH	2.17	0.57
1:B:343:ASN:ND2	1:B:356:TRP:HB2	2.20	0.57
1:C:191:PRO:HD2	1:C:213:TYR:CZ	2.39	0.57
1:C:598:SER:HB2	1:C:629:ALA:HB1	1.85	0.57
1:A:698:GLY:C	1:A:700:LEU:HB2	2.30	0.57
1:B:508:PHE:O	1:B:512:HIS:ND1	2.33	0.57
1:C:242:ARG:NH2	1:C:574:VAL:HG12	2.19	0.57
1:C:633:CYS:HA	1:C:653:TYR:CE2	2.40	0.57
1:C:640:TYR:CE1	1:C:649:TYR:HB2	2.39	0.57
1:C:666:THR:HG22	1:C:667:VAL:H	1.68	0.57
1:A:424:ILE:HD13	1:A:427:ARG:HH12	1.70	0.57
1:A:671:ILE:O	1:C:557:ARG:NH2	2.38	0.57
1:B:147:ALA:HB3	1:B:375:MET:HG3	1.87	0.57
1:C:199:ASP:OD2	1:C:204:LYS:NZ	2.32	0.57
1:C:436:VAL:O	1:C:453:GLN:NE2	2.38	0.57
1:A:165:TYR:HA	1:A:192:VAL:H	1.69	0.56
1:A:208:ARG:HD2	1:A:229:GLU:CD	2.30	0.56
1:A:297:MET:HG2	1:A:313:SER:H	1.69	0.56
1:A:372:VAL:O	1:A:375:MET:HG2	2.05	0.56
1:A:675:ILE:H	1:A:675:ILE:HD12	1.70	0.56
1:B:123:THR:H	1:B:126:GLN:CD	2.13	0.56
1:B:502:GLU:HA	1:B:505:ARG:HD3	1.86	0.56
1:C:171:SER:HA	1:C:184:GLY:O	2.05	0.56
1:C:618:GLY:N	1:C:622:GLU:O	2.38	0.56
1:A:590:SER:HA	1:A:594:GLY:H	1.69	0.56
1:B:286:GLU:HB2	1:B:294:PHE:CE1	2.40	0.56
1:C:385:ARG:HG3	1:C:396:THR:HA	1.85	0.56
1:B:437:GLY:O	1:B:453:GLN:NE2	2.30	0.56
1:C:164:TYR:HD1	1:C:273:VAL:HG22	1.70	0.56
1:C:185:ILE:HG23	1:C:253:LYS:HE3	1.87	0.56
1:C:639:ARG:NH2	1:C:696:ASP:OD2	2.37	0.56
1:C:646:GLY:O	1:C:661:ARG:NH1	2.39	0.56
1:B:149:VAL:HG13	1:B:370:GLN:H	1.70	0.56
1:B:635:VAL:N	1:B:693:GLU:OE1	2.39	0.56
1:B:328:ARG:NH1	1:B:333:LYS:O	2.28	0.56
1:B:144:GLU:OE1	1:B:144:GLU:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:PHE:HD1	1:C:228:HIS:HA	1.69	0.56
1:A:151:LYS:HG3	1:A:369:TRP:HE1	1.69	0.56
1:A:297:MET:HB2	1:A:314:TYR:CE2	2.41	0.56
1:A:319:PHE:CE1	1:A:343:ASN:HB3	2.41	0.56
1:B:279:ARG:O	1:B:288:VAL:HG22	2.06	0.56
1:B:296:TYR:HB2	1:B:313:SER:OG	2.06	0.56
1:B:329:ASP:OD1	1:B:331:THR:OG1	2.20	0.56
1:B:711:LEU:HA	1:B:714:LEU:HD12	1.88	0.56
1:C:680:ASP:OD1	1:C:681:HIS:N	2.38	0.56
1:A:140:GLN:O	1:A:379:GLU:HG2	2.05	0.56
1:B:256:PRO:HB2	1:B:264:ARG:NE	2.21	0.56
1:B:410:GLY:HA2	1:B:413:ILE:HD13	1.88	0.56
1:C:119:PRO:O	1:C:562:ARG:NE	2.37	0.56
1:C:564:LEU:HD21	1:C:569:ALA:HB2	1.87	0.56
1:A:117:PRO:HD2	1:A:560:SER:HB2	1.88	0.56
1:A:145:GLY:HA3	1:A:454:PRO:HA	1.88	0.56
1:A:174:TRP:N	1:A:181:GLN:O	2.33	0.56
1:A:540:ASN:O	1:A:544:LYS:HG3	2.06	0.56
1:A:639:ARG:HH11	1:C:565:GLY:H	1.54	0.56
1:B:498:THR:HG21	1:B:504:ALA:N	2.21	0.56
1:B:677:MET:HG3	1:B:678:LEU:H	1.70	0.56
1:C:703:THR:O	1:C:706:GLN:NE2	2.38	0.56
1:A:223:PHE:HD1	1:A:228:HIS:HA	1.70	0.56
1:A:713:ASP:HA	1:A:716:PHE:CE1	2.41	0.56
1:B:442:TYR:HB2	1:B:450:ILE:HB	1.88	0.56
1:B:592:ARG:HD3	1:B:593:PRO:HD2	1.88	0.56
1:B:598:SER:N	1:B:629:ALA:O	2.33	0.56
1:B:705:VAL:O	1:B:708:ARG:HG2	2.05	0.56
1:B:245:ARG:NH1	1:B:329:ASP:OD1	2.40	0.55
1:B:424:ILE:O	1:B:427:ARG:HG2	2.06	0.55
1:B:502:GLU:O	1:B:506:LEU:N	2.29	0.55
1:B:549:ALA:O	1:B:553:VAL:HG12	2.05	0.55
1:C:150:PHE:HB3	1:C:366:MET:HB3	1.87	0.55
1:A:136:ARG:CZ	1:A:526:ILE:HD12	2.36	0.55
1:A:237:ALA:HA	1:A:248:HIS:ND1	2.21	0.55
1:A:535:GLU:HA	1:A:538:LEU:HD13	1.88	0.55
1:A:665:THR:O	1:A:667:VAL:HG22	2.06	0.55
1:B:149:VAL:HG13	1:B:369:TRP:HB3	1.88	0.55
1:B:466:ARG:HD2	1:B:507:GLN:HB2	1.88	0.55
1:B:470:ARG:CZ	1:B:514:GLN:HE22	2.18	0.55
1:A:235:LYS:N	1:A:248:HIS:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:GLU:HA	1:A:707:ARG:HE	1.70	0.55
1:B:106:ALA:N	1:B:579:ASP:O	2.39	0.55
1:B:106:ALA:HA	1:B:643:PHE:HZ	1.72	0.55
1:B:452:TYR:HE2	1:B:454:PRO:HA	1.70	0.55
1:C:140:GLN:OE1	1:C:378:SER:HB2	2.06	0.55
1:A:404:LEU:HB3	1:A:410:GLY:HA3	1.89	0.55
1:A:631:GLU:HG3	1:A:632:PRO:HD2	1.89	0.55
1:B:146:ILE:HD13	1:B:421:MET:HG2	1.88	0.55
1:C:325:PHE:O	1:C:340:THR:OG1	2.20	0.55
1:A:258:ARG:NH2	1:A:260:GLU:OE2	2.31	0.55
1:A:284:TYR:CG	1:A:300:PHE:HE2	2.25	0.55
1:A:375:MET:SD	1:A:388:SER:HB2	2.46	0.55
1:A:702:TYR:O	1:A:706:GLN:NE2	2.40	0.55
1:B:302:GLY:HA3	1:B:356:TRP:CE2	2.41	0.55
1:B:209:SER:O	1:B:269:VAL:HB	2.07	0.55
1:B:558:ARG:HD3	1:B:559:VAL:H	1.72	0.55
1:C:297:MET:SD	1:C:312:THR:HA	2.46	0.55
1:C:415:LYS:HZ3	1:C:418:ARG:HD2	1.71	0.55
1:C:578:ALA:HB1	1:C:643:PHE:HE2	1.72	0.55
1:A:517:VAL:O	1:A:521:LEU:HG	2.06	0.55
1:A:676:THR:O	1:C:279:ARG:NH2	2.39	0.55
1:C:160:LYS:NZ	1:C:244:SER:OG	2.38	0.55
1:C:424:ILE:HG22	1:C:429:TYR:HE1	1.70	0.55
1:C:439:PRO:HB2	1:C:441:TYR:HE2	1.71	0.55
1:A:152:GLU:OE1	1:A:282:TYR:OH	2.16	0.55
1:B:538:LEU:H	1:B:538:LEU:HD12	1.72	0.55
1:B:702:TYR:O	1:B:705:VAL:HB	2.06	0.55
1:C:154:ILE:H	1:C:154:ILE:HD12	1.70	0.55
1:C:685:PRO:HG2	1:C:690:THR:HG21	1.89	0.55
1:A:242:ARG:N	1:A:606:TYR:OH	2.39	0.55
1:A:502:GLU:HB3	1:A:506:LEU:HD12	1.87	0.55
1:A:541:GLU:HA	1:A:544:LYS:HD3	1.88	0.55
1:C:116:CYS:O	1:C:118:PRO:HD3	2.06	0.55
1:B:154:ILE:HG13	1:B:156:PRO:HD3	1.89	0.55
1:A:300:PHE:CG	1:A:359:LYS:HA	2.42	0.54
1:A:301:TYR:CZ	1:A:312:THR:HB	2.42	0.54
1:A:672:ASP:OD1	1:A:672:ASP:N	2.35	0.54
1:B:537:THR:HA	1:B:540:ASN:OD1	2.06	0.54
1:A:704:GLU:HG3	1:A:707:ARG:CZ	2.38	0.54
1:B:142:TYR:CD1	1:B:376:LEU:HB3	2.43	0.54
1:C:297:MET:HE2	1:C:314:TYR:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HA	1:A:451:ALA:O	2.07	0.54
1:A:256:PRO:HB2	1:A:264:ARG:NE	2.21	0.54
1:A:701:ASP:O	1:A:704:GLU:N	2.40	0.54
1:B:150:PHE:HB3	1:B:366:MET:SD	2.48	0.54
1:B:587:MET:O	1:B:588:ARG:HG3	2.08	0.54
1:B:712:HIS:O	1:B:715:ARG:HD3	2.06	0.54
1:C:213:TYR:OH	1:C:348:PRO:O	2.25	0.54
1:C:583:VAL:HG22	1:C:602:VAL:HG12	1.90	0.54
1:C:711:LEU:HB2	1:C:715:ARG:NH2	2.22	0.54
1:B:562:ARG:HB3	1:C:699:LEU:HD23	1.88	0.54
1:B:710:GLN:NE2	1:B:713:ASP:HB3	2.20	0.54
1:C:146:ILE:O	1:C:452:TYR:HA	2.08	0.54
1:C:701:ASP:O	1:C:704:GLU:N	2.41	0.54
1:A:187:GLU:HG3	1:B:684:VAL:HG12	1.90	0.54
1:A:199:ASP:O	1:A:204:LYS:N	2.40	0.54
1:A:247:TRP:CD1	1:A:333:LYS:HZ1	2.26	0.54
1:B:105:LYS:HZ2	1:B:612:LEU:HD11	1.73	0.54
1:B:372:VAL:HG13	1:B:391:ILE:HG23	1.89	0.54
1:C:107:GLU:OE1	1:C:660:SER:OG	2.22	0.54
1:C:150:PHE:CE2	1:C:413:ILE:HG23	2.43	0.54
1:A:330:LEU:O	1:A:333:LYS:NZ	2.30	0.54
1:A:540:ASN:HA	1:A:543:ARG:HE	1.72	0.54
1:A:650:PHE:CZ	1:A:655:TYR:HB2	2.43	0.54
1:B:108:ASN:O	1:B:645:GLY:N	2.28	0.54
1:B:115:VAL:HG23	1:B:576:VAL:HG22	1.90	0.54
1:B:602:VAL:C	1:B:627:ARG:HH21	2.16	0.54
1:B:723:ILE:HA	1:C:181:GLN:NE2	2.22	0.54
1:C:559:VAL:HG12	1:C:572:THR:HA	1.89	0.54
1:C:589:ILE:N	1:C:595:ALA:O	2.30	0.54
1:A:133:CYS:HB3	1:A:526:ILE:HG23	1.90	0.54
1:A:151:LYS:HE2	1:A:369:TRP:CZ2	2.42	0.54
1:B:144:GLU:O	1:B:455:LEU:N	2.30	0.54
1:B:163:MET:HA	1:B:351:THR:O	2.07	0.54
1:B:235:LYS:HE2	1:B:250:THR:N	2.22	0.54
1:A:132:ARG:HD3	1:B:557:ARG:HH21	1.73	0.54
1:A:570:VAL:HG13	1:B:677:MET:HB2	1.90	0.54
1:A:616:GLN:HG3	1:A:626:THR:O	2.08	0.54
1:B:302:GLY:HA2	1:B:319:PHE:HZ	1.72	0.54
1:C:223:PHE:CD1	1:C:228:HIS:HA	2.43	0.54
1:C:560:SER:OG	1:C:571:SER:OG	2.25	0.54
1:A:199:ASP:HA	1:A:203:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HH12	1:A:212:LYS:HE2	1.73	0.54
1:A:615:GLY:O	1:A:627:ARG:NE	2.40	0.54
1:C:420:ALA:O	1:C:424:ILE:HG12	2.08	0.54
1:C:424:ILE:O	1:C:427:ARG:HG2	2.08	0.54
1:A:344:LEU:HA	1:A:352:VAL:O	2.08	0.53
1:A:369:TRP:HB3	1:A:370:GLN:OE1	2.08	0.53
1:A:500:SER:HB3	1:A:503:PHE:CE2	2.42	0.53
1:A:637:HIS:N	1:A:652:GLU:OE2	2.41	0.53
1:A:401:GLU:HA	1:A:441:TYR:O	2.07	0.53
1:B:114:TYR:O	1:B:622:GLU:HA	2.08	0.53
1:B:202:ASN:O	1:B:326:TYR:OH	2.16	0.53
1:C:215:ARG:O	1:C:218:LEU:HG	2.08	0.53
1:C:300:PHE:CG	1:C:359:LYS:HA	2.44	0.53
1:C:329:ASP:N	1:C:334:ALA:O	2.40	0.53
1:A:634:THR:OG1	1:A:692:HIS:O	2.19	0.53
1:B:499:SER:HB3	1:B:503:PHE:HE1	1.73	0.53
1:B:536:LEU:HA	1:B:539:TRP:HD1	1.74	0.53
1:C:256:PRO:HB2	1:C:264:ARG:NE	2.22	0.53
1:C:616:GLN:O	1:C:624:ARG:N	2.41	0.53
1:A:546:ASN:O	1:A:550:ILE:HG12	2.08	0.53
1:A:670:PHE:CD2	1:A:671:ILE:HB	2.43	0.53
1:C:523:ARG:HA	1:C:526:ILE:HD12	1.89	0.53
1:A:701:ASP:CB	1:A:704:GLU:HB2	2.37	0.53
1:A:709:ASN:HB2	1:B:710:GLN:OE1	2.08	0.53
1:B:245:ARG:O	1:B:275:GLU:HG2	2.08	0.53
1:B:402:TYR:N	1:B:441:TYR:HB2	2.24	0.53
1:A:150:PHE:CE1	1:A:368:LYS:HB3	2.43	0.53
1:A:162:THR:HG23	1:A:274:GLU:C	2.34	0.53
1:A:541:GLU:HG3	1:B:545:LEU:HD22	1.91	0.53
1:A:683:PHE:O	1:A:690:THR:HG21	2.09	0.53
1:B:119:PRO:HB3	1:B:560:SER:O	2.09	0.53
1:B:245:ARG:HH22	1:B:329:ASP:HA	1.74	0.53
1:B:634:THR:OG1	1:B:695:LYS:HE3	2.07	0.53
1:C:364:CYS:HA	1:C:409:LEU:HD13	1.91	0.53
1:A:287:PHE:CE1	1:A:295:VAL:HB	2.44	0.53
1:B:147:ALA:HA	1:B:451:ALA:O	2.09	0.53
1:B:235:LYS:HE3	1:B:248:HIS:NE2	2.23	0.53
1:B:243:THR:HG23	1:B:244:SER:O	2.08	0.53
1:B:467:GLU:OE1	1:B:471:GLU:HG2	2.08	0.53
1:A:136:ARG:HB3	1:A:137:PRO:CD	2.39	0.53
1:B:460:LEU:HD22	1:B:506:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:PHE:CZ	1:C:368:LYS:HB2	2.43	0.53
1:A:114:TYR:CE2	1:A:558:ARG:HA	2.44	0.53
1:A:143:THR:O	1:A:452:TYR:OH	2.27	0.53
1:A:586:SER:O	1:A:587:MET:HE2	2.09	0.53
1:B:146:ILE:HG22	1:B:453:GLN:HB3	1.91	0.53
1:B:527:ALA:O	1:B:531:LEU:HG	2.09	0.53
1:B:694:ILE:HG22	1:B:708:ARG:HH22	1.74	0.53
1:C:559:VAL:HA	1:C:572:THR:HA	1.91	0.53
1:C:704:GLU:HA	1:C:707:ARG:HG3	1.91	0.53
1:A:113:PHE:CE2	1:A:578:ALA:HA	2.44	0.53
1:A:702:TYR:OH	1:B:706:GLN:HB2	2.09	0.53
1:B:164:TYR:CD2	1:B:351:THR:HB	2.44	0.53
1:B:375:MET:SD	1:B:388:SER:HB2	2.49	0.53
1:C:144:GLU:HG2	1:C:455:LEU:HB2	1.91	0.53
1:A:344:LEU:HG	1:A:353:ALA:HB2	1.90	0.52
1:B:548:ASN:ND2	1:B:620:ASN:HB2	2.24	0.52
1:C:463:LEU:HG	1:C:506:LEU:HB3	1.90	0.52
1:A:297:MET:HA	1:A:311:HIS:HE1	1.74	0.52
1:A:301:TYR:CE1	1:A:312:THR:HB	2.44	0.52
1:A:345:LEU:O	1:A:351:THR:HA	2.09	0.52
1:A:682:GLU:HG2	1:C:165:TYR:HE1	1.74	0.52
1:C:130:PRO:HG3	1:C:536:LEU:HD22	1.91	0.52
1:A:151:LYS:HE2	1:A:369:TRP:HZ2	1.74	0.52
1:A:343:ASN:HB2	1:A:354:TRP:CE2	2.45	0.52
1:A:505:ARG:O	1:A:509:THR:HG23	2.09	0.52
1:A:677:MET:HG3	1:C:290:ALA:O	2.10	0.52
1:B:209:SER:HB2	1:B:224:HIS:HB2	1.91	0.52
1:B:297:MET:H	1:B:311:HIS:HE1	1.54	0.52
1:C:235:LYS:O	1:C:248:HIS:ND1	2.42	0.52
1:A:149:VAL:HG22	1:A:369:TRP:HD1	1.75	0.52
1:A:178:ARG:HE	1:A:258:ARG:HH12	1.56	0.52
1:A:589:ILE:O	1:A:595:ALA:N	2.29	0.52
1:B:559:VAL:HG11	1:B:622:GLU:OE2	2.09	0.52
1:C:113:PHE:HA	1:C:621:ASN:HB3	1.91	0.52
1:C:242:ARG:HH21	1:C:574:VAL:HG12	1.73	0.52
1:A:646:GLY:O	1:A:661:ARG:NH2	2.37	0.52
1:B:153:ASN:HA	1:C:670:PHE:CZ	2.44	0.52
1:B:198:ILE:HD11	1:B:322:VAL:HG21	1.90	0.52
1:A:324:GLY:HA2	1:A:339:PRO:HB2	1.92	0.52
1:A:380:TYR:C	1:A:385:ARG:HE	2.18	0.52
1:A:706:GLN:HA	1:A:709:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ARG:HH11	1:B:216:ASN:ND2	2.08	0.52
1:B:279:ARG:NH2	1:C:678:LEU:HA	2.25	0.52
1:A:598:SER:N	1:A:629:ALA:O	2.36	0.52
1:B:151:LYS:HE3	1:C:669:THR:H	1.74	0.52
1:B:288:VAL:HB	1:C:678:LEU:HD11	1.92	0.52
1:C:547:PRO:HB2	1:C:561:ALA:HB3	1.91	0.52
1:A:194:PHE:HD1	1:A:344:LEU:HD22	1.75	0.52
1:A:196:GLU:HA	1:A:200:LYS:CG	2.40	0.52
1:B:201:ILE:O	1:B:328:ARG:HD2	2.08	0.52
1:C:595:ALA:HB1	1:C:630:ILE:HD12	1.92	0.52
1:A:115:VAL:HA	1:A:623:LEU:HB2	1.92	0.52
1:A:132:ARG:NH1	1:A:133:CYS:O	2.43	0.52
1:A:583:VAL:HG23	1:A:600:PRO:HB3	1.91	0.52
1:A:602:VAL:HG23	1:A:604:PHE:HE1	1.75	0.52
1:A:646:GLY:HA2	1:A:661:ARG:HG2	1.91	0.52
1:B:224:HIS:CE1	1:B:268:THR:HG23	2.44	0.52
1:C:505:ARG:O	1:C:509:THR:HG23	2.10	0.52
1:C:598:SER:OG	1:C:630:ILE:O	2.28	0.52
1:A:132:ARG:HB2	1:B:557:ARG:NH2	2.25	0.52
1:A:369:TRP:HA	1:B:670:PHE:CD1	2.43	0.52
1:B:463:LEU:HD13	1:B:466:ARG:NH1	2.24	0.52
1:C:142:TYR:CD2	1:C:518:ASN:HB3	2.44	0.52
1:C:468:HIS:HD2	1:C:472:GLN:HE22	1.56	0.52
1:A:200:LYS:HA	1:A:204:LYS:HD3	1.92	0.51
1:A:709:ASN:HA	1:A:712:HIS:NE2	2.25	0.51
1:B:548:ASN:HD21	1:B:620:ASN:HB2	1.74	0.51
1:B:657:HIS:ND1	1:B:658:GLN:O	2.31	0.51
1:B:677:MET:HG3	1:B:678:LEU:HD12	1.92	0.51
1:B:700:LEU:HB3	1:B:701:ASP:C	2.35	0.51
1:C:235:LYS:O	1:C:248:HIS:N	2.26	0.51
1:C:691:ARG:HA	1:C:694:ILE:HD12	1.91	0.51
1:A:343:ASN:ND2	1:A:356:TRP:HB2	2.26	0.51
1:A:466:ARG:HH12	1:A:467:GLU:HG2	1.74	0.51
1:A:618:GLY:HA3	1:A:622:GLU:HB2	1.91	0.51
1:B:122:ALA:N	1:B:123:THR:HA	2.25	0.51
1:C:150:PHE:CD2	1:C:413:ILE:HG23	2.44	0.51
1:C:170:VAL:HG22	1:C:186:PHE:HB3	1.90	0.51
1:C:244:SER:HB2	1:C:275:GLU:HB2	1.92	0.51
1:A:467:GLU:OE1	1:A:471:GLU:HG2	2.10	0.51
1:A:583:VAL:HA	1:A:602:VAL:HG12	1.93	0.51
1:A:589:ILE:N	1:A:595:ALA:O	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:LEU:HB3	1:C:557:ARG:HH21	1.75	0.51
1:B:114:TYR:HB2	1:B:622:GLU:OE2	2.10	0.51
1:B:608:ASP:OD1	1:B:609:GLN:NE2	2.43	0.51
1:B:700:LEU:HB3	1:B:701:ASP:O	2.10	0.51
1:C:157:TYR:HB3	1:C:280:SER:HB3	1.92	0.51
1:C:326:TYR:HA	1:C:339:PRO:HA	1.91	0.51
1:C:649:TYR:HD1	1:C:656:SER:HB3	1.74	0.51
1:A:386:PHE:HE1	1:A:397:THR:OG1	1.93	0.51
1:A:439:PRO:HA	1:A:452:TYR:O	2.09	0.51
1:A:681:HIS:CG	1:A:682:GLU:N	2.79	0.51
1:B:359:LYS:NZ	1:B:361:PRO:HA	2.25	0.51
1:B:403:PRO:HD2	1:B:406:ARG:HE	1.75	0.51
1:B:587:MET:HB3	1:B:653:TYR:HB3	1.92	0.51
1:B:605:ARG:NH2	1:B:612:LEU:HG	2.25	0.51
1:B:710:GLN:O	1:B:714:LEU:HG	2.11	0.51
1:C:276:VAL:HB	1:C:290:ALA:HB3	1.92	0.51
1:A:341:THR:HG23	1:A:356:TRP:H	1.76	0.51
1:A:420:ALA:O	1:A:424:ILE:HG12	2.11	0.51
1:A:502:GLU:OE1	1:A:502:GLU:N	2.37	0.51
1:A:666:THR:O	1:A:667:VAL:HG13	2.10	0.51
1:B:212:LYS:NZ	1:B:229:GLU:OE2	2.38	0.51
1:A:147:ALA:HB2	1:A:452:TYR:HD1	1.76	0.51
1:A:175:PHE:HB2	1:A:260:GLU:HA	1.92	0.51
1:A:502:GLU:O	1:A:506:LEU:HB2	2.10	0.51
1:A:564:LEU:HD11	1:A:569:ALA:HB2	1.91	0.51
1:A:614:GLU:HB2	1:A:627:ARG:HG3	1.92	0.51
1:B:151:LYS:N	1:B:367:THR:O	2.31	0.51
1:B:183:MET:HG3	1:B:263:HIS:CE1	2.45	0.51
1:A:208:ARG:NH1	1:A:229:GLU:OE2	2.42	0.51
1:A:598:SER:OG	1:A:616:GLN:OE1	2.27	0.51
1:B:640:TYR:CE1	1:B:649:TYR:HB2	2.45	0.51
1:C:104:ILE:N	1:C:582:ILE:HG13	2.26	0.51
1:C:162:THR:HB	1:C:164:TYR:OH	2.09	0.51
1:C:537:THR:HA	1:C:540:ASN:ND2	2.25	0.51
1:C:605:ARG:NE	1:C:612:LEU:HG	2.25	0.51
1:A:234:LEU:HD13	1:A:273:VAL:HB	1.93	0.51
1:B:343:ASN:O	1:B:353:ALA:HA	2.11	0.51
1:B:389:ASP:HA	1:B:528:TRP:CE2	2.45	0.51
1:C:198:ILE:HG23	1:C:325:PHE:CE1	2.46	0.51
1:C:470:ARG:HH22	1:C:474:ARG:NH2	2.03	0.51
1:C:536:LEU:HA	1:C:539:TRP:CE3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ASP:HB2	1:A:270:ASN:OD1	2.11	0.51
1:B:636:GLY:N	1:B:652:GLU:OE1	2.43	0.51
1:C:302:GLY:HA2	1:C:319:PHE:CZ	2.46	0.51
1:C:680:ASP:O	1:C:681:HIS:ND1	2.44	0.51
1:A:421:MET:HE1	1:A:439:PRO:HB3	1.91	0.51
1:C:240:ALA:N	1:C:245:ARG:HD3	2.25	0.51
1:C:341:THR:HG1	1:C:356:TRP:HB3	1.76	0.51
1:A:425:PHE:HA	1:A:429:TYR:CD1	2.38	0.50
1:B:342:ARG:HH21	1:B:354:TRP:HA	1.77	0.50
1:B:358:PRO:HD2	1:B:360:ARG:NH2	2.27	0.50
1:B:699:LEU:CB	1:B:700:LEU:HG	2.40	0.50
1:A:134:PRO:HD2	1:A:526:ILE:HG12	1.93	0.50
1:A:208:ARG:NH1	1:A:212:LYS:HE2	2.26	0.50
1:A:701:ASP:O	1:A:705:VAL:N	2.36	0.50
1:B:115:VAL:O	1:B:117:PRO:HD3	2.11	0.50
1:C:105:LYS:HG3	1:C:579:ASP:H	1.76	0.50
1:C:208:ARG:HA	1:C:231:ASP:HA	1.93	0.50
1:C:285:ASP:O	1:C:311:HIS:ND1	2.44	0.50
1:C:716:PHE:CE2	1:C:718:ASP:HB3	2.46	0.50
1:A:348:PRO:HD2	1:A:349:LYS:NZ	2.26	0.50
1:A:442:TYR:HB2	1:A:450:ILE:HD12	1.93	0.50
1:B:150:PHE:HA	1:B:369:TRP:H	1.76	0.50
1:B:156:PRO:HB2	1:B:158:LYS:HZ3	1.76	0.50
1:B:165:TYR:HA	1:B:192:VAL:H	1.76	0.50
1:B:318:ARG:NE	1:B:346:THR:OG1	2.26	0.50
1:B:555:VAL:HG11	1:B:558:ARG:HB3	1.94	0.50
1:B:616:GLN:NE2	1:B:629:ALA:HB3	2.25	0.50
1:B:657:HIS:CE1	1:B:659:LEU:HG	2.46	0.50
1:C:296:TYR:C	1:C:314:TYR:HE2	2.19	0.50
1:A:599:ARG:NH1	1:A:641:PHE:HD2	2.09	0.50
1:B:240:ALA:HA	1:B:246:GLY:N	2.25	0.50
1:B:434:ILE:HB	1:B:456:LEU:HB2	1.93	0.50
1:C:279:ARG:HH12	1:C:290:ALA:HB2	1.75	0.50
1:C:534:HIS:O	1:C:538:LEU:HG	2.11	0.50
1:A:237:ALA:HA	1:A:248:HIS:HB3	1.93	0.50
1:A:678:LEU:HD12	1:C:243:THR:HB	1.93	0.50
1:B:121:GLY:N	1:B:569:ALA:HA	2.26	0.50
1:B:348:PRO:C	1:B:349:LYS:HD3	2.37	0.50
1:C:690:THR:HG21	1:C:692:HIS:ND1	2.26	0.50
1:A:141:ASN:HD21	1:A:470:ARG:HH12	1.59	0.50
1:A:704:GLU:O	1:A:708:ARG:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASN:HB3	1:B:377:ARG:HH12	1.76	0.50
1:B:291:THR:HG23	1:C:681:HIS:HB2	1.94	0.50
1:B:525:ALA:O	1:B:528:TRP:HB3	2.11	0.50
1:B:705:VAL:HA	1:B:708:ARG:HE	1.75	0.50
1:A:126:GLN:HA	1:A:568:MET:HE1	1.93	0.50
1:A:172:GLN:HE21	1:A:183:MET:HB3	1.77	0.50
1:C:287:PHE:CE1	1:C:295:VAL:HB	2.46	0.50
1:C:326:TYR:CZ	1:C:339:PRO:HD3	2.47	0.50
1:C:588:ARG:HH21	1:C:594:GLY:H	1.60	0.50
1:A:374:GLU:CD	1:A:389:ASP:HB2	2.36	0.50
1:A:589:ILE:HG22	1:A:630:ILE:HG21	1.93	0.50
1:A:636:GLY:N	1:A:652:GLU:OE2	2.41	0.50
1:B:143:THR:H	1:B:377:ARG:H	1.59	0.50
1:B:286:GLU:O	1:B:299:PRO:HD3	2.11	0.50
1:C:639:ARG:HH21	1:C:696:ASP:CG	2.19	0.50
1:C:707:ARG:NH1	1:C:708:ARG:HB3	2.27	0.50
1:A:185:ILE:HG21	1:A:253:LYS:NZ	2.26	0.50
1:A:701:ASP:OD2	1:A:707:ARG:NH2	2.43	0.50
1:B:348:PRO:HB2	1:B:349:LYS:HD3	1.94	0.50
1:B:614:GLU:HB3	1:B:627:ARG:HD2	1.93	0.50
1:C:374:GLU:OE1	1:C:390:ALA:HB2	2.12	0.50
1:A:142:TYR:CD2	1:A:518:ASN:HB3	2.47	0.49
1:A:153:ASN:N	1:A:365:THR:OG1	2.45	0.49
1:A:195:GLU:OE2	1:A:200:LYS:NZ	2.39	0.49
1:A:202:ASN:HA	1:A:328:ARG:HD2	1.94	0.49
1:B:546:ASN:O	1:B:550:ILE:HG12	2.12	0.49
1:B:194:PHE:CD2	1:B:320:LYS:HG2	2.46	0.49
1:B:347:THR:N	1:B:350:PHE:O	2.45	0.49
1:B:470:ARG:O	1:B:473:SER:OG	2.26	0.49
1:B:709:ASN:HA	1:B:712:HIS:CE1	2.46	0.49
1:C:196:GLU:O	1:C:201:ILE:N	2.45	0.49
1:C:464:TYR:O	1:C:468:HIS:ND1	2.43	0.49
1:C:501:ILE:O	1:C:505:ARG:HG3	2.12	0.49
1:A:302:GLY:HA2	1:A:319:PHE:CZ	2.47	0.49
1:A:465:VAL:O	1:A:469:LEU:HG	2.12	0.49
1:A:562:ARG:NH2	1:B:680:ASP:OD2	2.45	0.49
1:B:402:TYR:CE2	1:B:407:VAL:HB	2.47	0.49
1:B:723:ILE:HB	1:C:183:MET:HE1	1.94	0.49
1:C:149:VAL:O	1:C:369:TRP:N	2.41	0.49
1:C:343:ASN:HD21	1:C:356:TRP:CD1	2.29	0.49
1:C:466:ARG:HH12	1:C:470:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:TRP:HA	1:A:531:LEU:HD12	1.94	0.49
1:A:683:PHE:O	1:A:685:PRO:HD2	2.12	0.49
1:B:285:ASP:O	1:B:311:HIS:ND1	2.46	0.49
1:C:500:SER:HB3	1:C:503:PHE:CZ	2.47	0.49
1:C:555:VAL:HG23	1:C:557:ARG:H	1.77	0.49
1:C:588:ARG:CA	1:C:596:CYS:HA	2.39	0.49
1:A:109:THR:HA	1:A:578:ALA:HB3	1.94	0.49
1:A:225:ARG:HA	1:A:254:TYR:CD2	2.48	0.49
1:B:151:LYS:HE2	1:C:670:PHE:CD1	2.48	0.49
1:B:246:GLY:HA3	1:B:274:GLU:OE1	2.12	0.49
1:B:592:ARG:NH1	1:C:714:LEU:O	2.45	0.49
1:A:258:ARG:HH21	1:A:260:GLU:CD	2.20	0.49
1:A:469:LEU:HA	1:A:472:GLN:HG2	1.95	0.49
1:A:512:HIS:O	1:A:516:PRO:HD3	2.12	0.49
1:A:544:LYS:HE2	1:B:545:LEU:HD13	1.95	0.49
1:A:584:GLN:OE1	1:A:603:SER:N	2.45	0.49
1:B:200:LYS:O	1:B:205:GLY:N	2.45	0.49
1:B:243:THR:HG21	1:B:276:VAL:HG12	1.93	0.49
1:B:468:HIS:CE1	1:B:469:LEU:HG	2.48	0.49
1:B:624:ARG:H	1:B:624:ARG:HD3	1.78	0.49
1:C:195:GLU:OE1	1:C:208:ARG:NH2	2.34	0.49
1:C:616:GLN:OE1	1:C:629:ALA:HB3	2.12	0.49
1:B:234:LEU:HB3	1:B:247:TRP:HB3	1.95	0.49
1:C:466:ARG:O	1:C:470:ARG:N	2.36	0.49
1:A:119:PRO:HG2	1:A:569:ALA:CB	2.42	0.49
1:A:160:LYS:HG2	1:A:277:ASP:HA	1.94	0.49
1:A:225:ARG:HG2	1:A:254:TYR:HB2	1.94	0.49
1:A:465:VAL:O	1:A:468:HIS:HB3	2.13	0.49
1:A:549:ALA:O	1:A:553:VAL:HG12	2.12	0.49
1:B:199:ASP:O	1:B:204:LYS:N	2.46	0.49
1:B:208:ARG:HD2	1:B:229:GLU:OE2	2.12	0.49
1:C:140:GLN:HG2	1:C:380:TYR:HB2	1.94	0.49
1:C:520:MET:SD	1:C:521:LEU:HD23	2.52	0.49
1:C:618:GLY:H	1:C:623:LEU:HA	1.78	0.49
1:B:166:LYS:HB2	1:B:211:ALA:HB2	1.94	0.49
1:C:388:SER:O	1:C:392:SER:HA	2.13	0.49
1:C:636:GLY:HA2	1:C:638:ARG:HH21	1.77	0.49
1:A:172:GLN:HG3	1:A:263:HIS:HB3	1.95	0.49
1:A:183:MET:HG3	1:A:263:HIS:HE1	1.77	0.49
1:A:470:ARG:HD3	1:A:510:TYR:CE2	2.48	0.49
1:B:146:ILE:HG21	1:B:421:MET:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:ASN:HA	1:B:521:LEU:HD12	1.94	0.49
1:B:649:TYR:CD2	1:B:656:SER:HB2	2.48	0.49
1:C:580:ASN:O	1:C:604:PHE:HA	2.13	0.49
1:C:711:LEU:O	1:C:714:LEU:HB2	2.12	0.49
1:A:136:ARG:HB3	1:A:137:PRO:HD3	1.94	0.48
1:A:237:ALA:HA	1:A:248:HIS:HD1	1.76	0.48
1:A:670:PHE:O	1:A:670:PHE:CG	2.66	0.48
1:A:682:GLU:N	1:A:682:GLU:OE2	2.46	0.48
1:B:280:SER:HA	1:B:287:PHE:HA	1.94	0.48
1:B:282:TYR:HA	1:B:284:TYR:H	1.77	0.48
1:B:469:LEU:HD23	1:B:472:GLN:NE2	2.28	0.48
1:C:252:LEU:HD12	1:C:253:LYS:H	1.77	0.48
1:C:463:LEU:O	1:C:467:GLU:HB2	2.12	0.48
1:C:701:ASP:CG	1:C:704:GLU:HG2	2.37	0.48
1:A:498:THR:HG21	1:A:503:PHE:HB2	1.95	0.48
1:A:607:GLU:HG2	1:A:609:GLN:N	2.27	0.48
1:B:279:ARG:NH2	1:B:289:LEU:O	2.46	0.48
1:C:274:GLU:HG2	1:C:274:GLU:O	2.13	0.48
1:A:708:ARG:HE	1:A:711:LEU:HD11	1.78	0.48
1:B:191:PRO:HD2	1:B:213:TYR:CZ	2.49	0.48
1:B:210:THR:OG1	1:B:212:LYS:NZ	2.46	0.48
1:B:282:TYR:CG	1:B:283:PRO:HA	2.48	0.48
1:B:565:GLY:H	1:C:639:ARG:NH1	2.10	0.48
1:C:122:ALA:HB1	1:C:123:THR:HG22	1.94	0.48
1:C:134:PRO:HG2	1:C:526:ILE:HA	1.95	0.48
1:C:166:LYS:HZ1	1:C:208:ARG:HD2	1.77	0.48
1:C:201:ILE:O	1:C:205:GLY:N	2.44	0.48
1:A:215:ARG:NE	1:A:220:THR:OG1	2.47	0.48
1:A:304:ARG:HB2	1:A:356:TRP:CH2	2.49	0.48
1:A:602:VAL:HG23	1:A:604:PHE:CE1	2.48	0.48
1:B:264:ARG:HD2	1:B:265:TYR:H	1.78	0.48
1:C:169:THR:HG23	1:C:268:THR:HB	1.94	0.48
1:C:343:ASN:OD1	1:C:356:TRP:HB2	2.13	0.48
1:A:119:PRO:HG3	1:A:561:ALA:HA	1.94	0.48
1:A:286:GLU:HB2	1:A:294:PHE:CZ	2.48	0.48
1:B:120:THR:OG1	1:C:678:LEU:HB3	2.13	0.48
1:B:162:THR:HG23	1:B:275:GLU:N	2.27	0.48
1:B:201:ILE:HG21	1:B:273:VAL:HG21	1.94	0.48
1:C:301:TYR:CE1	1:C:312:THR:HB	2.48	0.48
1:A:343:ASN:HD22	1:A:354:TRP:NE1	2.11	0.48
1:A:463:LEU:HD21	1:A:506:LEU:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:THR:HG21	1:C:446:GLY:C	2.38	0.48
1:A:681:HIS:CG	1:A:682:GLU:H	2.31	0.48
1:B:247:TRP:N	1:B:274:GLU:OE2	2.45	0.48
1:B:634:THR:HG23	1:B:693:GLU:HA	1.94	0.48
1:C:233:GLU:OE1	1:C:234:LEU:N	2.46	0.48
1:C:711:LEU:HA	1:C:714:LEU:HD13	1.95	0.48
1:A:327:ALA:O	1:A:336:ALA:N	2.46	0.48
1:B:301:TYR:CE1	1:B:312:THR:HB	2.48	0.48
1:B:470:ARG:HD2	1:B:507:GLN:OE1	2.13	0.48
1:B:528:TRP:HA	1:B:531:LEU:HD12	1.96	0.48
1:B:599:ARG:HH22	1:B:619:GLU:HA	1.79	0.48
1:B:599:ARG:HG3	1:B:617:LEU:O	2.14	0.48
1:B:673:LEU:O	1:B:674:ASN:ND2	2.46	0.48
1:B:700:LEU:HD22	1:B:701:ASP:HB2	1.95	0.48
1:C:685:PRO:HG2	1:C:690:THR:CG2	2.44	0.48
1:A:164:TYR:HB2	1:A:351:THR:HB	1.95	0.48
1:A:402:TYR:HE1	1:A:443:LEU:HD22	1.78	0.48
1:A:415:LYS:HA	1:A:418:ARG:NH1	2.29	0.48
1:A:529:CYS:SG	1:A:533:ASN:ND2	2.87	0.48
1:B:157:TYR:H	1:B:284:TYR:HE2	1.61	0.48
1:B:589:ILE:HD13	1:B:597:TYR:HE1	1.79	0.48
1:C:177:HIS:CD2	1:C:178:ARG:N	2.82	0.48
1:C:198:ILE:HG23	1:C:325:PHE:HE1	1.79	0.48
1:C:237:ALA:HB2	1:C:248:HIS:HB3	1.95	0.48
1:C:303:TYR:CD2	1:C:321:GLN:HB3	2.49	0.48
1:A:285:ASP:HA	1:A:298:SER:HA	1.95	0.48
1:A:541:GLU:OE2	1:B:546:ASN:ND2	2.47	0.48
1:A:677:MET:HG2	1:C:120:THR:H	1.78	0.48
1:B:130:PRO:HG3	1:B:536:LEU:HD13	1.95	0.48
1:B:234:LEU:HD13	1:B:273:VAL:HB	1.96	0.48
1:B:297:MET:HG3	1:B:312:THR:HA	1.95	0.48
1:B:326:TYR:HB2	1:B:336:ALA:O	2.13	0.48
1:B:565:GLY:N	1:C:639:ARG:HH11	2.11	0.48
1:C:176:GLY:HA3	1:C:179:TYR:CE2	2.49	0.48
1:C:300:PHE:HB2	1:C:310:GLU:CD	2.39	0.48
1:C:704:GLU:HA	1:C:707:ARG:CG	2.44	0.48
1:A:119:PRO:HB3	1:A:571:SER:OG	2.13	0.48
1:A:162:THR:HG21	1:A:330:LEU:HD11	1.96	0.48
1:A:164:TYR:HD1	1:A:273:VAL:HG22	1.78	0.48
1:A:392:SER:OG	1:A:532:GLN:HG2	2.13	0.48
1:A:570:VAL:HG13	1:B:677:MET:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:CG	1:A:600:PRO:HD2	2.43	0.48
1:A:678:LEU:HG	1:A:679:GLU:H	1.78	0.48
1:B:319:PHE:CE2	1:B:321:GLN:HB2	2.49	0.48
1:B:401:GLU:OE1	1:B:440:GLN:HB3	2.14	0.48
1:C:223:PHE:HB3	1:C:227:ASP:O	2.13	0.48
1:C:564:LEU:HD11	1:C:569:ALA:HB2	1.94	0.48
1:C:641:PHE:O	1:C:648:VAL:HG12	2.13	0.48
1:C:651:GLU:OE2	1:C:651:GLU:N	2.44	0.48
1:A:138:GLU:HG3	1:A:515:ARG:HA	1.94	0.47
1:A:242:ARG:HE	1:A:625:LEU:HD23	1.78	0.47
1:A:297:MET:HA	1:A:311:HIS:CE1	2.48	0.47
1:A:436:VAL:O	1:A:454:PRO:HD2	2.13	0.47
1:A:502:GLU:OE2	1:A:505:ARG:NH1	2.48	0.47
1:A:592:ARG:HD2	1:A:593:PRO:HD2	1.96	0.47
1:B:208:ARG:HG3	1:B:210:THR:O	2.13	0.47
1:B:282:TYR:CD1	1:B:283:PRO:HA	2.49	0.47
1:B:582:ILE:N	1:B:602:VAL:HG13	2.28	0.47
1:C:700:LEU:HD21	1:C:708:ARG:NE	2.29	0.47
1:A:403:PRO:HG2	1:A:406:ARG:HG2	1.96	0.47
1:B:168:VAL:O	1:B:187:GLU:HA	2.14	0.47
1:B:197:VAL:HA	1:B:201:ILE:HB	1.95	0.47
1:B:642:THR:HA	1:B:647:TYR:CD1	2.49	0.47
1:B:706:GLN:HA	1:B:709:ASN:OD1	2.14	0.47
1:C:209:SER:HB2	1:C:224:HIS:HB2	1.96	0.47
1:C:529:CYS:HA	1:C:532:GLN:HG2	1.95	0.47
1:C:541:GLU:OE2	1:C:544:LYS:HB2	2.14	0.47
1:A:576:VAL:HG23	1:A:580:ASN:HB2	1.96	0.47
1:B:125:VAL:HG21	1:C:672:ASP:HB3	1.96	0.47
1:C:165:TYR:CA	1:C:192:VAL:HG23	2.44	0.47
1:C:605:ARG:HG3	1:C:612:LEU:HD23	1.96	0.47
1:A:167:ASP:HA	1:A:188:ASP:O	2.14	0.47
1:B:199:ASP:O	1:B:204:LYS:HG3	2.15	0.47
1:B:359:LYS:HZ3	1:B:361:PRO:HA	1.80	0.47
1:B:420:ALA:HA	1:B:423:ARG:CZ	2.45	0.47
1:C:198:ILE:O	1:C:202:ASN:HB3	2.15	0.47
1:A:348:PRO:HD2	1:A:349:LYS:HZ3	1.80	0.47
1:A:409:LEU:HG	1:A:412:CYS:HB3	1.96	0.47
1:A:560:SER:O	1:A:571:SER:OG	2.29	0.47
1:A:580:ASN:OD1	1:A:605:ARG:HG3	2.14	0.47
1:B:325:PHE:C	1:B:340:THR:H	2.23	0.47
1:B:564:LEU:HB3	1:C:639:ARG:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:LEU:N	1:B:700:LEU:HB2	2.18	0.47
1:C:467:GLU:OE2	1:C:470:ARG:HD3	2.14	0.47
1:A:420:ALA:HA	1:A:423:ARG:HH21	1.79	0.47
1:B:156:PRO:C	1:B:158:LYS:HZ3	2.22	0.47
1:B:196:GLU:HG3	1:B:200:LYS:HD2	1.96	0.47
1:B:517:VAL:O	1:B:521:LEU:HG	2.13	0.47
1:A:164:TYR:OH	1:A:353:ALA:HB3	2.15	0.47
1:A:192:VAL:HG13	1:A:196:GLU:HB2	1.97	0.47
1:A:208:ARG:NH2	1:A:212:LYS:HG2	2.29	0.47
1:A:381:GLY:HA3	1:A:385:ARG:NH2	2.14	0.47
1:A:540:ASN:O	1:A:543:ARG:NE	2.48	0.47
1:B:108:ASN:HB2	1:B:643:PHE:HD2	1.80	0.47
1:B:117:PRO:HD2	1:B:560:SER:CB	2.45	0.47
1:B:156:PRO:HB3	1:B:281:VAL:HA	1.95	0.47
1:B:172:GLN:O	1:B:183:MET:N	2.47	0.47
1:B:705:VAL:HG13	1:B:708:ARG:HH21	1.80	0.47
1:C:175:PHE:CG	1:C:258:ARG:HG3	2.49	0.47
1:C:328:ARG:HE	1:C:334:ALA:HA	1.80	0.47
1:C:402:TYR:CE2	1:C:407:VAL:HG13	2.49	0.47
1:C:438:GLN:HB2	1:C:475:LYS:NZ	2.29	0.47
1:C:555:VAL:HG23	1:C:557:ARG:N	2.30	0.47
1:C:706:GLN:O	1:C:710:GLN:HG3	2.15	0.47
1:A:105:LYS:HD2	1:A:579:ASP:O	2.14	0.47
1:A:154:ILE:HD12	1:A:282:TYR:CD2	2.50	0.47
1:A:171:SER:O	1:A:265:TYR:HA	2.15	0.47
1:A:273:VAL:HG12	1:A:330:LEU:CD1	2.44	0.47
1:A:706:GLN:HA	1:A:709:ASN:ND2	2.30	0.47
1:B:142:TYR:CE1	1:B:378:SER:HB3	2.50	0.47
1:C:166:LYS:NZ	1:C:208:ARG:HB2	2.29	0.47
1:C:242:ARG:HH21	1:C:606:TYR:HE1	1.63	0.47
1:C:514:GLN:HG2	1:C:518:ASN:ND2	2.22	0.47
1:C:540:ASN:O	1:C:543:ARG:HG3	2.15	0.47
1:C:588:ARG:NH2	1:C:589:ILE:O	2.48	0.47
1:C:659:LEU:HD23	1:C:659:LEU:HA	1.80	0.47
1:A:124:VAL:HG23	1:B:664:ILE:HD12	1.97	0.47
1:A:507:GLN:NE2	1:A:511:ASN:OD1	2.48	0.47
1:A:637:HIS:HE1	1:A:650:PHE:HB3	1.80	0.47
1:B:425:PHE:HA	1:B:429:TYR:HD1	1.80	0.47
1:B:522:GLY:O	1:B:526:ILE:HG13	2.15	0.47
1:C:243:THR:HG22	1:C:276:VAL:HA	1.97	0.47
1:C:318:ARG:O	1:C:320:LYS:NZ	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:LEU:O	1:C:535:GLU:HG2	2.15	0.47
1:C:546:ASN:O	1:C:550:ILE:HG12	2.14	0.47
1:C:617:LEU:HG	1:C:618:GLY:O	2.15	0.47
1:A:189:ARG:HG3	1:B:684:VAL:HG13	1.96	0.47
1:A:300:PHE:HB2	1:A:310:GLU:OE1	2.14	0.47
1:A:318:ARG:NH1	1:A:348:PRO:HD3	2.30	0.47
1:A:494:ARG:HB3	1:A:496:LYS:NZ	2.30	0.47
1:A:508:PHE:HA	1:A:511:ASN:ND2	2.30	0.47
1:B:141:ASN:O	1:B:377:ARG:NH1	2.48	0.47
1:B:392:SER:HB3	1:B:528:TRP:HZ2	1.80	0.47
1:B:532:GLN:HE21	1:B:536:LEU:HD11	1.79	0.47
1:C:166:LYS:NZ	1:C:208:ARG:HD2	2.30	0.47
1:C:552:SER:OG	1:C:558:ARG:HA	2.14	0.47
1:A:120:THR:O	1:B:678:LEU:HB2	2.15	0.46
1:A:130:PRO:HG3	1:A:536:LEU:HD13	1.97	0.46
1:A:368:LYS:O	1:B:670:PHE:HB3	2.14	0.46
1:A:582:ILE:HD13	1:A:612:LEU:HD11	1.97	0.46
1:C:109:THR:HA	1:C:644:GLY:HA3	1.97	0.46
1:C:165:TYR:O	1:C:272:ILE:HB	2.14	0.46
1:C:189:ARG:NH2	1:C:350:PHE:HB3	2.30	0.46
1:A:138:GLU:OE2	1:A:518:ASN:HB2	2.15	0.46
1:A:463:LEU:HD22	1:A:466:ARG:HH11	1.80	0.46
1:B:126:GLN:HB3	1:C:666:THR:HA	1.96	0.46
1:B:223:PHE:CD1	1:B:228:HIS:HA	2.51	0.46
1:B:318:ARG:HH21	1:B:346:THR:HG21	1.80	0.46
1:C:371:GLU:CD	1:C:420:ALA:HB1	2.40	0.46
1:C:599:ARG:HD3	1:C:624:ARG:HD2	1.96	0.46
1:A:144:GLU:OE1	1:A:455:LEU:HB2	2.15	0.46
1:A:163:MET:SD	1:A:352:VAL:HG22	2.54	0.46
1:A:164:TYR:CE1	1:A:273:VAL:HG13	2.50	0.46
1:A:342:ARG:NH2	1:A:354:TRP:HA	2.30	0.46
1:A:373:ASP:HB2	1:A:424:ILE:HG21	1.96	0.46
1:A:466:ARG:CZ	1:A:507:GLN:HB2	2.45	0.46
1:B:120:THR:HA	1:B:569:ALA:HB1	1.97	0.46
1:B:395:PHE:CD1	1:B:444:ALA:HB1	2.50	0.46
1:C:632:PRO:CB	1:C:695:LYS:HG3	2.44	0.46
1:A:131:ARG:NH2	1:A:532:GLN:OE1	2.48	0.46
1:A:175:PHE:CE1	1:A:264:ARG:HB3	2.50	0.46
1:B:136:ARG:HB3	1:B:137:PRO:HD3	1.96	0.46
1:C:108:ASN:O	1:C:646:GLY:N	2.48	0.46
1:C:150:PHE:CD1	1:C:449:LEU:HD22	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ARG:HH12	1:C:247:TRP:CD1	2.33	0.46
1:A:113:PHE:HB3	1:A:623:LEU:HD13	1.98	0.46
1:A:198:ILE:HD13	1:A:325:PHE:HE1	1.81	0.46
1:A:244:SER:HB2	1:A:276:VAL:HA	1.98	0.46
1:A:318:ARG:NH2	1:A:347:THR:HA	2.30	0.46
1:A:596:CYS:N	1:A:633:CYS:SG	2.88	0.46
1:B:164:TYR:O	1:B:350:PHE:HA	2.14	0.46
1:C:318:ARG:NH2	1:C:347:THR:HA	2.23	0.46
1:C:352:VAL:HB	1:C:354:TRP:CZ3	2.50	0.46
1:A:121:GLY:HA2	1:A:570:VAL:H	1.80	0.46
1:A:150:PHE:CZ	1:A:368:LYS:HB3	2.49	0.46
1:A:389:ASP:O	1:A:528:TRP:NE1	2.48	0.46
1:A:466:ARG:HD2	1:A:507:GLN:HB2	1.96	0.46
1:A:500:SER:O	1:A:503:PHE:N	2.22	0.46
1:B:105:LYS:HE3	1:B:580:ASN:HA	1.98	0.46
1:B:168:VAL:HG12	1:B:269:VAL:HG13	1.98	0.46
1:B:589:ILE:HB	1:B:597:TYR:CE1	2.51	0.46
1:B:699:LEU:HB3	1:B:700:LEU:CG	2.42	0.46
1:B:704:GLU:HB3	1:B:707:ARG:HE	1.81	0.46
1:C:341:THR:OG1	1:C:356:TRP:HB3	2.16	0.46
1:A:177:HIS:CD2	1:A:179:TYR:HE1	2.34	0.46
1:A:559:VAL:HG23	1:A:571:SER:O	2.16	0.46
1:A:640:TYR:HD1	1:A:649:TYR:HB2	1.81	0.46
1:B:345:LEU:HG	1:B:347:THR:HG22	1.98	0.46
1:B:616:GLN:CG	1:B:624:ARG:HH21	2.28	0.46
1:C:468:HIS:HD2	1:C:472:GLN:NE2	2.13	0.46
1:C:520:MET:O	1:C:524:VAL:HG13	2.16	0.46
1:A:240:ALA:HB1	1:A:246:GLY:H	1.80	0.46
1:A:672:ASP:HA	1:A:673:LEU:HB2	1.98	0.46
1:A:692:HIS:HA	1:A:695:LYS:CD	2.45	0.46
1:A:704:GLU:HG3	1:A:707:ARG:NE	2.31	0.46
1:B:234:LEU:HB3	1:B:247:TRP:CB	2.45	0.46
1:C:384:PHE:HZ	1:C:474:ARG:HB3	1.80	0.46
1:C:556:GLY:O	1:C:558:ARG:NH2	2.44	0.46
1:A:195:GLU:OE1	1:A:196:GLU:HG3	2.15	0.46
1:A:667:VAL:HG12	1:C:369:TRP:CZ3	2.50	0.46
1:C:156:PRO:CA	1:C:280:SER:O	2.63	0.46
1:C:156:PRO:HB3	1:C:281:VAL:HG22	1.97	0.46
1:C:215:ARG:HD2	1:C:216:ASN:ND2	2.31	0.46
1:C:233:GLU:O	1:C:249:THR:HG22	2.15	0.46
1:C:319:PHE:HE1	1:C:343:ASN:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:GLU:OE1	1:C:656:SER:HB2	2.16	0.46
1:A:273:VAL:HG12	1:A:330:LEU:HD11	1.98	0.46
1:A:511:ASN:O	1:A:514:GLN:HB2	2.15	0.46
1:A:631:GLU:HA	1:B:711:LEU:HD13	1.98	0.46
1:B:245:ARG:HD2	1:B:331:THR:HG21	1.96	0.46
1:B:247:TRP:HE1	1:B:331:THR:CG2	2.28	0.46
1:B:302:GLY:HA2	1:B:319:PHE:CZ	2.50	0.46
1:C:415:LYS:NZ	1:C:418:ARG:HD2	2.31	0.46
1:C:699:LEU:N	1:C:700:LEU:HB2	2.31	0.46
1:A:602:VAL:C	1:A:627:ARG:HH21	2.24	0.45
1:B:245:ARG:HH12	1:B:329:ASP:CG	2.24	0.45
1:B:300:PHE:O	1:B:310:GLU:HB3	2.17	0.45
1:C:142:TYR:CD1	1:C:376:LEU:HD13	2.51	0.45
1:C:150:PHE:HD2	1:C:366:MET:C	2.25	0.45
1:C:164:TYR:CB	1:C:192:VAL:HB	2.46	0.45
1:C:194:PHE:CD1	1:C:344:LEU:HD22	2.47	0.45
1:C:500:SER:HB3	1:C:503:PHE:CE2	2.51	0.45
1:C:605:ARG:HB3	1:C:607:GLU:O	2.16	0.45
1:C:709:ASN:O	1:C:715:ARG:NH1	2.47	0.45
1:C:711:LEU:O	1:C:715:ARG:HG3	2.16	0.45
1:B:157:TYR:N	1:B:284:TYR:OH	2.49	0.45
1:B:175:PHE:HB3	1:B:260:GLU:HG2	1.97	0.45
1:B:191:PRO:HD2	1:B:213:TYR:CE1	2.50	0.45
1:C:175:PHE:CE2	1:C:258:ARG:HA	2.52	0.45
1:C:380:TYR:O	1:C:385:ARG:NE	2.49	0.45
1:C:566:ASP:OD1	1:C:566:ASP:N	2.47	0.45
1:A:208:ARG:HA	1:A:231:ASP:HA	1.99	0.45
1:A:288:VAL:C	1:A:289:LEU:HD12	2.40	0.45
1:B:498:THR:HG23	1:B:500:SER:O	2.16	0.45
1:B:507:GLN:HE21	1:B:511:ASN:ND2	2.14	0.45
1:C:243:THR:CG2	1:C:277:ASP:H	2.29	0.45
1:C:300:PHE:CD2	1:C:359:LYS:HA	2.52	0.45
1:A:119:PRO:HG2	1:A:569:ALA:HB3	1.99	0.45
1:A:120:THR:HG21	1:A:292:GLY:HA2	1.98	0.45
1:A:250:THR:OG1	1:A:251:ASP:N	2.50	0.45
1:A:326:TYR:CE1	1:A:339:PRO:HB3	2.52	0.45
1:A:589:ILE:CG2	1:A:595:ALA:HB3	2.46	0.45
1:B:145:GLY:HA2	1:B:455:LEU:HG	1.97	0.45
1:B:168:VAL:HG22	1:B:188:ASP:HB2	1.99	0.45
1:B:235:LYS:O	1:B:248:HIS:N	2.37	0.45
1:B:558:ARG:NH1	1:B:574:VAL:HB	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:LEU:HD13	1:B:623:LEU:HA	1.80	0.45
1:C:581:VAL:HA	1:C:604:PHE:HA	1.97	0.45
1:A:141:ASN:HB2	1:A:379:GLU:OE1	2.16	0.45
1:A:165:TYR:HA	1:A:192:VAL:N	2.31	0.45
1:A:297:MET:SD	1:A:298:SER:N	2.89	0.45
1:A:365:THR:O	1:A:367:THR:HG23	2.17	0.45
1:B:105:LYS:HB2	1:B:107:GLU:OE1	2.15	0.45
1:B:106:ALA:HA	1:B:643:PHE:CZ	2.52	0.45
1:B:167:ASP:OD1	1:B:189:ARG:HG2	2.16	0.45
1:B:318:ARG:O	1:B:345:LEU:HA	2.17	0.45
1:B:320:LYS:HB2	1:B:344:LEU:HB2	1.98	0.45
1:C:105:LYS:HG3	1:C:579:ASP:N	2.31	0.45
1:C:113:PHE:HD2	1:C:576:VAL:O	2.00	0.45
1:C:113:PHE:HB2	1:C:576:VAL:HG22	1.98	0.45
1:C:151:LYS:HG2	1:C:369:TRP:HB2	1.99	0.45
1:C:319:PHE:CZ	1:C:321:GLN:HB2	2.51	0.45
1:C:322:VAL:O	1:C:325:PHE:HB3	2.16	0.45
1:C:348:PRO:HG2	1:C:349:LYS:NZ	2.31	0.45
1:A:189:ARG:HG3	1:B:684:VAL:CG1	2.47	0.45
1:A:286:GLU:O	1:A:299:PRO:HD3	2.17	0.45
1:A:377:ARG:NH2	1:A:471:GLU:OE2	2.50	0.45
1:A:667:VAL:HG23	1:A:670:PHE:CZ	2.52	0.45
1:A:670:PHE:HB3	1:C:369:TRP:HE1	1.79	0.45
1:B:147:ALA:HB1	1:B:450:ILE:HG23	1.98	0.45
1:B:196:GLU:CD	1:B:200:LYS:HD2	2.42	0.45
1:B:294:PHE:HE2	1:B:296:TYR:CZ	2.35	0.45
1:B:587:MET:HE3	1:B:654:ALA:HA	1.97	0.45
1:C:611:PRO:O	1:C:613:VAL:HG23	2.17	0.45
1:A:108:ASN:HB3	1:A:645:GLY:H	1.81	0.45
1:A:138:GLU:HG3	1:A:515:ARG:HG3	1.99	0.45
1:A:151:LYS:CG	1:A:369:TRP:HE1	2.28	0.45
1:B:237:ALA:HA	1:B:248:HIS:CE1	2.52	0.45
1:B:388:SER:HB3	1:B:393:THR:HG22	1.98	0.45
1:B:707:ARG:NH2	1:B:708:ARG:HB3	2.32	0.45
1:C:163:MET:HG3	1:C:291:THR:HG21	1.99	0.45
1:C:165:TYR:HA	1:C:192:VAL:H	1.81	0.45
1:C:379:GLU:HG3	1:C:384:PHE:CE1	2.41	0.45
1:C:700:LEU:HD22	1:C:705:VAL:CA	2.47	0.45
1:C:709:ASN:C	1:C:715:ARG:HH12	2.25	0.45
1:A:140:GLN:C	1:A:379:GLU:HG2	2.42	0.45
1:A:196:GLU:OE2	1:A:208:ARG:NH2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:O	1:A:288:VAL:HG22	2.15	0.45
1:A:379:GLU:OE1	1:A:474:ARG:HG2	2.17	0.45
1:B:108:ASN:HB2	1:B:643:PHE:CD2	2.52	0.45
1:B:119:PRO:HB2	1:B:569:ALA:C	2.42	0.45
1:B:469:LEU:HA	1:B:472:GLN:CD	2.42	0.45
1:B:471:GLU:OE1	1:B:474:ARG:NE	2.43	0.45
1:C:196:GLU:HG3	1:C:200:LYS:CB	2.45	0.45
1:A:513:ILE:O	1:A:517:VAL:HG12	2.16	0.45
1:A:634:THR:OG1	1:A:696:ASP:HB2	2.17	0.45
1:A:637:HIS:O	1:A:652:GLU:N	2.28	0.45
1:B:249:THR:OG1	1:B:270:ASN:HB3	2.16	0.45
1:B:541:GLU:HA	1:B:544:LYS:HG3	1.98	0.45
1:C:104:ILE:HG12	1:C:582:ILE:HG13	1.99	0.45
1:C:119:PRO:C	1:C:562:ARG:HH21	2.25	0.45
1:C:434:ILE:HB	1:C:456:LEU:HB3	1.99	0.45
1:C:649:TYR:CZ	1:C:651:GLU:HB3	2.51	0.45
1:A:194:PHE:CD1	1:A:344:LEU:HD22	2.51	0.45
1:A:428:ARG:NH1	1:A:429:TYR:OH	2.50	0.45
1:A:597:TYR:HB3	1:A:616:GLN:NE2	2.32	0.45
1:B:384:PHE:CZ	1:B:399:LEU:HG	2.52	0.45
1:B:700:LEU:HA	1:B:701:ASP:HB2	1.99	0.45
1:C:138:GLU:HG3	1:C:139:GLY:N	2.32	0.45
1:C:701:ASP:HB3	1:C:704:GLU:HB2	1.99	0.45
1:A:193:PRO:HB2	1:A:195:GLU:HG3	1.99	0.44
1:A:615:GLY:N	1:A:627:ARG:HE	2.15	0.44
1:B:429:TYR:HD2	1:B:432:THR:HB	1.81	0.44
1:B:685:PRO:HB2	1:B:690:THR:HG21	1.98	0.44
1:C:189:ARG:HE	1:C:189:ARG:HB3	1.47	0.44
1:C:546:ASN:OD1	1:C:549:ALA:N	2.30	0.44
1:A:166:LYS:NZ	1:A:208:ARG:O	2.49	0.44
1:A:374:GLU:OE2	1:A:390:ALA:N	2.50	0.44
1:A:562:ARG:HG2	1:A:569:ALA:HB3	1.98	0.44
1:B:326:TYR:CD2	1:B:335:ARG:HG3	2.53	0.44
1:B:710:GLN:HG3	1:B:714:LEU:HD11	1.98	0.44
1:C:424:ILE:HD13	1:C:427:ARG:CZ	2.48	0.44
1:C:651:GLU:HG2	1:C:651:GLU:O	2.16	0.44
1:B:124:VAL:HA	1:C:665:THR:OG1	2.17	0.44
1:B:520:MET:HE3	1:B:520:MET:HB3	1.83	0.44
1:C:117:PRO:HG3	1:C:242:ARG:HH22	1.83	0.44
1:C:208:ARG:H	1:C:208:ARG:HG3	1.55	0.44
1:C:712:HIS:ND1	1:C:715:ARG:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HA	1:A:201:ILE:HB	1.99	0.44
1:A:696:ASP:O	1:A:697:SER:OG	2.34	0.44
1:B:119:PRO:O	1:B:562:ARG:NE	2.49	0.44
1:B:550:ILE:O	1:B:554:THR:OG1	2.32	0.44
1:C:194:PHE:HB2	1:C:320:LYS:HE3	2.00	0.44
1:C:208:ARG:HB3	1:C:229:GLU:CG	2.46	0.44
1:C:412:CYS:SG	1:C:413:ILE:N	2.91	0.44
1:A:146:ILE:HG23	1:A:453:GLN:HB3	1.98	0.44
1:A:225:ARG:HA	1:A:254:TYR:CG	2.53	0.44
1:A:463:LEU:HD21	1:A:506:LEU:HB3	1.99	0.44
1:A:655:TYR:CZ	1:A:657:HIS:HA	2.52	0.44
1:B:132:ARG:HH11	1:B:133:CYS:H	1.65	0.44
1:B:325:PHE:HD2	1:B:342:ARG:HB2	1.83	0.44
1:B:345:LEU:O	1:B:351:THR:HA	2.17	0.44
1:B:497:THR:HB	1:B:501:ILE:HD13	1.99	0.44
1:C:116:CYS:SG	1:C:623:LEU:N	2.90	0.44
1:C:247:TRP:CG	1:C:333:LYS:HZ1	2.34	0.44
1:C:588:ARG:NH2	1:C:594:GLY:H	2.16	0.44
1:C:707:ARG:HD2	1:C:707:ARG:C	2.43	0.44
1:A:402:TYR:CE2	1:A:406:ARG:HB2	2.52	0.44
1:A:584:GLN:HG2	1:A:601:LEU:C	2.42	0.44
1:A:687:GLU:O	1:A:688:VAL:HG23	2.18	0.44
1:B:151:LYS:CE	1:C:669:THR:H	2.31	0.44
1:B:276:VAL:HG11	1:C:681:HIS:CD2	2.51	0.44
1:B:379:GLU:CD	1:B:474:ARG:HD3	2.42	0.44
1:B:710:GLN:NE2	1:B:710:GLN:O	2.50	0.44
1:C:176:GLY:HA3	1:C:179:TYR:CZ	2.53	0.44
1:C:302:GLY:HA3	1:C:356:TRP:NE1	2.33	0.44
1:C:402:TYR:HH	1:C:406:ARG:C	2.20	0.44
1:C:527:ALA:O	1:C:531:LEU:HG	2.17	0.44
1:C:620:ASN:OD1	1:C:642:THR:HG21	2.17	0.44
1:A:158:LYS:CD	1:A:279:ARG:HG3	2.47	0.44
1:A:197:VAL:HG11	1:A:344:LEU:HD21	2.00	0.44
1:A:318:ARG:HH12	1:A:348:PRO:HD3	1.82	0.44
1:B:126:GLN:CD	1:C:664:ILE:HD12	2.43	0.44
1:B:165:TYR:CA	1:B:192:VAL:HG23	2.48	0.44
1:B:335:ARG:HH12	1:B:339:PRO:HD3	1.83	0.44
1:B:565:GLY:N	1:C:639:ARG:NH1	2.66	0.44
1:C:201:ILE:O	1:C:328:ARG:HD2	2.17	0.44
1:C:322:VAL:O	1:C:322:VAL:HG13	2.17	0.44
1:C:345:LEU:HB2	1:C:354:TRP:HH2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LYS:HG3	1:A:107:GLU:OE2	2.18	0.44
1:A:686:LEU:HD23	1:A:690:THR:HA	2.00	0.44
1:B:144:GLU:OE2	1:B:456:LEU:HA	2.17	0.44
1:B:162:THR:C	1:B:163:MET:HE2	2.43	0.44
1:B:198:ILE:HD13	1:B:325:PHE:CE1	2.52	0.44
1:B:289:LEU:HD22	1:B:293:ASP:HB3	1.98	0.44
1:B:341:THR:HG23	1:B:356:TRP:H	1.83	0.44
1:B:604:PHE:O	1:B:612:LEU:CA	2.37	0.44
1:B:681:HIS:CG	1:B:682:GLU:N	2.86	0.44
1:C:666:THR:HG22	1:C:667:VAL:N	2.33	0.44
1:B:254:TYR:CE2	1:B:256:PRO:HA	2.53	0.44
1:C:117:PRO:HG3	1:C:242:ARG:NH2	2.32	0.44
1:C:203:ALA:HA	1:C:335:ARG:NH1	2.33	0.44
1:C:256:PRO:HB2	1:C:264:ARG:HE	1.82	0.44
1:C:320:LYS:NZ	1:C:346:THR:OG1	2.50	0.44
1:C:439:PRO:O	1:C:475:LYS:NZ	2.50	0.44
1:C:466:ARG:NH1	1:C:470:ARG:HG3	2.33	0.44
1:A:167:ASP:HB3	1:A:187:GLU:CD	2.43	0.43
1:A:178:ARG:NE	1:A:258:ARG:HH22	2.15	0.43
1:A:208:ARG:HB3	1:A:229:GLU:HG3	1.99	0.43
1:A:380:TYR:HB3	1:A:385:ARG:HD2	2.00	0.43
1:A:584:GLN:O	1:A:587:MET:HE3	2.18	0.43
1:A:676:THR:OG1	1:A:677:MET:N	2.51	0.43
1:B:164:TYR:CD1	1:B:273:VAL:HG22	2.46	0.43
1:B:281:VAL:N	1:B:286:GLU:OE2	2.26	0.43
1:C:163:MET:HE1	1:C:352:VAL:HG22	2.00	0.43
1:A:124:VAL:HG22	1:B:665:THR:HG23	2.00	0.43
1:A:499:SER:HG	1:A:503:PHE:HE1	1.65	0.43
1:A:501:ILE:O	1:A:505:ARG:HG3	2.18	0.43
1:B:168:VAL:HG11	1:B:211:ALA:HB3	2.00	0.43
1:B:326:TYR:CE2	1:B:335:ARG:HG3	2.53	0.43
1:C:175:PHE:CD1	1:C:180:SER:HB2	2.52	0.43
1:A:105:LYS:HZ1	1:A:107:GLU:CD	2.27	0.43
1:A:473:SER:HG	1:A:474:ARG:NH1	2.15	0.43
1:A:616:GLN:HB2	1:A:626:THR:OG1	2.17	0.43
1:B:175:PHE:HB3	1:B:260:GLU:HA	1.99	0.43
1:B:385:ARG:N	1:B:385:ARG:HD2	2.33	0.43
1:B:449:LEU:HD12	1:B:450:ILE:H	1.82	0.43
1:C:277:ASP:O	1:C:279:ARG:NH1	2.51	0.43
1:C:314:TYR:HB3	1:C:318:ARG:HH12	1.83	0.43
1:C:616:GLN:HE21	1:C:627:ARG:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:C	1:A:192:VAL:HG23	2.43	0.43
1:A:226:ASP:H	1:A:267:THR:HG22	1.82	0.43
1:A:368:LYS:NZ	1:A:416:ASP:HB3	2.32	0.43
1:A:383:SER:OG	1:A:396:THR:HG23	2.18	0.43
1:A:463:LEU:HD13	1:A:466:ARG:NH1	2.30	0.43
1:A:494:ARG:O	1:A:496:LYS:HG2	2.18	0.43
1:A:531:LEU:O	1:A:535:GLU:HG2	2.18	0.43
1:A:592:ARG:NH1	1:A:593:PRO:O	2.52	0.43
1:A:607:GLU:C	1:A:610:GLY:H	2.26	0.43
1:B:129:GLN:O	1:B:131:ARG:NE	2.50	0.43
1:B:189:ARG:HG3	1:C:684:VAL:CG1	2.48	0.43
1:B:553:VAL:HG13	1:B:554:THR:N	2.33	0.43
1:B:584:GLN:HG2	1:B:601:LEU:C	2.43	0.43
1:C:105:LYS:HA	1:C:578:ALA:HB3	2.00	0.43
1:C:193:PRO:HB2	1:C:195:GLU:OE2	2.18	0.43
1:C:304:ARG:HB2	1:C:356:TRP:CH2	2.54	0.43
1:A:150:PHE:CD2	1:A:366:MET:HG3	2.53	0.43
1:A:677:MET:HE3	1:C:290:ALA:C	2.43	0.43
1:B:564:LEU:O	1:B:567:VAL:HG12	2.18	0.43
1:B:601:LEU:HD12	1:B:616:GLN:HG3	2.00	0.43
1:C:201:ILE:C	1:C:205:GLY:H	2.27	0.43
1:C:210:THR:HG22	1:C:223:PHE:HA	1.99	0.43
1:A:165:TYR:CD2	1:A:350:PHE:HB3	2.54	0.43
1:A:568:MET:N	1:A:568:MET:SD	2.92	0.43
1:A:675:ILE:HD13	1:C:570:VAL:HG11	2.01	0.43
1:A:703:THR:C	1:C:702:TYR:HH	2.25	0.43
1:B:529:CYS:SG	1:B:533:ASN:ND2	2.91	0.43
1:B:536:LEU:HA	1:B:539:TRP:CD1	2.53	0.43
1:C:384:PHE:CZ	1:C:474:ARG:HB3	2.52	0.43
1:C:468:HIS:CG	1:C:469:LEU:N	2.86	0.43
1:C:507:GLN:NE2	1:C:511:ASN:OD1	2.52	0.43
1:C:636:GLY:CA	1:C:638:ARG:HH21	2.31	0.43
1:A:114:TYR:CZ	1:A:558:ARG:HA	2.53	0.43
1:A:153:ASN:OD1	1:B:671:ILE:HD13	2.18	0.43
1:A:402:TYR:CD1	1:A:443:LEU:HB2	2.53	0.43
1:A:592:ARG:HD2	1:A:592:ARG:HA	1.75	0.43
1:B:128:GLU:HB2	1:B:131:ARG:HH21	1.83	0.43
1:B:377:ARG:HD3	1:B:379:GLU:HB3	2.01	0.43
1:B:616:GLN:HB3	1:B:624:ARG:HH21	1.83	0.43
1:C:167:ASP:CG	1:C:189:ARG:HG2	2.42	0.43
1:C:243:THR:HG23	1:C:277:ASP:CG	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:GLU:N	1:C:274:GLU:OE2	2.51	0.43
1:C:377:ARG:HD2	1:C:384:PHE:CE1	2.53	0.43
1:C:402:TYR:CE2	1:C:406:ARG:HB2	2.54	0.43
1:A:280:SER:OG	1:A:281:VAL:N	2.52	0.43
1:A:402:TYR:H	1:A:441:TYR:HB2	1.83	0.43
1:A:493:GLU:OE2	1:A:495:ILE:HA	2.19	0.43
1:A:498:THR:O	1:A:500:SER:N	2.52	0.43
1:A:584:GLN:HG2	1:A:601:LEU:HB3	2.00	0.43
1:B:147:ALA:CB	1:B:375:MET:HG3	2.49	0.43
1:B:174:TRP:CE3	1:B:181:GLN:HB2	2.50	0.43
1:B:377:ARG:HH11	1:B:379:GLU:HG2	1.84	0.43
1:B:440:GLN:OE1	1:B:452:TYR:HB3	2.19	0.43
1:B:466:ARG:NH1	1:B:467:GLU:HG2	2.34	0.43
1:B:564:LEU:HD23	1:B:569:ALA:HB2	2.00	0.43
1:C:144:GLU:HA	1:C:375:MET:O	2.19	0.43
1:C:162:THR:HG23	1:C:274:GLU:C	2.44	0.43
1:C:275:GLU:OE2	1:C:330:LEU:HB2	2.19	0.43
1:C:342:ARG:HD3	1:C:342:ARG:HA	1.73	0.43
1:C:466:ARG:O	1:C:469:LEU:CB	2.65	0.43
1:C:634:THR:H	1:C:653:TYR:HE2	1.66	0.43
1:A:106:ALA:O	1:A:579:ASP:HA	2.19	0.43
1:A:138:GLU:HB3	1:A:139:GLY:H	1.70	0.43
1:A:201:ILE:O	1:A:205:GLY:N	2.51	0.43
1:A:320:LYS:NZ	1:A:346:THR:OG1	2.31	0.43
1:B:589:ILE:HD12	1:B:589:ILE:HA	1.88	0.43
1:B:635:VAL:HG22	1:B:693:GLU:OE1	2.19	0.43
1:C:401:GLU:HG2	1:C:442:TYR:CE1	2.54	0.43
1:A:146:ILE:HA	1:A:373:ASP:HA	2.01	0.43
1:A:200:LYS:O	1:A:205:GLY:N	2.52	0.43
1:A:209:SER:HB3	1:A:230:THR:HB	2.01	0.43
1:A:711:LEU:HD21	1:C:631:GLU:OE1	2.19	0.43
1:B:104:ILE:N	1:B:582:ILE:HG23	2.33	0.43
1:B:202:ASN:O	1:B:328:ARG:HB2	2.18	0.43
1:B:412:CYS:SG	1:B:413:ILE:N	2.92	0.43
1:B:515:ARG:HE	1:B:515:ARG:HB2	1.63	0.43
1:B:641:PHE:O	1:B:648:VAL:HG12	2.19	0.43
1:C:230:THR:O	1:C:232:MET:HG3	2.19	0.43
1:A:132:ARG:HH11	1:A:133:CYS:H	1.67	0.42
1:A:162:THR:HB	1:A:164:TYR:OH	2.18	0.42
1:A:183:MET:HG3	1:A:263:HIS:CE1	2.54	0.42
1:A:581:VAL:HG13	1:A:604:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:HD3	1:A:624:ARG:HH12	1.84	0.42
1:B:194:PHE:CG	1:B:320:LYS:HG2	2.54	0.42
1:B:551:ALA:O	1:B:555:VAL:CB	2.63	0.42
1:B:561:ALA:CA	1:B:569:ALA:O	2.61	0.42
1:C:414:GLY:C	1:C:418:ARG:HE	2.26	0.42
1:A:704:GLU:HA	1:A:707:ARG:HB2	2.00	0.42
1:B:119:PRO:HD2	1:B:562:ARG:CZ	2.49	0.42
1:B:151:LYS:NZ	1:B:369:TRP:HA	2.25	0.42
1:B:160:LYS:HA	1:B:160:LYS:HD3	1.79	0.42
1:B:200:LYS:O	1:B:204:LYS:HB2	2.19	0.42
1:B:342:ARG:NH2	1:B:354:TRP:HA	2.33	0.42
1:B:672:ASP:CA	1:B:673:LEU:HB3	2.35	0.42
1:C:162:THR:HA	1:C:275:GLU:HA	2.00	0.42
1:C:242:ARG:HH12	1:C:573:CYS:HA	1.84	0.42
1:C:567:VAL:O	1:C:568:MET:HE2	2.19	0.42
1:C:600:PRO:O	1:C:602:VAL:HG13	2.19	0.42
1:C:690:THR:OG1	1:C:691:ARG:N	2.52	0.42
1:A:193:PRO:O	1:A:197:VAL:HG23	2.20	0.42
1:A:289:LEU:HB2	1:A:293:ASP:O	2.20	0.42
1:A:384:PHE:HB3	1:A:386:PHE:CZ	2.53	0.42
1:A:466:ARG:NE	1:A:507:GLN:HB2	2.34	0.42
1:A:664:ILE:C	1:A:666:THR:H	2.26	0.42
1:B:631:GLU:OE1	1:B:695:LYS:HE2	2.19	0.42
1:C:150:PHE:CB	1:C:366:MET:HB3	2.48	0.42
1:C:307:SER:O	1:C:310:GLU:HB2	2.19	0.42
1:C:321:GLN:HA	1:C:343:ASN:HA	2.00	0.42
1:C:324:GLY:C	1:C:339:PRO:HB2	2.45	0.42
1:C:425:PHE:O	1:C:429:TYR:N	2.38	0.42
1:C:552:SER:OG	1:C:558:ARG:NH1	2.52	0.42
1:C:599:ARG:NH1	1:C:619:GLU:OE2	2.52	0.42
1:A:150:PHE:O	1:A:151:LYS:HG2	2.20	0.42
1:A:190:ALA:HB1	1:A:213:TYR:CB	2.49	0.42
1:A:233:GLU:O	1:A:249:THR:HG22	2.20	0.42
1:A:288:VAL:HG12	1:A:294:PHE:CE2	2.55	0.42
1:B:121:GLY:HA2	1:B:570:VAL:HG12	2.01	0.42
1:B:127:PHE:CE1	1:B:568:MET:HG2	2.54	0.42
1:B:189:ARG:HG3	1:C:684:VAL:HB	2.00	0.42
1:B:424:ILE:HD13	1:B:427:ARG:CZ	2.49	0.42
1:B:605:ARG:CZ	1:B:612:LEU:HG	2.49	0.42
1:B:695:LYS:HD2	1:B:695:LYS:O	2.19	0.42
1:C:224:HIS:HE1	1:C:268:THR:HG23	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PHE:CE2	1:A:354:TRP:HB2	2.54	0.42
1:A:168:VAL:N	1:A:187:GLU:OE2	2.53	0.42
1:A:284:TYR:C	1:A:299:PRO:HD2	2.45	0.42
1:A:460:LEU:HD22	1:A:506:LEU:HD22	2.01	0.42
1:A:500:SER:HB3	1:A:503:PHE:CZ	2.54	0.42
1:A:703:THR:HG21	1:C:545:LEU:CD1	2.48	0.42
1:B:498:THR:HG21	1:B:503:PHE:HB2	2.01	0.42
1:B:543:ARG:HD3	1:B:568:MET:HE1	2.01	0.42
1:B:570:VAL:HG11	1:C:677:MET:HG2	2.01	0.42
1:C:115:VAL:O	1:C:625:LEU:HD21	2.20	0.42
1:C:191:PRO:HB3	1:C:350:PHE:C	2.44	0.42
1:C:509:THR:O	1:C:513:ILE:HG12	2.19	0.42
1:A:164:TYR:HB3	1:A:192:VAL:HB	2.01	0.42
1:A:289:LEU:HD13	1:A:294:PHE:HA	2.01	0.42
1:A:651:GLU:CD	1:A:656:SER:HB2	2.43	0.42
1:C:329:ASP:O	1:C:333:LYS:N	2.52	0.42
1:C:599:ARG:NE	1:C:618:GLY:HA2	2.35	0.42
1:C:707:ARG:HD2	1:C:708:ARG:N	2.34	0.42
1:A:162:THR:C	1:A:163:MET:HE2	2.45	0.42
1:A:209:SER:H	1:A:230:THR:C	2.26	0.42
1:A:392:SER:OG	1:A:528:TRP:HD1	2.00	0.42
1:A:401:GLU:OE2	1:A:440:GLN:HB3	2.19	0.42
1:B:700:LEU:HA	1:B:700:LEU:HD23	1.80	0.42
1:C:165:TYR:HA	1:C:192:VAL:HG23	2.01	0.42
1:A:154:ILE:HG22	1:B:671:ILE:HD11	2.01	0.42
1:A:302:GLY:HA2	1:A:319:PHE:HZ	1.85	0.42
1:A:412:CYS:SG	1:A:413:ILE:N	2.92	0.42
1:A:699:LEU:HD11	1:C:626:THR:HG22	2.02	0.42
1:A:699:LEU:N	1:A:700:LEU:HB2	2.35	0.42
1:B:128:GLU:OE1	1:B:131:ARG:NH2	2.51	0.42
1:B:146:ILE:CG2	1:B:453:GLN:HB3	2.50	0.42
1:B:241:THR:C	1:B:243:THR:H	2.27	0.42
1:B:290:ALA:O	1:C:679:GLU:HG2	2.19	0.42
1:B:599:ARG:HB3	1:B:616:GLN:CD	2.44	0.42
1:C:104:ILE:N	1:C:579:ASP:HA	2.35	0.42
1:C:280:SER:HB2	1:C:299:PRO:HB3	2.02	0.42
1:C:327:ALA:H	1:C:337:THR:HG21	1.85	0.42
1:A:141:ASN:ND2	1:A:471:GLU:OE2	2.53	0.42
1:A:178:ARG:NE	1:A:258:ARG:HH12	2.17	0.42
1:A:209:SER:O	1:A:269:VAL:HB	2.20	0.42
1:A:404:LEU:HD22	1:A:410:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ARG:HB3	1:A:596:CYS:SG	2.60	0.42
1:A:630:ILE:HG13	1:B:711:LEU:HD21	2.02	0.42
1:A:666:THR:O	1:A:666:THR:HG22	2.19	0.42
1:A:700:LEU:HG	1:A:705:VAL:HG22	2.02	0.42
1:B:369:TRP:HE1	1:C:669:THR:HG23	1.84	0.42
1:B:502:GLU:CA	1:B:505:ARG:HB2	2.41	0.42
1:B:580:ASN:ND2	1:B:608:ASP:HA	2.35	0.42
1:B:648:VAL:HG23	1:B:658:GLN:HE22	1.84	0.42
1:B:648:VAL:HG23	1:B:658:GLN:NE2	2.34	0.42
1:C:128:GLU:H	1:C:128:GLU:CD	2.27	0.42
1:C:236:PRO:HA	1:C:247:TRP:CD1	2.54	0.42
1:C:286:GLU:OE1	1:C:296:TYR:HB3	2.20	0.42
1:C:635:VAL:HG23	1:C:635:VAL:O	2.20	0.42
1:A:224:HIS:HE2	1:A:252:LEU:HD21	1.85	0.42
1:A:514:GLN:O	1:A:518:ASN:ND2	2.53	0.42
1:A:626:THR:HA	1:B:689:TYR:OH	2.20	0.42
1:B:355:ASP:OD1	1:B:355:ASP:N	2.51	0.42
1:B:381:GLY:HA3	1:B:385:ARG:NH2	2.35	0.42
1:B:700:LEU:CD2	1:B:701:ASP:HB2	2.50	0.42
1:C:392:SER:HB2	1:C:528:TRP:CD1	2.55	0.42
1:A:257:SER:HB2	1:A:264:ARG:NH1	2.35	0.41
1:B:352:VAL:HB	1:B:354:TRP:CZ3	2.55	0.41
1:B:392:SER:HA	1:B:528:TRP:NE1	2.30	0.41
1:B:704:GLU:HA	1:B:707:ARG:HB3	2.01	0.41
1:C:155:ALA:HA	1:C:156:PRO:HD3	1.93	0.41
1:C:178:ARG:NE	1:C:178:ARG:HA	2.35	0.41
1:C:440:GLN:H	1:C:452:TYR:H	1.66	0.41
1:A:154:ILE:HD12	1:A:282:TYR:HD2	1.83	0.41
1:A:155:ALA:O	1:A:281:VAL:HA	2.20	0.41
1:A:497:THR:HB	1:A:501:ILE:HD13	2.02	0.41
1:B:173:VAL:HA	1:B:182:PHE:HA	2.02	0.41
1:B:298:SER:HB2	1:B:311:HIS:HB3	2.01	0.41
1:B:342:ARG:HA	1:B:342:ARG:HD2	1.69	0.41
1:B:365:THR:O	1:B:367:THR:HG23	2.20	0.41
1:B:620:ASN:O	1:B:622:GLU:HG2	2.20	0.41
1:B:701:ASP:HB3	1:B:704:GLU:HG3	2.01	0.41
1:C:441:TYR:HA	1:C:450:ILE:O	2.20	0.41
1:C:463:LEU:HD11	1:C:506:LEU:O	2.20	0.41
1:C:633:CYS:HA	1:C:653:TYR:HE2	1.84	0.41
1:C:664:ILE:O	1:C:665:THR:OG1	2.35	0.41
1:A:141:ASN:ND2	1:A:470:ARG:HH12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HA	1:A:360:ARG:NE	2.35	0.41
1:A:564:LEU:HD21	1:A:569:ALA:HB2	2.02	0.41
1:B:119:PRO:HG2	1:B:562:ARG:HG2	2.02	0.41
1:B:183:MET:HG3	1:B:263:HIS:HE1	1.83	0.41
1:B:371:GLU:CD	1:B:423:ARG:HH21	2.29	0.41
1:B:385:ARG:HG3	1:B:396:THR:HG23	2.02	0.41
1:C:138:GLU:CG	1:C:139:GLY:N	2.82	0.41
1:C:193:PRO:O	1:C:197:VAL:HG23	2.20	0.41
1:C:280:SER:HA	1:C:287:PHE:CB	2.49	0.41
1:C:692:HIS:HD2	1:C:695:LYS:NZ	2.18	0.41
1:A:257:SER:HB2	1:A:264:ARG:HH12	1.85	0.41
1:A:635:VAL:HG22	1:A:692:HIS:CB	2.50	0.41
1:A:701:ASP:O	1:A:702:TYR:C	2.63	0.41
1:B:188:ASP:O	1:C:684:VAL:HG21	2.19	0.41
1:B:194:PHE:CE1	1:B:198:ILE:HD11	2.56	0.41
1:B:297:MET:HB2	1:B:314:TYR:CD2	2.55	0.41
1:B:317:ASP:O	1:B:318:ARG:HD2	2.19	0.41
1:B:327:ALA:N	1:B:337:THR:OG1	2.33	0.41
1:B:369:TRP:HD1	1:C:669:THR:OG1	2.03	0.41
1:B:419:ASP:HA	1:B:422:ASP:OD1	2.20	0.41
1:B:574:VAL:HG12	1:B:576:VAL:HG23	2.03	0.41
1:C:140:GLN:HB3	1:C:379:GLU:N	2.36	0.41
1:C:167:ASP:HB3	1:C:187:GLU:OE1	2.20	0.41
1:C:167:ASP:HB2	1:C:270:ASN:HD21	1.85	0.41
1:C:308:HIS:CE1	1:C:309:THR:HG23	2.56	0.41
1:C:469:LEU:HA	1:C:472:GLN:OE1	2.21	0.41
1:C:515:ARG:HB3	1:C:516:PRO:HD3	2.02	0.41
1:A:111:ALA:HB3	1:A:644:GLY:O	2.20	0.41
1:A:200:LYS:HA	1:A:204:LYS:HB2	2.01	0.41
1:A:302:GLY:H	1:A:356:TRP:CD1	2.38	0.41
1:A:494:ARG:HB3	1:A:496:LYS:HZ3	1.85	0.41
1:A:639:ARG:NH1	1:C:565:GLY:H	2.19	0.41
1:A:649:TYR:CD2	1:A:656:SER:HB3	2.55	0.41
1:B:328:ARG:HG2	1:B:330:LEU:HD22	2.02	0.41
1:B:376:LEU:HA	1:B:376:LEU:HD23	1.79	0.41
1:B:634:THR:OG1	1:B:696:ASP:OD1	2.39	0.41
1:C:167:ASP:OD2	1:C:189:ARG:HG2	2.20	0.41
1:C:300:PHE:HD1	1:C:357:VAL:HG13	1.84	0.41
1:C:365:THR:OG1	1:C:408:ASP:HB2	2.21	0.41
1:C:513:ILE:C	1:C:516:PRO:HD2	2.46	0.41
1:C:709:ASN:OD1	1:C:710:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:HE	1:A:258:ARG:NH2	2.15	0.41
1:A:208:ARG:NH1	1:A:210:THR:O	2.54	0.41
1:A:323:ASP:OD2	1:A:324:GLY:N	2.49	0.41
1:A:372:VAL:HG22	1:A:390:ALA:HB3	2.03	0.41
1:A:694:ILE:HA	1:A:698:GLY:HA3	2.02	0.41
1:A:702:TYR:O	1:A:705:VAL:HB	2.20	0.41
1:B:104:ILE:C	1:B:582:ILE:HG13	2.44	0.41
1:B:187:GLU:CD	1:C:685:PRO:HA	2.45	0.41
1:B:285:ASP:HA	1:B:311:HIS:HB3	2.02	0.41
1:B:424:ILE:HD13	1:B:427:ARG:NE	2.35	0.41
1:B:543:ARG:HG2	1:B:547:PRO:HA	2.01	0.41
1:B:583:VAL:HA	1:B:602:VAL:HG22	2.03	0.41
1:B:599:ARG:HB3	1:B:616:GLN:CG	2.50	0.41
1:B:640:TYR:CD1	1:B:649:TYR:HB2	2.55	0.41
1:B:640:TYR:HB3	1:B:647:TYR:HB3	2.01	0.41
1:B:701:ASP:HB3	1:B:704:GLU:CG	2.51	0.41
1:C:119:PRO:HD2	1:C:562:ARG:HG2	2.02	0.41
1:C:436:VAL:C	1:C:453:GLN:HE22	2.28	0.41
1:C:439:PRO:HA	1:C:452:TYR:C	2.46	0.41
1:C:560:SER:N	1:C:571:SER:O	2.33	0.41
1:A:115:VAL:HG13	1:A:242:ARG:HD2	2.02	0.41
1:A:126:GLN:OE1	1:A:126:GLN:N	2.54	0.41
1:A:234:LEU:HD21	1:A:271:CYS:SG	2.61	0.41
1:A:413:ILE:H	1:A:413:ILE:HD12	1.85	0.41
1:B:116:CYS:SG	1:B:622:GLU:HB3	2.60	0.41
1:B:128:GLU:OE1	1:B:131:ARG:NE	2.51	0.41
1:B:237:ALA:HB2	1:B:248:HIS:CG	2.55	0.41
1:B:375:MET:HB3	1:B:452:TYR:HE1	1.85	0.41
1:B:391:ILE:O	1:B:392:SER:OG	2.37	0.41
1:B:436:VAL:HG11	1:B:456:LEU:HD11	2.02	0.41
1:B:558:ARG:CD	1:B:559:VAL:H	2.33	0.41
1:B:611:PRO:O	1:B:613:VAL:HG23	2.21	0.41
1:C:385:ARG:NE	1:C:396:THR:HG23	2.36	0.41
1:C:671:ILE:HD12	1:C:675:ILE:HD13	2.03	0.41
1:C:712:HIS:CD2	1:C:715:ARG:HD2	2.56	0.41
1:A:254:TYR:CE2	1:A:256:PRO:HA	2.56	0.41
1:A:722:VAL:O	1:B:181:GLN:HG3	2.21	0.41
1:B:130:PRO:N	1:B:536:LEU:HD22	2.36	0.41
1:C:171:SER:O	1:C:171:SER:OG	2.33	0.41
1:C:191:PRO:HB3	1:C:350:PHE:O	2.21	0.41
1:C:234:LEU:HB3	1:C:247:TRP:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:HIS:CD2	1:A:179:TYR:CE1	3.09	0.41
1:A:237:ALA:HB3	1:A:240:ALA:HB2	2.02	0.41
1:A:320:LYS:HB2	1:A:320:LYS:HE2	1.88	0.41
1:A:343:ASN:HB2	1:A:354:TRP:CZ2	2.56	0.41
1:A:649:TYR:HD2	1:A:657:HIS:HD1	1.68	0.41
1:B:116:CYS:HB2	1:B:624:ARG:HA	2.02	0.41
1:B:158:LYS:CD	1:B:279:ARG:HG2	2.51	0.41
1:B:160:LYS:HD2	1:B:244:SER:OG	2.21	0.41
1:B:177:HIS:CE1	1:B:178:ARG:HB3	2.56	0.41
1:B:197:VAL:O	1:B:202:ASN:N	2.48	0.41
1:B:198:ILE:HA	1:B:325:PHE:HZ	1.86	0.41
1:B:224:HIS:HE2	1:B:252:LEU:HD13	1.86	0.41
1:B:323:ASP:OD2	1:B:324:GLY:N	2.54	0.41
1:B:404:LEU:HD22	1:B:410:GLY:O	2.21	0.41
1:C:172:GLN:HG3	1:C:265:TYR:CE1	2.55	0.41
1:C:321:GLN:HG3	1:C:343:ASN:OD1	2.20	0.41
1:C:404:LEU:HB2	1:C:410:GLY:CA	2.44	0.41
1:A:321:GLN:HG3	1:A:343:ASN:OD1	2.21	0.41
1:A:699:LEU:HD12	1:A:699:LEU:O	2.21	0.41
1:A:704:GLU:CA	1:A:707:ARG:HE	2.31	0.41
1:B:149:VAL:HG21	1:B:369:TRP:HE3	1.84	0.41
1:B:541:GLU:O	1:B:544:LYS:HB2	2.20	0.41
1:C:552:SER:O	1:C:558:ARG:NH2	2.54	0.41
1:C:690:THR:HG23	1:C:692:HIS:H	1.86	0.41
1:A:121:GLY:CA	1:A:570:VAL:H	2.34	0.40
1:A:136:ARG:NH2	1:A:526:ILE:HD12	2.37	0.40
1:A:208:ARG:HH22	1:A:212:LYS:HG2	1.86	0.40
1:A:359:LYS:H	1:A:359:LYS:HG2	1.72	0.40
1:B:104:ILE:O	1:B:582:ILE:HA	2.21	0.40
1:B:392:SER:HB3	1:B:528:TRP:CZ2	2.55	0.40
1:B:553:VAL:HG13	1:B:554:THR:H	1.86	0.40
1:C:136:ARG:HB3	1:C:137:PRO:HD2	2.03	0.40
1:C:321:GLN:HG3	1:C:343:ASN:CG	2.46	0.40
1:C:551:ALA:O	1:C:555:VAL:HG13	2.20	0.40
1:A:114:TYR:HE2	1:A:552:SER:OG	2.04	0.40
1:A:628:ASP:O	1:A:630:ILE:HG12	2.22	0.40
1:B:117:PRO:O	1:B:119:PRO:HD3	2.21	0.40
1:B:193:PRO:O	1:B:197:VAL:HG23	2.21	0.40
1:B:469:LEU:HA	1:B:472:GLN:NE2	2.37	0.40
1:C:119:PRO:HG2	1:C:569:ALA:O	2.22	0.40
1:C:199:ASP:O	1:C:204:LYS:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LEU:HA	1:C:333:LYS:HA	2.03	0.40
1:C:529:CYS:O	1:C:532:GLN:HG3	2.21	0.40
1:C:637:HIS:N	1:C:652:GLU:OE1	2.50	0.40
1:C:651:GLU:CD	1:C:656:SER:HB2	2.46	0.40
1:C:690:THR:OG1	1:C:691:ARG:HD3	2.21	0.40
1:A:326:TYR:HE1	1:A:339:PRO:HB3	1.85	0.40
1:A:535:GLU:HB3	1:A:539:TRP:CE2	2.56	0.40
1:A:661:ARG:NH1	1:C:129:GLN:OE1	2.55	0.40
1:B:158:LYS:HD3	1:B:279:ARG:HG2	2.03	0.40
1:B:413:ILE:H	1:B:413:ILE:HD12	1.87	0.40
1:B:465:VAL:HA	1:B:468:HIS:NE2	2.35	0.40
1:C:128:GLU:O	1:C:536:LEU:HD11	2.21	0.40
1:C:192:VAL:HA	1:C:193:PRO:HD3	1.91	0.40
1:C:214:VAL:HA	1:C:219:GLU:HA	2.03	0.40
1:A:166:LYS:HE3	1:A:211:ALA:HB2	2.03	0.40
1:A:191:PRO:HD3	1:A:349:LYS:HA	2.04	0.40
1:A:318:ARG:CZ	1:A:347:THR:HA	2.52	0.40
1:A:349:LYS:HE2	1:A:350:PHE:CE2	2.56	0.40
1:A:604:PHE:O	1:A:612:LEU:HD12	2.21	0.40
1:A:614:GLU:HB2	1:A:627:ARG:CZ	2.51	0.40
1:A:672:ASP:HA	1:A:673:LEU:CB	2.51	0.40
1:B:140:GLN:OE1	1:B:140:GLN:HA	2.22	0.40
1:B:226:ASP:HB2	1:B:254:TYR:CZ	2.57	0.40
1:B:320:LYS:HB2	1:B:320:LYS:HE2	1.91	0.40
1:C:521:LEU:O	1:C:524:VAL:HG22	2.22	0.40
1:A:123:THR:HG21	1:A:568:MET:H	1.87	0.40
1:A:286:GLU:HB2	1:A:294:PHE:HZ	1.86	0.40
1:B:105:LYS:NZ	1:B:612:LEU:HD21	2.36	0.40
1:B:194:PHE:CE1	1:B:344:LEU:HD13	2.57	0.40
1:B:258:ARG:NH1	1:B:260:GLU:OE2	2.45	0.40
1:B:297:MET:CG	1:B:312:THR:HA	2.52	0.40
1:B:466:ARG:CD	1:B:507:GLN:HB2	2.50	0.40
1:B:691:ARG:HD3	1:B:691:ARG:H	1.86	0.40
1:C:141:ASN:HB2	1:C:379:GLU:HB2	2.04	0.40
1:C:349:LYS:HE2	1:C:350:PHE:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	602/904 (67%)	513 (85%)	85 (14%)	4 (1%)	18	56
1	B	602/904 (67%)	484 (80%)	115 (19%)	3 (0%)	24	63
1	C	602/904 (67%)	494 (82%)	102 (17%)	6 (1%)	12	49
All	All	1806/2712 (67%)	1491 (83%)	302 (17%)	13 (1%)	20	56

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PRO
1	A	671	ILE
1	C	137	PRO
1	C	687	GLU
1	C	688	VAL
1	C	138	GLU
1	B	700	LEU
1	A	138	GLU
1	C	689	TYR
1	B	139	GLY
1	B	685	PRO
1	C	139	GLY
1	A	136	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	529/746 (71%)	524 (99%)	5 (1%)	70	79
1	B	529/746 (71%)	526 (99%)	3 (1%)	78	83
1	C	529/746 (71%)	528 (100%)	1 (0%)	87	87
All	All	1587/2238 (71%)	1578 (99%)	9 (1%)	76	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	VAL
1	A	282	TYR
1	A	412	CYS
1	A	667	VAL
1	A	673	LEU
1	B	177	HIS
1	B	394	THR
1	B	656	SER
1	C	352	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	HIS
1	A	202	ASN
1	A	255	ASN
1	A	263	HIS
1	A	458	ASN
1	A	532	GLN
1	A	534	HIS
1	A	674	ASN
1	A	692	HIS
1	A	706	GLN
1	A	712	HIS
1	B	172	GLN
1	B	216	ASN
1	B	263	HIS
1	B	514	GLN
1	B	532	GLN
1	B	580	ASN
1	B	658	GLN
1	B	710	GLN
1	C	177	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	C	181	GLN
1	C	216	ASN
1	C	308	HIS
1	C	398	ASN
1	C	468	HIS
1	C	507	GLN
1	C	511	ASN
1	C	514	GLN
1	C	518	ASN
1	C	692	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

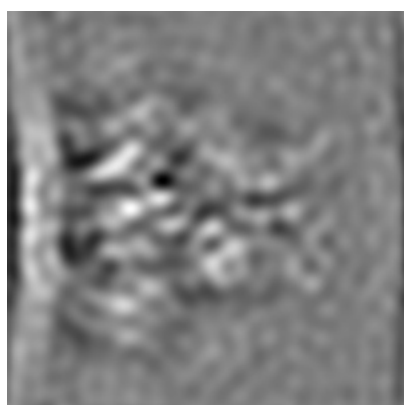
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11123. These allow visual inspection of the internal detail of the map and identification of artifacts.

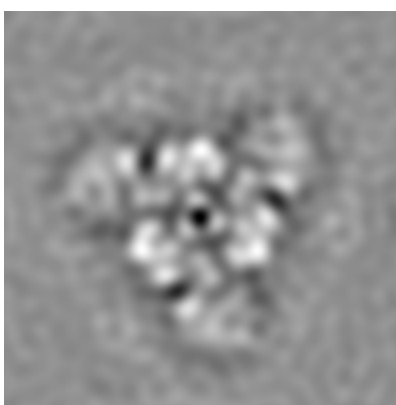
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

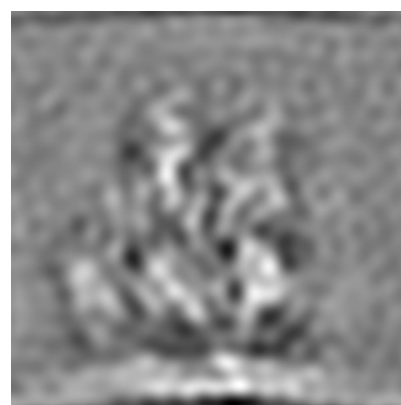
6.1.1 Primary map



X



Y

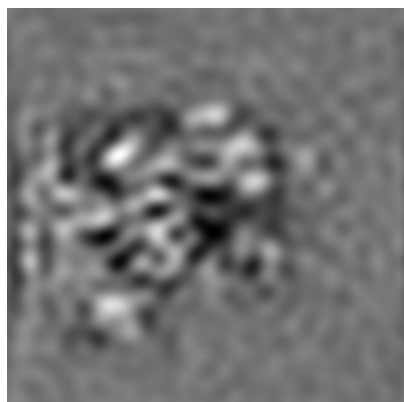


Z

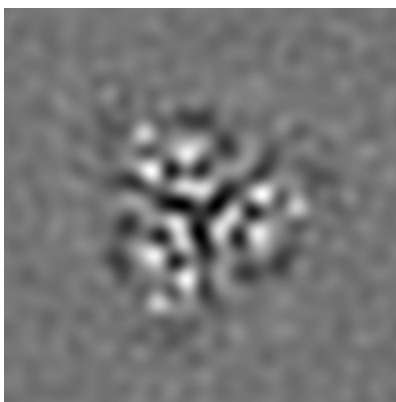
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

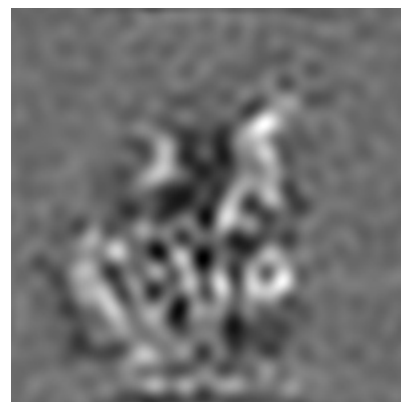
6.2.1 Primary map



X Index: 50



Y Index: 50

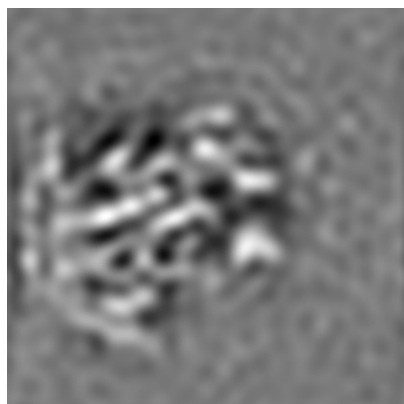


Z Index: 50

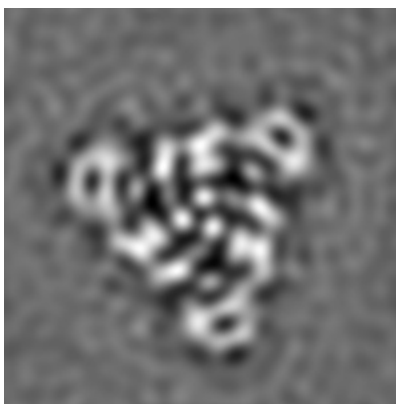
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

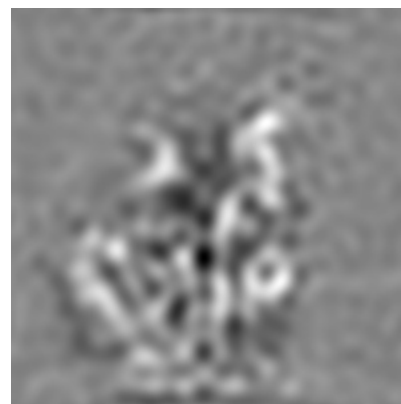
6.3.1 Primary map



X Index: 52



Y Index: 29

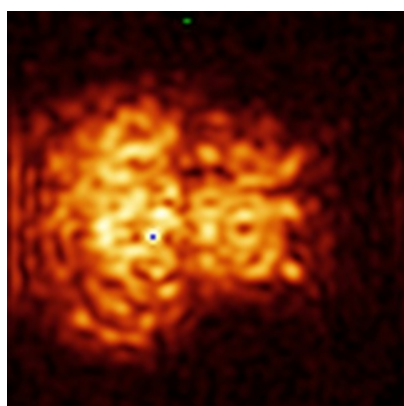


Z Index: 49

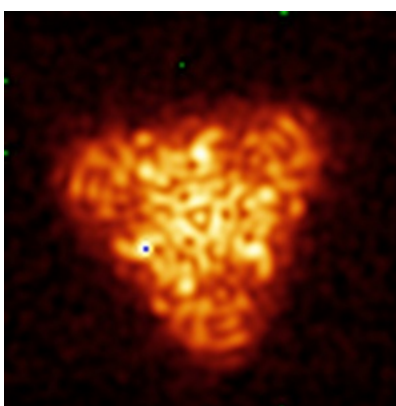
The images above show the largest variance slices of the map in three orthogonal directions.

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

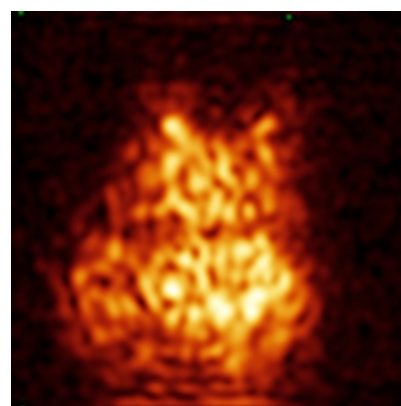
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

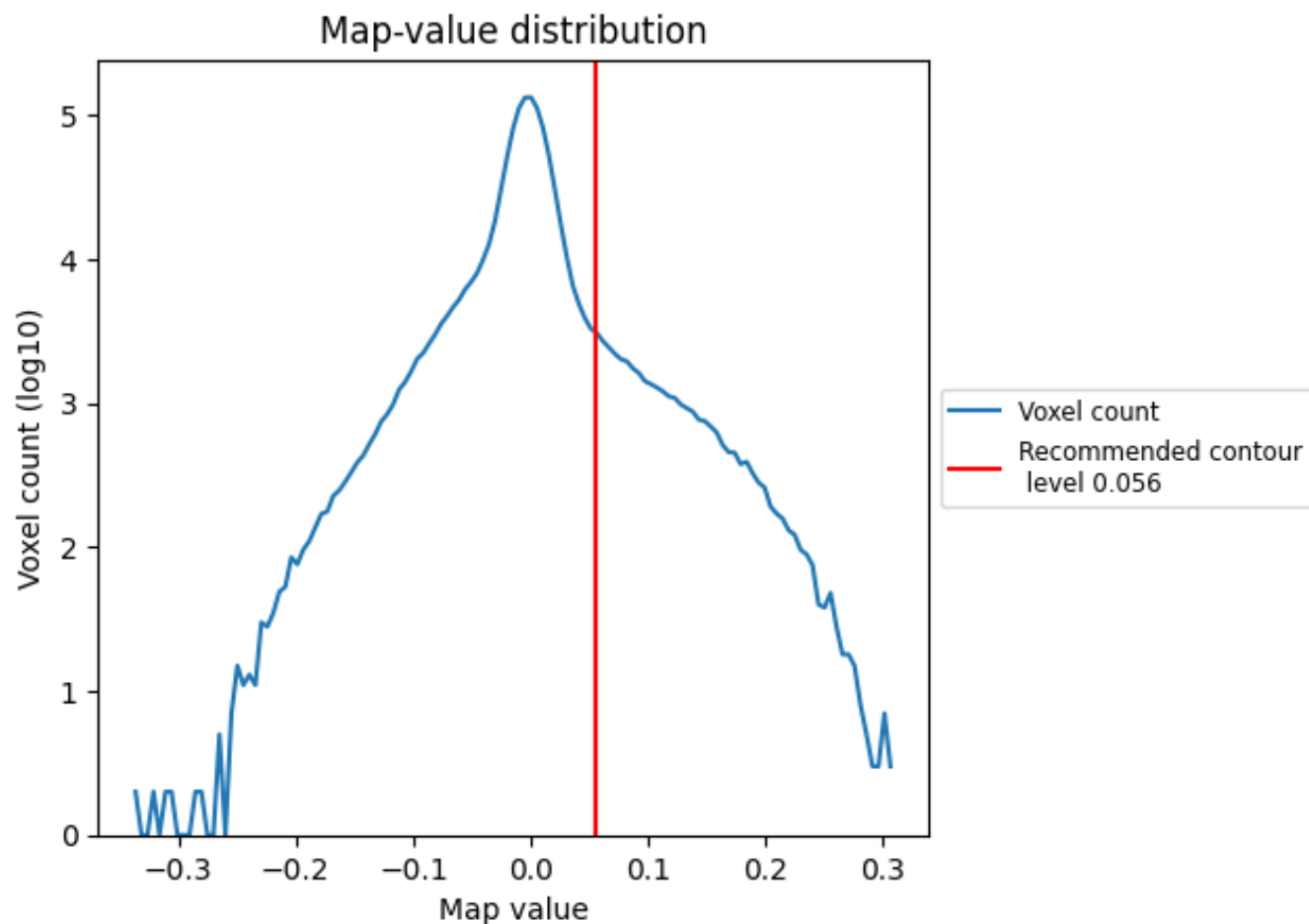
6.6 Mask visualisation

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

7 Map analysis [i](#)

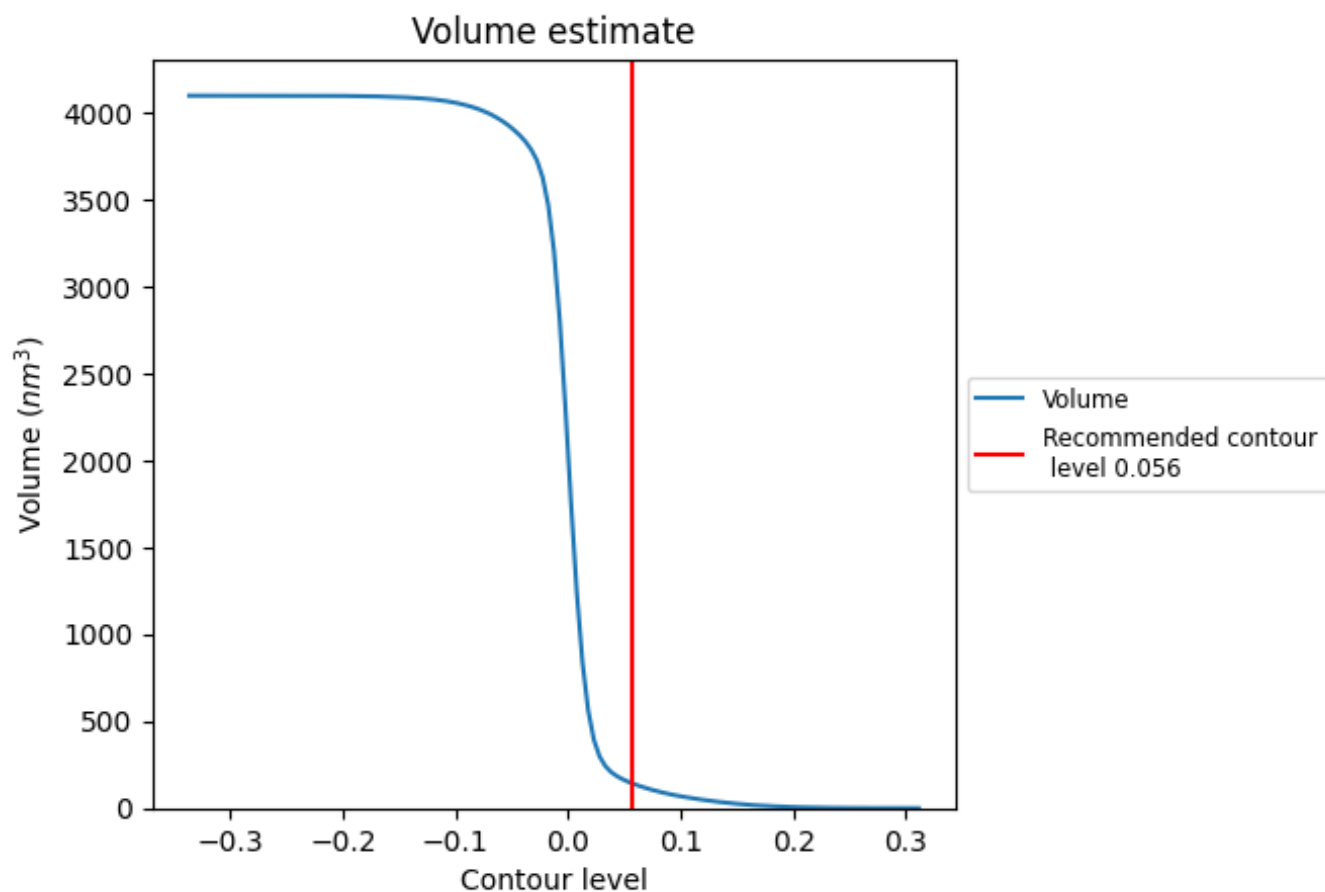
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

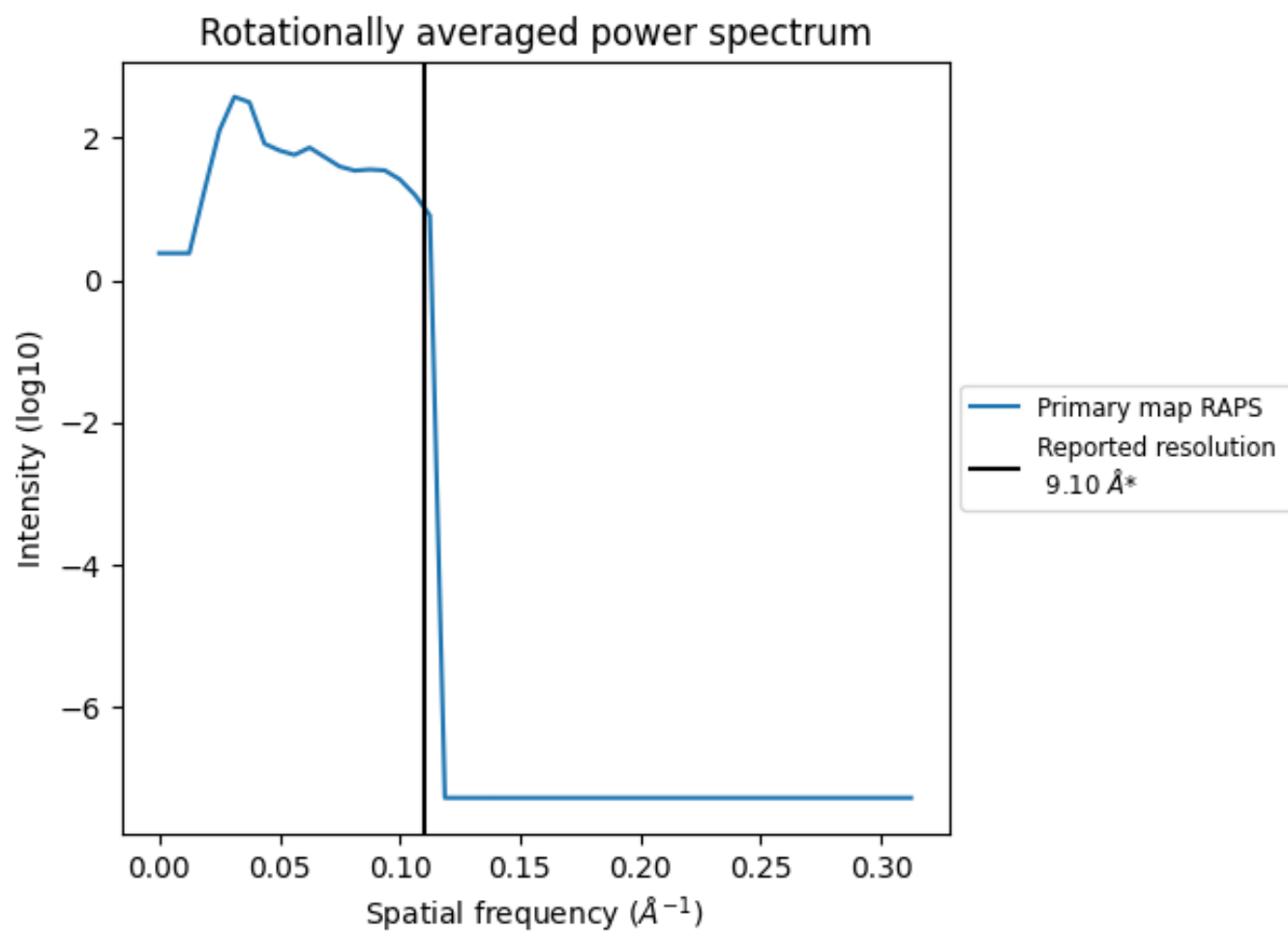
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145 nm³; this corresponds to an approximate mass of 131 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 ⓘ

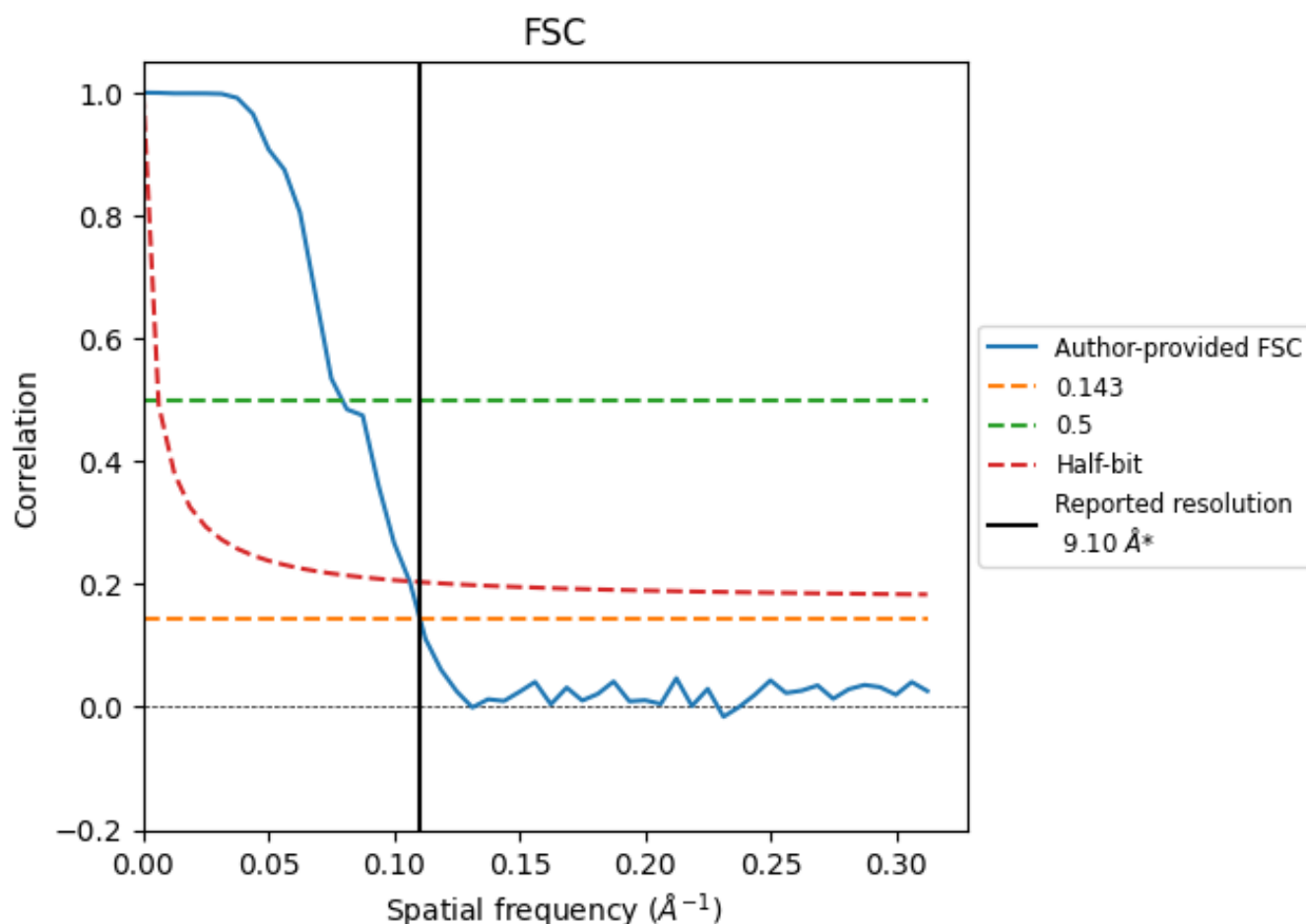


*Reported resolution corresponds to spatial frequency of 0.110 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.110 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	9.07	12.61	9.43
Unmasked-calculated*	-	-	-

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

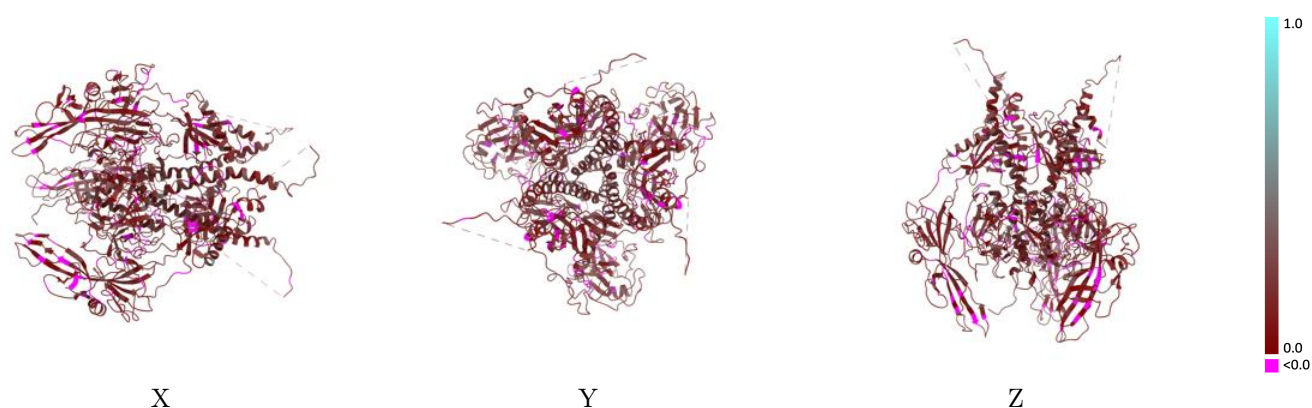
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11123 and PDB model 6Z9M. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)

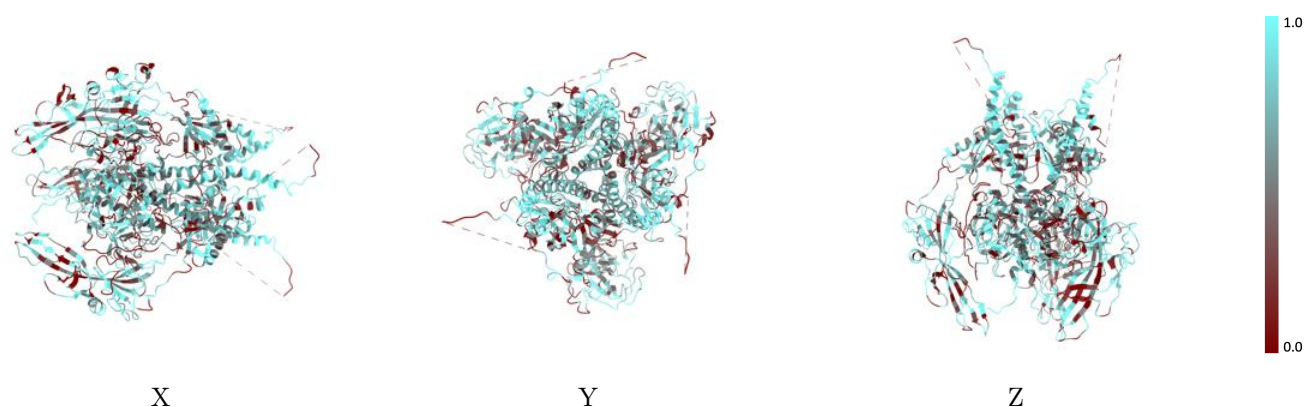
This section was not generated.

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



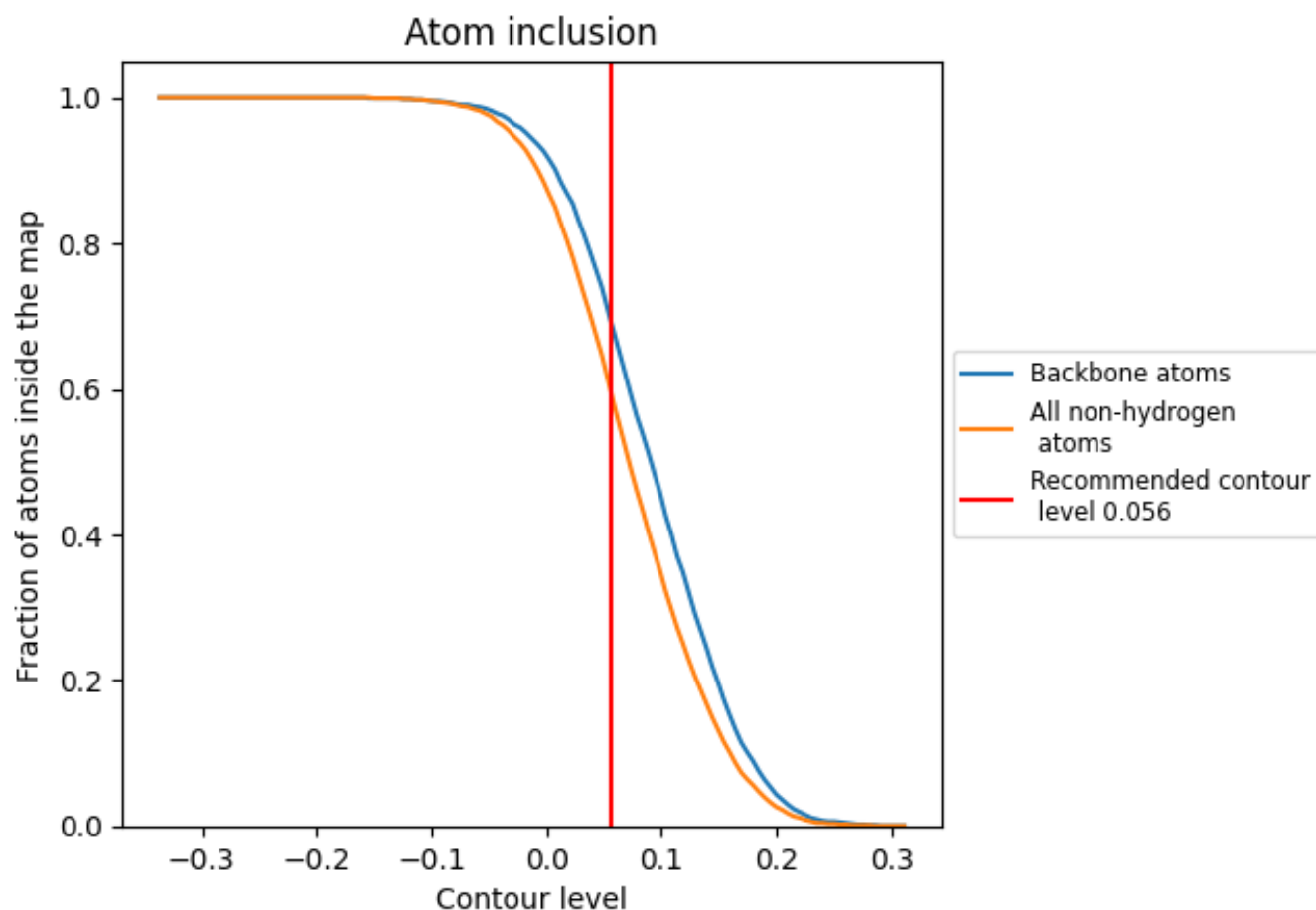
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.056).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.056) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5970	0.1550
A	0.6000	0.1540
B	0.6020	0.1540
C	0.5900	0.1580

