



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:06 AM UTC

PDB ID : 9CLN / pdb_00009cln
EMDB ID : EMD-45726
Title : Cryo-EM model derived from localized reconstruction of human adenovirus 5 (Ad5)-hexon-FII complex at 3.9Å resolution
Authors : Reddy, V.S.; Ma, O.X.
Deposited on : 2024-07-11
Resolution : 4.13 Å(reported)
Based on initial model : 6B1T

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

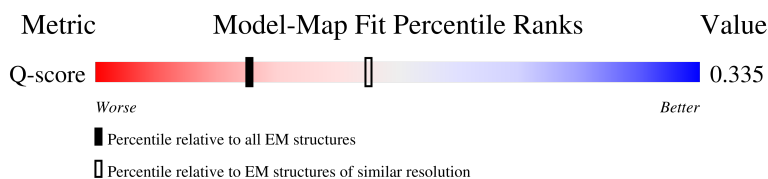
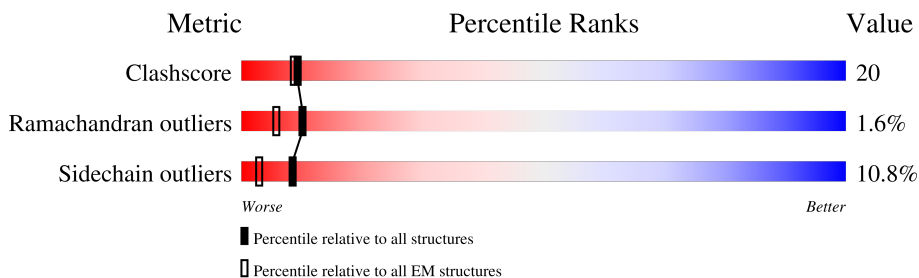
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.13 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	5607 (3.63 - 4.63)

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	J	952	
1	K	952	
1	L	952	
2	Z	622	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CGU	Z	16	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26799 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	J	925	Total	C	N	O	S	0	0
			7401	4703	1253	1409	36		
1	K	922	Total	C	N	O	S	0	0
			7382	4691	1250	1405	36		
1	L	924	Total	C	N	O	S	0	0
			7394	4699	1252	1407	36		

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	579	Total	C	N	O	S	0	0
			4615	2868	805	910	32		

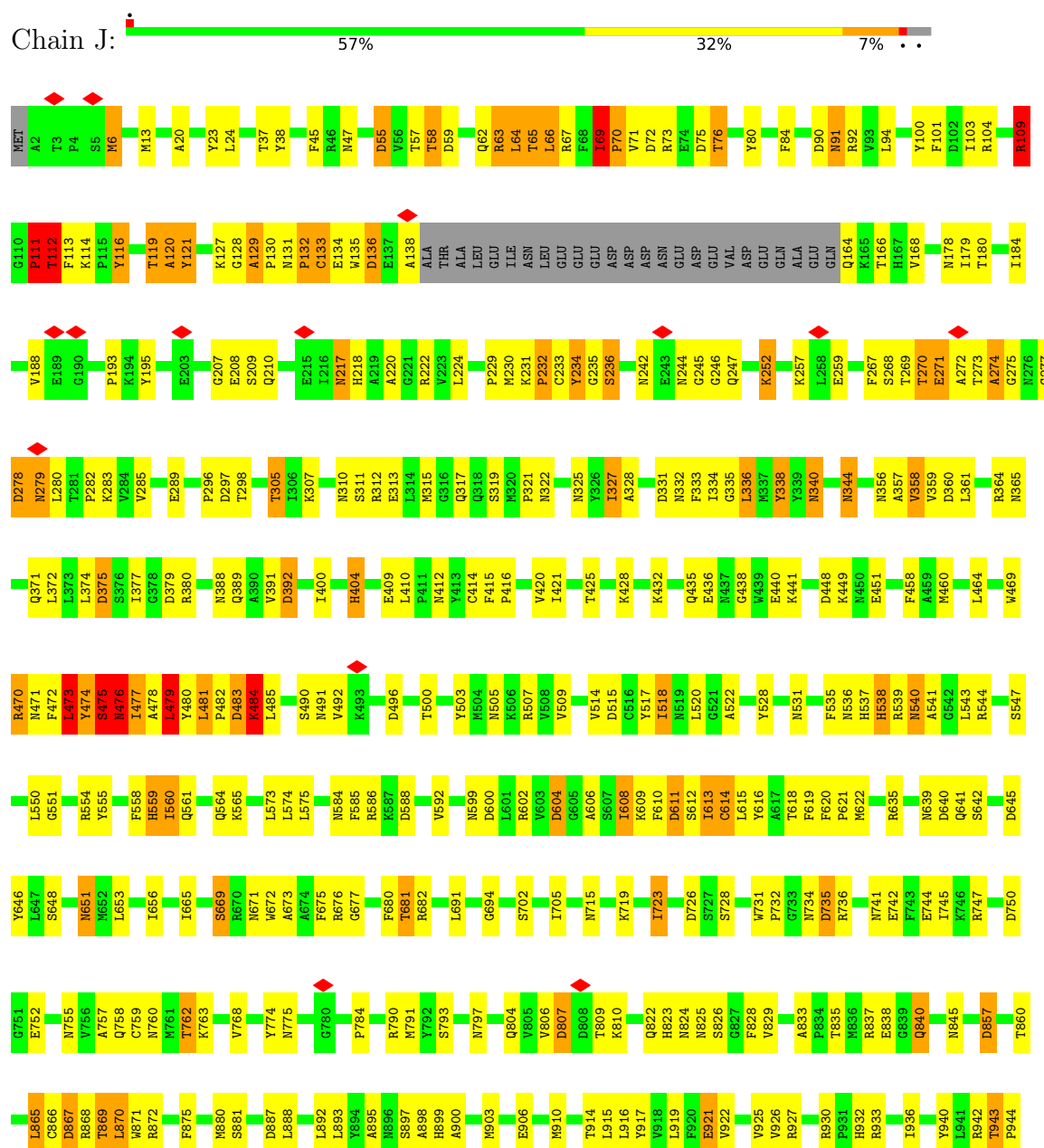
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	K	1	Total	Ca	0
			1	1	
3	Z	6	Total	Ca	0
			6	6	

3 Residue-property plots

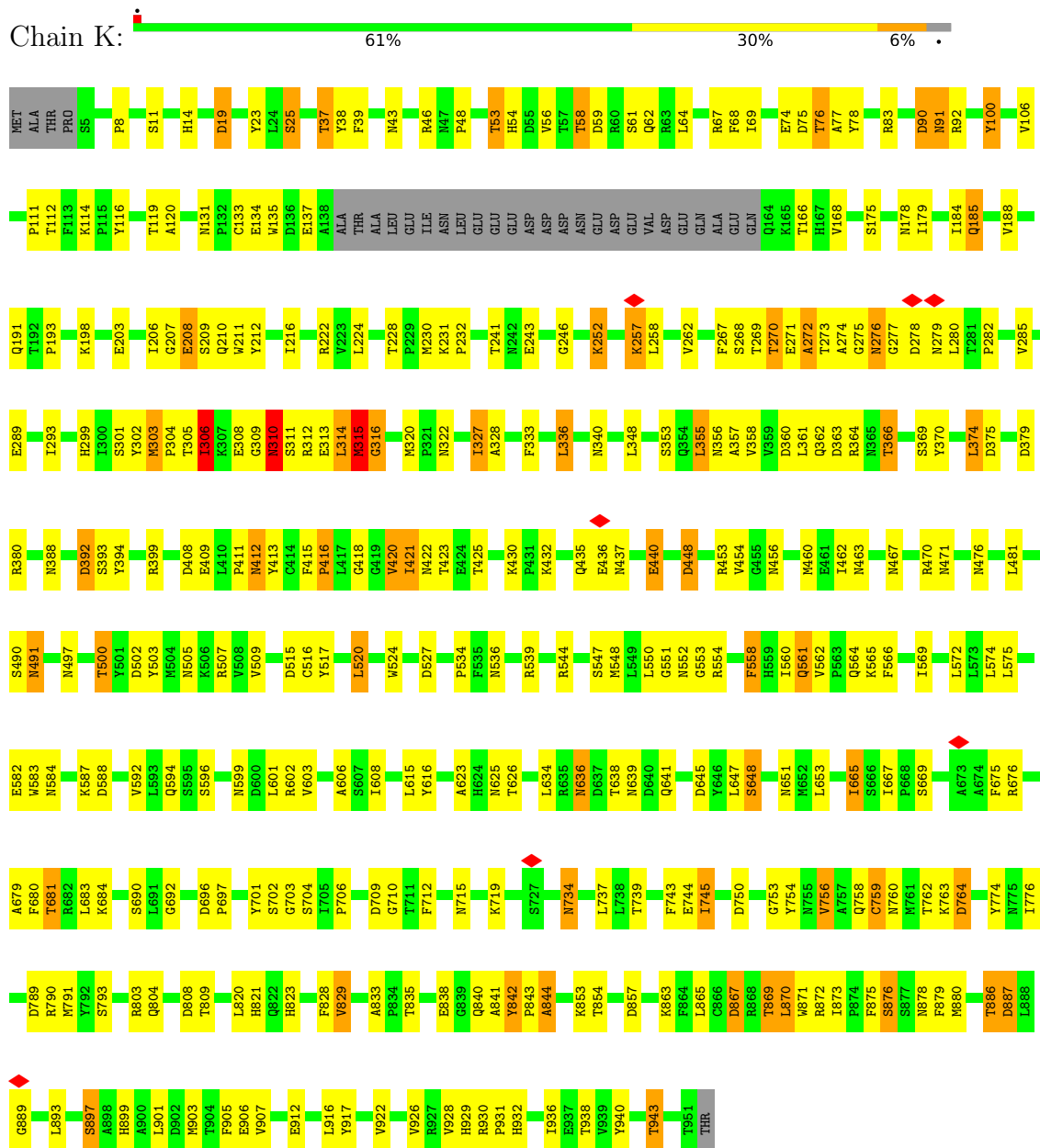
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Hexon protein

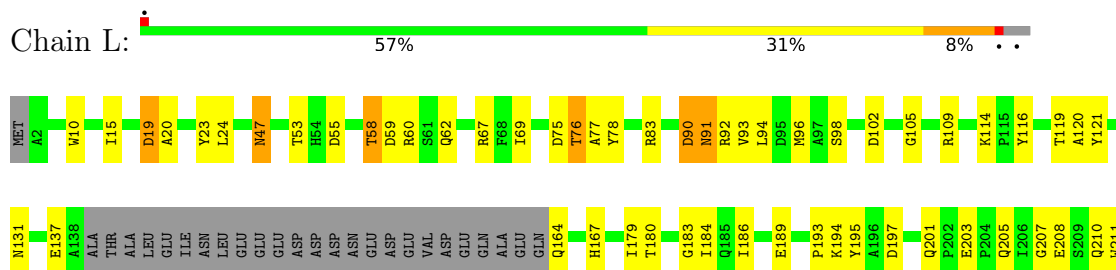


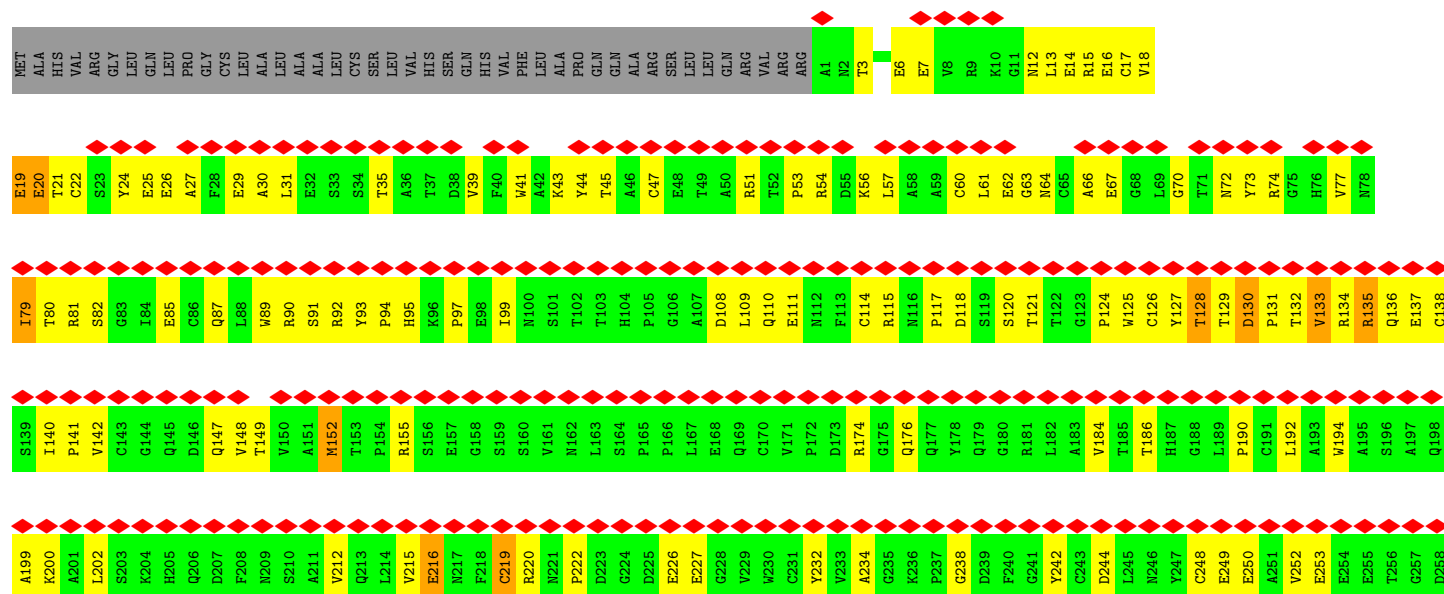


• Molecule 1: Hexon protein



• Molecule 1: Hexon protein





F559	I499	C439	L379	G319	G259
Y560	R500	L440	L380	R320	L260
T561	I501	P441	V381	I321	D261
H562	T502	D442	R382	V322	E262
V563	D503	R443	I383	E323	D263
F564	N504	E444	G384	G324	S264
R565	M505	T445	K385	S325	D265
L566	F506	A446	H386	D326	R266
K567	C507	A447	K387	A327	A267
K568	A508	S448	R388	E328	I268
W569	G509	L449	T389	I329	E269
I570	Y510	L450	R390	G330	G270
Q571	K511	Q451	Y391	M331	R271
K572	P512	A452	E392	S332	T272
V573	D513	G453	R393	P333	A273
I574	E514	Y454	K394	K334	T274
D575	G515	K455	I395	Q335	S275
Q576	K516	G456	E396	V336	E276
F577	R517	R457	K397	M337	Y277
G578	G518	V458	I398	L338	Q278
E579	D519	T459	R399	F339	T279
	A520	G460	M400	R340	F280
	C521	W461	L401	K341	I281
	E522	G462	E402	S342	N282
	G523	M463	K403	P283	P283
	D524	L464	I404	Q344	R284
	S525	K465	Y405	E345	T285
G526	E466	S466	I406	L346	F286
G527	T467	H467	H407	L347	G287
P528	W468	W468	P408	C348	S288
F529	T469	T469	R409	G349	G289
V530	A470	A470	Y410	A350	E290
M531	M471	M471	M411	S351	A291
K532	W472	W472	W412	L352	D292
S533	S473	G473	R413	I353	C293
F534	K474	K474	E414	S354	G294
F535	G475	G475	M415	D355	L295
N536	Q476	Q476	L416	R356	R296
N537	P477	P477	D417	W357	P297
R538	S478	S478	R418	V358	L298
W539	W479	W479	D419	L359	F299
Y540	L480	L480	T420	T360	E300
Q541	Q481	Q481	A421	A361	K301
M542	W482	W482	L422	A362	K302
G543	W483	W483	M423	H363	S303
I544	W484	W484	K424	C364	L304
V545	L485	L485	L425	L365	E305
S546	E486	E486	K426	L366	D306
W547	T487	T487	K427	Y367	K307
G548	W488	W488	P428	P368	T308
E549	E489	E489	W429	P369	E309
G550	R490	R490	A430	W370	R310
C551	P491	P491	F431	D371	E311
D552	W492	W492	S432	K372	L312
R553	C493	C493	D433	N373	L313
D554	K494	K494	Y434	F374	E314
G555	D495	D495	I435	T375	S315
K556	S496	S496	H436	E376	Y316
F557	T497	T497	P437	N377	I317
G558	R498	R498	W438	D378	D318

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	81	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	129.536, 211.2, 111.232	wwPDB
Map dimensions	150, 79, 92	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.408, 1.408, 1.408	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CGU

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	J	0.55	8/7600 (0.1%)	0.61	10/10336 (0.1%)
1	K	0.40	1/7580 (0.0%)	0.47	2/10307 (0.0%)
1	L	0.53	1/7593 (0.0%)	0.63	17/10326 (0.2%)
2	Z	0.17	0/4597	0.45	0/6220
All	All	0.46	10/27370 (0.0%)	0.55	29/37189 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	476	ASN	C-O	7.36	1.33	1.24
1	J	129	ALA	CA-C	-6.84	1.44	1.52
1	K	416	PRO	CA-C	-6.41	1.44	1.52
1	J	473	LEU	CA-C	-6.33	1.44	1.52
1	J	120	ALA	CA-C	-5.54	1.46	1.53
1	J	119	THR	CA-C	-5.52	1.45	1.52
1	L	716	HIS	CA-C	-5.27	1.46	1.53
1	J	475	SER	C-O	5.06	1.30	1.24
1	J	69	ILE	CA-CB	-5.01	1.50	1.54
1	J	69	ILE	CA-C	-5.00	1.48	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	109	ARG	N-CA-C	9.35	122.66	111.82
1	L	370	TYR	N-CA-C	-8.77	101.62	111.71
1	J	536	ASN	N-CA-C	-8.33	99.81	111.81
1	L	502	ASP	CA-C-N	-8.05	108.86	120.29
1	L	502	ASP	C-N-CA	-8.05	108.86	120.29
1	L	713	TYR	N-CA-C	6.55	120.61	112.03
1	L	368	LEU	N-CA-C	-6.48	103.91	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	362	GLN	N-CA-C	6.45	119.65	110.68
1	L	688	THR	N-CA-C	6.42	116.98	109.60
1	L	501	TYR	N-CA-C	-5.92	104.73	111.07
1	L	378	GLY	N-CA-C	5.74	117.91	110.45
1	J	473	LEU	N-CA-C	-5.72	101.99	111.37
1	J	470	ARG	N-CA-C	-5.59	104.19	111.02
1	L	287	TYR	N-CA-C	-5.57	100.32	109.40
1	K	844	ALA	N-CA-C	5.54	118.45	109.86
1	L	291	VAL	CA-C-N	-5.54	113.85	122.16
1	L	291	VAL	C-N-CA	-5.54	113.85	122.16
1	J	69	ILE	CB-CA-C	-5.46	104.65	110.16
1	L	411	PRO	O-C-N	-5.44	116.37	123.06
1	J	121	TYR	CA-C-N	-5.43	114.81	122.63
1	J	121	TYR	C-N-CA	-5.43	114.81	122.63
1	J	111	PRO	N-CA-C	-5.41	101.32	112.47
1	L	363	ASP	N-CA-C	-5.35	99.40	110.80
1	L	871	TRP	N-CA-C	-5.24	103.23	110.35
1	J	116	TYR	N-CA-C	5.23	117.04	108.52
1	K	276	ASN	N-CA-C	5.18	115.08	108.24
1	L	717	THR	CB-CA-C	-5.17	102.76	111.24
1	J	63	ARG	N-CA-C	5.16	118.15	110.52
1	L	426	LEU	N-CA-C	5.05	115.86	107.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	7401	0	7105	321	0
1	K	7382	0	7084	260	0
1	L	7394	0	7098	359	0
2	Z	4615	0	4343	186	0
3	K	1	0	0	0	0
3	Z	6	0	0	0	0
All	All	26799	0	25630	1066	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 20.

All (1066) 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)
2:Z:130:ASP:OD2	2:Z:133:VAL:CG2	1.73	1.36
1:K:276:ASN:HA	1:K:279:ASN:HB3	1.46	0.97
2:Z:130:ASP:OD2	2:Z:133:VAL:HG23	0.79	0.95
1:L:683:LEU:CD1	1:L:707:TYR:HB2	1.97	0.93
1:L:340:ASN:HD21	1:L:366:THR:H	1.13	0.92
2:Z:130:ASP:CG	2:Z:133:VAL:HG23	1.97	0.90
1:K:230:MET:HE2	1:K:310:ASN:HD22	1.35	0.90
1:K:421:ILE:HD12	1:K:422:ASN:H	1.40	0.87
1:J:127:LYS:HE3	1:J:234:TYR:CE2	2.10	0.86
1:K:269:THR:HA	1:L:426:LEU:HD21	1.57	0.86
1:K:759:CYS:SG	1:K:760:ASN:N	2.49	0.85
1:L:683:LEU:HD13	1:L:707:TYR:HB2	1.57	0.84
1:J:484:LYS:O	1:J:485:LEU:HD23	1.77	0.83
1:L:340:ASN:ND2	1:L:366:THR:H	1.76	0.83
1:L:365:ASN:HD21	1:L:368:LEU:HB2	1.42	0.82
1:L:759:CYS:SG	1:L:760:ASN:N	2.52	0.81
1:J:474:TYR:O	1:J:475:SER:C	2.18	0.81
1:L:421:ILE:HD11	1:L:458:PHE:HB3	1.63	0.80
1:K:276:ASN:CA	1:K:279:ASN:HB3	2.11	0.80
1:J:130:PRO:HG3	1:J:315:MET:HE1	1.63	0.80
1:L:492:VAL:HG12	1:L:493:LYS:H	1.46	0.80
2:Z:120:SER:HB2	2:Z:135:ARG:HH22	1.47	0.79
1:J:111:PRO:HD2	1:J:112:THR:HG22	1.64	0.79
1:J:537:HIS:CG	1:J:538:HIS:H	2.00	0.79
1:J:759:CYS:SG	1:J:760:ASN:N	2.51	0.78
1:L:717:THR:HB	1:L:908:ASP:HB2	1.66	0.78
1:L:364:ARG:HA	1:L:651:ASN:HD21	1.47	0.77
1:L:683:LEU:HD11	1:L:707:TYR:HB2	1.66	0.77
1:J:483:ASP:C	1:J:485:LEU:H	1.93	0.77
2:Z:67:GLU:HB3	2:Z:72:ASN:HD21	1.49	0.77
1:J:804:GLN:HE22	1:K:551:GLY:HA3	1.49	0.77
1:J:109:ARG:HE	1:J:327:ILE:HG22	1.49	0.77
1:L:704:SER:O	1:L:705:ILE:C	2.27	0.76
1:K:314:LEU:O	1:K:315:MET:C	2.27	0.76
1:J:65:THR:HG22	1:J:618:THR:HG22	1.66	0.76
1:K:276:ASN:HA	1:K:279:ASN:CB	2.16	0.75
1:K:453:ARG:NH1	1:K:454:VAL:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:775:ASN:HD21	1:J:881:SER:HB3	1.49	0.75
1:K:269:THR:HG22	1:K:271:GLU:H	1.52	0.75
1:J:333:PHE:HE1	1:J:388:ASN:HB3	1.52	0.75
1:J:551:GLY:HA3	1:L:804:GLN:HE22	1.48	0.75
1:K:230:MET:HE2	1:K:310:ASN:ND2	2.02	0.74
1:J:116:TYR:CD2	1:L:520:LEU:HD13	2.23	0.74
1:L:490:SER:O	1:L:492:VAL:HG23	1.87	0.74
2:Z:90:ARG:HH22	2:Z:111:GLU:HB3	1.54	0.73
1:K:131:ASN:ND2	1:K:231:LYS:O	2.23	0.72
1:L:340:ASN:HD21	1:L:366:THR:N	1.86	0.72
1:L:701:TYR:CG	1:L:702:SER:N	2.58	0.72
1:J:273:THR:O	1:J:274:ALA:C	2.30	0.72
1:L:269:THR:HG22	1:L:272:ALA:H	1.52	0.72
1:J:392:ASP:OD1	1:J:392:ASP:N	2.13	0.72
2:Z:60:CYS:SG	2:Z:72:ASN:ND2	2.62	0.72
2:Z:124:PRO:HB2	2:Z:140:ILE:HG13	1.72	0.71
1:J:478:ALA:O	1:J:480:TYR:N	2.23	0.71
1:L:687:GLU:HG2	1:L:701:TYR:CZ	2.25	0.71
1:L:764:ASP:OD1	1:L:764:ASP:N	2.22	0.71
2:Z:460:GLY:HA3	2:Z:523:GLY:HA2	1.71	0.71
1:K:497:ASN:ND2	1:K:500:THR:OG1	2.23	0.71
1:L:705:ILE:HD12	1:L:705:ILE:H	1.55	0.71
1:J:111:PRO:HD2	1:J:604:ASP:HB3	1.71	0.70
1:J:333:PHE:HE2	1:J:560:ILE:HD12	1.55	0.70
2:Z:73:TYR:O	2:Z:74:ARG:NH1	2.24	0.70
1:K:363:ASP:O	1:K:651:ASN:ND2	2.23	0.70
1:K:100:TYR:HE1	1:K:616:TYR:HB2	1.55	0.70
1:K:276:ASN:O	1:K:278:ASP:N	2.24	0.70
1:K:356:ASN:ND2	1:K:358:VAL:O	2.25	0.70
1:J:269:THR:HB	1:J:272:ALA:HB2	1.73	0.70
1:J:231:LYS:HA	1:J:317:GLN:OE1	1.91	0.70
1:J:824:ASN:OD1	1:J:825:ASN:ND2	2.25	0.70
1:L:701:TYR:CZ	1:L:703:GLY:N	2.60	0.70
1:J:867:ASP:N	1:J:867:ASP:OD1	2.25	0.70
1:K:411:PRO:HB2	1:K:413:TYR:CE1	2.26	0.70
1:J:273:THR:HG22	1:J:280:LEU:HD21	1.74	0.69
1:L:807:ASP:OD1	1:L:808:ASP:N	2.25	0.69
2:Z:39:VAL:HG12	2:Z:43:LYS:HE3	1.74	0.69
1:L:533:ASN:HB2	1:L:713:TYR:CE2	2.28	0.69
2:Z:90:ARG:NH1	2:Z:111:GLU:OE1	2.23	0.69
1:L:707:TYR:CG	1:L:707:TYR:O	2.45	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:ILE:HG13	1:L:218:HIS:HD2	1.56	0.69
1:L:538:HIS:O	1:L:544:ARG:NH2	2.26	0.69
1:J:268:SER:HB2	1:J:282:PRO:HA	1.75	0.68
1:K:311:SER:O	1:K:312:ARG:C	2.34	0.68
1:J:233:CYS:O	1:J:235:GLY:N	2.27	0.68
1:J:134:GLU:CD	1:J:168:VAL:HG22	2.17	0.68
1:L:276:ASN:C	1:L:278:ASP:H	2.02	0.68
2:Z:15:ARG:NH2	2:Z:16:CGU:OE22	2.26	0.68
1:L:685:THR:O	1:L:687:GLU:N	2.27	0.68
1:J:130:PRO:CG	1:J:315:MET:HE1	2.24	0.68
1:J:653:LEU:HD21	1:J:917:TYR:HD1	1.58	0.68
2:Z:109:LEU:HA	2:Z:115:ARG:HG3	1.75	0.67
2:Z:458:VAL:HG21	2:Z:485:LEU:HD12	1.75	0.67
1:J:131:ASN:O	1:J:132:PRO:C	2.35	0.67
1:L:374:LEU:O	1:L:375:ASP:C	2.35	0.67
1:J:483:ASP:C	1:J:485:LEU:N	2.51	0.67
1:J:613:ILE:HG22	1:J:614:CYS:H	1.58	0.67
1:L:701:TYR:OH	1:L:703:GLY:HA3	1.93	0.67
2:Z:192:LEU:HD11	2:Z:234:ALA:HB2	1.77	0.67
1:K:83:ARG:NH1	1:K:582:GLU:OE1	2.27	0.67
1:J:331:ASP:OD2	1:J:371:GLN:NE2	2.28	0.67
1:L:121:TYR:HB2	1:L:235:GLY:HA2	1.76	0.67
1:L:480:TYR:HH	1:L:538:HIS:HD1	1.41	0.67
1:L:588:ASP:OD2	1:L:602:ARG:NH2	2.28	0.67
2:Z:219:CYS:O	2:Z:220:ARG:NH1	2.28	0.67
1:J:234:TYR:HB3	1:J:319:SER:OG	1.95	0.67
1:J:837:ARG:HB3	1:L:413:TYR:CE2	2.30	0.67
1:L:364:ARG:HA	1:L:651:ASN:ND2	2.09	0.67
1:L:497:ASN:O	1:L:499:ASN:N	2.27	0.67
1:K:750:ASP:OD2	1:K:754:TYR:N	2.28	0.66
1:L:367:GLU:C	1:L:369:SER:N	2.45	0.66
1:L:706:PRO:C	1:L:708:LEU:H	2.02	0.66
1:J:483:ASP:O	1:J:485:LEU:N	2.27	0.66
1:K:276:ASN:HA	1:K:279:ASN:ND2	2.10	0.66
1:L:367:GLU:C	1:L:369:SER:H	2.03	0.66
1:L:536:ASN:HD21	1:L:703:GLY:C	2.04	0.66
1:J:897:SER:OG	1:J:898:ALA:N	2.29	0.66
1:L:384:PHE:CE2	1:L:386:MET:HB3	2.31	0.66
1:L:83:ARG:NH1	1:L:582:GLU:OE1	2.28	0.66
2:Z:400:MET:SD	2:Z:400:MET:N	2.69	0.66
1:J:232:PRO:HG3	1:J:317:GLN:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:356:ASN:ND2	1:J:358:VAL:O	2.30	0.65
1:L:714:LEU:C	1:L:716:HIS:H	2.04	0.65
2:Z:401:LEU:HD22	2:Z:423:MET:HB3	1.79	0.65
1:J:471:ASN:ND2	1:L:410:LEU:HB2	2.10	0.65
1:L:706:PRO:O	1:L:708:LEU:N	2.29	0.65
1:J:269:THR:O	1:J:273:THR:HG23	1.97	0.65
1:J:804:GLN:HG3	1:J:860:THR:HG22	1.78	0.65
1:L:384:PHE:HB3	1:L:389:GLN:HB3	1.79	0.65
1:J:360:ASP:OD1	1:J:364:ARG:NH1	2.29	0.65
1:J:757:ALA:H	1:K:561:GLN:HE22	1.43	0.65
1:K:280:LEU:HB2	1:L:439:TRP:HB3	1.78	0.65
1:J:242:ASN:ND2	1:J:246:GLY:O	2.29	0.65
1:K:76:THR:O	1:K:587:LYS:NZ	2.30	0.64
1:K:267:PHE:HB3	1:L:426:LEU:CD1	2.27	0.64
1:J:620:PHE:O	1:J:621:PRO:C	2.37	0.64
1:K:379:ASP:OD1	1:K:380:ARG:N	2.29	0.64
1:K:392:ASP:OD1	1:K:392:ASP:N	2.30	0.64
1:J:333:PHE:CE1	1:J:388:ASN:HB3	2.32	0.64
1:L:131:ASN:ND2	1:L:231:LYS:O	2.30	0.64
1:J:72:ASP:OD1	1:J:73:ARG:N	2.30	0.64
1:J:554:ARG:NH2	1:J:555:TYR:OH	2.30	0.64
1:L:364:ARG:CA	1:L:651:ASN:HD21	2.10	0.64
1:K:432:LYS:NZ	1:K:440:GLU:OE1	2.30	0.64
1:J:471:ASN:HD21	1:L:410:LEU:HB2	1.61	0.64
1:K:340:ASN:ND2	1:K:364:ARG:O	2.30	0.64
1:L:715:ASN:ND2	1:L:869:THR:O	2.31	0.64
1:K:536:ASN:HD21	1:K:704:SER:H	1.46	0.64
1:J:80:TYR:CE2	1:J:613:ILE:HD11	2.33	0.63
1:K:111:PRO:HD3	1:K:554:ARG:HH11	1.63	0.63
1:K:311:SER:OG	1:K:313:GLU:HB2	1.98	0.63
2:Z:91:SER:HA	2:Z:469:THR:HA	1.80	0.63
1:J:230:MET:SD	1:J:315:MET:HG2	2.38	0.63
1:K:272:ALA:O	1:K:273:THR:C	2.40	0.63
1:J:472:PHE:O	1:J:473:LEU:C	2.40	0.63
1:J:121:TYR:HE2	1:J:296:PRO:HG3	1.62	0.63
1:L:697:PRO:O	1:L:699:TYR:N	2.32	0.63
1:L:625:ASN:OD1	1:L:626:THR:N	2.31	0.63
2:Z:194:TRP:N	2:Z:216:GLU:O	2.26	0.63
2:Z:479:VAL:O	2:Z:481:GLN:NE2	2.32	0.63
1:K:463:ASN:O	1:K:467:ASN:ND2	2.27	0.62
1:J:415:PHE:CE2	1:K:828:PHE:HD1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:279:ASN:OD1	1:K:280:LEU:N	2.31	0.62
1:J:277:GLY:O	1:J:279:ASN:N	2.31	0.62
2:Z:73:TYR:O	2:Z:115:ARG:NH1	2.33	0.62
1:L:271:GLU:C	1:L:273:THR:H	2.07	0.62
1:J:80:TYR:HE2	1:J:613:ILE:HD11	1.63	0.62
1:J:217:ASN:OD1	1:J:217:ASN:N	2.30	0.62
1:J:359:VAL:H	1:J:940:TYR:HE2	1.47	0.62
1:L:701:TYR:CZ	1:L:703:GLY:HA3	2.35	0.62
1:J:208:GLU:OE2	1:J:210:GLN:NE2	2.27	0.62
1:J:340:ASN:ND2	1:J:364:ARG:O	2.32	0.62
1:K:53:THR:O	1:K:54:HIS:ND1	2.33	0.62
1:K:867:ASP:OD1	1:K:867:ASP:N	2.32	0.62
1:L:210:GLN:OE1	1:L:210:GLN:N	2.29	0.62
1:L:365:ASN:ND2	1:L:368:LEU:HB2	2.14	0.62
1:J:332:ASN:OD1	1:J:371:GLN:NE2	2.33	0.62
2:Z:422:LEU:HD23	2:Z:573:VAL:HG11	1.81	0.62
1:K:393:SER:OG	1:K:394:TYR:N	2.33	0.61
1:L:367:GLU:O	1:L:368:LEU:C	2.42	0.61
1:J:503:TYR:OH	1:J:507:ARG:NH2	2.34	0.61
1:J:537:HIS:CG	1:J:538:HIS:N	2.64	0.61
1:J:726:ASP:HA	1:J:900:ALA:HB3	1.82	0.61
1:K:299:HIS:NE2	1:K:320:MET:SD	2.73	0.61
1:L:705:ILE:CG2	1:L:708:LEU:HB2	2.31	0.61
2:Z:3:THR:O	2:Z:6:CGU:N	2.32	0.61
1:L:595:SER:OG	1:L:596:SER:N	2.29	0.61
1:J:104:ARG:HG2	1:J:559:HIS:HB2	1.82	0.61
1:L:364:ARG:CA	1:L:651:ASN:ND2	2.63	0.61
1:K:114:LYS:NZ	1:K:116:TYR:O	2.33	0.61
1:K:314:LEU:O	1:K:316:GLY:N	2.34	0.61
1:L:409:GLU:OE1	1:L:409:GLU:N	2.34	0.61
2:Z:517:ARG:NH1	2:Z:550:GLY:O	2.32	0.61
1:J:642:SER:OG	1:K:46:ARG:N	2.34	0.61
1:K:185:GLN:HG3	1:K:193:PRO:HB3	1.84	0.60
1:K:422:ASN:O	1:K:453:ARG:HD3	2.01	0.60
1:K:684:LYS:NZ	1:K:912:GLU:OE1	2.31	0.60
1:L:383:TYR:HD1	1:L:390:ALA:HA	1.66	0.60
1:J:271:GLU:HA	1:J:274:ALA:HB2	1.83	0.60
1:K:709:ASP:OD1	1:K:710:GLY:N	2.35	0.60
1:J:335:GLY:O	1:J:586:ARG:NH1	2.33	0.60
1:K:804:GLN:HE22	1:L:551:GLY:HA3	1.65	0.60
1:L:416:PRO:O	1:L:417:LEU:C	2.43	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:478:ALA:C	1:J:480:TYR:H	2.08	0.60
1:L:90:ASP:OD1	1:L:90:ASP:N	2.34	0.60
1:L:709:ASP:OD1	1:L:710:GLY:N	2.34	0.60
1:L:714:LEU:O	1:L:716:HIS:N	2.34	0.60
1:L:671:ASN:OD1	1:L:672:TRP:N	2.35	0.60
1:J:109:ARG:O	1:J:606:ALA:HB2	2.01	0.60
1:J:604:ASP:OD1	1:J:604:ASP:N	2.33	0.60
1:L:813:ASP:N	1:L:813:ASP:OD1	2.35	0.60
2:Z:43:LYS:HB3	2:Z:61:LEU:HD22	1.82	0.60
1:J:111:PRO:CD	1:J:604:ASP:HB3	2.31	0.60
1:J:120:ALA:O	1:J:121:TYR:CG	2.54	0.60
1:L:750:ASP:OD1	1:L:753:GLY:N	2.35	0.60
2:Z:109:LEU:HD21	2:Z:117:PRO:HG3	1.83	0.60
1:J:298:THR:HG22	1:J:321:PRO:HA	1.84	0.59
1:J:539:ARG:O	1:J:541:ALA:N	2.35	0.59
1:K:267:PHE:HB3	1:L:426:LEU:HD12	1.83	0.59
1:L:213:GLU:N	1:L:213:GLU:OE1	2.33	0.59
1:L:717:THR:HB	1:L:908:ASP:CB	2.32	0.59
1:L:203:GLU:OE1	1:L:205:GLN:NE2	2.35	0.59
1:J:470:ARG:O	1:J:471:ASN:C	2.43	0.59
1:K:409:GLU:N	1:K:409:GLU:OE1	2.33	0.59
1:K:842:TYR:CE1	1:L:224:LEU:HD21	2.37	0.59
1:L:887:ASP:OD1	1:L:888:LEU:N	2.35	0.59
2:Z:382:ARG:HB2	2:Z:385:LYS:HD2	1.84	0.59
1:J:179:ILE:HG13	1:J:218:HIS:HD2	1.67	0.59
1:J:242:ASN:OD1	1:J:245:GLY:N	2.35	0.59
1:L:684:LYS:O	1:L:685:THR:C	2.44	0.59
2:Z:250:GLU:O	2:Z:565:ARG:NH2	2.35	0.59
1:J:415:PHE:CZ	1:K:828:PHE:HD1	2.20	0.59
1:J:131:ASN:O	1:J:133:CYS:N	2.36	0.59
1:J:322:ASN:OD1	1:J:505:ASN:ND2	2.35	0.59
1:K:515:ASP:OD1	1:K:516:CYS:N	2.34	0.59
1:J:344:ASN:O	1:J:584:ASN:ND2	2.35	0.59
1:L:270:THR:O	1:L:273:THR:N	2.35	0.59
1:L:497:ASN:HD21	1:L:499:ASN:HB2	1.68	0.59
1:J:540:ASN:O	1:J:543:LEU:N	2.36	0.58
1:L:502:ASP:CG	1:L:506:LYS:HE3	2.27	0.58
1:L:667:ILE:HB	1:L:901:LEU:HB3	1.85	0.58
1:K:312:ARG:O	1:K:313:GLU:C	2.45	0.58
1:K:100:TYR:CE1	1:K:616:TYR:HB2	2.38	0.58
1:K:175:SER:HB2	1:K:216:ILE:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:564:GLN:OE1	1:K:565:LYS:N	2.37	0.58
1:L:205:GLN:N	1:L:205:GLN:OE1	2.35	0.58
1:L:367:GLU:HB2	1:L:708:LEU:HD23	1.85	0.58
1:L:535:PHE:O	1:L:540:ASN:ND2	2.37	0.58
2:Z:19:CGU:OE11	2:Z:54:ARG:HB3	2.02	0.58
1:J:575:LEU:HG	1:J:930:ARG:HH21	1.69	0.58
1:J:620:PHE:CD1	1:J:620:PHE:C	2.78	0.58
2:Z:297:PRO:HA	2:Z:301:LYS:HB2	1.85	0.58
1:J:269:THR:O	1:J:272:ALA:HB3	2.03	0.58
1:J:435:GLN:NE2	1:J:436:GLU:O	2.37	0.58
1:J:635:ARG:HH22	1:J:933:ARG:HA	1.68	0.58
1:K:641:GLN:HG3	1:K:930:ARG:HH22	1.68	0.58
1:J:130:PRO:HG3	1:J:315:MET:CE	2.32	0.58
1:K:37:THR:OG1	1:K:38:TYR:N	2.37	0.58
1:K:358:VAL:HG13	1:K:566:PHE:HE2	1.68	0.58
1:L:685:THR:O	1:L:686:LYS:C	2.46	0.58
1:K:53:THR:O	1:K:53:THR:OG1	2.18	0.58
1:L:367:GLU:O	1:L:369:SER:N	2.37	0.58
1:J:755:ASN:O	1:J:763:LYS:NZ	2.38	0.57
1:K:230:MET:SD	1:K:315:MET:SD	3.02	0.57
1:J:233:CYS:O	1:J:234:TYR:C	2.47	0.57
1:J:297:ASP:OD1	1:J:297:ASP:N	2.36	0.57
1:J:473:LEU:O	1:J:474:TYR:O	2.23	0.57
1:K:887:ASP:N	1:K:887:ASP:OD1	2.23	0.57
2:Z:293:CYS:O	2:Z:538:ARG:NH1	2.34	0.57
1:K:8:PRO:HG2	1:K:11:SER:HB3	1.86	0.57
1:K:257:LYS:H	1:K:257:LYS:HD3	1.69	0.57
1:L:372:LEU:O	1:L:375:ASP:HB3	2.04	0.57
1:L:842:TYR:HD1	1:L:843:PRO:HD2	1.68	0.57
2:Z:108:ASP:O	2:Z:115:ARG:NH2	2.35	0.57
1:L:189:GLU:HB2	1:L:194:LYS:HD2	1.86	0.57
2:Z:12:ASN:OD1	2:Z:13:LEU:N	2.37	0.57
1:K:922:VAL:HB	1:K:943:THR:O	2.04	0.57
1:L:340:ASN:N	1:L:340:ASN:OD1	2.38	0.57
1:J:379:ASP:OD1	1:J:380:ARG:N	2.38	0.57
1:L:58:THR:OG1	1:L:59:ASP:N	2.38	0.57
1:L:365:ASN:N	1:L:651:ASN:ND2	2.53	0.57
1:L:427:THR:OG1	1:L:448:ASP:O	2.22	0.57
2:Z:85:GLU:OE2	2:Z:553:ARG:NH2	2.37	0.57
1:J:332:ASN:HD21	1:J:389:GLN:HG3	1.70	0.57
2:Z:131:PRO:HB3	2:Z:367:TYR:OH	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:311:SER:O	1:K:313:GLU:N	2.38	0.57
1:K:690:SER:N	1:K:696:ASP:OD2	2.35	0.57
1:L:564:GLN:OE1	1:L:565:LYS:N	2.38	0.57
1:L:701:TYR:CZ	1:L:703:GLY:CA	2.88	0.57
2:Z:125:TRP:CZ3	2:Z:135:ARG:HG2	2.40	0.57
1:J:272:ALA:O	1:J:273:THR:C	2.46	0.56
1:L:501:TYR:CE1	1:L:505:ASN:HB2	2.40	0.56
1:J:715:ASN:OD1	1:J:871:TRP:NE1	2.39	0.56
1:K:230:MET:HG3	1:K:310:ASN:HD21	1.70	0.56
2:Z:132:THR:HG22	2:Z:412:TRP:HZ3	1.69	0.56
2:Z:174:ARG:NH1	2:Z:250:GLU:OE1	2.34	0.56
1:K:415:PHE:HB3	1:K:416:PRO:HD2	1.87	0.56
1:K:527:ASP:OD1	1:K:863:LYS:NZ	2.38	0.56
2:Z:433:ASP:OD1	2:Z:433:ASP:N	2.36	0.56
2:Z:550:GLY:HA2	2:Z:556:LYS:HB2	1.86	0.56
1:J:121:TYR:HE2	1:J:296:PRO:CG	2.16	0.56
1:J:305:THR:HG22	1:J:307:LYS:H	1.70	0.56
1:J:823:HIS:O	1:J:823:HIS:ND1	2.38	0.56
1:K:208:GLU:OE1	1:K:209:SER:N	2.39	0.56
1:K:683:LEU:HD21	1:K:706:PRO:HB2	1.88	0.56
1:K:905:PHE:CD2	1:K:916:LEU:HD21	2.40	0.56
2:Z:308:THR:OG1	2:Z:457:ARG:NH2	2.39	0.56
2:Z:388:ARG:HH21	2:Z:461:TRP:HD1	1.54	0.56
1:J:69:ILE:O	1:J:70:PRO:C	2.47	0.56
1:L:363:ASP:O	1:L:651:ASN:ND2	2.39	0.56
1:K:702:SER:O	1:K:702:SER:OG	2.23	0.56
1:L:114:LYS:NZ	1:L:116:TYR:O	2.39	0.56
1:L:897:SER:OG	1:L:898:ALA:N	2.38	0.56
1:J:116:TYR:HD1	1:J:116:TYR:O	1.89	0.56
1:J:473:LEU:O	1:J:474:TYR:C	2.49	0.56
1:J:608:ILE:HD11	1:J:610:PHE:CE1	2.41	0.56
1:L:432:LYS:H	1:L:438:GLY:HA3	1.71	0.56
2:Z:252:VAL:HG23	2:Z:443:ARG:HG3	1.88	0.56
1:K:62:GLN:OE1	1:K:92:ARG:NE	2.39	0.56
1:L:867:ASP:OD1	1:L:867:ASP:N	2.37	0.56
2:Z:226:GLU:HB2	2:Z:565:ARG:HB3	1.86	0.55
2:Z:296:ARG:NH2	2:Z:306:ASP:OD1	2.37	0.55
1:J:70:PRO:O	1:J:71:VAL:C	2.48	0.55
1:L:340:ASN:ND2	1:L:364:ARG:O	2.38	0.55
1:L:376:SER:O	1:L:378:GLY:N	2.38	0.55
1:L:298:THR:HG22	1:L:321:PRO:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:90:ARG:HH12	2:Z:111:GLU:HA	1.71	0.55
1:J:757:ALA:H	1:K:561:GLN:NE2	2.05	0.55
1:L:330:ARG:HH12	1:L:705:ILE:HD13	1.72	0.55
1:L:365:ASN:H	1:L:651:ASN:ND2	2.04	0.55
1:K:241:THR:OG1	1:K:246:GLY:O	2.21	0.55
1:K:276:ASN:HA	1:K:279:ASN:CG	2.31	0.55
1:L:421:ILE:HD11	1:L:458:PHE:CB	2.34	0.55
1:J:892:LEU:HA	1:J:895:ALA:HB3	1.89	0.55
1:K:67:ARG:HB2	1:K:616:TYR:HE1	1.70	0.55
1:K:328:ALA:HB2	1:K:547:SER:HA	1.89	0.55
1:L:531:ASN:HD22	1:L:910:MET:HE3	1.70	0.55
1:L:697:PRO:O	1:L:698:TYR:C	2.49	0.55
1:J:409:GLU:OE1	1:J:409:GLU:N	2.35	0.55
1:J:807:ASP:OD2	1:J:809:THR:OG1	2.23	0.55
1:K:268:SER:OG	1:K:282:PRO:HA	2.07	0.55
2:Z:43:LYS:O	2:Z:47:CYS:N	2.39	0.55
1:K:878:ASN:HD22	1:K:880:MET:HG3	1.71	0.55
1:L:369:SER:O	1:L:370:TYR:C	2.47	0.55
1:L:683:LEU:HD21	1:L:712:PHE:HE1	1.72	0.55
1:J:822:GLN:HA	1:J:845:ASN:HD21	1.72	0.55
1:L:428:LYS:HD2	1:L:446:PHE:HD2	1.72	0.55
2:Z:51:ARG:HA	2:Z:57:LEU:HD13	1.89	0.55
1:J:365:ASN:H	1:J:651:ASN:HD21	1.54	0.54
1:J:432:LYS:HE2	1:J:438:GLY:HA3	1.89	0.54
1:K:178:ASN:OD1	1:K:179:ILE:N	2.40	0.54
1:K:179:ILE:HD13	1:K:285:VAL:HG23	1.88	0.54
1:J:47:ASN:OD1	1:J:47:ASN:N	2.40	0.54
1:J:338:TYR:OH	1:J:694:GLY:O	2.26	0.54
1:L:685:THR:HG22	1:L:686:LYS:N	2.22	0.54
2:Z:80:THR:HB	2:Z:136:GLN:HB3	1.88	0.54
1:K:90:ASP:OD1	1:K:90:ASP:N	2.40	0.54
1:L:408:ASP:OD1	1:L:408:ASP:N	2.38	0.54
1:J:208:GLU:O	1:K:456:ASN:ND2	2.41	0.54
1:L:706:PRO:C	1:L:708:LEU:N	2.65	0.54
2:Z:13:LEU:O	2:Z:17:CYS:HB2	2.06	0.54
2:Z:497:THR:HG21	2:Z:549:GLU:HG3	1.89	0.54
2:Z:545:VAL:HA	2:Z:560:TYR:HD1	1.72	0.54
1:J:676:ARG:NH1	1:J:922:VAL:O	2.40	0.54
1:K:420:VAL:HG21	1:K:453:ARG:HG2	1.89	0.54
1:K:544:ARG:HG3	1:K:548:MET:HE3	1.90	0.54
1:K:665:ILE:HG13	1:K:903:MET:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:719:LYS:HB3	1:K:906:GLU:HG2	1.88	0.54
1:L:599:ASN:OD1	1:L:599:ASN:N	2.39	0.54
1:L:707:TYR:HE1	1:L:917:TYR:HE2	1.56	0.54
1:J:484:LYS:C	1:J:485:LEU:HD23	2.33	0.54
1:J:744:GLU:O	1:J:762:THR:OG1	2.21	0.54
1:L:365:ASN:H	1:L:651:ASN:HD21	1.56	0.54
1:J:414:CYS:O	1:J:415:PHE:CG	2.61	0.54
1:J:474:TYR:O	1:J:475:SER:O	2.25	0.54
1:L:276:ASN:C	1:L:278:ASP:N	2.66	0.54
2:Z:15:ARG:HH21	2:Z:16:CGU:CD2	2.20	0.54
2:Z:141:PRO:HA	2:Z:148:VAL:HA	1.90	0.54
1:J:69:ILE:O	1:J:71:VAL:N	2.40	0.54
1:J:111:PRO:HD3	1:J:604:ASP:O	2.07	0.54
1:J:887:ASP:OD1	1:J:888:LEU:N	2.41	0.54
1:L:515:ASP:OD1	1:L:516:CYS:N	2.35	0.54
2:Z:94:PRO:HG3	2:Z:129:THR:C	2.33	0.54
2:Z:529:PHE:N	2:Z:543:GLY:O	2.38	0.54
1:J:220:ALA:HA	1:J:285:VAL:O	2.08	0.54
1:J:311:SER:OG	1:J:312:ARG:N	2.41	0.54
1:K:360:ASP:HA	1:K:364:ARG:HH22	1.73	0.54
1:K:448:ASP:N	1:K:448:ASP:OD1	2.40	0.54
1:L:710:GLY:O	1:L:711:THR:C	2.47	0.54
1:L:775:ASN:HD21	1:L:881:SER:HB3	1.72	0.54
2:Z:138:CYS:O	2:Z:149:THR:OG1	2.26	0.54
1:J:103:ILE:HG12	1:J:613:ILE:HG23	1.90	0.54
1:L:94:LEU:HD13	1:L:619:PHE:HE1	1.72	0.54
1:L:318:GLN:OE1	1:L:836:MET:HB2	2.08	0.54
1:L:367:GLU:HB2	1:L:708:LEU:CD2	2.38	0.54
2:Z:89:TRP:CZ2	2:Z:126:CYS:HA	2.43	0.54
1:J:273:THR:OG1	1:J:274:ALA:N	2.41	0.53
2:Z:43:LYS:HE2	2:Z:61:LEU:O	2.08	0.53
1:J:564:GLN:OE1	1:J:565:LYS:N	2.41	0.53
1:K:599:ASN:OD1	1:K:599:ASN:N	2.36	0.53
1:J:94:LEU:HD22	1:J:619:PHE:HE1	1.73	0.53
1:K:333:PHE:HB3	1:K:336:LEU:HD12	1.89	0.53
1:J:828:PHE:HD1	1:L:415:PHE:CE1	2.25	0.53
1:K:133:CYS:SG	1:K:315:MET:SD	3.03	0.53
1:K:134:GLU:HG2	1:K:168:VAL:HG13	1.91	0.53
2:Z:253:GLU:OE2	2:Z:490:ARG:NH1	2.41	0.53
1:J:496:ASP:OD1	1:J:496:ASP:N	2.40	0.53
1:K:91:ASN:OD1	1:K:91:ASN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:774:TYR:OH	1:K:789:ASP:OD1	2.26	0.53
1:K:838:GLU:OE1	1:L:207:GLY:N	2.41	0.53
1:K:764:ASP:N	1:K:764:ASP:OD1	2.42	0.53
1:K:841:ALA:O	1:K:842:TYR:HB2	2.08	0.53
1:L:369:SER:OG	1:L:370:TYR:N	2.37	0.53
2:Z:16:CGU:HA	2:Z:20:CGU:HB3	1.91	0.53
1:J:109:ARG:NE	1:J:327:ILE:HG22	2.21	0.53
1:J:269:THR:HB	1:J:272:ALA:CB	2.38	0.53
1:L:365:ASN:N	1:L:651:ASN:HD21	2.07	0.53
1:K:715:ASN:ND2	1:K:869:THR:O	2.28	0.53
1:K:68:PHE:HB2	1:K:615:LEU:HB3	1.91	0.53
1:K:734:ASN:OD1	1:K:734:ASN:N	2.40	0.53
1:K:744:GLU:O	1:K:762:THR:OG1	2.27	0.53
1:L:705:ILE:HG22	1:L:708:LEU:HB2	1.91	0.53
1:J:127:LYS:HE3	1:J:234:TYR:CZ	2.43	0.52
1:J:267:PHE:O	1:J:283:LYS:N	2.41	0.52
1:J:723:ILE:HG22	1:J:903:MET:HG2	1.90	0.52
1:L:421:ILE:O	1:L:422:ASN:C	2.51	0.52
1:L:818:GLY:O	1:L:822:GLN:NE2	2.39	0.52
1:L:432:LYS:HG2	1:L:438:GLY:HA2	1.92	0.52
1:L:695:TYR:C	1:L:695:TYR:CD2	2.87	0.52
1:J:414:CYS:SG	1:K:460:MET:HE2	2.50	0.52
1:K:208:GLU:OE2	1:K:210:GLN:NE2	2.43	0.52
1:L:769:GLN:HE22	1:L:872:ARG:H	1.57	0.52
1:J:55:ASP:N	1:J:55:ASP:OD1	2.43	0.52
2:Z:336:VAL:HG22	2:Z:383:ILE:HG23	1.90	0.52
1:J:559:HIS:O	1:J:559:HIS:ND1	2.41	0.52
2:Z:125:TRP:CE3	2:Z:135:ARG:HB3	2.44	0.52
1:J:538:HIS:O	1:J:538:HIS:CD2	2.63	0.52
1:K:135:TRP:NE1	1:K:137:GLU:OE2	2.38	0.52
1:K:276:ASN:HA	1:K:279:ASN:HD22	1.75	0.52
1:L:611:ASP:OD1	1:L:611:ASP:N	2.43	0.52
1:J:179:ILE:HG13	1:J:218:HIS:CD2	2.44	0.52
1:K:536:ASN:OD1	1:K:701:TYR:OH	2.28	0.52
1:K:680:PHE:CE1	1:K:871:TRP:HB2	2.45	0.52
2:Z:17:CYS:O	2:Z:44:TYR:OH	2.28	0.52
2:Z:417:ASP:OD2	2:Z:418:ARG:NH1	2.41	0.52
2:Z:554:ASP:N	2:Z:554:ASP:OD1	2.43	0.52
1:J:273:THR:O	1:J:275:GLY:N	2.43	0.52
1:K:303:MET:O	1:K:304:PRO:C	2.53	0.52
1:K:928:VAL:HG22	1:K:938:THR:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:362:ALA:N	2:Z:419:ASP:OD1	2.42	0.52
1:J:412:ASN:ND2	1:J:464:LEU:HD12	2.25	0.52
1:L:707:TYR:CE1	1:L:917:TYR:HE2	2.28	0.52
2:Z:66:ALA:N	2:Z:141:PRO:O	2.36	0.52
2:Z:184:VAL:HA	2:Z:190:PRO:HA	1.92	0.52
1:K:311:SER:HG	1:K:313:GLU:HB2	1.74	0.51
1:L:279:ASN:C	1:L:281:THR:N	2.68	0.51
2:Z:114:CYS:SG	2:Z:126:CYS:HB3	2.50	0.51
1:L:705:ILE:H	1:L:705:ILE:CD1	2.22	0.51
1:K:467:ASN:O	1:K:471:ASN:ND2	2.33	0.51
1:K:515:ASP:HB3	1:K:517:TYR:CE2	2.45	0.51
1:J:922:VAL:HB	1:J:943:THR:O	2.10	0.51
1:K:366:THR:O	1:K:369:SER:OG	2.25	0.51
1:J:57:THR:HG21	1:L:877:SER:HB2	1.91	0.51
1:K:575:LEU:HG	1:K:930:ARG:HE	1.74	0.51
1:L:823:HIS:O	1:L:823:HIS:ND1	2.42	0.51
2:Z:81:ARG:N	2:Z:137:GLU:O	2.43	0.51
1:J:37:THR:OG1	1:J:38:TYR:N	2.43	0.51
1:K:276:ASN:N	1:K:279:ASN:HB3	2.25	0.51
1:L:271:GLU:C	1:L:273:THR:N	2.68	0.51
1:K:669:SER:HA	1:K:899:HIS:O	2.11	0.51
1:J:535:PHE:O	1:J:540:ASN:ND2	2.44	0.51
1:L:75:ASP:OD1	1:L:76:THR:N	2.44	0.51
1:L:675:PHE:HB3	1:L:875:PHE:HD2	1.76	0.51
2:Z:16:CGU:C	2:Z:22:CYS:HB3	2.41	0.51
1:K:19:ASP:N	1:K:19:ASP:OD1	2.44	0.51
1:L:330:ARG:NH1	1:L:705:ILE:HD13	2.25	0.51
1:J:328:ALA:HB2	1:J:547:SER:HA	1.92	0.50
1:J:514:VAL:HG13	1:J:518:ILE:HD13	1.92	0.50
1:J:791:MET:SD	1:J:868:ARG:NH2	2.84	0.50
1:K:476:ASN:OD1	1:K:539:ARG:NH2	2.37	0.50
1:K:520:LEU:HD13	1:L:116:TYR:CD2	2.46	0.50
1:L:253:GLN:OE1	1:L:255:ASN:N	2.44	0.50
1:L:361:LEU:H	1:L:364:ARG:HH12	1.59	0.50
2:Z:335:GLN:HG2	2:Z:461:TRP:HZ3	1.76	0.50
1:J:236:SER:HB2	1:L:843:PRO:HB3	1.92	0.50
1:K:191:GLN:N	1:K:191:GLN:OE1	2.44	0.50
1:K:361:LEU:H	1:K:364:ARG:NH2	2.10	0.50
1:L:313:GLU:OE1	1:L:313:GLU:N	2.39	0.50
1:L:330:ARG:HH12	1:L:705:ILE:CD1	2.24	0.50
1:J:333:PHE:HD2	1:J:336:LEU:HD12	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:681:THR:HG22	1:J:682:ARG:H	1.76	0.50
1:K:361:LEU:HG	1:K:364:ARG:HH21	1.77	0.50
1:K:413:TYR:CD2	1:L:837:ARG:HG2	2.46	0.50
2:Z:95:HIS:HB3	2:Z:134:ARG:NH1	2.25	0.50
2:Z:545:VAL:HA	2:Z:560:TYR:CD1	2.45	0.50
1:J:113:PHE:O	1:J:113:PHE:CG	2.62	0.50
1:J:677:GLY:O	1:J:921:GLU:HG3	2.11	0.50
1:K:843:PRO:HD3	1:L:131:ASN:OD1	2.11	0.50
1:L:384:PHE:CZ	1:L:386:MET:HB3	2.46	0.50
2:Z:63:GLY:C	2:Z:74:ARG:H	2.15	0.50
1:J:109:ARG:HG2	1:J:327:ILE:CG2	2.41	0.50
1:J:669:SER:HA	1:J:899:HIS:O	2.11	0.50
1:J:797:ASN:HD21	1:J:868:ARG:HD3	1.77	0.50
1:K:58:THR:OG1	1:K:59:ASP:N	2.44	0.50
1:L:376:SER:C	1:L:378:GLY:H	2.19	0.50
2:Z:99:ILE:HG21	2:Z:118:ASP:HB3	1.93	0.50
1:K:653:LEU:HD21	1:K:917:TYR:HD1	1.77	0.50
1:L:413:TYR:HB2	1:L:415:PHE:CZ	2.45	0.50
2:Z:95:HIS:CG	2:Z:369:PRO:HB3	2.47	0.50
2:Z:97:PRO:HB3	2:Z:127:TYR:CE2	2.47	0.50
2:Z:573:VAL:HA	2:Z:576:GLN:HE21	1.77	0.50
1:L:179:ILE:HG13	1:L:218:HIS:CD2	2.41	0.50
1:L:270:THR:O	1:L:271:GLU:C	2.53	0.50
1:L:645:ASP:OD1	1:L:647:LEU:N	2.45	0.50
2:Z:485:LEU:HD13	2:Z:509:GLY:HA2	1.93	0.50
1:J:475:SER:O	1:J:476:ASN:C	2.54	0.50
1:J:540:ASN:O	1:J:541:ALA:C	2.54	0.50
2:Z:6:CGU:OE22	2:Z:15:ARG:NH1	2.45	0.50
1:J:671:ASN:OD1	1:J:672:TRP:N	2.45	0.49
1:K:210:GLN:CD	1:K:210:GLN:H	2.20	0.49
1:L:91:ASN:N	1:L:91:ASN:OD1	2.42	0.49
1:L:501:TYR:O	1:L:505:ASN:N	2.42	0.49
1:J:380:ARG:HH12	1:J:389:GLN:HG2	1.76	0.49
1:J:475:SER:O	1:J:479:LEU:HG	2.13	0.49
1:J:491:ASN:O	1:J:491:ASN:ND2	2.45	0.49
1:L:501:TYR:O	1:L:502:ASP:C	2.53	0.49
2:Z:309:GLU:OE2	2:Z:532:LYS:NZ	2.30	0.49
1:J:91:ASN:OD1	1:J:91:ASN:N	2.43	0.49
1:L:670:ARG:NH2	1:L:945:PHE:HA	2.28	0.49
1:L:705:ILE:HG21	1:L:708:LEU:HB2	1.94	0.49
1:J:482:PRO:CD	1:J:528:TYR:HB3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:635:ARG:HH12	1:J:932:HIS:C	2.20	0.49
2:Z:124:PRO:HD2	2:Z:149:THR:HG21	1.94	0.49
1:K:491:ASN:OD1	1:K:491:ASN:N	2.44	0.49
1:K:524:TRP:CE3	1:K:803:ARG:HB3	2.47	0.49
2:Z:238:GLY:HA3	2:Z:576:GLN:HG2	1.93	0.49
1:J:80:TYR:CE1	1:J:585:PHE:HB2	2.47	0.49
1:J:119:THR:OG1	1:J:120:ALA:N	2.44	0.49
1:J:837:ARG:O	1:J:837:ARG:NH1	2.44	0.49
1:K:645:ASP:OD1	1:K:648:SER:N	2.43	0.49
1:L:380:ARG:HG3	1:L:391:VAL:HB	1.95	0.49
2:Z:110:GLN:HG2	2:Z:115:ARG:NH2	2.28	0.49
1:J:640:ASP:OD2	1:J:927:ARG:NE	2.37	0.49
1:L:531:ASN:HA	1:L:714:LEU:HD21	1.95	0.49
2:Z:15:ARG:HE	2:Z:16:CGU:HG	1.78	0.49
2:Z:82:SER:O	2:Z:155:ARG:N	2.46	0.49
2:Z:299:PHE:O	2:Z:304:LEU:N	2.43	0.49
2:Z:338:LEU:HD21	2:Z:379:LEU:HD13	1.95	0.49
2:Z:414:GLU:OE2	2:Z:415:ASN:ND2	2.45	0.49
1:J:790:ARG:N	1:J:793:SER:OG	2.46	0.49
1:L:305:THR:HG22	1:L:307:LYS:H	1.78	0.49
1:L:615:LEU:HD12	1:L:616:TYR:H	1.78	0.49
2:Z:27:ALA:HA	2:Z:30:ALA:HB3	1.95	0.49
1:J:651:ASN:OD1	1:J:651:ASN:N	2.45	0.49
1:J:869:THR:OG1	1:J:870:LEU:N	2.45	0.49
2:Z:13:LEU:HB2	2:Z:30:ALA:O	2.13	0.49
2:Z:338:LEU:HD11	2:Z:379:LEU:HB3	1.95	0.49
2:Z:341:LYS:HG3	2:Z:377:ASN:O	2.13	0.49
1:J:804:GLN:OE1	1:K:552:ASN:N	2.38	0.49
1:K:804:GLN:OE1	1:L:553:GLY:N	2.38	0.49
1:L:707:TYR:CE1	1:L:917:TYR:CE2	3.01	0.49
1:L:197:ASP:N	1:L:201:GLN:OE1	2.32	0.48
1:L:279:ASN:O	1:L:280:LEU:C	2.54	0.48
1:L:362:GLN:HG3	1:L:362:GLN:O	2.13	0.48
2:Z:73:TYR:OH	2:Z:77:VAL:N	2.46	0.48
1:J:252:LYS:HA	1:J:257:LYS:HA	1.94	0.48
1:K:209:SER:OG	1:K:210:GLN:OE1	2.31	0.48
1:K:322:ASN:CG	1:K:505:ASN:HD21	2.21	0.48
1:K:853:LYS:HG3	1:K:854:THR:HG23	1.95	0.48
1:L:62:GLN:HE22	1:L:92:ARG:HG2	1.78	0.48
1:L:76:THR:HG22	1:L:77:ALA:H	1.78	0.48
1:L:109:ARG:NH2	1:L:550:LEU:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:320:MET:HG3	1:L:321:PRO:HD2	1.95	0.48
1:K:305:THR:HB	1:K:306:ILE:H	1.46	0.48
1:K:679:ALA:HB1	1:K:870:LEU:HD12	1.95	0.48
1:L:60:ARG:HD2	1:L:624:HIS:CE1	2.48	0.48
1:L:361:LEU:H	1:L:364:ARG:NH1	2.11	0.48
1:L:774:TYR:HB2	1:L:776:ILE:HG13	1.94	0.48
1:J:134:GLU:O	1:J:135:TRP:HB3	2.11	0.48
1:L:497:ASN:O	1:L:497:ASN:CG	2.54	0.48
1:J:58:THR:OG1	1:J:59:ASP:N	2.45	0.48
1:J:112:THR:O	1:J:325:ASN:ND2	2.46	0.48
1:J:130:PRO:HB2	1:J:315:MET:SD	2.54	0.48
1:K:276:ASN:C	1:K:279:ASN:H	2.21	0.48
1:K:311:SER:C	1:K:313:GLU:N	2.67	0.48
1:K:356:ASN:CG	1:K:358:VAL:H	2.21	0.48
1:J:270:THR:C	1:J:272:ALA:N	2.69	0.48
1:J:484:LYS:HB3	1:J:484:LYS:HE2	1.44	0.48
1:J:639:ASN:HD21	1:K:25:SER:HB3	1.79	0.48
1:K:166:THR:HB	1:L:446:PHE:CD1	2.48	0.48
1:K:252:LYS:HA	1:K:258:LEU:HA	1.94	0.48
1:K:470:ARG:NH1	1:K:829:VAL:HG21	2.28	0.48
1:K:804:GLN:CD	1:L:553:GLY:H	2.21	0.48
1:L:868:ARG:O	1:L:869:THR:HB	2.14	0.48
2:Z:186:THR:HG21	2:Z:409:ARG:HD3	1.96	0.48
1:J:90:ASP:OD1	1:J:933:ARG:NH1	2.47	0.48
1:L:373:LEU:HD11	1:L:377:ILE:HD13	1.96	0.48
2:Z:53:PRO:HD2	2:Z:56:LYS:HD2	1.96	0.48
1:J:134:GLU:C	1:J:135:TRP:HE3	2.22	0.48
1:J:360:ASP:OD1	1:J:361:LEU:N	2.45	0.48
1:J:731:TRP:CG	1:J:732:PRO:HA	2.49	0.48
1:L:501:TYR:CD1	1:L:505:ASN:HB2	2.49	0.48
1:J:474:TYR:CE2	1:J:479:LEU:HD21	2.49	0.48
1:J:554:ARG:HD3	1:J:555:TYR:CE1	2.48	0.48
1:L:20:ALA:HA	1:L:23:TYR:CE2	2.49	0.48
1:L:137:GLU:OE1	1:L:167:HIS:NE2	2.47	0.48
1:L:421:ILE:O	1:L:423:THR:N	2.47	0.48
1:L:681:THR:HG22	1:L:682:ARG:H	1.78	0.48
2:Z:212:VAL:HG21	2:Z:222:PRO:HA	1.96	0.48
2:Z:227:GLU:OE2	2:Z:407:HIS:NE2	2.47	0.48
1:K:270:THR:C	1:K:272:ALA:N	2.68	0.47
1:K:302:TYR:O	1:K:304:PRO:HD3	2.14	0.47
1:L:217:ASN:HB2	1:L:218:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:497:ASN:ND2	1:L:499:ASN:HD22	2.12	0.47
1:J:613:ILE:O	1:J:614:CYS:SG	2.71	0.47
1:K:415:PHE:CE2	1:L:828:PHE:HD2	2.31	0.47
1:L:232:PRO:HD3	1:L:317:GLN:NE2	2.28	0.47
1:L:276:ASN:O	1:L:278:ASP:N	2.47	0.47
1:L:653:LEU:HD21	1:L:917:TYR:HD2	1.79	0.47
1:L:790:ARG:N	1:L:793:SER:OG	2.47	0.47
2:Z:87:GLN:NE2	2:Z:95:HIS:O	2.39	0.47
2:Z:95:HIS:ND1	2:Z:134:ARG:HD2	2.29	0.47
2:Z:186:THR:HG22	2:Z:244:ASP:H	1.79	0.47
2:Z:337:MET:HB2	2:Z:385:LYS:HD3	1.96	0.47
2:Z:418:ARG:NH1	2:Z:504:ASN:HB2	2.29	0.47
1:J:114:LYS:O	1:J:325:ASN:N	2.34	0.47
1:J:588:ASP:OD2	1:J:602:ARG:NH2	2.30	0.47
1:J:833:ALA:HB1	1:J:835:THR:HG23	1.96	0.47
2:Z:461:TRP:CH2	2:Z:480:LEU:HD13	2.50	0.47
1:J:356:ASN:OD1	1:J:357:ALA:N	2.48	0.47
1:K:520:LEU:HD13	1:L:116:TYR:CG	2.49	0.47
1:L:299:HIS:HE1	1:L:320:MET:HG2	1.78	0.47
2:Z:128:THR:OG1	2:Z:133:VAL:HB	2.14	0.47
1:J:472:PHE:HE1	1:J:476:ASN:ND2	2.13	0.47
1:J:804:GLN:OE1	1:K:553:GLY:N	2.47	0.47
1:L:656:ILE:HD11	1:L:916:LEU:HB2	1.95	0.47
1:L:718:PHE:CD1	1:L:907:VAL:HG12	2.49	0.47
2:Z:13:LEU:HD22	2:Z:31:LEU:HD21	1.96	0.47
2:Z:35:THR:O	2:Z:39:VAL:HG23	2.14	0.47
1:J:270:THR:O	1:J:272:ALA:N	2.48	0.47
1:J:535:PHE:C	1:J:537:HIS:H	2.22	0.47
1:J:734:ASN:OD1	1:K:61:SER:OG	2.28	0.47
1:J:735:ASP:N	1:J:735:ASP:OD1	2.47	0.47
1:J:826:SER:OG	1:J:840:GLN:O	2.26	0.47
1:J:857:ASP:N	1:J:857:ASP:OD1	2.46	0.47
1:K:222:ARG:NE	1:K:289:GLU:OE2	2.34	0.47
1:K:636:ASN:OD1	1:K:636:ASN:N	2.48	0.47
1:L:62:GLN:CD	1:L:92:ARG:HE	2.22	0.47
1:L:137:GLU:O	1:L:164:GLN:HA	2.15	0.47
1:L:280:LEU:O	1:L:281:THR:C	2.55	0.47
1:L:685:THR:C	1:L:687:GLU:N	2.73	0.47
1:J:561:GLN:HE22	1:L:757:ALA:H	1.62	0.47
1:L:502:ASP:OD1	1:L:506:LYS:HE3	2.14	0.47
2:Z:90:ARG:NH1	2:Z:111:GLU:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:457:ARG:HB3	2:Z:530:VAL:HG22	1.95	0.47
1:L:684:LYS:HA	1:L:914:THR:HG22	1.97	0.47
1:L:704:SER:O	1:L:706:PRO:N	2.48	0.47
1:L:785:GLU:OE1	1:L:785:GLU:N	2.44	0.47
1:L:876:SER:OG	1:L:879:PHE:N	2.46	0.47
1:L:368:LEU:HD12	1:L:368:LEU:O	2.15	0.47
1:L:818:GLY:C	1:L:822:GLN:HE21	2.22	0.47
1:J:897:SER:HG	1:J:898:ALA:N	2.11	0.46
1:K:645:ASP:O	1:K:648:SER:OG	2.33	0.46
1:L:697:PRO:HG2	1:L:698:TYR:HD1	1.79	0.46
2:Z:504:ASN:O	2:Z:562:HIS:N	2.31	0.46
2:Z:573:VAL:O	2:Z:576:GLN:HB2	2.15	0.46
1:J:121:TYR:CE2	1:J:296:PRO:HG3	2.47	0.46
1:J:838:GLU:OE1	1:K:207:GLY:N	2.49	0.46
1:K:353:SER:HB2	1:K:355:LEU:HD12	1.97	0.46
1:K:356:ASN:OD1	1:K:357:ALA:N	2.49	0.46
1:L:194:LYS:HE3	1:L:194:LYS:HB3	1.78	0.46
1:L:375:ASP:CG	1:L:376:SER:N	2.70	0.46
1:L:566:PHE:HD1	1:L:568:ALA:H	1.61	0.46
1:L:922:VAL:HB	1:L:943:THR:O	2.16	0.46
2:Z:505:MET:HG2	2:Z:561:THR:HA	1.95	0.46
1:J:715:ASN:ND2	1:J:869:THR:O	2.48	0.46
1:L:328:ALA:HB2	1:L:547:SER:HA	1.98	0.46
1:L:428:LYS:HD2	1:L:446:PHE:CD2	2.51	0.46
2:Z:333:PRO:HB2	2:Z:436:HIS:N	2.31	0.46
2:Z:465:LYS:HE2	2:Z:517:ARG:HH21	1.80	0.46
1:J:473:LEU:HD13	1:J:518:ILE:HD11	1.97	0.46
1:J:490:SER:O	1:J:492:VAL:HG23	2.15	0.46
2:Z:41:TRP:O	2:Z:45:THR:OG1	2.27	0.46
1:J:478:ALA:C	1:J:480:TYR:N	2.70	0.46
1:J:758:GLN:HE21	1:K:560:ILE:HG22	1.81	0.46
1:J:774:TYR:CE2	1:J:784:PRO:HG3	2.50	0.46
1:K:399:ARG:HE	1:K:865:LEU:HD21	1.80	0.46
1:L:346:GLY:HA3	1:L:583:TRP:CE3	2.50	0.46
2:Z:74:ARG:HA	2:Z:115:ARG:HH12	1.81	0.46
1:J:64:LEU:HD13	1:J:621:PRO:HD3	1.97	0.46
1:K:857:ASP:OD1	1:K:857:ASP:N	2.46	0.46
1:L:370:TYR:CD1	1:L:565:LYS:HG2	2.50	0.46
1:L:421:ILE:CD1	1:L:422:ASN:H	2.29	0.46
1:L:842:TYR:HD1	1:L:843:PRO:CD	2.29	0.46
1:K:348:LEU:HD23	1:K:569:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:701:TYR:CD2	1:L:702:SER:N	2.83	0.46
1:L:717:THR:HB	1:L:908:ASP:CG	2.41	0.46
2:Z:544:ILE:HG13	2:Z:563:VAL:HG11	1.98	0.46
1:J:116:TYR:O	1:J:116:TYR:CD1	2.69	0.46
1:J:128:GLY:O	1:J:129:ALA:C	2.54	0.46
1:J:791:MET:HE3	1:J:791:MET:HB2	1.86	0.46
1:K:67:ARG:HB2	1:K:616:TYR:CE1	2.50	0.46
1:K:558:PHE:HD1	1:K:558:PHE:H	1.64	0.46
1:L:98:SER:O	1:L:98:SER:OG	2.29	0.46
1:L:575:LEU:O	1:L:579:TYR:OH	2.30	0.46
1:L:595:SER:HB3	1:L:702:SER:OG	2.16	0.46
2:Z:60:CYS:HB2	2:Z:67:GLU:HG2	1.97	0.46
1:J:247:GLN:H	1:J:247:GLN:HG2	1.51	0.46
1:K:842:TYR:O	1:K:843:PRO:C	2.59	0.46
1:L:277:GLY:C	1:L:279:ASN:N	2.71	0.46
1:L:494:ILE:HD11	1:L:502:ASP:O	2.16	0.46
1:L:755:ASN:N	1:L:755:ASN:OD1	2.47	0.46
2:Z:404:ILE:HG12	2:Z:423:MET:HG2	1.97	0.46
1:K:302:TYR:CD1	1:K:302:TYR:C	2.92	0.46
1:L:676:ARG:HB2	1:L:921:GLU:HB2	1.98	0.46
1:L:705:ILE:HD12	1:L:705:ILE:N	2.26	0.46
1:L:869:THR:C	1:L:870:LEU:HD23	2.40	0.46
1:J:702:SER:O	1:J:702:SER:OG	2.28	0.45
1:L:707:TYR:O	1:L:707:TYR:CD2	2.69	0.45
1:L:713:TYR:CD1	1:L:713:TYR:O	2.69	0.45
1:L:718:PHE:HD1	1:L:907:VAL:HG12	1.80	0.45
2:Z:63:GLY:HA3	2:Z:74:ARG:HG2	1.98	0.45
1:J:279:ASN:N	1:J:279:ASN:OD1	2.48	0.45
1:K:681:THR:HG21	1:K:712:PHE:CD2	2.52	0.45
1:L:78:TYR:HA	1:L:587:LYS:HB2	1.98	0.45
1:L:119:THR:OG1	1:L:120:ALA:N	2.50	0.45
2:Z:62:GLU:OE2	2:Z:64:ASN:ND2	2.48	0.45
1:J:538:HIS:CD2	1:J:538:HIS:C	2.94	0.45
1:K:588:ASP:OD1	1:K:602:ARG:NH2	2.39	0.45
1:K:602:ARG:HH12	1:K:697:PRO:HA	1.82	0.45
1:L:833:ALA:HB1	1:L:835:THR:HG23	1.97	0.45
2:Z:87:GLN:HB2	2:Z:94:PRO:HD2	1.98	0.45
1:J:441:LYS:HD3	1:L:273:THR:HG21	1.98	0.45
1:J:927:ARG:NH1	1:K:14:HIS:HE1	2.15	0.45
1:L:370:TYR:CG	1:L:565:LYS:HD2	2.52	0.45
2:Z:70:GLY:HA3	2:Z:124:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:72:ASN:HA	2:Z:74:ARG:NH2	2.31	0.45
2:Z:92:ARG:O	2:Z:370:TRP:NE1	2.49	0.45
2:Z:115:ARG:N	2:Z:125:TRP:O	2.47	0.45
2:Z:353:ILE:HD13	2:Z:359:LEU:HB2	1.97	0.45
1:K:360:ASP:OD1	1:K:364:ARG:NH1	2.50	0.45
1:L:432:LYS:N	1:L:438:GLY:O	2.49	0.45
2:Z:142:VAL:N	2:Z:147:GLN:O	2.32	0.45
1:K:412:ASN:OD1	1:K:412:ASN:N	2.50	0.45
1:L:524:TRP:NE1	1:L:525:SER:O	2.50	0.45
2:Z:415:ASN:OD1	2:Z:415:ASN:N	2.50	0.45
1:J:100:TYR:CE1	1:J:616:TYR:HB2	2.52	0.45
1:J:133:CYS:SG	1:J:135:TRP:CE3	3.10	0.45
1:J:178:ASN:OD1	1:J:179:ILE:N	2.49	0.45
1:J:745:ILE:O	1:J:762:THR:OG1	2.35	0.45
1:K:14:HIS:CD2	1:K:23:TYR:CZ	3.04	0.45
1:L:232:PRO:HG3	1:L:317:GLN:HG3	1.99	0.45
1:L:377:ILE:O	1:L:377:ILE:HG13	2.15	0.45
1:J:193:PRO:HB2	1:J:195:TYR:CE1	2.52	0.45
2:Z:74:ARG:HD3	2:Z:115:ARG:NH2	2.32	0.45
2:Z:407:HIS:CE1	2:Z:409:ARG:HB2	2.51	0.45
2:Z:549:GLU:HB2	2:Z:559:PHE:HE1	1.82	0.45
2:Z:295:LEU:HB3	2:Z:301:LYS:HE2	1.99	0.45
1:J:338:TYR:CE2	1:J:586:ARG:HG2	2.52	0.45
1:K:327:ILE:HA	1:K:594:GLN:O	2.17	0.45
1:K:625:ASN:OD1	1:K:626:THR:N	2.50	0.45
1:L:268:SER:OG	1:L:282:PRO:HA	2.17	0.45
1:L:277:GLY:O	1:L:279:ASN:N	2.50	0.45
1:J:109:ARG:HG2	1:J:327:ILE:HG21	1.98	0.44
1:J:404:HIS:HE1	1:K:544:ARG:HD3	1.82	0.44
1:K:411:PRO:HB2	1:K:413:TYR:HE1	1.81	0.44
1:L:695:TYR:CG	1:L:696:ASP:N	2.83	0.44
2:Z:327:ALA:HB1	2:Z:331:MET:SD	2.57	0.44
1:J:62:GLN:OE1	1:J:92:ARG:NE	2.48	0.44
1:J:410:LEU:HD13	1:K:470:ARG:NH2	2.32	0.44
1:J:550:LEU:HD23	1:J:550:LEU:HA	1.78	0.44
1:J:942:ARG:HH21	1:J:945:PHE:HB3	1.82	0.44
1:K:303:MET:O	1:K:305:THR:N	2.50	0.44
1:L:323:ARG:CZ	1:L:479:LEU:HD22	2.47	0.44
1:L:713:TYR:O	1:L:714:LEU:HD23	2.16	0.44
2:Z:80:THR:HA	2:Z:138:CYS:HA	1.99	0.44
1:J:375:ASP:OD1	1:J:790:ARG:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:544:ARG:HD3	1:L:404:HIS:NE2	2.32	0.44
1:K:399:ARG:HH21	1:K:865:LEU:HD11	1.80	0.44
1:K:399:ARG:CZ	1:K:534:PRO:HG3	2.47	0.44
1:K:823:HIS:CE1	1:K:844:ALA:HA	2.52	0.44
1:L:670:ARG:NH2	1:L:944:PRO:O	2.40	0.44
1:J:414:CYS:SG	1:J:460:MET:HB2	2.58	0.44
1:J:744:GLU:CD	1:J:747:ARG:HE	2.26	0.44
1:K:701:TYR:CZ	1:K:703:GLY:HA3	2.53	0.44
1:K:931:PRO:HB2	1:K:932:HIS:HD1	1.82	0.44
1:L:392:ASP:N	1:L:392:ASP:OD1	2.50	0.44
1:L:492:VAL:HG12	1:L:493:LYS:N	2.20	0.44
1:L:645:ASP:OD1	1:L:648:SER:N	2.50	0.44
1:J:460:MET:HG3	1:K:460:MET:HE1	2.00	0.44
1:J:481:LEU:O	1:J:482:PRO:C	2.55	0.44
1:J:538:HIS:O	1:J:538:HIS:HD2	2.01	0.44
1:L:271:GLU:O	1:L:273:THR:N	2.51	0.44
1:L:370:TYR:CE1	1:L:565:LYS:HG2	2.53	0.44
1:L:536:ASN:ND2	1:L:703:GLY:C	2.73	0.44
1:L:707:TYR:HE1	1:L:917:TYR:CE2	2.34	0.44
1:J:231:LYS:CA	1:J:317:GLN:OE1	2.62	0.44
1:J:432:LYS:HB3	1:J:438:GLY:HA3	2.00	0.44
1:J:448:ASP:OD1	1:J:449:LYS:N	2.51	0.44
1:J:656:ILE:HD11	1:J:916:LEU:HB2	2.00	0.44
1:L:524:TRP:CE2	1:L:803:ARG:HD3	2.53	0.44
1:L:685:THR:H	1:L:914:THR:HA	1.83	0.44
1:J:622:MET:HE1	1:K:39:PHE:HD2	1.83	0.44
1:K:58:THR:HB	1:K:623:ALA:HA	1.99	0.44
1:J:797:ASN:ND2	1:J:867:ASP:O	2.46	0.44
1:J:828:PHE:HD1	1:L:415:PHE:CD1	2.36	0.44
1:J:828:PHE:HD1	1:L:415:PHE:CZ	2.36	0.44
1:K:745:ILE:H	1:K:745:ILE:HG13	1.55	0.44
1:L:535:PHE:CD1	1:L:711:THR:HB	2.53	0.44
1:J:75:ASP:OD1	1:J:76:THR:N	2.50	0.44
1:J:112:THR:O	1:J:112:THR:OG1	2.32	0.44
1:J:138:ALA:HA	1:J:164:GLN:HB3	2.00	0.44
1:J:224:LEU:HD21	1:L:842:TYR:HE1	1.82	0.44
1:K:333:PHE:O	1:K:336:LEU:HB2	2.18	0.44
1:K:408:ASP:N	1:K:408:ASP:OD1	2.50	0.44
1:K:808:ASP:OD1	1:K:809:THR:N	2.51	0.44
1:L:211:TRP:CZ3	1:L:418:GLY:HA3	2.53	0.44
1:L:484:LYS:HB2	1:L:484:LYS:HE3	1.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:675:PHE:HB3	1:L:875:PHE:CD2	2.52	0.44
1:L:783:ILE:H	1:L:783:ILE:HG12	1.56	0.44
1:J:599:ASN:OD1	1:J:599:ASN:N	2.51	0.43
1:K:75:ASP:OD1	1:K:76:THR:N	2.51	0.43
1:L:558:PHE:HD1	1:L:558:PHE:H	1.65	0.43
2:Z:194:TRP:CE3	2:Z:199:ALA:HB1	2.53	0.43
1:J:230:MET:HB2	1:J:310:ASN:OD1	2.18	0.43
1:J:270:THR:O	1:J:271:GLU:C	2.61	0.43
1:J:736:ARG:O	1:K:64:LEU:HB2	2.19	0.43
1:K:739:THR:HG21	1:K:744:GLU:HG3	2.00	0.43
1:K:876:SER:OG	1:K:879:PHE:N	2.51	0.43
1:J:101:PHE:O	1:J:561:GLN:HA	2.18	0.43
1:J:448:ASP:CG	1:J:449:LYS:HG3	2.42	0.43
1:J:469:TRP:NE1	1:J:473:LEU:HG	2.33	0.43
1:J:520:LEU:HD13	1:K:116:TYR:CG	2.53	0.43
1:L:330:ARG:NE	1:L:591:MET:O	2.30	0.43
1:L:437:ASN:O	1:L:439:TRP:N	2.51	0.43
1:L:724:THR:OG1	1:L:902:ASP:HB2	2.18	0.43
1:J:66:LEU:HD23	1:J:66:LEU:HA	1.76	0.43
1:J:70:PRO:HD3	1:J:84:PHE:HE2	1.84	0.43
1:K:550:LEU:HD23	1:K:550:LEU:HA	1.88	0.43
1:K:601:LEU:HD12	1:K:606:ALA:HB2	2.00	0.43
1:L:401:ILE:HG22	1:L:403:ASN:HB2	1.99	0.43
1:L:686:LYS:HB2	1:L:686:LYS:HZ3	1.82	0.43
1:L:880:MET:HE2	1:L:880:MET:HB3	1.81	0.43
2:Z:114:CYS:HB3	2:Z:125:TRP:C	2.43	0.43
1:K:268:SER:HG	1:K:282:PRO:HA	1.83	0.43
1:K:435:GLN:C	1:K:437:ASN:H	2.26	0.43
1:L:367:GLU:HG3	1:L:708:LEU:HD21	2.01	0.43
2:Z:334:TRP:CE3	2:Z:438:VAL:HB	2.53	0.43
2:Z:340:ARG:HA	2:Z:379:LEU:HD23	2.01	0.43
2:Z:493:CYS:O	2:Z:496:SER:OG	2.30	0.43
1:L:96:MET:HG2	1:L:572:LEU:O	2.18	0.43
1:L:867:ASP:O	1:L:868:ARG:HB2	2.19	0.43
2:Z:249:GLU:HA	2:Z:503:ASP:HB3	2.01	0.43
1:J:20:ALA:HA	1:J:23:TYR:CZ	2.53	0.43
2:Z:449:LEU:HD11	2:Z:533:SER:HB2	2.01	0.43
1:J:280:LEU:HD12	1:J:280:LEU:HA	1.81	0.43
1:K:363:ASP:OD1	1:K:363:ASP:N	2.49	0.43
2:Z:194:TRP:O	2:Z:200:LYS:HG3	2.19	0.43
2:Z:382:ARG:CB	2:Z:385:LYS:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:105:GLY:HA2	1:L:611:ASP:OD1	2.18	0.43
1:L:367:GLU:CB	1:L:708:LEU:CD2	2.96	0.43
1:L:545:TYR:HE1	1:L:549:LEU:HD22	1.84	0.43
1:L:697:PRO:C	1:L:699:TYR:N	2.77	0.43
1:L:718:PHE:O	1:L:746:LYS:HE2	2.19	0.43
2:Z:93:TYR:CG	2:Z:94:PRO:HA	2.54	0.43
2:Z:436:HIS:ND1	2:Z:437:PRO:HD2	2.33	0.43
2:Z:485:LEU:HD22	2:Z:509:GLY:HA2	2.00	0.43
1:J:675:PHE:HB3	1:J:875:PHE:CD2	2.53	0.43
1:K:269:THR:HG22	1:K:271:GLU:N	2.27	0.43
1:K:303:MET:HE3	1:K:303:MET:HB3	1.59	0.43
1:K:756:VAL:HG21	1:K:763:LYS:HA	2.00	0.43
1:L:19:ASP:OD1	1:L:19:ASP:N	2.47	0.43
1:L:653:LEU:HD21	1:L:917:TYR:CD2	2.54	0.43
1:L:701:TYR:OH	1:L:703:GLY:CA	2.65	0.43
2:Z:341:LYS:HA	2:Z:380:LEU:HD23	2.00	0.43
1:J:331:ASP:O	1:J:334:ILE:HG13	2.18	0.42
1:K:198:LYS:HD2	1:K:262:VAL:HB	2.01	0.42
1:K:820:LEU:HB2	1:K:821:HIS:CE1	2.53	0.42
1:L:421:ILE:HD12	1:L:421:ILE:H	1.83	0.42
1:L:684:LYS:HE2	1:L:912:GLU:OE2	2.18	0.42
1:J:6:MET:HE2	1:J:6:MET:HA	2.01	0.42
1:J:270:THR:HB	1:J:271:GLU:H	1.66	0.42
1:L:369:SER:C	1:L:371:GLN:N	2.70	0.42
1:L:928:VAL:HG22	1:L:938:THR:HG22	2.01	0.42
2:Z:92:ARG:N	2:Z:468:TRP:O	2.51	0.42
2:Z:132:THR:HG22	2:Z:412:TRP:CZ3	2.52	0.42
1:K:683:LEU:HD23	1:K:683:LEU:HA	1.78	0.42
1:L:498:PRO:HA	1:L:503:TYR:CD2	2.54	0.42
2:Z:227:GLU:OE1	2:Z:242:TYR:OH	2.35	0.42
2:Z:508:ALA:HB3	2:Z:560:TYR:CE2	2.54	0.42
1:J:136:ASP:OD1	1:J:136:ASP:N	2.51	0.42
1:K:564:GLN:OE1	1:K:566:PHE:N	2.30	0.42
1:K:737:LEU:HD23	1:K:737:LEU:HA	1.89	0.42
1:K:774:TYR:O	1:K:776:ILE:HG13	2.18	0.42
1:L:746:LYS:NZ	1:L:908:ASP:OD2	2.38	0.42
2:Z:22:CYS:SG	2:Z:27:ALA:HB2	2.58	0.42
2:Z:541:GLN:HG2	2:Z:563:VAL:HG21	2.00	0.42
1:J:470:ARG:HH12	1:J:829:VAL:HG21	1.83	0.42
1:J:807:ASP:CG	1:J:809:THR:H	2.27	0.42
1:K:276:ASN:O	1:K:279:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:THR:HG23	1:L:183:GLY:H	1.84	0.42
1:L:252:LYS:HZ2	1:L:252:LYS:HB3	1.85	0.42
1:L:656:ILE:HG12	1:L:663:VAL:HG21	2.01	0.42
2:Z:295:LEU:HG	2:Z:538:ARG:HG2	2.01	0.42
2:Z:448:SER:O	2:Z:452:ALA:N	2.52	0.42
1:L:331:ASP:O	1:L:334:ILE:HG13	2.19	0.42
2:Z:94:PRO:HG3	2:Z:129:THR:O	2.18	0.42
2:Z:441:PRO:HD3	2:Z:540:TYR:HB3	2.01	0.42
2:Z:457:ARG:HD2	2:Z:539:TRP:HZ3	1.85	0.42
1:J:13:MET:HG3	1:L:941:LEU:HD23	2.01	0.42
1:J:24:LEU:HD23	1:J:24:LEU:HA	1.90	0.42
1:J:574:LEU:HD23	1:J:574:LEU:HA	1.85	0.42
1:J:759:CYS:HG	1:J:760:ASN:H	1.62	0.42
1:J:824:ASN:OD1	1:J:825:ASN:N	2.53	0.42
1:K:639:ASN:OD1	1:L:24:LEU:HD22	2.19	0.42
1:L:526:LEU:HD23	1:L:526:LEU:HA	1.92	0.42
1:L:673:ALA:O	1:L:944:PRO:HG3	2.20	0.42
2:Z:321:ILE:HA	2:Z:510:TYR:CZ	2.54	0.42
1:J:209:SER:HB2	1:L:302:TYR:HE2	1.85	0.42
1:J:231:LYS:C	1:J:232:PRO:O	2.61	0.42
1:J:719:LYS:HB2	1:J:906:GLU:O	2.19	0.42
1:J:865:LEU:HD12	1:J:865:LEU:HA	1.83	0.42
1:K:14:HIS:O	1:K:48:PRO:HB3	2.20	0.42
1:K:758:GLN:HE21	1:K:758:GLN:HB2	1.61	0.42
1:L:47:ASN:OD1	1:L:47:ASN:N	2.51	0.42
1:L:441:LYS:HE2	1:L:441:LYS:HB3	1.92	0.42
1:L:493:LYS:HE3	1:L:493:LYS:HB3	1.61	0.42
1:L:808:ASP:N	1:L:808:ASP:OD1	2.53	0.42
1:J:112:THR:HG21	1:J:604:ASP:OD2	2.19	0.42
1:J:611:ASP:HB3	1:J:612:SER:H	1.74	0.42
1:L:67:ARG:HD2	1:L:616:TYR:OH	2.19	0.42
1:L:426:LEU:HD23	1:L:426:LEU:HA	1.66	0.42
1:L:468:LEU:HD23	1:L:468:LEU:HA	1.88	0.42
2:Z:66:ALA:HB2	2:Z:140:ILE:HG22	2.02	0.42
2:Z:95:HIS:HB3	2:Z:134:ARG:HH11	1.85	0.42
2:Z:358:VAL:O	2:Z:422:LEU:HD12	2.19	0.42
2:Z:422:LEU:HB2	2:Z:569:TRP:HH2	1.84	0.42
2:Z:508:ALA:HB3	2:Z:560:TYR:HE2	1.84	0.42
1:J:207:GLY:HA3	1:L:838:GLU:HB2	2.01	0.42
1:J:917:TYR:CZ	1:J:919:LEU:HD21	2.54	0.42
1:K:791:MET:HE3	1:K:791:MET:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:929:HIS:CD2	1:K:931:PRO:HD3	2.55	0.42
1:L:212:TYR:HD1	1:L:212:TYR:H	1.67	0.42
1:L:217:ASN:HB2	1:L:218:HIS:ND1	2.35	0.42
1:L:415:PHE:CD2	1:L:415:PHE:N	2.88	0.42
1:L:520:LEU:HD23	1:L:520:LEU:HA	1.75	0.42
1:L:866:CYS:O	1:L:869:THR:HG22	2.20	0.42
2:Z:573:VAL:HA	2:Z:576:GLN:NE2	2.34	0.42
1:J:121:TYR:HD1	1:J:121:TYR:HA	1.73	0.41
1:J:680:PHE:CE1	1:J:871:TRP:HB2	2.55	0.41
1:J:807:ASP:OD1	1:J:810:LYS:N	2.53	0.41
1:K:78:TYR:C	1:K:587:LYS:HD3	2.45	0.41
1:K:886:THR:OG1	1:K:889:GLY:N	2.50	0.41
1:L:10:TRP:CD1	1:L:15:ILE:HD12	2.55	0.41
1:L:470:ARG:HE	1:L:515:ASP:CG	2.28	0.41
1:L:836:MET:HE3	1:L:837:ARG:NH1	2.35	0.41
1:L:850:LEU:HA	1:L:850:LEU:HD23	1.81	0.41
2:Z:95:HIS:CG	2:Z:134:ARG:HA	2.54	0.41
1:J:121:TYR:CE2	1:J:296:PRO:CG	3.01	0.41
1:J:271:GLU:O	1:J:274:ALA:HB2	2.20	0.41
1:K:203:GLU:HB2	1:K:206:ILE:HG13	2.02	0.41
1:K:252:LYS:N	1:K:258:LEU:HD13	2.35	0.41
1:K:503:TYR:OH	1:K:507:ARG:NH2	2.52	0.41
1:J:178:ASN:HA	1:J:218:HIS:CD2	2.56	0.41
1:J:522:ALA:HB2	1:K:552:ASN:CG	2.44	0.41
1:J:645:ASP:OD1	1:J:646:TYR:N	2.54	0.41
1:K:615:LEU:HD12	1:K:616:TYR:H	1.85	0.41
1:K:743:PHE:HE2	1:K:873:ILE:HD13	1.85	0.41
1:K:893:LEU:O	1:K:897:SER:OG	2.38	0.41
1:L:53:THR:O	1:L:53:THR:OG1	2.30	0.41
1:L:531:ASN:OD1	1:L:531:ASN:N	2.54	0.41
1:L:775:ASN:OD1	1:L:881:SER:N	2.53	0.41
2:Z:497:THR:OG1	2:Z:549:GLU:OE2	2.29	0.41
1:J:416:PRO:HG3	1:J:458:PHE:HB3	2.02	0.41
1:J:531:ASN:HD22	1:J:910:MET:HE3	1.85	0.41
1:K:76:THR:HG22	1:K:77:ALA:H	1.85	0.41
1:K:583:TRP:CD1	1:K:584:ASN:H	2.38	0.41
1:K:833:ALA:HB1	1:K:835:THR:HG23	2.02	0.41
1:K:926:VAL:HG22	1:K:940:TYR:HD1	1.85	0.41
1:L:105:GLY:HA2	1:L:611:ASP:CG	2.46	0.41
1:L:684:LYS:HG2	1:L:912:GLU:OE2	2.20	0.41
1:L:687:GLU:HG2	1:L:701:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:721:VAL:O	1:L:742:GLU:HB2	2.21	0.41
1:J:410:LEU:HD23	1:J:410:LEU:HA	1.93	0.41
1:J:665:ILE:HG13	1:J:903:MET:HB2	2.03	0.41
1:K:435:GLN:O	1:K:436:GLU:HB3	2.20	0.41
1:L:225:LYS:HE2	1:L:288:SER:OG	2.20	0.41
1:L:714:LEU:HD23	1:L:714:LEU:HA	1.86	0.41
2:Z:16:CGU:O	2:Z:22:CYS:N	2.53	0.41
1:J:340:ASN:OD1	1:J:340:ASN:N	2.50	0.41
1:J:535:PHE:C	1:J:537:HIS:N	2.76	0.41
1:J:673:ALA:O	1:J:944:PRO:HG3	2.21	0.41
1:K:675:PHE:HD2	1:K:875:PHE:CD2	2.39	0.41
1:L:750:ASP:OD1	1:L:752:GLU:N	2.40	0.41
2:Z:72:ASN:OD1	2:Z:72:ASN:N	2.52	0.41
2:Z:176:GLN:O	2:Z:212:VAL:HG13	2.20	0.41
1:J:231:LYS:HA	1:J:231:LYS:HD3	1.80	0.41
1:J:428:LYS:HE2	1:L:265:GLN:HG3	2.02	0.41
1:J:615:LEU:HD12	1:J:616:TYR:N	2.35	0.41
1:K:111:PRO:CD	1:K:554:ARG:HH11	2.31	0.41
1:K:257:LYS:HB2	1:K:257:LYS:HE2	1.70	0.41
1:L:373:LEU:O	1:L:377:ILE:HG12	2.20	0.41
1:L:541:ALA:HA	1:L:544:ARG:HG2	2.03	0.41
2:Z:457:ARG:HD2	2:Z:539:TRP:CZ3	2.56	0.41
1:K:119:THR:OG1	1:K:120:ALA:N	2.53	0.41
1:K:131:ASN:HD21	1:K:232:PRO:C	2.29	0.41
1:K:333:PHE:CD2	1:K:562:VAL:HG22	2.56	0.41
1:K:750:ASP:OD1	1:K:753:GLY:N	2.53	0.41
1:L:373:LEU:O	1:L:373:LEU:HD12	2.20	0.41
2:Z:20:CGU:HB2	2:Z:21:THR:H	1.64	0.41
1:J:133:CYS:HB3	1:J:315:MET:SD	2.60	0.41
1:J:134:GLU:CG	1:J:168:VAL:HG22	2.50	0.41
1:J:242:ASN:HD21	1:J:246:GLY:H	1.68	0.41
1:J:515:ASP:HB3	1:J:517:TYR:CE2	2.56	0.41
1:J:797:ASN:O	1:J:866:CYS:HA	2.21	0.41
1:J:880:MET:HE2	1:J:880:MET:HB3	1.93	0.41
1:K:302:TYR:CE1	1:K:304:PRO:HA	2.56	0.41
1:K:374:LEU:HD23	1:K:374:LEU:HA	1.80	0.41
1:L:375:ASP:HB2	1:L:792:TYR:CD1	2.56	0.41
1:L:497:ASN:C	1:L:499:ASN:N	2.78	0.41
1:L:640:ASP:OD2	1:L:927:ARG:NE	2.44	0.41
1:L:683:LEU:HD21	1:L:712:PHE:CE1	2.55	0.41
1:L:684:LYS:HB3	1:L:687:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:688:THR:HA	1:L:689:PRO:HD3	1.87	0.41
1:L:701:TYR:CE2	1:L:703:GLY:N	2.88	0.41
1:L:911:ASP:OD1	1:L:911:ASP:N	2.49	0.41
2:Z:314:GLU:HA	2:Z:455:LYS:HE3	2.02	0.41
1:J:133:CYS:SG	1:J:315:MET:SD	3.19	0.41
1:J:271:GLU:O	1:J:274:ALA:CB	2.69	0.41
1:K:362:GLN:HE21	1:K:692:GLY:HA3	1.86	0.41
1:K:380:ARG:HD2	1:K:380:ARG:HA	1.70	0.41
1:K:415:PHE:CZ	1:L:828:PHE:HB3	2.56	0.41
1:L:371:GLN:OE1	1:L:380:ARG:NH2	2.48	0.41
1:L:379:ASP:OD1	1:L:381:THR:HG23	2.21	0.41
1:L:542:GLY:O	1:L:546:ARG:HG3	2.21	0.41
1:J:222:ARG:HH21	1:J:289:GLU:CD	2.28	0.40
1:K:645:ASP:OD1	1:K:647:LEU:N	2.55	0.40
2:Z:63:GLY:O	2:Z:74:ARG:N	2.29	0.40
2:Z:519:ASP:HB3	2:Z:522:GLU:HG3	2.03	0.40
1:J:914:THR:O	1:J:915:LEU:HD23	2.22	0.40
1:K:211:TRP:CZ3	1:K:418:GLY:HA3	2.56	0.40
1:L:372:LEU:N	1:L:372:LEU:HD23	2.36	0.40
1:L:415:PHE:O	1:L:416:PRO:C	2.64	0.40
1:L:432:LYS:H	1:L:438:GLY:CA	2.32	0.40
2:Z:79:ILE:HD12	2:Z:152:MET:HE3	2.02	0.40
2:Z:127:TYR:HE1	2:Z:134:ARG:NE	2.18	0.40
1:J:414:CYS:SG	1:K:460:MET:CE	3.09	0.40
1:J:561:GLN:NE2	1:L:756:VAL:HA	2.35	0.40
1:K:43:ASN:OD1	1:K:43:ASN:N	2.54	0.40
1:K:358:VAL:HG13	1:K:566:PHE:CE2	2.51	0.40
1:K:370:TYR:HE1	1:K:374:LEU:HD12	1.87	0.40
1:K:430:LYS:HE3	1:K:440:GLU:HG3	2.03	0.40
1:K:840:GLN:HE21	1:K:840:GLN:HB2	1.79	0.40
1:L:575:LEU:HB2	1:L:930:ARG:HD2	2.03	0.40
2:Z:494:LYS:HG2	2:Z:501:ILE:HG13	2.03	0.40
1:J:476:ASN:O	1:J:477:ILE:C	2.62	0.40
1:J:741:ASN:HB3	1:J:742:GLU:OE1	2.21	0.40
1:J:926:VAL:HG22	1:J:940:TYR:CD1	2.56	0.40
1:L:193:PRO:HB2	1:L:195:TYR:CZ	2.57	0.40
1:J:415:PHE:CE2	1:K:828:PHE:CD1	3.05	0.40
1:K:309:GLY:O	1:K:310:ASN:CG	2.64	0.40
1:K:667:ILE:HB	1:K:901:LEU:HB3	2.04	0.40
1:K:790:ARG:N	1:K:793:SER:HG	2.19	0.40
1:L:277:GLY:O	1:L:278:ASP:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:806:VAL:HG22	1:L:807:ASP:O	2.21	0.40
2:Z:120:SER:HB3	2:Z:125:TRP:CD1	2.56	0.40
2:Z:202:LEU:HD13	2:Z:232:TYR:CG	2.56	0.40
2:Z:297:PRO:HA	2:Z:301:LYS:HD2	2.02	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	J	921/952 (97%)	807 (88%)	96 (10%)	18 (2%)	6	33
1	K	918/952 (96%)	818 (89%)	90 (10%)	10 (1%)	11	44
1	L	920/952 (97%)	798 (87%)	98 (11%)	24 (3%)	4	28
2	Z	567/622 (91%)	525 (93%)	42 (7%)	0	100	100
All	All	3326/3478 (96%)	2948 (89%)	326 (10%)	52 (2%)	10	37

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	70	PRO
1	J	111	PRO
1	J	234	TYR
1	J	274	ALA
1	J	474	TYR
1	J	475	SER
1	K	277	GLY
1	K	315	MET
1	L	377	ILE
1	L	685	THR
1	L	697	PRO

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Mol	Chain	Res	Type
1	L	698	TYR
1	L	707	TYR
1	L	715	ASN
1	J	112	THR
1	J	270	THR
1	J	278	ASP
1	J	476	ASN
1	J	479	LEU
1	J	484	LYS
1	J	540	ASN
1	K	272	ALA
1	K	274	ALA
1	K	310	ASN
1	K	314	LEU
1	L	272	ALA
1	L	416	PRO
1	L	495	SER
1	L	686	LYS
1	L	702	SER
1	L	703	GLY
1	L	709	ASP
1	K	275	GLY
1	L	363	ASP
1	L	422	ASN
1	L	701	TYR
1	L	869	THR
1	J	611	ASP
1	K	316	GLY
1	L	278	ASP
1	J	232	PRO
1	J	614	CYS
1	L	270	THR
1	L	489	PRO
1	J	132	PRO
1	J	229	PRO
1	K	306	ILE
1	L	689	PRO
1	L	706	PRO
1	L	421	ILE
1	L	498	PRO
1	K	842	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	805/829 (97%)	708 (88%)	97 (12%)	5	20
1	K	803/829 (97%)	716 (89%)	87 (11%)	6	23
1	L	804/829 (97%)	709 (88%)	95 (12%)	5	20
2	Z	486/521 (93%)	453 (93%)	33 (7%)	14	38
All	All	2898/3008 (96%)	2586 (89%)	312 (11%)	8	23

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	6	MET
1	J	45	PHE
1	J	55	ASP
1	J	58	THR
1	J	63	ARG
1	J	64	LEU
1	J	65	THR
1	J	66	LEU
1	J	67	ARG
1	J	69	ILE
1	J	76	THR
1	J	91	ASN
1	J	109	ARG
1	J	112	THR
1	J	133	CYS
1	J	136	ASP
1	J	166	THR
1	J	180	THR
1	J	184	ILE
1	J	188	VAL
1	J	217	ASN
1	J	236	SER
1	J	244	ASN
1	J	252	LYS

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Mol	Chain	Res	Type
1	J	259	GLU
1	J	271	GLU
1	J	278	ASP
1	J	279	ASN
1	J	305	THR
1	J	313	GLU
1	J	327	ILE
1	J	336	LEU
1	J	338	TYR
1	J	340	ASN
1	J	344	ASN
1	J	358	VAL
1	J	372	LEU
1	J	374	LEU
1	J	375	ASP
1	J	377	ILE
1	J	391	VAL
1	J	392	ASP
1	J	400	ILE
1	J	404	HIS
1	J	420	VAL
1	J	421	ILE
1	J	425	THR
1	J	440	GLU
1	J	451	GLU
1	J	473	LEU
1	J	477	ILE
1	J	479	LEU
1	J	481	LEU
1	J	483	ASP
1	J	484	LYS
1	J	500	THR
1	J	509	VAL
1	J	518	ILE
1	J	538	HIS
1	J	558	PHE
1	J	559	HIS
1	J	560	ILE
1	J	573	LEU
1	J	592	VAL
1	J	600	ASP
1	J	604	ASP

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Mol	Chain	Res	Type
1	J	608	ILE
1	J	609	LYS
1	J	613	ILE
1	J	641	GLN
1	J	648	SER
1	J	651	ASN
1	J	669	SER
1	J	681	THR
1	J	691	LEU
1	J	705	ILE
1	J	723	ILE
1	J	728	SER
1	J	735	ASP
1	J	750	ASP
1	J	752	GLU
1	J	762	THR
1	J	768	VAL
1	J	806	VAL
1	J	807	ASP
1	J	840	GLN
1	J	857	ASP
1	J	865	LEU
1	J	867	ASP
1	J	869	THR
1	J	870	LEU
1	J	872	ARG
1	J	893	LEU
1	J	921	GLU
1	J	925	VAL
1	J	936	ILE
1	J	943	THR
1	K	19	ASP
1	K	25	SER
1	K	37	THR
1	K	53	THR
1	K	56	VAL
1	K	58	THR
1	K	69	ILE
1	K	74	GLU
1	K	76	THR
1	K	90	ASP
1	K	91	ASN

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Mol	Chain	Res	Type
1	K	100	TYR
1	K	106	VAL
1	K	112	THR
1	K	184	ILE
1	K	185	GLN
1	K	188	VAL
1	K	208	GLU
1	K	212	TYR
1	K	224	LEU
1	K	228	THR
1	K	243	GLU
1	K	252	LYS
1	K	257	LYS
1	K	270	THR
1	K	293	ILE
1	K	301	SER
1	K	303	MET
1	K	306	ILE
1	K	308	GLU
1	K	310	ASN
1	K	315	MET
1	K	327	ILE
1	K	336	LEU
1	K	355	LEU
1	K	366	THR
1	K	374	LEU
1	K	375	ASP
1	K	388	ASN
1	K	392	ASP
1	K	412	ASN
1	K	420	VAL
1	K	421	ILE
1	K	423	THR
1	K	425	THR
1	K	440	GLU
1	K	448	ASP
1	K	462	ILE
1	K	481	LEU
1	K	490	SER
1	K	491	ASN
1	K	500	THR
1	K	502	ASP

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Mol	Chain	Res	Type
1	K	509	VAL
1	K	520	LEU
1	K	558	PHE
1	K	561	GLN
1	K	572	LEU
1	K	574	LEU
1	K	592	VAL
1	K	596	SER
1	K	603	VAL
1	K	608	ILE
1	K	634	LEU
1	K	636	ASN
1	K	638	THR
1	K	648	SER
1	K	665	ILE
1	K	676	ARG
1	K	681	THR
1	K	734	ASN
1	K	745	ILE
1	K	756	VAL
1	K	759	CYS
1	K	764	ASP
1	K	829	VAL
1	K	867	ASP
1	K	869	THR
1	K	870	LEU
1	K	872	ARG
1	K	876	SER
1	K	886	THR
1	K	887	ASP
1	K	897	SER
1	K	907	VAL
1	K	936	ILE
1	K	943	THR
1	L	19	ASP
1	L	47	ASN
1	L	55	ASP
1	L	58	THR
1	L	69	ILE
1	L	76	THR
1	L	90	ASP
1	L	91	ASN

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Mol	Chain	Res	Type
1	L	93	VAL
1	L	102	ASP
1	L	184	ILE
1	L	186	ILE
1	L	208	GLU
1	L	212	TYR
1	L	224	LEU
1	L	227	THR
1	L	234	TYR
1	L	251	VAL
1	L	252	LYS
1	L	257	LYS
1	L	269	THR
1	L	273	THR
1	L	280	LEU
1	L	290	ASP
1	L	291	VAL
1	L	308	GLU
1	L	327	ILE
1	L	336	LEU
1	L	338	TYR
1	L	340	ASN
1	L	342	THR
1	L	348	LEU
1	L	360	ASP
1	L	365	ASN
1	L	368	LEU
1	L	369	SER
1	L	373	LEU
1	L	374	LEU
1	L	375	ASP
1	L	381	THR
1	L	391	VAL
1	L	406	THR
1	L	414	CYS
1	L	417	LEU
1	L	421	ILE
1	L	423	THR
1	L	425	THR
1	L	426	LEU
1	L	432	LYS
1	L	445	GLU

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Mol	Chain	Res	Type
1	L	451	GLU
1	L	452	ILE
1	L	491	ASN
1	L	493	LYS
1	L	494	ILE
1	L	497	ASN
1	L	500	THR
1	L	509	VAL
1	L	514	VAL
1	L	558	PHE
1	L	561	GLN
1	L	569	ILE
1	L	574	LEU
1	L	592	VAL
1	L	595	SER
1	L	600	ASP
1	L	611	ASP
1	L	648	SER
1	L	651	ASN
1	L	681	THR
1	L	684	LYS
1	L	686	LYS
1	L	691	LEU
1	L	695	TYR
1	L	696	ASP
1	L	708	LEU
1	L	738	LEU
1	L	742	GLU
1	L	745	ILE
1	L	755	ASN
1	L	756	VAL
1	L	764	ASP
1	L	783	ILE
1	L	787	TYR
1	L	806	VAL
1	L	813	ASP
1	L	822	GLN
1	L	857	ASP
1	L	860	THR
1	L	867	ASP
1	L	872	ARG
1	L	876	SER

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Mol	Chain	Res	Type
1	L	888	LEU
1	L	935	VAL
1	L	936	ILE
2	Z	18	VAL
2	Z	24	TYR
2	Z	79	ILE
2	Z	121	THR
2	Z	128	THR
2	Z	130	ASP
2	Z	133	VAL
2	Z	135	ARG
2	Z	152	MET
2	Z	215	VAL
2	Z	216	GLU
2	Z	219	CYS
2	Z	248	CYS
2	Z	316	TYR
2	Z	317	ILE
2	Z	329	ILE
2	Z	348	CYS
2	Z	394	ASN
2	Z	409	ARG
2	Z	414	GLU
2	Z	415	ASN
2	Z	431	PHE
2	Z	433	ASP
2	Z	436	HIS
2	Z	454	TYR
2	Z	479	VAL
2	Z	480	LEU
2	Z	499	ILE
2	Z	504	ASN
2	Z	507	CYS
2	Z	530	VAL
2	Z	554	ASP
2	Z	563	VAL

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

Mol	Chain	Res	Type
1	J	255	ASN
1	J	332	ASN

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Mol	Chain	Res	Type
1	J	371	GLN
1	J	404	HIS
1	J	435	GLN
1	J	467	ASN
1	J	471	ASN
1	J	538	HIS
1	J	540	ASN
1	J	561	GLN
1	J	651	ASN
1	J	662	ASN
1	J	758	GLN
1	J	769	GLN
1	J	815	GLN
1	K	310	ASN
1	K	317	GLN
1	K	332	ASN
1	K	351	GLN
1	K	389	GLN
1	K	422	ASN
1	K	505	ASN
1	K	538	HIS
1	K	561	GLN
1	L	218	HIS
1	L	247	GLN
1	L	279	ASN
1	L	491	ASN
1	L	499	ASN
1	L	651	ASN
1	L	769	GLN
2	Z	136	GLN
2	Z	179	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CGU	Z	16	3,2	9,11,12	1.14	0	10,14,16	0.85	0
2	CGU	Z	19	2	9,11,12	1.49	1 (11%)	10,14,16	0.82	0
2	CGU	Z	6	3,2	9,11,12	1.31	0	10,14,16	0.84	0
2	CGU	Z	7	3,2	9,11,12	1.47	1 (11%)	10,14,16	0.82	0
2	CGU	Z	20	3,2	9,11,12	1.45	1 (11%)	10,14,16	0.86	0
2	CGU	Z	25	3,2	9,11,12	1.46	1 (11%)	10,14,16	0.84	0
2	CGU	Z	26	3,2	9,11,12	1.50	1 (11%)	10,14,16	0.81	0
2	CGU	Z	14	3,2	9,11,12	1.48	1 (11%)	10,14,16	0.83	0
2	CGU	Z	32	2	9,11,12	1.46	0	10,14,16	0.88	0
2	CGU	Z	29	3,2	9,11,12	1.47	1 (11%)	10,14,16	1.00	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CGU	Z	16	3,2	-	1/13/14/16	-
2	CGU	Z	19	2	-	3/13/14/16	-
2	CGU	Z	6	3,2	-	3/13/14/16	-
2	CGU	Z	7	3,2	-	2/13/14/16	-
2	CGU	Z	20	3,2	-	2/13/14/16	-
2	CGU	Z	25	3,2	-	4/13/14/16	-
2	CGU	Z	26	3,2	-	3/13/14/16	-
2	CGU	Z	14	3,2	-	8/13/14/16	-
2	CGU	Z	32	2	-	3/13/14/16	-
2	CGU	Z	29	3,2	-	3/13/14/16	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	14	CGU	CG-CD2	2.33	1.55	1.52
2	Z	20	CGU	CG-CD2	2.33	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	19	CGU	CG-CD1	2.28	1.55	1.52
2	Z	26	CGU	CG-CD2	2.21	1.54	1.52
2	Z	7	CGU	CG-CD2	2.14	1.54	1.52
2	Z	25	CGU	CG-CD2	2.11	1.54	1.52
2	Z	29	CGU	CG-CD2	2.05	1.54	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	7	CGU	N-CA-CB-CG
2	Z	7	CGU	C-CA-CB-CG
2	Z	14	CGU	C-CA-CB-CG
2	Z	14	CGU	CA-CB-CG-CD1
2	Z	14	CGU	CA-CB-CG-CD2
2	Z	20	CGU	O-C-CA-CB
2	Z	20	CGU	CA-CB-CG-CD1
2	Z	25	CGU	CA-CB-CG-CD2
2	Z	29	CGU	CA-CB-CG-CD1
2	Z	19	CGU	N-CA-CB-CG
2	Z	29	CGU	N-CA-CB-CG
2	Z	14	CGU	OE11-CD1-CG-CB
2	Z	25	CGU	OE11-CD1-CG-CB
2	Z	25	CGU	OE12-CD1-CG-CB
2	Z	26	CGU	OE11-CD1-CG-CB
2	Z	26	CGU	OE12-CD1-CG-CB
2	Z	29	CGU	CA-CB-CG-CD2
2	Z	14	CGU	N-CA-CB-CG
2	Z	6	CGU	OE21-CD2-CG-CB
2	Z	6	CGU	OE22-CD2-CG-CB
2	Z	14	CGU	OE12-CD1-CG-CB
2	Z	16	CGU	OE12-CD1-CG-CB
2	Z	32	CGU	OE21-CD2-CG-CB
2	Z	32	CGU	OE22-CD2-CG-CB
2	Z	6	CGU	OE11-CD1-CG-CD2
2	Z	14	CGU	OE11-CD1-CG-CD2
2	Z	14	CGU	OE21-CD2-CG-CD1
2	Z	19	CGU	OE21-CD2-CG-CD1
2	Z	19	CGU	OE22-CD2-CG-CD1
2	Z	25	CGU	OE12-CD1-CG-CD2

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Mol	Chain	Res	Type	Atoms
2	Z	26	CGU	OE21-CD2-CG-CD1
2	Z	32	CGU	OE11-CD1-CG-CD2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	16	CGU	6	0
2	Z	19	CGU	1	0
2	Z	6	CGU	2	0
2	Z	20	CGU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

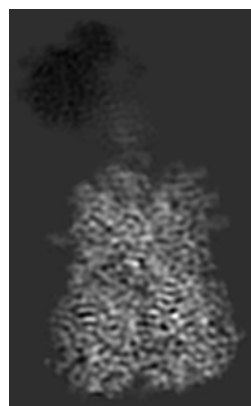
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45726. These allow visual inspection of the internal detail of the map and identification of artifacts.

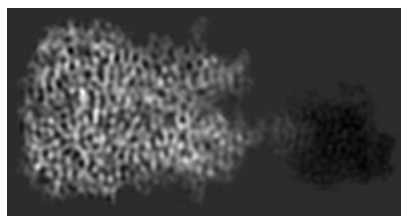
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

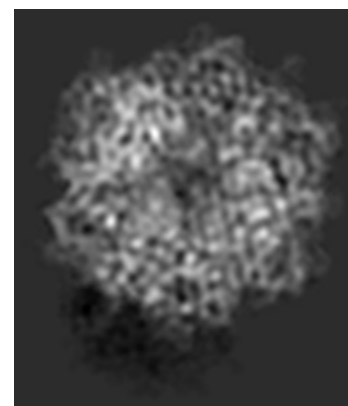
6.1.1 Primary map



X

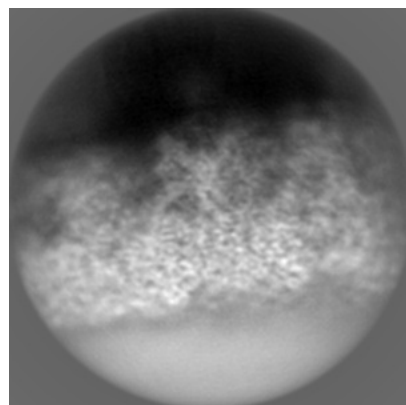


Y

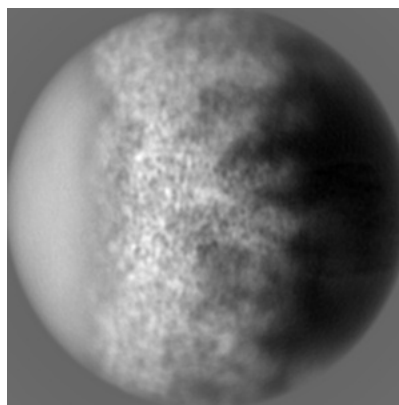


Z

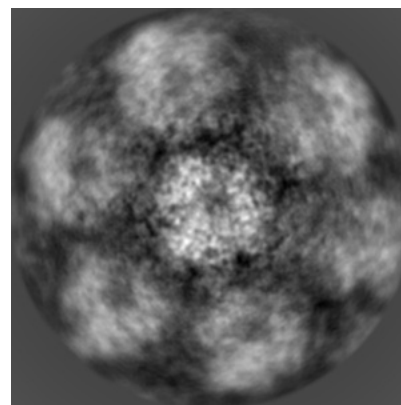
6.1.2 Raw map



X



Y

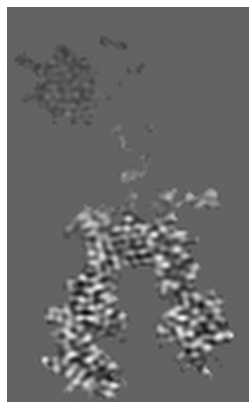


Z

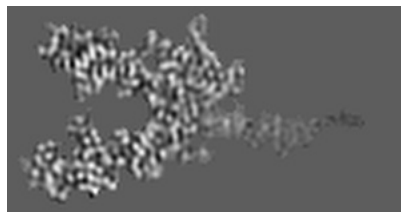
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

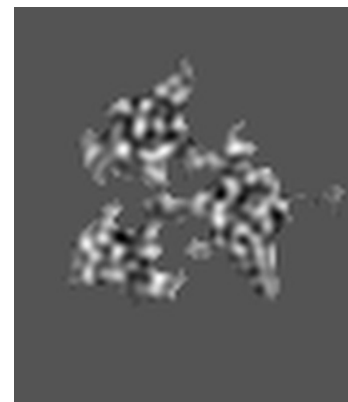
6.2.1 Primary map



X Index: 39

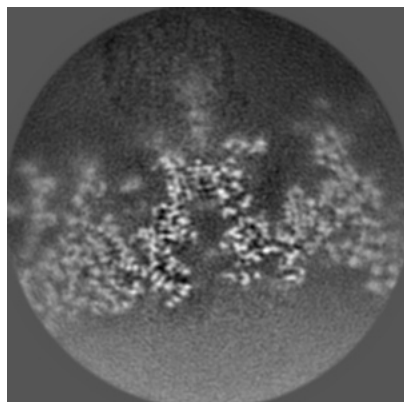


Y Index: 46

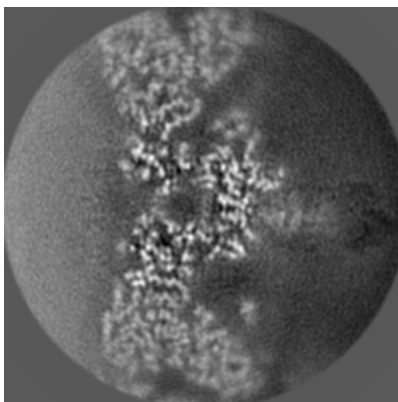


Z Index: 75

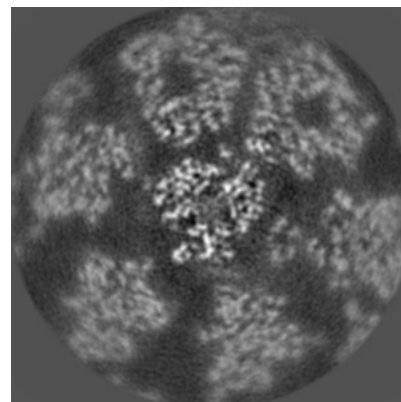
6.2.2 Raw map



X Index: 100



Y Index: 100

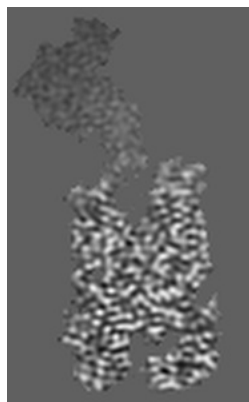


Z Index: 100

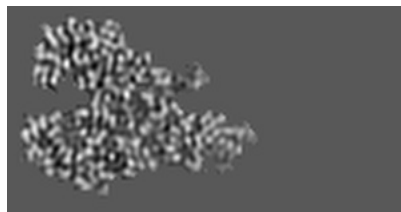
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

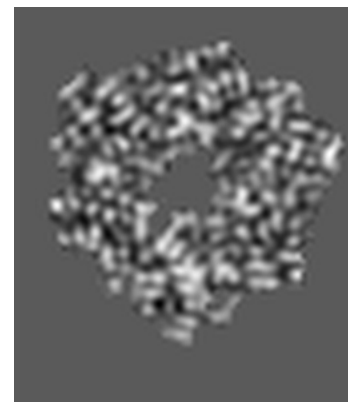
6.3.1 Primary map



X Index: 28

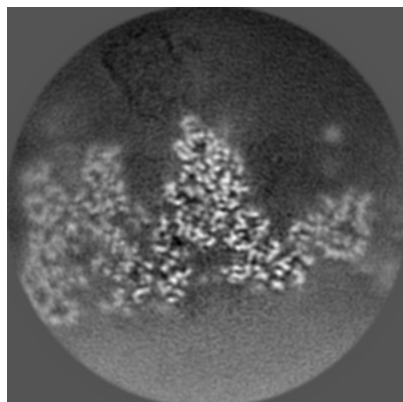


Y Index: 64

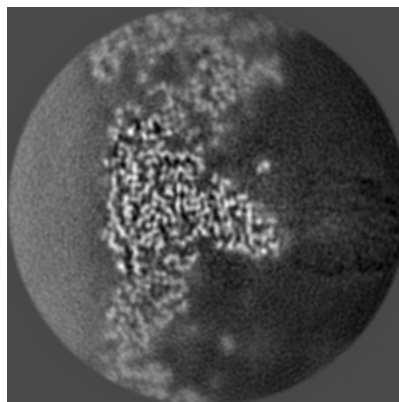


Z Index: 33

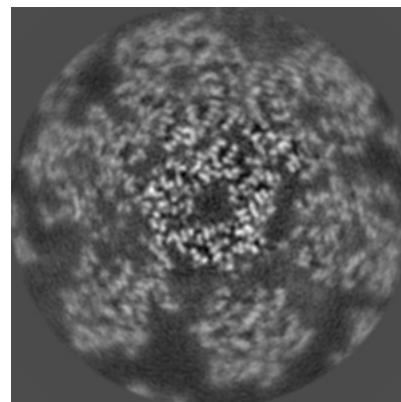
6.3.2 Raw map



X Index: 112



Y Index: 81



Z Index: 91

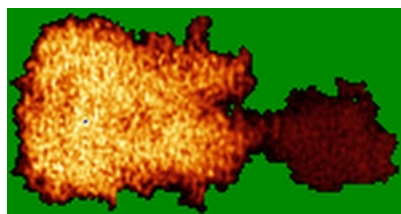
The images above show the largest variance slices of the map in three orthogonal directions.

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

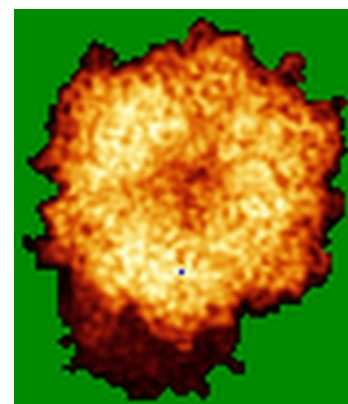
6.4.1 Primary map



X

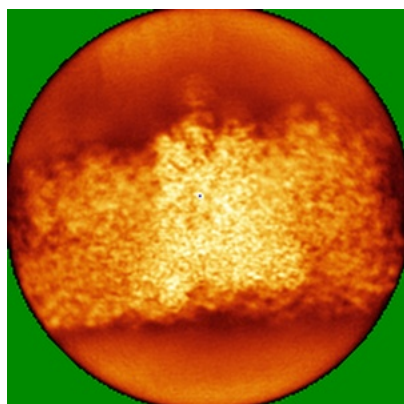


Y

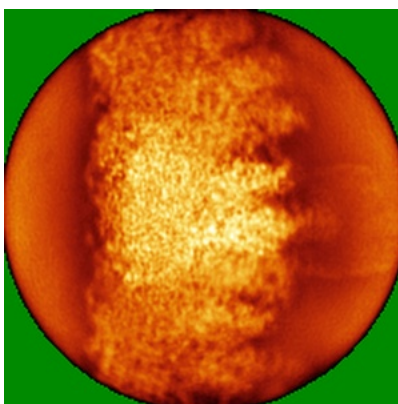


Z

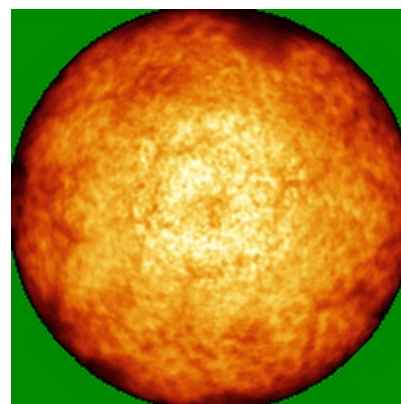
6.4.2 Raw map



X



Y



Z

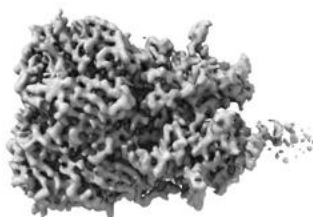
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

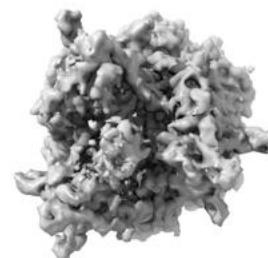
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

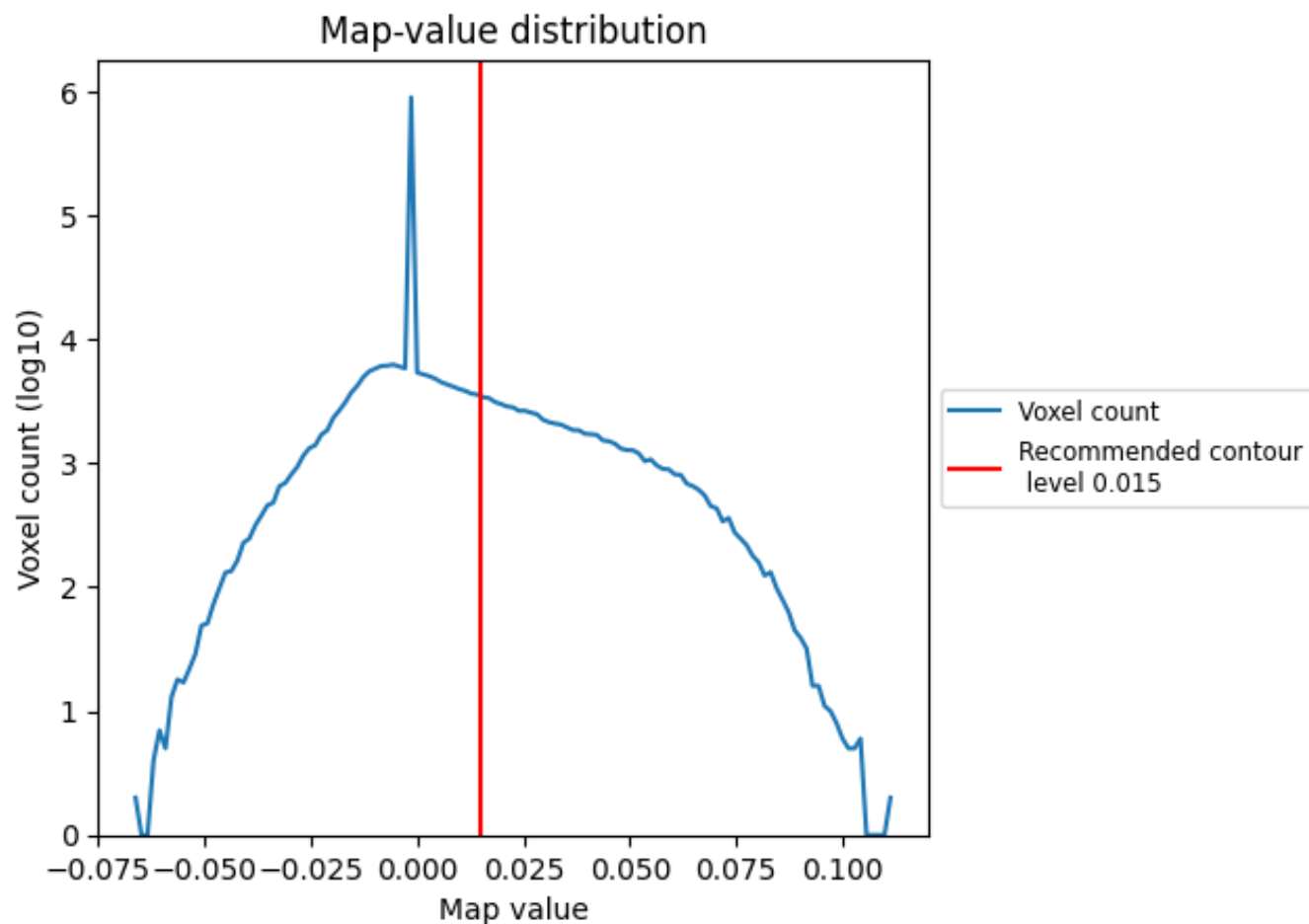
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

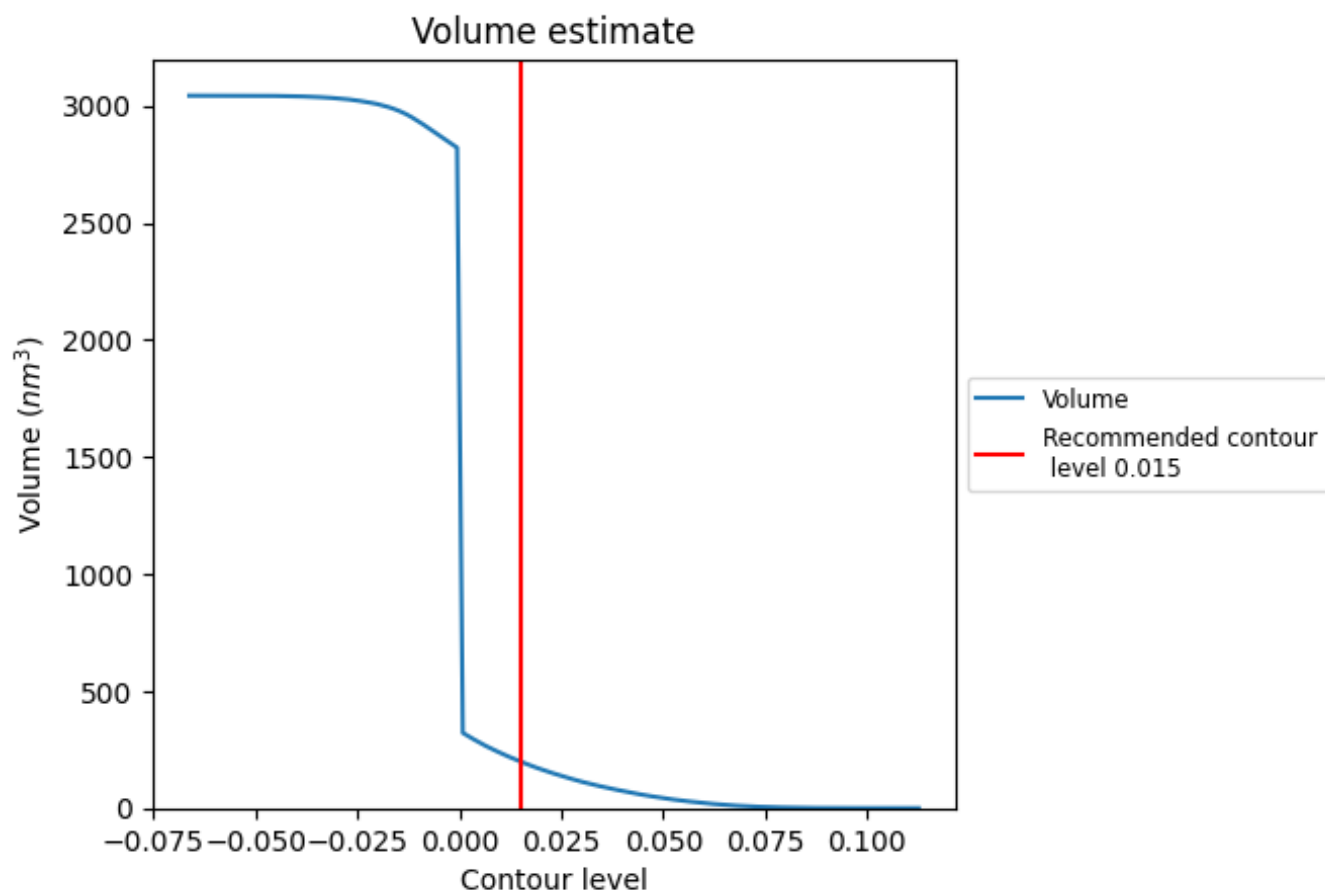
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 199 nm³; this corresponds to an approximate mass of 180 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.

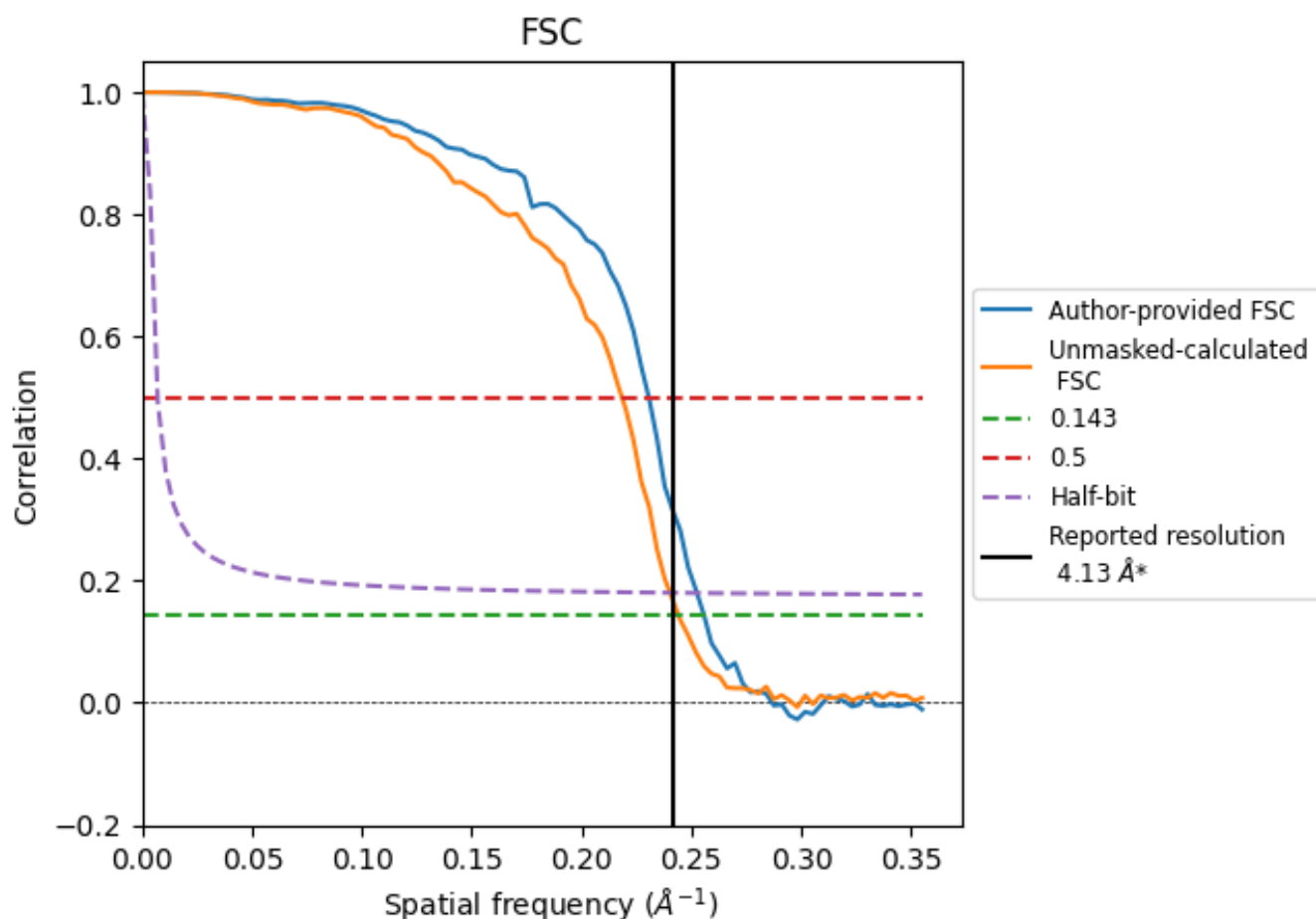
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

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 0.242 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

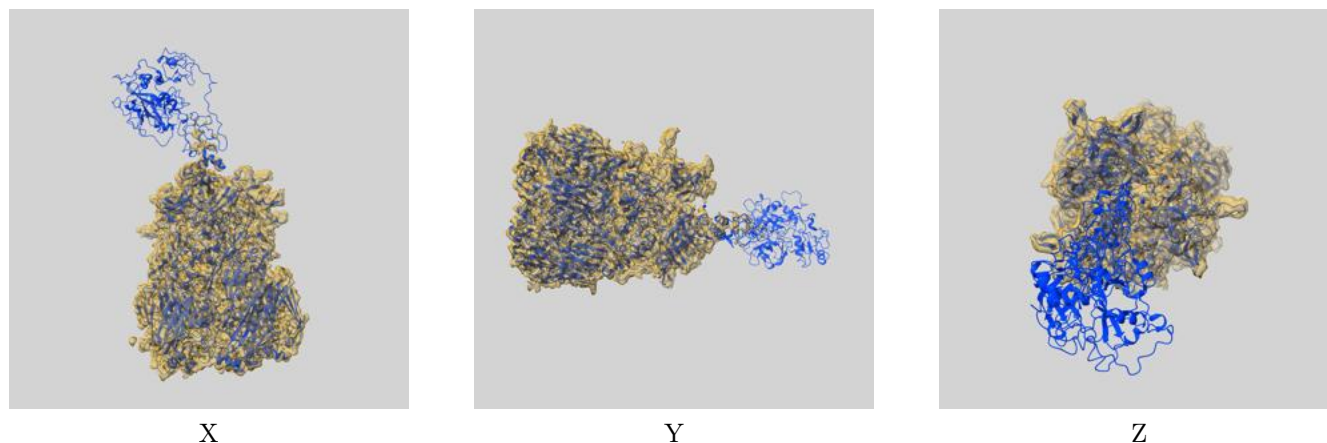
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.13	-	-
Author-provided FSC curve	3.91	4.33	3.96
Unmasked-calculated*	4.10	4.58	4.16

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

9 Map-model fit [i](#)

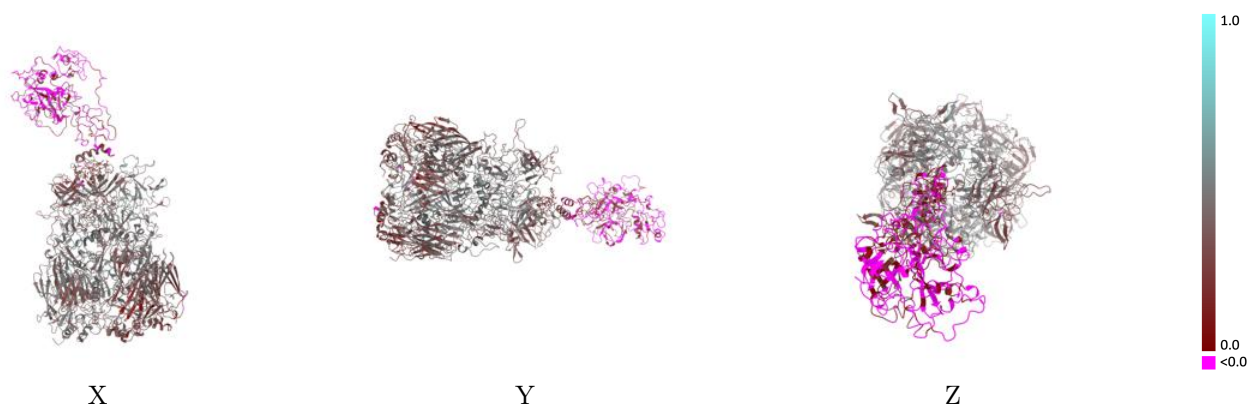
This section contains information regarding the fit between EMDB map EMD-45726 and PDB model 9CLN. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



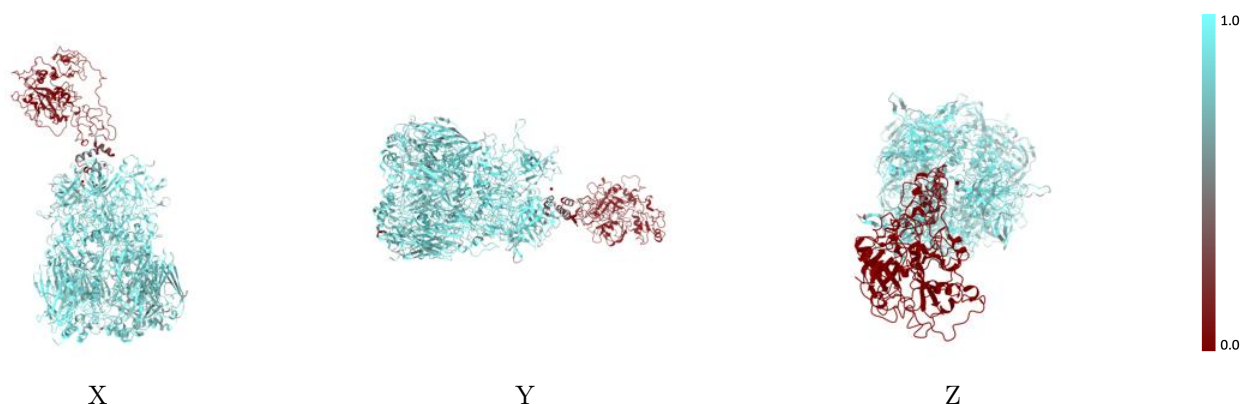
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



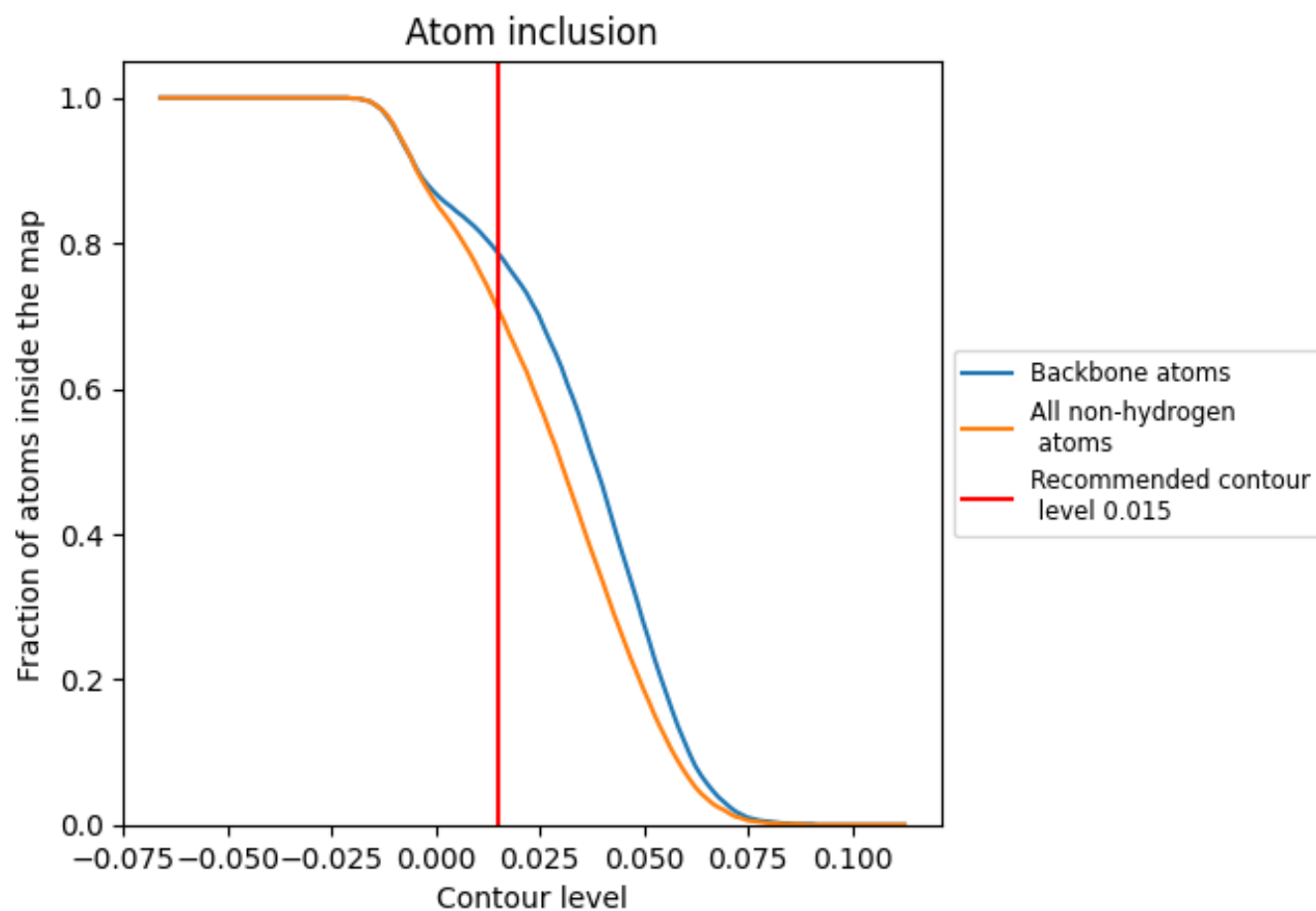
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.3350
J	0.8560	0.4210
K	0.8360	0.3920
L	0.8480	0.4040
Z	0.0470	-0.0040

