



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:35 AM UTC

PDB ID : 9ZPC / pdb_00009zpc
EMDB ID : EMD-74526
Title : Cryo-EM structure of human PI3KC3-C2
Authors : Chen, M.; Joiner, A.; Hurley, J.H.
Deposited on : 2025-12-16
Resolution : 3.83 Å(reported)
Based on initial model : .

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:

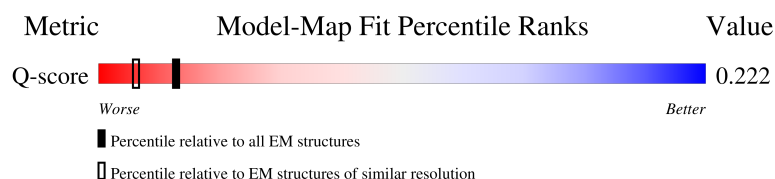
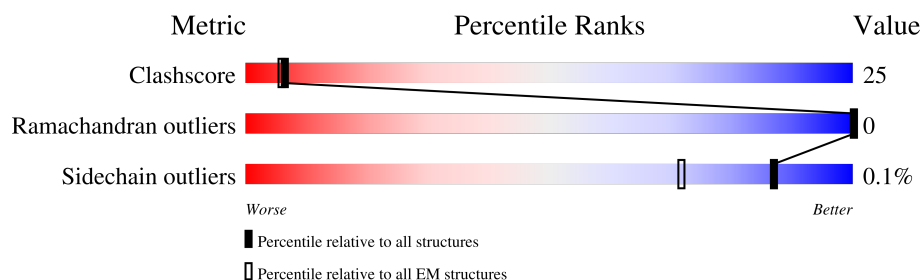
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.83 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	9087 (3.33 - 4.33)

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	1445	26% 36% 37% 28%
2	B	887	7% 16% 12% 72%
3	C	699	27% 33% 22% 45%
4	D	450	31% 41% 32% 27%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16275 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 Phosphoinositide 3-kinase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1045	8350	5349	1449	1511	41	0	0

There are 87 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	expression tag	UNP A0JP11
A	-34	PHE	-	expression tag	UNP A0JP11
A	-33	MET	-	expression tag	UNP A0JP11
A	-32	PRO	-	expression tag	UNP A0JP11
A	-31	SER	-	expression tag	UNP A0JP11
A	-30	SER	-	expression tag	UNP A0JP11
A	-29	PHE	-	expression tag	UNP A0JP11
A	-28	SER	-	expression tag	UNP A0JP11
A	-27	TYR	-	expression tag	UNP A0JP11
A	-26	SER	-	expression tag	UNP A0JP11
A	-25	SER	-	expression tag	UNP A0JP11
A	-24	TRP	-	expression tag	UNP A0JP11
A	-23	ALA	-	expression tag	UNP A0JP11
A	-22	THR	-	expression tag	UNP A0JP11
A	-21	CYS	-	expression tag	UNP A0JP11
A	-20	TRP	-	expression tag	UNP A0JP11
A	-19	LEU	-	expression tag	UNP A0JP11
A	-18	LEU	-	expression tag	UNP A0JP11
A	-17	CYS	-	expression tag	UNP A0JP11
A	-16	CYS	-	expression tag	UNP A0JP11
A	-15	LEU	-	expression tag	UNP A0JP11
A	-14	ILE	-	expression tag	UNP A0JP11
A	-13	ILE	-	expression tag	UNP A0JP11
A	-12	LEU	-	expression tag	UNP A0JP11
A	-11	ALA	-	expression tag	UNP A0JP11
A	-10	LYS	-	expression tag	UNP A0JP11
A	-9	ASN	-	expression tag	UNP A0JP11
A	-8	SER	-	expression tag	UNP A0JP11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP A0JP11
A	-6	ILE	-	expression tag	UNP A0JP11
A	-5	ASP	-	expression tag	UNP A0JP11
A	-4	GLY	-	expression tag	UNP A0JP11
A	-3	ILE	-	expression tag	UNP A0JP11
A	-2	GLU	-	expression tag	UNP A0JP11
A	-1	ALA	-	expression tag	UNP A0JP11
A	0	THR	-	expression tag	UNP A0JP11
A	1359	GLY	-	expression tag	UNP A0JP11
A	1360	THR	-	expression tag	UNP A0JP11
A	1361	GLU	-	expression tag	UNP A0JP11
A	1362	ASN	-	expression tag	UNP A0JP11
A	1363	LEU	-	expression tag	UNP A0JP11
A	1364	TYR	-	expression tag	UNP A0JP11
A	1365	PHE	-	expression tag	UNP A0JP11
A	1366	GLN	-	expression tag	UNP A0JP11
A	1367	SER	-	expression tag	UNP A0JP11
A	1368	GLY	-	expression tag	UNP A0JP11
A	1369	MET	-	expression tag	UNP A0JP11
A	1370	ALA	-	expression tag	UNP A0JP11
A	1371	ALA	-	expression tag	UNP A0JP11
A	1372	TRP	-	expression tag	UNP A0JP11
A	1373	SER	-	expression tag	UNP A0JP11
A	1374	HIS	-	expression tag	UNP A0JP11
A	1375	PRO	-	expression tag	UNP A0JP11
A	1376	GLN	-	expression tag	UNP A0JP11
A	1377	PHE	-	expression tag	UNP A0JP11
A	1378	GLU	-	expression tag	UNP A0JP11
A	1379	LYS	-	expression tag	UNP A0JP11
A	1380	GLY	-	expression tag	UNP A0JP11
A	1381	GLY	-	expression tag	UNP A0JP11
A	1382	GLY	-	expression tag	UNP A0JP11
A	1383	ALA	-	expression tag	UNP A0JP11
A	1384	ARG	-	expression tag	UNP A0JP11
A	1385	GLY	-	expression tag	UNP A0JP11
A	1386	GLY	-	expression tag	UNP A0JP11
A	1387	SER	-	expression tag	UNP A0JP11
A	1388	GLY	-	expression tag	UNP A0JP11
A	1389	GLY	-	expression tag	UNP A0JP11
A	1390	GLY	-	expression tag	UNP A0JP11
A	1391	SER	-	expression tag	UNP A0JP11
A	1392	TRP	-	expression tag	UNP A0JP11

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1393	SER	-	expression tag	UNP A0JP11
A	1394	HIS	-	expression tag	UNP A0JP11
A	1395	PRO	-	expression tag	UNP A0JP11
A	1396	GLN	-	expression tag	UNP A0JP11
A	1397	PHE	-	expression tag	UNP A0JP11
A	1398	GLU	-	expression tag	UNP A0JP11
A	1399	LYS	-	expression tag	UNP A0JP11
A	1400	GLY	-	expression tag	UNP A0JP11
A	1401	PHE	-	expression tag	UNP A0JP11
A	1402	ASP	-	expression tag	UNP A0JP11
A	1403	TYR	-	expression tag	UNP A0JP11
A	1404	LYS	-	expression tag	UNP A0JP11
A	1405	ASP	-	expression tag	UNP A0JP11
A	1406	ASP	-	expression tag	UNP A0JP11
A	1407	ASP	-	expression tag	UNP A0JP11
A	1408	ASP	-	expression tag	UNP A0JP11
A	1409	LYS	-	expression tag	UNP A0JP11

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	250	Total	C	N	O	S	0	0
			2034	1304	344	371	15		

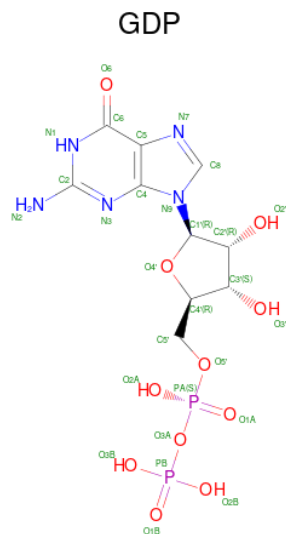
- Molecule 3 is a protein called UV radiation resistance-associated gene protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	385	Total	C	N	O	S	0	0
			3153	2014	566	563	10		

- Molecule 4 is a protein called Beclin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	328	Total	C	N	O	S	0	0
			2708	1701	467	524	16		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Mg 1	0

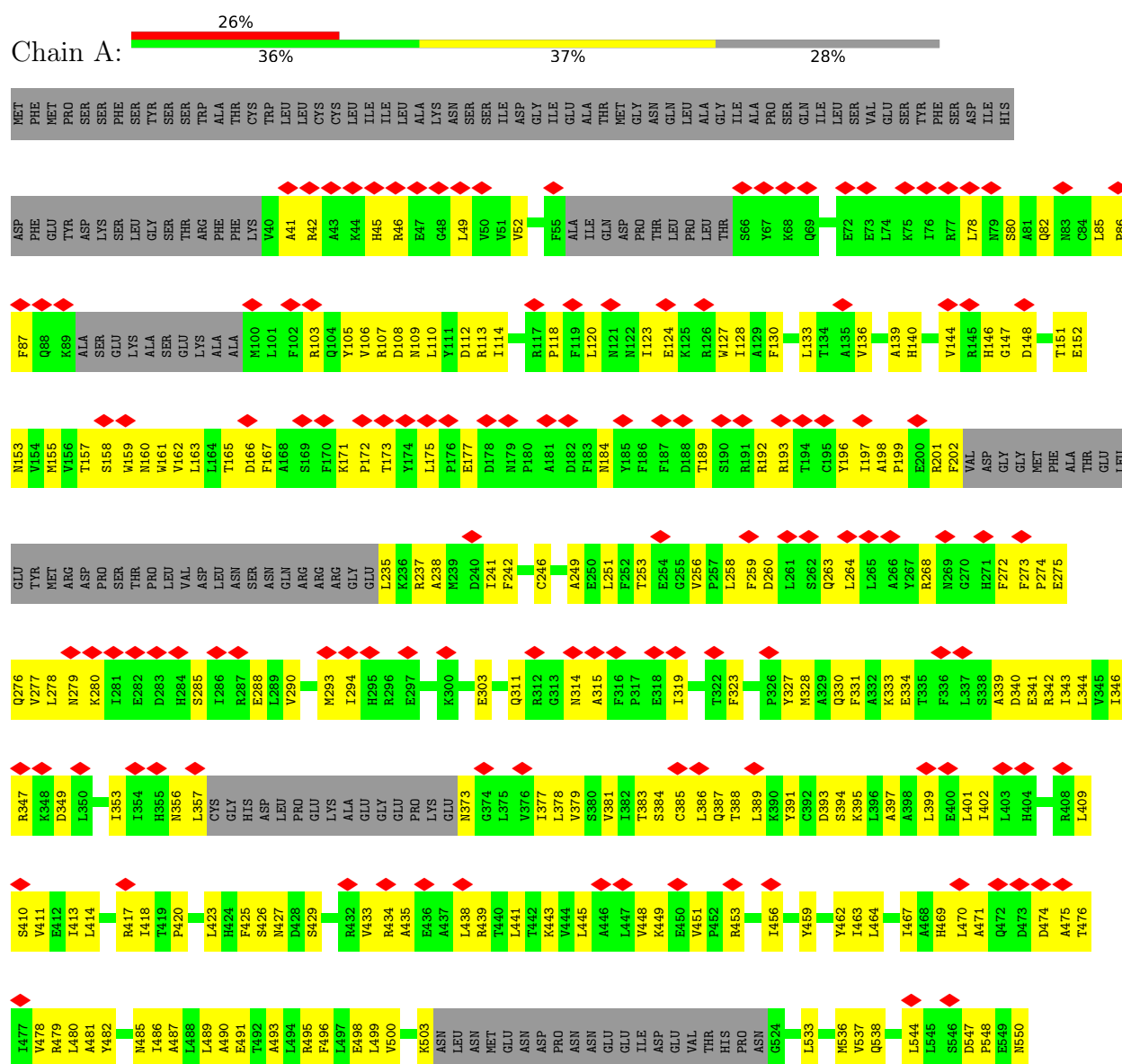
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

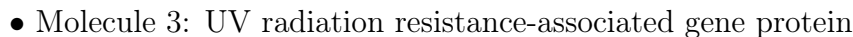
3 Residue-property plots

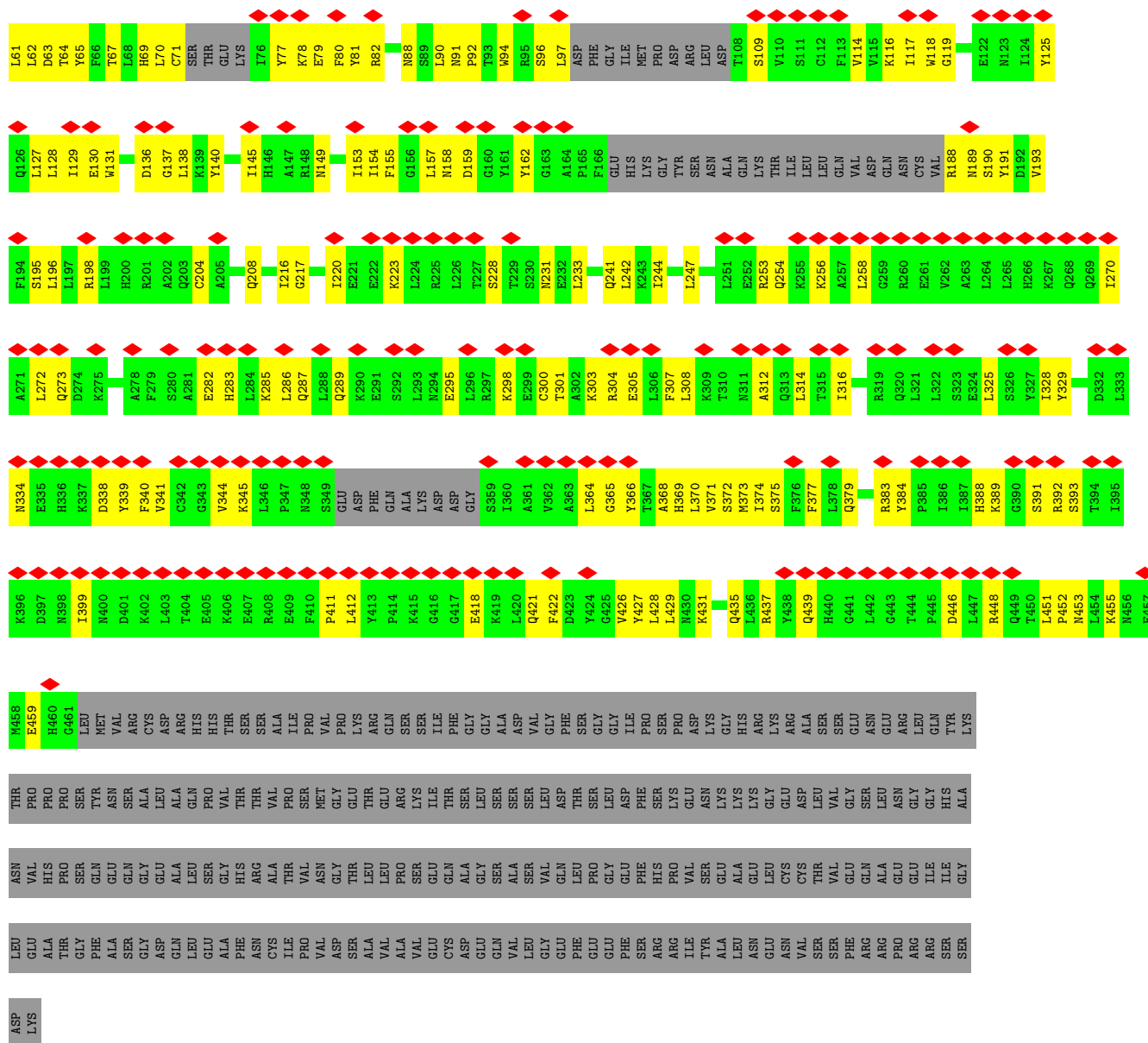
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Phosphoinositide 3-kinase regulatory subunit 4

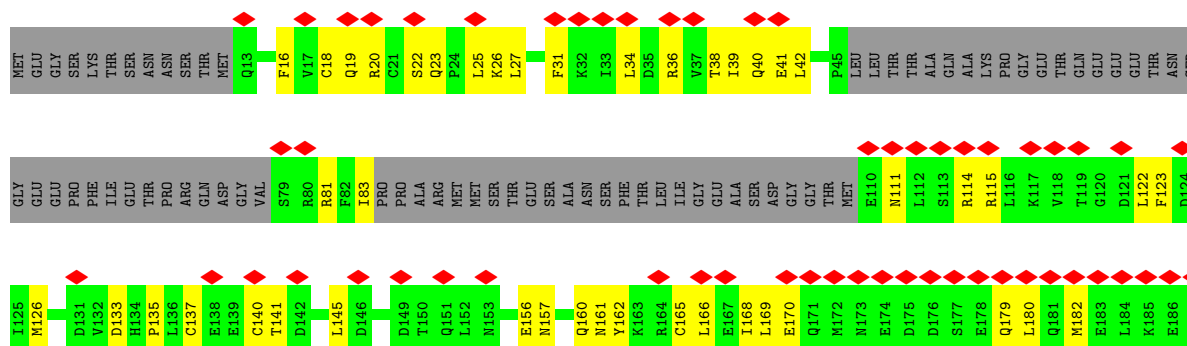








• Molecule 4: Beclin-1



E192	R193	L194	L198	E199	D200	V201	E202	K203	N204	R205	K206	I207	E213	K214	E218	R221	Q224	Y229	Q230	R231	E232	Y233	S234	E235	F236	K237	R238	Q239	Q240	L241	E242	E246	L247	K248	S249	N252	R255	Y256	A257	Q258	T259	Q260	L261	D262	K263	L264	K265	K266	T267	N268								
V269	F270	N271	A272	T273	F274	H275	I276	H277	H278	S279	G280	Q281	F282	G283	T284	I285	N286	N287	F288	R289	L290	G291	R292	L293	P294	S295	V296	P297	V298	E299	W300	N301	E302	I303	N304	Q309	T310	V311	L312	L313	L314	H315	A316	L317	A318	N319	K320	M321	G322	L323	K324	F325	Q326	R327	Y328	R329	L330	V331
P332	Y333	G334	ASN	HIS	SER	TYR	LEU	GLU	SER	LEU	THR	ASP	LYS	SER	GLY	LEU	PRO	GLY	TYR	CYS	SER	GLY	GLY	LEU	ARG	PHE	PHE	TRP	ASP	ASN	LYS	PHE	D366	H367	A371	F372	L373	D374	Q377	Q378	F379	K380	E381	E382	V383	E384	K385	G386	E387	T388	R389	F390	C391	L392	P393	Y394		
R395	M396	D397	V398	E399	K400	G401	K402	T403	E404	D405	T406	GLY	GLY	SER	GLY	GLY	SER	TYR	SER	ILE	LYS	THR	GLN	PHE	ASN	SER	SER	GLU	GLU	Q424	W425	T426	K427	A428	L429	K430	F431	M432	L433	T434	M435	L436	K437	W438	G439	L440	A441	W442	W443	S444	S445	Q446	F447	TYR	ASN	LYS		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	234920	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.842	Depositor
Minimum map value	-0.469	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.19	Depositor
Map size (Å)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: GDP, ZN, MG

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	0.42	0/8539	0.60	0/11579
2	B	0.39	0/2084	0.51	0/2812
3	C	0.30	0/3208	0.50	0/4314
4	D	0.27	0/2749	0.47	0/3699
All	All	0.37	0/16580	0.55	0/22404

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8350	0	8405	519	0
2	B	2034	0	2020	109	0
3	C	3153	0	3241	142	0
4	D	2708	0	2659	149	0
5	A	28	0	12	1	0
6	A	1	0	0	0	0
7	D	1	0	0	0	0
All	All	16275	0	16337	825	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 25.

All (825) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:HD3	1:A:166:ASP:OD1	1.61	0.98
1:A:1017:VAL:CG2	1:A:1045:VAL:HG11	1.96	0.96
1:A:103:ARG:HD3	1:A:166:ASP:CG	1.92	0.94
1:A:106:VAL:HG21	1:A:155:MET:HB3	1.46	0.93
1:A:999:ILE:HD13	1:A:1346:VAL:HG12	1.51	0.91
1:A:1188:ARG:HD3	1:A:1243:HIS:HB3	1.51	0.91
1:A:1060:ALA:HB2	1:A:1101:MET:HE3	1.52	0.90
1:A:1017:VAL:HG11	1:A:1059:ILE:HD12	1.56	0.87
3:C:188:ARG:NH1	4:D:18:CYS:SG	2.47	0.86
2:B:18:ASN:HD22	2:B:92:LYS:HE2	1.41	0.84
1:A:1066:VAL:HG13	1:A:1101:MET:HE1	1.59	0.84
1:A:1196:TYR:HB3	1:A:1199:TRP:CD1	2.13	0.83
3:C:49:ALA:HB1	3:C:51:ARG:HH22	1.45	0.81
1:A:705:GLN:H	1:A:719:VAL:HG13	1.46	0.80
4:D:315:HIS:CD2	4:D:332:PRO:HD3	2.17	0.80
3:C:228:SER:HA	3:C:231:ASN:HB3	1.63	0.79
1:A:386:LEU:HD11	1:A:402:ILE:HD11	1.65	0.79
1:A:1017:VAL:HG22	1:A:1045:VAL:HG11	1.64	0.78
2:B:76:THR:HA	2:B:91:LEU:HD21	1.64	0.78
3:C:69:HIS:HB2	3:C:114:VAL:HB	1.66	0.78
4:D:315:HIS:CG	4:D:332:PRO:HD3	2.19	0.78
1:A:411:VAL:HG13	1:A:448:VAL:HG13	1.67	0.77
3:C:47:ASN:HA	3:C:96:SER:HB3	1.67	0.77
1:A:640:THR:HG23	1:A:681:VAL:HG21	1.69	0.75
1:A:676:VAL:HG13	1:A:716:LEU:HD23	1.67	0.75
2:B:112:ASP:OD1	2:B:113:VAL:N	2.18	0.75
3:C:71:CYS:HB2	3:C:114:VAL:HG23	1.67	0.75
1:A:570:ARG:HH12	3:C:46:ARG:CB	2.00	0.75
1:A:1202:ALA:HB3	1:A:1213:TRP:HZ3	1.52	0.74
1:A:113:ARG:NH2	1:A:118:PRO:O	2.20	0.74
1:A:667:PRO:HA	1:A:723:PRO:HB2	1.70	0.74
1:A:691:VAL:O	1:A:695:LEU:HB2	1.87	0.74
3:C:216:ILE:HG23	4:D:166:LEU:HD11	1.70	0.73
4:D:31:PHE:HA	4:D:34:LEU:HD23	1.70	0.73
1:A:679:ILE:HD13	1:A:699:LEU:HD21	1.70	0.73
1:A:997:ASN:HB2	1:A:1046:LYS:HB2	1.70	0.73
3:C:223:LYS:NZ	4:D:170:GLU:OE1	2.22	0.73
1:A:570:ARG:HH12	3:C:46:ARG:HB3	1.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:383:ARG:NH1	3:C:384:TYR:OH	2.23	0.72
1:A:1017:VAL:HG21	1:A:1059:ILE:HG21	1.70	0.72
1:A:1163:GLY:HA2	1:A:1187:ILE:HG13	1.71	0.72
1:A:1090:LEU:HB3	1:A:1095:ASP:HB2	1.71	0.72
2:B:57:LEU:HB2	2:B:87:TRP:CZ2	2.25	0.72
1:A:147:GLY:O	1:A:201:ARG:NH2	2.23	0.71
3:C:289:GLN:HB3	4:D:236:PHE:CZ	2.25	0.71
1:A:420:PRO:HB2	2:B:265:LEU:HD23	1.73	0.71
1:A:639:LEU:HB3	1:A:678:PHE:CE1	2.26	0.71
1:A:747:MET:HA	1:A:750:LYS:HE2	1.72	0.71
1:A:427:ASN:OD1	1:A:469:HIS:NE2	2.24	0.70
1:A:724:VAL:HG12	1:A:783:GLU:HG2	1.72	0.70
4:D:330:LEU:HD13	4:D:333:TYR:HE1	1.56	0.70
2:B:30:ARG:HH11	2:B:122:VAL:HG11	1.56	0.70
2:B:21:LEU:HD21	2:B:108:LEU:HD21	1.74	0.70
1:A:1113:ALA:HB1	1:A:1121:LEU:HD21	1.73	0.69
3:C:43:ARG:NH1	4:D:133:ASP:OD1	2.26	0.69
1:A:1199:TRP:CH2	1:A:1221:ARG:HB2	2.28	0.69
4:D:289:ARG:HH21	4:D:298:VAL:HG22	1.56	0.69
1:A:435:ALA:HB1	1:A:439:ARG:HH12	1.57	0.69
2:B:142:ASP:H	2:B:162:ARG:HH11	1.39	0.69
4:D:378:GLN:O	4:D:382:GLU:N	2.23	0.69
1:A:448:VAL:O	1:A:495:ARG:NH1	2.25	0.69
4:D:235:GLU:OE2	4:D:239:GLN:NE2	2.25	0.68
1:A:487:ALA:HB2	1:A:560:GLY:HA2	1.75	0.68
1:A:109:ASN:ND2	1:A:112:ASP:OD2	2.27	0.68
1:A:439:ARG:HG2	1:A:443:LYS:HE3	1.74	0.68
3:C:412:LEU:HD13	3:C:429:LEU:HD22	1.75	0.68
1:A:387:GLN:HE22	2:B:263:GLU:H	1.40	0.68
1:A:1172:PHE:CD1	2:B:197:THR:HG21	2.28	0.68
3:C:116:LYS:HD2	3:C:127:LEU:HD11	1.74	0.68
4:D:213:GLU:OE2	4:D:214:LYS:NZ	2.25	0.68
4:D:436:LEU:O	4:D:440:LEU:N	2.24	0.68
2:B:57:LEU:HB2	2:B:87:TRP:HZ2	1.56	0.68
1:A:594:ARG:NH2	1:A:626:ASP:OD2	2.25	0.67
3:C:233:LEU:HD22	4:D:180:LEU:HB3	1.76	0.67
1:A:198:ALA:HB3	1:A:201:ARG:HG3	1.74	0.67
1:A:1155:TRP:HE3	1:A:1167:CYS:HG	1.43	0.67
2:B:199:ARG:O	2:B:203:MET:HG2	1.94	0.67
1:A:487:ALA:O	1:A:563:ARG:NH1	2.28	0.67
1:A:684:ARG:NH1	1:A:711:GLU:O	2.23	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLN:O	1:A:161:TRP:NE1	2.27	0.67
1:A:327:TYR:CZ	1:A:353:ILE:HD11	2.30	0.66
3:C:116:LYS:NZ	3:C:130:GLU:OE1	2.28	0.66
3:C:44:HIS:ND1	3:C:158:ASN:OD1	2.28	0.66
1:A:159:TRP:HB2	1:A:381:VAL:HG22	1.76	0.66
2:B:60:THR:HG1	2:B:111:TRP:CD1	2.13	0.66
1:A:1196:TYR:HB3	1:A:1199:TRP:HD1	1.57	0.66
4:D:314:LEU:HD12	4:D:372:PHE:CZ	2.29	0.66
1:A:1243:HIS:CD2	1:A:1333:THR:HA	2.31	0.66
1:A:482:TYR:HE2	1:A:486:ILE:HD12	1.60	0.66
1:A:1047:THR:HB	1:A:1060:ALA:HB3	1.76	0.66
1:A:1046:LYS:O	1:A:1047:THR:OG1	2.13	0.65
2:B:129:LEU:HB3	2:B:136:PHE:HE1	1.59	0.65
1:A:708:ILE:HG21	3:C:231:ASN:HD21	1.62	0.65
1:A:237:ARG:NH2	1:A:303:GLU:OE1	2.29	0.65
1:A:533:LEU:HA	1:A:536:MET:HE2	1.78	0.65
1:A:572:LYS:H	1:A:572:LYS:HD2	1.61	0.65
1:A:160:ASN:HD22	1:A:377:ILE:HA	1.62	0.65
4:D:114:ARG:HH12	4:D:115:ARG:HH11	1.45	0.65
1:A:1017:VAL:HG11	1:A:1059:ILE:CD1	2.26	0.64
1:A:1099:VAL:HG11	1:A:1144:ILE:O	1.96	0.64
4:D:314:LEU:HD12	4:D:372:PHE:CE1	2.32	0.64
1:A:602:VAL:HG21	1:A:641:CYS:HB2	1.79	0.64
3:C:418:GLU:HB3	3:C:421:GLN:HB2	1.80	0.64
1:A:1244:GLY:O	1:A:1258:THR:HA	1.96	0.64
4:D:165:CYS:HA	4:D:168:ILE:HG22	1.79	0.64
1:A:78:LEU:HD11	1:A:144:VAL:HG11	1.78	0.64
1:A:498:GLU:OE1	3:C:90:LEU:N	2.24	0.64
1:A:1143:LEU:O	1:A:1161:SER:N	2.26	0.64
2:B:60:THR:HA	2:B:74:VAL:O	1.97	0.64
3:C:188:ARG:HH22	4:D:137:CYS:HA	1.63	0.64
1:A:1266:ARG:HG2	1:A:1278:VAL:HG22	1.80	0.64
1:A:1151:ILE:O	1:A:1153:GLN:NE2	2.31	0.63
1:A:668:ASN:OD1	1:A:669:LEU:N	2.31	0.63
1:A:172:PRO:O	1:A:201:ARG:NH1	2.30	0.63
1:A:1212:MET:HB2	1:A:1222:PHE:HB3	1.81	0.63
2:B:106:VAL:HG23	2:B:129:LEU:HD11	1.80	0.63
1:A:1202:ALA:HB3	1:A:1213:TRP:CZ3	2.33	0.63
1:A:103:ARG:HD2	1:A:165:THR:HB	1.81	0.63
1:A:682:VAL:HG12	1:A:695:LEU:HD21	1.80	0.62
2:B:59:VAL:HG22	2:B:110:ILE:HG13	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:270:PHE:HE2	4:D:316:ALA:HB1	1.64	0.62
1:A:984:LEU:HD21	3:C:399:ILE:HD12	1.81	0.62
1:A:1172:PHE:CZ	2:B:187:MET:HE1	2.33	0.62
1:A:1245:ILE:HG23	1:A:1256:LEU:HD11	1.81	0.62
4:D:270:PHE:O	4:D:274:PHE:N	2.27	0.62
1:A:41:ALA:HB3	1:A:52:VAL:O	1.98	0.62
1:A:334:GLU:OE1	1:A:334:GLU:N	2.28	0.62
3:C:365:GLY:HA3	3:C:391:SER:HA	1.80	0.62
1:A:290:VAL:HG12	1:A:294:ILE:HD13	1.81	0.62
1:A:1328:HIS:ND1	1:A:1349:SER:HB2	2.13	0.62
1:A:1172:PHE:HA	2:B:174:ARG:HH11	1.64	0.62
1:A:110:LEU:HD11	1:A:251:LEU:HD13	1.82	0.62
1:A:323:PHE:CZ	1:A:353:ILE:HG12	2.35	0.62
1:A:342:ARG:NH1	2:B:256:PRO:O	2.33	0.62
2:B:76:THR:HG22	2:B:91:LEU:HD11	1.82	0.62
4:D:431:PHE:O	4:D:435:ASN:N	2.30	0.62
2:B:192:TRP:H	2:B:192:TRP:CD1	2.16	0.61
1:A:474:ASP:OD1	1:A:475:ALA:N	2.33	0.61
1:A:331:PHE:HB3	1:A:342:ARG:NH2	2.15	0.61
2:B:33:LYS:O	3:C:253:ARG:NH1	2.33	0.61
1:A:109:ASN:OD1	1:A:155:MET:HE1	2.00	0.61
1:A:561:ILE:HG23	1:A:577:LEU:HD21	1.83	0.61
4:D:377:GLN:NE2	4:D:381:GLU:OE2	2.33	0.61
4:D:273:THR:O	4:D:286:ASN:ND2	2.34	0.61
1:A:701:PRO:HG2	1:A:702:TYR:CE2	2.36	0.61
1:A:1104:PHE:HZ	1:A:1133:TRP:HZ2	1.49	0.61
1:A:146:HIS:ND1	1:A:167:PHE:HA	2.15	0.60
1:A:651:PRO:O	1:A:655:GLU:HG2	2.01	0.60
2:B:142:ASP:OD1	2:B:162:ARG:NH1	2.34	0.60
4:D:221:ARG:HH11	4:D:224:GLN:HG2	1.66	0.60
4:D:111:ASN:HA	4:D:114:ARG:HG2	1.84	0.60
4:D:315:HIS:ND1	4:D:331:VAL:HA	2.16	0.60
1:A:199:PRO:HD3	1:A:242:PHE:CE2	2.37	0.60
1:A:791:LYS:O	1:A:795:MET:HG3	2.01	0.60
1:A:1017:VAL:HG22	1:A:1045:VAL:CG1	2.29	0.60
3:C:286:LEU:HD13	4:D:233:TYR:HD1	1.66	0.60
1:A:996:VAL:HB	1:A:1348:ALA:HB1	1.84	0.60
1:A:686:ILE:HD11	1:A:695:LEU:HD11	1.84	0.60
1:A:1101:MET:HG2	1:A:1114:TYR:HB3	1.83	0.60
1:A:1288:VAL:HG12	1:A:1305:GLN:HA	1.84	0.60
2:B:101:PRO:HD2	2:B:104:ALA:HB2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:ASP:OD1	4:D:238:ARG:NH1	2.33	0.59
4:D:387:GLU:OE1	4:D:442:TRP:NE1	2.25	0.59
1:A:1172:PHE:CE2	2:B:187:MET:HE1	2.37	0.59
1:A:1292:ARG:HH11	1:A:1299:GLU:CD	2.10	0.59
1:A:342:ARG:HH11	2:B:256:PRO:HB2	1.67	0.59
1:A:747:MET:HG2	1:A:756:LEU:HD22	1.83	0.59
1:A:1005:HIS:CE1	1:A:1055:HIS:HA	2.37	0.59
3:C:128:LEU:O	3:C:129:ILE:HG12	2.02	0.59
3:C:325:LEU:HD22	3:C:377:PHE:HE2	1.67	0.59
4:D:392:LEU:HB3	4:D:435:ASN:OD1	2.01	0.59
1:A:381:VAL:O	1:A:384:SER:OG	2.21	0.59
1:A:547:ASP:O	1:A:553:LYS:HE3	2.03	0.59
1:A:588:LYS:NZ	1:A:626:ASP:OD1	2.27	0.59
1:A:1199:TRP:CZ3	1:A:1221:ARG:HB2	2.37	0.59
2:B:35:TYR:HE1	4:D:202:GLU:HG3	1.68	0.59
1:A:688:THR:HA	1:A:691:VAL:HB	1.85	0.59
2:B:129:LEU:HB3	2:B:136:PHE:CE1	2.38	0.59
1:A:1155:TRP:HE3	1:A:1167:CYS:SG	2.26	0.59
1:A:568:PHE:HE2	1:A:577:LEU:HD22	1.68	0.59
1:A:1081:LYS:HE2	1:A:1083:HIS:HD2	1.66	0.59
2:B:26:LEU:HD21	2:B:215:MET:HE3	1.85	0.59
1:A:1017:VAL:CG1	1:A:1059:ILE:HD12	2.32	0.58
3:C:340:PHE:HA	3:C:344:VAL:O	2.02	0.58
1:A:110:LEU:HD23	1:A:151:THR:HG23	1.85	0.58
1:A:438:LEU:HD11	1:A:489:LEU:HD11	1.84	0.58
1:A:557:MET:HE1	1:A:597:PHE:HA	1.86	0.58
1:A:1257:LEU:HD23	1:A:1335:VAL:HG11	1.86	0.58
4:D:313:LEU:HD21	4:D:440:LEU:HD12	1.85	0.58
1:A:420:PRO:HB3	2:B:269:LYS:HB2	1.85	0.58
1:A:690:ASP:OD1	4:D:162:TYR:OH	2.22	0.58
1:A:445:LEU:HD13	1:A:459:TYR:HE1	1.69	0.58
1:A:413:ILE:HA	1:A:417:ARG:HH22	1.69	0.58
1:A:557:MET:CE	1:A:597:PHE:HA	2.34	0.58
1:A:762:PRO:HD2	1:A:768:ALA:HB2	1.86	0.58
1:A:414:LEU:HD23	1:A:418:ILE:HD12	1.86	0.58
4:D:317:LEU:HD22	4:D:443:VAL:HG21	1.86	0.58
1:A:481:ALA:O	1:A:485:ASN:ND2	2.32	0.57
1:A:985:LEU:HD22	1:A:1326:VAL:HB	1.85	0.57
1:A:253:THR:HB	1:A:256:VAL:HB	1.85	0.57
1:A:434:ARG:HD2	1:A:478:VAL:HG21	1.86	0.57
2:B:191:ASP:HB3	2:B:195:ARG:NH1	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:191:TYR:CE2	3:C:196:LEU:HB2	2.38	0.57
1:A:1201:ILE:HG12	1:A:1212:MET:HG2	1.86	0.57
1:A:664:LEU:HD21	1:A:679:ILE:HD12	1.84	0.57
1:A:680:THR:HG22	1:A:710:ILE:O	2.04	0.57
1:A:1261:SER:HA	1:A:1331:ILE:HG23	1.86	0.57
1:A:989:LEU:HD13	1:A:1020:TRP:CZ3	2.40	0.57
1:A:1292:ARG:NH1	1:A:1299:GLU:OE1	2.38	0.57
3:C:228:SER:HA	3:C:231:ASN:CB	2.35	0.57
4:D:381:GLU:O	4:D:385:LYS:N	2.22	0.57
1:A:1155:TRP:HA	1:A:1168:TRP:O	2.05	0.57
1:A:238:ALA:O	1:A:241:ILE:HG22	2.05	0.56
2:B:63:VAL:HG21	2:B:95:VAL:HG21	1.86	0.56
1:A:1090:LEU:HD13	1:A:1095:ASP:HB3	1.85	0.56
2:B:52:GLU:OE1	3:C:256:LYS:NZ	2.38	0.56
3:C:254:GLN:OE1	4:D:205:ARG:NH2	2.37	0.56
1:A:49:LEU:N	2:B:260:MET:HE2	2.21	0.56
1:A:479:ARG:HH22	1:A:548:PRO:HD2	1.69	0.56
1:A:704:THR:N	1:A:719:VAL:O	2.36	0.56
1:A:1064:GLY:HA2	1:A:1097:CYS:HA	1.87	0.56
1:A:1330:ASP:OD1	4:D:252:ASN:ND2	2.25	0.56
4:D:36:ARG:NE	4:D:40:GLN:OE1	2.37	0.56
4:D:292:ARG:HG3	4:D:298:VAL:HB	1.86	0.56
1:A:1017:VAL:HG21	1:A:1059:ILE:CG2	2.36	0.56
3:C:370:LEU:O	3:C:374:ILE:HG12	2.05	0.56
1:A:557:MET:HE3	1:A:581:MET:HG2	1.87	0.56
1:A:1021:ASN:HD22	1:A:1035:ILE:HD12	1.71	0.56
1:A:1068:LEU:O	1:A:1069:LEU:HD12	2.05	0.56
1:A:148:ASP:OD2	1:A:171:LYS:NZ	2.38	0.56
3:C:69:HIS:CD2	3:C:79:GLU:HB3	2.40	0.56
1:A:550:ASN:HB3	1:A:593:LEU:HB2	1.88	0.56
4:D:311:VAL:HA	4:D:372:PHE:HE2	1.70	0.56
1:A:629:GLU:CD	1:A:726:ARG:HH12	2.14	0.56
1:A:495:ARG:HG3	3:C:88:ASN:HB3	1.88	0.56
1:A:346:ILE:HG22	1:A:401:LEU:HD11	1.88	0.55
1:A:670:TRP:CZ2	2:B:58:TYR:HE2	2.23	0.55
3:C:340:PHE:HE1	3:C:345:LYS:HG2	1.71	0.55
4:D:179:GLN:HA	4:D:182:MET:HE3	1.88	0.55
2:B:70:LEU:HD21	2:B:99:ASP:O	2.05	0.55
1:A:1086:GLN:HE21	1:A:1087:SER:H	1.54	0.55
3:C:364:LEU:HD23	3:C:451:LEU:HD11	1.89	0.55
4:D:276:ILE:HG23	4:D:433:LEU:HB3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:TRP:HE3	1:A:631:VAL:HG23	1.71	0.55
1:A:673:TYR:HD2	2:B:113:VAL:HG21	1.70	0.55
2:B:55:SER:H	2:B:85:TRP:HE1	1.53	0.55
1:A:459:TYR:CE1	1:A:463:ILE:HG21	2.41	0.55
1:A:1169:ASP:OD2	1:A:1171:ARG:NH1	2.29	0.55
1:A:1181:HIS:CD2	1:A:1204:VAL:HG11	2.42	0.55
1:A:133:LEU:HD21	1:A:293:MET:HE1	1.89	0.55
1:A:462:TYR:HB2	2:B:273:LEU:HD21	1.89	0.55
1:A:1072:GLU:HB2	1:A:1081:LYS:HB3	1.87	0.55
3:C:217:GLY:O	3:C:220:ILE:HG22	2.07	0.55
4:D:221:ARG:NH1	4:D:224:GLN:HG2	2.21	0.55
1:A:1001:VAL:CG1	1:A:1338:PHE:HB3	2.36	0.55
1:A:1002:SER:HB3	1:A:1050:PHE:CG	2.41	0.55
2:B:90:TRP:CZ3	2:B:222:ARG:HB2	2.42	0.55
3:C:70:LEU:HD21	3:C:80:PHE:HE2	1.72	0.55
3:C:94:TRP:HH2	3:C:117:ILE:HD13	1.72	0.55
1:A:1156:LEU:HD23	1:A:1170:MET:SD	2.47	0.55
3:C:270:ILE:O	3:C:273:GLN:HG2	2.07	0.55
1:A:746:HIS:C	1:A:750:LYS:HZ3	2.15	0.54
3:C:190:SER:HB3	4:D:25:LEU:HD12	1.89	0.54
1:A:471:ALA:HB2	1:A:482:TYR:CZ	2.43	0.54
1:A:702:TYR:OH	1:A:789:ALA:HB1	2.07	0.54
1:A:1172:PHE:HD1	2:B:197:THR:HG21	1.72	0.54
1:A:1051:CYS:HA	1:A:1103:HIS:ND1	2.22	0.54
1:A:1213:TRP:NE1	1:A:1220:ARG:HB2	2.22	0.54
1:A:87:PHE:CZ	1:A:166:ASP:HB3	2.41	0.54
1:A:353:ILE:HG21	1:A:378:LEU:HD22	1.90	0.54
1:A:598:PHE:HE1	1:A:620:LEU:HG	1.73	0.54
3:C:369:HIS:CD2	3:C:373:MET:HG2	2.42	0.54
4:D:16:PHE:HD2	4:D:27:LEU:HD11	1.72	0.54
1:A:413:ILE:HA	1:A:417:ARG:NH2	2.23	0.54
2:B:105:GLN:NE2	2:B:153:GLY:O	2.37	0.54
3:C:129:ILE:HG23	3:C:131:TRP:CD1	2.43	0.54
1:A:114:ILE:HD13	1:A:120:LEU:HD12	1.89	0.54
1:A:581:MET:SD	1:A:604:VAL:HG21	2.48	0.54
1:A:1085:LEU:HD12	1:A:1085:LEU:O	2.08	0.54
1:A:1230:PRO:HB2	1:A:1233:SER:HB2	1.90	0.54
2:B:199:ARG:O	2:B:202:GLU:HG3	2.06	0.54
4:D:292:ARG:NE	4:D:298:VAL:O	2.41	0.54
1:A:276:GLN:HG2	1:A:277:VAL:N	2.23	0.54
1:A:343:ILE:HG13	1:A:389:LEU:HD21	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ILE:HD12	1:A:377:ILE:H	1.72	0.54
1:A:629:GLU:O	1:A:633:VAL:HG23	2.08	0.54
1:A:1001:VAL:HG11	1:A:1338:PHE:HB3	1.89	0.54
1:A:1213:TRP:CD1	1:A:1220:ARG:HB2	2.42	0.54
2:B:107:ALA:HB1	2:B:151:ALA:HB3	1.90	0.54
1:A:1118:ASN:HD22	4:D:231:ARG:HG2	1.72	0.54
4:D:274:PHE:CE2	4:D:309:GLN:HG2	2.43	0.54
1:A:78:LEU:HG	1:A:144:VAL:HG21	1.90	0.53
1:A:285:SER:HB3	1:A:315:ALA:HB2	1.90	0.53
1:A:157:THR:HG22	1:A:158:SER:H	1.73	0.53
2:B:264:ASN:ND2	2:B:267:GLU:OE1	2.41	0.53
3:C:193:VAL:HG11	4:D:34:LEU:HD21	1.89	0.53
4:D:16:PHE:CD2	4:D:27:LEU:HD11	2.43	0.53
1:A:441:LEU:HD11	1:A:463:ILE:HD11	1.90	0.53
1:A:105:TYR:HD1	2:B:260:MET:HE3	1.73	0.53
1:A:275:GLU:HA	1:A:278:LEU:HB2	1.90	0.53
1:A:453:ARG:HG2	1:A:503:LYS:HD2	1.91	0.53
1:A:989:LEU:HD22	1:A:1020:TRP:HZ3	1.73	0.53
4:D:374:ASP:HA	4:D:377:GLN:HB3	1.89	0.53
1:A:456:ILE:HD12	1:A:500:VAL:HG13	1.89	0.53
3:C:300:CYS:SG	3:C:303:LYS:NZ	2.73	0.53
1:A:1077:PRO:HG2	1:A:1079:SER:O	2.08	0.53
3:C:384:TYR:CE2	3:C:428:LEU:HD22	2.43	0.53
1:A:399:LEU:HD21	1:A:425:PHE:HD2	1.74	0.53
1:A:471:ALA:HB2	1:A:482:TYR:CE1	2.44	0.53
2:B:63:VAL:HG22	2:B:106:VAL:HG22	1.90	0.53
4:D:380:LYS:HB2	4:D:392:LEU:HD12	1.91	0.53
3:C:191:TYR:HE2	3:C:196:LEU:HB2	1.72	0.52
1:A:1226:ALA:HA	1:A:1303:GLU:HB3	1.91	0.52
3:C:435:GLN:O	3:C:439:GLN:HG2	2.09	0.52
4:D:390:PHE:CE2	4:D:438:TRP:HB3	2.44	0.52
1:A:482:TYR:CD2	1:A:544:LEU:HD11	2.44	0.52
1:A:1199:TRP:HH2	1:A:1221:ARG:HB2	1.73	0.52
1:A:1164:THR:OG1	1:A:1180:CYS:SG	2.63	0.52
1:A:1242:VAL:HG11	1:A:1258:THR:HB	1.91	0.52
1:A:1300:VAL:HG12	1:A:1302:GLN:HG3	1.91	0.52
2:B:136:PHE:HB3	2:B:233:ILE:HB	1.91	0.52
1:A:314:ASN:OD1	1:A:315:ALA:N	2.42	0.52
1:A:413:ILE:HG23	1:A:417:ARG:NH2	2.23	0.52
1:A:972:SER:HB2	1:A:974:PRO:HD2	1.92	0.52
1:A:565:CYS:HB3	1:A:607:TYR:CG	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:274:PHE:HD1	4:D:313:LEU:HD13	1.75	0.52
1:A:340:ASP:O	1:A:344:LEU:HG	2.10	0.52
1:A:570:ARG:HH12	3:C:46:ARG:HB2	1.73	0.52
1:A:664:LEU:O	1:A:672:ARG:HD3	2.10	0.52
1:A:328:MET:HE3	1:A:377:ILE:HG22	1.91	0.51
3:C:295:GLU:O	3:C:298:LYS:HG2	2.10	0.51
3:C:411:PRO:O	3:C:412:LEU:HD23	2.10	0.51
1:A:136:VAL:HG12	1:A:140:HIS:CE1	2.45	0.51
1:A:629:GLU:HB3	1:A:671:ILE:HD11	1.92	0.51
1:A:1223:THR:HG21	1:A:1232:LEU:HD21	1.90	0.51
1:A:1050:PHE:CD2	1:A:1057:LEU:HD13	2.46	0.51
3:C:188:ARG:O	4:D:26:LYS:N	2.26	0.51
4:D:271:ASN:HB2	4:D:440:LEU:HD21	1.90	0.51
1:A:105:TYR:O	2:B:260:MET:HE1	2.10	0.51
1:A:451:VAL:HG11	1:A:500:VAL:HG22	1.92	0.51
1:A:637:TYR:CZ	2:B:117:GLY:HA2	2.45	0.51
2:B:44:LEU:HD22	2:B:50:TYR:HE2	1.74	0.51
3:C:258:LEU:HD11	4:D:201:VAL:HG13	1.92	0.51
1:A:731:TYR:HB3	1:A:774:LEU:CD2	2.41	0.51
1:A:1290:TYR:HA	1:A:1302:GLN:O	2.10	0.51
2:B:128:SER:O	2:B:137:ARG:NE	2.36	0.51
1:A:103:ARG:HD3	1:A:166:ASP:OD2	2.10	0.51
1:A:499:LEU:HD22	3:C:61:LEU:CD1	2.41	0.51
1:A:579:SER:O	1:A:583:THR:HG23	2.11	0.51
1:A:724:VAL:HG23	1:A:729:PHE:HB2	1.92	0.51
2:B:25:SER:HA	2:B:85:TRP:O	2.11	0.51
3:C:117:ILE:H	3:C:129:ILE:HB	1.74	0.51
3:C:149:ASN:CG	4:D:81:ARG:HH22	2.18	0.51
1:A:184:ASN:OD1	1:A:193:ARG:NH2	2.34	0.51
1:A:996:VAL:HG22	1:A:1012:SER:HB3	1.91	0.51
3:C:314:LEU:HD11	3:C:379:GLN:HE22	1.75	0.51
4:D:274:PHE:CZ	4:D:312:LEU:HD22	2.45	0.51
1:A:80:SER:O	1:A:82:GLN:NE2	2.43	0.51
1:A:969:GLU:C	1:A:1151:ILE:HG21	2.36	0.51
2:B:130:PHE:CD2	2:B:235:TYR:HB2	2.46	0.51
3:C:45:LEU:HD12	3:C:157:LEU:HD11	1.93	0.51
3:C:303:LYS:HE2	4:D:247:LEU:HG	1.92	0.51
4:D:38:THR:O	4:D:41:GLU:HG3	2.11	0.51
1:A:1186:ARG:HD2	4:D:241:LEU:HD13	1.94	0.50
4:D:18:CYS:O	4:D:22:SER:N	2.37	0.50
1:A:387:GLN:NE2	2:B:262:MET:HB3	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:ARG:HH21	4:D:145:LEU:HD13	1.76	0.50
4:D:273:THR:C	4:D:286:ASN:HD21	2.18	0.50
1:A:612:SER:HA	1:A:615:ILE:HD13	1.92	0.50
1:A:659:ASP:O	1:A:662:PRO:HD2	2.11	0.50
1:A:1139:LEU:HB3	4:D:230:GLN:HB3	1.94	0.50
1:A:328:MET:HE1	1:A:378:LEU:HD12	1.93	0.50
1:A:341:GLU:N	1:A:341:GLU:OE1	2.44	0.50
2:B:182:HIS:ND1	2:B:198:PHE:HZ	2.10	0.50
1:A:1108:ALA:O	1:A:1127:ARG:HD2	2.12	0.50
1:A:1113:ALA:HA	1:A:1122:VAL:O	2.10	0.50
3:C:189:ASN:HA	4:D:26:LYS:HB3	1.94	0.50
1:A:487:ALA:HB2	1:A:560:GLY:CA	2.41	0.50
1:A:557:MET:HB3	1:A:600:SER:OG	2.12	0.50
1:A:746:HIS:CD2	1:A:750:LYS:HZ3	2.29	0.50
1:A:1169:ASP:O	1:A:1173:GLN:N	2.44	0.50
2:B:55:SER:N	2:B:85:TRP:HE1	2.09	0.50
1:A:196:TYR:CE1	1:A:246:CYS:HB3	2.46	0.49
1:A:650:LYS:HG2	1:A:654:TYR:CE2	2.47	0.49
1:A:740:SER:HB3	1:A:767:ILE:HG13	1.94	0.49
1:A:997:ASN:HB2	1:A:1046:LYS:CB	2.39	0.49
1:A:1137:HIS:HE2	1:A:1141:SER:HB2	1.77	0.49
2:B:146:TRP:CG	2:B:159:THR:HG22	2.47	0.49
3:C:129:ILE:HG13	3:C:153:ILE:HD11	1.93	0.49
1:A:49:LEU:H	2:B:260:MET:HE2	1.77	0.49
1:A:602:VAL:HG11	1:A:641:CYS:HB3	1.94	0.49
1:A:662:PRO:HA	1:A:702:TYR:CZ	2.47	0.49
1:A:1207:ASN:HA	1:A:1238:SER:HB3	1.93	0.49
2:B:198:PHE:HA	2:B:201:ILE:HD12	1.94	0.49
4:D:274:PHE:HD2	4:D:286:ASN:OD1	1.94	0.49
1:A:476:THR:O	1:A:480:LEU:HG	2.13	0.49
3:C:272:LEU:HD21	4:D:218:GLU:HG2	1.93	0.49
3:C:341:VAL:O	3:C:344:VAL:HG12	2.12	0.49
4:D:281:GLN:OE1	4:D:281:GLN:N	2.35	0.49
1:A:42:ARG:HG3	1:A:49:LEU:HD23	1.94	0.49
1:A:1038:TYR:HB2	1:A:1082:ILE:HD11	1.94	0.49
1:A:1104:PHE:HZ	1:A:1133:TRP:CZ2	2.28	0.49
3:C:40:ARG:NH2	3:C:162:TYR:HE2	2.11	0.49
1:A:999:ILE:HG12	1:A:1010:THR:HG22	1.94	0.49
1:A:1011:CYS:HB2	1:A:1045:VAL:HG12	1.94	0.49
1:A:1255:ILE:HD12	1:A:1267:PHE:CZ	2.48	0.49
3:C:437:ARG:NH2	3:C:453:ASN:O	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:311:VAL:HG22	4:D:372:PHE:CE2	2.47	0.49
1:A:1137:HIS:NE2	1:A:1141:SER:HB2	2.27	0.49
1:A:1350:ARG:NH1	4:D:246:GLU:OE1	2.40	0.49
3:C:283:HIS:O	3:C:287:GLN:HG2	2.13	0.49
3:C:341:VAL:HG21	3:C:451:LEU:HD22	1.94	0.49
1:A:1020:TRP:N	1:A:1020:TRP:CD1	2.78	0.49
1:A:1160:THR:OG1	1:A:1164:THR:O	2.28	0.49
3:C:40:ARG:NH1	3:C:136:ASP:HA	2.28	0.49
3:C:282:GLU:HB3	4:D:229:TYR:CZ	2.47	0.49
1:A:467:ILE:HD13	1:A:489:LEU:HD13	1.94	0.49
1:A:585:LEU:HD21	1:A:598:PHE:CE2	2.47	0.49
1:A:703:ILE:HD12	1:A:705:GLN:O	2.13	0.49
1:A:1158:ILE:HB	1:A:1166:ALA:HB3	1.94	0.49
1:A:1181:HIS:CD2	1:A:1204:VAL:HG21	2.48	0.49
1:A:1243:HIS:HE2	1:A:1331:ILE:HG22	1.78	0.49
2:B:58:TYR:CE1	2:B:75:ARG:HG2	2.47	0.49
1:A:490:ALA:HB1	1:A:567:PHE:CE2	2.48	0.49
1:A:679:ILE:HG21	1:A:699:LEU:HD11	1.94	0.49
3:C:329:TYR:CD2	3:C:366:TYR:HB3	2.47	0.49
2:B:200:GLU:O	2:B:204:ILE:HG13	2.13	0.49
1:A:155:MET:CG	1:A:165:THR:HG21	2.43	0.48
1:A:319:ILE:HG22	1:A:357:LEU:HD23	1.95	0.48
1:A:591:TRP:CE3	1:A:631:VAL:HG23	2.47	0.48
1:A:1125:ASP:O	1:A:1129:SER:N	2.46	0.48
1:A:349:ASP:O	1:A:353:ILE:HG13	2.12	0.48
1:A:426:SER:HB2	1:A:470:LEU:HD11	1.96	0.48
1:A:1224:LEU:HD23	1:A:1301:VAL:HB	1.95	0.48
3:C:328:ILE:HG21	4:D:312:LEU:HD21	1.95	0.48
3:C:384:TYR:CD2	3:C:428:LEU:HB3	2.48	0.48
4:D:157:ASN:O	4:D:161:ASN:ND2	2.44	0.48
1:A:420:PRO:HB2	2:B:265:LEU:CD2	2.42	0.48
1:A:733:LEU:HB2	1:A:794:MET:CE	2.43	0.48
1:A:1064:GLY:HA3	1:A:1092:GLN:HE22	1.78	0.48
1:A:1199:TRP:CH2	1:A:1214:ASP:HB2	2.48	0.48
1:A:1225:TRP:HB3	1:A:1302:GLN:HG2	1.94	0.48
3:C:282:GLU:O	3:C:285:LYS:HG2	2.14	0.48
3:C:371:VAL:HG21	3:C:429:LEU:HD11	1.94	0.48
4:D:394:TYR:CG	4:D:431:PHE:HB3	2.48	0.48
1:A:409:LEU:HD22	1:A:413:ILE:HG21	1.95	0.48
1:A:1243:HIS:HD2	1:A:1333:THR:HA	1.78	0.48
2:B:140:MET:HG2	2:B:218:MET:SD	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:307:PHE:HE1	4:D:257:ALA:HB2	1.77	0.48
1:A:160:ASN:ND2	1:A:377:ILE:HA	2.29	0.48
1:A:1149:VAL:HG13	1:A:1156:LEU:HB3	1.96	0.48
3:C:303:LYS:HZ3	4:D:247:LEU:HA	1.78	0.48
1:A:78:LEU:HB2	1:A:86:PRO:HG3	1.95	0.48
1:A:499:LEU:HD22	3:C:61:LEU:HD11	1.95	0.48
1:A:568:PHE:CE2	1:A:577:LEU:HB2	2.48	0.48
3:C:64:THR:O	3:C:94:TRP:NE1	2.41	0.48
4:D:39:ILE:HD12	4:D:122:LEU:HD22	1.95	0.48
1:A:625:SER:HB2	1:A:793:PHE:HA	1.96	0.48
4:D:367:HIS:O	4:D:371:ALA:N	2.33	0.48
1:A:1097:CYS:O	1:A:1116:THR:HA	2.14	0.48
3:C:373:MET:HB3	3:C:377:PHE:CE2	2.49	0.48
1:A:1068:LEU:HB2	1:A:1086:GLN:HB2	1.95	0.48
2:B:35:TYR:HB2	4:D:198:LEU:HD21	1.95	0.48
3:C:52:ASN:H	3:C:91:ASN:CG	2.21	0.48
3:C:80:PHE:O	3:C:80:PHE:CG	2.67	0.48
1:A:276:GLN:HG2	1:A:277:VAL:H	1.78	0.48
3:C:334:ASN:OD1	3:C:338:ASP:N	2.45	0.48
4:D:199:GLU:O	4:D:203:LYS:HG2	2.14	0.48
4:D:324:LYS:HG3	4:D:326:GLN:NE2	2.29	0.48
4:D:396:MET:HB3	4:D:396:MET:HE2	1.79	0.48
4:D:274:PHE:CE1	4:D:312:LEU:HD22	2.48	0.47
4:D:390:PHE:CZ	4:D:438:TRP:HB3	2.48	0.47
4:D:430:LYS:O	4:D:434:THR:OG1	2.21	0.47
1:A:249:ALA:HB2	1:A:290:VAL:HG11	1.96	0.47
2:B:194:ASP:OD2	2:B:195:ARG:N	2.47	0.47
1:A:153:ASN:ND2	1:A:165:THR:OG1	2.47	0.47
1:A:258:LEU:HD11	1:A:278:LEU:HD22	1.95	0.47
1:A:750:LYS:O	1:A:754:GLY:N	2.45	0.47
3:C:289:GLN:HB3	4:D:236:PHE:CE2	2.49	0.47
1:A:197:ILE:O	1:A:264:LEU:HD21	2.15	0.47
1:A:636:LEU:HD11	1:A:671:ILE:HG23	1.96	0.47
3:C:188:ARG:C	4:D:26:LYS:HB3	2.39	0.47
4:D:157:ASN:OD1	4:D:161:ASN:ND2	2.48	0.47
1:A:746:HIS:CD2	1:A:750:LYS:NZ	2.82	0.47
2:B:110:ILE:HD11	2:B:217:LEU:HD22	1.97	0.47
3:C:188:ARG:NH2	4:D:137:CYS:HA	2.29	0.47
1:A:198:ALA:HA	1:A:242:PHE:CD2	2.50	0.47
1:A:1150:ASP:HB2	1:A:1155:TRP:CD1	2.49	0.47
3:C:301:THR:HA	3:C:304:ARG:NH2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:VAL:HB	1:A:1088:ARG:HD2	1.96	0.47
1:A:1157:CYS:SG	1:A:1200:VAL:HG11	2.54	0.47
1:A:1172:PHE:CE2	2:B:178:LEU:HB3	2.49	0.47
2:B:19:VAL:HG22	2:B:97:TYR:CE2	2.48	0.47
2:B:39:LEU:HD11	3:C:247:LEU:HD21	1.96	0.47
2:B:206:GLU:O	2:B:210:ARG:HG2	2.14	0.47
3:C:305:GLU:HA	3:C:308:LEU:HD12	1.97	0.47
1:A:498:GLU:HB3	3:C:61:LEU:HD13	1.97	0.47
1:A:591:TRP:CD1	1:A:628:GLU:HG2	2.49	0.47
2:B:59:VAL:H	2:B:76:THR:HG23	1.80	0.47
4:D:137:CYS:HB3	4:D:140:CYS:H	1.80	0.47
4:D:270:PHE:HB3	4:D:313:LEU:CD1	2.45	0.47
1:A:570:ARG:NH1	3:C:46:ARG:HB3	2.24	0.47
1:A:691:VAL:HA	1:A:695:LEU:HD22	1.97	0.47
1:A:1012:SER:OG	1:A:1014:ASP:OD1	2.23	0.47
1:A:1211:SER:HB2	1:A:1213:TRP:CZ3	2.50	0.47
2:B:210:ARG:HA	2:B:210:ARG:HH21	1.79	0.47
1:A:275:GLU:HA	1:A:278:LEU:HD23	1.95	0.47
1:A:495:ARG:HG3	3:C:88:ASN:CB	2.44	0.47
3:C:300:CYS:HA	3:C:303:LYS:HE3	1.96	0.47
4:D:424:GLN:HG3	4:D:425:TRP:H	1.80	0.47
1:A:108:ASP:O	1:A:155:MET:HE3	2.13	0.46
1:A:383:THR:HA	1:A:386:LEU:HD12	1.96	0.46
2:B:41:ASP:HB2	2:B:44:LEU:HD12	1.97	0.46
1:A:568:PHE:CE2	1:A:577:LEU:HD22	2.49	0.46
1:A:1203:ALA:HB2	1:A:1245:ILE:HD11	1.97	0.46
4:D:162:TYR:O	4:D:166:LEU:HG	2.15	0.46
2:B:19:VAL:HG22	2:B:97:TYR:CZ	2.50	0.46
3:C:118:TRP:CE3	3:C:127:LEU:HB2	2.51	0.46
4:D:383:VAL:HG22	4:D:442:TRP:CZ3	2.50	0.46
1:A:553:LYS:HD3	1:A:584:PHE:CE1	2.50	0.46
1:A:630:PHE:HE1	1:A:670:TRP:CD1	2.34	0.46
1:A:691:VAL:HG13	1:A:695:LEU:HD22	1.97	0.46
2:B:41:ASP:O	2:B:44:LEU:HB2	2.15	0.46
1:A:1181:HIS:HB3	1:A:1184:ARG:H	1.81	0.46
1:A:1292:ARG:HE	1:A:1299:GLU:HB3	1.79	0.46
2:B:142:ASP:H	2:B:162:ARG:NH1	2.09	0.46
4:D:190:GLU:OE1	4:D:193:ARG:NH2	2.45	0.46
1:A:199:PRO:HD3	1:A:242:PHE:CD2	2.51	0.46
1:A:347:ARG:HD3	1:A:397:ALA:O	2.15	0.46
1:A:742:PHE:HE2	1:A:795:MET:HG2	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:MET:HG3	2:B:118:LYS:HZ3	1.79	0.46
2:B:182:HIS:HD1	2:B:198:PHE:HZ	1.63	0.46
2:B:210:ARG:HA	2:B:210:ARG:NH2	2.31	0.46
3:C:97:LEU:HD23	3:C:97:LEU:H	1.81	0.46
3:C:241:GLN:HA	3:C:244:ILE:HD12	1.98	0.46
1:A:256:VAL:HG11	1:A:280:LYS:HD2	1.97	0.46
1:A:676:VAL:O	1:A:680:THR:HG23	2.16	0.46
1:A:496:PHE:O	1:A:500:VAL:HG23	2.15	0.46
3:C:191:TYR:HB2	3:C:195:SER:HB3	1.98	0.46
1:A:128:ILE:HG23	1:A:162:VAL:CG2	2.46	0.46
1:A:258:LEU:HG	1:A:259:PHE:CD1	2.51	0.46
1:A:272:PHE:CE2	1:A:274:PRO:HG3	2.51	0.46
2:B:145:VAL:HB	2:B:215:MET:HB2	1.98	0.46
3:C:188:ARG:C	3:C:188:ARG:HD2	2.41	0.46
1:A:449:LYS:NZ	1:A:499:LEU:HD21	2.31	0.46
1:A:1100:ASP:H	1:A:1115:ALA:HB3	1.81	0.46
3:C:190:SER:CB	4:D:25:LEU:HD12	2.45	0.46
4:D:274:PHE:HA	4:D:286:ASN:OD1	2.16	0.46
4:D:374:ASP:OD1	4:D:378:GLN:HG3	2.16	0.46
3:C:372:SER:O	3:C:375:SER:OG	2.33	0.45
1:A:123:ILE:HG12	1:A:373:ASN:O	2.17	0.45
1:A:591:TRP:HB2	1:A:631:VAL:HG23	1.99	0.45
1:A:984:LEU:HD21	3:C:399:ILE:CD1	2.45	0.45
4:D:19:GLN:HB2	4:D:133:ASP:O	2.15	0.45
4:D:431:PHE:O	4:D:434:THR:HB	2.15	0.45
1:A:152:GLU:CD	1:A:192:ARG:HH11	2.24	0.45
1:A:459:TYR:O	1:A:463:ILE:HG22	2.17	0.45
1:A:482:TYR:CE2	1:A:486:ILE:HD12	2.47	0.45
1:A:970:TRP:HE1	1:A:1249:PRO:HD3	1.81	0.45
1:A:1190:LEU:HA	1:A:1201:ILE:O	2.16	0.45
3:C:40:ARG:HH11	3:C:136:ASP:HA	1.81	0.45
3:C:117:ILE:HG13	3:C:129:ILE:HG13	1.97	0.45
1:A:175:LEU:HD12	1:A:197:ILE:HG21	1.97	0.45
1:A:582:ILE:HG12	1:A:619:LEU:HD13	1.99	0.45
1:A:970:TRP:N	1:A:1151:ILE:HG21	2.32	0.45
1:A:1151:ILE:H	1:A:1151:ILE:HD12	1.81	0.45
1:A:1236:GLN:N	1:A:1237:PRO:HD3	2.32	0.45
3:C:128:LEU:O	3:C:128:LEU:HG	2.16	0.45
3:C:312:ALA:O	3:C:316:ILE:HG12	2.17	0.45
4:D:331:VAL:HB	4:D:332:PRO:HD2	1.97	0.45
1:A:453:ARG:HG2	1:A:503:LYS:HZ3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ALA:HA	1:A:797:SER:OG	2.16	0.45
1:A:975:PRO:O	1:A:1339:GLN:NE2	2.49	0.45
3:C:325:LEU:HD22	3:C:377:PHE:CE2	2.50	0.45
4:D:276:ILE:HD12	4:D:440:LEU:HD13	1.98	0.45
1:A:1190:LEU:HD22	1:A:1200:VAL:CG1	2.47	0.45
1:A:598:PHE:O	1:A:638:ALA:HB2	2.17	0.45
1:A:669:LEU:HG	1:A:673:TYR:CE2	2.52	0.45
1:A:731:TYR:HB3	1:A:774:LEU:HD21	1.97	0.45
1:A:1060:ALA:HB1	1:A:1098:VAL:HB	1.98	0.45
3:C:43:ARG:HH11	4:D:133:ASP:CG	2.25	0.45
3:C:369:HIS:HB2	3:C:388:HIS:CE1	2.52	0.45
3:C:422:PHE:O	3:C:426:VAL:HG23	2.17	0.45
4:D:42:LEU:HB3	4:D:126:MET:HE3	1.98	0.45
4:D:311:VAL:HG11	4:D:333:TYR:CD1	2.51	0.45
1:A:45:HIS:CG	1:A:46:ARG:N	2.85	0.45
1:A:107:ARG:NH1	2:B:259:GLN:HE22	2.15	0.45
1:A:479:ARG:NH2	1:A:547:ASP:HB3	2.32	0.45
1:A:616:LEU:HB3	1:A:620:LEU:HD13	1.98	0.45
1:A:633:VAL:HA	1:A:636:LEU:HD12	1.98	0.45
1:A:1049:THR:O	1:A:1057:LEU:HD12	2.17	0.45
3:C:286:LEU:HB2	4:D:229:TYR:HE1	1.82	0.45
1:A:707:ILE:HG23	1:A:719:VAL:HG11	1.97	0.45
1:A:139:ALA:HB1	1:A:144:VAL:HB	1.99	0.45
1:A:177:GLU:OE2	1:A:268:ARG:HD3	2.16	0.45
1:A:605:ALA:HB3	1:A:642:MET:HE2	1.99	0.45
1:A:769:GLN:O	1:A:769:GLN:NE2	2.50	0.45
1:A:972:SER:CB	1:A:974:PRO:HD2	2.46	0.45
3:C:389:LYS:O	3:C:393:SER:HB2	2.17	0.45
1:A:273:PHE:HB3	1:A:275:GLU:OE1	2.17	0.44
1:A:585:LEU:HD23	1:A:585:LEU:HA	1.75	0.44
1:A:683:ALA:HA	1:A:691:VAL:HG22	2.00	0.44
1:A:742:PHE:CE2	1:A:795:MET:HG2	2.52	0.44
1:A:1021:ASN:O	1:A:1025:MET:HG2	2.17	0.44
4:D:156:GLU:O	4:D:160:GLN:HG2	2.17	0.44
1:A:323:PHE:CE1	1:A:353:ILE:HG12	2.52	0.44
1:A:574:ASN:HB2	1:A:608:VAL:HG13	1.99	0.44
1:A:661:ALA:HB3	1:A:662:PRO:HD3	1.99	0.44
1:A:680:THR:HG21	1:A:713:LYS:HG2	1.99	0.44
1:A:1045:VAL:HG13	1:A:1060:ALA:O	2.16	0.44
1:A:1339:GLN:HB3	1:A:1343:GLY:HA2	1.99	0.44
1:A:459:TYR:CD1	1:A:463:ILE:HG21	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ARG:NE	2:B:49:LEU:HG	2.32	0.44
2:B:35:TYR:CE1	4:D:202:GLU:HG3	2.49	0.44
3:C:368:ALA:HB2	3:C:412:LEU:HD12	2.00	0.44
1:A:423:LEU:HD21	1:A:463:ILE:CD1	2.46	0.44
1:A:1214:ASP:HB3	1:A:1217:THR:HG22	1.99	0.44
2:B:26:LEU:O	2:B:85:TRP:HE3	2.01	0.44
2:B:64:PHE:O	2:B:104:ALA:HA	2.17	0.44
1:A:1268:TRP:HA	1:A:1276:SER:HB3	1.99	0.44
3:C:63:ASP:O	3:C:125:TYR:HE1	2.00	0.44
3:C:140:TYR:OH	3:C:159:ASP:O	2.27	0.44
4:D:204:ASN:HA	4:D:207:ILE:HG22	2.00	0.44
1:A:85:LEU:HB2	1:A:163:LEU:HD23	1.98	0.44
1:A:384:SER:O	2:B:259:GLN:HB2	2.18	0.44
1:A:429:SER:O	1:A:434:ARG:NH1	2.50	0.44
1:A:482:TYR:HD2	1:A:544:LEU:HD11	1.83	0.44
2:B:138:GLN:OE1	2:B:232:GLY:HA2	2.17	0.44
2:B:182:HIS:NE2	2:B:189:LYS:HD2	2.32	0.44
4:D:111:ASN:HA	4:D:114:ARG:NE	2.33	0.44
1:A:85:LEU:CB	1:A:163:LEU:HD23	2.48	0.44
1:A:463:ILE:O	1:A:467:ILE:HG23	2.17	0.44
1:A:1124:TRP:HA	1:A:1131:ASN:HA	1.99	0.44
1:A:1199:TRP:CZ3	1:A:1214:ASP:HB2	2.52	0.44
2:B:60:THR:OG1	2:B:111:TRP:NE1	2.50	0.44
3:C:204:CYS:O	3:C:208:GLN:HG2	2.18	0.44
4:D:283:GLY:N	4:D:430:LYS:HG3	2.32	0.44
1:A:701:PRO:HG2	1:A:702:TYR:CD2	2.52	0.44
1:A:124:GLU:OE1	1:A:160:ASN:ND2	2.51	0.44
1:A:538:GLN:HG3	1:A:568:PHE:HE1	1.83	0.44
1:A:973:LYS:HB2	1:A:1003:ASP:HB2	2.00	0.44
3:C:392:ARG:HH22	4:D:301:ASN:CG	2.24	0.44
4:D:200:ASP:O	4:D:204:ASN:ND2	2.43	0.44
4:D:429:LEU:HA	4:D:432:MET:HG3	1.99	0.44
1:A:323:PHE:HD2	1:A:356:ASN:HD22	1.64	0.43
1:A:970:TRP:CD1	1:A:1194:PRO:HB3	2.52	0.43
1:A:988:HIS:CE1	1:A:1353:ILE:HD13	2.53	0.43
1:A:1193:HIS:ND1	1:A:1196:TYR:HB2	2.33	0.43
4:D:402:LYS:NZ	4:D:404:GLU:HG3	2.32	0.43
1:A:260:ASP:N	1:A:263:GLN:OE1	2.51	0.43
1:A:629:GLU:HB3	1:A:671:ILE:CD1	2.48	0.43
2:B:32:GLN:HB3	3:C:253:ARG:HH22	1.84	0.43
2:B:32:GLN:NE2	2:B:52:GLU:OE2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:268:ASN:CG	4:D:444:SER:HB2	2.44	0.43
1:A:331:PHE:HB3	1:A:342:ARG:HH22	1.82	0.43
1:A:664:LEU:O	1:A:720:LEU:HD13	2.18	0.43
1:A:750:LYS:CG	1:A:755:SER:HB2	2.47	0.43
1:A:983:GLY:HA3	1:A:1279:VAL:HB	2.01	0.43
1:A:984:LEU:O	1:A:1357:TRP:HA	2.18	0.43
1:A:1246:TYR:O	1:A:1256:LEU:HD12	2.19	0.43
1:A:127:TRP:O	1:A:130:PHE:HB3	2.18	0.43
1:A:155:MET:HG2	1:A:165:THR:CG2	2.48	0.43
1:A:347:ARG:HA	1:A:347:ARG:HH21	1.82	0.43
1:A:584:PHE:HB3	1:A:593:LEU:HG	2.01	0.43
1:A:687:SER:O	1:A:691:VAL:HG23	2.19	0.43
1:A:733:LEU:HB2	1:A:794:MET:HE3	2.00	0.43
1:A:1068:LEU:C	1:A:1069:LEU:HD12	2.43	0.43
1:A:451:VAL:HG11	1:A:500:VAL:HA	1.99	0.43
1:A:1020:TRP:HB3	1:A:1025:MET:HE3	2.01	0.43
1:A:1144:ILE:O	1:A:1144:ILE:HG13	2.18	0.43
3:C:368:ALA:CB	3:C:412:LEU:HD12	2.48	0.43
1:A:139:ALA:O	1:A:144:VAL:N	2.34	0.43
1:A:464:LEU:HA	1:A:467:ILE:HG12	2.01	0.43
1:A:550:ASN:OD1	1:A:593:LEU:HD22	2.19	0.43
1:A:1011:CYS:SG	1:A:1046:LYS:HA	2.59	0.43
3:C:65:TYR:OH	3:C:82:ARG:NH2	2.52	0.43
4:D:289:ARG:NH2	4:D:298:VAL:HG22	2.27	0.43
1:A:565:CYS:SG	1:A:604:VAL:HG22	2.58	0.43
1:A:630:PHE:CE1	1:A:670:TRP:CD1	3.06	0.43
1:A:691:VAL:HA	1:A:695:LEU:HD13	2.00	0.43
1:A:1246:TYR:CZ	1:A:1248:SER:HB2	2.54	0.43
1:A:114:ILE:CD1	1:A:120:LEU:HD12	2.48	0.43
1:A:155:MET:HG3	1:A:165:THR:HG21	2.01	0.43
1:A:276:GLN:HA	1:A:279:ASN:OD1	2.18	0.43
1:A:491:GLU:OE1	1:A:491:GLU:N	2.50	0.43
1:A:544:LEU:HB2	1:A:556:LEU:HD22	2.01	0.43
1:A:1350:ARG:HD3	4:D:249:SER:HB2	2.00	0.43
2:B:91:LEU:HD23	2:B:91:LEU:HA	1.74	0.43
3:C:62:LEU:HD13	3:C:119:GLY:HA3	2.00	0.43
3:C:289:GLN:OE1	4:D:240:GLN:NE2	2.44	0.43
1:A:114:ILE:HD11	1:A:251:LEU:HD12	2.01	0.43
1:A:379:VAL:HG21	1:A:409:LEU:HD11	2.01	0.43
1:A:388:THR:HG22	1:A:388:THR:O	2.18	0.43
1:A:189:THR:HG21	5:A:1501:GDP:O3A	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:446:ASP:OD1	3:C:448:ARG:HG2	2.19	0.42
1:A:339:ALA:HB1	1:A:385:CYS:HB3	2.01	0.42
1:A:439:ARG:CZ	1:A:439:ARG:HB2	2.49	0.42
1:A:538:GLN:HG3	1:A:568:PHE:CE1	2.53	0.42
1:A:1019:ILE:HD13	1:A:1071:ILE:HD12	2.01	0.42
2:B:174:ARG:HD2	2:B:174:ARG:O	2.19	0.42
4:D:18:CYS:N	4:D:23:GLN:O	2.38	0.42
1:A:395:LYS:HD2	1:A:433:VAL:HG21	2.02	0.42
1:A:459:TYR:CD2	1:A:493:ALA:HB2	2.54	0.42
2:B:197:THR:O	2:B:201:ILE:HG13	2.19	0.42
4:D:114:ARG:HH12	4:D:115:ARG:NH1	2.15	0.42
1:A:197:ILE:HG23	1:A:201:ARG:HD3	2.02	0.42
1:A:410:SER:OG	1:A:413:ILE:HG12	2.19	0.42
1:A:581:MET:HE1	1:A:601:ILE:HA	2.01	0.42
1:A:591:TRP:CH2	1:A:630:PHE:HB3	2.55	0.42
1:A:649:GLN:HB2	1:A:652:HIS:CG	2.54	0.42
4:D:267:THR:HG21	4:D:272:ALA:HB2	2.00	0.42
4:D:393:PRO:HG2	4:D:438:TRP:NE1	2.34	0.42
1:A:654:TYR:CE2	1:A:694:LYS:HE3	2.54	0.42
1:A:705:GLN:H	1:A:719:VAL:CG1	2.26	0.42
1:A:1186:ARG:HD3	4:D:241:LEU:HD22	2.01	0.42
3:C:45:LEU:HD11	3:C:155:PHE:HD2	1.85	0.42
1:A:537:VAL:HG21	1:A:567:PHE:CD2	2.55	0.42
1:A:613:SER:OG	1:A:649:GLN:HG2	2.20	0.42
1:A:643:CYS:SG	1:A:682:VAL:HG22	2.59	0.42
3:C:427:TYR:OH	3:C:431:LYS:NZ	2.29	0.42
4:D:424:GLN:HG3	4:D:425:TRP:N	2.34	0.42
1:A:120:LEU:HD22	1:A:124:GLU:HG2	2.01	0.42
1:A:128:ILE:HG23	1:A:162:VAL:HG21	2.00	0.42
1:A:487:ALA:HB1	1:A:563:ARG:CZ	2.49	0.42
3:C:41:ARG:NE	3:C:109:SER:O	2.51	0.42
4:D:137:CYS:O	4:D:141:THR:N	2.41	0.42
4:D:393:PRO:HG2	4:D:438:TRP:CD1	2.55	0.42
1:A:146:HIS:CE1	1:A:166:ASP:O	2.72	0.42
1:A:490:ALA:O	1:A:493:ALA:HB3	2.19	0.42
1:A:1331:ILE:HB	1:A:1350:ARG:HG3	2.00	0.42
4:D:274:PHE:HB3	4:D:285:ILE:CG1	2.49	0.42
1:A:557:MET:O	1:A:600:SER:HB3	2.19	0.42
1:A:653:VAL:HG11	1:A:686:ILE:HD13	2.01	0.42
1:A:1118:ASN:O	1:A:1139:LEU:HD21	2.19	0.42
1:A:1118:ASN:ND2	4:D:231:ARG:HG2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:ILE:HA	1:A:1160:THR:HA	2.02	0.42
1:A:1211:SER:HB2	1:A:1213:TRP:CH2	2.54	0.42
3:C:286:LEU:HD13	4:D:233:TYR:CD1	2.51	0.42
1:A:173:THR:OG1	1:A:235:LEU:HG	2.20	0.42
1:A:311:GLN:OE1	1:A:314:ASN:ND2	2.43	0.42
1:A:330:GLN:O	1:A:333:LYS:HG2	2.20	0.42
1:A:617:LYS:HA	1:A:656:PHE:HZ	1.85	0.42
3:C:190:SER:HA	4:D:25:LEU:HD12	2.01	0.42
4:D:286:ASN:HB2	4:D:288:PHE:CE1	2.54	0.42
1:A:347:ARG:HG3	1:A:397:ALA:HB1	2.01	0.41
1:A:479:ARG:HH21	1:A:547:ASP:HB3	1.85	0.41
1:A:574:ASN:HB2	1:A:608:VAL:CG1	2.50	0.41
2:B:228:ASP:OD1	2:B:228:ASP:N	2.51	0.41
3:C:189:ASN:OD1	3:C:189:ASN:N	2.52	0.41
4:D:18:CYS:HB2	4:D:23:GLN:H	1.85	0.41
1:A:175:LEU:O	1:A:202:PHE:HA	2.20	0.41
1:A:565:CYS:HB3	1:A:607:TYR:CD2	2.55	0.41
1:A:1172:PHE:HE2	2:B:178:LEU:HB3	1.85	0.41
1:A:1198:SER:HB3	2:B:192:TRP:CZ2	2.55	0.41
1:A:124:GLU:OE1	1:A:377:ILE:HG13	2.19	0.41
1:A:393:ASP:OD1	1:A:394:SER:N	2.53	0.41
1:A:629:GLU:OE1	1:A:668:ASN:HB2	2.21	0.41
1:A:85:LEU:HD22	1:A:163:LEU:HD23	2.01	0.41
1:A:459:TYR:CZ	1:A:463:ILE:HG21	2.55	0.41
1:A:677:GLY:O	1:A:680:THR:OG1	2.36	0.41
1:A:1196:TYR:CB	1:A:1199:TRP:CD1	2.94	0.41
2:B:192:TRP:O	2:B:195:ARG:HG2	2.20	0.41
3:C:77:TYR:OH	3:C:78:LYS:NZ	2.31	0.41
1:A:676:VAL:HG21	1:A:717:LEU:HD23	2.01	0.41
1:A:985:LEU:HD13	1:A:1355:LYS:HD3	2.02	0.41
1:A:1046:LYS:HE3	4:D:242:GLU:OE1	2.21	0.41
1:A:319:ILE:CG2	1:A:357:LEU:HD23	2.51	0.41
1:A:629:GLU:CB	1:A:671:ILE:HD11	2.49	0.41
1:A:983:GLY:CA	1:A:1279:VAL:HB	2.50	0.41
1:A:985:LEU:H	1:A:985:LEU:HD23	1.86	0.41
3:C:138:LEU:HD13	3:C:162:TYR:HB3	2.03	0.41
4:D:262:ASP:O	4:D:266:LYS:HE2	2.20	0.41
1:A:161:TRP:HD1	1:A:163:LEU:CD1	2.33	0.41
1:A:423:LEU:HD21	1:A:463:ILE:HD11	2.02	0.41
1:A:1172:PHE:CE1	2:B:197:THR:HG21	2.55	0.41
1:A:105:TYR:CD1	2:B:260:MET:HE3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:PHE:HZ	1:A:794:MET:HG2	1.86	0.41
1:A:748:ARG:HG2	1:A:759:CYS:SG	2.61	0.41
1:A:992:HIS:HB2	1:A:1352:GLY:O	2.20	0.41
1:A:1240:HIS:HA	1:A:1261:SER:OG	2.20	0.41
2:B:30:ARG:CZ	2:B:49:LEU:HG	2.50	0.41
1:A:391:TYR:HB2	1:A:393:ASP:OD1	2.21	0.41
1:A:441:LEU:HD21	1:A:463:ILE:HD11	2.02	0.41
1:A:553:LYS:O	1:A:557:MET:HG3	2.21	0.41
1:A:625:SER:HA	1:A:793:PHE:HD1	1.86	0.41
1:A:692:TYR:CZ	4:D:169:LEU:HD21	2.56	0.41
1:A:970:TRP:HA	1:A:1151:ILE:HG12	2.01	0.41
1:A:1330:ASP:HB3	1:A:1349:SER:OG	2.21	0.41
1:A:1335:VAL:HG13	1:A:1345:ILE:HG23	2.02	0.41
2:B:21:LEU:HD23	2:B:61:CYS:SG	2.61	0.41
2:B:48:GLY:HA3	2:B:112:ASP:OD2	2.21	0.41
2:B:74:VAL:HG23	2:B:94:PRO:HD3	2.03	0.41
3:C:45:LEU:HA	3:C:157:LEU:HG	2.02	0.41
3:C:67:THR:HA	3:C:81:TYR:O	2.21	0.41
3:C:145:ILE:HG23	3:C:154:ILE:HD12	2.02	0.41
3:C:188:ARG:CZ	4:D:137:CYS:SG	3.09	0.41
4:D:20:ARG:NH2	4:D:133:ASP:H	2.19	0.41
4:D:311:VAL:HA	4:D:372:PHE:CE2	2.53	0.41
1:A:285:SER:O	1:A:288:GLU:HG2	2.20	0.41
1:A:557:MET:HE2	1:A:600:SER:OG	2.21	0.41
1:A:667:PRO:HB2	1:A:726:ARG:HD2	2.03	0.41
1:A:718:SER:OG	3:C:242:LEU:HD12	2.21	0.41
2:B:74:VAL:CG2	2:B:94:PRO:HD3	2.51	0.41
3:C:92:PRO:HG3	3:C:94:TRP:CZ2	2.55	0.41
4:D:374:ASP:O	4:D:378:GLN:N	2.31	0.41
4:D:432:MET:O	4:D:436:LEU:N	2.35	0.41
3:C:339:TYR:CD2	3:C:452:PRO:HG3	2.56	0.40
1:A:658:SER:HB2	1:A:698:TYR:CE2	2.56	0.40
1:A:988:HIS:CD2	1:A:1355:LYS:HE2	2.57	0.40
1:A:1211:SER:HB3	1:A:1220:ARG:HD3	2.02	0.40
1:A:1291:TYR:O	1:A:1301:VAL:HA	2.21	0.40
2:B:212:SER:OG	2:B:214:PHE:HB2	2.20	0.40
3:C:46:ARG:NH2	3:C:97:LEU:O	2.42	0.40
3:C:455:LYS:HE2	3:C:459:GLU:HG3	2.02	0.40
4:D:123:PHE:CZ	4:D:135:PRO:HB3	2.57	0.40
4:D:314:LEU:HA	4:D:314:LEU:HD23	1.84	0.40
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:CG2	1:A:699:LEU:HD11	2.51	0.40
2:B:136:PHE:CB	2:B:233:ILE:HB	2.51	0.40
3:C:137:GLY:O	4:D:83:ILE:HG21	2.22	0.40
4:D:274:PHE:HB3	4:D:285:ILE:HD11	2.02	0.40
1:A:445:LEU:HD13	1:A:459:TYR:CE1	2.51	0.40
1:A:598:PHE:HB3	1:A:638:ALA:HB2	2.04	0.40
1:A:1196:TYR:CG	1:A:1199:TRP:CD1	3.10	0.40
1:A:1232:LEU:HG	1:A:1300:VAL:HG21	2.03	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	939/1445 (65%)	880 (94%)	59 (6%)	0	100	100
2	B	244/887 (28%)	220 (90%)	24 (10%)	0	100	100
3	C	375/699 (54%)	351 (94%)	24 (6%)	0	100	100
4	D	318/450 (71%)	308 (97%)	10 (3%)	0	100	100
All	All	1876/3481 (54%)	1759 (94%)	117 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	922/1270 (73%)	921 (100%)	1 (0%)	88	89
2	B	224/799 (28%)	224 (100%)	0	100	100
3	C	348/607 (57%)	348 (100%)	0	100	100
4	D	301/405 (74%)	301 (100%)	0	100	100
All	All	1795/3081 (58%)	1794 (100%)	1 (0%)	87	89

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	733	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	131	GLN
1	A	140	HIS
1	A	146	HIS
1	A	160	ASN
1	A	387	GLN
1	A	652	HIS
1	A	705	GLN
1	A	746	HIS
1	A	749	GLN
1	A	1005	HIS
1	A	1092	GLN
1	A	1118	ASN
1	A	1302	GLN
1	A	1329	HIS
2	B	18	ASN
2	B	141	HIS
2	B	148	ASN
2	B	259	GLN
3	C	151	ASN
3	C	214	GLN
3	C	266	HIS
3	C	283	HIS
3	C	313	GLN
3	C	379	GLN
4	D	23	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	179	GLN
4	D	271	ASN
4	D	319	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GDP	A	1501	-	29,30,30	1.16	3 (10%)	45,47,47	1.85	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	A	1501	-	-	8/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1501	GDP	C5-C4	2.96	1.46	1.38
5	A	1501	GDP	C6-N1	-2.86	1.33	1.38
5	A	1501	GDP	C5-N7	-2.43	1.34	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1501	GDP	C5-C4-N3	-6.59	117.91	128.39
5	A	1501	GDP	N9-C4-N3	5.11	136.17	125.95
5	A	1501	GDP	C2-N3-C4	5.03	120.97	112.30
5	A	1501	GDP	O6-C6-C5	-2.66	119.52	126.53
5	A	1501	GDP	C3'-C2'-C1'	2.46	106.11	101.46
5	A	1501	GDP	C6-C5-N7	2.38	134.63	130.29
5	A	1501	GDP	C5-C6-N1	2.02	118.39	113.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1501	GDP	C5'-O5'-PA-O3A
5	A	1501	GDP	C5'-O5'-PA-O1A
5	A	1501	GDP	C5'-O5'-PA-O2A
5	A	1501	GDP	PA-O3A-PB-O1B
5	A	1501	GDP	PA-O3A-PB-O2B
5	A	1501	GDP	PA-O3A-PB-O3B
5	A	1501	GDP	C4'-C5'-O5'-PA
5	A	1501	GDP	O4'-C4'-C5'-O5'

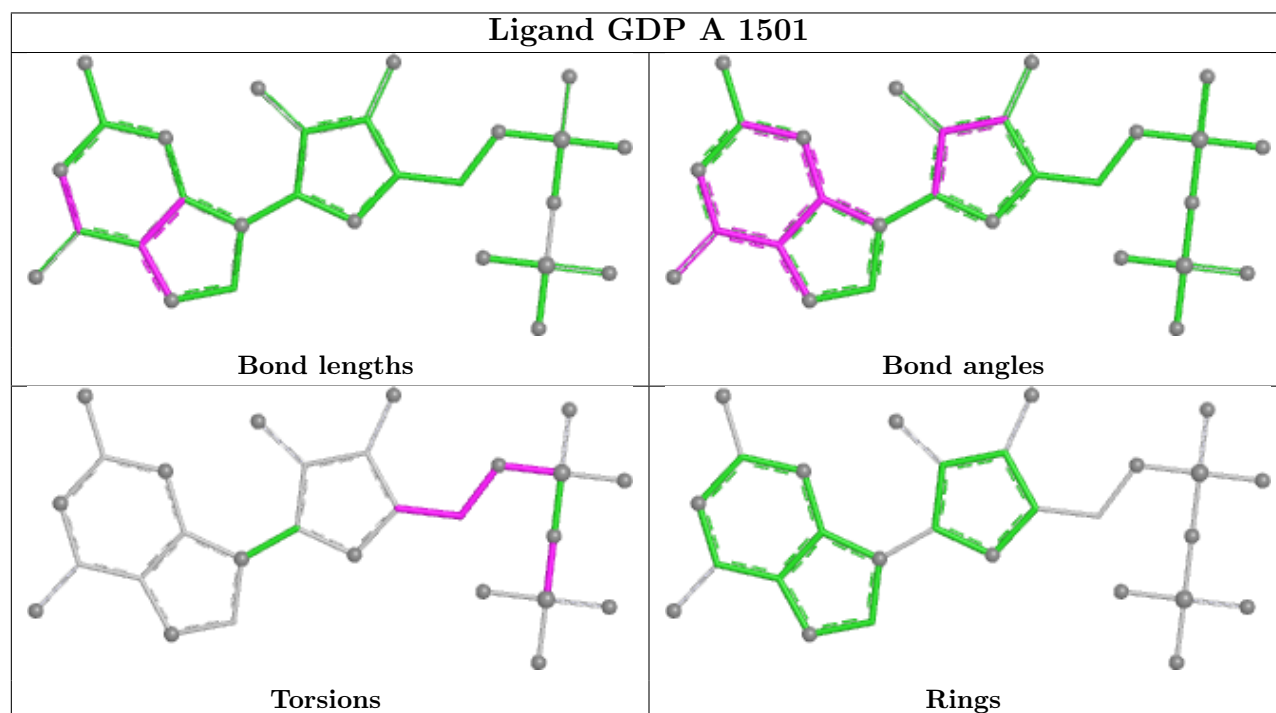
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1501	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

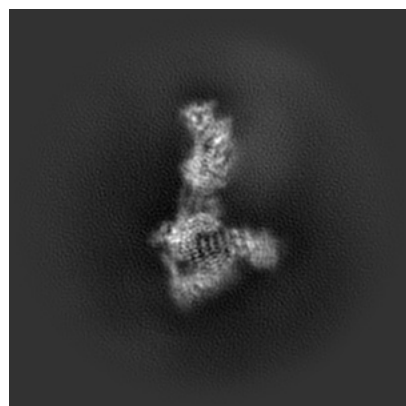
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-74526. These allow visual inspection of the internal detail of the map and identification of artifacts.

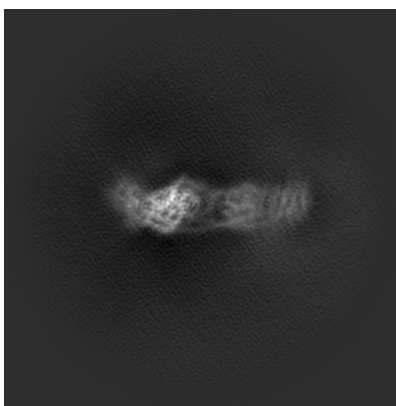
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

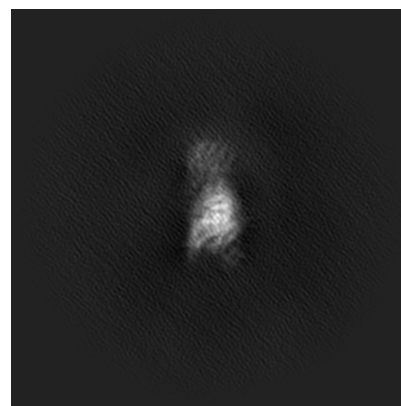
6.1.1 Primary map



X

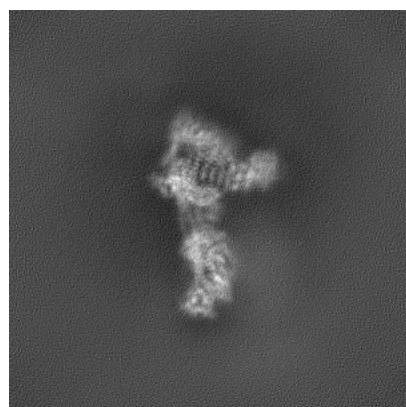


Y

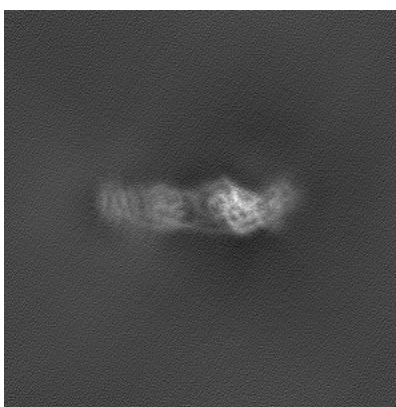


Z

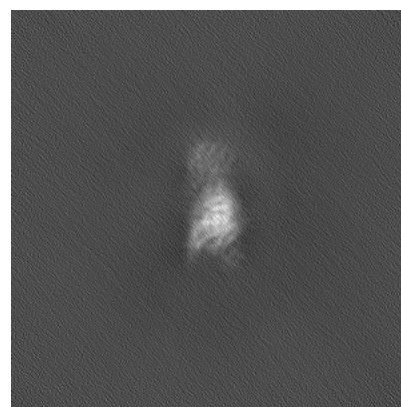
6.1.2 Raw map



X



Y

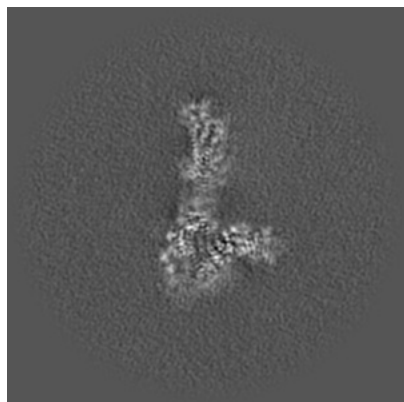


Z

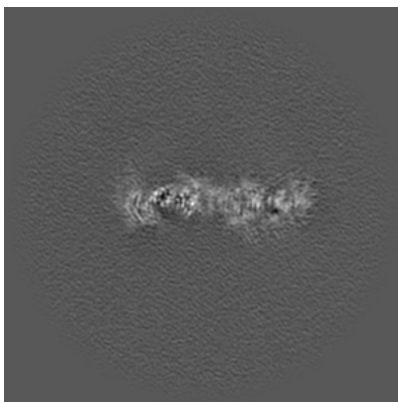
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

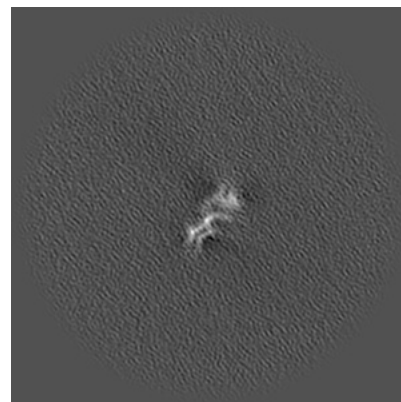
6.2.1 Primary map



X Index: 200

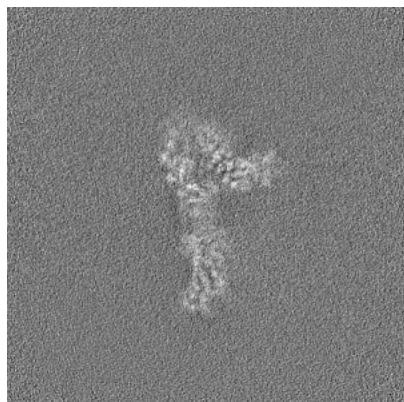


Y Index: 200

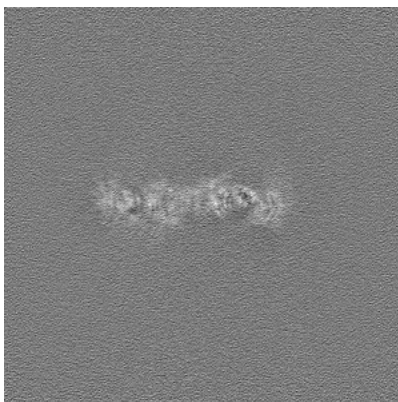


Z Index: 200

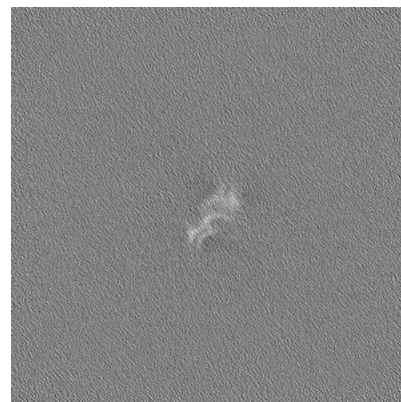
6.2.2 Raw map



X Index: 200



Y Index: 200

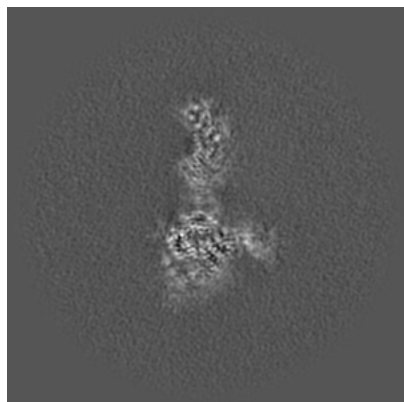


Z Index: 200

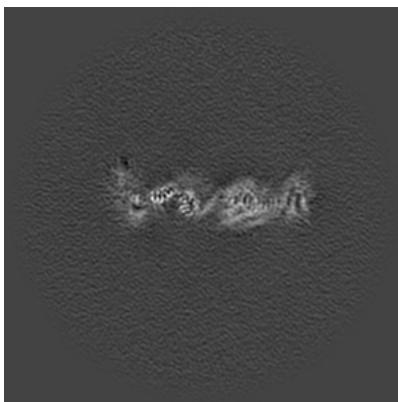
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

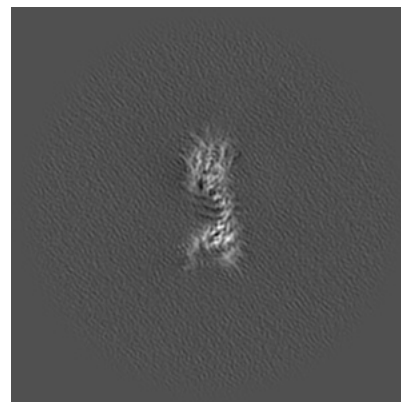
6.3.1 Primary map



X Index: 205

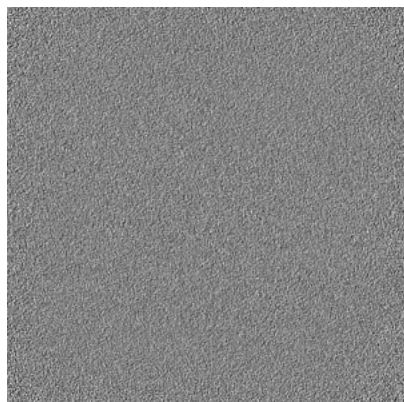


Y Index: 187

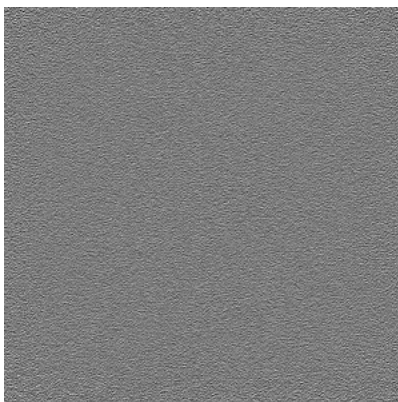


Z Index: 168

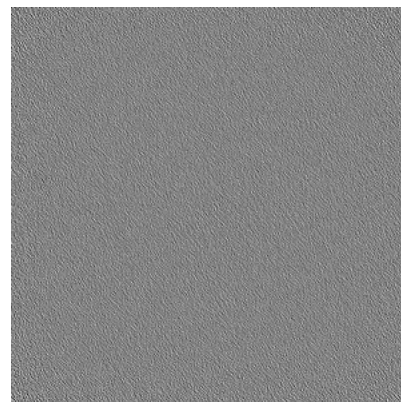
6.3.2 Raw map



X Index: 0



Y Index: 0

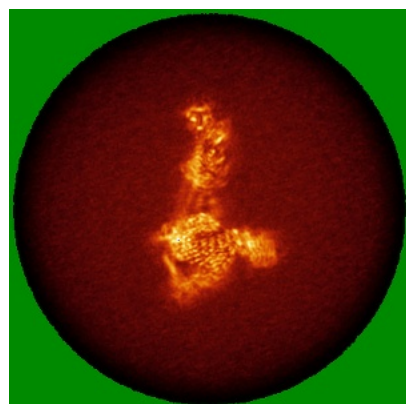


Z Index: 0

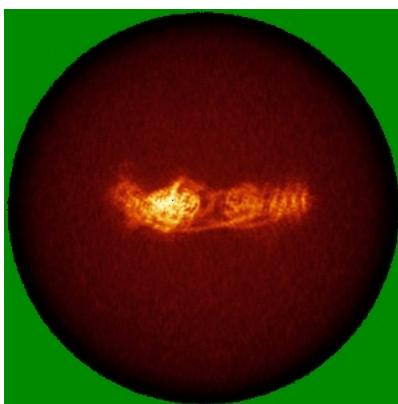
The images above show the largest variance slices of the map in three orthogonal directions.

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

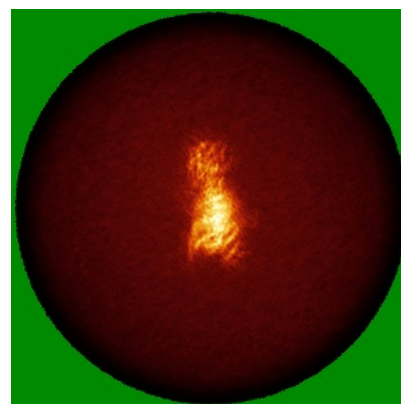
6.4.1 Primary map



X

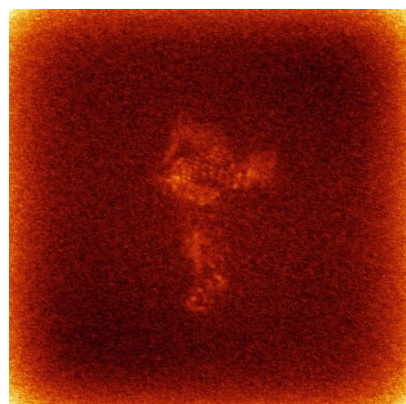


Y

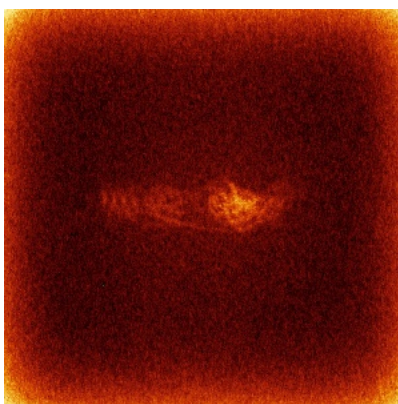


Z

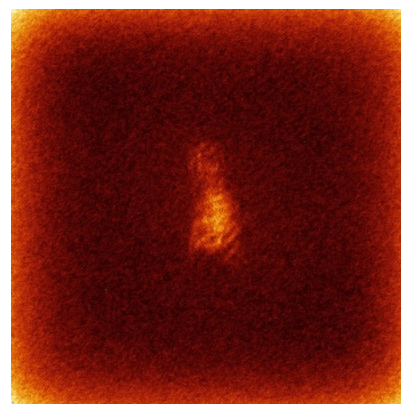
6.4.2 Raw map



X



Y



Z

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

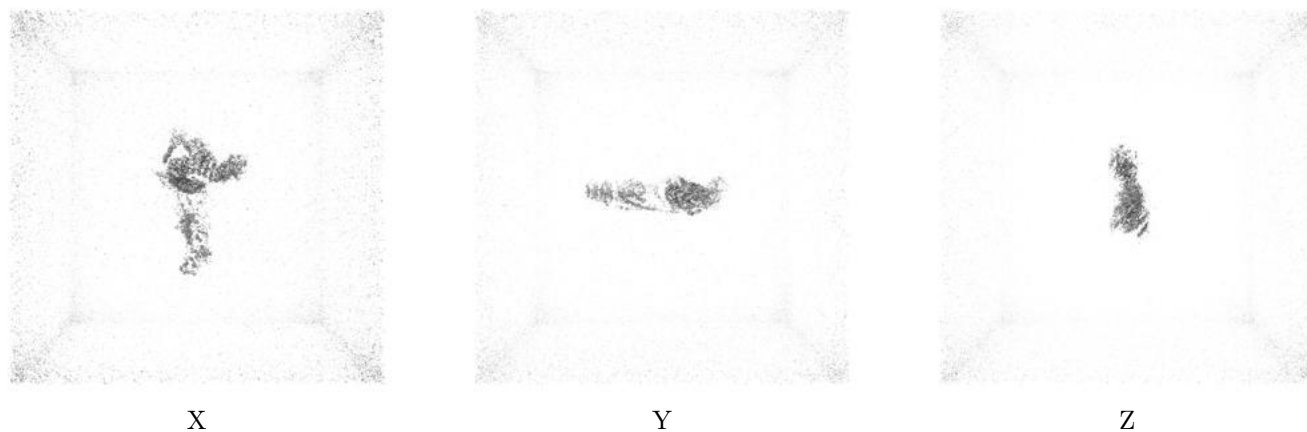
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.19. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

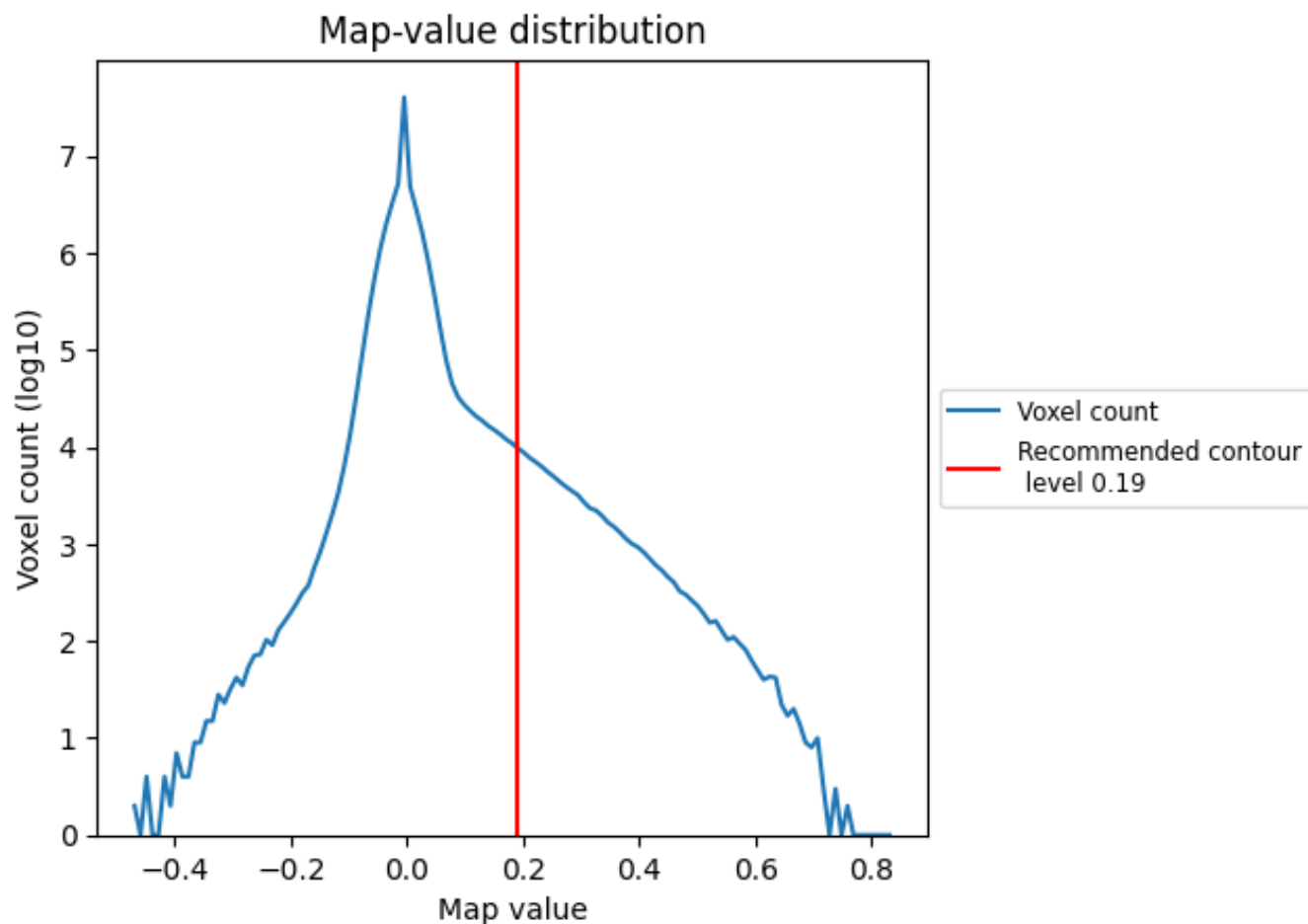
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

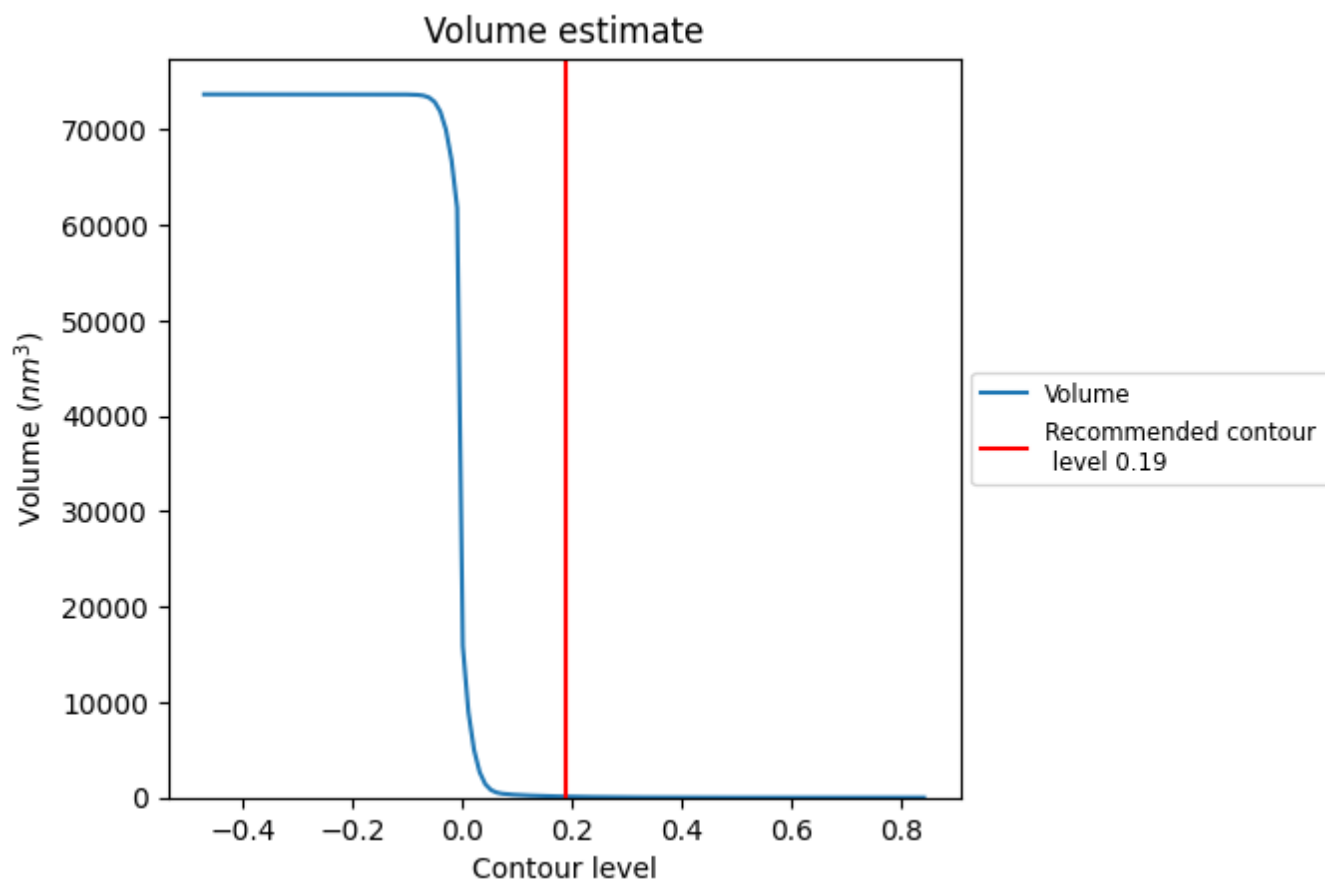
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

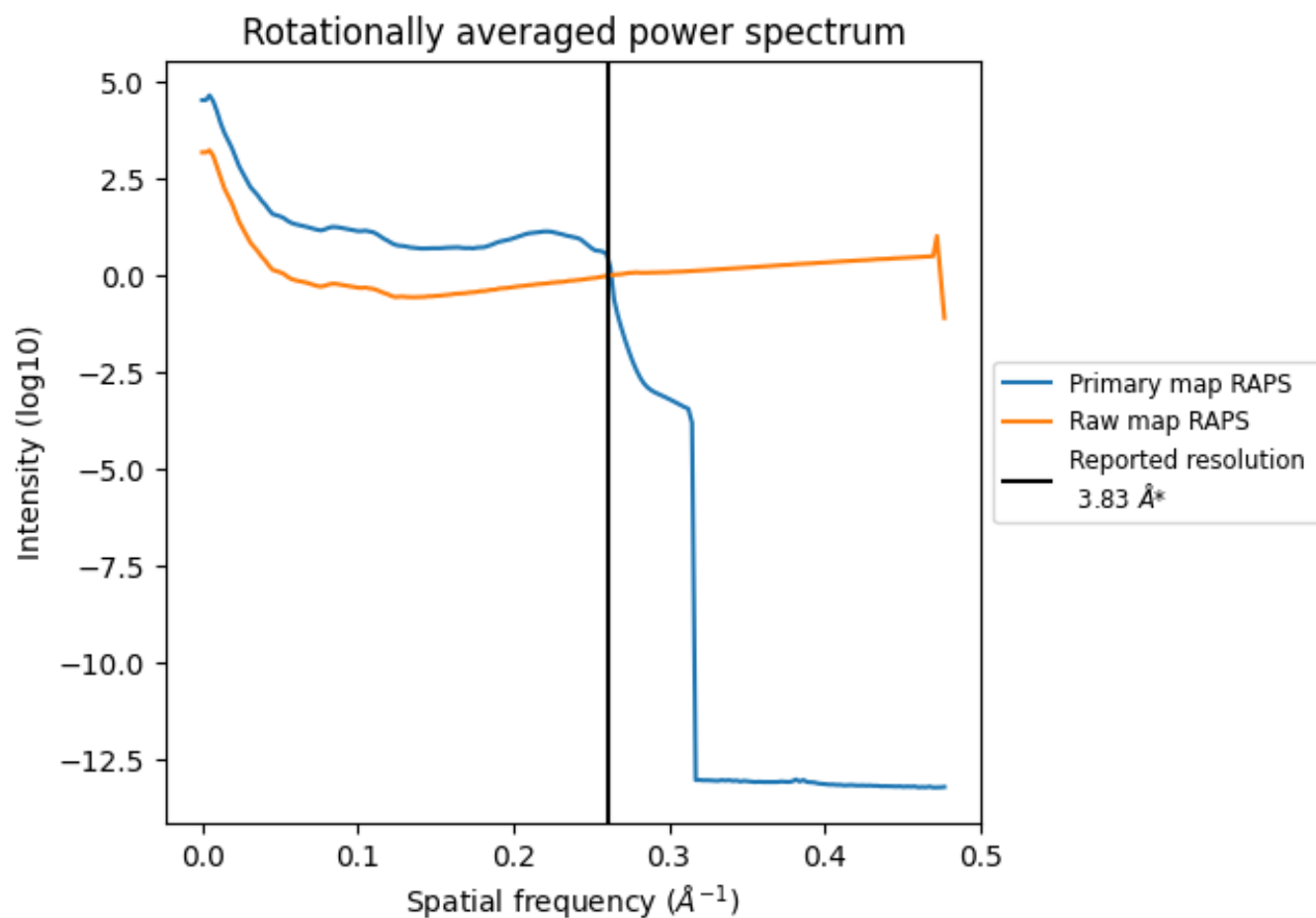
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 103 nm³; this corresponds to an approximate mass of 93 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 ⓘ

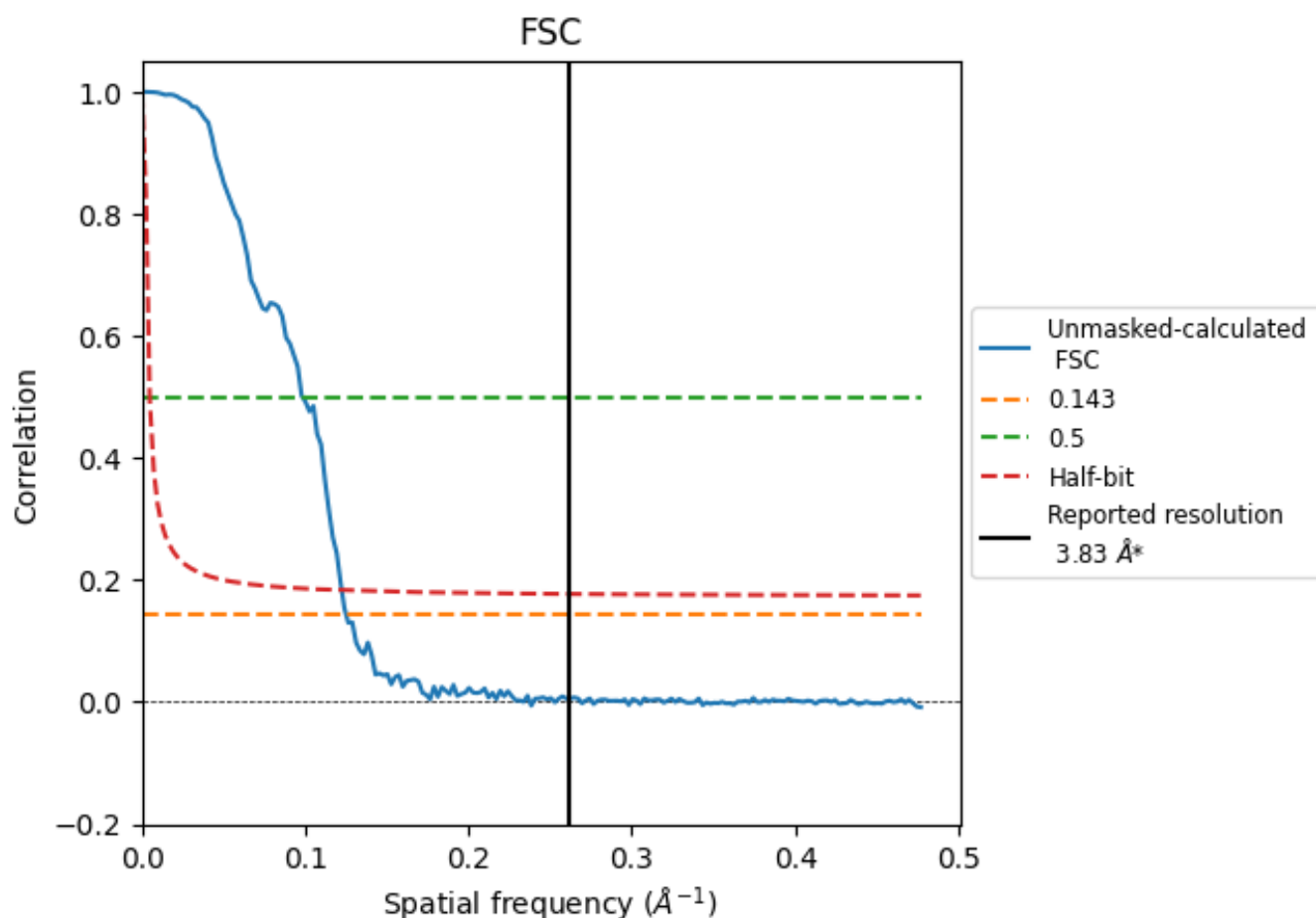


*Reported resolution corresponds to spatial frequency of 0.261 Å⁻¹

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 0.261 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

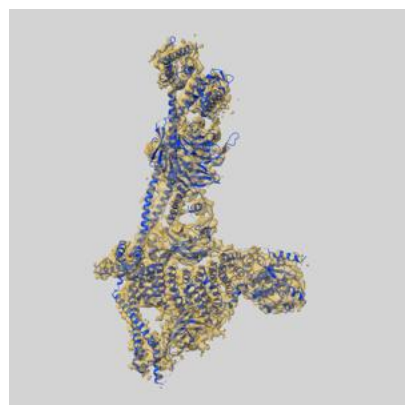
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.83	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.99	10.18	8.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.99 differs from the reported value 3.83 by more than 10 %

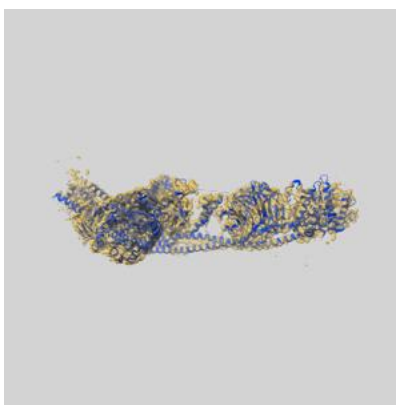
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-74526 and PDB model 9ZPC. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

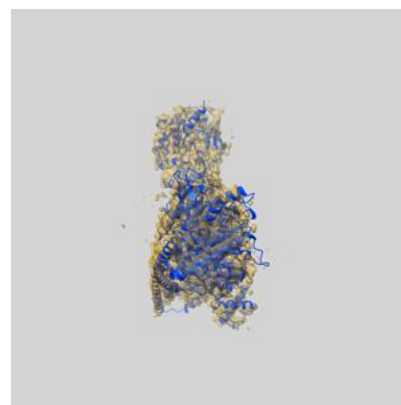
9.1 Map-model overlay [i](#)



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.19 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](#)

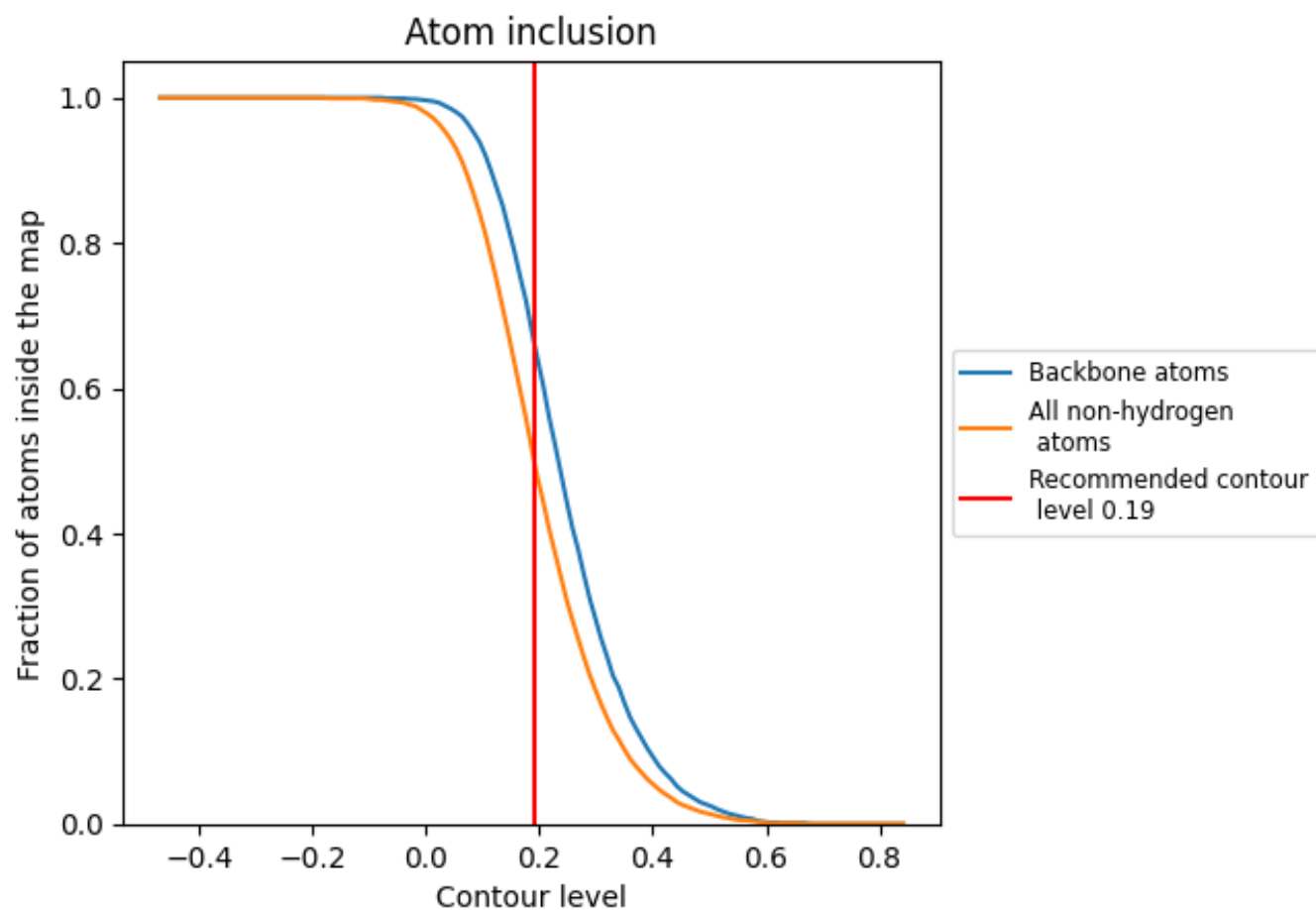


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 50% 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 (0.19) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5010	0.2220
A	0.5280	0.2450
B	0.6020	0.2650
C	0.4240	0.1830
D	0.4340	0.1650

