



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:58 AM UTC

PDB ID : 7F5T / pdb_00007f5t
EMDB ID : EMD-31466
Title : Drosophila P5CS filament with glutamate
Authors : Liu, J.L.; Zhong, J.; Guo, C.J.; Zhou, X.
Deposited on : 2021-06-22
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
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

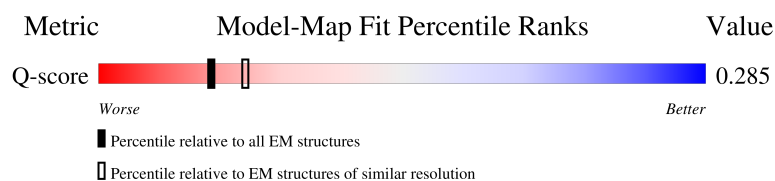
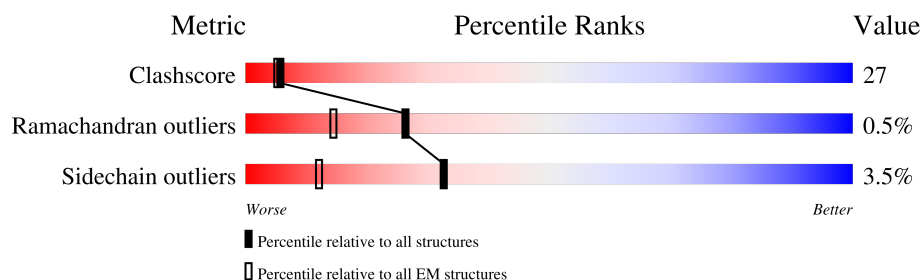
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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

Mol	Chain	Length	Quality of chain
1	A	776	5% 42% 44% 13%
1	B	776	5% 42% 44% 13%
1	C	776	5% 42% 43% 13%
1	D	776	5% 42% 43% 13%

2 Entry composition [i](#)

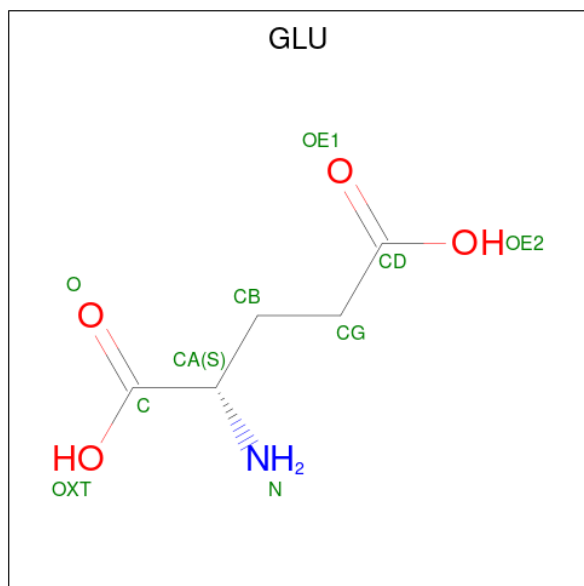
There are 2 unique types of molecules in this entry. The entry contains 20436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Delta-1-pyrroline-5-carboxylate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	674	Total	C	N	O	S	0	0
			5099	3195	904	972	28		
1	B	674	Total	C	N	O	S	0	0
			5099	3195	904	972	28		
1	C	674	Total	C	N	O	S	0	0
			5099	3195	904	972	28		
1	D	674	Total	C	N	O	S	0	0
			5099	3195	904	972	28		

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			10	5	1	4	
2	B	1	Total	C	N	O	0
			10	5	1	4	

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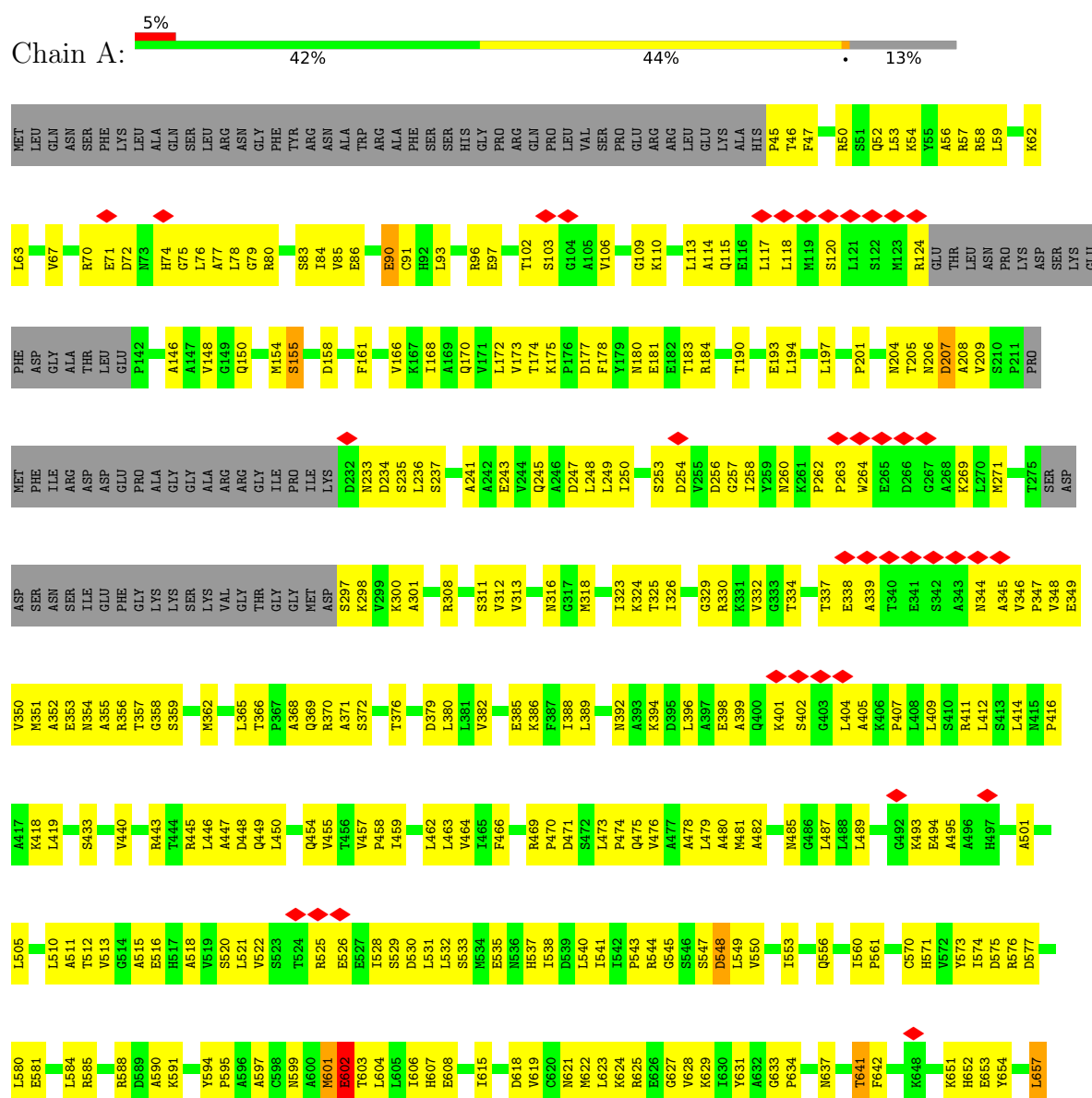
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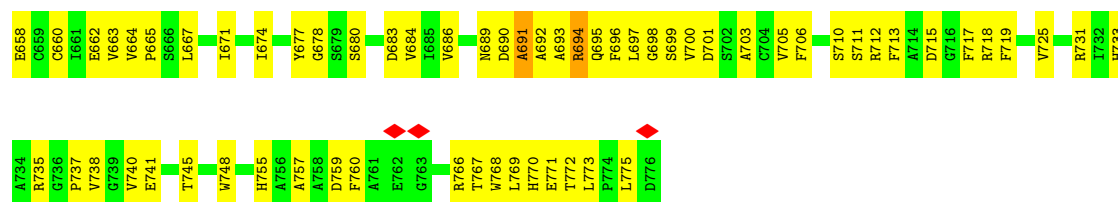
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			10	5	1	4	
2	D	1	Total	C	N	O	0
			10	5	1	4	

3 Residue-property plots

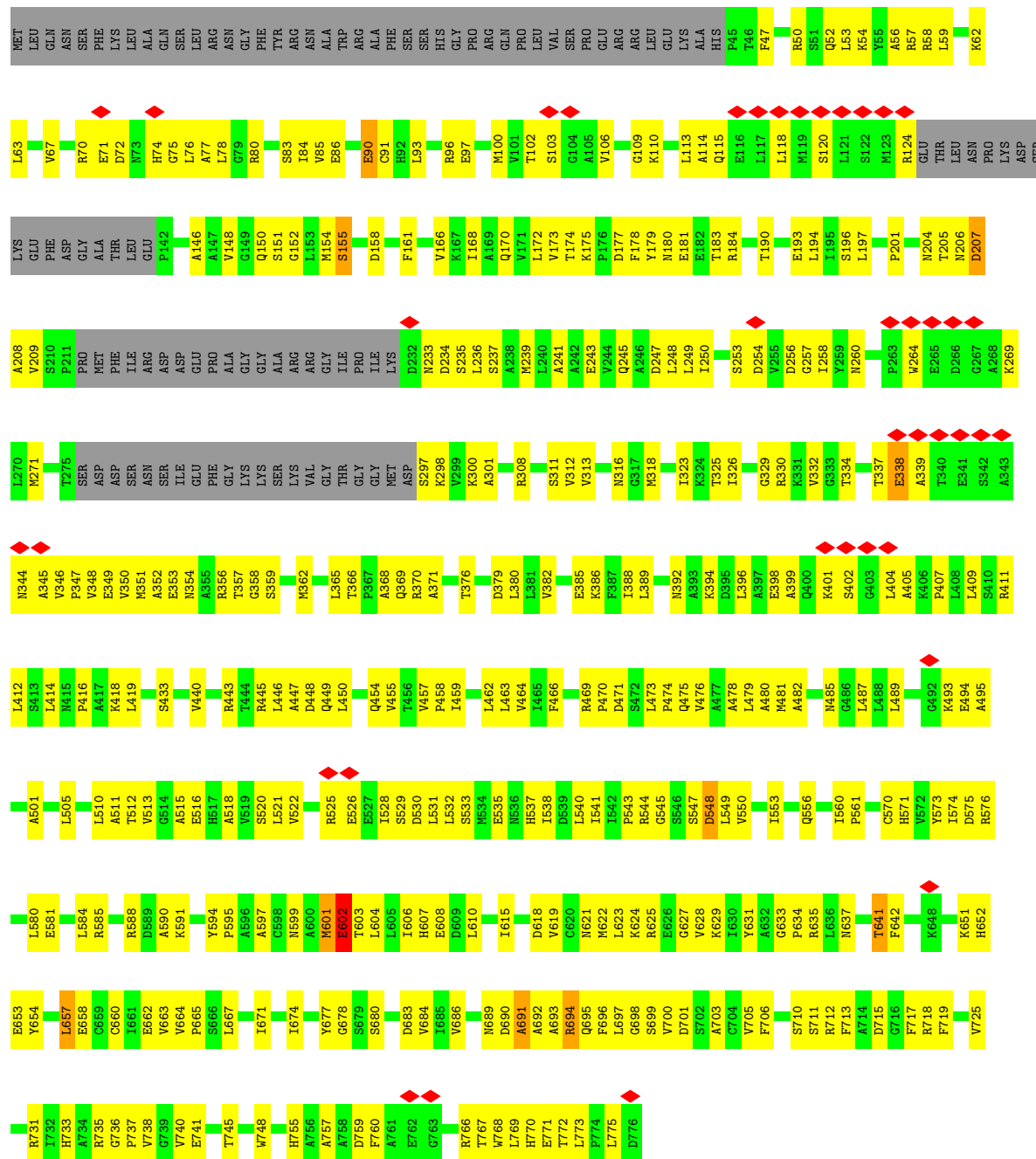
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Delta-1-pyrroline-5-carboxylate synthase

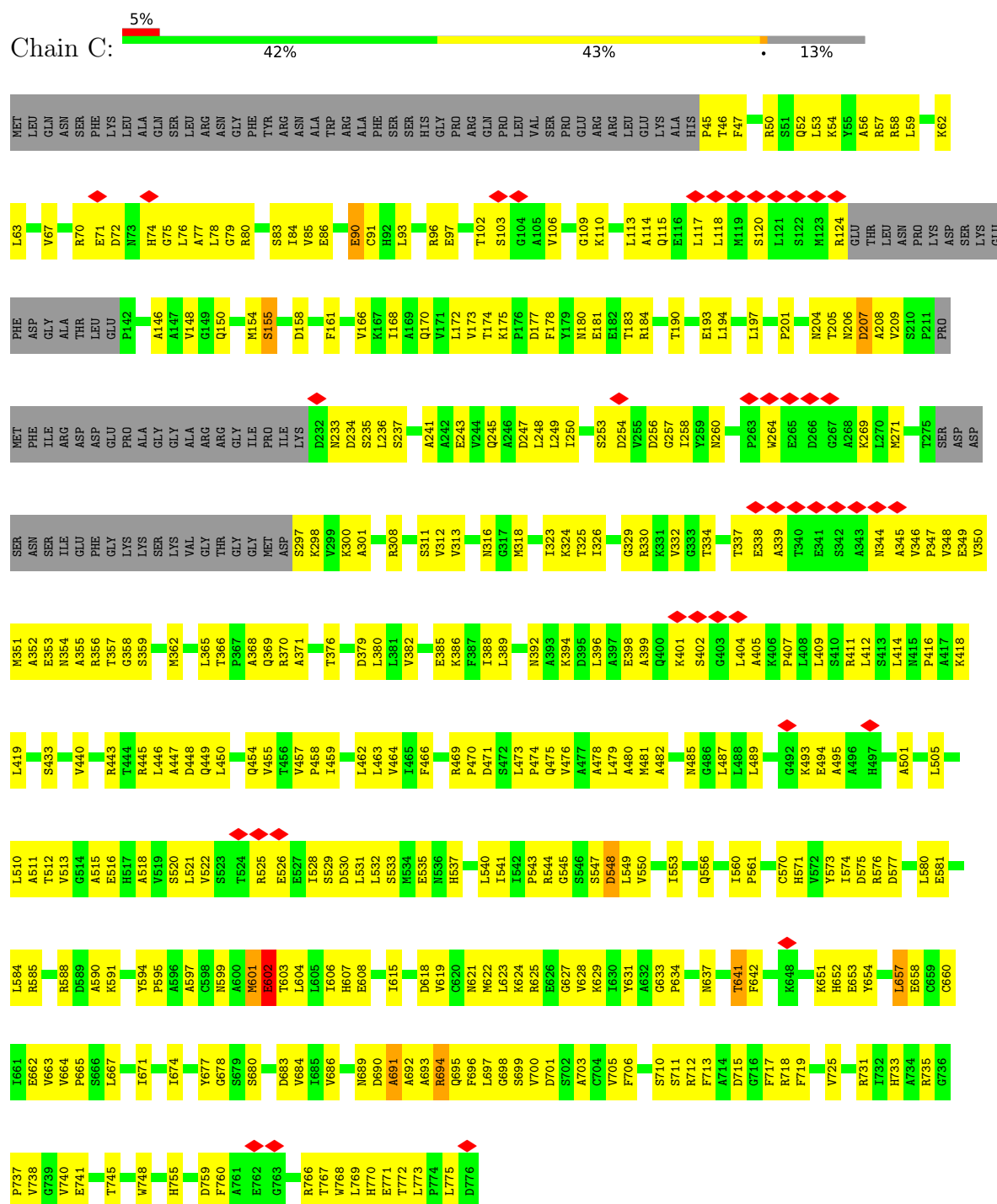




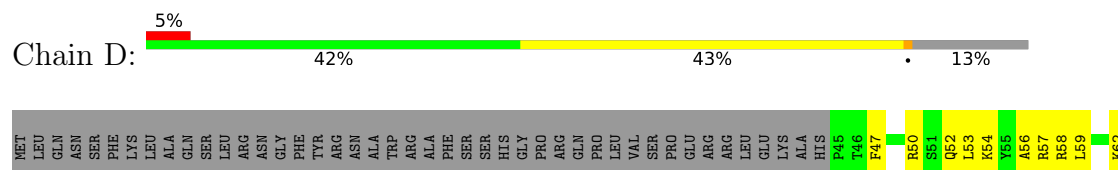
• Molecule 1: Delta-1-pyrroline-5-carboxylate synthase



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L63	PHE	S210	V346	L414	L505	E581	E658	A734
V67	ASP	P211	P347	M415	L510	L584	G659	R735
R70	GLY	MET	E349	P416	A511	R585	C660	G736
E71	ALA	ASP	M351	A417	T512	R588	I661	P737
D72	THR	ILE	A352	L419	V513	D589	V663	G738
M73	LEU	ARG	E353	S433	G514	A590	V664	V740
H74	GLU	ASP	N354	V440	A515	K591	P665	E741
G75	P142	ASP	A355	V440	E516	L594	L667	T745
L76	A146	GLU	R356	R443	H517	P595	I671	M748
A77	A147	PRU	T357	T444	A518	A596	L674	H755
G78	V148	ALA	G358	R445	V519	C598	A756	A756
L79	G149	GLY	S359	L446	S520	N599	A757	A757
G79	Q150	GLY	M362	L447	V522	A600	G678	A758
R80	S151	ALA	L365	Q449	D448	M601	S679	D759
S83	L153	ARG	T366	L450	L452	E602	S680	F760
I84	M154	GLY	F367	Q454	E526	T603	D683	A761
V85	S155	ILE	A368	V455	E527	L604	V684	E762
E86	S156	PRO	Q369	T456	S529	L606	I685	G763
E90	D158	ILE	R370	P458	L531	E608	V686	R766
C91	F161	LYS	A371	T459	L532	P609	N689	M768
H92	V166	D232	T376	L462	M534	L610	D690	L769
L93	K167	N233	D379	V463	E535	L615	A692	H770
R96	I168	D234	L380	V464	H536	V619	A693	E771
E97	A169	S235	V382	T465	L538	G620	R694	T772
T102	Q170	S236	E385	F466	D539	M621	Q695	Q695
S103	V171	A238	F387	R469	L540	N622	P696	P696
G104	L172	M239	I388	D471	T541	L623	N622	L697
A105	V173	L240	L389	S472	P543	R625	G629	G698
V106	T174	A241	I389	L473	R544	E626	A632	S699
G109	K175	E244	N392	L477	G545	G627	L632	V700
K110	D177	V244	A393	Q475	S546	V628	A632	D701
L113	F178	Q245	K331	V476	R547	A703	F642	S702
A114	M180	L248	T323	A477	D548	V705	R648	C704
Q115	E182	L249	T325	L478	V550	F706	K651	V706
E116	R184	I250	I326	L479	L553	G633	H652	S710
L117	T190	S253	G329	A480	P556	P634	E653	S711
L118	E193	D254	R330	M481	Q556	N637	V654	R712
M119	E194	V255	K332	A482	P561	L644	R657	F713
S120	L194	G256	V332	M485	C570	F642	L657	A714
L121	I195	I258	T334	L487	H571	K648		D715
S122	S196	N260	T337	L488	V572	K651		G716
M123	L197	P263	E338	L489	H573	H652		F717
R124	P201	V264	A339	G492	Y573	E654		R718
GLU	N204	E265	T340	K493	L574			F719
THR	T205	D266	E341	A495	R576			V725
LEU	N206	G267	S342	L411	L580			R731
ASN	D207	A268	N344	L412				I732
PRO	A208	K269	A343	S413				H733
LYS	A208	L270	N344					
ASP	LYS	M271						
SER	LYS							
GLU								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432746	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.006	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/5173	0.56	3/6996 (0.0%)
1	B	0.41	0/5173	0.56	3/6996 (0.0%)
1	C	0.41	0/5173	0.56	3/6996 (0.0%)
1	D	0.41	0/5173	0.56	3/6996 (0.0%)
All	All	0.41	0/20692	0.56	12/27984 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	ALA	CA-C-N	-5.40	118.63	123.33
1	D	345	ALA	C-N-CA	-5.40	118.63	123.33
1	C	345	ALA	CA-C-N	-5.39	118.64	123.33
1	C	345	ALA	C-N-CA	-5.39	118.64	123.33
1	A	345	ALA	CA-C-N	-5.38	118.65	123.33
1	A	345	ALA	C-N-CA	-5.38	118.65	123.33
1	B	345	ALA	CA-C-N	-5.36	118.67	123.33
1	B	345	ALA	C-N-CA	-5.36	118.67	123.33
1	A	691	ALA	N-CA-C	-5.29	105.16	111.03
1	D	691	ALA	N-CA-C	-5.28	105.17	111.03
1	B	691	ALA	N-CA-C	-5.27	105.18	111.03
1	C	691	ALA	N-CA-C	-5.26	105.19	111.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5099	0	5173	282	0
1	B	5099	0	5173	288	0
1	C	5099	0	5173	278	0
1	D	5099	0	5173	286	0
2	A	10	0	5	0	0
2	B	10	0	5	0	0
2	C	10	0	5	0	0
2	D	10	0	5	0	0
All	All	20436	0	20712	1119	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 27.

All (1119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:HIS:HB2	1:D:733:HIS:HB2	1.46	0.97
1:D:346:VAL:HG22	1:D:350:VAL:HG13	1.62	0.81
1:B:346:VAL:HG22	1:B:350:VAL:HG13	1.62	0.81
1:A:346:VAL:HG22	1:A:350:VAL:HG13	1.62	0.80
1:C:346:VAL:HG22	1:C:350:VAL:HG13	1.62	0.80
1:D:522:VAL:HB	1:D:526:GLU:HG3	1.65	0.79
1:B:522:VAL:HB	1:B:526:GLU:HG3	1.65	0.79
1:C:522:VAL:HB	1:C:526:GLU:HG3	1.65	0.79
1:A:256:ASP:HA	1:A:316:ASN:HB2	1.65	0.78
1:C:256:ASP:HA	1:C:316:ASN:HB2	1.65	0.78
1:A:522:VAL:HB	1:A:526:GLU:HG3	1.65	0.78
1:D:545:GLY:H	1:D:549:LEU:HD22	1.49	0.77
1:B:545:GLY:H	1:B:549:LEU:HD22	1.49	0.77
1:B:256:ASP:HA	1:B:316:ASN:HB2	1.65	0.77
1:D:256:ASP:HA	1:D:316:ASN:HB2	1.65	0.77
1:A:545:GLY:H	1:A:549:LEU:HD22	1.49	0.76
1:C:545:GLY:H	1:C:549:LEU:HD22	1.49	0.76
1:A:511:ALA:HA	1:A:515:ALA:HA	1.69	0.74
1:C:511:ALA:HA	1:C:515:ALA:HA	1.69	0.74
1:B:446:LEU:HB2	1:B:450:LEU:HD23	1.70	0.74
1:D:446:LEU:HB2	1:D:450:LEU:HD23	1.70	0.74
1:D:392:ASN:HD22	1:D:414:LEU:HB3	1.53	0.73
1:A:392:ASN:HD22	1:A:414:LEU:HB3	1.53	0.73
1:B:392:ASN:HD22	1:B:414:LEU:HB3	1.54	0.73
1:C:392:ASN:HD22	1:C:414:LEU:HB3	1.53	0.73
1:A:446:LEU:HB2	1:A:450:LEU:HD23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HA	1:A:53:LEU:HD23	1.71	0.73
1:B:50:ARG:HA	1:B:53:LEU:HD23	1.71	0.73
1:C:50:ARG:HA	1:C:53:LEU:HD23	1.71	0.73
1:C:446:LEU:HB2	1:C:450:LEU:HD23	1.70	0.73
1:D:50:ARG:HA	1:D:53:LEU:HD23	1.71	0.72
1:B:511:ALA:HA	1:B:515:ALA:HA	1.69	0.72
1:C:50:ARG:NH2	1:C:332:VAL:O	2.23	0.72
1:D:511:ALA:HA	1:D:515:ALA:HA	1.69	0.72
1:A:50:ARG:NH2	1:A:332:VAL:O	2.23	0.72
1:D:50:ARG:NH2	1:D:332:VAL:O	2.23	0.72
1:D:178:PHE:O	1:D:184:ARG:NH1	2.21	0.72
1:B:50:ARG:NH2	1:B:332:VAL:O	2.23	0.72
1:D:254:ASP:HA	1:D:318:MET:HE1	1.72	0.71
1:B:254:ASP:HA	1:B:318:MET:HE1	1.73	0.71
1:A:178:PHE:O	1:A:184:ARG:NH1	2.21	0.71
1:A:106:VAL:HG12	1:A:146:ALA:HB2	1.73	0.70
1:C:106:VAL:HG12	1:C:146:ALA:HB2	1.73	0.70
1:B:106:VAL:HG12	1:B:146:ALA:HB2	1.73	0.70
1:D:106:VAL:HG12	1:D:146:ALA:HB2	1.73	0.70
1:C:178:PHE:O	1:C:184:ARG:NH1	2.21	0.70
1:B:337:THR:HG22	1:B:339:ALA:H	1.56	0.70
1:D:337:THR:HG22	1:D:339:ALA:H	1.56	0.70
1:A:541:ILE:HG22	1:A:543:PRO:HD3	1.74	0.70
1:C:541:ILE:HG22	1:C:543:PRO:HD3	1.74	0.70
1:B:541:ILE:HG22	1:B:543:PRO:HD3	1.74	0.70
1:C:254:ASP:HA	1:C:318:MET:HE1	1.72	0.70
1:A:254:ASP:HA	1:A:318:MET:HE1	1.72	0.69
1:D:541:ILE:HG22	1:D:543:PRO:HD3	1.74	0.69
1:B:253:SER:OG	1:B:298:LYS:NZ	2.26	0.69
1:D:253:SER:OG	1:D:298:LYS:NZ	2.26	0.69
1:C:591:LYS:HE2	1:C:595:PRO:HB3	1.75	0.69
1:B:67:VAL:O	1:B:80:ARG:NE	2.25	0.69
1:D:67:VAL:O	1:D:80:ARG:NE	2.26	0.69
1:A:591:LYS:HE2	1:A:595:PRO:HB3	1.75	0.69
1:C:260:ASN:HA	1:C:271:MET:HE3	1.76	0.69
1:A:260:ASN:HA	1:A:271:MET:HE3	1.76	0.68
1:D:260:ASN:HA	1:D:271:MET:HE3	1.76	0.68
1:B:260:ASN:HA	1:B:271:MET:HE3	1.76	0.68
1:D:447:ALA:HA	1:D:769:LEU:HD13	1.76	0.68
1:A:253:SER:OG	1:A:298:LYS:NZ	2.26	0.68
1:B:447:ALA:HA	1:B:769:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:THR:HG22	1:C:339:ALA:H	1.56	0.68
1:B:588:ARG:HG3	1:B:622:MET:HE2	1.76	0.67
1:C:253:SER:OG	1:C:298:LYS:NZ	2.26	0.67
1:A:337:THR:HG22	1:A:339:ALA:H	1.56	0.67
1:D:588:ARG:HG3	1:D:622:MET:HE2	1.76	0.67
1:D:591:LYS:HE2	1:D:595:PRO:HB3	1.75	0.67
1:B:56:ALA:O	1:B:96:ARG:NH2	2.28	0.67
1:B:591:LYS:HE2	1:B:595:PRO:HB3	1.75	0.67
1:D:56:ALA:O	1:D:96:ARG:NH2	2.28	0.67
1:A:56:ALA:O	1:A:96:ARG:NH2	2.28	0.67
1:C:56:ALA:O	1:C:96:ARG:NH2	2.28	0.67
1:B:90:GLU:OE1	1:B:90:GLU:HA	1.95	0.67
1:C:297:SER:N	1:C:300:LYS:HG3	2.10	0.67
1:A:447:ALA:HA	1:A:769:LEU:HD13	1.76	0.67
1:A:543:PRO:HB2	1:A:550:VAL:HG12	1.77	0.67
1:B:358:GLY:HA3	1:B:518:ALA:HB2	1.77	0.67
1:C:543:PRO:HB2	1:C:550:VAL:HG12	1.77	0.67
1:D:90:GLU:HA	1:D:90:GLU:OE1	1.95	0.67
1:A:297:SER:N	1:A:300:LYS:HG3	2.10	0.66
1:C:254:ASP:O	1:C:316:ASN:ND2	2.28	0.66
1:A:358:GLY:HA3	1:A:518:ALA:HB2	1.77	0.66
1:B:581:GLU:HA	1:B:584:LEU:HD12	1.77	0.66
1:C:447:ALA:HA	1:C:769:LEU:HD13	1.76	0.66
1:D:358:GLY:HA3	1:D:518:ALA:HB2	1.77	0.66
1:D:581:GLU:HA	1:D:584:LEU:HD12	1.76	0.66
1:A:254:ASP:O	1:A:316:ASN:ND2	2.28	0.66
1:C:358:GLY:HA3	1:C:518:ALA:HB2	1.77	0.66
1:A:581:GLU:HA	1:A:584:LEU:HD12	1.76	0.66
1:B:297:SER:N	1:B:300:LYS:HG3	2.10	0.66
1:C:67:VAL:O	1:C:80:ARG:NE	2.25	0.66
1:C:581:GLU:HA	1:C:584:LEU:HD12	1.77	0.66
1:D:297:SER:N	1:D:300:LYS:HG3	2.10	0.66
1:B:543:PRO:HB2	1:B:550:VAL:HG12	1.77	0.66
1:D:543:PRO:HB2	1:D:550:VAL:HG12	1.77	0.66
1:A:588:ARG:HG3	1:A:622:MET:HE2	1.76	0.66
1:C:588:ARG:HG3	1:C:622:MET:HE2	1.76	0.66
1:B:254:ASP:O	1:B:316:ASN:ND2	2.28	0.66
1:D:254:ASP:O	1:D:316:ASN:ND2	2.28	0.66
1:A:67:VAL:O	1:A:80:ARG:NE	2.26	0.65
1:B:178:PHE:O	1:B:184:ARG:NH1	2.21	0.65
1:B:574:ILE:HD12	1:B:606:ILE:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:ILE:HD12	1:D:606:ILE:HG12	1.78	0.65
1:C:90:GLU:HA	1:C:90:GLU:OE1	1.95	0.65
1:A:90:GLU:HA	1:A:90:GLU:OE1	1.95	0.65
1:A:325:THR:HG23	1:A:330:ARG:HD3	1.79	0.65
1:C:325:THR:HG23	1:C:330:ARG:HD3	1.79	0.65
1:D:325:THR:HG23	1:D:330:ARG:HD3	1.79	0.65
1:B:325:THR:HG23	1:B:330:ARG:HD3	1.79	0.65
1:A:601:MET:C	1:A:603:THR:H	2.05	0.64
1:C:535:GLU:O	1:C:537:HIS:ND1	2.30	0.64
1:C:601:MET:C	1:C:603:THR:H	2.05	0.64
1:C:741:GLU:OE1	1:C:741:GLU:N	2.27	0.64
1:A:535:GLU:O	1:A:537:HIS:ND1	2.31	0.64
1:A:733:HIS:HB2	1:C:733:HIS:HB2	1.80	0.64
1:A:741:GLU:OE1	1:A:741:GLU:N	2.27	0.64
1:D:466:PHE:HB3	1:D:544:ARG:HB3	1.79	0.64
1:B:466:PHE:HB3	1:B:544:ARG:HB3	1.79	0.64
1:B:601:MET:C	1:B:603:THR:H	2.05	0.64
1:A:386:LYS:H	1:A:386:LYS:HD2	1.63	0.64
1:C:386:LYS:H	1:C:386:LYS:HD2	1.63	0.64
1:D:601:MET:C	1:D:603:THR:H	2.05	0.64
1:A:54:LYS:O	1:A:96:ARG:NH1	2.31	0.64
1:C:54:LYS:O	1:C:96:ARG:NH1	2.31	0.64
1:C:466:PHE:HB3	1:C:544:ARG:HB3	1.78	0.64
1:B:54:LYS:O	1:B:96:ARG:NH1	2.31	0.63
1:B:641:THR:HG23	1:B:642:PHE:H	1.63	0.63
1:D:54:LYS:O	1:D:96:ARG:NH1	2.31	0.63
1:D:641:THR:HG23	1:D:642:PHE:H	1.64	0.63
1:A:466:PHE:HB3	1:A:544:ARG:HB3	1.79	0.63
1:B:623:LEU:HB3	1:B:628:VAL:HB	1.81	0.63
1:D:623:LEU:HB3	1:D:628:VAL:HB	1.81	0.63
1:B:386:LYS:H	1:B:386:LYS:HD2	1.63	0.63
1:C:574:ILE:HD12	1:C:606:ILE:HG12	1.78	0.63
1:A:574:ILE:HD12	1:A:606:ILE:HG12	1.78	0.63
1:D:535:GLU:O	1:D:537:HIS:ND1	2.30	0.63
1:D:386:LYS:H	1:D:386:LYS:HD2	1.63	0.63
1:A:346:VAL:HG21	1:A:351:MET:HG3	1.81	0.63
1:B:365:LEU:O	1:B:369:GLN:HB2	1.99	0.63
1:B:535:GLU:O	1:B:537:HIS:ND1	2.31	0.63
1:D:365:LEU:O	1:D:369:GLN:HB2	1.99	0.63
1:C:346:VAL:HG21	1:C:351:MET:HG3	1.81	0.63
1:A:57:ARG:N	1:A:247:ASP:OD2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:N	1:C:247:ASP:OD2	2.32	0.62
1:A:365:LEU:O	1:A:369:GLN:HB2	1.99	0.62
1:B:57:ARG:N	1:B:247:ASP:OD2	2.32	0.62
1:C:365:LEU:O	1:C:369:GLN:HB2	1.99	0.62
1:C:58:ARG:N	1:C:247:ASP:OD2	2.31	0.62
1:D:57:ARG:N	1:D:247:ASP:OD2	2.32	0.62
1:D:346:VAL:HG21	1:D:351:MET:HG3	1.81	0.62
1:A:58:ARG:N	1:A:247:ASP:OD2	2.31	0.62
1:B:346:VAL:HG21	1:B:351:MET:HG3	1.81	0.62
1:D:349:GLU:O	1:D:352:ALA:N	2.33	0.62
1:A:623:LEU:HB3	1:A:628:VAL:HB	1.81	0.62
1:A:625:ARG:CZ	1:A:625:ARG:HA	2.30	0.62
1:B:349:GLU:O	1:B:352:ALA:N	2.33	0.62
1:C:623:LEU:HB3	1:C:628:VAL:HB	1.81	0.62
1:C:625:ARG:HA	1:C:625:ARG:CZ	2.30	0.62
1:C:520:SER:OG	1:C:521:LEU:N	2.32	0.61
1:A:520:SER:OG	1:A:521:LEU:N	2.32	0.61
1:D:405:ALA:O	1:D:409:LEU:N	2.28	0.61
1:C:641:THR:HG23	1:C:642:PHE:H	1.63	0.61
1:A:376:THR:HG21	1:A:512:THR:HG21	1.83	0.61
1:B:405:ALA:O	1:B:409:LEU:N	2.28	0.61
1:C:376:THR:HG21	1:C:512:THR:HG21	1.83	0.61
1:B:625:ARG:CZ	1:B:625:ARG:HA	2.30	0.61
1:C:405:ALA:O	1:C:409:LEU:N	2.29	0.61
1:A:641:THR:HG23	1:A:642:PHE:H	1.63	0.61
1:D:625:ARG:CZ	1:D:625:ARG:HA	2.30	0.61
1:A:470:PRO:HG3	1:A:495:ALA:HB1	1.83	0.61
1:C:470:PRO:HG3	1:C:495:ALA:HB1	1.83	0.61
1:C:349:GLU:O	1:C:352:ALA:N	2.33	0.61
1:A:405:ALA:O	1:A:409:LEU:N	2.28	0.60
1:A:349:GLU:O	1:A:352:ALA:N	2.33	0.60
1:B:680:SER:O	1:B:703:ALA:N	2.26	0.60
1:D:520:SER:OG	1:D:521:LEU:N	2.32	0.60
1:D:680:SER:O	1:D:703:ALA:N	2.26	0.60
1:B:520:SER:OG	1:B:521:LEU:N	2.32	0.60
1:D:470:PRO:HG3	1:D:495:ALA:HB1	1.83	0.60
1:B:376:THR:HG21	1:B:512:THR:HG21	1.83	0.60
1:B:470:PRO:HG3	1:B:495:ALA:HB1	1.83	0.60
1:D:376:THR:HG21	1:D:512:THR:HG21	1.83	0.60
1:C:680:SER:O	1:C:703:ALA:N	2.26	0.60
1:A:694:ARG:HG2	1:A:695:GLN:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:SER:O	1:A:703:ALA:N	2.26	0.59
1:C:694:ARG:HG2	1:C:695:GLN:N	2.17	0.59
1:D:58:ARG:N	1:D:247:ASP:OD2	2.31	0.59
1:A:462:LEU:HD13	1:A:485:ASN:HD22	1.68	0.59
1:B:58:ARG:N	1:B:247:ASP:OD2	2.31	0.59
1:C:462:LEU:HD13	1:C:485:ASN:HD22	1.68	0.59
1:B:694:ARG:HG2	1:B:695:GLN:N	2.17	0.59
1:D:694:ARG:HG2	1:D:695:GLN:N	2.17	0.59
1:B:462:LEU:HD13	1:B:485:ASN:HD22	1.68	0.58
1:B:680:SER:OG	1:B:701:ASP:O	2.21	0.58
1:D:462:LEU:HD13	1:D:485:ASN:HD22	1.68	0.58
1:D:680:SER:OG	1:D:701:ASP:O	2.21	0.58
1:B:760:PHE:HA	1:B:766:ARG:HB2	1.84	0.58
1:D:760:PHE:HA	1:D:766:ARG:HB2	1.84	0.58
1:B:260:ASN:HB2	1:B:269:LYS:HB3	1.85	0.58
1:D:741:GLU:OE1	1:D:741:GLU:N	2.27	0.58
1:B:741:GLU:OE1	1:B:741:GLU:N	2.27	0.58
1:C:680:SER:OG	1:C:701:ASP:O	2.21	0.58
1:D:260:ASN:HB2	1:D:269:LYS:HB3	1.86	0.58
1:A:680:SER:OG	1:A:701:ASP:O	2.21	0.58
1:A:63:LEU:HD21	1:A:84:ILE:HG21	1.86	0.57
1:C:63:LEU:HD21	1:C:84:ILE:HG21	1.86	0.57
1:C:696:PHE:O	1:C:700:VAL:HG22	2.05	0.57
1:A:696:PHE:O	1:A:700:VAL:HG22	2.05	0.57
1:C:549:LEU:O	1:C:553:ILE:HG12	2.05	0.57
1:C:576:ARG:HB3	1:C:607:HIS:CD2	2.39	0.57
1:C:760:PHE:HA	1:C:766:ARG:HB2	1.84	0.57
1:A:475:GLN:O	1:A:479:LEU:HG	2.05	0.57
1:B:356:ARG:O	1:B:359:SER:OG	2.22	0.57
1:B:407:PRO:O	1:B:411:ARG:HG2	2.05	0.57
1:B:457:VAL:HG23	1:B:745:THR:HG23	1.87	0.57
1:C:475:GLN:O	1:C:479:LEU:HG	2.05	0.57
1:D:356:ARG:O	1:D:359:SER:OG	2.22	0.57
1:D:407:PRO:O	1:D:411:ARG:HG2	2.05	0.57
1:D:457:VAL:HG23	1:D:745:THR:HG23	1.87	0.57
1:A:549:LEU:O	1:A:553:ILE:HG12	2.05	0.57
1:A:576:ARG:HB3	1:A:607:HIS:CD2	2.39	0.57
1:A:760:PHE:HA	1:A:766:ARG:HB2	1.84	0.57
1:B:530:ASP:O	1:B:533:SER:OG	2.22	0.57
1:B:576:ARG:HB3	1:B:607:HIS:CD2	2.39	0.57
1:D:576:ARG:HB3	1:D:607:HIS:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:TYR:HB3	1:A:712:ARG:HH21	1.69	0.57
1:B:70:ARG:NH2	1:B:76:LEU:O	2.38	0.57
1:C:594:TYR:HB3	1:C:712:ARG:HH21	1.70	0.57
1:D:70:ARG:NH2	1:D:76:LEU:O	2.38	0.57
1:A:407:PRO:O	1:A:411:ARG:HG2	2.05	0.57
1:B:80:ARG:O	1:B:84:ILE:HG12	2.05	0.57
1:D:80:ARG:O	1:D:84:ILE:HG12	2.05	0.57
1:C:260:ASN:HB2	1:C:269:LYS:HB3	1.86	0.57
1:A:260:ASN:HB2	1:A:269:LYS:HB3	1.86	0.56
1:B:475:GLN:O	1:B:479:LEU:HG	2.05	0.56
1:C:356:ARG:O	1:C:359:SER:OG	2.22	0.56
1:C:407:PRO:O	1:C:411:ARG:HG2	2.05	0.56
1:A:457:VAL:HG23	1:A:745:THR:HG23	1.87	0.56
1:B:690:ASP:HA	1:B:693:ALA:CB	2.35	0.56
1:C:457:VAL:HG23	1:C:745:THR:HG23	1.87	0.56
1:D:475:GLN:O	1:D:479:LEU:HG	2.05	0.56
1:D:690:ASP:HA	1:D:693:ALA:CB	2.35	0.56
1:A:70:ARG:NH2	1:A:76:LEU:O	2.38	0.56
1:A:180:ASN:HB3	1:A:183:THR:HG22	1.88	0.56
1:A:356:ARG:O	1:A:359:SER:OG	2.22	0.56
1:B:63:LEU:HD21	1:B:84:ILE:HG21	1.86	0.56
1:B:696:PHE:O	1:B:700:VAL:HG22	2.05	0.56
1:D:250:ILE:HD13	1:D:323:ILE:HD12	1.88	0.56
1:D:696:PHE:O	1:D:700:VAL:HG22	2.05	0.56
1:A:233:ASN:HB2	1:A:236:LEU:HD12	1.88	0.56
1:A:690:ASP:HA	1:A:693:ALA:CB	2.35	0.56
1:B:250:ILE:HD13	1:B:323:ILE:HD12	1.88	0.56
1:C:70:ARG:NH2	1:C:76:LEU:O	2.38	0.56
1:C:180:ASN:HB3	1:C:183:THR:HG22	1.87	0.56
1:C:690:ASP:HA	1:C:693:ALA:CB	2.35	0.56
1:D:63:LEU:HD21	1:D:84:ILE:HG21	1.86	0.56
1:B:71:GLU:N	1:B:71:GLU:OE1	2.39	0.56
1:D:207:ASP:O	1:D:208:ALA:C	2.47	0.56
1:D:549:LEU:O	1:D:553:ILE:HG12	2.05	0.56
1:A:80:ARG:O	1:A:84:ILE:HG12	2.04	0.56
1:B:207:ASP:O	1:B:208:ALA:C	2.47	0.56
1:C:233:ASN:HB2	1:C:236:LEU:HD12	1.88	0.56
1:D:71:GLU:N	1:D:71:GLU:OE1	2.39	0.56
1:D:594:TYR:HB3	1:D:712:ARG:HH21	1.69	0.56
1:B:70:ARG:HA	1:B:77:ALA:HB2	1.88	0.56
1:C:80:ARG:O	1:C:84:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:LEU:O	1:B:553:ILE:HG12	2.05	0.56
1:D:70:ARG:HA	1:D:77:ALA:HB2	1.88	0.56
1:B:594:TYR:HB3	1:B:712:ARG:HH21	1.69	0.56
1:B:731:ARG:HE	1:B:735:ARG:HH12	1.54	0.56
1:D:731:ARG:HE	1:D:735:ARG:HH12	1.54	0.56
1:C:207:ASP:O	1:C:208:ALA:C	2.47	0.55
1:A:433:SER:OG	1:A:482:ALA:HB1	2.07	0.55
1:A:634:PRO:HA	1:A:637:ASN:HD22	1.71	0.55
1:D:180:ASN:HB3	1:D:183:THR:HG22	1.88	0.55
1:A:674:ILE:O	1:A:678:GLY:N	2.38	0.55
1:A:731:ARG:HE	1:A:735:ARG:HH12	1.54	0.55
1:B:180:ASN:HB3	1:B:183:THR:HG22	1.88	0.55
1:C:71:GLU:OE1	1:C:71:GLU:N	2.39	0.55
1:C:433:SER:OG	1:C:482:ALA:HB1	2.07	0.55
1:C:530:ASP:O	1:C:533:SER:OG	2.22	0.55
1:A:71:GLU:N	1:A:71:GLU:OE1	2.39	0.55
1:A:207:ASP:O	1:A:208:ALA:C	2.47	0.55
1:C:545:GLY:N	1:C:549:LEU:HD22	2.20	0.55
1:A:70:ARG:HA	1:A:77:ALA:HB2	1.88	0.55
1:A:530:ASP:O	1:A:533:SER:OG	2.22	0.55
1:A:591:LYS:HB2	1:A:601:MET:SD	2.47	0.55
1:B:433:SER:OG	1:B:482:ALA:HB1	2.07	0.55
1:C:591:LYS:HB2	1:C:601:MET:SD	2.47	0.55
1:C:634:PRO:HA	1:C:637:ASN:HD22	1.71	0.55
1:B:47:PHE:CD2	1:B:52:GLN:HB3	2.42	0.55
1:B:264:TRP:CD1	1:B:264:TRP:H	2.23	0.55
1:C:731:ARG:HE	1:C:735:ARG:HH12	1.54	0.55
1:D:433:SER:OG	1:D:482:ALA:HB1	2.07	0.55
1:C:70:ARG:HA	1:C:77:ALA:HB2	1.88	0.55
1:D:47:PHE:CD2	1:D:52:GLN:HB3	2.42	0.55
1:D:264:TRP:H	1:D:264:TRP:CD1	2.23	0.55
1:A:545:GLY:N	1:A:549:LEU:HD22	2.21	0.55
1:B:233:ASN:HB2	1:B:236:LEU:HD12	1.88	0.55
1:B:591:LYS:HB2	1:B:601:MET:SD	2.47	0.55
1:B:634:PRO:HA	1:B:637:ASN:HD22	1.71	0.55
1:D:591:LYS:HB2	1:D:601:MET:SD	2.47	0.55
1:A:398:GLU:O	1:A:401:LYS:NZ	2.28	0.54
1:D:233:ASN:HB2	1:D:236:LEU:HD12	1.88	0.54
1:D:634:PRO:HA	1:D:637:ASN:HD22	1.71	0.54
1:A:47:PHE:CD2	1:A:52:GLN:HB3	2.42	0.54
1:B:580:LEU:HD22	1:B:615:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ILE:HD13	1:C:323:ILE:HD12	1.88	0.54
1:C:599:ASN:ND2	1:C:712:ARG:HA	2.23	0.54
1:D:580:LEU:HD22	1:D:615:ILE:HG13	1.90	0.54
1:A:599:ASN:ND2	1:A:712:ARG:HA	2.23	0.54
1:C:398:GLU:O	1:C:401:LYS:NZ	2.28	0.54
1:B:398:GLU:O	1:B:401:LYS:NZ	2.27	0.54
1:B:599:ASN:HD21	1:B:712:ARG:HD2	1.72	0.54
1:C:47:PHE:CD2	1:C:52:GLN:HB3	2.42	0.54
1:D:599:ASN:HD21	1:D:712:ARG:HD2	1.72	0.54
1:A:250:ILE:HD13	1:A:323:ILE:HD12	1.88	0.54
1:A:624:LYS:NZ	1:A:625:ARG:HD2	2.23	0.54
1:B:47:PHE:HD2	1:B:52:GLN:HB3	1.73	0.54
1:C:354:ASN:O	1:C:357:THR:OG1	2.14	0.54
1:C:624:LYS:NZ	1:C:625:ARG:HD2	2.23	0.54
1:D:398:GLU:O	1:D:401:LYS:NZ	2.27	0.54
1:A:580:LEU:HD22	1:A:615:ILE:HG13	1.90	0.54
1:C:580:LEU:HD22	1:C:615:ILE:HG13	1.90	0.54
1:D:47:PHE:HD2	1:D:52:GLN:HB3	1.73	0.54
1:A:354:ASN:O	1:A:357:THR:OG1	2.14	0.54
1:C:264:TRP:H	1:C:264:TRP:CD1	2.23	0.54
1:A:47:PHE:HD2	1:A:52:GLN:HB3	1.73	0.54
1:A:194:LEU:HD13	1:A:201:PRO:HB3	1.89	0.54
1:A:264:TRP:H	1:A:264:TRP:CD1	2.23	0.54
1:B:624:LYS:NZ	1:B:625:ARG:HD2	2.23	0.54
1:A:174:THR:N	1:A:177:ASP:OD2	2.41	0.54
1:C:174:THR:N	1:C:177:ASP:OD2	2.41	0.54
1:B:174:THR:N	1:B:177:ASP:OD2	2.41	0.53
1:C:47:PHE:HD2	1:C:52:GLN:HB3	1.73	0.53
1:C:489:LEU:O	1:C:522:VAL:HG22	2.08	0.53
1:D:174:THR:N	1:D:177:ASP:OD2	2.41	0.53
1:D:624:LYS:NZ	1:D:625:ARG:HD2	2.23	0.53
1:A:489:LEU:O	1:A:522:VAL:HG22	2.08	0.53
1:B:323:ILE:HA	1:B:326:ILE:HG22	1.91	0.53
1:B:599:ASN:ND2	1:B:712:ARG:HA	2.23	0.53
1:C:194:LEU:HD13	1:C:201:PRO:HB3	1.89	0.53
1:D:712:ARG:O	1:D:718:ARG:NH1	2.41	0.53
1:B:712:ARG:O	1:B:718:ARG:NH1	2.41	0.53
1:D:194:LEU:HD13	1:D:201:PRO:HB3	1.89	0.53
1:D:392:ASN:ND2	1:D:414:LEU:HB3	2.22	0.53
1:D:599:ASN:ND2	1:D:712:ARG:HA	2.23	0.53
1:A:689:ASN:OD1	1:A:691:ALA:N	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HD13	1:B:201:PRO:HB3	1.89	0.53
1:B:392:ASN:ND2	1:B:414:LEU:HB3	2.22	0.53
1:B:489:LEU:O	1:B:522:VAL:HG22	2.08	0.53
1:B:621:ASN:O	1:B:625:ARG:HG2	2.09	0.53
1:C:362:MET:HA	1:C:365:LEU:HD13	1.91	0.53
1:C:323:ILE:HA	1:C:326:ILE:HG22	1.91	0.53
1:D:323:ILE:HA	1:D:326:ILE:HG22	1.91	0.53
1:D:489:LEU:O	1:D:522:VAL:HG22	2.08	0.53
1:D:621:ASN:O	1:D:625:ARG:HG2	2.09	0.53
1:A:323:ILE:HA	1:A:326:ILE:HG22	1.91	0.53
1:A:362:MET:HA	1:A:365:LEU:HD13	1.91	0.53
1:A:712:ARG:O	1:A:718:ARG:NH1	2.41	0.53
1:B:109:GLY:O	1:B:113:LEU:HG	2.08	0.53
1:C:109:GLY:O	1:C:113:LEU:HG	2.08	0.53
1:C:494:GLU:OE1	1:C:494:GLU:N	2.30	0.53
1:C:689:ASN:OD1	1:C:691:ALA:N	2.37	0.53
1:C:599:ASN:HD21	1:C:712:ARG:HD2	1.72	0.53
1:C:621:ASN:O	1:C:625:ARG:HG2	2.09	0.53
1:D:109:GLY:O	1:D:113:LEU:HG	2.08	0.53
1:D:545:GLY:N	1:D:549:LEU:HD22	2.21	0.53
1:A:109:GLY:O	1:A:113:LEU:HG	2.08	0.53
1:A:599:ASN:HD21	1:A:712:ARG:HD2	1.72	0.53
1:A:667:LEU:HD21	1:A:692:ALA:HB1	1.91	0.53
1:C:667:LEU:HD21	1:C:692:ALA:HB1	1.91	0.53
1:D:690:ASP:HA	1:D:693:ALA:HB3	1.90	0.53
1:A:621:ASN:O	1:A:625:ARG:HG2	2.09	0.53
1:B:545:GLY:N	1:B:549:LEU:HD22	2.21	0.53
1:B:690:ASP:HA	1:B:693:ALA:HB3	1.91	0.53
1:C:712:ARG:O	1:C:718:ARG:NH1	2.41	0.53
1:B:362:MET:HA	1:B:365:LEU:HD13	1.91	0.53
1:D:362:MET:HA	1:D:365:LEU:HD13	1.91	0.53
1:B:608:GLU:HB2	1:B:665:PRO:HA	1.90	0.52
1:D:608:GLU:HB2	1:D:665:PRO:HA	1.90	0.52
1:A:608:GLU:HB2	1:A:665:PRO:HA	1.90	0.52
1:B:667:LEU:HD21	1:B:692:ALA:HB1	1.91	0.52
1:C:608:GLU:HB2	1:C:665:PRO:HA	1.90	0.52
1:D:667:LEU:HD21	1:D:692:ALA:HB1	1.91	0.52
1:A:346:VAL:HG11	1:A:351:MET:H	1.75	0.52
1:B:731:ARG:NH2	1:D:459:ILE:O	2.42	0.52
1:C:674:ILE:O	1:C:678:GLY:N	2.38	0.52
1:B:346:VAL:HG11	1:B:351:MET:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:VAL:HG11	1:C:351:MET:H	1.75	0.52
1:C:318:MET:SD	1:C:318:MET:N	2.83	0.52
1:C:388:ILE:HG22	1:C:501:ALA:HB1	1.91	0.52
1:C:690:ASP:HA	1:C:693:ALA:HB3	1.91	0.52
1:A:318:MET:SD	1:A:318:MET:N	2.83	0.52
1:A:690:ASP:HA	1:A:693:ALA:HB3	1.90	0.52
1:B:248:LEU:HD12	1:B:311:SER:O	2.10	0.52
1:B:414:LEU:HD12	1:B:418:LYS:HB2	1.92	0.52
1:D:346:VAL:HG11	1:D:351:MET:H	1.75	0.52
1:D:414:LEU:HD12	1:D:418:LYS:HB2	1.92	0.52
1:A:388:ILE:HG22	1:A:501:ALA:HB1	1.91	0.52
1:A:560:ILE:HD12	1:A:561:PRO:HD2	1.92	0.52
1:B:318:MET:SD	1:B:318:MET:N	2.83	0.52
1:D:248:LEU:HD12	1:D:311:SER:O	2.10	0.52
1:B:651:LYS:NZ	1:B:677:TYR:O	2.42	0.51
1:C:560:ILE:HD12	1:C:561:PRO:HD2	1.92	0.51
1:D:318:MET:SD	1:D:318:MET:N	2.83	0.51
1:D:651:LYS:NZ	1:D:677:TYR:O	2.43	0.51
1:A:414:LEU:HD12	1:A:418:LYS:HB2	1.92	0.51
1:A:628:VAL:HG22	1:A:657:LEU:HD12	1.93	0.51
1:C:628:VAL:HG22	1:C:657:LEU:HD12	1.92	0.51
1:A:370:ARG:HD2	1:A:481:MET:O	2.11	0.51
1:B:388:ILE:HG22	1:B:501:ALA:HB1	1.91	0.51
1:C:370:ARG:HD2	1:C:481:MET:O	2.11	0.51
1:C:414:LEU:HD12	1:C:418:LYS:HB2	1.92	0.51
1:C:478:ALA:HA	1:C:481:MET:HG2	1.93	0.51
1:D:388:ILE:HG22	1:D:501:ALA:HB1	1.91	0.51
1:D:448:ASP:O	1:D:755:HIS:NE2	2.34	0.51
1:A:478:ALA:HA	1:A:481:MET:HG2	1.93	0.51
1:B:448:ASP:O	1:B:755:HIS:NE2	2.34	0.51
1:C:348:VAL:HB	1:C:349:GLU:CD	2.36	0.51
1:D:693:ALA:O	1:D:697:LEU:HG	2.11	0.51
1:A:348:VAL:HB	1:A:349:GLU:CD	2.36	0.51
1:B:693:ALA:O	1:B:697:LEU:HG	2.11	0.51
1:D:368:ALA:HA	1:D:371:ALA:HB3	1.93	0.51
1:A:50:ARG:HB3	1:A:329:GLY:HA2	1.93	0.51
1:B:368:ALA:HA	1:B:371:ALA:HB3	1.93	0.51
1:C:50:ARG:HB3	1:C:329:GLY:HA2	1.93	0.51
1:B:370:ARG:HD2	1:B:481:MET:O	2.11	0.51
1:B:493:LYS:HG2	1:B:525:ARG:HH22	1.75	0.51
1:B:560:ILE:HD12	1:B:561:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:PHE:CE2	1:B:737:PRO:HG2	2.46	0.51
1:C:248:LEU:HD12	1:C:311:SER:O	2.10	0.51
1:D:370:ARG:HD2	1:D:481:MET:O	2.11	0.51
1:D:493:LYS:HG2	1:D:525:ARG:HH22	1.75	0.51
1:D:674:ILE:O	1:D:678:GLY:N	2.38	0.51
1:D:719:PHE:CE2	1:D:737:PRO:HG2	2.46	0.51
1:A:248:LEU:HD12	1:A:311:SER:O	2.10	0.51
1:A:693:ALA:O	1:A:697:LEU:HG	2.11	0.51
1:B:346:VAL:HG11	1:B:351:MET:HB2	1.92	0.51
1:B:348:VAL:HB	1:B:349:GLU:CD	2.36	0.51
1:C:693:ALA:O	1:C:697:LEU:HG	2.11	0.51
1:A:719:PHE:CE2	1:A:737:PRO:HG2	2.46	0.51
1:C:651:LYS:NZ	1:C:677:TYR:O	2.42	0.51
1:C:719:PHE:CE2	1:C:737:PRO:HG2	2.46	0.51
1:D:346:VAL:HG11	1:D:351:MET:HB2	1.92	0.51
1:D:348:VAL:HB	1:D:349:GLU:CD	2.36	0.51
1:D:560:ILE:HD12	1:D:561:PRO:HD2	1.92	0.51
1:D:731:ARG:NE	1:D:735:ARG:HH12	2.09	0.51
1:B:683:ASP:OD1	1:B:684:VAL:N	2.45	0.50
1:B:731:ARG:NE	1:B:735:ARG:HH12	2.08	0.50
1:D:628:VAL:HG22	1:D:657:LEU:HD12	1.92	0.50
1:D:683:ASP:OD1	1:D:684:VAL:N	2.45	0.50
1:A:651:LYS:NZ	1:A:677:TYR:O	2.42	0.50
1:B:62:LYS:HG3	1:B:237:SER:HB3	1.94	0.50
1:B:674:ILE:O	1:B:678:GLY:N	2.38	0.50
1:D:62:LYS:HG3	1:D:237:SER:HB3	1.94	0.50
1:A:493:LYS:HG2	1:A:525:ARG:HH22	1.75	0.50
1:A:731:ARG:NE	1:A:735:ARG:HH12	2.08	0.50
1:B:628:VAL:HG22	1:B:657:LEU:HD12	1.93	0.50
1:C:493:LYS:HB2	1:C:525:ARG:HH12	1.76	0.50
1:C:731:ARG:NE	1:C:735:ARG:HH12	2.08	0.50
1:A:392:ASN:ND2	1:A:414:LEU:HB3	2.22	0.50
1:A:493:LYS:HB2	1:A:525:ARG:HH12	1.76	0.50
1:B:493:LYS:HB2	1:B:525:ARG:HH12	1.76	0.50
1:B:601:MET:O	1:B:603:THR:N	2.44	0.50
1:B:667:LEU:HD12	1:B:667:LEU:H	1.77	0.50
1:D:50:ARG:HB3	1:D:329:GLY:HA2	1.92	0.50
1:D:493:LYS:HB2	1:D:525:ARG:HH12	1.76	0.50
1:D:667:LEU:HD12	1:D:667:LEU:H	1.77	0.50
1:C:683:ASP:OD1	1:C:684:VAL:N	2.45	0.50
1:A:62:LYS:HG3	1:A:237:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ALA:HB2	1:A:487:LEU:HD22	1.94	0.50
1:A:683:ASP:OD1	1:A:684:VAL:N	2.45	0.50
1:B:50:ARG:HB3	1:B:329:GLY:HA2	1.93	0.50
1:B:691:ALA:HA	1:B:694:ARG:HD2	1.93	0.50
1:C:62:LYS:HG3	1:C:237:SER:HB3	1.94	0.50
1:C:493:LYS:HG2	1:C:525:ARG:HH22	1.75	0.50
1:D:691:ALA:HA	1:D:694:ARG:HD2	1.94	0.50
1:A:368:ALA:HA	1:A:371:ALA:HB3	1.93	0.50
1:A:667:LEU:H	1:A:667:LEU:HD12	1.77	0.50
1:C:308:ARG:HD2	1:C:308:ARG:N	2.26	0.50
1:C:368:ALA:HA	1:C:371:ALA:HB3	1.93	0.50
1:C:480:ALA:HB2	1:C:487:LEU:HD22	1.94	0.50
1:C:667:LEU:HD12	1:C:667:LEU:H	1.77	0.50
1:A:308:ARG:HD2	1:A:308:ARG:N	2.26	0.50
1:B:308:ARG:N	1:B:308:ARG:HD2	2.26	0.50
1:C:392:ASN:ND2	1:C:414:LEU:HB3	2.22	0.50
1:D:480:ALA:HB2	1:D:487:LEU:HD22	1.94	0.50
1:B:478:ALA:HA	1:B:481:MET:HG2	1.93	0.50
1:B:480:ALA:HB2	1:B:487:LEU:HD22	1.94	0.50
1:B:601:MET:C	1:B:603:THR:N	2.70	0.50
1:C:346:VAL:HG11	1:C:351:MET:HB2	1.92	0.50
1:D:308:ARG:N	1:D:308:ARG:HD2	2.26	0.50
1:D:478:ALA:HA	1:D:481:MET:HG2	1.93	0.50
1:D:601:MET:C	1:D:603:THR:N	2.70	0.50
1:A:78:LEU:HB3	1:C:86:GLU:OE1	2.12	0.49
1:B:654:TYR:HB3	1:B:658:GLU:HB2	1.94	0.49
1:D:654:TYR:HB3	1:D:658:GLU:HB2	1.94	0.49
1:A:346:VAL:HG11	1:A:351:MET:HB2	1.92	0.49
1:A:601:MET:O	1:A:603:THR:N	2.44	0.49
1:B:459:ILE:O	1:D:731:ARG:NH2	2.45	0.49
1:C:601:MET:O	1:C:603:THR:N	2.44	0.49
1:A:206:ASN:O	1:A:207:ASP:C	2.55	0.49
1:A:757:ALA:HB2	1:C:710:SER:OG	2.13	0.49
1:B:297:SER:OG	1:B:298:LYS:N	2.44	0.49
1:B:522:VAL:HG23	1:B:522:VAL:O	2.13	0.49
1:C:206:ASN:O	1:C:207:ASP:C	2.55	0.49
1:D:206:ASN:O	1:D:207:ASP:C	2.55	0.49
1:D:601:MET:O	1:D:603:THR:N	2.43	0.49
1:A:297:SER:OG	1:A:298:LYS:N	2.44	0.49
1:B:206:ASN:O	1:B:207:ASP:C	2.55	0.49
1:D:70:ARG:NH1	1:D:75:GLY:HA3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:SER:OG	1:D:298:LYS:N	2.44	0.49
1:D:522:VAL:HG23	1:D:522:VAL:O	2.13	0.49
1:B:70:ARG:NH1	1:B:75:GLY:HA3	2.28	0.49
1:B:689:ASN:OD1	1:B:691:ALA:N	2.37	0.49
1:A:601:MET:C	1:A:603:THR:N	2.70	0.49
1:C:297:SER:OG	1:C:298:LYS:N	2.44	0.49
1:C:601:MET:C	1:C:603:THR:N	2.70	0.49
1:D:689:ASN:OD1	1:D:691:ALA:N	2.37	0.49
1:A:366:THR:HG22	1:A:370:ARG:HH22	1.78	0.49
1:B:440:VAL:HA	1:B:455:VAL:HA	1.95	0.49
1:D:530:ASP:O	1:D:533:SER:OG	2.22	0.49
1:A:70:ARG:NH1	1:A:75:GLY:HA3	2.28	0.49
1:A:440:VAL:HA	1:A:455:VAL:HA	1.95	0.49
1:B:712:ARG:HB3	1:D:757:ALA:HB2	1.95	0.49
1:C:70:ARG:NH1	1:C:75:GLY:HA3	2.28	0.49
1:C:440:VAL:HA	1:C:455:VAL:HA	1.95	0.49
1:B:696:PHE:O	1:B:697:LEU:C	2.55	0.48
1:C:366:THR:HG22	1:C:370:ARG:HH22	1.78	0.48
1:D:440:VAL:HA	1:D:455:VAL:HA	1.95	0.48
1:A:63:LEU:HD11	1:A:84:ILE:HG21	1.95	0.48
1:A:113:LEU:O	1:A:115:GLN:N	2.46	0.48
1:B:113:LEU:O	1:B:115:GLN:N	2.46	0.48
1:A:624:LYS:HZ2	1:A:625:ARG:HD2	1.78	0.48
1:B:399:ALA:O	1:B:402:SER:OG	2.20	0.48
1:C:63:LEU:HD11	1:C:84:ILE:HG21	1.95	0.48
1:C:113:LEU:O	1:C:115:GLN:N	2.46	0.48
1:D:113:LEU:O	1:D:115:GLN:N	2.46	0.48
1:D:696:PHE:O	1:D:697:LEU:C	2.55	0.48
1:A:654:TYR:HB3	1:A:658:GLU:HB2	1.94	0.48
1:A:696:PHE:O	1:A:697:LEU:C	2.55	0.48
1:C:356:ARG:NH1	1:C:537:HIS:HA	2.29	0.48
1:A:356:ARG:NH1	1:A:537:HIS:HA	2.29	0.48
1:A:577:ASP:OD1	1:A:577:ASP:N	2.45	0.48
1:B:356:ARG:NH1	1:B:537:HIS:HA	2.29	0.48
1:B:494:GLU:OE1	1:B:494:GLU:N	2.30	0.48
1:C:522:VAL:HG23	1:C:522:VAL:O	2.13	0.48
1:C:654:TYR:HB3	1:C:658:GLU:HB2	1.94	0.48
1:A:353:GLU:O	1:A:357:THR:HG23	2.14	0.48
1:A:358:GLY:O	1:A:362:MET:HG2	2.13	0.48
1:A:522:VAL:O	1:A:522:VAL:HG23	2.13	0.48
1:B:63:LEU:HD11	1:B:84:ILE:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:757:ALA:HB2	1:D:712:ARG:HB3	1.95	0.48
1:C:353:GLU:O	1:C:357:THR:HG23	2.14	0.48
1:C:358:GLY:O	1:C:362:MET:HG2	2.13	0.48
1:D:356:ARG:NH1	1:D:537:HIS:HA	2.29	0.48
1:D:399:ALA:O	1:D:402:SER:OG	2.20	0.48
1:A:113:LEU:C	1:A:115:GLN:H	2.22	0.48
1:A:358:GLY:HA2	1:A:516:GLU:OE1	2.14	0.48
1:A:691:ALA:HA	1:A:694:ARG:HD2	1.93	0.48
1:B:700:VAL:HG21	1:B:705:VAL:HG11	1.96	0.48
1:C:113:LEU:C	1:C:115:GLN:H	2.22	0.48
1:C:358:GLY:HA2	1:C:516:GLU:OE1	2.13	0.48
1:C:577:ASP:OD1	1:C:577:ASP:N	2.46	0.48
1:C:691:ALA:HA	1:C:694:ARG:HD2	1.94	0.48
1:C:696:PHE:O	1:C:697:LEU:C	2.55	0.48
1:D:63:LEU:HD11	1:D:84:ILE:HG21	1.95	0.48
1:D:494:GLU:OE1	1:D:494:GLU:N	2.30	0.48
1:A:170:GLN:HE22	1:A:172:LEU:HG	1.79	0.48
1:B:52:GLN:N	1:B:52:GLN:OE1	2.47	0.48
1:C:170:GLN:HE22	1:C:172:LEU:HG	1.79	0.48
1:D:52:GLN:N	1:D:52:GLN:OE1	2.47	0.48
1:D:700:VAL:HG21	1:D:705:VAL:HG11	1.96	0.48
1:B:113:LEU:C	1:B:115:GLN:H	2.22	0.48
1:B:446:LEU:O	1:B:769:LEU:N	2.45	0.48
1:A:667:LEU:O	1:A:671:ILE:HG12	2.14	0.48
1:B:170:GLN:HE22	1:B:172:LEU:HG	1.79	0.48
1:C:667:LEU:O	1:C:671:ILE:HG12	2.14	0.48
1:A:454:GLN:HB2	1:A:748:TRP:CZ3	2.49	0.47
1:B:353:GLU:O	1:B:357:THR:HG23	2.14	0.47
1:B:366:THR:HG22	1:B:370:ARG:HH22	1.78	0.47
1:D:170:GLN:HE22	1:D:172:LEU:HG	1.79	0.47
1:D:353:GLU:O	1:D:357:THR:HG23	2.14	0.47
1:D:446:LEU:O	1:D:769:LEU:N	2.45	0.47
1:D:633:GLY:O	1:D:637:ASN:N	2.35	0.47
1:A:86:GLU:OE1	1:C:78:LEU:HB3	2.14	0.47
1:B:358:GLY:HA2	1:B:516:GLU:OE1	2.14	0.47
1:B:633:GLY:O	1:B:637:ASN:N	2.35	0.47
1:C:450:LEU:HD13	1:C:755:HIS:CD2	2.49	0.47
1:D:113:LEU:C	1:D:115:GLN:H	2.22	0.47
1:D:358:GLY:HA2	1:D:516:GLU:OE1	2.14	0.47
1:D:366:THR:HG22	1:D:370:ARG:HH22	1.78	0.47
1:A:52:GLN:OE1	1:A:52:GLN:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:HD13	1:A:755:HIS:CD2	2.49	0.47
1:B:450:LEU:HD13	1:B:755:HIS:CD2	2.49	0.47
1:B:667:LEU:O	1:B:671:ILE:HG12	2.14	0.47
1:C:52:GLN:OE1	1:C:52:GLN:N	2.47	0.47
1:D:667:LEU:O	1:D:671:ILE:HG12	2.14	0.47
1:B:102:THR:O	1:B:204:ASN:ND2	2.47	0.47
1:B:454:GLN:HB2	1:B:748:TRP:CZ3	2.49	0.47
1:C:102:THR:O	1:C:204:ASN:ND2	2.48	0.47
1:C:454:GLN:HB2	1:C:748:TRP:CZ3	2.49	0.47
1:D:454:GLN:HB2	1:D:748:TRP:CZ3	2.49	0.47
1:A:102:THR:O	1:A:204:ASN:ND2	2.48	0.47
1:A:469:ARG:NH1	1:A:545:GLY:O	2.47	0.47
1:A:573:TYR:OH	1:A:575:ASP:OD1	2.31	0.47
1:B:354:ASN:O	1:B:357:THR:OG1	2.14	0.47
1:C:469:ARG:NH1	1:C:545:GLY:O	2.47	0.47
1:D:102:THR:O	1:D:204:ASN:ND2	2.48	0.47
1:D:354:ASN:O	1:D:357:THR:OG1	2.14	0.47
1:D:358:GLY:O	1:D:362:MET:HG2	2.13	0.47
1:D:450:LEU:HD13	1:D:755:HIS:CD2	2.49	0.47
1:B:358:GLY:O	1:B:362:MET:HG2	2.13	0.47
1:B:573:TYR:OH	1:B:575:ASP:OD1	2.31	0.47
1:A:494:GLU:OE1	1:A:494:GLU:N	2.30	0.47
1:B:548:ASP:O	1:B:549:LEU:C	2.57	0.47
1:B:615:ILE:O	1:B:619:VAL:HG13	2.15	0.47
1:C:573:TYR:OH	1:C:575:ASP:OD1	2.31	0.47
1:D:548:ASP:O	1:D:549:LEU:C	2.57	0.47
1:D:573:TYR:OH	1:D:575:ASP:OD1	2.31	0.47
1:D:615:ILE:O	1:D:619:VAL:HG13	2.15	0.47
1:B:206:ASN:OD1	1:B:208:ALA:HB3	2.14	0.47
1:D:476:VAL:HA	1:D:479:LEU:HD12	1.97	0.47
1:A:654:TYR:HE2	1:A:660:CYS:H	1.63	0.47
1:B:476:VAL:HA	1:B:479:LEU:HD12	1.97	0.47
1:D:543:PRO:HB2	1:D:549:LEU:HD23	1.97	0.47
1:A:349:GLU:OE1	1:A:349:GLU:N	2.48	0.47
1:A:570:CYS:O	1:A:571:HIS:ND1	2.48	0.47
1:B:543:PRO:HB2	1:B:549:LEU:HD23	1.97	0.47
1:B:570:CYS:O	1:B:571:HIS:ND1	2.48	0.47
1:C:74:HIS:HA	1:C:110:LYS:HD2	1.97	0.47
1:C:654:TYR:HE2	1:C:660:CYS:H	1.63	0.47
1:C:700:VAL:HG21	1:C:705:VAL:HG11	1.96	0.47
1:D:206:ASN:OD1	1:D:208:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:CYS:O	1:D:571:HIS:ND1	2.48	0.47
1:A:74:HIS:HA	1:A:110:LYS:HD2	1.97	0.46
1:A:346:VAL:CG1	1:A:351:MET:H	2.28	0.46
1:C:349:GLU:N	1:C:349:GLU:OE1	2.48	0.46
1:C:570:CYS:O	1:C:571:HIS:ND1	2.48	0.46
1:B:346:VAL:CG1	1:B:351:MET:H	2.28	0.46
1:B:458:PRO:HB3	1:B:485:ASN:HB3	1.98	0.46
1:C:206:ASN:OD1	1:C:208:ALA:HB3	2.15	0.46
1:C:346:VAL:CG1	1:C:351:MET:H	2.28	0.46
1:C:624:LYS:HZ2	1:C:625:ARG:HD2	1.80	0.46
1:D:652:HIS:HD2	1:D:654:TYR:CE1	2.33	0.46
1:A:700:VAL:HG21	1:A:705:VAL:HG11	1.96	0.46
1:B:652:HIS:HD2	1:B:654:TYR:CE1	2.33	0.46
1:C:241:ALA:O	1:C:245:GLN:N	2.48	0.46
1:C:385:GLU:HA	1:C:388:ILE:HG12	1.96	0.46
1:C:548:ASP:O	1:C:549:LEU:C	2.57	0.46
1:D:241:ALA:O	1:D:245:GLN:N	2.48	0.46
1:D:458:PRO:HB3	1:D:485:ASN:HB3	1.98	0.46
1:A:206:ASN:OD1	1:A:208:ALA:HB3	2.15	0.46
1:A:241:ALA:O	1:A:245:GLN:N	2.48	0.46
1:A:385:GLU:HA	1:A:388:ILE:HG12	1.96	0.46
1:B:193:GLU:O	1:B:197:LEU:HD23	2.15	0.46
1:B:241:ALA:O	1:B:245:GLN:N	2.48	0.46
1:B:349:GLU:N	1:B:349:GLU:OE1	2.48	0.46
1:D:193:GLU:O	1:D:197:LEU:HD23	2.15	0.46
1:D:346:VAL:CG1	1:D:351:MET:H	2.28	0.46
1:D:349:GLU:N	1:D:349:GLU:OE1	2.48	0.46
1:A:193:GLU:O	1:A:197:LEU:HD23	2.15	0.46
1:C:458:PRO:HB3	1:C:485:ASN:HB3	1.98	0.46
1:D:624:LYS:HZ2	1:D:625:ARG:HD2	1.80	0.46
1:A:543:PRO:HB2	1:A:549:LEU:HD23	1.97	0.46
1:A:548:ASP:O	1:A:549:LEU:C	2.57	0.46
1:A:652:HIS:HD2	1:A:654:TYR:CE1	2.33	0.46
1:B:100:MET:HE2	1:B:100:MET:HB3	1.78	0.46
1:B:385:GLU:HA	1:B:388:ILE:HG12	1.96	0.46
1:B:725:VAL:HG12	1:B:738:VAL:O	2.16	0.46
1:C:652:HIS:HD2	1:C:654:TYR:CE1	2.33	0.46
1:C:697:LEU:O	1:C:700:VAL:HG22	2.16	0.46
1:D:725:VAL:HG12	1:D:738:VAL:O	2.16	0.46
1:A:234:ASP:OD1	1:A:235:SER:N	2.45	0.46
1:A:458:PRO:HB3	1:A:485:ASN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:LEU:O	1:A:700:VAL:HG22	2.16	0.46
1:C:193:GLU:O	1:C:197:LEU:HD23	2.15	0.46
1:C:543:PRO:HB2	1:C:549:LEU:HD23	1.97	0.46
1:D:385:GLU:HA	1:D:388:ILE:HG12	1.96	0.46
1:D:532:LEU:HD11	1:D:556:GLN:HG3	1.98	0.46
1:D:652:HIS:CG	1:D:653:GLU:N	2.84	0.46
1:B:532:LEU:HD11	1:B:556:GLN:HG3	1.98	0.46
1:B:624:LYS:HZ2	1:B:625:ARG:HD2	1.81	0.46
1:B:652:HIS:CG	1:B:653:GLU:N	2.84	0.46
1:B:654:TYR:HE2	1:B:660:CYS:H	1.63	0.45
1:C:248:LEU:HD11	1:C:313:VAL:HG12	1.98	0.45
1:D:574:ILE:HA	1:D:686:VAL:HG23	1.98	0.45
1:A:161:PHE:HB3	1:A:166:VAL:HG13	1.98	0.45
1:B:74:HIS:HA	1:B:110:LYS:HD2	1.97	0.45
1:B:471:ASP:O	1:B:474:PRO:HD2	2.17	0.45
1:C:59:LEU:N	1:C:97:GLU:O	2.27	0.45
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.87	0.45
1:C:234:ASP:OD1	1:C:235:SER:N	2.46	0.45
1:D:74:HIS:HA	1:D:110:LYS:HD2	1.97	0.45
1:D:248:LEU:HD11	1:D:313:VAL:HG12	1.98	0.45
1:D:471:ASP:O	1:D:474:PRO:HD2	2.17	0.45
1:A:248:LEU:HD11	1:A:313:VAL:HG12	1.98	0.45
1:B:248:LEU:HD11	1:B:313:VAL:HG12	1.98	0.45
1:B:574:ILE:HA	1:B:686:VAL:HG23	1.98	0.45
1:D:654:TYR:HE2	1:D:660:CYS:H	1.63	0.45
1:B:697:LEU:O	1:B:700:VAL:HG22	2.16	0.45
1:C:161:PHE:HB3	1:C:166:VAL:HG13	1.98	0.45
1:C:180:ASN:OD1	1:C:181:GLU:N	2.50	0.45
1:C:532:LEU:HD11	1:C:556:GLN:HG3	1.98	0.45
1:D:445:ARG:NE	1:D:771:GLU:OE2	2.33	0.45
1:D:697:LEU:O	1:D:700:VAL:HG22	2.16	0.45
1:A:180:ASN:OD1	1:A:181:GLU:N	2.50	0.45
1:A:476:VAL:HA	1:A:479:LEU:HD12	1.97	0.45
1:A:532:LEU:HD11	1:A:556:GLN:HG3	1.98	0.45
1:A:652:HIS:CG	1:A:653:GLU:H	2.35	0.45
1:A:725:VAL:HG12	1:A:738:VAL:O	2.16	0.45
1:B:86:GLU:OE1	1:D:78:LEU:HB3	2.16	0.45
1:B:601:MET:HB2	1:B:601:MET:HE2	1.66	0.45
1:C:256:ASP:OD1	1:C:257:GLY:N	2.50	0.45
1:C:476:VAL:HA	1:C:479:LEU:HD12	1.97	0.45
1:C:652:HIS:CG	1:C:653:GLU:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:725:VAL:HG12	1:C:738:VAL:O	2.16	0.45
1:A:67:VAL:C	1:A:80:ARG:HH21	2.25	0.45
1:A:256:ASP:OD1	1:A:257:GLY:N	2.50	0.45
1:C:459:ILE:HG21	1:C:540:LEU:HD23	1.98	0.45
1:C:694:ARG:O	1:C:695:GLN:C	2.58	0.45
1:D:161:PHE:HB3	1:D:166:VAL:HG13	1.98	0.45
1:D:601:MET:HE2	1:D:601:MET:HB2	1.66	0.45
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.87	0.45
1:A:459:ILE:HG21	1:A:540:LEU:HD23	1.98	0.45
1:B:396:LEU:HD13	1:B:412:LEU:HD21	1.99	0.45
1:B:710:SER:H	1:B:713:PHE:HD2	1.64	0.45
1:C:471:ASP:O	1:C:474:PRO:HD2	2.17	0.45
1:C:652:HIS:CG	1:C:653:GLU:N	2.84	0.45
1:D:469:ARG:NH1	1:D:545:GLY:O	2.47	0.45
1:D:652:HIS:CG	1:D:653:GLU:H	2.35	0.45
1:D:710:SER:H	1:D:713:PHE:HD2	1.64	0.45
1:A:471:ASP:O	1:A:474:PRO:HD2	2.17	0.45
1:A:652:HIS:CG	1:A:653:GLU:N	2.84	0.45
1:B:652:HIS:CG	1:B:653:GLU:H	2.35	0.45
1:B:768:TRP:HB3	1:B:770:HIS:NE2	2.32	0.45
1:C:67:VAL:C	1:C:80:ARG:HH21	2.25	0.45
1:D:768:TRP:HB3	1:D:770:HIS:NE2	2.32	0.45
1:A:623:LEU:O	1:A:628:VAL:HG23	2.17	0.45
1:A:694:ARG:O	1:A:695:GLN:C	2.58	0.45
1:B:161:PHE:HB3	1:B:166:VAL:HG13	1.98	0.45
1:B:260:ASN:N	1:B:269:LYS:O	2.50	0.45
1:B:450:LEU:HD12	1:B:450:LEU:HA	1.74	0.45
1:D:396:LEU:HD13	1:D:412:LEU:HD21	1.99	0.45
1:B:469:ARG:NH1	1:B:545:GLY:O	2.47	0.45
1:B:684:VAL:HG23	1:B:706:PHE:HB2	1.99	0.45
1:D:684:VAL:HG23	1:D:706:PHE:HB2	1.99	0.45
1:A:59:LEU:N	1:A:97:GLU:O	2.27	0.44
1:A:446:LEU:O	1:A:769:LEU:N	2.45	0.44
1:A:574:ILE:HA	1:A:686:VAL:HG23	1.98	0.44
1:A:615:ILE:O	1:A:619:VAL:HG13	2.15	0.44
1:B:594:TYR:HD2	1:B:597:ALA:HB2	1.82	0.44
1:B:623:LEU:O	1:B:628:VAL:HG23	2.17	0.44
1:C:574:ILE:HA	1:C:686:VAL:HG23	1.98	0.44
1:C:615:ILE:O	1:C:619:VAL:HG13	2.15	0.44
1:C:623:LEU:O	1:C:628:VAL:HG23	2.17	0.44
1:D:67:VAL:C	1:D:80:ARG:HH21	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ASN:N	1:D:269:LYS:O	2.50	0.44
1:D:528:ILE:HG13	1:D:529:SER:N	2.32	0.44
1:A:85:VAL:HG23	1:A:161:PHE:CZ	2.52	0.44
1:A:399:ALA:O	1:A:402:SER:OG	2.20	0.44
1:A:684:VAL:HG23	1:A:706:PHE:HB2	1.99	0.44
1:A:768:TRP:HB3	1:A:770:HIS:NE2	2.32	0.44
1:B:78:LEU:HB3	1:D:86:GLU:OE1	2.17	0.44
1:B:180:ASN:OD1	1:B:181:GLU:N	2.50	0.44
1:B:445:ARG:NE	1:B:771:GLU:OE2	2.33	0.44
1:C:684:VAL:HG23	1:C:706:PHE:HB2	1.99	0.44
1:C:768:TRP:HB3	1:C:770:HIS:NE2	2.32	0.44
1:D:150:GLN:NE2	1:D:170:GLN:HG3	2.32	0.44
1:D:180:ASN:OD1	1:D:181:GLU:N	2.50	0.44
1:D:256:ASP:OD1	1:D:257:GLY:N	2.50	0.44
1:D:594:TYR:HD2	1:D:597:ALA:HB2	1.82	0.44
1:D:623:LEU:O	1:D:628:VAL:HG23	2.17	0.44
1:A:120:SER:O	1:A:124:ARG:N	2.48	0.44
1:A:594:TYR:HD2	1:A:597:ALA:HB2	1.82	0.44
1:B:67:VAL:C	1:B:80:ARG:HH21	2.25	0.44
1:B:150:GLN:NE2	1:B:170:GLN:HG3	2.32	0.44
1:B:172:LEU:HD22	1:B:205:THR:C	2.42	0.44
1:B:528:ILE:HG13	1:B:529:SER:N	2.32	0.44
1:B:623:LEU:O	1:B:627:GLY:N	2.51	0.44
1:C:85:VAL:HG23	1:C:161:PHE:CZ	2.52	0.44
1:C:260:ASN:N	1:C:269:LYS:O	2.50	0.44
1:D:59:LEU:N	1:D:97:GLU:O	2.27	0.44
1:D:450:LEU:HD12	1:D:450:LEU:HA	1.74	0.44
1:A:623:LEU:O	1:A:627:GLY:N	2.51	0.44
1:B:256:ASP:OD1	1:B:257:GLY:N	2.50	0.44
1:C:120:SER:O	1:C:124:ARG:N	2.48	0.44
1:C:594:TYR:HD2	1:C:597:ALA:HB2	1.82	0.44
1:C:623:LEU:O	1:C:627:GLY:N	2.51	0.44
1:D:172:LEU:HD22	1:D:205:THR:C	2.42	0.44
1:D:623:LEU:O	1:D:627:GLY:N	2.51	0.44
1:A:260:ASN:N	1:A:269:LYS:O	2.50	0.44
1:A:396:LEU:HD13	1:A:412:LEU:HD21	1.99	0.44
1:B:239:MET:HE3	1:B:239:MET:HB2	1.61	0.44
1:B:449:GLN:HB2	1:B:755:HIS:CE1	2.53	0.44
1:C:396:LEU:HD13	1:C:412:LEU:HD21	1.99	0.44
1:C:470:PRO:O	1:C:474:PRO:HD3	2.18	0.44
1:D:535:GLU:C	1:D:537:HIS:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:SER:O	1:D:548:ASP:C	2.60	0.44
1:A:470:PRO:O	1:A:474:PRO:HD3	2.18	0.44
1:B:535:GLU:C	1:B:537:HIS:H	2.25	0.44
1:B:547:SER:O	1:B:548:ASP:C	2.60	0.44
1:C:446:LEU:O	1:C:769:LEU:N	2.45	0.44
1:D:85:VAL:HG23	1:D:161:PHE:CZ	2.52	0.44
1:D:449:GLN:HB2	1:D:755:HIS:CE1	2.53	0.44
1:B:59:LEU:N	1:B:97:GLU:O	2.27	0.44
1:B:85:VAL:HG23	1:B:161:PHE:CZ	2.53	0.44
1:B:459:ILE:HG21	1:B:540:LEU:HD23	1.99	0.44
1:C:399:ALA:O	1:C:402:SER:OG	2.20	0.44
1:C:662:GLU:OE1	1:C:664:VAL:HG13	2.18	0.44
1:D:72:ASP:HB3	1:D:74:HIS:HB3	1.99	0.44
1:D:459:ILE:HG21	1:D:540:LEU:HD23	1.99	0.44
1:A:86:GLU:OE1	1:C:79:GLY:N	2.51	0.44
1:A:300:LYS:O	1:A:301:ALA:C	2.58	0.44
1:B:72:ASP:HB3	1:B:74:HIS:HB3	2.00	0.44
1:B:470:PRO:O	1:B:474:PRO:HD3	2.18	0.44
1:C:150:GLN:NE2	1:C:170:GLN:HG3	2.32	0.44
1:D:239:MET:HB2	1:D:239:MET:HE3	1.61	0.44
1:A:535:GLU:C	1:A:537:HIS:H	2.25	0.44
1:A:662:GLU:OE1	1:A:664:VAL:HG13	2.18	0.44
1:C:622:MET:O	1:C:625:ARG:HB2	2.18	0.44
1:C:710:SER:H	1:C:713:PHE:HD2	1.64	0.44
1:D:470:PRO:O	1:D:474:PRO:HD3	2.18	0.44
1:C:528:ILE:HG13	1:C:529:SER:N	2.32	0.43
1:C:535:GLU:C	1:C:537:HIS:H	2.26	0.43
1:A:150:GLN:NE2	1:A:170:GLN:HG3	2.32	0.43
1:A:172:LEU:HD22	1:A:205:THR:C	2.43	0.43
1:A:622:MET:O	1:A:625:ARG:HB2	2.18	0.43
1:C:300:LYS:O	1:C:301:ALA:C	2.58	0.43
1:C:602:GLU:H	1:C:602:GLU:HG2	1.51	0.43
1:A:72:ASP:HB3	1:A:74:HIS:HB3	1.99	0.43
1:A:394:LYS:O	1:A:398:GLU:HG3	2.18	0.43
1:A:528:ILE:HG13	1:A:529:SER:N	2.32	0.43
1:C:394:LYS:O	1:C:398:GLU:HG3	2.18	0.43
1:A:710:SER:H	1:A:713:PHE:HD2	1.64	0.43
1:C:72:ASP:HB3	1:C:74:HIS:HB3	2.00	0.43
1:C:172:LEU:HD22	1:C:205:THR:C	2.43	0.43
1:C:449:GLN:HB2	1:C:755:HIS:CE1	2.53	0.43
1:A:380:LEU:HB3	1:A:505:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:GLN:HB2	1:A:755:HIS:CE1	2.53	0.43
1:D:300:LYS:O	1:D:301:ALA:C	2.58	0.43
1:A:447:ALA:HB2	1:A:767:THR:O	2.18	0.43
1:B:300:LYS:O	1:B:301:ALA:C	2.58	0.43
1:C:380:LEU:HB3	1:C:505:LEU:HG	2.01	0.43
1:D:662:GLU:OE1	1:D:664:VAL:HG13	2.18	0.43
1:D:694:ARG:O	1:D:695:GLN:C	2.58	0.43
1:A:173:VAL:O	1:A:205:THR:HA	2.19	0.43
1:B:380:LEU:HB3	1:B:505:LEU:HG	2.00	0.43
1:B:653:GLU:N	1:B:653:GLU:OE1	2.52	0.43
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.80	0.43
1:C:447:ALA:HB2	1:C:767:THR:O	2.18	0.43
1:A:591:LYS:HD2	1:A:591:LYS:HA	1.79	0.43
1:B:318:MET:HE2	1:B:318:MET:H	1.84	0.43
1:B:662:GLU:OE1	1:B:664:VAL:HG13	2.18	0.43
1:B:698:GLY:O	1:B:699:SER:C	2.61	0.43
1:C:70:ARG:NH1	1:C:76:LEU:H	2.17	0.43
1:C:173:VAL:O	1:C:205:THR:HA	2.19	0.43
1:C:249:LEU:HD22	1:C:312:VAL:HG13	2.00	0.43
1:D:380:LEU:HB3	1:D:505:LEU:HG	2.01	0.43
1:D:653:GLU:N	1:D:653:GLU:OE1	2.52	0.43
1:D:698:GLY:O	1:D:699:SER:C	2.61	0.43
1:A:70:ARG:NH1	1:A:76:LEU:H	2.17	0.43
1:A:318:MET:HE2	1:A:318:MET:H	1.84	0.43
1:A:445:ARG:NE	1:A:771:GLU:OE2	2.33	0.43
1:A:625:ARG:HA	1:A:625:ARG:NH2	2.34	0.43
1:B:599:ASN:ND2	1:B:712:ARG:HD2	2.34	0.43
1:B:694:ARG:O	1:B:695:GLN:C	2.58	0.43
1:C:625:ARG:HA	1:C:625:ARG:NH2	2.34	0.43
1:D:318:MET:HE2	1:D:318:MET:H	1.84	0.43
1:D:599:ASN:ND2	1:D:712:ARG:HD2	2.34	0.43
1:A:170:GLN:NE2	1:A:172:LEU:HG	2.34	0.42
1:A:379:ASP:HA	1:A:382:VAL:HG12	2.01	0.42
1:A:599:ASN:ND2	1:A:712:ARG:HD2	2.34	0.42
1:A:633:GLY:O	1:A:637:ASN:N	2.35	0.42
1:B:258:ILE:O	1:B:271:MET:N	2.50	0.42
1:B:394:LYS:O	1:B:398:GLU:HG3	2.19	0.42
1:B:591:LYS:HD2	1:B:591:LYS:HA	1.79	0.42
1:C:170:GLN:NE2	1:C:172:LEU:HG	2.34	0.42
1:C:599:ASN:ND2	1:C:712:ARG:HD2	2.34	0.42
1:D:258:ILE:O	1:D:271:MET:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:LYS:O	1:D:398:GLU:HG3	2.19	0.42
1:A:249:LEU:HD22	1:A:312:VAL:HG13	2.00	0.42
1:A:602:GLU:H	1:A:602:GLU:HG2	1.50	0.42
1:B:625:ARG:HA	1:B:625:ARG:NH2	2.34	0.42
1:C:113:LEU:HD21	1:C:148:VAL:HG11	2.02	0.42
1:C:318:MET:HE2	1:C:318:MET:H	1.84	0.42
1:C:379:ASP:HA	1:C:382:VAL:HG12	2.01	0.42
1:D:447:ALA:HB2	1:D:767:THR:O	2.18	0.42
1:D:625:ARG:HA	1:D:625:ARG:NH2	2.34	0.42
1:A:113:LEU:HD21	1:A:148:VAL:HG11	2.02	0.42
1:A:547:SER:O	1:A:548:ASP:C	2.60	0.42
1:A:653:GLU:N	1:A:653:GLU:OE1	2.52	0.42
1:C:405:ALA:H	1:C:409:LEU:HG	1.84	0.42
1:C:547:SER:O	1:C:548:ASP:C	2.60	0.42
1:C:653:GLU:N	1:C:653:GLU:OE1	2.52	0.42
1:C:698:GLY:O	1:C:699:SER:C	2.61	0.42
1:D:150:GLN:HE22	1:D:154:MET:HG2	1.84	0.42
1:D:591:LYS:HA	1:D:591:LYS:HD2	1.79	0.42
1:A:405:ALA:H	1:A:409:LEU:HG	1.84	0.42
1:A:443:ARG:HG3	1:A:775:LEU:HA	2.02	0.42
1:B:443:ARG:HB3	1:B:773:LEU:HB2	2.01	0.42
1:B:447:ALA:HB2	1:B:767:THR:O	2.19	0.42
1:C:443:ARG:HG3	1:C:775:LEU:HA	2.02	0.42
1:D:70:ARG:NH1	1:D:76:LEU:H	2.17	0.42
1:D:622:MET:O	1:D:625:ARG:HB2	2.18	0.42
1:A:690:ASP:HA	1:A:693:ALA:HB2	2.02	0.42
1:B:70:ARG:NH1	1:B:76:LEU:H	2.17	0.42
1:B:150:GLN:HE22	1:B:154:MET:HG2	1.84	0.42
1:B:170:GLN:NE2	1:B:172:LEU:HG	2.34	0.42
1:B:173:VAL:O	1:B:205:THR:HA	2.19	0.42
1:B:389:LEU:HD11	1:B:416:PRO:HG3	2.01	0.42
1:B:622:MET:O	1:B:625:ARG:HB2	2.18	0.42
1:C:591:LYS:HD2	1:C:591:LYS:HA	1.79	0.42
1:C:633:GLY:O	1:C:637:ASN:N	2.35	0.42
1:C:690:ASP:HA	1:C:693:ALA:HB2	2.02	0.42
1:D:173:VAL:O	1:D:205:THR:HA	2.19	0.42
1:A:538:ILE:H	1:A:538:ILE:HG12	1.60	0.42
1:A:698:GLY:O	1:A:699:SER:C	2.61	0.42
1:B:629:LYS:HD2	1:B:631:TYR:HE1	1.84	0.42
1:B:690:ASP:HA	1:B:693:ALA:HB2	2.02	0.42
1:D:170:GLN:NE2	1:D:172:LEU:HG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:LEU:HD11	1:D:416:PRO:HG3	2.01	0.42
1:D:443:ARG:HB3	1:D:773:LEU:HB2	2.01	0.42
1:D:602:GLU:H	1:D:602:GLU:HG2	1.51	0.42
1:D:629:LYS:HD2	1:D:631:TYR:HE1	1.84	0.42
1:A:368:ALA:O	1:A:372:SER:OG	2.32	0.42
1:B:249:LEU:HD22	1:B:312:VAL:HG13	2.00	0.42
1:C:150:GLN:HE22	1:C:154:MET:HG2	1.84	0.42
1:D:271:MET:O	1:D:334:THR:HG23	2.20	0.42
1:D:462:LEU:HD22	1:D:485:ASN:HD21	1.85	0.42
1:D:690:ASP:HA	1:D:693:ALA:HB2	2.02	0.42
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.85	0.42
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.80	0.42
1:A:271:MET:O	1:A:334:THR:HG23	2.20	0.42
1:B:269:LYS:NZ	1:B:271:MET:HA	2.35	0.42
1:B:271:MET:O	1:B:334:THR:HG23	2.20	0.42
1:B:449:GLN:HB2	1:B:755:HIS:HE1	1.84	0.42
1:B:462:LEU:HD22	1:B:485:ASN:HD21	1.85	0.42
1:C:258:ILE:O	1:C:271:MET:N	2.50	0.42
1:C:271:MET:O	1:C:334:THR:HG23	2.20	0.42
1:D:120:SER:O	1:D:124:ARG:N	2.48	0.42
1:D:249:LEU:HD22	1:D:312:VAL:HG13	2.00	0.42
1:D:449:GLN:HB2	1:D:755:HIS:HE1	1.84	0.42
1:A:150:GLN:HE22	1:A:154:MET:HG2	1.84	0.42
1:A:629:LYS:HD2	1:A:631:TYR:HE1	1.84	0.42
1:B:120:SER:O	1:B:124:ARG:N	2.48	0.42
1:B:175:LYS:HB2	1:B:236:LEU:HD21	2.02	0.42
1:C:448:ASP:O	1:C:755:HIS:NE2	2.34	0.42
1:D:269:LYS:NZ	1:D:271:MET:HA	2.35	0.42
1:D:712:ARG:HD2	1:D:712:ARG:HA	1.95	0.42
1:A:56:ALA:O	1:A:96:ARG:HD3	2.20	0.42
1:A:258:ILE:O	1:A:271:MET:N	2.50	0.42
1:A:449:GLN:HB2	1:A:755:HIS:HE1	1.84	0.42
1:B:161:PHE:CD2	1:B:168:ILE:HD13	2.55	0.42
1:C:56:ALA:O	1:C:96:ARG:HD3	2.20	0.42
1:D:161:PHE:CD2	1:D:168:ILE:HD13	2.55	0.42
1:D:463:LEU:HD11	1:D:531:LEU:HD21	2.01	0.42
1:B:602:GLU:H	1:B:602:GLU:HG2	1.50	0.41
1:B:712:ARG:HD2	1:B:712:ARG:HA	1.95	0.41
1:C:445:ARG:NE	1:C:771:GLU:OE2	2.33	0.41
1:C:629:LYS:HD2	1:C:631:TYR:HE1	1.84	0.41
1:D:175:LYS:HB2	1:D:236:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:HA	1:A:158:ASP:OD2	2.21	0.41
1:A:416:PRO:HA	1:A:419:LEU:HD13	2.03	0.41
1:A:759:ASP:CG	1:A:766:ARG:HE	2.29	0.41
1:C:161:PHE:CD2	1:C:168:ILE:HD13	2.55	0.41
1:C:416:PRO:HA	1:C:419:LEU:HD13	2.02	0.41
1:C:443:ARG:HB3	1:C:773:LEU:HB2	2.01	0.41
1:C:574:ILE:HD11	1:C:604:LEU:HD11	2.02	0.41
1:C:759:ASP:CG	1:C:766:ARG:HE	2.29	0.41
1:D:538:ILE:H	1:D:538:ILE:HG12	1.60	0.41
1:A:161:PHE:CD2	1:A:168:ILE:HD13	2.55	0.41
1:A:269:LYS:NZ	1:A:271:MET:HA	2.35	0.41
1:A:443:ARG:HB3	1:A:773:LEU:HB2	2.01	0.41
1:A:574:ILE:HD11	1:A:604:LEU:HD11	2.02	0.41
1:B:463:LEU:HD11	1:B:531:LEU:HD21	2.01	0.41
1:C:115:GLN:O	1:C:118:LEU:HB3	2.21	0.41
1:C:150:GLN:HE22	1:C:170:GLN:HG3	1.85	0.41
1:C:449:GLN:HB2	1:C:755:HIS:HE1	1.84	0.41
1:C:512:THR:OG1	1:C:513:VAL:N	2.53	0.41
1:D:379:ASP:HA	1:D:382:VAL:HG12	2.01	0.41
1:D:405:ALA:H	1:D:409:LEU:HG	1.84	0.41
1:D:416:PRO:HA	1:D:419:LEU:HD13	2.03	0.41
1:A:115:GLN:O	1:A:118:LEU:HB3	2.21	0.41
1:A:150:GLN:HE22	1:A:170:GLN:HG3	1.85	0.41
1:A:448:ASP:O	1:A:755:HIS:NE2	2.34	0.41
1:A:512:THR:OG1	1:A:513:VAL:N	2.53	0.41
1:A:590:ALA:HB1	1:A:601:MET:HG2	2.02	0.41
1:B:379:ASP:HA	1:B:382:VAL:HG12	2.01	0.41
1:B:416:PRO:HA	1:B:419:LEU:HD13	2.03	0.41
1:B:538:ILE:H	1:B:538:ILE:HG12	1.60	0.41
1:B:718:ARG:O	1:D:446:LEU:HD13	2.21	0.41
1:C:155:SER:HA	1:C:158:ASP:OD2	2.21	0.41
1:C:463:LEU:HD11	1:C:531:LEU:HD21	2.01	0.41
1:A:462:LEU:HD22	1:A:485:ASN:HD21	1.85	0.41
1:A:463:LEU:HD11	1:A:531:LEU:HD21	2.01	0.41
1:B:512:THR:OG1	1:B:513:VAL:N	2.53	0.41
1:B:759:ASP:CG	1:B:766:ARG:HE	2.28	0.41
1:C:93:LEU:HD23	1:C:93:LEU:HA	1.85	0.41
1:C:269:LYS:NZ	1:C:271:MET:HA	2.35	0.41
1:C:346:VAL:HG11	1:C:351:MET:CB	2.50	0.41
1:C:462:LEU:HD22	1:C:485:ASN:HD21	1.85	0.41
1:C:590:ALA:HB1	1:C:601:MET:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:HA	1:A:86:GLU:OE2	2.21	0.41
1:A:346:VAL:HG11	1:A:351:MET:CB	2.50	0.41
1:B:405:ALA:H	1:B:409:LEU:HG	1.84	0.41
1:C:581:GLU:O	1:C:585:ARG:HG2	2.20	0.41
1:D:150:GLN:HE22	1:D:170:GLN:HG3	1.85	0.41
1:D:512:THR:OG1	1:D:513:VAL:N	2.53	0.41
1:D:590:ALA:HB1	1:D:601:MET:HG2	2.02	0.41
1:D:759:ASP:CG	1:D:766:ARG:HE	2.28	0.41
1:A:103:SER:HB3	1:A:233:ASN:HD21	1.85	0.41
1:B:113:LEU:HD21	1:B:148:VAL:HG11	2.02	0.41
1:B:443:ARG:HG3	1:B:775:LEU:HA	2.02	0.41
1:B:590:ALA:HB1	1:B:601:MET:HG2	2.02	0.41
1:C:83:SER:HA	1:C:86:GLU:OE2	2.21	0.41
1:D:473:LEU:HB3	1:D:474:PRO:HD3	2.02	0.41
1:A:197:LEU:HD12	1:D:116:GLU:HB3	2.02	0.41
1:B:150:GLN:HE22	1:B:170:GLN:HG3	1.85	0.41
1:B:473:LEU:HB3	1:B:474:PRO:HD3	2.02	0.41
1:B:510:LEU:HD13	1:B:516:GLU:O	2.21	0.41
1:B:584:LEU:HD23	1:B:619:VAL:HG12	2.03	0.41
1:B:719:PHE:N	1:B:719:PHE:CD1	2.89	0.41
1:C:103:SER:HB3	1:C:233:ASN:HD21	1.85	0.41
1:D:443:ARG:HG3	1:D:775:LEU:HA	2.02	0.41
1:D:719:PHE:N	1:D:719:PHE:CD1	2.89	0.41
1:A:354:ASN:O	1:A:355:ALA:C	2.63	0.41
1:A:471:ASP:OD1	1:A:471:ASP:N	2.53	0.41
1:A:581:GLU:O	1:A:585:ARG:HG2	2.20	0.41
1:B:83:SER:HA	1:B:86:GLU:OE2	2.21	0.41
1:B:344:ASN:O	1:B:346:VAL:N	2.54	0.41
1:B:581:GLU:O	1:B:585:ARG:HG2	2.20	0.41
1:C:184:ARG:HG3	1:C:243:GLU:CD	2.46	0.41
1:C:473:LEU:HB3	1:C:474:PRO:HD3	2.02	0.41
1:D:83:SER:HA	1:D:86:GLU:OE2	2.21	0.41
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.85	0.41
1:D:113:LEU:HD21	1:D:148:VAL:HG11	2.02	0.41
1:D:115:GLN:O	1:D:118:LEU:HB3	2.20	0.41
1:D:155:SER:HA	1:D:158:ASP:OD2	2.21	0.41
1:D:510:LEU:HD13	1:D:516:GLU:O	2.21	0.41
1:D:581:GLU:O	1:D:585:ARG:HG2	2.20	0.41
1:D:584:LEU:HD23	1:D:619:VAL:HG12	2.03	0.41
1:A:184:ARG:HG3	1:A:243:GLU:CD	2.46	0.41
1:A:197:LEU:HD13	1:A:197:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LEU:HD11	1:A:416:PRO:HG3	2.01	0.41
1:A:473:LEU:HB3	1:A:474:PRO:HD3	2.02	0.41
1:B:115:GLN:O	1:B:118:LEU:HB3	2.21	0.41
1:B:234:ASP:OD1	1:B:235:SER:N	2.45	0.41
1:D:344:ASN:O	1:D:346:VAL:N	2.54	0.41
1:D:576:ARG:HA	1:D:610:LEU:HD11	2.03	0.41
1:A:510:LEU:HD13	1:A:516:GLU:O	2.21	0.40
1:B:58:ARG:C	1:B:59:LEU:HD22	2.46	0.40
1:C:70:ARG:C	1:C:72:ASP:H	2.29	0.40
1:C:389:LEU:HD11	1:C:416:PRO:HG3	2.01	0.40
1:C:510:LEU:HD13	1:C:516:GLU:O	2.21	0.40
1:C:715:ASP:O	1:C:717:PHE:N	2.54	0.40
1:D:58:ARG:C	1:D:59:LEU:HD22	2.46	0.40
1:A:45:PRO:HB2	1:A:46:THR:H	1.75	0.40
1:A:70:ARG:C	1:A:72:ASP:H	2.29	0.40
1:A:344:ASN:O	1:A:346:VAL:N	2.54	0.40
1:B:155:SER:HA	1:B:158:ASP:OD2	2.21	0.40
1:B:574:ILE:HD11	1:B:604:LEU:HD11	2.01	0.40
1:B:576:ARG:HA	1:B:610:LEU:HD11	2.04	0.40
1:C:344:ASN:O	1:C:346:VAL:N	2.54	0.40
1:C:354:ASN:O	1:C:355:ALA:C	2.63	0.40
1:C:471:ASP:OD1	1:C:471:ASP:N	2.53	0.40
1:D:346:VAL:HG11	1:D:351:MET:CB	2.50	0.40
1:D:392:ASN:HD22	1:D:414:LEU:CB	2.29	0.40
1:D:574:ILE:HD11	1:D:604:LEU:HD11	2.02	0.40
1:D:715:ASP:O	1:D:717:PHE:N	2.54	0.40
1:A:79:GLY:N	1:C:86:GLU:OE1	2.55	0.40
1:A:324:LYS:HB2	1:A:324:LYS:HE3	1.88	0.40
1:A:584:LEU:HD23	1:A:619:VAL:HG12	2.03	0.40
1:A:715:ASP:O	1:A:717:PHE:N	2.54	0.40
1:B:93:LEU:HA	1:B:93:LEU:HD23	1.85	0.40
1:B:184:ARG:HG3	1:B:243:GLU:CD	2.46	0.40
1:B:338:GLU:O	1:B:339:ALA:C	2.64	0.40
1:B:346:VAL:HG11	1:B:351:MET:CB	2.50	0.40
1:B:443:ARG:O	1:B:773:LEU:N	2.55	0.40
1:B:715:ASP:O	1:B:717:PHE:N	2.54	0.40
1:C:197:LEU:HD13	1:C:197:LEU:HA	1.91	0.40
1:C:615:ILE:HA	1:C:618:ASP:OD2	2.21	0.40
1:D:338:GLU:O	1:D:339:ALA:C	2.64	0.40
1:D:443:ARG:O	1:D:773:LEU:N	2.55	0.40
1:A:615:ILE:HA	1:A:618:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:SER:HB3	1:B:233:ASN:HD21	1.85	0.40
1:B:175:LYS:HE2	1:B:179:TYR:OH	2.22	0.40
1:B:193:GLU:O	1:B:196:SER:OG	2.39	0.40
1:B:445:ARG:HA	1:B:450:LEU:O	2.21	0.40
1:C:45:PRO:HB2	1:C:46:THR:H	1.76	0.40
1:C:175:LYS:HB2	1:C:236:LEU:HD21	2.02	0.40
1:C:324:LYS:HB2	1:C:324:LYS:HE3	1.88	0.40
1:C:584:LEU:HD23	1:C:619:VAL:HG12	2.03	0.40
1:C:671:ILE:HA	1:C:674:ILE:HD12	2.04	0.40
1:D:175:LYS:HE2	1:D:179:TYR:OH	2.22	0.40
1:D:184:ARG:HG3	1:D:243:GLU:CD	2.46	0.40
1:D:445:ARG:HA	1:D:450:LEU:O	2.21	0.40
1:D:736:GLY:HA3	1:D:737:PRO:HD3	1.95	0.40
1:A:175:LYS:HB2	1:A:236:LEU:HD21	2.02	0.40
1:A:262:PRO:HA	1:A:263:PRO:HD3	1.91	0.40
1:A:671:ILE:HA	1:A:674:ILE:HD12	2.04	0.40
1:B:56:ALA:O	1:B:96:ARG:HD3	2.20	0.40
1:B:151:SER:OG	1:B:152:GLY:N	2.55	0.40
1:B:392:ASN:HD22	1:B:414:LEU:CB	2.29	0.40
1:B:615:ILE:HA	1:B:618:ASP:OD2	2.21	0.40
1:B:635:ARG:CZ	1:B:665:PRO:HD3	2.51	0.40
1:B:736:GLY:HA3	1:B:737:PRO:HD3	1.95	0.40
1:D:56:ALA:O	1:D:96:ARG:HD3	2.20	0.40
1:D:151:SER:OG	1:D:152:GLY:N	2.55	0.40
1:D:193:GLU:O	1:D:196:SER:OG	2.39	0.40
1:D:234:ASP:OD1	1:D:235:SER:N	2.46	0.40
1:D:485:ASN:OD1	1:D:485:ASN:N	2.50	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	666/776 (86%)	574 (86%)	89 (13%)	3 (0%)	24	61
1	B	666/776 (86%)	575 (86%)	88 (13%)	3 (0%)	24	61
1	C	666/776 (86%)	575 (86%)	88 (13%)	3 (0%)	24	61
1	D	666/776 (86%)	575 (86%)	88 (13%)	3 (0%)	24	61
All	All	2664/3104 (86%)	2299 (86%)	353 (13%)	12 (0%)	26	61

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	602	GLU
1	B	602	GLU
1	C	602	GLU
1	D	602	GLU
1	A	114	ALA
1	B	114	ALA
1	C	114	ALA
1	D	114	ALA
1	A	347	PRO
1	B	347	PRO
1	C	347	PRO
1	D	347	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	545/630 (86%)	526 (96%)	19 (4%)	32	54
1	B	545/630 (86%)	526 (96%)	19 (4%)	32	54
1	C	545/630 (86%)	526 (96%)	19 (4%)	32	54
1	D	545/630 (86%)	526 (96%)	19 (4%)	32	54
All	All	2180/2520 (86%)	2104 (96%)	76 (4%)	32	54

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	91	CYS
1	A	155	SER
1	A	190	THR
1	A	207	ASP
1	A	209	VAL
1	A	338	GLU
1	A	404	LEU
1	A	464	VAL
1	A	548	ASP
1	A	601	MET
1	A	602	GLU
1	A	641	THR
1	A	657	LEU
1	A	663	VAL
1	A	694	ARG
1	A	711	SER
1	A	740	VAL
1	A	772	THR
1	B	90	GLU
1	B	91	CYS
1	B	155	SER
1	B	190	THR
1	B	207	ASP
1	B	209	VAL
1	B	338	GLU
1	B	404	LEU
1	B	464	VAL
1	B	548	ASP
1	B	601	MET
1	B	602	GLU
1	B	641	THR
1	B	657	LEU
1	B	663	VAL
1	B	694	ARG
1	B	711	SER
1	B	740	VAL
1	B	772	THR
1	C	90	GLU
1	C	91	CYS
1	C	155	SER
1	C	190	THR
1	C	207	ASP

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Mol	Chain	Res	Type
1	C	209	VAL
1	C	338	GLU
1	C	404	LEU
1	C	464	VAL
1	C	548	ASP
1	C	601	MET
1	C	602	GLU
1	C	641	THR
1	C	657	LEU
1	C	663	VAL
1	C	694	ARG
1	C	711	SER
1	C	740	VAL
1	C	772	THR
1	D	90	GLU
1	D	91	CYS
1	D	155	SER
1	D	190	THR
1	D	207	ASP
1	D	209	VAL
1	D	338	GLU
1	D	404	LEU
1	D	464	VAL
1	D	548	ASP
1	D	601	MET
1	D	602	GLU
1	D	641	THR
1	D	657	LEU
1	D	663	VAL
1	D	694	ARG
1	D	711	SER
1	D	740	VAL
1	D	772	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	170	GLN
1	A	204	ASN
1	A	363	GLN
1	A	369	GLN

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Mol	Chain	Res	Type
1	A	392	ASN
1	A	607	HIS
1	A	637	ASN
1	A	652	HIS
1	A	673	HIS
1	A	695	GLN
1	A	707	HIS
1	B	150	GLN
1	B	170	GLN
1	B	204	ASN
1	B	363	GLN
1	B	369	GLN
1	B	392	ASN
1	B	607	HIS
1	B	652	HIS
1	B	695	GLN
1	B	707	HIS
1	C	150	GLN
1	C	170	GLN
1	C	204	ASN
1	C	363	GLN
1	C	369	GLN
1	C	392	ASN
1	C	607	HIS
1	C	637	ASN
1	C	652	HIS
1	C	695	GLN
1	C	707	HIS
1	D	150	GLN
1	D	170	GLN
1	D	204	ASN
1	D	363	GLN
1	D	369	GLN
1	D	392	ASN
1	D	607	HIS
1	D	652	HIS
1	D	695	GLN
1	D	707	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	GLU	D	801	-	8,9,9	1.08	1 (12%)	8,11,11	1.18	1 (12%)
2	GLU	B	801	-	8,9,9	1.10	1 (12%)	8,11,11	1.18	1 (12%)
2	GLU	C	801	-	8,9,9	1.08	1 (12%)	8,11,11	1.18	1 (12%)
2	GLU	A	801	-	8,9,9	1.08	1 (12%)	8,11,11	1.18	1 (12%)

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
2	GLU	D	801	-	-	3/9/9/9	-
2	GLU	B	801	-	-	3/9/9/9	-
2	GLU	C	801	-	-	3/9/9/9	-
2	GLU	A	801	-	-	3/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	GLU	OXT-C	-2.26	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	GLU	OXT-C	-2.17	1.23	1.30
2	A	801	GLU	OXT-C	-2.17	1.23	1.30
2	C	801	GLU	OXT-C	-2.17	1.23	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	GLU	OXT-C-O	-2.62	118.13	124.08
2	A	801	GLU	OXT-C-O	-2.62	118.13	124.08
2	C	801	GLU	OXT-C-O	-2.62	118.13	124.08
2	B	801	GLU	OXT-C-O	-2.62	118.14	124.08

There are no chirality outliers.

All (12) torsion outliers are listed below:

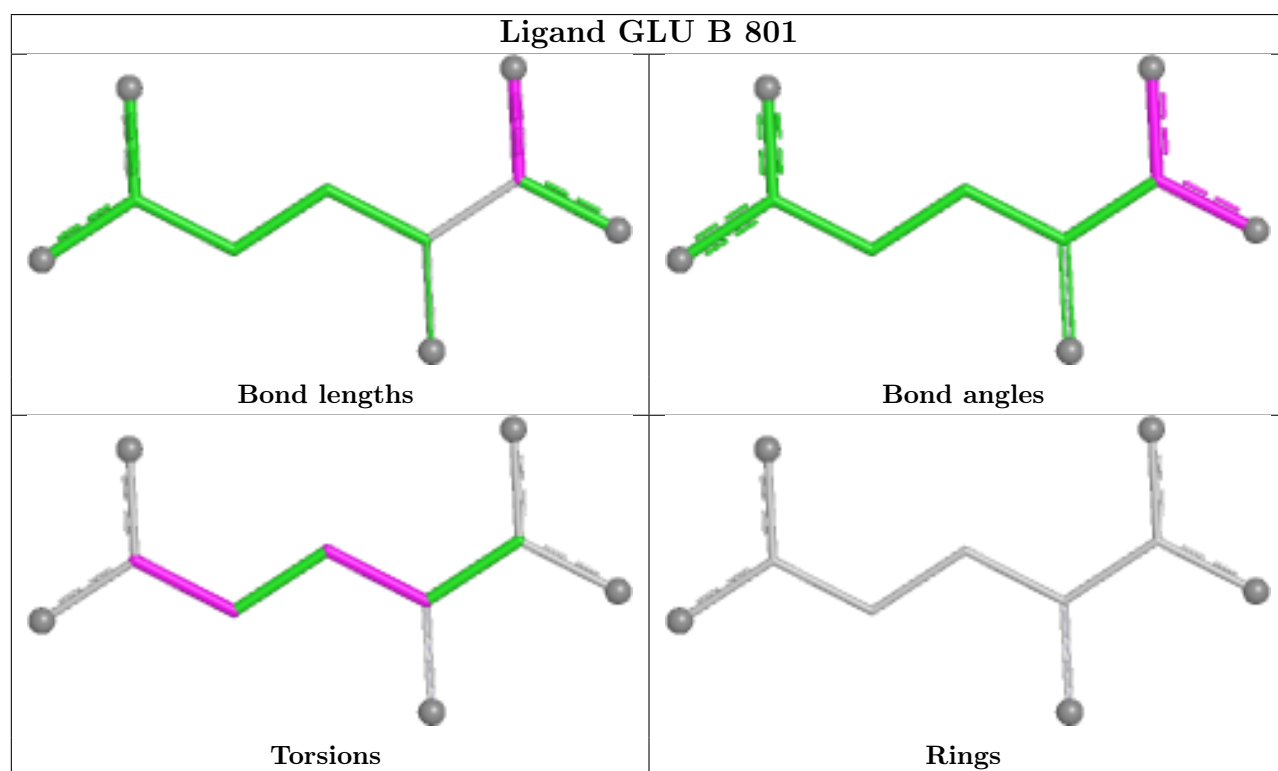
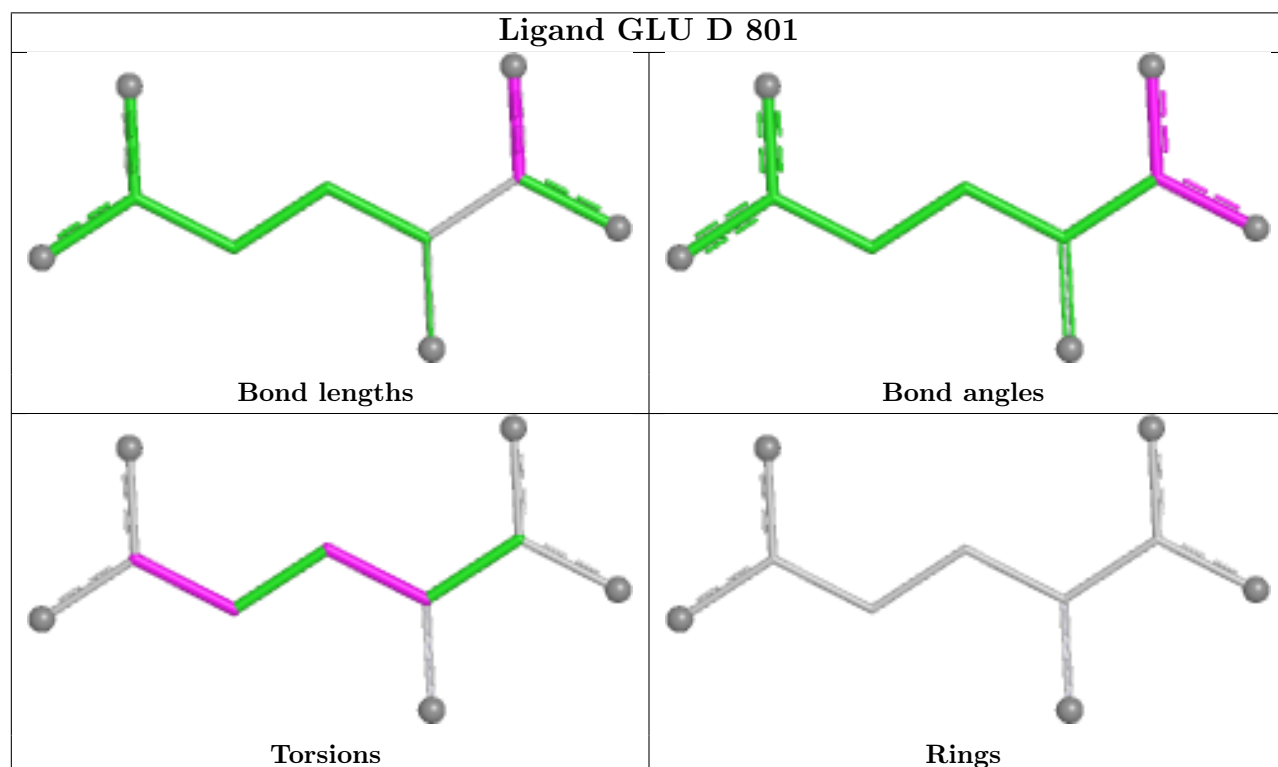
Mol	Chain	Res	Type	Atoms
2	A	801	GLU	OE2-CD-CG-CB
2	C	801	GLU	OE2-CD-CG-CB
2	D	801	GLU	OE2-CD-CG-CB
2	A	801	GLU	OE1-CD-CG-CB
2	C	801	GLU	OE1-CD-CG-CB
2	D	801	GLU	OE1-CD-CG-CB
2	B	801	GLU	OE1-CD-CG-CB
2	B	801	GLU	OE2-CD-CG-CB
2	A	801	GLU	N-CA-CB-CG
2	B	801	GLU	N-CA-CB-CG
2	C	801	GLU	N-CA-CB-CG
2	D	801	GLU	N-CA-CB-CG

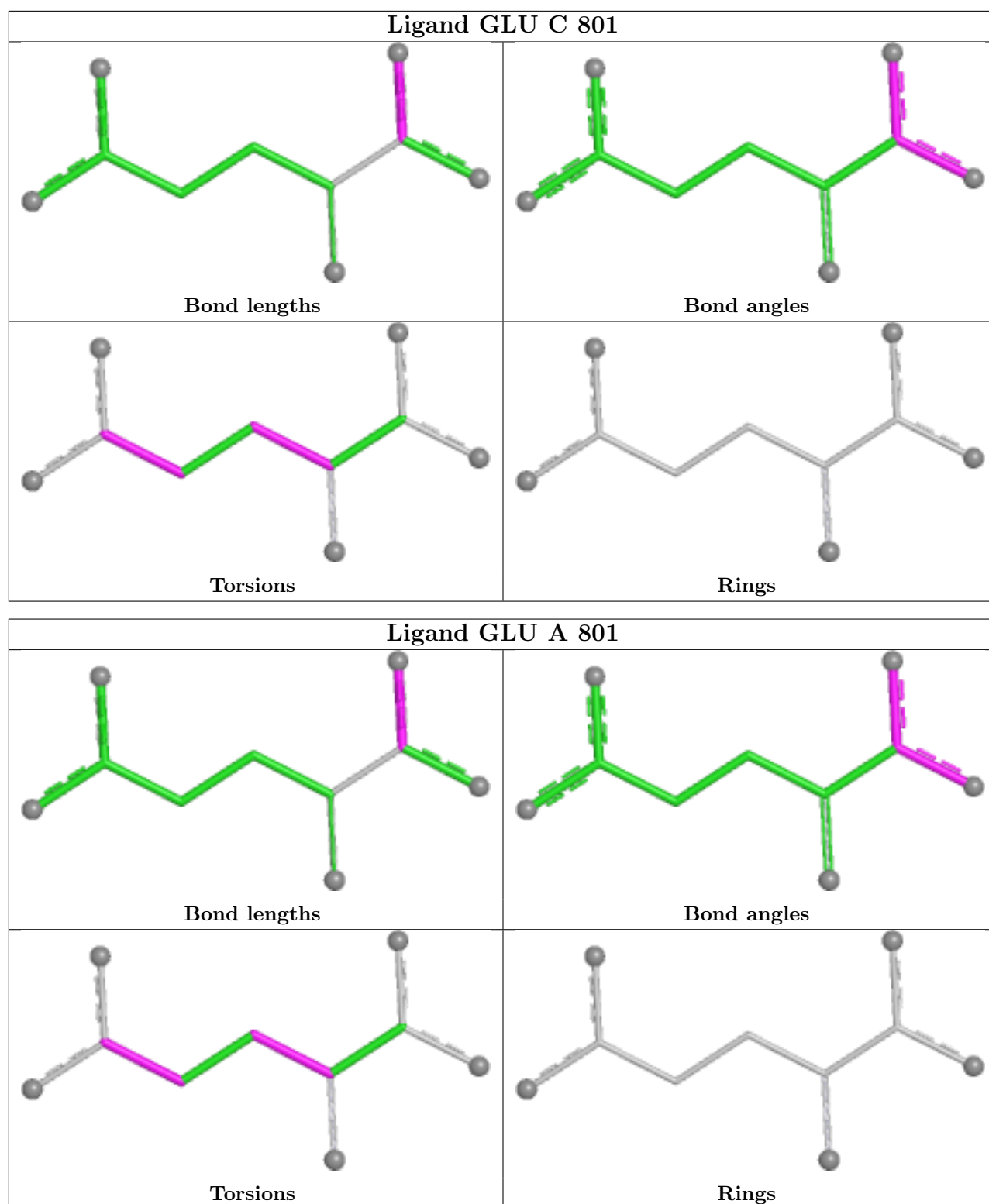
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no chain breaks in this entry.

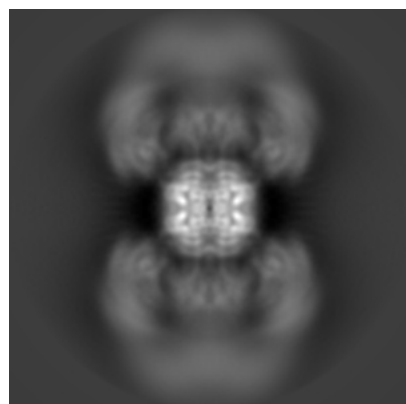
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31466. These allow visual inspection of the internal detail of the map and identification of artifacts.

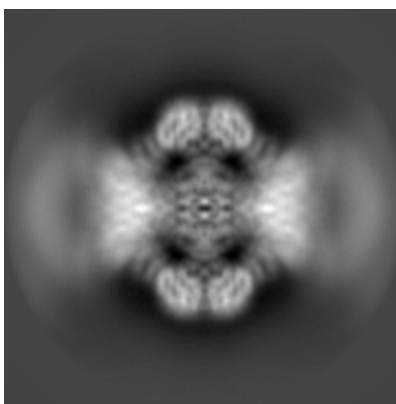
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

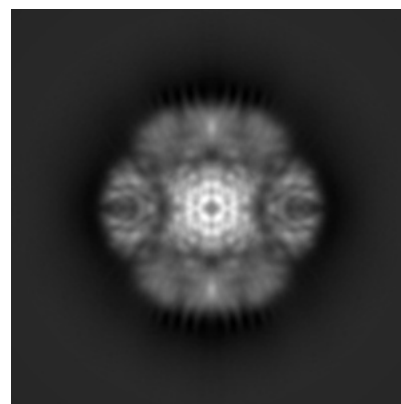
6.1.1 Primary map



X

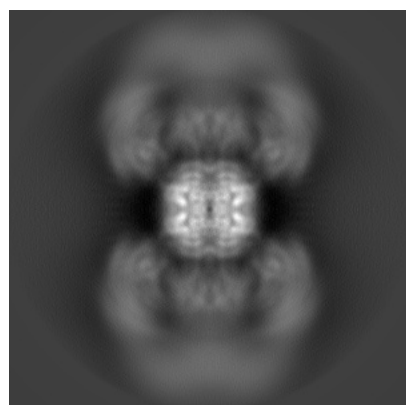


Y

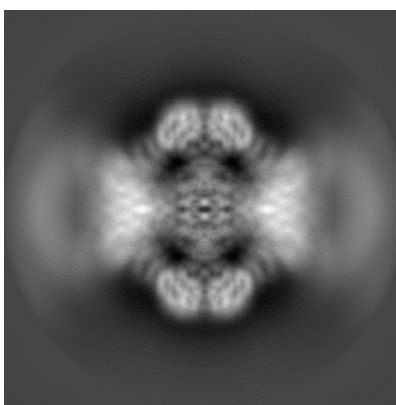


Z

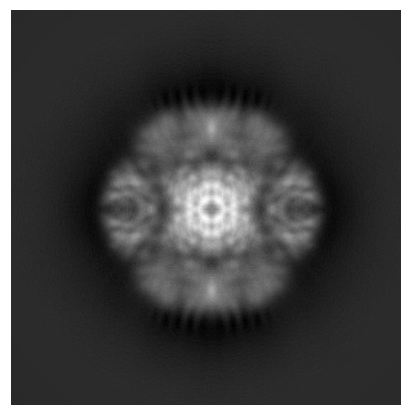
6.1.2 Raw map



X



Y

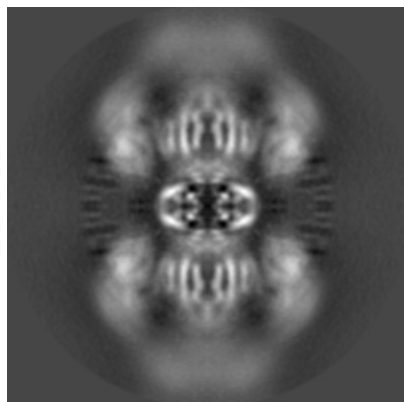


Z

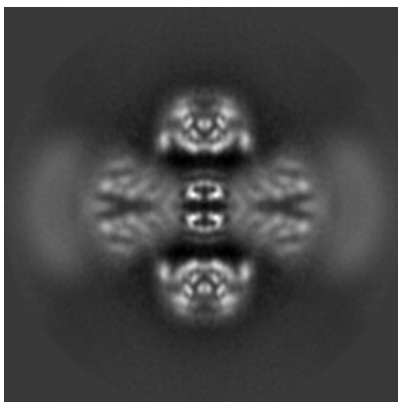
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

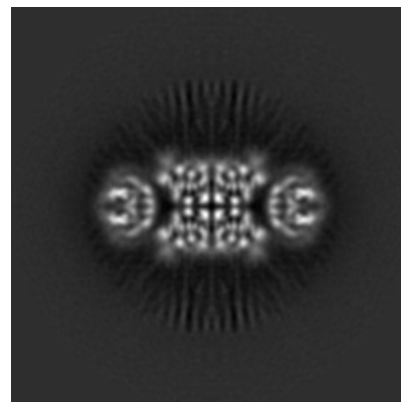
6.2.1 Primary map



X Index: 150

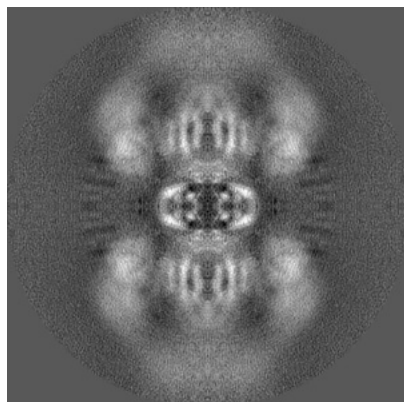


Y Index: 150

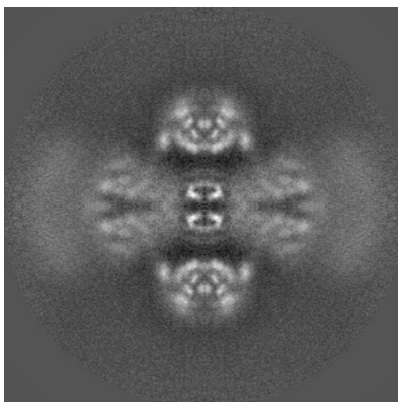


Z Index: 150

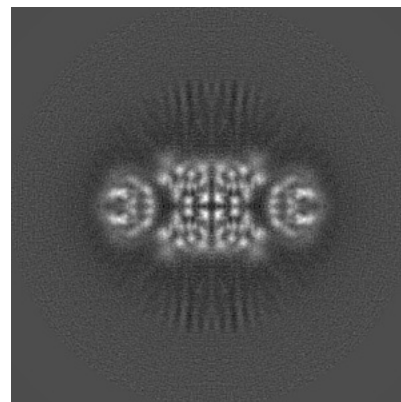
6.2.2 Raw map



X Index: 150



Y Index: 150

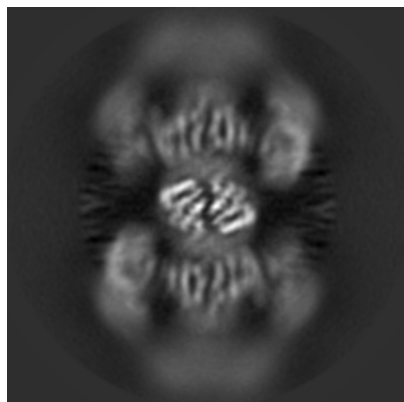


Z Index: 150

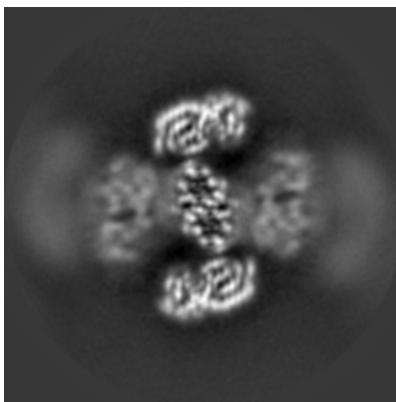
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

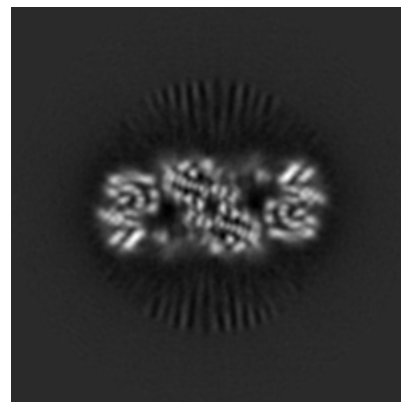
6.3.1 Primary map



X Index: 146

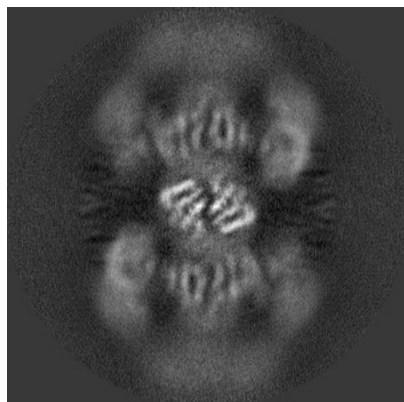


Y Index: 140

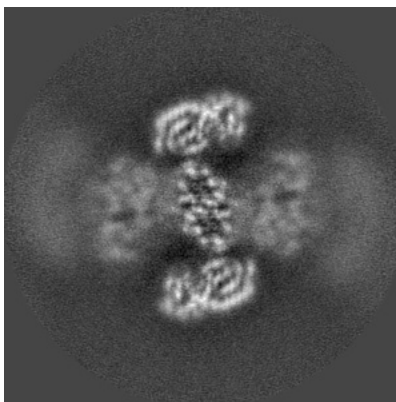


Z Index: 142

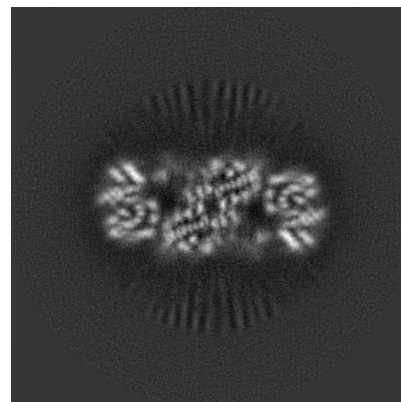
6.3.2 Raw map



X Index: 146



Y Index: 140

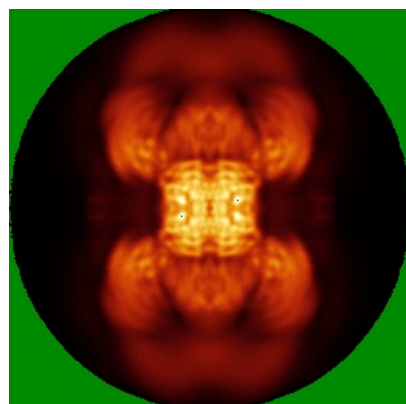


Z Index: 158

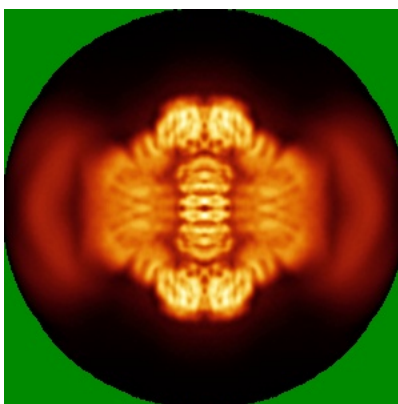
The images above show the largest variance slices of the map in three orthogonal directions.

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

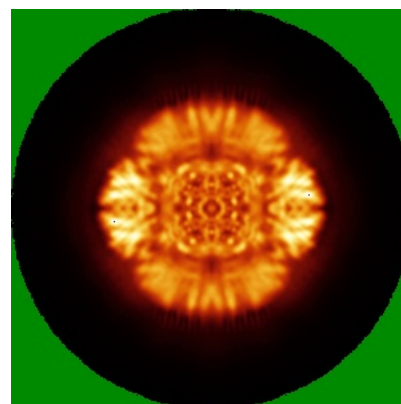
6.4.1 Primary map



X

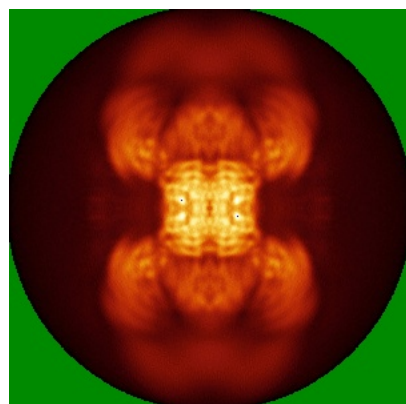


Y

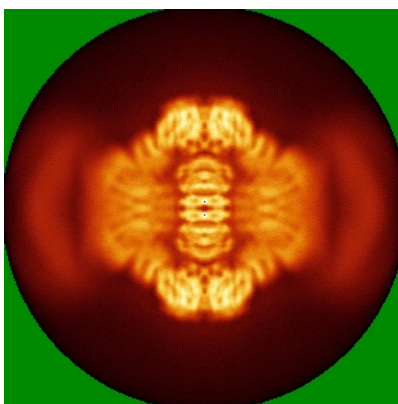


Z

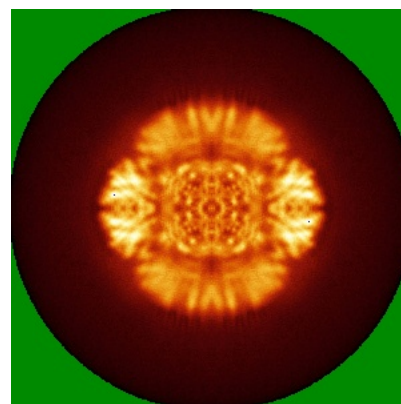
6.4.2 Raw map



X



Y

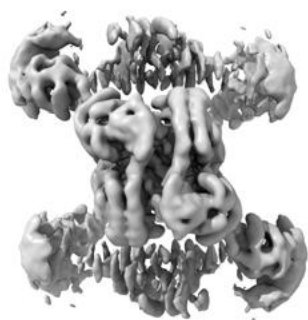


Z

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](#)

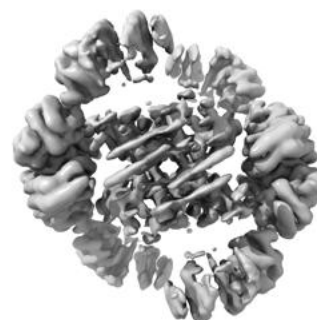
6.5.1 Primary map



X



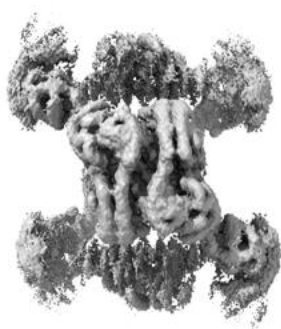
Y



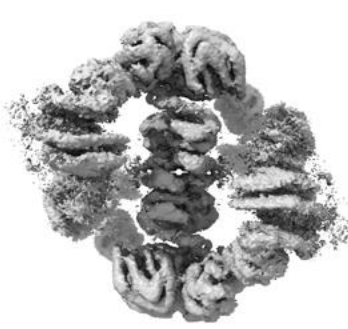
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

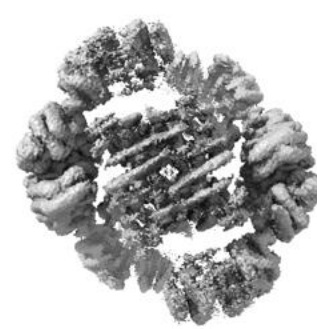
6.5.2 Raw map



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.

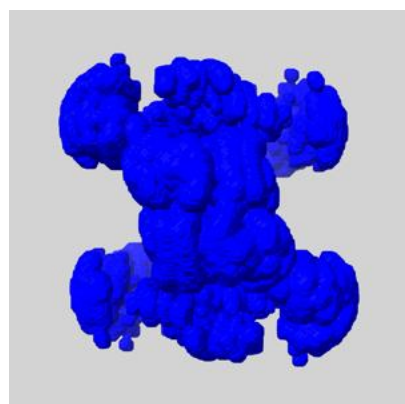
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

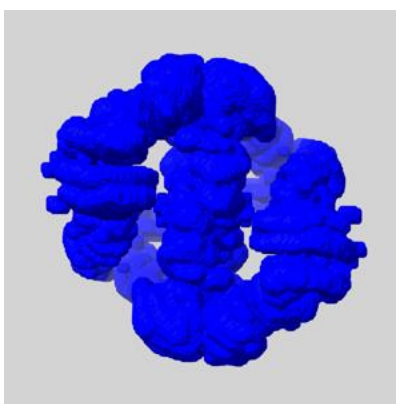
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

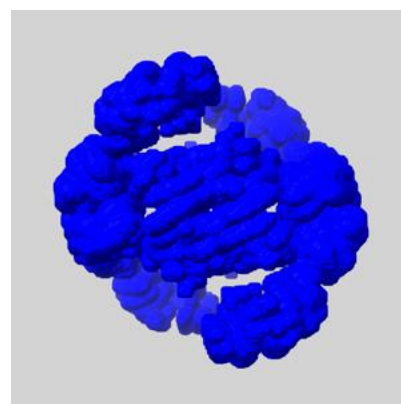
6.6.1 emd_31466_msk_1.map [i](#)



X



Y

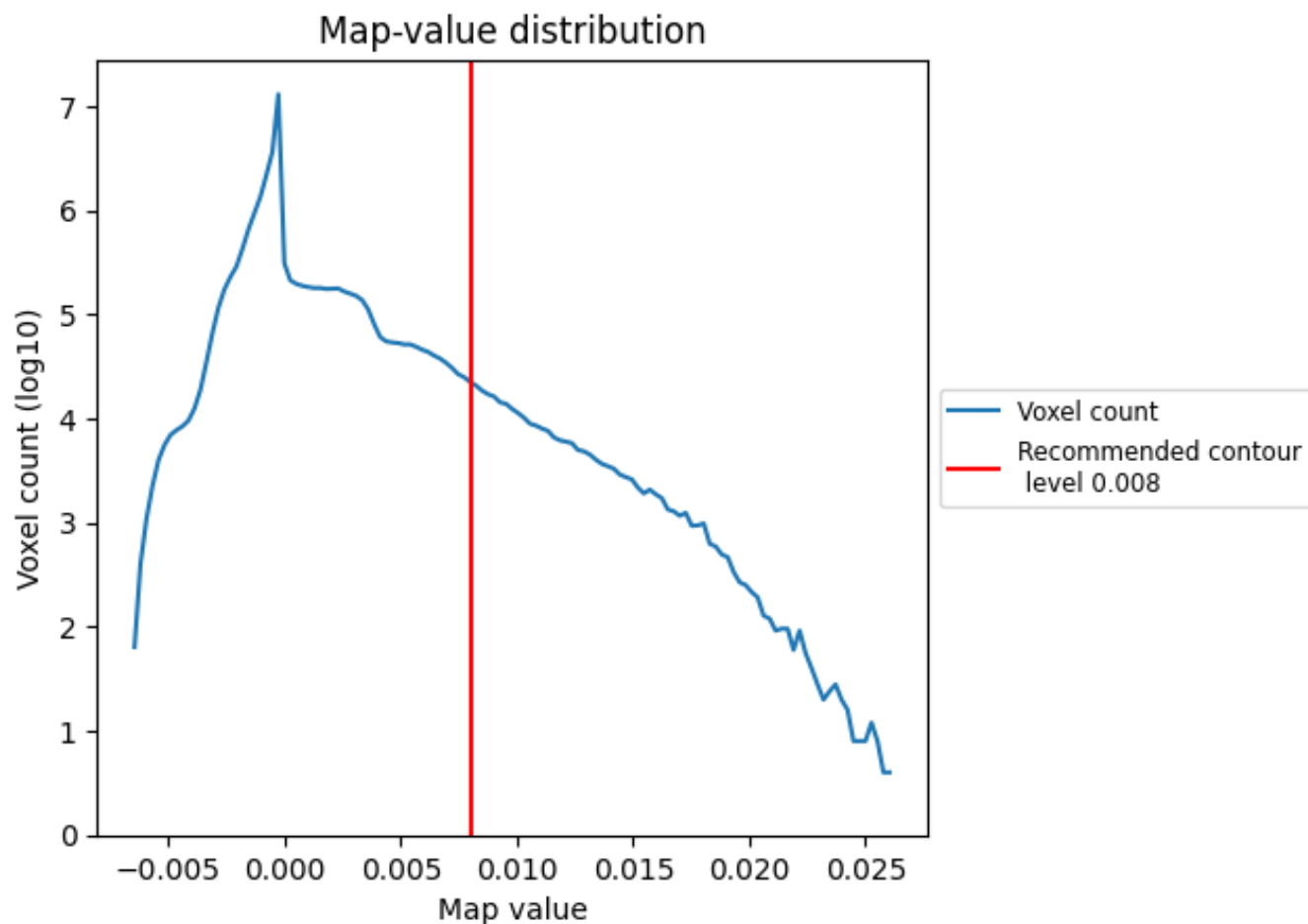


Z

7 Map analysis [i](#)

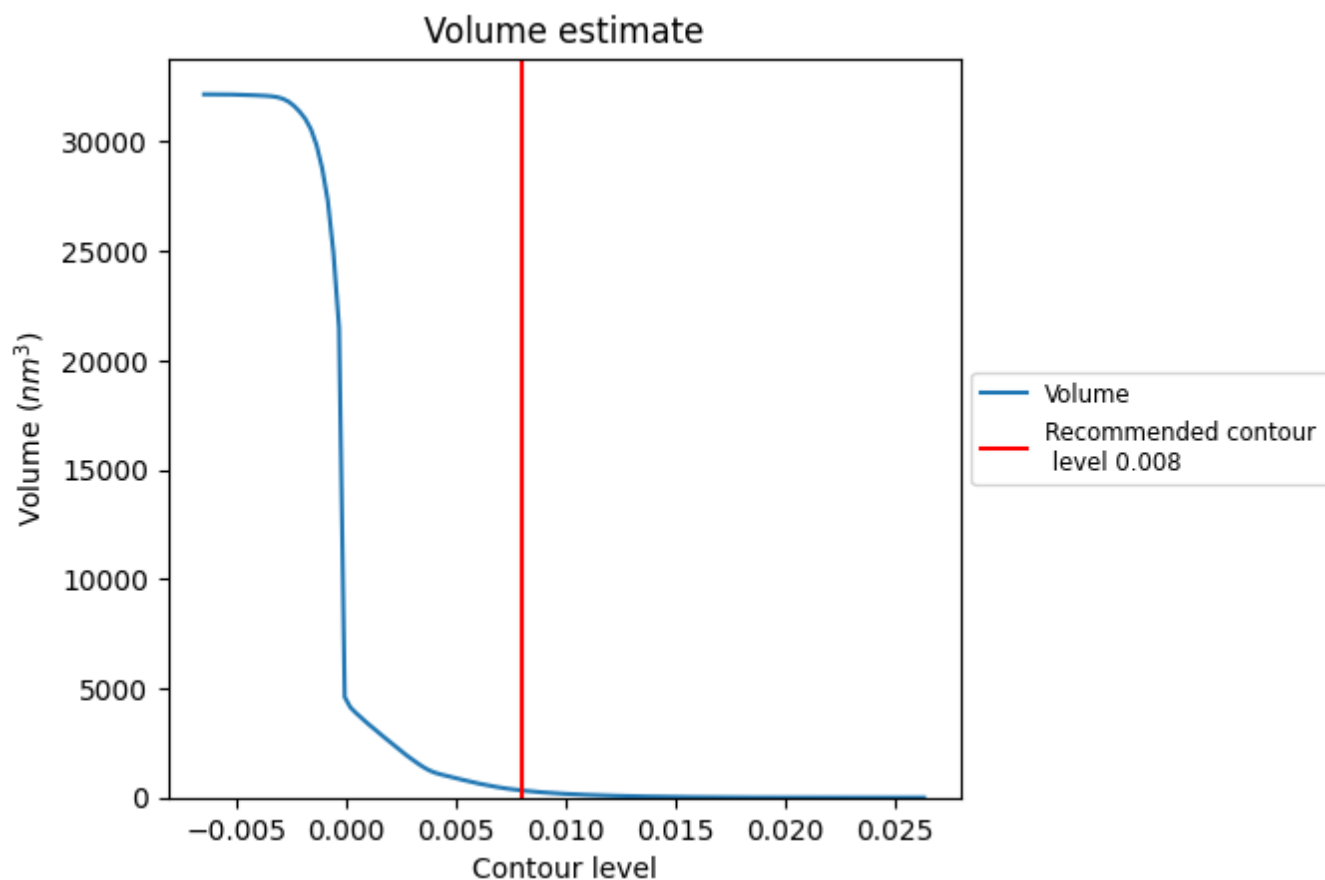
This section contains the results of statistical analysis of the map.

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.

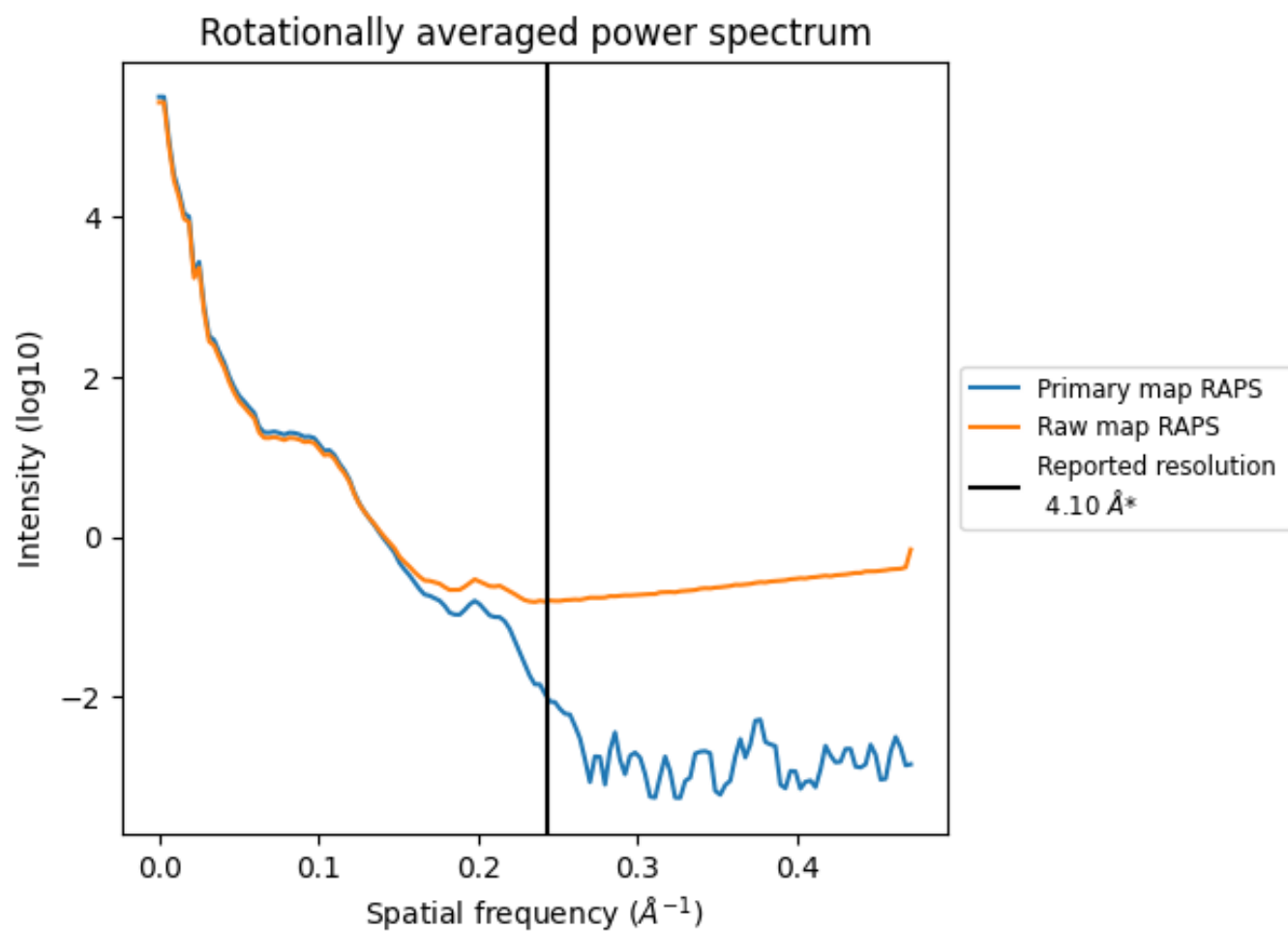
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 325 nm³; this corresponds to an approximate mass of 294 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 ⓘ

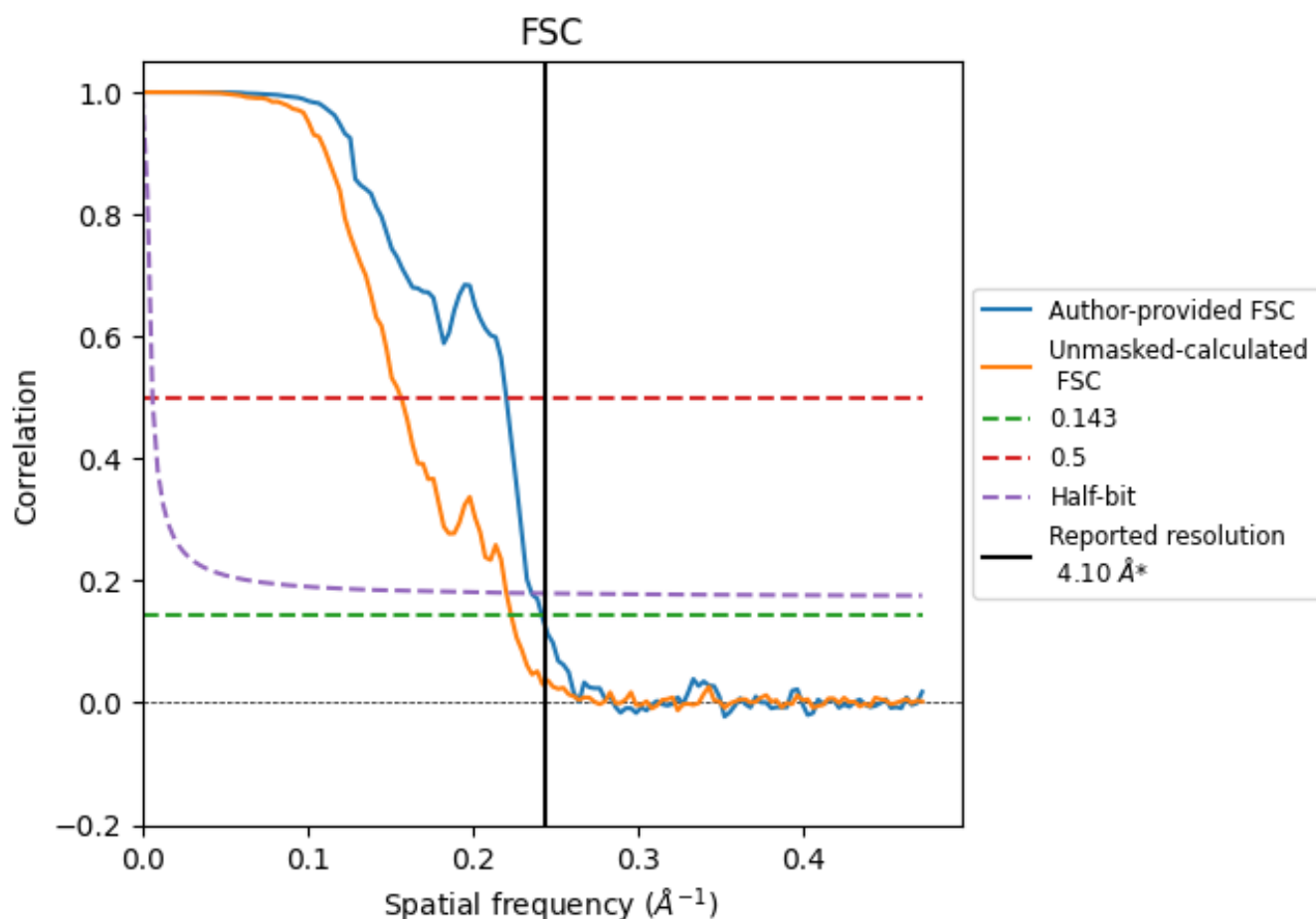


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

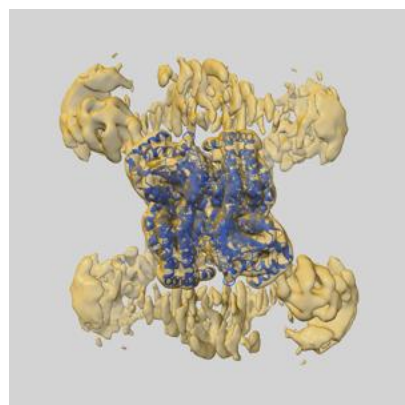
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	4.54	4.24
Unmasked-calculated*	4.48	6.39	4.54

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

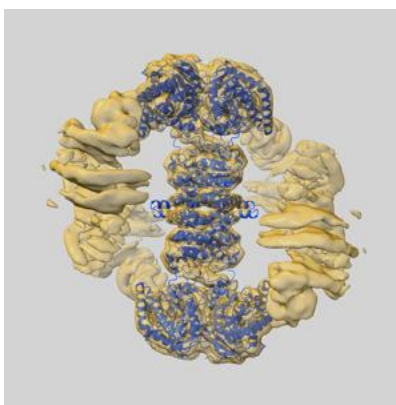
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31466 and PDB model 7F5T. Per-residue inclusion information can be found in section [3](#) on page [5](#).

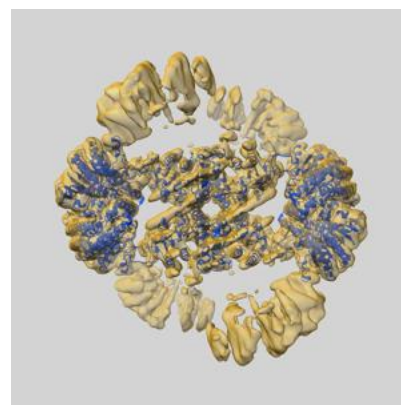
9.1 Map-model overlay [i](#)



X



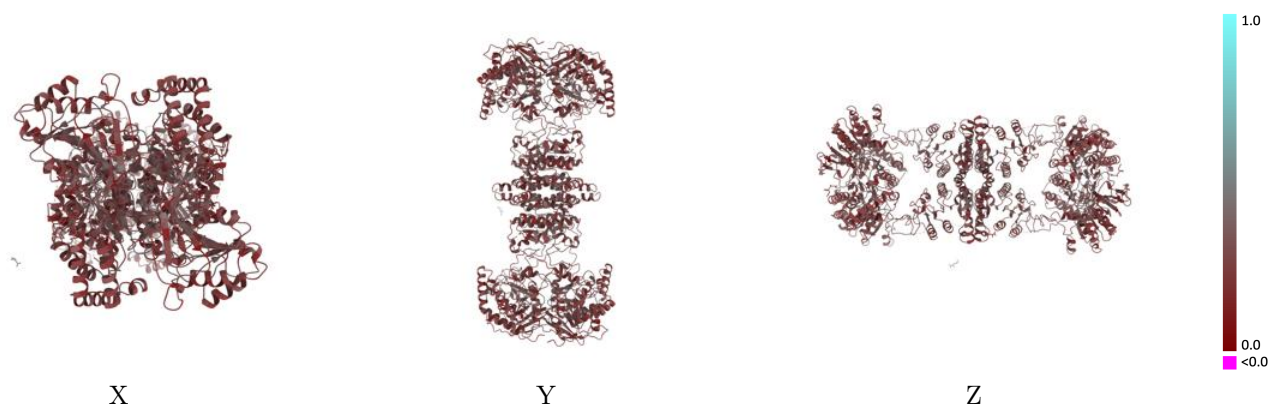
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

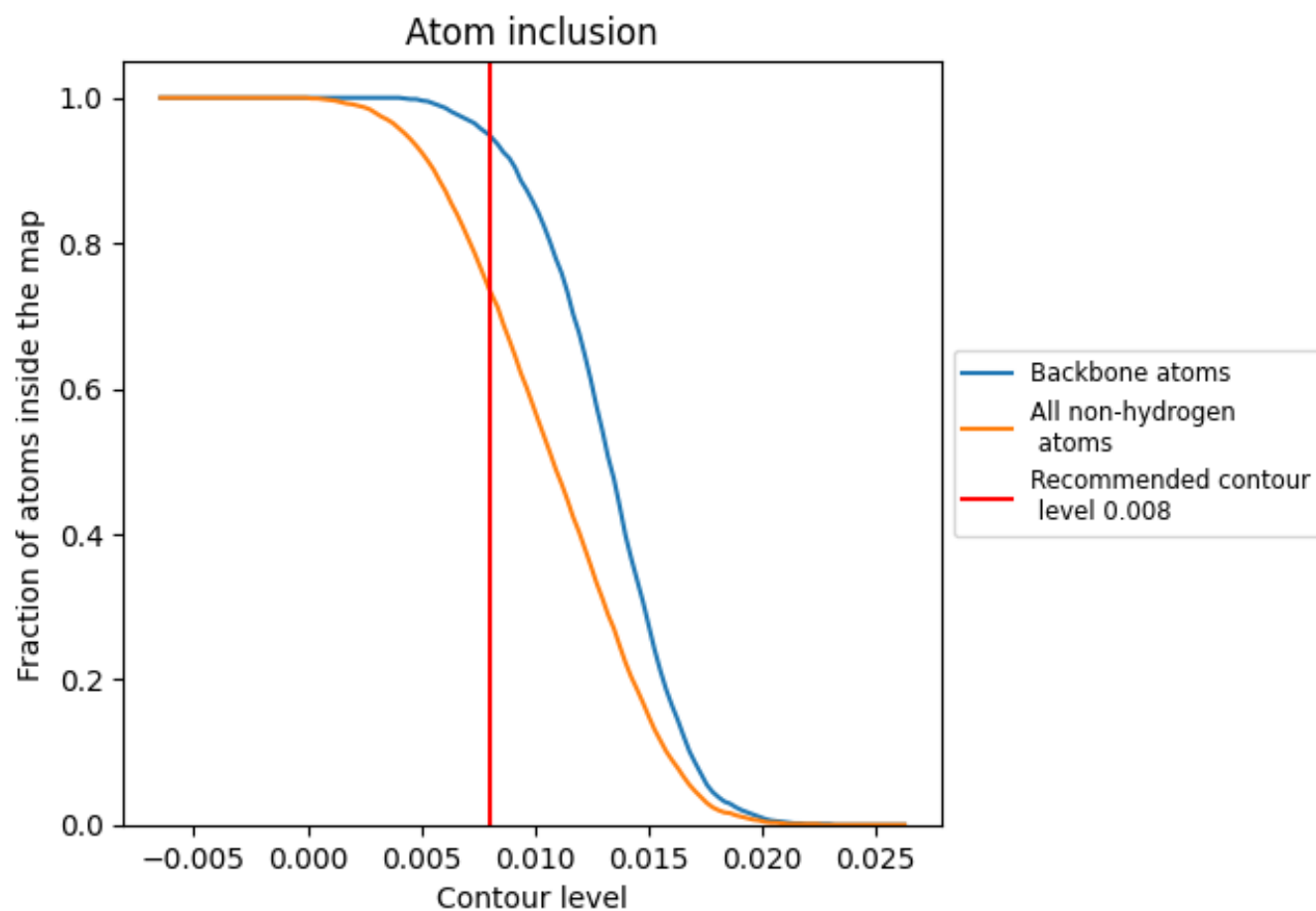


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 74% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7370	0.2850
A	0.7350	0.2850
B	0.7380	0.2840
C	0.7370	0.2860
D	0.7400	0.2850

