



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:05 AM UTC

PDB ID : 7YR3 / pdb_00007yr3
EMDB ID : EMD-34044
Title : SARS-CoV-2 BA.2.75 S Trimer in complex with ACE2(state2)
Authors : Wang, L.
Deposited on : 2022-08-08
Resolution : 3.52 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:

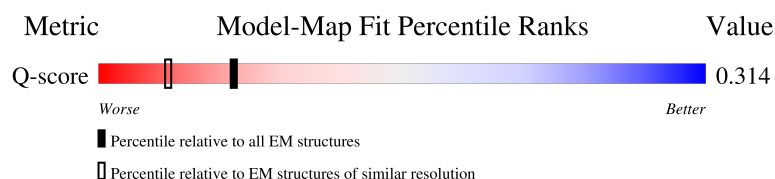
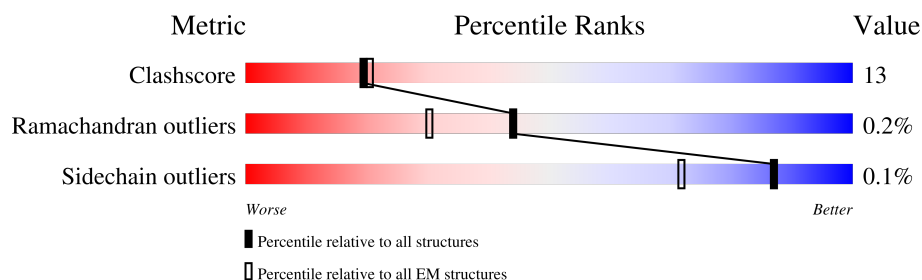
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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

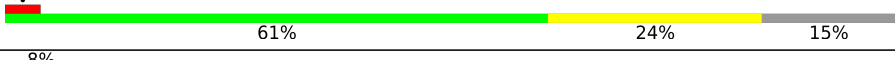
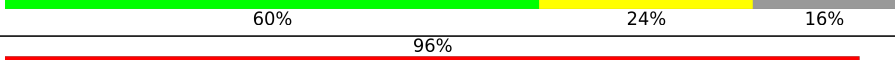
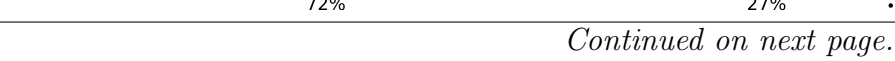
The reported resolution of this entry is 3.52 Å.

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	13017 (3.02 - 4.02)

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	B	1270	
1	C	1270	
1	F	1270	
2	D	603	

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Mol	Chain	Length	Quality of chain
2	G	603	
3	A	2	
3	E	2	
3	H	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	G	902	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35899 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1058	Total	C	N	O	S	0	0
			8258	5271	1380	1571	36		
1	C	1080	Total	C	N	O	S	0	0
			8426	5380	1407	1603	36		
1	F	1068	Total	C	N	O	S	0	0
			8335	5323	1392	1583	37		

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	147	GLU	LYS	variant	UNP P0DTC2
B	152	ARG	TRP	variant	UNP P0DTC2
B	157	LEU	PHE	variant	UNP P0DTC2
B	210	VAL	ILE	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	257	SER	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	683	ALA	ARG	engineered mutation	UNP P0DTC2
B	685	ALA	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	147	GLU	LYS	variant	UNP P0DTC2
C	152	ARG	TRP	variant	UNP P0DTC2
C	157	LEU	PHE	variant	UNP P0DTC2
C	210	VAL	ILE	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	257	SER	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	683	ALA	ARG	engineered mutation	UNP P0DTC2
C	685	ALA	ARG	engineered mutation	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
F	22	ILE	THR	variant	UNP P0DTC2
F	?	-	LEU	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	?	-	PRO	deletion	UNP P0DTC2
F	27	SER	ALA	variant	UNP P0DTC2
F	142	ASP	GLY	variant	UNP P0DTC2
F	147	GLU	LYS	variant	UNP P0DTC2
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F	210	VAL	ILE	variant	UNP P0DTC2
F	213	GLY	VAL	variant	UNP P0DTC2
F	257	SER	GLY	variant	UNP P0DTC2
F	339	HIS	GLY	variant	UNP P0DTC2
F	371	PHE	SER	variant	UNP P0DTC2
F	373	PRO	SER	variant	UNP P0DTC2
F	375	PHE	SER	variant	UNP P0DTC2
F	376	ALA	THR	variant	UNP P0DTC2
F	405	ASN	ASP	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	408	SER	ARG	variant	UNP P0DTC2
F	417	ASN	LYS	variant	UNP P0DTC2
F	440	LYS	ASN	variant	UNP P0DTC2
F	446	SER	GLY	variant	UNP P0DTC2
F	460	LYS	ASN	variant	UNP P0DTC2
F	477	ASN	SER	variant	UNP P0DTC2
F	478	LYS	THR	variant	UNP P0DTC2
F	484	ALA	GLU	variant	UNP P0DTC2
F	498	ARG	GLN	variant	UNP P0DTC2
F	501	TYR	ASN	variant	UNP P0DTC2
F	505	HIS	TYR	variant	UNP P0DTC2
F	614	GLY	ASP	variant	UNP P0DTC2
F	655	TYR	HIS	variant	UNP P0DTC2
F	679	LYS	ASN	variant	UNP P0DTC2
F	681	HIS	PRO	variant	UNP P0DTC2
F	683	ALA	ARG	engineered mutation	UNP P0DTC2
F	685	ALA	ARG	engineered mutation	UNP P0DTC2
F	764	LYS	ASN	variant	UNP P0DTC2
F	796	TYR	ASP	variant	UNP P0DTC2
F	817	PRO	PHE	engineered mutation	UNP P0DTC2
F	892	PRO	ALA	engineered mutation	UNP P0DTC2
F	899	PRO	ALA	engineered mutation	UNP P0DTC2
F	942	PRO	ALA	engineered mutation	UNP P0DTC2
F	954	HIS	GLN	variant	UNP P0DTC2
F	969	LYS	ASN	variant	UNP P0DTC2
F	986	PRO	LYS	engineered mutation	UNP P0DTC2
F	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		
2	G	597	Total	C	N	O	S	0	0
			4870	3115	806	920	29		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	616	HIS	-	expression tag	UNP Q9BYF1
D	617	HIS	-	expression tag	UNP Q9BYF1
D	618	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
G	616	HIS	-	expression tag	UNP Q9BYF1
G	617	HIS	-	expression tag	UNP Q9BYF1
G	618	HIS	-	expression tag	UNP Q9BYF1
G	619	HIS	-	expression tag	UNP Q9BYF1
G	620	HIS	-	expression tag	UNP Q9BYF1
G	621	HIS	-	expression tag	UNP Q9BYF1

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	
4	G	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		AltConf
5	G	1	Total	Zn	0
			1	1	

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total	Cl	0
			1	1	
6	G	1	Total	Cl	0
			1	1	

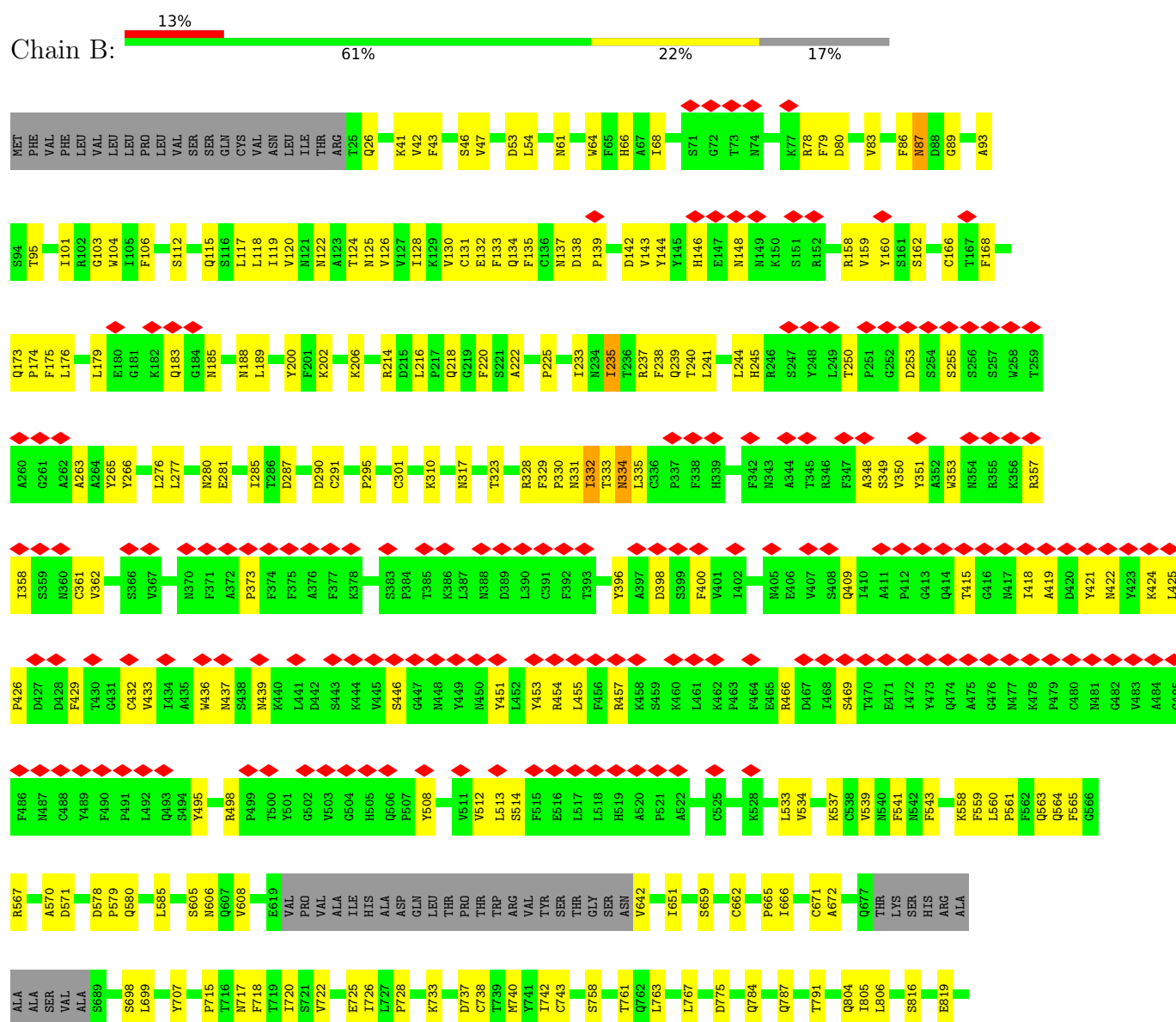
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	D	71	Total	O	0
			71	71	
7	G	71	Total	O	0
			71	71	

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.

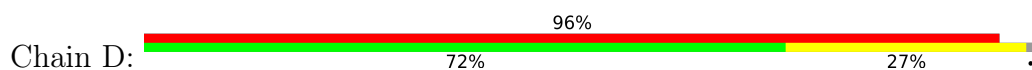
• Molecule 1: Spike glycoprotein



L1049	L1050	S1051	F1052	P1053	Q1054	H1064	V1065	E1072	F1075	I1081	K1086	F1089	G1093	V1096	S1097	W1102	F1103	R1107	V1122	V1133	N1134	N1135	D1139	E1144	LEU	ASP	ASP	PHE	GLN	TYR	GLU	GLU	LEU	ASP	TRP	TRP	TYR	PHE	LYS	TRP	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP
LEU	GLY	ASP	ILE	ILE	GLY	THR	ILE	ASN	ALA	SER	VAL	THR	ASN	ILE	GLN	LYS	GLY	ARG	LEU	ASP	ILE	GLN	ASN	VAL	ALA	LYS	ASN	LEU	ASP	GLY	GLN	TYR	GLU	GLU	LEU	ASP	TRP	TRP	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	VAL	ASP

ALA	ILE	VAL	MET	VAL	THR	ILE	MET	LEU	CYS	VAL	THR	SER	CYS	CYS	CYS	LYS	GLY	CYS	SER	CYS	GLY	ASP	GLU	PRO	VAL	LEU	LYS	GLY	VAL	LYS	LEU	HIS	TYR	THR
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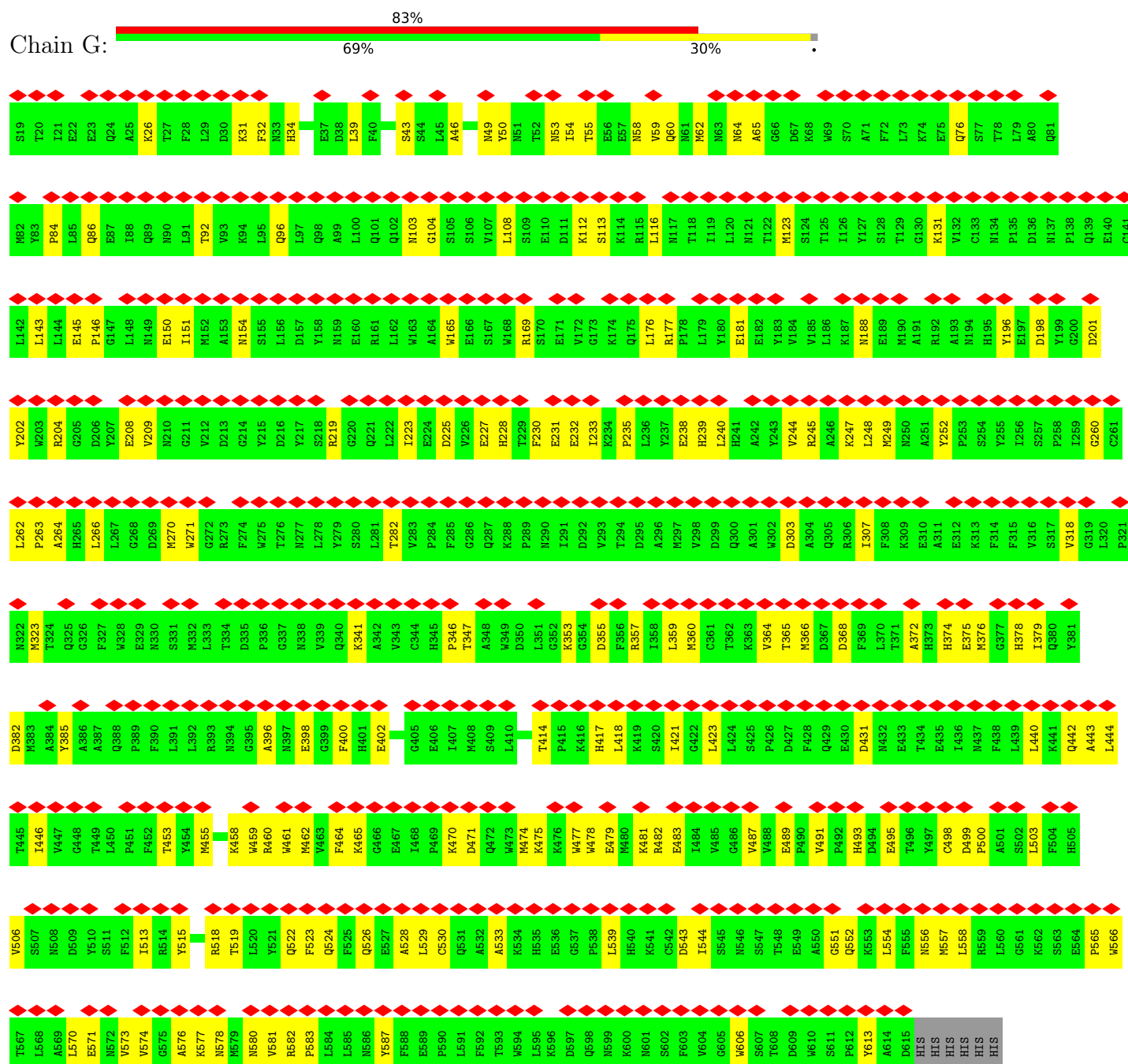
● Molecule 2: Angiotensin-converting enzyme 2



S59	T20	T21	E22	E23	Q24	A25	K26	T27	F28	L29	D30	F31	K32	R33	H34	E35	A36	E37	D38	L39	F40	Y41	Q42	S43	S44	L45	A46	S47	W48	Y49	Y50	N51	T52	N53	I54	T55	E56	E57	N58	Y59	Q60	N61	H62	N63	H64	A65	G66	D67	K68	S69	A70	F71	L72	K73	E74	Q75	S76	T77	T78
L79	A80	Q81	M82	Y83	P84	L85	Q86	E87	T88	Q89	N90	L91	T92	V93	K94	L95	Q96	L97	Q98	A99	L100	Q101	Q102	N103	G104	S105	S106	V107	L108	S109	D110	D111	K112	S113	K114	R115	L116	M117	T118	I119	L120	T122	M123	S124	T125	I126	Y127	S128	T129	G130	K131	V132	C133	N134	P135	D136	M137	P138	
Q139	E140	C141	L142	L143	L144	E145	P146	G147	L148	M149	E150	I151	M152	A153	H154	S155	L156	D157	L158	M159	E160	R161	L162	W163	A164	W165	E166	S167	W168	R169	S170	E171	V172	G173	K174	Q175	L176	R177	L178	L179	Y180	E181	E182	Y183	V184	V185	L186	K187	N188	E189	M190	A191	R192	A193	N194	H195	Y196	E197	D198
Y199	G200	D201	Y202	W203	R204	G205	D206	Y207	E208	V209	N210	G211	V212	D213	Q214	Y215	D216	Y217	S218	Q219	Q220	Q221	L222	I223	E224	D225	Y226	E227	H228	T229	E230	E231	E232	I233	K234	P235	L236	Y237	E238	H239	L240	H241	A242	Y243	A244	R245	A246	K247	M249	N250	A251	Y252	P253	F314	E254	E255	I256	S257	P258
I259	G260	C261	L262	E263	A264	H265	L266	L267	D268	E269	W270	W271	G272	R273	F274	W275	T276	N277	L278	Y279	S280	L281	T282	V283	P284	F285	G286	Q287	K288	P289	N290	E291	G292	V293	T294	D295	A296	M297	V298	D299	Q300	A301	W302	D303	V304	T305	K306	I307	F308	K309	E310	A311	K312	K313	H314	E315	V316	S317	V318
G319	L320	F321	M322	M323	T324	Q325	G326	F327	Q328	E329	N330	S331	M332	L333	T334	D335	P336	G337	N338	V339	Q340	K341	A342	V343	C344	H345	P346	T347	A348	W349	D350	L351	G352	K353	D354	F355	R356	I357	L358	L359	M360	C361	T362	K363	V364	T365	M366	D367	D368	F369	L370	T371	A372	H373	H374	E375	M376	G377	H378
I379	Q380	Y381	M382	A383	A384	Y385	A386	A387	Q388	P389	F390	L391	L392	R393	N394	G395	A396	N397	E398	F400	H401	E402	A403	V404	G405	A406	I407	M408	S409	L410	S411	A412	A413	T414	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426	D427	F428	Q429	E430	D431	N432	E433	T434	E435	E436	I437	N438	F439
L439	L440	K441	Q442	A443	L444	T445	I446	V447	G448	T449	L450	P451	F452	T453	Y454	M455	L456	E457	K458	W459	R460	W461	M462	V463	F464	K465	G466	E467	I468	P469	K470	D471	Q472	W473	M474	K475	K476	W477	W478	E479	M480	K481	R482	E483	I484	V485	G486	V487	V488	E489	P490	W491	P492	H493	D494	E495	T496	Y497	C498
D499	P500	A501	S502	L503	F504	H505	V506	S507	N508	D509	Y510	S511	F512	I513	R514	Y515	Y516	T517	R518	T519	L520	Y521	Q522	F523	Q524	F525	G526	E527	A528	L529	C530	Q531	A532	A533	K534	H535	E536	G537	P538	L539	H540	K541	C542	D543	I544	S545	N546	S547	T548	E549	A550	G551	Q552	K553	L554	F555	N556	M557	L558
R559	L560	G561	K562	S563	E564	P565	W566	T567	L568	A569	L570	E571	N572	V573	V574	G575	A576	K577	N578	M579	N580	V581	R582	P583	L584	L585	N586	Y587	F588	E589	P590	L591	F592	T593	W594	L595	K596	D597	Q598	N599	K600	N601	S602	F603	V604	G605	W606	S607	T608	D609	W610	S611	P612	Y613	A614	D615	HIS	HIS	HIS

HIS
HIS
HIS

- Molecule 2: Angiotensin-converting enzyme 2



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%

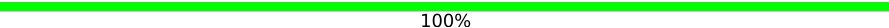


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  50% 100%

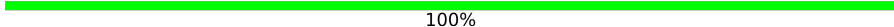


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

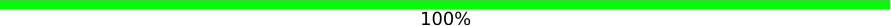


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50% 50%

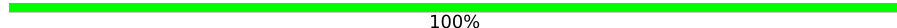


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	313740	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.894	Depositor
Minimum map value	-0.423	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	332.8, 332.8, 332.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	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: NAG, ZN, CL

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	B	0.16	0/8455	0.34	1/11509 (0.0%)
1	C	0.16	0/8631	0.35	0/11756
1	F	0.16	0/8534	0.34	0/11617
2	D	0.12	0/5007	0.31	0/6803
2	G	0.11	0/5007	0.29	0/6803
All	All	0.15	0/35634	0.33	1/48488 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1135	ASN	CB-CA-C	-5.21	109.59	115.79

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	B	8258	0	8044	204	0
1	C	8426	0	8195	239	0
1	F	8335	0	8129	232	0
2	D	4870	0	4639	109	0
2	G	4870	0	4639	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	28	0	25	2	0
3	E	28	0	25	0	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
4	B	210	0	192	7	0
4	C	238	0	221	3	0
4	D	56	0	52	0	0
4	F	182	0	169	3	0
4	G	56	0	52	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	2	0
7	D	71	0	0	8	0
7	G	71	0	0	13	0
All	All	35899	0	34557	883	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 13.

All (883) 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:332:ILE:HG23	1:B:334:ASN:H	1.26	0.98
1:F:335:LEU:HG	1:F:338:PHE:HB2	1.47	0.97
1:B:740:MET:HE1	1:F:319:ARG:HE	1.44	0.82
1:B:331:ASN:HD21	4:B:1308:NAG:HN2	1.28	0.80
1:C:89:GLY:HA2	1:C:194:PHE:O	1.82	0.80
1:F:332:ILE:HD12	1:F:332:ILE:H	1.46	0.80
1:B:912:THR:OG1	1:B:1106:GLN:NE2	2.15	0.79
1:C:402:ILE:HG13	1:C:403:ARG:H	1.47	0.78
1:F:560:LEU:HB2	1:F:563:GLN:HE21	1.49	0.78
1:B:419:ALA:HB3	4:B:1309:NAG:H3	1.65	0.76
1:F:78:ARG:HG2	1:F:80:ASP:H	1.51	0.75
1:F:112:SER:HA	1:F:132:GLU:HG2	1.69	0.75
1:B:103:GLY:HA3	1:B:241:LEU:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:TYR:O	1:B:466:ARG:NH2	2.20	0.74
1:F:28:TYR:HB2	1:F:258:TRP:HA	1.70	0.74
1:C:130:VAL:HB	1:C:168:PHE:HB2	1.69	0.74
1:F:335:LEU:O	1:F:336:CYS:C	2.30	0.73
1:F:106:PHE:HB3	1:F:235:ILE:HG12	1.70	0.73
1:C:447:GLY:HA3	1:C:497:PHE:H	1.55	0.72
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.71	0.71
1:F:96:GLU:HG2	1:F:100:ILE:HB	1.70	0.71
1:F:119:ILE:HG12	1:F:128:ILE:HG12	1.73	0.71
2:D:529:LEU:HD11	2:D:554:LEU:HD22	1.72	0.71
1:C:755:GLN:C	1:C:757:GLY:H	1.98	0.71
1:C:802:PHE:HB3	1:C:806:LEU:HD23	1.71	0.71
2:D:381:TYR:HD1	2:D:558:LEU:HG	1.54	0.71
1:B:361:CYS:SG	1:B:362:VAL:N	2.61	0.71
1:B:737:ASP:OD2	1:F:317:ASN:ND2	2.24	0.70
1:C:26:GLN:HE21	1:C:63:THR:HB	1.56	0.70
2:D:293:VAL:HG23	2:D:297:MET:HE1	1.72	0.70
1:B:139:PRO:HG3	1:B:244:LEU:HD23	1.72	0.69
1:C:659:SER:HB3	1:C:698:SER:HB3	1.74	0.69
1:C:214:ARG:HH21	1:C:218:GLN:HG2	1.57	0.69
1:C:425:LEU:HD12	1:C:426:PRO:HD2	1.75	0.69
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.74	0.69
2:G:262:LEU:HD12	2:G:263:PRO:HD2	1.75	0.69
2:G:574:VAL:HG23	2:G:576:ALA:H	1.55	0.69
1:F:472:ILE:HG13	1:F:482:GLY:HA2	1.75	0.69
1:B:332:ILE:HG13	1:B:333:THR:H	1.56	0.68
1:C:475:ALA:O	1:C:487:ASN:ND2	2.26	0.68
1:B:131:CYS:SG	1:B:132:GLU:N	2.67	0.68
1:F:338:PHE:HE1	1:F:358:ILE:HD13	1.59	0.68
2:G:453:THR:HG22	2:G:513:ILE:HD12	1.76	0.68
1:F:117:LEU:HD21	1:F:119:ILE:HG13	1.75	0.67
1:C:634:ARG:O	1:C:636:TYR:N	2.27	0.67
2:G:54:ILE:HB	2:G:341:LYS:HB2	1.74	0.67
2:G:225:ASP:OD2	2:G:578:ASN:ND2	2.27	0.67
2:D:320:LEU:HD13	2:D:380:GLN:HG2	1.77	0.67
2:D:419:LYS:NZ	2:D:425:SER:O	2.28	0.67
1:B:446:SER:O	1:B:498:ARG:NH2	2.27	0.67
1:C:755:GLN:O	1:C:757:GLY:N	2.28	0.67
1:C:534:VAL:HG21	1:C:539:VAL:HG11	1.77	0.67
1:B:331:ASN:OD1	4:B:1308:NAG:H82	1.94	0.66
1:C:605:SER:OG	1:C:607:GLN:OE1	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:ILE:HG22	2:D:123:MET:HE1	1.77	0.66
2:G:31:LYS:HA	2:G:34:HIS:CD2	2.31	0.66
1:B:454:ARG:HD3	1:B:457:ARG:HB3	1.78	0.66
1:C:1090:PRO:HG3	1:C:1095:PHE:HB2	1.77	0.66
2:G:378:HIS:HE1	2:G:402:GLU:HA	1.60	0.66
1:B:83:VAL:HA	1:B:237:ARG:HH21	1.60	0.66
1:F:34:ARG:NH2	1:F:217:PRO:O	2.29	0.66
1:F:68:ILE:HA	1:F:250:THR:HB	1.78	0.66
1:F:366:SER:OG	1:F:388:ASN:ND2	2.28	0.66
1:B:237:ARG:HH12	1:B:239:GLN:HB2	1.60	0.66
1:F:804:GLN:NE2	1:F:935:GLN:OE1	2.29	0.66
1:B:87:ASN:ND2	1:B:87:ASN:O	2.29	0.65
1:C:131:CYS:SG	1:C:132:GLU:N	2.70	0.65
2:D:204:ARG:HH12	2:D:223:ILE:HG13	1.61	0.65
2:D:529:LEU:HD21	2:D:554:LEU:HB2	1.79	0.65
2:G:414:THR:HG23	2:G:417:HIS:H	1.61	0.65
1:C:96:GLU:O	1:C:190:ARG:NH2	2.28	0.65
1:C:394:ASN:ND2	1:F:200:TYR:OH	2.30	0.65
1:B:104:TRP:HB3	1:B:106:PHE:HE2	1.62	0.65
1:C:454:ARG:NH2	1:C:467:ASP:O	2.29	0.65
1:C:1097:SER:HB2	1:C:1102:TRP:CE3	2.32	0.65
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.78	0.65
2:D:131:LYS:HB3	2:D:143:LEU:HD23	1.79	0.65
1:F:596:SER:HB3	1:F:611:LEU:HB3	1.77	0.65
2:D:539:LEU:HD23	2:D:587:TYR:HB2	1.79	0.65
1:C:112:SER:HA	1:C:132:GLU:HG2	1.79	0.64
1:B:124:THR:HA	1:B:174:PRO:HG3	1.79	0.64
1:C:318:PHE:HE2	1:C:620:VAL:HG11	1.62	0.64
1:C:560:LEU:O	1:C:563:GLN:NE2	2.30	0.64
1:B:331:ASN:ND2	4:B:1308:NAG:HN2	1.95	0.64
1:C:1019:ARG:NH1	1:C:1023:ASN:OD1	2.31	0.64
2:G:204:ARG:NH2	7:G:1011:HOH:O	2.29	0.64
2:D:103:ASN:ND2	2:D:106:SER:OG	2.29	0.64
1:B:328:ARG:NE	1:B:578:ASP:OD2	2.31	0.63
1:C:26:GLN:HA	1:C:64:TRP:O	1.99	0.63
1:C:759:PHE:O	1:C:763:LEU:HD23	1.98	0.63
1:B:53:ASP:OD2	1:B:54:LEU:N	2.30	0.63
2:G:479:GLU:HA	2:G:482:ARG:HD2	1.80	0.63
2:D:346:PRO:HG2	2:D:371:THR:HG21	1.79	0.63
1:C:124:THR:HA	1:C:174:PRO:HG3	1.81	0.63
1:F:144:TYR:O	1:F:150:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:247:LYS:HD2	2:G:282:THR:HG22	1.79	0.63
2:D:293:VAL:HG12	2:D:424:LEU:HD13	1.80	0.62
2:D:196:TYR:HB3	2:D:201:ASP:HB3	1.79	0.62
1:B:333:THR:HB	1:B:362:VAL:HG21	1.80	0.62
2:D:574:VAL:HG23	2:D:576:ALA:H	1.62	0.62
1:F:214:ARG:NH1	1:F:215:ASP:O	2.32	0.62
1:C:656:VAL:HG12	1:C:658:ASN:H	1.65	0.62
1:F:26:GLN:HA	1:F:64:TRP:O	1.98	0.62
2:G:374:HIS:NE2	2:G:378:HIS:CE1	2.68	0.62
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.81	0.62
1:F:349:SER:HA	1:F:401:VAL:HG12	1.82	0.62
2:G:526:GLN:NE2	2:G:530:CYS:SG	2.73	0.62
2:D:518:ARG:NH1	7:D:1017:HOH:O	2.33	0.62
2:D:184:VAL:HG22	2:D:464:PHE:HE1	1.65	0.61
2:D:356:PHE:HD2	2:D:379:ILE:HG23	1.65	0.61
2:D:267:LEU:HD11	2:D:487:VAL:HG21	1.82	0.61
1:F:446:SER:O	1:F:498:ARG:NE	2.27	0.61
1:B:805:ILE:HD12	1:B:878:LEU:HD11	1.83	0.61
2:G:169:ARG:NH2	2:G:270:MET:O	2.34	0.61
2:G:398:GLU:OE2	7:G:1001:HOH:O	2.16	0.61
1:B:93:ALA:HB1	1:B:189:LEU:HD11	1.82	0.61
2:D:168:TRP:HE1	2:D:271:TRP:HE1	1.47	0.61
2:G:188:ASN:ND2	7:G:1018:HOH:O	2.34	0.61
2:G:365:THR:HG23	2:G:368:ASP:H	1.66	0.61
1:C:571:ASP:HB2	1:F:967:SER:HB2	1.82	0.61
1:C:816:SER:HB2	1:C:819:GLU:HG3	1.81	0.61
2:D:607:SER:OG	2:D:609:ASP:OD1	2.16	0.61
1:B:323:THR:OG1	1:B:537:LYS:NZ	2.34	0.61
1:C:93:ALA:HB1	1:C:189:LEU:HD11	1.83	0.61
1:C:403:ARG:HA	1:C:507:PRO:HA	1.83	0.61
1:F:426:PRO:HG2	1:F:429:PHE:HB2	1.83	0.61
1:F:1097:SER:HB3	1:F:1102:TRP:CD2	2.36	0.60
1:F:327:VAL:HG11	1:F:528:LYS:HD3	1.82	0.60
1:B:115:GLN:HB3	1:B:233:ILE:HD13	1.81	0.60
1:B:357:ARG:HD3	1:C:167:THR:HG22	1.84	0.60
1:B:1076:THR:O	1:B:1097:SER:OG	2.19	0.60
2:G:414:THR:HG21	2:G:543:ASP:HB2	1.83	0.60
2:G:573:VAL:HG13	2:G:574:VAL:HG13	1.82	0.60
2:G:177:ARG:NH2	2:G:181:GLU:OE2	2.34	0.60
1:B:699:LEU:HB3	1:C:873:TYR:HE1	1.66	0.60
1:C:882:ILE:HG13	1:C:883:THR:HG23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:971:GLY:O	1:C:995:ARG:NH1	2.35	0.59
1:F:365:TYR:N	1:F:388:ASN:OD1	2.29	0.59
1:F:780:GLU:O	1:F:784:GLN:NE2	2.33	0.59
1:F:412:PRO:HB3	1:F:427:ASP:HA	1.83	0.59
2:G:150:GLU:OE1	7:G:1002:HOH:O	2.17	0.59
2:G:204:ARG:HH12	2:G:465:LYS:HZ1	1.48	0.59
1:F:159:VAL:HG22	1:F:160:TYR:H	1.66	0.59
1:F:656:VAL:HG12	1:F:658:ASN:H	1.67	0.59
2:G:481:LYS:HB3	2:G:487:VAL:HG23	1.83	0.59
1:F:523:THR:HG22	1:F:524:VAL:HG23	1.83	0.59
1:B:422:ASN:HD21	1:B:453:TYR:HD2	1.50	0.59
1:C:596:SER:HB2	1:C:611:LEU:HB3	1.83	0.59
1:C:616:ASN:OD1	1:C:644:GLN:NE2	2.35	0.59
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.28	0.59
1:C:412:PRO:HB3	1:C:427:ASP:HA	1.85	0.59
1:C:661:GLU:O	1:C:695:TYR:OH	2.21	0.59
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.84	0.59
2:D:527:GLU:OE1	2:D:582:ARG:NH2	2.35	0.59
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.84	0.59
1:B:559:PHE:HB3	1:B:563:GLN:HG3	1.85	0.59
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.34	0.59
1:B:61:ASN:HD21	4:B:1301:NAG:HN2	1.51	0.59
1:C:188:ASN:HA	1:C:209:PRO:HA	1.84	0.59
1:C:547:THR:HG23	1:F:978:ASN:HB3	1.84	0.59
2:G:477:TRP:CD2	2:G:500:PRO:HG3	2.37	0.59
1:B:421:TYR:HD1	1:B:457:ARG:HG2	1.68	0.58
1:F:335:LEU:HG	1:F:338:PHE:CB	2.29	0.58
1:F:347:PHE:CG	1:F:509:ARG:HD3	2.38	0.58
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.34	0.58
1:F:122:ASN:HB3	1:F:125:ASN:HB3	1.85	0.58
1:C:358:ILE:HB	1:C:395:VAL:HB	1.86	0.58
1:C:560:LEU:N	1:C:563:GLN:HE22	2.00	0.58
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.36	0.58
2:D:315:PHE:HA	2:D:318:VAL:HG22	1.84	0.58
2:G:131:LYS:HB3	2:G:143:LEU:HD23	1.85	0.58
2:G:245:ARG:NH1	2:G:260:GLY:O	2.37	0.58
1:C:415:THR:HG22	1:C:417:ASN:H	1.68	0.58
1:F:124:THR:HA	1:F:174:PRO:HG3	1.85	0.58
1:F:204:TYR:HB3	1:F:223:LEU:HB3	1.85	0.58
2:G:43:SER:HA	2:G:65:ALA:HB1	1.85	0.58
1:B:132:GLU:N	1:B:166:CYS:SG	2.76	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:TYR:H	1:F:230:PRO:HA	1.68	0.58
2:G:177:ARG:HB2	2:G:498:CYS:HB2	1.86	0.57
2:G:108:LEU:HD22	2:G:112:LYS:HD2	1.85	0.57
1:B:738:CYS:O	1:B:742:ILE:N	2.37	0.57
2:D:137:ASN:HD21	2:D:139:GLN:HE21	1.51	0.57
2:G:528:ALA:HB2	2:G:574:VAL:HG12	1.86	0.57
1:B:816:SER:HB2	1:B:819:GLU:HG3	1.85	0.57
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.38	0.57
1:F:168:PHE:HZ	1:F:229:LEU:HD11	1.69	0.57
1:F:335:LEU:O	1:F:338:PHE:N	2.37	0.57
2:G:244:VAL:HA	2:G:247:LYS:HE3	1.85	0.57
1:F:802:PHE:HB3	1:F:806:LEU:HD23	1.85	0.57
2:G:382:ASP:HA	2:G:385:TYR:CZ	2.39	0.57
2:D:443:ALA:O	2:D:448:GLY:N	2.38	0.57
1:F:350:VAL:HA	1:F:400:PHE:HB2	1.86	0.57
2:G:458:LYS:O	2:G:462:MET:HG2	2.04	0.57
1:C:405:ASN:HB2	1:C:504:GLY:O	2.05	0.57
1:F:406:GLU:HG2	1:F:409:GLN:HE22	1.69	0.57
1:C:760:CYS:O	1:C:761:THR:C	2.46	0.56
1:C:1106:GLN:HE21	1:C:1109:PHE:HB3	1.70	0.56
2:G:396:ALA:HB3	2:G:400:PHE:HE1	1.69	0.56
2:G:571:GLU:HB2	2:G:577:LYS:HA	1.85	0.56
2:G:165:TRP:O	2:G:169:ARG:HG2	2.06	0.56
1:B:143:VAL:HG13	1:B:144:TYR:HD1	1.70	0.56
1:C:157:LEU:HG	1:C:159:VAL:HG22	1.87	0.56
1:F:725:GLU:OE1	1:F:1064:HIS:NE2	2.35	0.56
1:B:122:ASN:HB3	1:B:125:ASN:HB2	1.88	0.56
1:B:882:ILE:HG13	1:B:883:THR:HG23	1.86	0.56
1:C:916:LEU:HD12	1:C:923:ILE:HD12	1.86	0.56
1:B:804:GLN:NE2	1:B:935:GLN:OE1	2.32	0.56
2:G:227:GLU:OE2	2:G:458:LYS:NZ	2.30	0.56
2:G:528:ALA:HB1	2:G:573:VAL:HG22	1.87	0.56
1:B:214:ARG:HH22	1:B:218:GLN:H	1.54	0.56
4:C:1312:NAG:H83	4:C:1312:NAG:H3	1.88	0.56
2:D:90:ASN:HB3	2:D:93:VAL:HG22	1.88	0.56
1:F:328:ARG:NH2	1:F:580:GLN:HE21	2.03	0.56
1:B:47:VAL:HG13	1:F:569:ILE:HG22	1.87	0.56
1:B:914:ASN:HA	1:F:1089:PHE:HE2	1.71	0.56
1:C:183:GLN:HG3	1:C:185:ASN:H	1.71	0.56
1:C:422:ASN:OD1	1:C:454:ARG:N	2.37	0.56
1:F:106:PHE:HD1	1:F:235:ILE:HG21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.87	0.55
1:C:97:LYS:HD2	1:C:98:SER:N	2.20	0.55
1:F:131:CYS:SG	1:F:132:GLU:N	2.80	0.55
1:C:438:SER:HB3	1:C:509:ARG:HG3	1.88	0.55
1:F:105:ILE:HB	1:F:239:GLN:HB3	1.89	0.55
4:F:1310:NAG:H3	4:F:1310:NAG:H83	1.87	0.55
2:G:318:VAL:HB	2:G:551:GLY:HA3	1.87	0.55
1:B:743:CYS:HA	1:B:977:LEU:HD11	1.88	0.55
2:D:356:PHE:CD2	2:D:379:ILE:HG23	2.41	0.55
1:F:173:GLN:HG2	1:F:174:PRO:HD2	1.87	0.55
2:G:235:PRO:O	2:G:239:HIS:ND1	2.40	0.55
2:D:107:VAL:HG13	2:D:108:LEU:HD12	1.87	0.55
2:G:248:LEU:O	2:G:252:TYR:N	2.38	0.55
2:G:323:MET:SD	7:G:1051:HOH:O	2.58	0.55
1:C:1039:ARG:NE	1:F:1031:GLU:OE2	2.36	0.55
1:C:96:GLU:H	1:C:190:ARG:HH12	1.53	0.55
1:C:120:VAL:HB	1:C:127:VAL:HB	1.89	0.55
1:B:130:VAL:HB	1:B:168:PHE:HB2	1.88	0.55
2:D:161:ARG:NH2	7:D:1008:HOH:O	2.39	0.55
1:F:437:ASN:ND2	1:F:506:GLN:OE1	2.32	0.55
1:B:329:PHE:O	1:B:580:GLN:NE2	2.38	0.55
1:C:1095:PHE:HD1	1:C:1104:VAL:HG12	1.72	0.55
1:F:78:ARG:HD3	1:F:78:ARG:H	1.71	0.55
1:B:666:ILE:HD11	1:B:672:ALA:HB2	1.89	0.55
1:B:763:LEU:HD22	1:B:1008:VAL:HG21	1.88	0.55
1:C:144:TYR:HB3	1:C:150:LYS:HD3	1.89	0.55
1:C:619:GLU:OE2	1:C:620:VAL:HG23	2.07	0.55
2:G:524:GLN:NE2	7:G:1028:HOH:O	2.39	0.55
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.22	0.54
1:B:225:PRO:HD2	1:F:562:PHE:CE2	2.41	0.54
2:D:228:HIS:O	2:D:232:GLU:HG2	2.08	0.54
2:G:26:LYS:NZ	2:G:92:THR:OG1	2.40	0.54
1:C:42:VAL:HG23	1:C:44:ARG:HE	1.71	0.54
1:C:104:TRP:HB2	1:C:119:ILE:HB	1.90	0.54
2:G:123:MET:HE1	2:G:176:LEU:HD13	1.89	0.54
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.90	0.54
1:F:64:TRP:HZ2	1:F:215:ASP:HB3	1.71	0.54
1:F:126:VAL:HG12	1:F:172:SER:H	1.73	0.54
1:B:26:GLN:HA	1:B:64:TRP:O	2.08	0.54
4:B:1312:NAG:H3	4:B:1312:NAG:H83	1.89	0.54
1:C:462:LYS:HE3	1:C:463:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:619:GLU:HB2	1:F:621:PRO:HD2	1.89	0.54
2:G:526:GLN:HE22	2:G:539:LEU:HG	1.72	0.54
1:C:635:VAL:HG23	1:C:636:TYR:H	1.72	0.54
2:D:401:HIS:CE1	2:D:402:GLU:HG2	2.43	0.54
1:F:134:GLN:OE1	1:F:162:SER:OG	2.23	0.54
1:F:411:ALA:HB3	1:F:414:GLN:HG3	1.89	0.54
2:G:208:GLU:OE1	2:G:219:ARG:NH1	2.41	0.54
2:G:245:ARG:NH2	7:G:1029:HOH:O	2.39	0.54
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.88	0.54
1:C:96:GLU:OE1	1:C:101:ILE:N	2.34	0.54
1:F:850:ILE:HG12	1:F:853:GLN:HG2	1.89	0.54
2:G:582:ARG:NH2	7:G:1024:HOH:O	2.36	0.54
1:B:119:ILE:HD12	1:B:128:ILE:HG12	1.89	0.53
1:F:357:ARG:NH1	1:F:359:SER:OG	2.41	0.53
1:F:403:ARG:HD3	1:F:505:HIS:HA	1.90	0.53
1:F:676:THR:HG22	1:F:690:GLN:HE22	1.71	0.53
1:B:173:GLN:HG3	1:B:174:PRO:HD2	1.91	0.53
1:C:402:ILE:HG13	1:C:403:ARG:N	2.19	0.53
2:D:528:ALA:HB2	2:D:574:VAL:HG12	1.91	0.53
1:F:146:HIS:NE2	1:F:148:ASN:HB2	2.24	0.53
2:D:468:ILE:HG22	2:D:473:TRP:HD1	1.74	0.53
1:F:1096:VAL:O	1:F:1103:PHE:N	2.41	0.53
1:C:307:THR:HA	1:C:602:THR:HG21	1.89	0.53
1:C:760:CYS:O	1:C:763:LEU:N	2.42	0.53
1:B:665:PRO:HB3	1:C:864:LEU:HD13	1.90	0.53
1:B:945:LEU:HD23	1:B:948:LEU:HD12	1.91	0.53
1:C:931:ILE:O	1:C:934:ILE:HG22	2.09	0.53
2:D:370:LEU:HA	2:D:373:HIS:CD2	2.44	0.53
2:G:570:LEU:O	2:G:574:VAL:HG22	2.08	0.53
2:G:552:GLN:NE2	2:G:556:ASN:OD1	2.40	0.53
1:F:125:ASN:OD1	1:F:126:VAL:N	2.42	0.53
1:F:613:GLN:HA	1:F:648:GLY:HA3	1.92	0.53
1:B:134:GLN:NE2	1:B:162:SER:OG	2.35	0.52
1:F:398:ASP:HB2	1:F:512:VAL:HG22	1.91	0.52
1:C:1095:PHE:CD1	1:C:1104:VAL:HG12	2.45	0.52
1:F:183:GLN:HG3	1:F:185:ASN:H	1.74	0.52
1:C:296:LEU:HB2	1:C:608:VAL:HG11	1.91	0.52
2:D:50:TYR:HA	2:D:58:ASN:HB3	1.92	0.52
1:F:336:CYS:O	1:F:337:PRO:C	2.53	0.52
1:B:68:ILE:HA	1:B:250:THR:HB	1.92	0.52
1:F:290:ASP:O	1:F:297:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1050:MET:HE2	1:F:1052:PHE:CE1	2.44	0.52
1:B:558:LYS:HE2	4:C:1307:NAG:H61	1.91	0.52
1:C:919:ASN:O	1:C:923:ILE:HG13	2.09	0.52
2:D:37:GLU:OE1	2:D:393:ARG:NH1	2.35	0.52
2:D:152:MET:SD	2:D:269:ASP:HA	2.50	0.52
1:B:894:LEU:HD13	1:F:715:PRO:HD3	1.91	0.52
1:F:661:GLU:O	1:F:695:TYR:OH	2.26	0.52
2:G:238:GLU:HG2	2:G:606:TRP:CZ3	2.45	0.52
2:G:470:LYS:NZ	7:G:1027:HOH:O	2.37	0.52
1:B:131:CYS:HB3	1:B:133:PHE:CE2	2.45	0.52
1:C:502:GLY:O	1:C:506:GLN:N	2.38	0.51
1:C:984:LEU:HB3	1:C:988:GLU:HG3	1.91	0.51
2:D:519:THR:O	2:D:522:GLN:HG2	2.10	0.51
1:F:107:GLY:H	1:F:235:ILE:HG23	1.74	0.51
1:F:442:ASP:OD2	1:F:509:ARG:NH2	2.43	0.51
1:F:1102:TRP:HB2	1:F:1135:ASN:ND2	2.25	0.51
1:B:707:TYR:HE1	1:C:897:PRO:HA	1.75	0.51
1:B:87:ASN:C	1:B:87:ASN:HD22	2.15	0.51
1:C:328:ARG:NH2	1:C:578:ASP:OD1	2.33	0.51
1:C:1104:VAL:HG13	1:C:1115:ILE:HG13	1.93	0.51
1:F:99:ASN:HB2	1:F:102:ARG:HD3	1.91	0.51
1:F:902:MET:HE1	1:F:1050:MET:SD	2.51	0.51
1:B:146:HIS:NE2	1:B:148:ASN:HB2	2.26	0.51
1:B:914:ASN:HA	1:F:1089:PHE:CE2	2.46	0.51
2:G:519:THR:O	2:G:522:GLN:HG2	2.11	0.51
1:B:424:LYS:NZ	1:B:425:LEU:O	2.35	0.51
1:B:567:ARG:NH1	1:B:571:ASP:OD1	2.44	0.51
1:C:318:PHE:CE2	1:C:620:VAL:HG11	2.44	0.51
1:C:327:VAL:HG11	1:C:528:LYS:HE2	1.92	0.51
1:C:501:TYR:HD2	1:C:505:HIS:HB3	1.76	0.51
2:D:415:PRO:O	2:D:419:LYS:HG2	2.11	0.51
1:F:86:PHE:HB2	1:F:238:PHE:HB2	1.93	0.51
2:G:374:HIS:NE2	2:G:402:GLU:OE2	2.39	0.51
1:C:436:TRP:HE1	1:C:509:ARG:HD3	1.74	0.51
1:F:106:PHE:HD2	1:F:117:LEU:HD22	1.75	0.51
1:F:586:ASP:OD1	1:F:587:ILE:N	2.43	0.51
2:D:351:LEU:HB2	2:D:355:ASP:HB3	1.91	0.51
1:F:106:PHE:HB2	1:F:117:LEU:HB3	1.91	0.51
1:F:307:THR:HA	1:F:602:THR:HG21	1.93	0.51
2:G:60:GLN:NE2	2:G:64:ASN:OD1	2.44	0.50
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HG23	1:C:160:TYR:CD1	2.47	0.50
1:F:41:LYS:HG3	1:F:41:LYS:O	2.12	0.50
1:C:69:HIS:CE1	1:C:78:ARG:HB3	2.47	0.50
1:C:569:ILE:HG21	1:F:853:GLN:HG3	1.92	0.50
2:D:269:ASP:OD2	2:D:274:PHE:N	2.39	0.50
1:F:645:THR:HG22	1:F:647:ALA:H	1.76	0.50
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.94	0.50
2:D:120:LEU:HA	2:D:123:MET:SD	2.51	0.50
2:D:269:ASP:OD2	2:D:273:ARG:N	2.45	0.50
1:B:642:VAL:HG22	1:B:651:ILE:HG22	1.93	0.50
1:C:1029:MET:HE2	1:C:1053:PRO:HB3	1.94	0.50
1:C:1083:HIS:CD2	1:C:1136:THR:HA	2.46	0.50
2:G:474:MET:N	2:G:495:GLU:OE1	2.42	0.50
1:B:95:THR:HG22	1:B:189:LEU:HA	1.93	0.50
1:B:659:SER:HB3	1:B:698:SER:HB3	1.94	0.50
1:B:985:ASP:N	1:B:985:ASP:OD1	2.44	0.50
1:C:403:ARG:HG3	1:C:405:ASN:H	1.76	0.50
1:C:96:GLU:N	1:C:190:ARG:HH12	2.10	0.50
1:C:707:TYR:HE1	1:F:897:PRO:HA	1.76	0.50
2:D:453:THR:HA	2:D:512:PHE:HE2	1.76	0.50
2:D:573:VAL:HG23	2:D:574:VAL:HG13	1.93	0.50
1:B:396:TYR:HB2	1:B:514:SER:HB3	1.93	0.50
1:C:48:LEU:HD12	1:C:276:LEU:HD21	1.94	0.50
1:F:335:LEU:HD21	1:F:368:LEU:HB3	1.93	0.50
1:F:986:PRO:N	1:F:987:PRO:HD2	2.26	0.50
1:B:183:GLN:HG3	1:B:185:ASN:H	1.76	0.49
1:C:103:GLY:HA3	1:C:241:LEU:HB3	1.93	0.49
2:D:570:LEU:O	2:D:574:VAL:HG22	2.12	0.49
1:C:878:LEU:O	1:C:882:ILE:HG12	2.12	0.49
1:F:188:ASN:HA	1:F:209:PRO:HA	1.94	0.49
1:B:1107:ARG:HG2	1:C:904:TYR:OH	2.13	0.49
1:C:401:VAL:HG12	1:C:509:ARG:HG2	1.94	0.49
2:G:264:ALA:O	7:G:1003:HOH:O	2.20	0.49
1:C:108:THR:HB	1:C:114:THR:HG21	1.93	0.49
1:C:350:VAL:HB	1:C:402:ILE:HG22	1.93	0.49
1:C:635:VAL:HG23	1:C:636:TYR:CD1	2.47	0.49
1:C:729:VAL:HG13	1:C:781:VAL:HG21	1.94	0.49
1:F:65:PHE:O	1:F:265:TYR:HB3	2.12	0.49
1:C:403:ARG:HG3	1:C:405:ASN:N	2.27	0.49
1:C:130:VAL:HG21	1:C:231:ILE:HG21	1.94	0.49
1:F:93:ALA:HB3	1:F:266:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:471:ASP:OD1	2:G:471:ASP:N	2.45	0.49
1:B:168:PHE:HD1	1:F:357:ARG:CZ	2.26	0.49
1:B:533:LEU:HD11	1:B:585:LEU:HD11	1.93	0.49
2:G:266:LEU:O	2:G:266:LEU:HD23	2.13	0.49
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.30	0.49
2:D:452:PHE:HZ	2:D:503:LEU:HD21	1.78	0.49
1:F:403:ARG:HH11	1:F:405:ASN:HD21	1.61	0.49
1:C:565:PHE:HB2	1:F:42:VAL:HG12	1.94	0.49
1:F:328:ARG:NH1	1:F:533:LEU:HB2	2.28	0.49
1:C:86:PHE:HB2	1:C:238:PHE:HB2	1.96	0.48
1:C:403:ARG:HD2	1:C:405:ASN:HB3	1.94	0.48
1:F:386:LYS:HE3	1:F:390:LEU:HD21	1.95	0.48
1:B:101:ILE:HD11	1:B:240:THR:OG1	2.13	0.48
1:B:128:ILE:HD11	1:B:175:PHE:HZ	1.78	0.48
1:B:290:ASP:OD1	1:B:291:CYS:N	2.46	0.48
1:B:349:SER:HB2	1:B:351:TYR:CD1	2.48	0.48
2:D:481:LYS:HD3	2:D:485:VAL:HB	1.96	0.48
2:G:198:ASP:HB2	2:G:464:PHE:HB3	1.95	0.48
1:B:563:GLN:OE1	1:C:41:LYS:HG3	2.14	0.48
1:C:393:THR:HB	1:C:516:GLU:HB2	1.95	0.48
1:B:106:PHE:HB2	1:B:117:LEU:HD23	1.94	0.48
1:B:200:TYR:O	1:B:202:LYS:HD2	2.13	0.48
1:B:1094:VAL:O	1:B:1104:VAL:HA	2.12	0.48
1:F:109:THR:OG1	1:F:111:ASP:OD1	2.31	0.48
1:F:421:TYR:CD1	1:F:457:ARG:HB3	2.49	0.48
1:F:905:ARG:HD2	1:F:1049:LEU:O	2.13	0.48
2:G:55:THR:O	2:G:59:VAL:HG23	2.14	0.48
2:D:54:ILE:HB	2:D:341:LYS:HB2	1.95	0.48
1:B:138:ASP:HB3	1:B:158:ARG:HD2	1.95	0.48
1:B:433:VAL:HG12	1:B:512:VAL:HA	1.95	0.48
1:F:126:VAL:HG22	1:F:128:ILE:HG13	1.95	0.48
1:F:237:ARG:HH11	1:F:237:ARG:HG3	1.79	0.48
1:C:126:VAL:HG22	1:C:128:ILE:HG13	1.96	0.48
2:D:152:MET:SD	2:D:277:ASN:ND2	2.86	0.48
1:B:699:LEU:HB3	1:C:873:TYR:CE1	2.47	0.48
2:D:165:TRP:HA	2:D:270:MET:HE2	1.95	0.48
1:F:922:LEU:HG	1:F:926:GLN:HE21	1.78	0.48
1:B:1082:CYS:HB2	1:B:1126:CYS:HB2	1.71	0.48
2:D:248:LEU:O	2:D:252:TYR:N	2.40	0.48
2:G:46:ALA:HA	2:G:49:ASN:ND2	2.29	0.48
1:B:348:ALA:O	1:B:400:PHE:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ARG:HG2	1:C:406:GLU:HG2	1.95	0.48
1:B:784:GLN:OE1	1:B:1030:SER:OG	2.32	0.47
1:B:1089:PHE:HE2	1:C:917:TYR:HD2	1.61	0.47
1:B:1135:ASN:CG	1:B:1136:THR:H	2.20	0.47
1:F:89:GLY:HA3	1:F:270:LEU:HD12	1.96	0.47
1:F:474:GLN:NE2	1:F:478:LYS:O	2.47	0.47
2:G:442:GLN:O	2:G:446:ILE:N	2.29	0.47
1:B:280:ASN:OD1	1:B:281:GLU:N	2.46	0.47
1:B:1104:VAL:HG11	1:B:1119:ASN:HD22	1.79	0.47
1:B:159:VAL:HG13	1:B:160:TYR:CD1	2.49	0.47
1:B:1010:GLN:OE1	1:B:1014:ARG:NH2	2.47	0.47
1:B:1027:THR:O	1:B:1031:GLU:HG3	2.15	0.47
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.94	0.47
1:C:295:PRO:HG3	1:C:633:TRP:CZ3	2.49	0.47
1:C:555:SER:OG	1:C:586:ASP:N	2.46	0.47
2:D:96:GLN:HG2	2:D:391:LEU:HB2	1.95	0.47
1:F:462:LYS:N	1:F:465:GLU:OE1	2.43	0.47
1:F:560:LEU:HB2	1:F:563:GLN:NE2	2.25	0.47
1:F:985:ASP:OD1	1:F:985:ASP:N	2.44	0.47
1:B:78:ARG:HG2	1:B:80:ASP:H	1.79	0.47
1:B:717:ASN:ND2	3:A:1:NAG:O5	2.47	0.47
1:C:318:PHE:HZ	1:C:615:VAL:HG11	1.80	0.47
1:C:1092:GLU:OE2	1:C:1107:ARG:NH1	2.47	0.47
1:F:770:ILE:HD11	1:F:1012:LEU:HD23	1.95	0.47
1:B:42:VAL:HG12	1:F:565:PHE:HB2	1.97	0.47
1:C:666:ILE:HD11	1:C:672:ALA:HB2	1.97	0.47
1:C:755:GLN:C	1:C:757:GLY:N	2.63	0.47
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.44	0.47
1:F:332:ILE:HG22	1:F:333:THR:N	2.30	0.47
1:B:46:SER:OG	1:B:281:GLU:OE1	2.30	0.47
1:C:905:ARG:HD2	1:C:1049:LEU:O	2.15	0.47
2:D:176:LEU:HB3	2:D:180:TYR:CD2	2.50	0.47
2:D:187:LYS:HA	2:D:190:MET:HE3	1.95	0.47
1:F:420:ASP:OD1	4:F:1307:NAG:O3	2.26	0.47
1:F:569:ILE:O	1:F:569:ILE:HG13	2.14	0.47
1:F:906:PHE:CD2	1:F:916:LEU:HB2	2.50	0.47
1:C:211:ASN:OD1	1:C:217:PRO:HG3	2.15	0.47
1:C:290:ASP:OD1	1:C:291:CYS:N	2.47	0.47
1:C:350:VAL:HG21	1:C:418:ILE:HD11	1.96	0.47
1:C:506:GLN:HE21	1:C:508:TYR:HE1	1.63	0.47
1:C:676:THR:OG1	1:C:689:SER:O	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:501:ALA:HA	2:D:506:VAL:HG11	1.97	0.47
1:F:40:ASP:OD1	1:F:40:ASP:N	2.46	0.47
1:F:118:LEU:HD22	1:F:133:PHE:CE2	2.49	0.47
1:F:318:PHE:HZ	1:F:615:VAL:HG11	1.80	0.47
1:F:332:ILE:HG22	1:F:333:THR:H	1.79	0.47
1:F:421:TYR:HD1	1:F:457:ARG:HB3	1.79	0.47
1:F:722:VAL:HG22	1:F:1065:VAL:HG22	1.97	0.47
2:G:455:MET:HE1	2:G:477:TRP:CH2	2.50	0.47
1:B:605:SER:OG	1:B:606:ASN:N	2.48	0.47
2:D:360:MET:HE3	2:D:362:THR:HA	1.96	0.47
2:G:209:VAL:HG11	2:G:565:PRO:HB3	1.97	0.47
2:G:366:MET:HE1	2:G:418:LEU:HD11	1.96	0.47
2:G:431:ASP:OD1	2:G:431:ASP:N	2.47	0.47
1:B:276:LEU:HD11	1:B:301:CYS:HA	1.97	0.47
1:C:619:GLU:CD	1:C:620:VAL:HG23	2.39	0.47
2:G:539:LEU:HD23	2:G:587:TYR:HD2	1.80	0.47
1:B:565:PHE:HB2	1:C:42:VAL:HG12	1.97	0.47
1:B:717:ASN:HD21	3:A:1:NAG:H61	1.80	0.47
1:C:439:ASN:ND2	1:C:506:GLN:OE1	2.48	0.47
1:C:468:ILE:O	1:C:468:ILE:HG13	2.15	0.47
1:C:562:PHE:CZ	1:F:41:LYS:HE3	2.50	0.47
2:D:580:ASN:O	7:D:1001:HOH:O	2.21	0.47
1:F:433:VAL:HG12	1:F:512:VAL:HA	1.97	0.47
1:B:541:PHE:HB2	1:B:543:PHE:CE1	2.50	0.46
1:B:819:GLU:OE1	1:B:1055:SER:OG	2.31	0.46
1:F:715:PRO:HA	1:F:1072:GLU:HA	1.96	0.46
1:B:720:ILE:HG13	1:B:923:ILE:HG23	1.97	0.46
2:D:381:TYR:CD1	2:D:558:LEU:HG	2.44	0.46
2:D:389:PRO:O	2:D:393:ARG:HG3	2.14	0.46
1:F:906:PHE:HE1	1:F:1049:LEU:HD11	1.80	0.46
2:G:375:GLU:O	2:G:379:ILE:HG12	2.16	0.46
1:B:331:ASN:O	1:B:334:ASN:ND2	2.49	0.46
1:C:44:ARG:HH11	1:C:49:HIS:HB2	1.80	0.46
1:C:69:HIS:CD2	1:C:78:ARG:HB3	2.50	0.46
2:G:177:ARG:HE	2:G:181:GLU:HG3	1.80	0.46
1:B:560:LEU:HB2	1:B:561:PRO:HD2	1.98	0.46
1:B:1046:GLY:HA2	1:C:890:ALA:HA	1.98	0.46
1:C:83:VAL:HB	1:C:237:ARG:NH1	2.31	0.46
2:D:19:SER:OG	2:D:20:THR:N	2.47	0.46
2:G:493:HIS:ND1	2:G:499:ASP:OD2	2.43	0.46
1:B:787:GLN:OE1	1:F:703:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ILE:HG12	1:C:242:LEU:HD13	1.98	0.46
1:C:196:ASN:ND2	1:C:201:PHE:CD1	2.81	0.46
2:G:248:LEU:HD12	2:G:266:LEU:HD21	1.97	0.46
1:B:906:PHE:CD2	1:B:916:LEU:HB2	2.50	0.46
2:D:276:THR:N	7:D:1024:HOH:O	2.47	0.46
1:F:69:HIS:CG	1:F:78:ARG:HB3	2.51	0.46
1:F:451:TYR:O	1:F:495:TYR:HB3	2.15	0.46
2:G:382:ASP:OD1	2:G:385:TYR:OH	2.25	0.46
1:C:396:TYR:HB2	1:C:514:SER:OG	2.16	0.46
1:C:941:THR:HG21	1:C:944:ALA:HB2	1.97	0.46
2:D:43:SER:HA	2:D:65:ALA:HB1	1.96	0.46
1:F:424:LYS:NZ	1:F:425:LEU:O	2.30	0.46
2:G:459:TRP:HE3	2:G:460:ARG:HD2	1.80	0.46
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.50	0.46
2:D:374:HIS:CD2	2:D:374:HIS:C	2.93	0.46
1:F:403:ARG:HG3	1:F:497:PHE:CZ	2.51	0.46
1:B:1045:LYS:O	1:B:1066:THR:HG21	2.15	0.46
2:D:446:ILE:O	2:D:449:THR:HG22	2.16	0.46
1:F:97:LYS:HG3	1:F:98:SER:H	1.79	0.46
2:G:524:GLN:NE2	7:G:1024:HOH:O	2.49	0.46
1:B:570:ALA:HB1	1:C:963:VAL:HG11	1.97	0.46
1:C:402:ILE:HD12	1:C:406:GLU:CB	2.46	0.46
1:C:537:LYS:HB2	1:C:537:LYS:HE3	1.74	0.46
2:D:170:SER:HA	2:D:497:TYR:CD2	2.51	0.46
2:G:230:PHE:HA	2:G:233:ILE:HG22	1.98	0.46
2:G:375:GLU:HA	2:G:378:HIS:CD2	2.51	0.46
1:B:93:ALA:HB3	1:B:266:TYR:HB2	1.97	0.45
1:B:233:ILE:HG23	1:B:235:ILE:HG13	1.99	0.45
1:B:454:ARG:HH11	1:B:457:ARG:HA	1.82	0.45
1:B:823:PHE:CD2	1:B:1057:PRO:HG3	2.51	0.45
1:B:902:MET:HE1	1:B:1049:LEU:HD13	1.97	0.45
2:D:294:THR:HG23	2:D:364:VAL:O	2.17	0.45
2:D:555:PHE:HA	2:D:558:LEU:HB2	1.98	0.45
1:F:106:PHE:CD2	1:F:117:LEU:HD22	2.52	0.45
1:F:612:TYR:CD2	1:F:621:PRO:HB3	2.50	0.45
1:F:903:ALA:HB1	1:F:913:GLN:HG2	1.99	0.45
2:G:271:TRP:NE1	2:G:503:LEU:HD13	2.32	0.45
1:B:118:LEU:HG	1:B:120:VAL:HG23	1.98	0.45
1:B:1083:HIS:CG	1:B:1137:VAL:HG22	2.52	0.45
1:C:1087:ALA:O	1:C:1088:HIS:ND1	2.49	0.45
1:F:101:ILE:HD11	1:F:240:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.98	0.45
1:C:621:PRO:HA	1:C:624:ILE:HD12	1.97	0.45
2:D:37:GLU:HG3	2:D:353:LYS:HE3	1.98	0.45
2:D:378:HIS:CD2	2:D:401:HIS:HB2	2.52	0.45
1:F:612:TYR:O	1:F:649:CYS:N	2.40	0.45
1:B:432:CYS:H	1:B:513:LEU:HB2	1.81	0.45
1:C:93:ALA:HA	1:C:190:ARG:O	2.15	0.45
1:F:69:HIS:CE1	1:F:141:LEU:HD13	2.52	0.45
2:G:53:ASN:O	2:G:58:ASN:ND2	2.43	0.45
2:G:396:ALA:HB3	2:G:400:PHE:CE1	2.51	0.45
1:B:41:LYS:NZ	1:F:563:GLN:HE22	2.15	0.45
1:B:86:PHE:HB2	1:B:238:PHE:HB2	1.98	0.45
1:B:564:GLN:HG3	1:C:41:LYS:HB3	1.98	0.45
1:C:69:HIS:CG	1:C:78:ARG:HB3	2.52	0.45
2:D:201:ASP:HA	2:D:204:ARG:HG2	1.99	0.45
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.85	0.45
1:C:1100:THR:HG23	1:C:1101:HIS:ND1	2.31	0.45
1:F:379:CYS:CB	1:F:432:CYS:HA	2.46	0.45
2:G:145:GLU:HA	2:G:146:PRO:HA	1.80	0.45
2:G:196:TYR:CD2	2:G:202:TYR:HA	2.52	0.45
1:B:560:LEU:N	1:B:563:GLN:HE21	2.14	0.45
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.99	0.45
1:C:318:PHE:HB2	1:C:629:LEU:HD12	1.99	0.45
1:C:404:GLY:O	1:C:407:VAL:HG12	2.17	0.45
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.99	0.45
2:G:198:ASP:OD1	2:G:201:ASP:HB2	2.17	0.45
1:B:1067:TYR:O	1:B:1067:TYR:CD1	2.69	0.45
1:C:295:PRO:HG2	1:C:636:TYR:HE1	1.81	0.45
1:C:401:VAL:CG1	1:C:509:ARG:HG2	2.47	0.45
1:F:212:LEU:HD23	1:F:212:LEU:H	1.82	0.45
2:G:355:ASP:OD2	2:G:357:ARG:NH2	2.50	0.45
2:G:580:ASN:OD1	2:G:581:VAL:N	2.50	0.45
1:B:662:CYS:HB2	1:B:671:CYS:HB3	1.70	0.44
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.99	0.44
1:C:392:PHE:HB2	1:C:524:VAL:HG13	1.98	0.44
1:C:671:CYS:SG	1:C:697:MET:HB3	2.57	0.44
2:D:187:LYS:NZ	7:D:1023:HOH:O	2.44	0.44
2:D:396:ALA:HB3	2:D:400:PHE:CE2	2.52	0.44
1:F:540:ASN:HA	1:F:549:THR:HA	1.97	0.44
1:F:951:VAL:O	1:F:955:ASN:ND2	2.42	0.44
2:G:364:VAL:O	2:G:364:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PHE:CZ	1:B:137:ASN:HB2	2.53	0.44
1:F:321:GLN:OE1	1:F:322:PRO:HD2	2.17	0.44
1:B:83:VAL:HA	1:B:237:ARG:NH2	2.30	0.44
1:B:373:PRO:HD2	1:B:436:TRP:CD1	2.52	0.44
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.80	0.44
1:B:791:THR:HG21	1:B:806:LEU:HD22	1.99	0.44
1:B:1095:PHE:HE1	1:B:1115:ILE:HD12	1.83	0.44
1:C:69:HIS:O	1:C:247:SER:OG	2.26	0.44
2:G:150:GLU:HG2	2:G:154:ASN:ND2	2.32	0.44
2:G:461:TRP:O	2:G:465:LYS:HG3	2.17	0.44
1:C:196:ASN:ND2	1:C:201:PHE:CE1	2.85	0.44
1:C:369:TYR:HA	1:C:374:PHE:CE2	2.53	0.44
2:D:57:GLU:O	2:D:61:ASN:ND2	2.33	0.44
2:D:462:MET:HA	2:D:462:MET:HE2	1.98	0.44
2:G:478:TRP:CE2	2:G:489:GLU:HB3	2.52	0.44
1:C:289:VAL:HG23	1:C:306:PHE:CZ	2.53	0.44
1:C:331:ASN:HB3	4:C:1308:NAG:H3	2.00	0.44
1:C:1140:PRO:O	1:C:1143:PRO:HD3	2.17	0.44
1:F:310:LYS:HG3	1:F:600:PRO:HA	1.98	0.44
1:F:424:LYS:HG3	1:F:463:PRO:HA	1.99	0.44
1:F:611:LEU:HD21	1:F:666:ILE:HG23	2.00	0.44
1:F:659:SER:HB3	1:F:698:SER:HB2	1.99	0.44
2:G:247:LYS:HG3	2:G:248:LEU:HD22	1.99	0.44
2:G:303:ASP:O	2:G:307:ILE:HG13	2.17	0.44
2:G:460:ARG:HH21	2:G:506:VAL:HG11	1.81	0.44
1:B:78:ARG:HH11	1:B:79:PHE:H	1.64	0.44
1:B:86:PHE:CZ	1:B:89:GLY:HA2	2.53	0.44
1:B:206:LYS:HD2	1:B:222:ALA:O	2.17	0.44
1:B:240:THR:HG21	1:B:265:TYR:HE2	1.82	0.44
1:B:558:LYS:HD2	1:B:558:LYS:HA	1.76	0.44
1:C:96:GLU:HB3	1:C:100:ILE:HB	1.99	0.44
1:C:759:PHE:CD1	1:C:1001:LEU:HD21	2.52	0.44
1:F:1075:PHE:HB3	1:F:1096:VAL:HG13	1.99	0.44
2:G:483:GLU:O	2:G:606:TRP:NE1	2.31	0.44
1:C:78:ARG:HH11	1:C:79:PHE:H	1.64	0.44
1:C:142:ASP:OD2	1:C:150:LYS:NZ	2.50	0.44
1:F:344:ALA:HB3	1:F:347:PHE:CE1	2.52	0.44
1:F:1139:ASP:OD1	1:F:1139:ASP:N	2.42	0.44
2:G:151:ILE:HG13	7:G:1002:HOH:O	2.18	0.44
2:G:460:ARG:HH12	2:G:500:PRO:HB3	1.81	0.44
1:C:41:LYS:HD2	1:C:41:LYS:HA	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:LEU:HD23	1:F:176:LEU:H	1.82	0.44
1:F:327:VAL:HG13	1:F:542:ASN:HB3	1.99	0.44
2:G:84:PRO:HB2	2:G:86:GLN:HG3	2.00	0.44
2:G:489:GLU:HG2	2:G:613:TYR:HE2	1.82	0.44
1:B:985:ASP:C	1:B:987:PRO:HD2	2.42	0.43
1:C:27:SER:HB2	1:C:259:THR:O	2.18	0.43
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.82	0.43
1:F:365:TYR:HD2	1:F:368:LEU:HD21	1.82	0.43
1:F:396:TYR:HD2	1:F:514:SER:HB3	1.83	0.43
2:G:372:ALA:HA	2:G:375:GLU:HG2	2.00	0.43
1:B:422:ASN:ND2	1:B:453:TYR:HB2	2.32	0.43
1:B:567:ARG:HA	1:B:567:ARG:HD3	1.77	0.43
1:B:931:ILE:O	1:B:934:ILE:HG22	2.19	0.43
1:C:127:VAL:HG12	1:C:127:VAL:O	2.18	0.43
1:C:394:ASN:OD1	1:C:395:VAL:N	2.51	0.43
2:D:22:GLU:HG2	2:D:88:ILE:HD11	1.99	0.43
2:D:72:PHE:O	2:D:76:GLN:HG2	2.17	0.43
2:D:170:SER:HA	2:D:497:TYR:HD2	1.83	0.43
1:F:159:VAL:HG13	1:F:160:TYR:CD2	2.53	0.43
1:F:403:ARG:HD2	1:F:405:ASN:OD1	2.18	0.43
2:G:460:ARG:NH1	2:G:500:PRO:HB3	2.33	0.43
1:C:122:ASN:OD1	1:C:123:ALA:N	2.45	0.43
1:C:984:LEU:HB2	1:C:989:ALA:HB2	2.01	0.43
1:F:878:LEU:HD11	1:F:1054:GLN:HE22	1.82	0.43
1:B:718:PHE:HA	1:B:1069:PRO:HA	2.00	0.43
1:B:1102:TRP:HB2	1:B:1135:ASN:HD21	1.83	0.43
1:C:486:PHE:HE1	1:F:377:PHE:HB2	1.82	0.43
2:D:237:TYR:CD1	2:D:451:PRO:HG2	2.52	0.43
2:D:463:VAL:HG23	2:D:468:ILE:HD12	2.00	0.43
1:F:773:GLU:OE2	1:F:1019:ARG:NE	2.51	0.43
1:F:865:LEU:HD22	1:F:869:MET:HE2	2.00	0.43
2:G:240:LEU:HD22	2:G:443:ALA:HB1	2.01	0.43
2:G:515:TYR:HD1	2:G:518:ARG:HH21	1.65	0.43
2:G:529:LEU:O	2:G:533:ALA:N	2.52	0.43
1:C:976:VAL:HG12	1:C:979:ASP:H	1.84	0.43
2:G:400:PHE:CZ	2:G:566:TRP:HB2	2.54	0.43
2:G:554:LEU:O	2:G:558:LEU:HG	2.18	0.43
1:B:200:TYR:OH	1:F:522:ALA:O	2.31	0.43
1:B:451:TYR:O	1:B:495:TYR:HB3	2.18	0.43
1:B:43:PHE:HB3	1:F:566:GLY:HA2	2.01	0.43
1:B:357:ARG:NH2	1:C:169:GLU:H	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:PRO:HD3	1:C:425:LEU:HD23	2.00	0.43
1:C:424:LYS:HZ1	1:C:463:PRO:HD3	1.82	0.43
2:D:177:ARG:NH1	2:D:495:GLU:O	2.52	0.43
1:F:175:PHE:CE2	1:F:203:ILE:HG21	2.54	0.43
1:B:437:ASN:HA	1:B:508:TYR:CD1	2.53	0.43
1:B:453:TYR:HE2	1:B:455:LEU:HD13	1.84	0.43
1:B:1096:VAL:N	1:B:1103:PHE:O	2.52	0.43
1:C:25:THR:N	1:C:66:HIS:HB3	2.33	0.43
2:D:45:LEU:HD12	2:D:45:LEU:HA	1.89	0.43
1:F:78:ARG:HH11	1:F:79:PHE:H	1.66	0.43
1:F:432:CYS:H	1:F:513:LEU:HB2	1.84	0.43
1:F:546:LEU:HD11	1:F:573:THR:HG21	2.00	0.43
2:G:50:TYR:CE1	2:G:59:VAL:HG22	2.54	0.43
2:G:59:VAL:O	2:G:62:MET:HG3	2.18	0.43
2:G:198:ASP:OD2	2:G:465:LYS:HG2	2.18	0.43
2:G:228:HIS:O	2:G:232:GLU:HG3	2.19	0.43
1:B:41:LYS:HD2	1:B:41:LYS:HA	1.59	0.43
1:B:277:LEU:HD22	1:B:285:ILE:HD13	2.01	0.43
1:C:53:ASP:HB2	1:C:55:PHE:CE1	2.54	0.43
1:C:104:TRP:HB3	1:C:106:PHE:HE1	1.84	0.43
1:C:402:ILE:O	1:C:403:ARG:HB3	2.18	0.43
1:C:821:LEU:HD13	1:C:935:GLN:HG3	2.01	0.43
1:C:977:LEU:HD23	1:C:977:LEU:HA	1.84	0.43
2:D:257:SER:HB2	2:D:610:TRP:CE2	2.54	0.43
1:F:69:HIS:ND1	1:F:78:ARG:HB3	2.33	0.43
1:F:763:LEU:HD11	1:F:1004:LEU:HG	2.01	0.43
1:F:989:ALA:O	1:F:993:ILE:HG12	2.19	0.43
1:B:905:ARG:HD3	1:B:1049:LEU:O	2.19	0.43
1:C:26:GLN:NE2	1:C:63:THR:HB	2.30	0.43
1:C:568:ASP:OD1	1:C:569:ILE:N	2.50	0.43
2:D:105:SER:OG	2:D:116:LEU:HD11	2.19	0.43
2:D:371:THR:O	2:D:375:GLU:HG2	2.18	0.43
2:G:523:PHE:HB3	2:G:583:PRO:HB2	2.01	0.43
1:B:763:LEU:HD23	1:B:763:LEU:HA	1.89	0.42
1:F:69:HIS:CE1	1:F:78:ARG:HB3	2.54	0.42
1:F:458:LYS:HB2	1:F:458:LYS:HE2	1.81	0.42
1:F:931:ILE:O	1:F:934:ILE:HG22	2.19	0.42
1:F:1086:LYS:HE2	1:F:1122:VAL:HG21	1.99	0.42
2:G:398:GLU:O	7:G:1004:HOH:O	2.21	0.42
1:B:179:LEU:HG	1:B:188:ASN:HD22	1.83	0.42
1:B:310:LYS:HE3	1:B:310:LYS:HB3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASN:OD1	1:B:317:ASN:N	2.52	0.42
2:D:176:LEU:HD13	2:D:180:TYR:HE2	1.82	0.42
2:D:459:TRP:NE1	2:D:477:TRP:HB2	2.34	0.42
1:F:423:TYR:HE1	1:F:425:LEU:HG	1.84	0.42
1:B:66:HIS:ND1	1:B:263:ALA:O	2.53	0.42
1:C:40:ASP:N	1:C:40:ASP:OD1	2.50	0.42
1:C:83:VAL:HA	1:C:237:ARG:HH22	1.85	0.42
1:C:406:GLU:OE1	1:C:409:GLN:NE2	2.52	0.42
1:C:1073:LYS:HB3	1:C:1073:LYS:HE2	1.78	0.42
1:C:1106:GLN:NE2	1:C:1109:PHE:HB3	2.33	0.42
2:D:165:TRP:HZ3	2:D:491:VAL:HB	1.83	0.42
2:D:323:MET:HE3	2:D:323:MET:HA	2.02	0.42
2:D:587:TYR:O	7:D:1002:HOH:O	2.22	0.42
1:F:65:PHE:O	1:F:263:ALA:HB1	2.19	0.42
1:F:89:GLY:HA2	1:F:194:PHE:O	2.19	0.42
1:F:101:ILE:HD12	1:F:241:LEU:O	2.19	0.42
1:F:541:PHE:CZ	1:F:587:ILE:HD13	2.54	0.42
1:F:767:LEU:HD23	1:F:767:LEU:HA	1.87	0.42
1:F:878:LEU:HD11	1:F:1054:GLN:NE2	2.35	0.42
2:G:113:SER:O	2:G:116:LEU:HG	2.19	0.42
2:G:204:ARG:HH21	2:G:461:TRP:CG	2.37	0.42
2:G:376:MET:HE3	2:G:376:MET:HB2	1.77	0.42
1:B:117:LEU:HD21	1:B:119:ILE:HD11	2.01	0.42
2:G:245:ARG:O	2:G:249:MET:HG3	2.18	0.42
1:B:358:ILE:HG23	1:B:361:CYS:HB3	2.02	0.42
1:C:339:HIS:HB3	1:C:371:PHE:CZ	2.54	0.42
1:C:359:SER:OG	1:C:360:ASN:N	2.53	0.42
1:C:501:TYR:CD2	1:C:505:HIS:HB3	2.54	0.42
2:D:450:LEU:HB2	2:D:451:PRO:HD3	2.01	0.42
2:D:461:TRP:HZ2	2:D:513:ILE:HG21	1.85	0.42
2:D:535:HIS:NE2	2:D:538:PRO:O	2.47	0.42
1:F:195:LYS:HE2	1:F:204:TYR:HE2	1.85	0.42
1:F:202:LYS:C	1:F:203:ILE:HD13	2.44	0.42
1:F:335:LEU:CG	1:F:338:PHE:HB2	2.35	0.42
1:F:821:LEU:HD11	1:F:935:GLN:HG3	2.01	0.42
1:B:823:PHE:HD2	1:B:1057:PRO:HG3	1.84	0.42
1:C:362:VAL:HG13	1:C:362:VAL:O	2.19	0.42
2:D:236:LEU:HB2	2:D:592:PHE:CZ	2.54	0.42
2:D:382:ASP:HA	2:D:385:TYR:CZ	2.55	0.42
1:F:48:LEU:HD12	1:F:276:LEU:HD21	2.02	0.42
1:F:334:ASN:HB3	1:F:339:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:LEU:O	1:F:336:CYS:O	2.36	0.42
1:F:364:ASP:OD1	1:F:364:ASP:N	2.52	0.42
2:G:440:LEU:O	2:G:444:LEU:HG	2.20	0.42
1:C:586:ASP:OD1	1:C:587:ILE:N	2.53	0.42
2:D:184:VAL:HG22	2:D:464:PHE:CE1	2.51	0.42
1:B:112:SER:HB3	1:B:134:GLN:HB3	2.02	0.42
1:B:176:LEU:H	1:B:176:LEU:HD23	1.85	0.42
1:C:53:ASP:HB2	1:C:55:PHE:HE1	1.84	0.42
1:F:346:ARG:HD2	1:F:346:ARG:HA	1.95	0.42
1:F:798:GLY:HA3	1:F:899:PRO:HG3	2.02	0.42
2:G:204:ARG:CZ	2:G:223:ILE:HD11	2.49	0.42
1:B:220:PHE:HD1	1:B:287:ASP:HA	1.84	0.42
1:C:365:TYR:HD2	1:C:387:LEU:HD13	1.84	0.42
1:C:1097:SER:OG	1:C:1101:HIS:O	2.32	0.42
1:F:914:ASN:C	1:F:914:ASN:HD22	2.27	0.42
1:F:1093:GLY:H	1:F:1107:ARG:NH1	2.18	0.42
2:G:460:ARG:NH2	2:G:506:VAL:HG21	2.34	0.42
1:C:131:CYS:HB3	1:C:133:PHE:CE2	2.54	0.42
1:C:383:SER:HB2	1:F:985:ASP:H	1.84	0.42
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.55	0.41
1:C:142:ASP:HB2	1:C:245:HIS:CD2	2.55	0.41
1:C:231:ILE:HG13	1:C:232:GLY:H	1.85	0.41
1:C:310:LYS:HG3	1:C:600:PRO:HA	2.02	0.41
1:C:563:GLN:HG3	1:F:41:LYS:HG3	2.02	0.41
1:C:598:ILE:HB	1:C:609:ALA:HB3	2.02	0.41
1:C:661:GLU:N	1:C:661:GLU:OE2	2.53	0.41
1:F:90:VAL:HG12	1:F:194:PHE:HB2	2.02	0.41
1:F:131:CYS:HB3	1:F:133:PHE:CE2	2.55	0.41
1:F:454:ARG:NH2	1:F:469:SER:H	2.18	0.41
2:G:346:PRO:HG3	2:G:360:MET:SD	2.60	0.41
1:B:426:PRO:HG2	1:B:429:PHE:HB2	2.02	0.41
1:B:971:GLY:O	1:B:995:ARG:NH1	2.42	0.41
1:B:987:PRO:HD3	1:C:413:GLY:HA3	2.02	0.41
2:D:346:PRO:HA	2:D:359:LEU:O	2.20	0.41
2:D:374:HIS:O	2:D:378:HIS:HB2	2.20	0.41
1:F:338:PHE:HB3	1:F:342:PHE:CE2	2.55	0.41
1:F:338:PHE:CE1	1:F:358:ILE:HD13	2.48	0.41
2:G:165:TRP:HZ3	2:G:491:VAL:HB	1.84	0.41
2:G:475:LYS:N	2:G:495:GLU:OE2	2.53	0.41
1:B:454:ARG:NH2	1:B:469:SER:O	2.53	0.41
1:B:758:SER:HB2	1:B:761:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:THR:HG22	2:D:31:LYS:HE2	2.01	0.41
2:D:404:VAL:O	2:D:408:MET:HG2	2.20	0.41
1:F:202:LYS:HB3	1:F:204:TYR:CE2	2.54	0.41
1:F:336:CYS:HB2	1:F:362:VAL:O	2.20	0.41
1:F:456:PHE:HD2	1:F:491:PRO:HA	1.86	0.41
1:F:728:PRO:HB3	1:F:951:VAL:HG21	2.00	0.41
2:G:227:GLU:O	2:G:231:GLU:HG2	2.20	0.41
2:G:347:THR:OG1	2:G:359:LEU:HB3	2.20	0.41
1:B:332:ILE:HG23	1:B:333:THR:N	2.35	0.41
1:C:537:LYS:C	1:C:551:VAL:HG12	2.46	0.41
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.86	0.41
2:D:460:ARG:HH22	2:D:512:PHE:HB2	1.85	0.41
2:D:474:MET:HA	2:D:477:TRP:HB3	2.02	0.41
2:G:39:LEU:HD23	2:G:39:LEU:HA	1.81	0.41
1:B:104:TRP:HB3	1:B:106:PHE:CE2	2.49	0.41
1:B:253:ASP:OD2	1:B:255:SER:OG	2.30	0.41
1:C:202:LYS:O	1:C:203:ILE:HD13	2.21	0.41
1:C:368:LEU:H	1:C:368:LEU:HD23	1.85	0.41
1:C:457:ARG:HH22	1:C:461:LEU:HA	1.85	0.41
2:D:381:TYR:OH	7:D:1003:HOH:O	2.22	0.41
2:D:398:GLU:OE1	7:D:1004:HOH:O	2.22	0.41
2:D:557:MET:HG2	2:D:569:ALA:HB1	2.03	0.41
1:F:501:TYR:OH	2:G:353:LYS:NZ	2.43	0.41
1:F:605:SER:OG	1:F:606:ASN:N	2.52	0.41
1:F:945:LEU:HD22	1:F:948:LEU:HD12	2.03	0.41
1:C:592:PHE:HZ	1:F:855:PHE:O	2.02	0.41
1:C:902:MET:HE1	1:C:1049:LEU:HD13	2.01	0.41
2:D:366:MET:HA	2:D:366:MET:HE2	2.01	0.41
1:F:108:THR:O	1:F:109:THR:OG1	2.35	0.41
2:G:459:TRP:CD1	2:G:477:TRP:HE3	2.38	0.41
2:G:557:MET:HE2	2:G:573:VAL:HG11	2.02	0.41
1:C:282:ASN:C	1:C:282:ASN:HD22	2.26	0.41
1:F:595:VAL:HG12	1:F:612:TYR:CE1	2.56	0.41
1:F:906:PHE:HB3	1:F:911:VAL:HG13	2.03	0.41
2:G:32:PHE:HB2	2:G:76:GLN:OE1	2.19	0.41
2:G:92:THR:O	2:G:96:GLN:HG2	2.20	0.41
1:B:415:THR:C	4:B:1309:NAG:H4	2.45	0.41
1:C:422:ASN:ND2	1:C:453:TYR:HB2	2.35	0.41
1:C:452:LEU:HB2	1:C:492:LEU:HD12	2.03	0.41
1:F:703:ASN:OD1	1:F:704:SER:N	2.53	0.41
1:F:867:ASP:OD1	1:F:867:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLN:NE2	1:B:418:ILE:H	2.18	0.41
1:B:1088:HIS:CE1	1:B:1122:VAL:HG12	2.56	0.41
1:C:146:HIS:CD2	1:C:148:ASN:HB2	2.56	0.41
1:C:183:GLN:NE2	1:C:185:ASN:HB3	2.36	0.41
1:C:390:LEU:HD21	1:F:983:ARG:HG3	2.02	0.41
1:C:555:SER:HB2	1:C:584:ILE:HG13	2.03	0.41
1:C:620:VAL:O	1:C:624:ILE:HG13	2.20	0.41
2:D:468:ILE:HG23	2:D:476:LYS:HD3	2.03	0.41
1:F:97:LYS:HG3	1:F:98:SER:N	2.36	0.41
1:F:335:LEU:HD23	1:F:371:PHE:CE2	2.55	0.41
1:F:858:LEU:HD21	1:F:962:LEU:HD23	2.02	0.41
2:G:169:ARG:HD2	6:G:902:CL:CL	2.58	0.41
2:G:471:ASP:O	2:G:495:GLU:HG3	2.21	0.41
2:G:477:TRP:CE3	2:G:500:PRO:HG3	2.55	0.41
1:B:331:ASN:O	1:B:332:ILE:C	2.64	0.41
1:B:353:TRP:HB2	1:B:398:ASP:HB3	2.02	0.41
1:B:560:LEU:O	1:B:563:GLN:HG2	2.20	0.41
1:B:728:PRO:HB3	1:B:951:VAL:HG21	2.03	0.41
1:B:1095:PHE:CE1	1:B:1115:ILE:HD12	2.56	0.41
1:C:558:LYS:NZ	4:F:1305:NAG:O6	2.35	0.41
1:F:437:ASN:HA	1:F:508:TYR:CD1	2.56	0.41
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.91	0.40
1:C:519:HIS:HA	1:C:565:PHE:HE2	1.85	0.40
2:D:177:ARG:O	2:D:181:GLU:HG3	2.21	0.40
1:F:429:PHE:HE1	1:F:514:SER:HB2	1.86	0.40
1:F:714:ILE:HD12	1:F:1096:VAL:HG21	2.02	0.40
1:F:919:ASN:O	1:F:923:ILE:HD12	2.21	0.40
2:G:459:TRP:HA	2:G:462:MET:HE2	2.03	0.40
1:B:869:MET:HB2	1:F:699:LEU:HD21	2.02	0.40
1:C:383:SER:HB3	1:C:386:LYS:HB2	2.02	0.40
1:C:445:VAL:O	1:C:498:ARG:NE	2.55	0.40
1:F:111:ASP:OD1	1:F:111:ASP:N	2.53	0.40
1:F:1081:ILE:HD13	1:F:1133:VAL:HG23	2.01	0.40
2:G:421:ILE:HG13	2:G:423:LEU:HG	2.03	0.40
2:G:460:ARG:HH22	2:G:500:PRO:C	2.29	0.40
2:G:543:ASP:OD1	2:G:544:ILE:N	2.55	0.40
1:C:457:ARG:NH1	1:C:467:ASP:OD2	2.52	0.40
1:F:425:LEU:HD23	1:F:425:LEU:HA	1.96	0.40
1:F:431:GLY:HA3	1:F:513:LEU:O	2.22	0.40
1:B:142:ASP:HB2	1:B:245:HIS:CE1	2.56	0.40
1:B:330:PRO:HA	1:B:579:PRO:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:VAL:HG22	1:B:422:ASN:HB3	2.04	0.40
1:C:878:LEU:HA	1:C:881:THR:HG22	2.03	0.40
2:D:478:TRP:CD2	2:D:489:GLU:HB3	2.57	0.40
2:G:103:ASN:OD1	2:G:104:GLY:N	2.55	0.40
2:G:169:ARG:NH1	6:G:902:CL:CL	2.92	0.40
2:G:524:GLN:HG3	2:G:574:VAL:HG11	2.04	0.40
1:C:78:ARG:HG2	1:C:79:PHE:N	2.35	0.40
1:C:329:PHE:CE2	1:C:528:LYS:HB2	2.56	0.40
1:C:436:TRP:NE1	1:C:509:ARG:HD3	2.36	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	B	1050/1270 (83%)	934 (89%)	113 (11%)	3 (0%)	36	66
1	C	1074/1270 (85%)	976 (91%)	96 (9%)	2 (0%)	43	74
1	F	1060/1270 (84%)	964 (91%)	94 (9%)	2 (0%)	43	74
2	D	595/603 (99%)	578 (97%)	17 (3%)	0	100	100
2	G	595/603 (99%)	573 (96%)	22 (4%)	0	100	100
All	All	4374/5016 (87%)	4025 (92%)	342 (8%)	7 (0%)	44	74

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	635	VAL
1	F	337	PRO
1	B	332	ILE
1	C	756	TYR
1	B	334	ASN

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Mol	Chain	Res	Type
1	F	235	ILE
1	B	235	ILE

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	B	921/1111 (83%)	918 (100%)	3 (0%)	86	83
1	C	939/1111 (84%)	939 (100%)	0	100	100
1	F	930/1111 (84%)	928 (100%)	2 (0%)	87	85
2	D	527/533 (99%)	527 (100%)	0	100	100
2	G	527/533 (99%)	527 (100%)	0	100	100
All	All	3844/4399 (87%)	3839 (100%)	5 (0%)	87	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ASN
1	B	335	LEU
1	B	439	ASN
1	F	333	THR
1	F	335	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	HIS
1	B	81	ASN
1	B	87	ASN
1	B	211	ASN
1	B	239	GLN
1	B	271	GLN
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	331	ASN
1	B	334	ASN
1	B	675	GLN
1	B	751	ASN
1	C	26	GLN
1	C	81	ASN
1	C	115	GLN
1	C	121	ASN
1	C	370	ASN
1	C	409	GLN
1	C	439	ASN
1	C	450	ASN
1	C	519	HIS
1	C	580	GLN
1	C	625	HIS
1	C	641	ASN
1	C	644	GLN
1	C	1106	GLN
2	D	139	GLN
2	D	154	ASN
2	D	290	ASN
2	D	345	HIS
2	D	442	GLN
2	D	524	GLN
2	D	572	ASN
1	F	69	HIS
1	F	115	GLN
1	F	121	ASN
1	F	165	ASN
1	F	370	ASN
1	F	414	GLN
1	F	450	ASN
1	F	481	ASN
1	F	505	HIS
1	F	563	GLN
1	F	580	GLN
1	F	607	GLN
1	F	690	GLN
1	F	853	GLN
1	F	960	ASN
1	F	1036	GLN
1	F	1054	GLN

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Mol	Chain	Res	Type
2	G	60	GLN
2	G	64	ASN
2	G	81	GLN
2	G	175	GLN
2	G	194	ASN
2	G	290	ASN
2	G	345	HIS
2	G	437	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](#)

18 monosaccharides 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	$\# Z > 2$
3	NAG	A	1	3	14,14,15	0.17	0	17,19,21	0.46	0
3	NAG	A	2	3	14,14,15	0.24	0	17,19,21	0.43	0
3	NAG	E	1	3	14,14,15	0.21	0	17,19,21	0.52	0
3	NAG	E	2	3	14,14,15	0.27	0	17,19,21	0.60	1 (5%)
3	NAG	H	1	3,1	14,14,15	0.38	0	17,19,21	0.63	0
3	NAG	H	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	I	1	3,1	14,14,15	0.23	0	17,19,21	0.56	0
3	NAG	I	2	3	14,14,15	0.22	0	17,19,21	0.41	0
3	NAG	J	1	3	14,14,15	0.17	0	17,19,21	0.60	0
3	NAG	J	2	3	14,14,15	0.25	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	1	3,1	14,14,15	0.87	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	K	2	3	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	L	1	3	14,14,15	0.32	0	17,19,21	0.41	0
3	NAG	L	2	3	14,14,15	0.18	0	17,19,21	0.47	0
3	NAG	M	1	3	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.26	0	17,19,21	0.52	0
3	NAG	N	1	3,1	14,14,15	0.88	1 (7%)	17,19,21	1.27	1 (5%)
3	NAG	N	2	3	14,14,15	0.22	0	17,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1	3	-	1/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	N	2	3	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	1	NAG	O5-C1	3.06	1.48	1.43
3	K	1	NAG	O5-C1	2.95	1.48	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	NAG	C1-O5-C5	4.77	118.58	112.19
3	K	1	NAG	C1-O5-C5	4.77	118.58	112.19
3	E	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

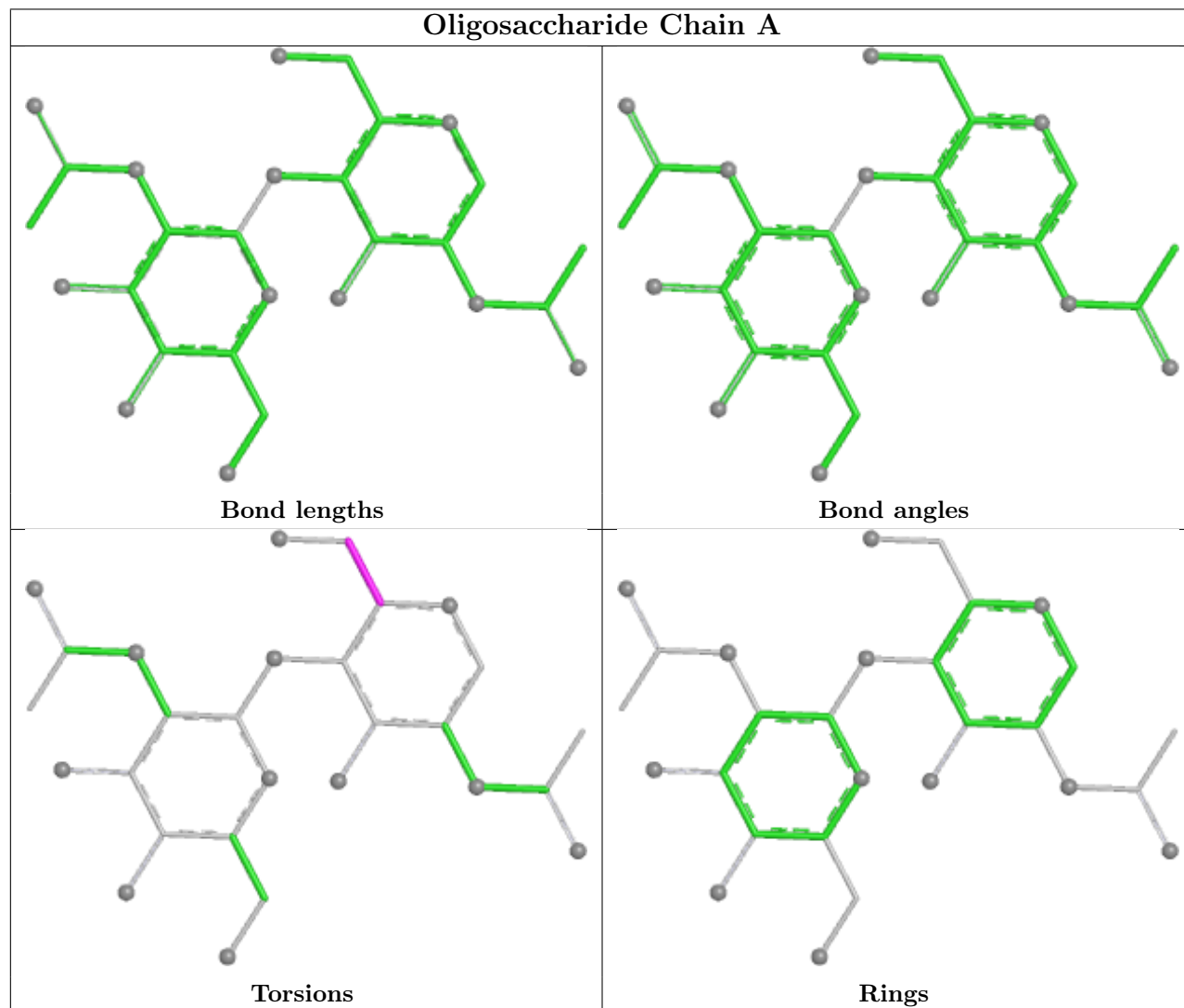
Mol	Chain	Res	Type	Atoms
3	K	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	M	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	A	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	H	1	NAG	C1-C2-N2-C7
3	K	1	NAG	C1-C2-N2-C7
3	N	1	NAG	C1-C2-N2-C7
3	L	2	NAG	C4-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	N	1	NAG	C4-C5-C6-O6
3	N	1	NAG	C3-C2-N2-C7
3	H	1	NAG	C3-C2-N2-C7
3	K	1	NAG	C3-C2-N2-C7
3	K	1	NAG	C4-C5-C6-O6

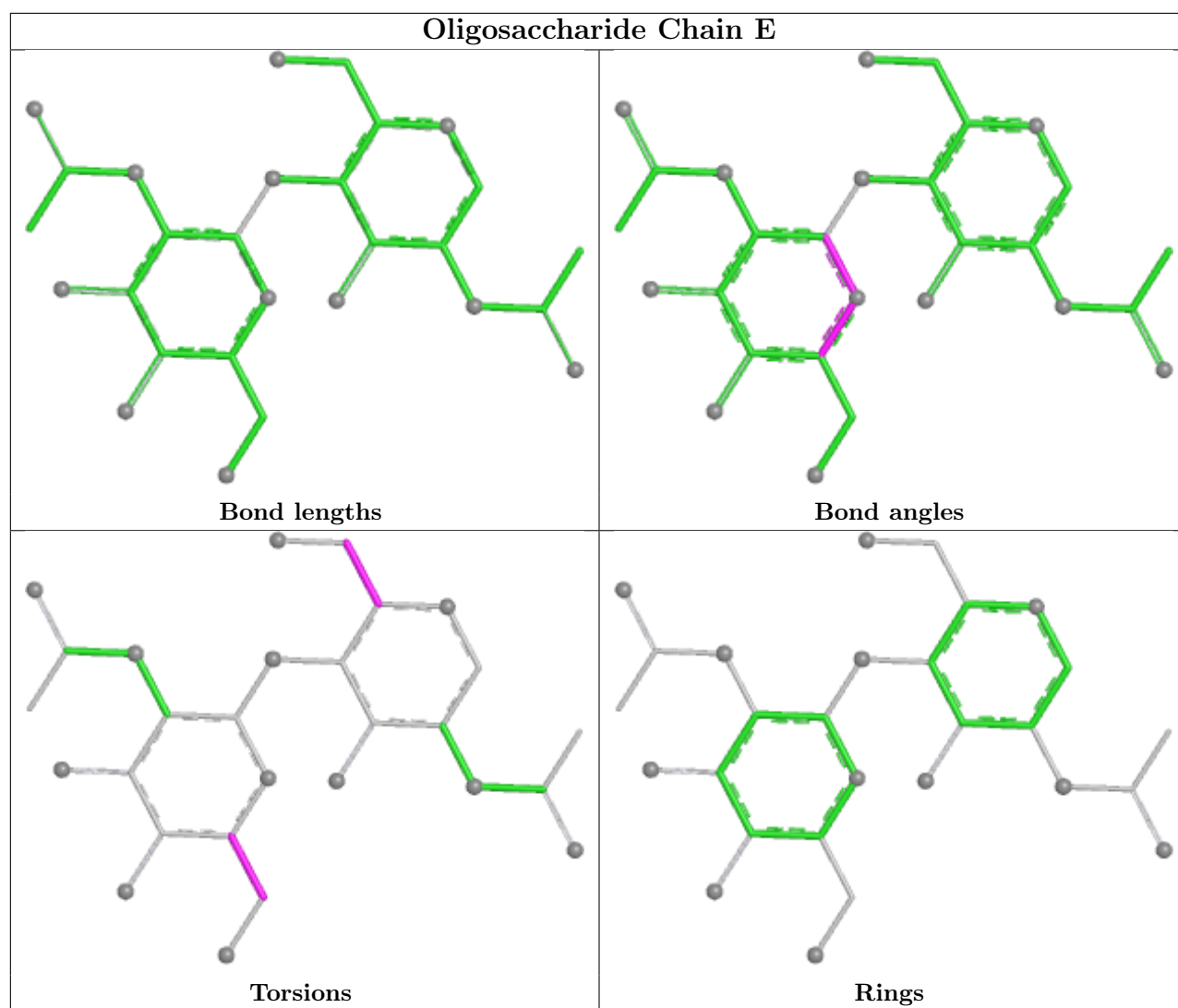
There are no ring outliers.

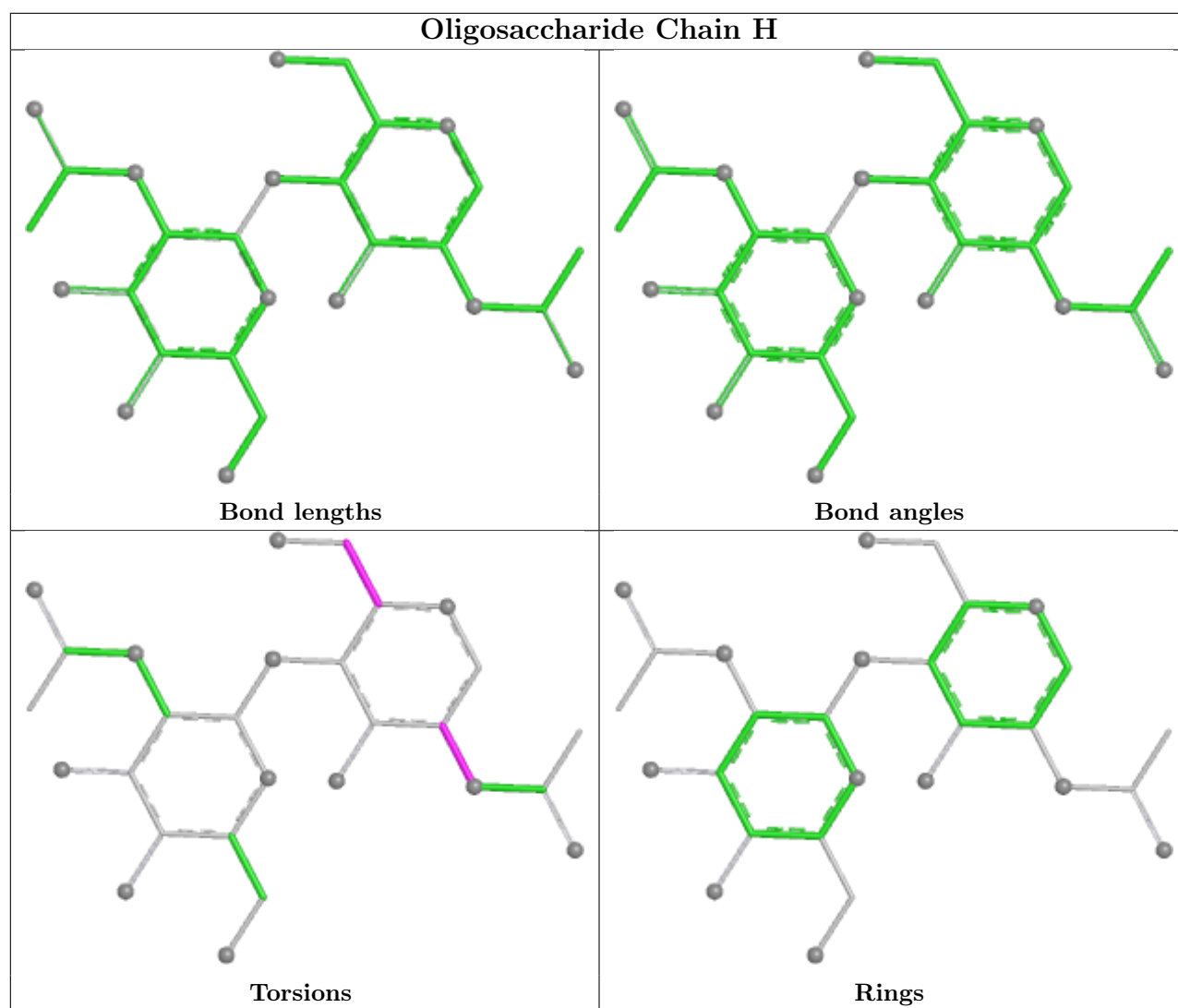
1 monomer is involved in 2 short contacts:

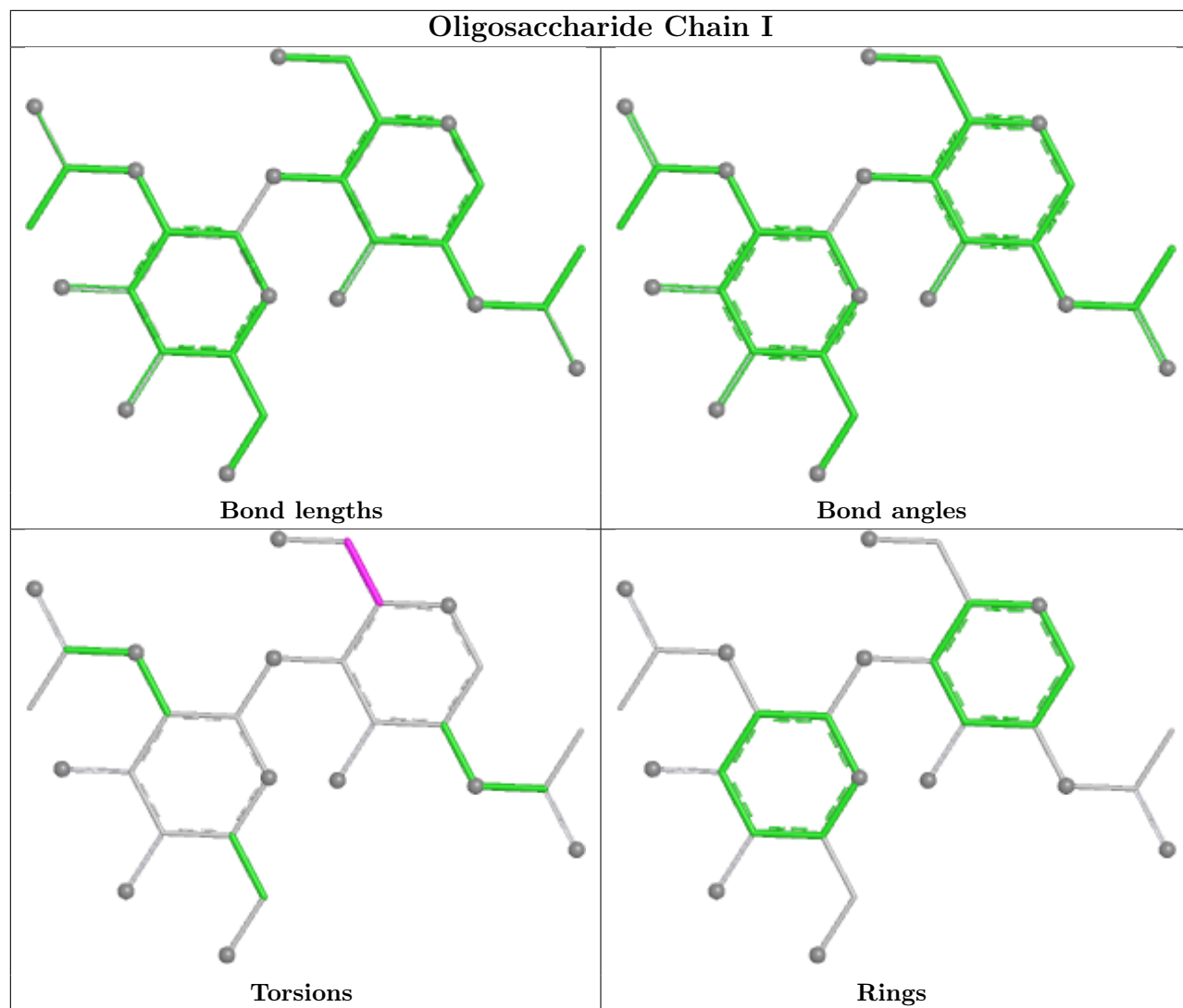
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	2	0

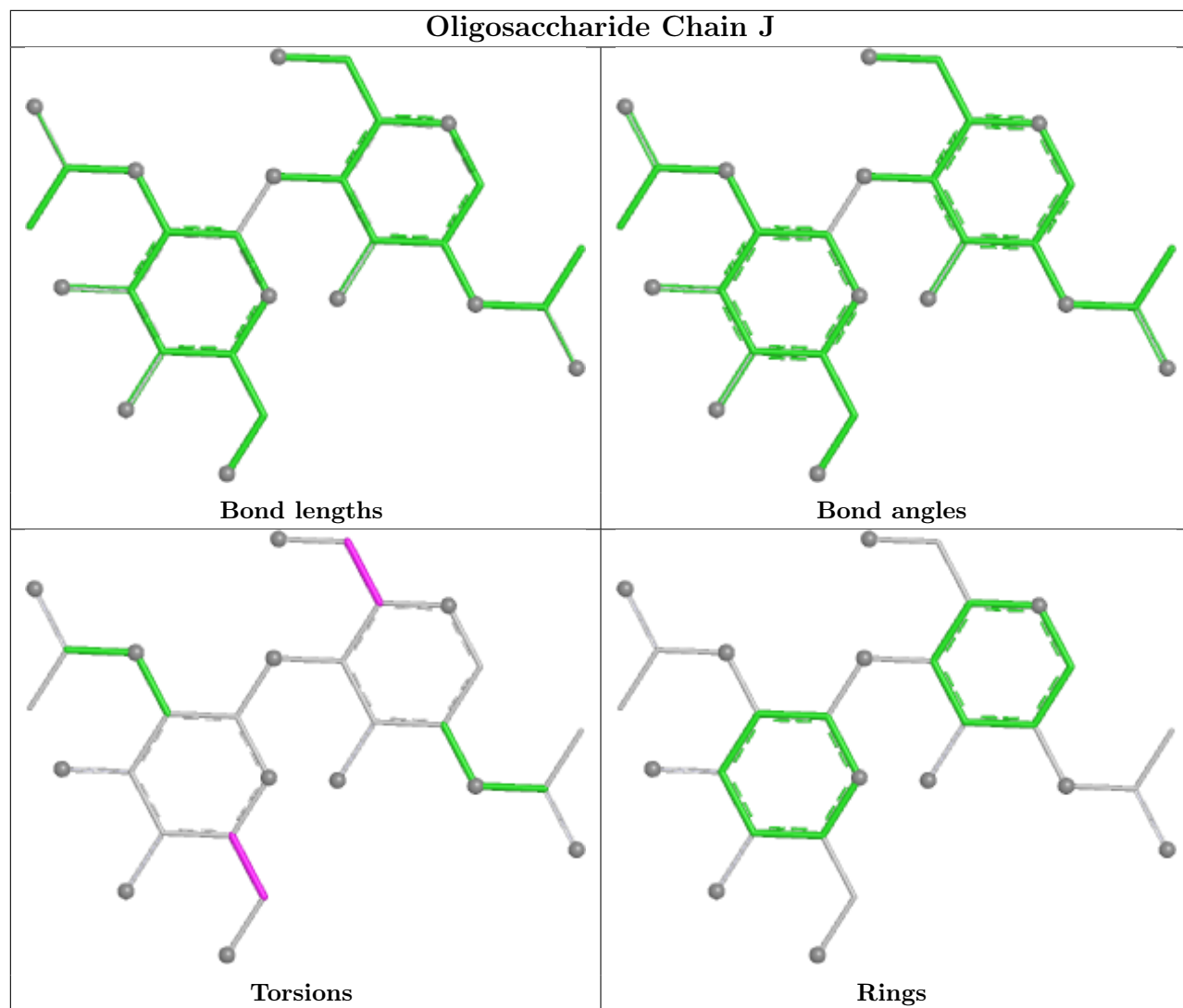
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

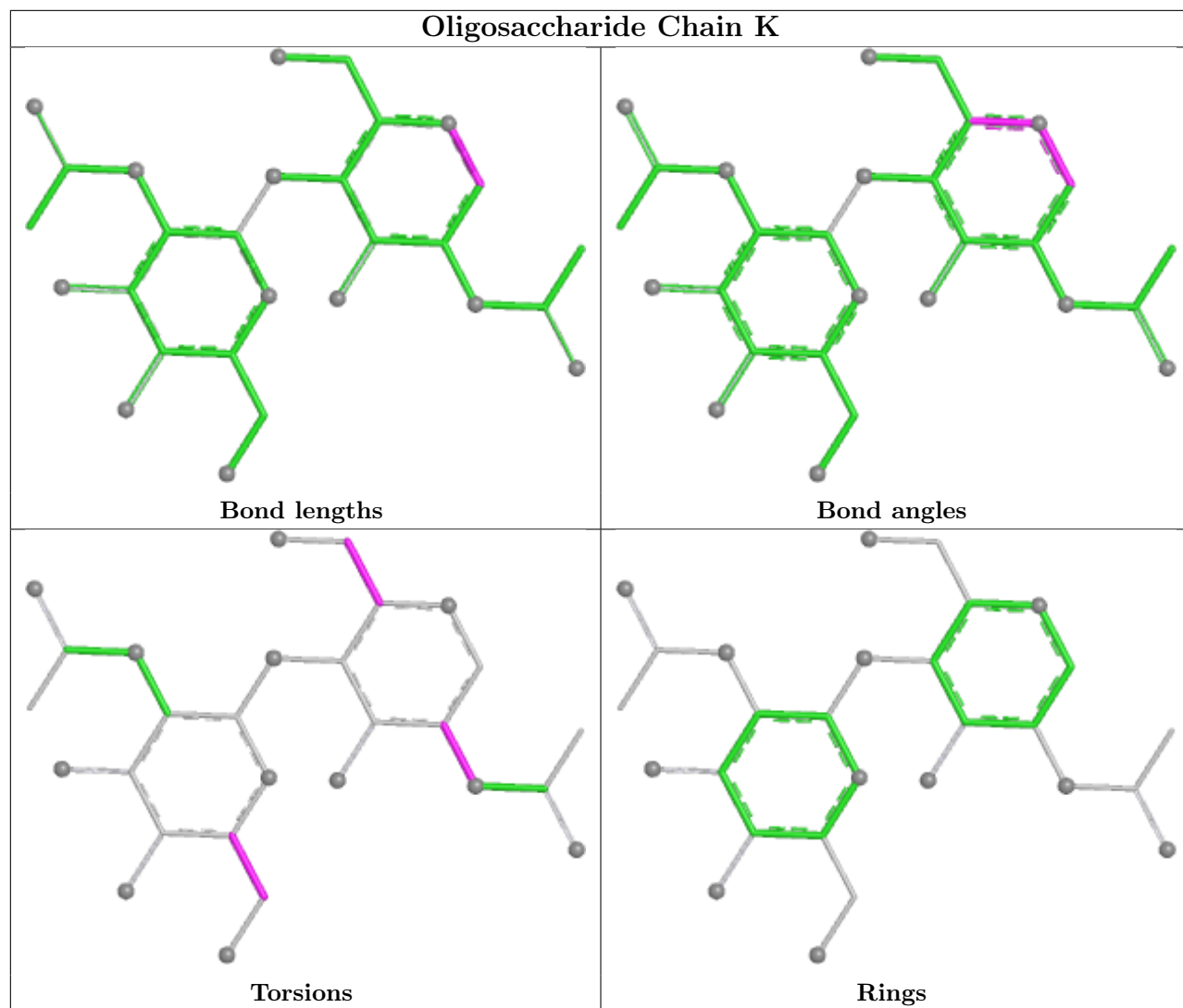


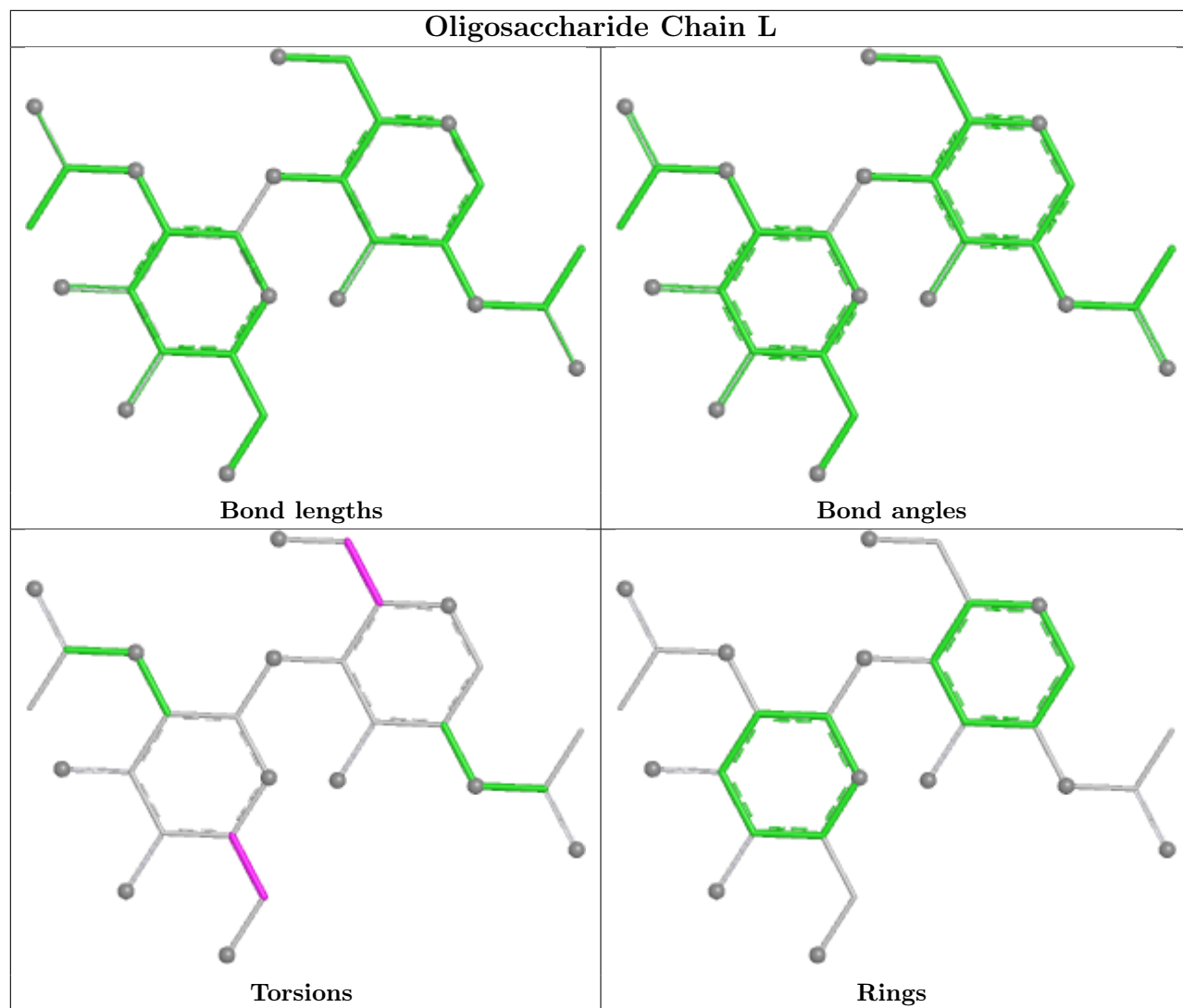


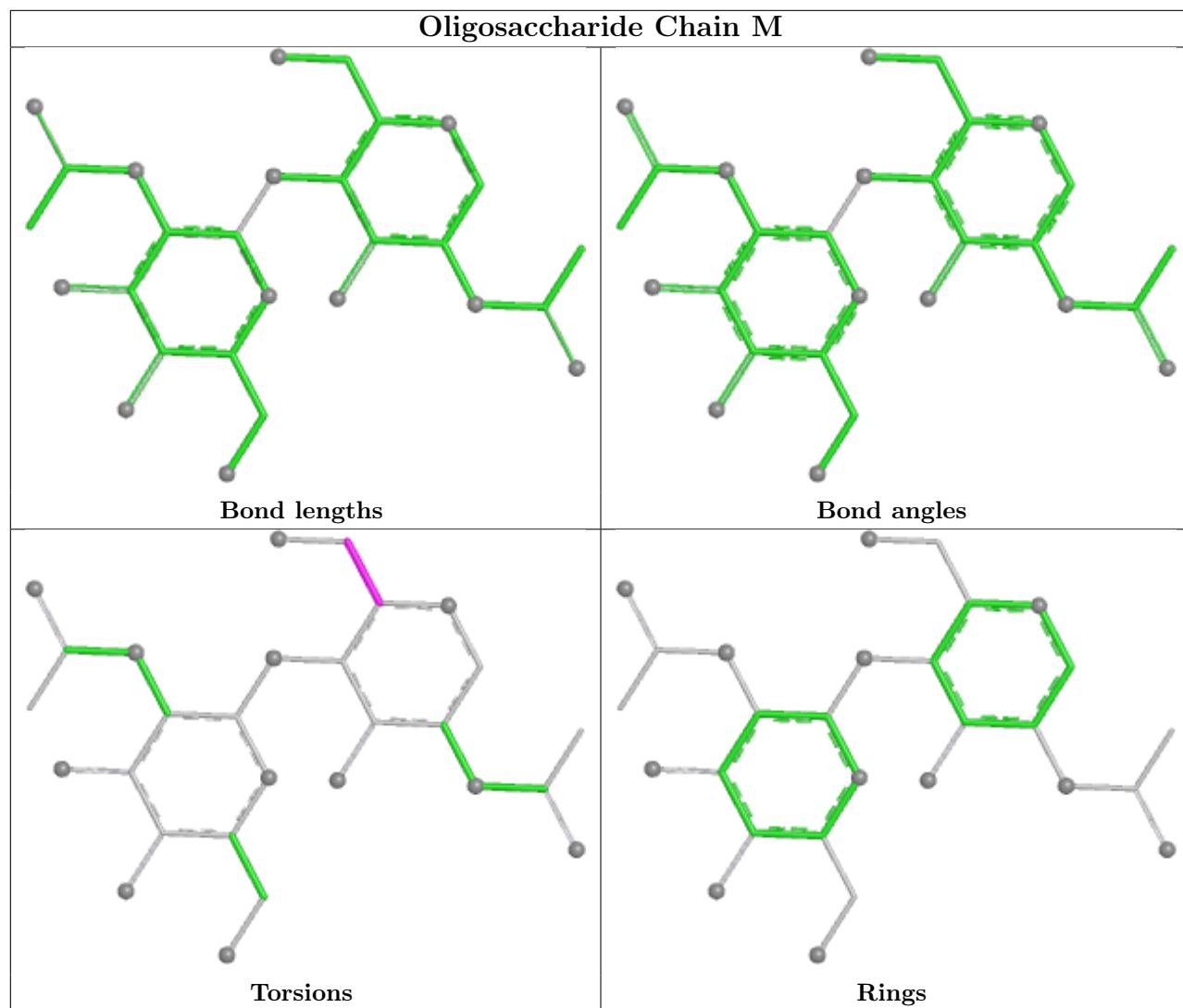


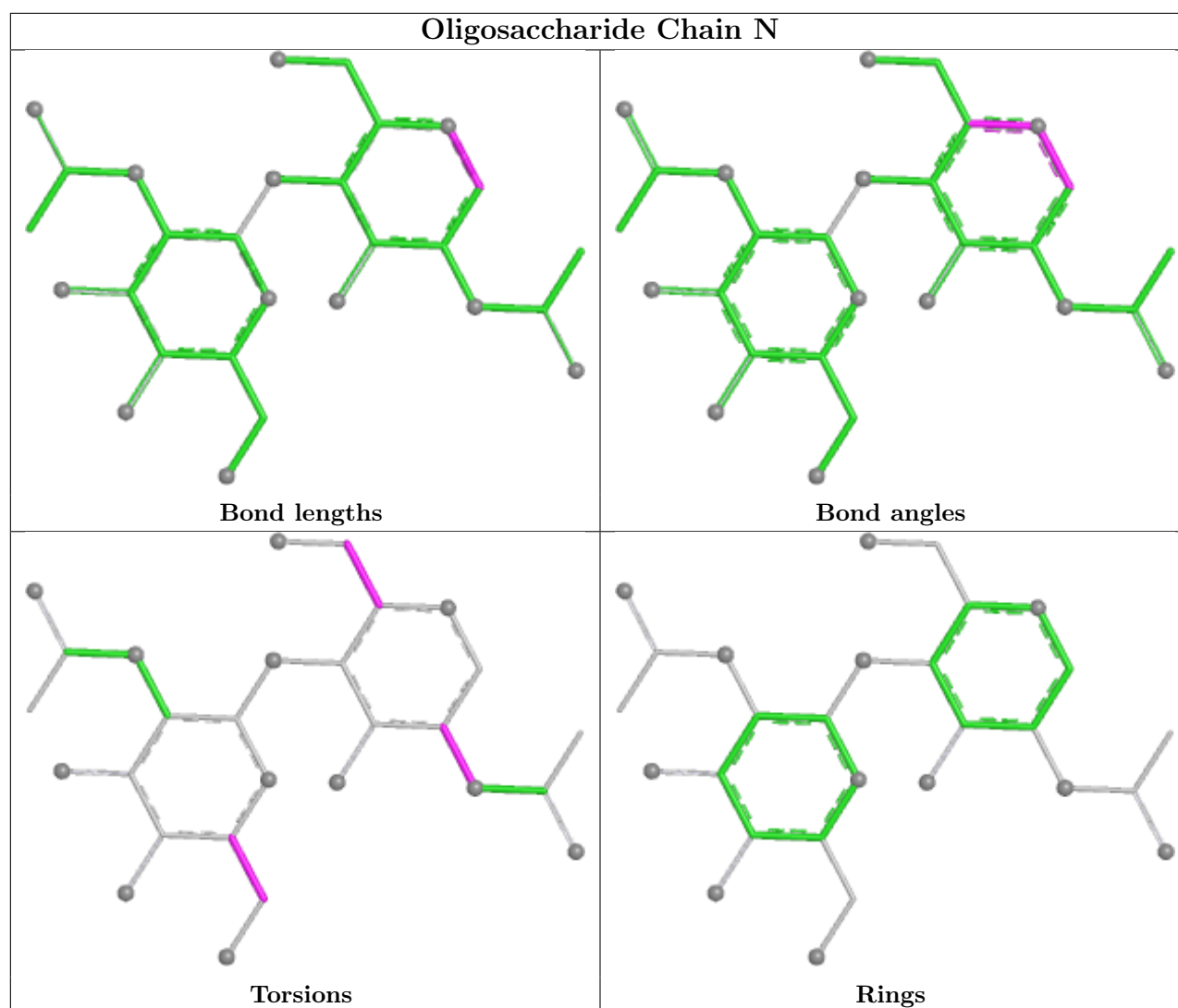












5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 4 are monoatomic - leaving 53 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	$\# Z > 2$
4	NAG	F	1305	-	14,14,15	0.23	0	17,19,21	0.42	0
4	NAG	G	906	2	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	C	1303	-	14,14,15	0.23	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1304	-	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	C	1307	-	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	1311	1	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	B	1307	-	14,14,15	0.44	0	17,19,21	0.78	1 (5%)
4	NAG	D	905	2	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	C	1312	1	14,14,15	0.47	0	17,19,21	1.35	2 (11%)
4	NAG	C	1315	1	14,14,15	0.25	0	17,19,21	0.47	0
4	NAG	B	1314	-	14,14,15	0.22	0	17,19,21	0.56	0
4	NAG	B	1303	-	14,14,15	0.28	0	17,19,21	0.43	0
4	NAG	F	1302	-	14,14,15	0.18	0	17,19,21	0.47	0
4	NAG	C	1313	1	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	B	1305	-	14,14,15	0.27	0	17,19,21	0.57	0
4	NAG	C	1308	-	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	F	1308	-	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	F	1304	-	14,14,15	0.21	0	17,19,21	0.59	0
4	NAG	C	1306	-	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	B	1302	-	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	B	1315	-	14,14,15	0.19	0	17,19,21	0.47	0
4	NAG	B	1313	1	14,14,15	0.18	0	17,19,21	0.44	0
4	NAG	B	1301	-	14,14,15	0.24	0	17,19,21	0.54	0
4	NAG	B	1311	1	14,14,15	0.23	0	17,19,21	0.44	0
4	NAG	F	1303	-	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	F	1311	1	14,14,15	0.18	0	17,19,21	0.42	0
4	NAG	B	1304	-	14,14,15	0.30	0	17,19,21	0.54	0
4	NAG	G	905	2	14,14,15	0.25	0	17,19,21	0.41	0
4	NAG	B	1306	-	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	F	1312	-	14,14,15	0.26	0	17,19,21	0.53	0
4	NAG	F	1309	1	14,14,15	0.20	0	17,19,21	0.47	0
4	NAG	C	1310	1	14,14,15	0.21	0	17,19,21	0.40	0
4	NAG	F	1313	1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	F	1306	-	14,14,15	0.60	0	17,19,21	1.04	2 (11%)
4	NAG	C	1317	-	14,14,15	0.20	0	17,19,21	0.45	0
4	NAG	D	903	2	14,14,15	0.22	0	17,19,21	0.39	0
4	NAG	C	1305	-	14,14,15	0.24	0	17,19,21	0.56	0
4	NAG	D	904	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	1312	1	14,14,15	0.42	0	17,19,21	1.34	2 (11%)
4	NAG	G	904	2	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	B	1310	1	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	C	1316	-	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	D	906	2	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1309	-	14,14,15	0.37	0	17,19,21	0.66	0
4	NAG	F	1307	-	14,14,15	0.29	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1314	-	14,14,15	0.22	0	17,19,21	0.54	0
4	NAG	G	903	2	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	C	1301	-	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	F	1301	-	14,14,15	0.20	0	17,19,21	0.44	0
4	NAG	F	1310	-	14,14,15	0.44	0	17,19,21	1.35	2 (11%)
4	NAG	C	1309	-	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	C	1302	-	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	B	1308	-	14,14,15	0.21	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	G	906	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1311	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1307	-	-	4/6/23/26	0/1/1/1
4	NAG	D	905	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1312	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1314	-	-	3/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	0/6/23/26	0/1/1/1
4	NAG	F	1302	-	-	1/6/23/26	0/1/1/1
4	NAG	C	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1308	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1308	-	-	1/6/23/26	0/1/1/1
4	NAG	F	1304	-	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1315	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1301	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	-	-	3/6/23/26	0/1/1/1
4	NAG	G	905	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1312	-	-	3/6/23/26	0/1/1/1
4	NAG	F	1309	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1313	1	-	0/6/23/26	0/1/1/1
4	NAG	F	1306	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1317	-	-	2/6/23/26	0/1/1/1
4	NAG	D	903	2	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	D	904	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	6/6/23/26	0/1/1/1
4	NAG	G	904	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1316	-	-	2/6/23/26	0/1/1/1
4	NAG	D	906	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1309	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1307	-	-	0/6/23/26	0/1/1/1
4	NAG	C	1314	-	-	4/6/23/26	0/1/1/1
4	NAG	G	903	2	-	3/6/23/26	0/1/1/1
4	NAG	C	1301	-	-	1/6/23/26	0/1/1/1
4	NAG	F	1301	-	-	2/6/23/26	0/1/1/1
4	NAG	F	1310	-	-	6/6/23/26	0/1/1/1
4	NAG	C	1309	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1308	-	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1312	NAG	C2-N2-C7	4.61	129.07	122.90
4	C	1312	NAG	C2-N2-C7	4.59	129.06	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1310	NAG	C2-N2-C7	4.57	129.02	122.90
4	F	1306	NAG	C1-O5-C5	3.02	116.24	112.19
4	B	1307	NAG	C1-O5-C5	2.89	116.06	112.19
4	F	1306	NAG	C3-C4-C5	2.38	114.54	110.23
4	C	1312	NAG	C1-C2-N2	2.27	114.01	110.43
4	B	1312	NAG	C1-C2-N2	2.24	113.96	110.43
4	F	1310	NAG	C1-C2-N2	2.19	113.88	110.43

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1302	NAG	C4-C5-C6-O6
4	C	1315	NAG	C4-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	B	1312	NAG	C4-C5-C6-O6
4	C	1317	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	C	1315	NAG	O5-C5-C6-O6
4	B	1306	NAG	C4-C5-C6-O6
4	F	1301	NAG	C4-C5-C6-O6
4	C	1314	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	D	905	NAG	C4-C5-C6-O6
4	F	1303	NAG	C4-C5-C6-O6
4	B	1310	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	G	906	NAG	O5-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	F	1310	NAG	C4-C5-C6-O6
4	B	1315	NAG	O5-C5-C6-O6
4	F	1304	NAG	C4-C5-C6-O6
4	F	1311	NAG	C4-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	G	903	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1314	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	B	1312	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1317	NAG	O5-C5-C6-O6
4	F	1311	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	C	1310	NAG	O5-C5-C6-O6
4	F	1301	NAG	O5-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	B	1315	NAG	C4-C5-C6-O6
4	D	905	NAG	O5-C5-C6-O6
4	F	1306	NAG	O5-C5-C6-O6
4	F	1303	NAG	O5-C5-C6-O6
4	G	905	NAG	O5-C5-C6-O6
4	D	903	NAG	O5-C5-C6-O6
4	B	1310	NAG	C4-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	G	903	NAG	C4-C5-C6-O6
4	G	906	NAG	C4-C5-C6-O6
4	D	903	NAG	C4-C5-C6-O6
4	G	905	NAG	C4-C5-C6-O6
4	B	1307	NAG	C8-C7-N2-C2
4	B	1307	NAG	O7-C7-N2-C2
4	B	1312	NAG	C8-C7-N2-C2
4	B	1312	NAG	O7-C7-N2-C2
4	C	1307	NAG	C8-C7-N2-C2
4	C	1307	NAG	O7-C7-N2-C2
4	C	1312	NAG	C8-C7-N2-C2
4	C	1312	NAG	O7-C7-N2-C2
4	F	1305	NAG	C8-C7-N2-C2
4	F	1305	NAG	O7-C7-N2-C2
4	F	1310	NAG	C8-C7-N2-C2
4	F	1310	NAG	O7-C7-N2-C2
4	F	1310	NAG	O5-C5-C6-O6
4	D	906	NAG	O5-C5-C6-O6
4	C	1310	NAG	C4-C5-C6-O6
4	B	1314	NAG	O5-C5-C6-O6
4	F	1304	NAG	O5-C5-C6-O6
4	B	1313	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	D	906	NAG	C4-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	1311	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	F	1302	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	F	1306	NAG	C4-C5-C6-O6
4	F	1305	NAG	O5-C5-C6-O6
4	F	1312	NAG	O5-C5-C6-O6
4	B	1304	NAG	C1-C2-N2-C7
4	B	1305	NAG	C1-C2-N2-C7
4	C	1304	NAG	C1-C2-N2-C7
4	C	1314	NAG	C1-C2-N2-C7
4	C	1316	NAG	C1-C2-N2-C7
4	F	1304	NAG	C1-C2-N2-C7
4	F	1312	NAG	C1-C2-N2-C7
4	C	1306	NAG	O5-C5-C6-O6
4	B	1301	NAG	C3-C2-N2-C7
4	B	1314	NAG	C3-C2-N2-C7
4	C	1304	NAG	C3-C2-N2-C7
4	C	1305	NAG	C3-C2-N2-C7
4	C	1314	NAG	C3-C2-N2-C7
4	C	1316	NAG	C3-C2-N2-C7
4	F	1304	NAG	C3-C2-N2-C7
4	B	1309	NAG	C4-C5-C6-O6
4	B	1304	NAG	C4-C5-C6-O6
4	B	1301	NAG	C1-C2-N2-C7
4	B	1312	NAG	C1-C2-N2-C7
4	B	1314	NAG	C1-C2-N2-C7
4	C	1305	NAG	C1-C2-N2-C7
4	C	1312	NAG	C1-C2-N2-C7
4	F	1308	NAG	C1-C2-N2-C7
4	F	1310	NAG	C1-C2-N2-C7
4	G	903	NAG	C1-C2-N2-C7
4	B	1304	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	B	1312	NAG	C3-C2-N2-C7
4	C	1312	NAG	C3-C2-N2-C7
4	F	1310	NAG	C3-C2-N2-C7
4	F	1312	NAG	C3-C2-N2-C7

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1305	NAG	1	0
4	C	1307	NAG	1	0
4	C	1312	NAG	1	0
4	C	1308	NAG	1	0
4	B	1301	NAG	1	0
4	B	1312	NAG	1	0
4	B	1309	NAG	2	0
4	F	1307	NAG	1	0
4	F	1310	NAG	1	0
4	B	1308	NAG	3	0

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.

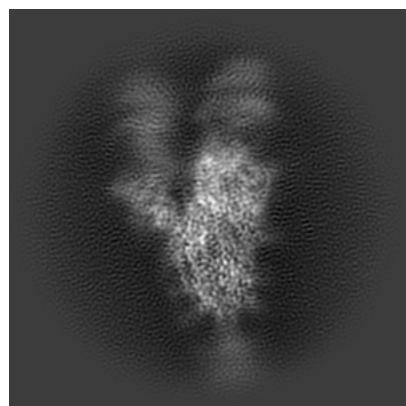
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34044. These allow visual inspection of the internal detail of the map and identification of artifacts.

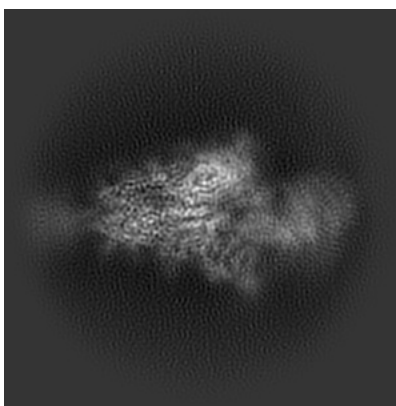
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

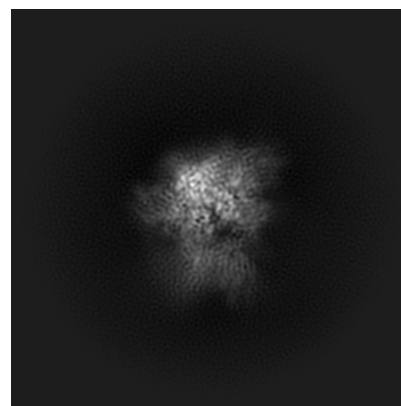
6.1.1 Primary map



X

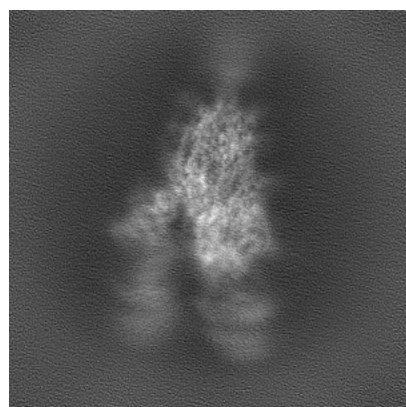


Y

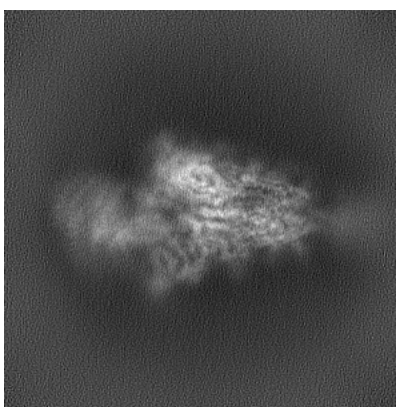


Z

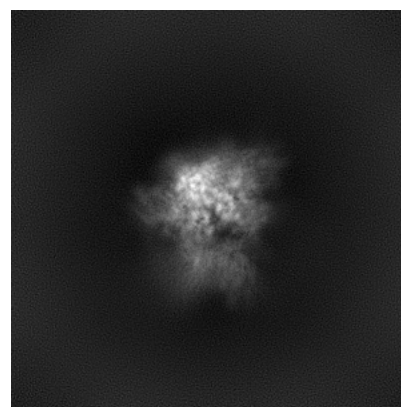
6.1.2 Raw map



X



Y

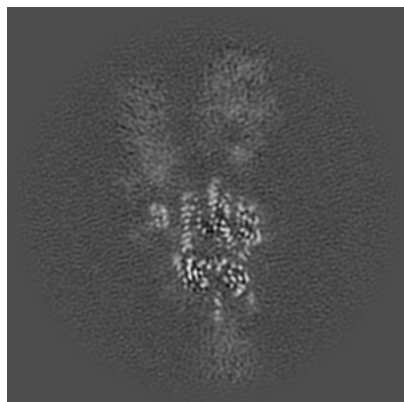


Z

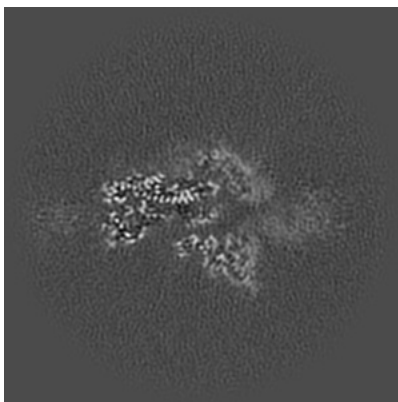
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

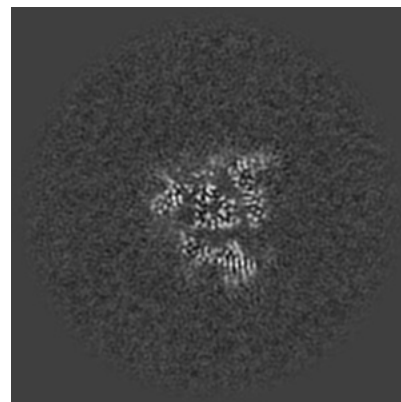
6.2.1 Primary map



X Index: 160

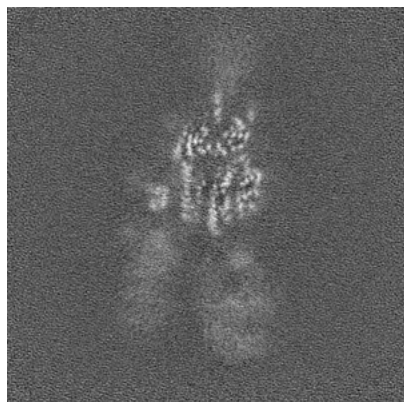


Y Index: 160

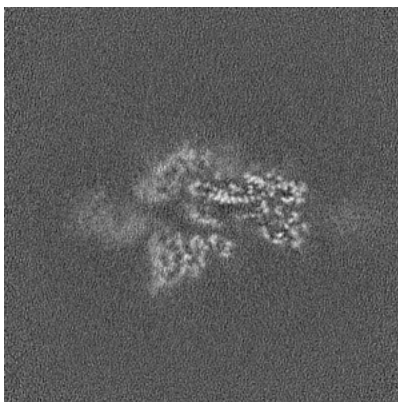


Z Index: 160

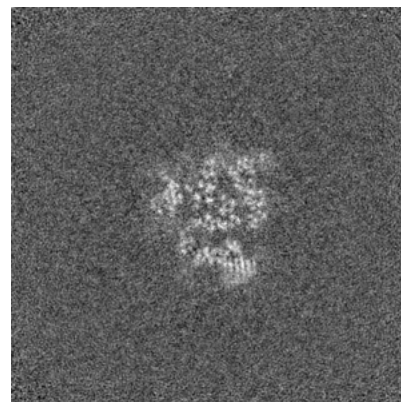
6.2.2 Raw map



X Index: 160



Y Index: 160

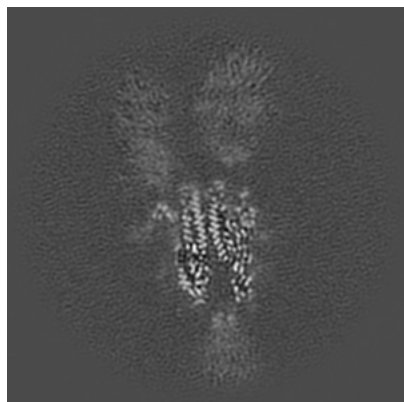


Z Index: 160

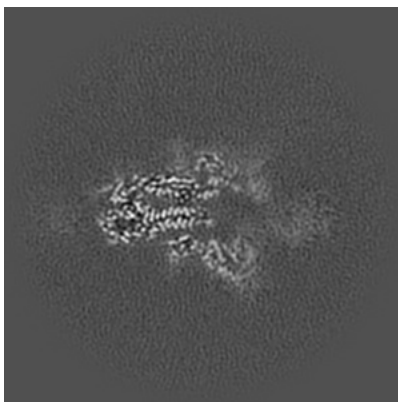
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

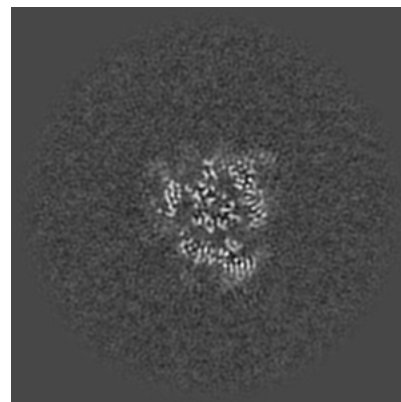
6.3.1 Primary map



X Index: 156

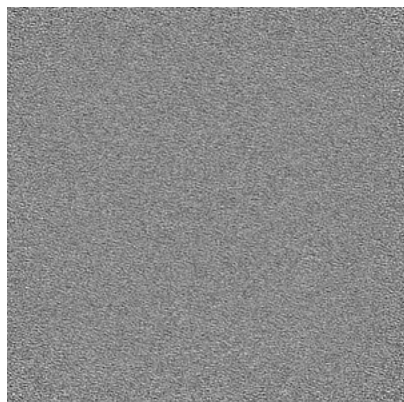


Y Index: 155

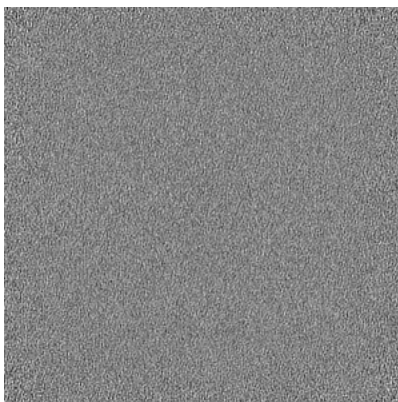


Z Index: 158

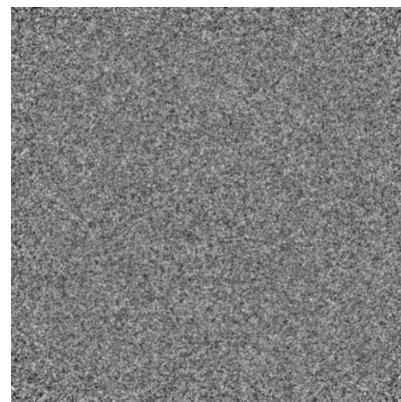
6.3.2 Raw map



X Index: 0



Y Index: 0

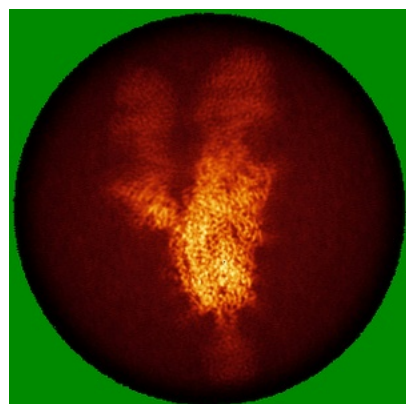


Z Index: 0

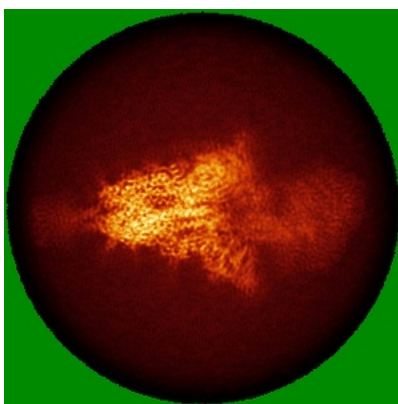
The images above show the largest variance slices of the map in three orthogonal directions.

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

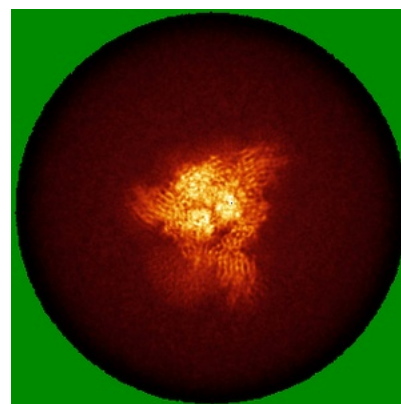
6.4.1 Primary map



X

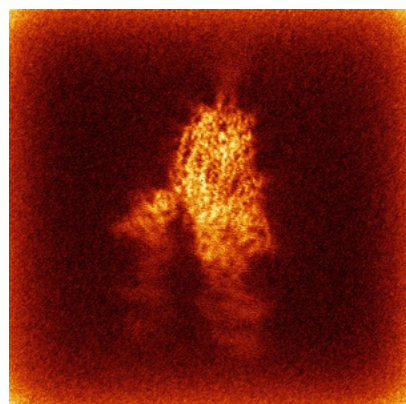


Y

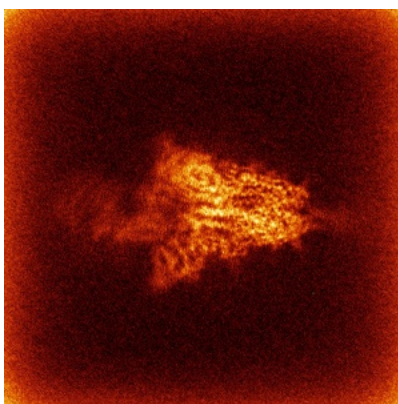


Z

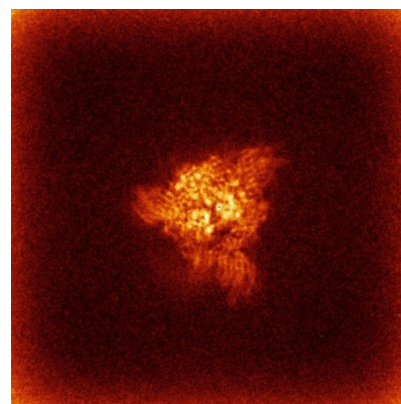
6.4.2 Raw map



X



Y

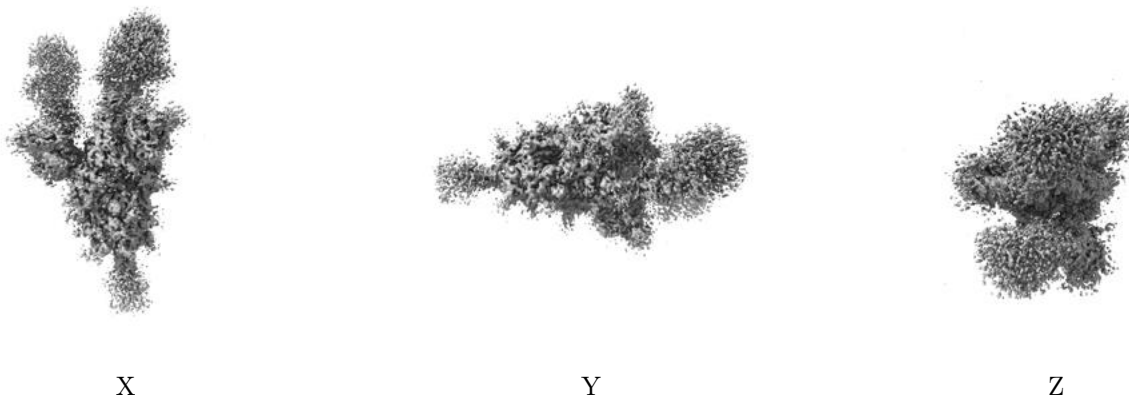


Z

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.

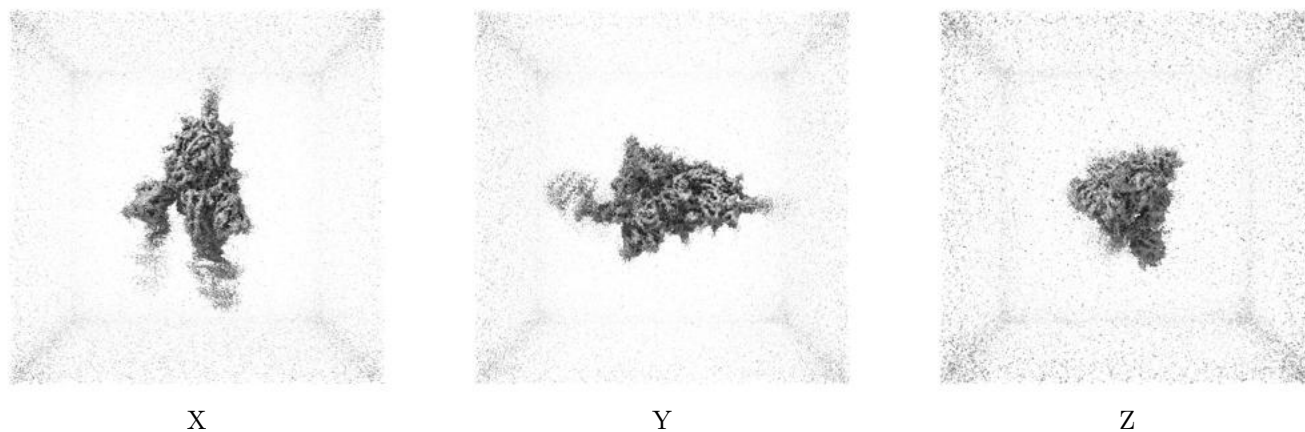
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

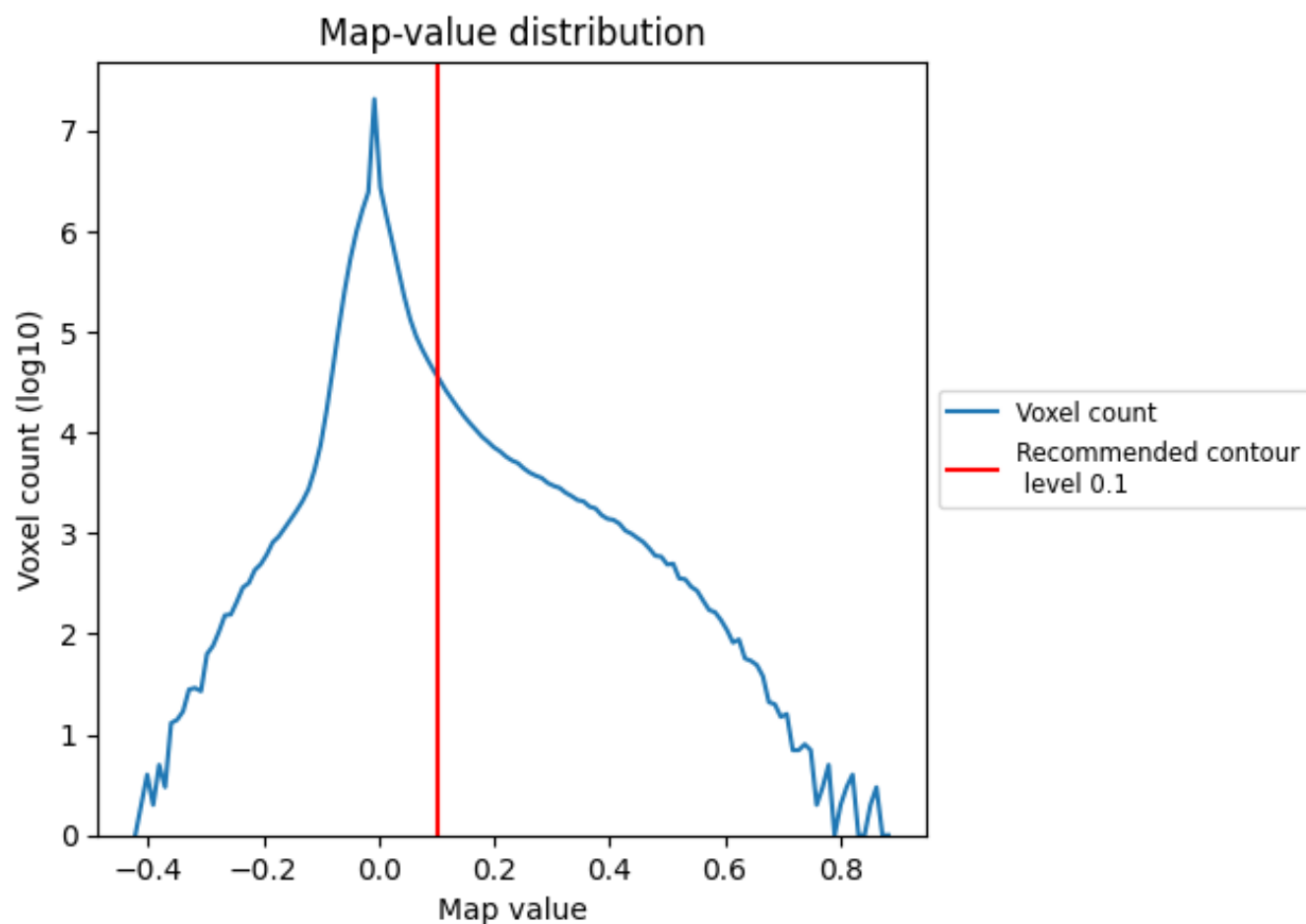
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

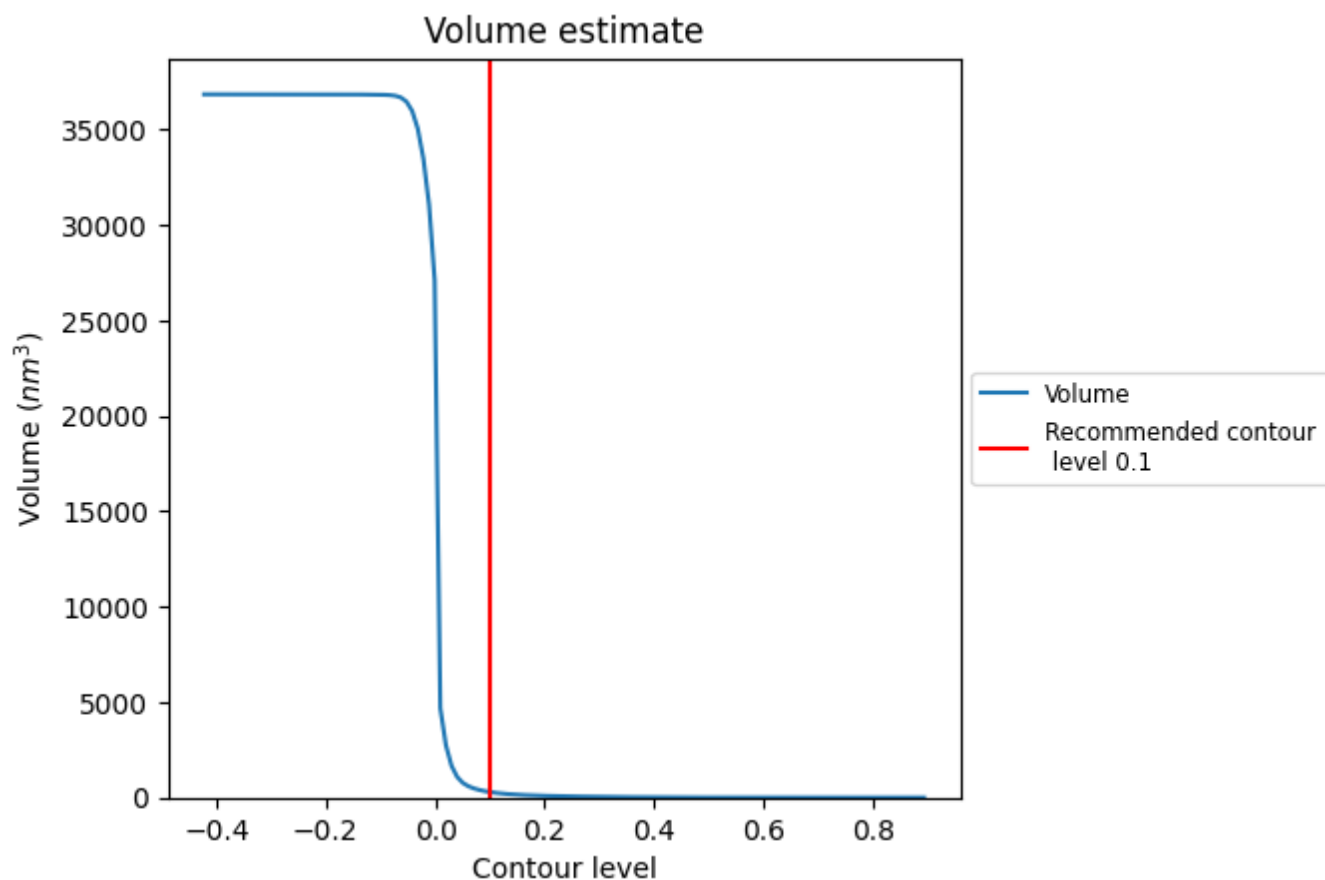
This section contains the results of statistical analysis of the map.

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.

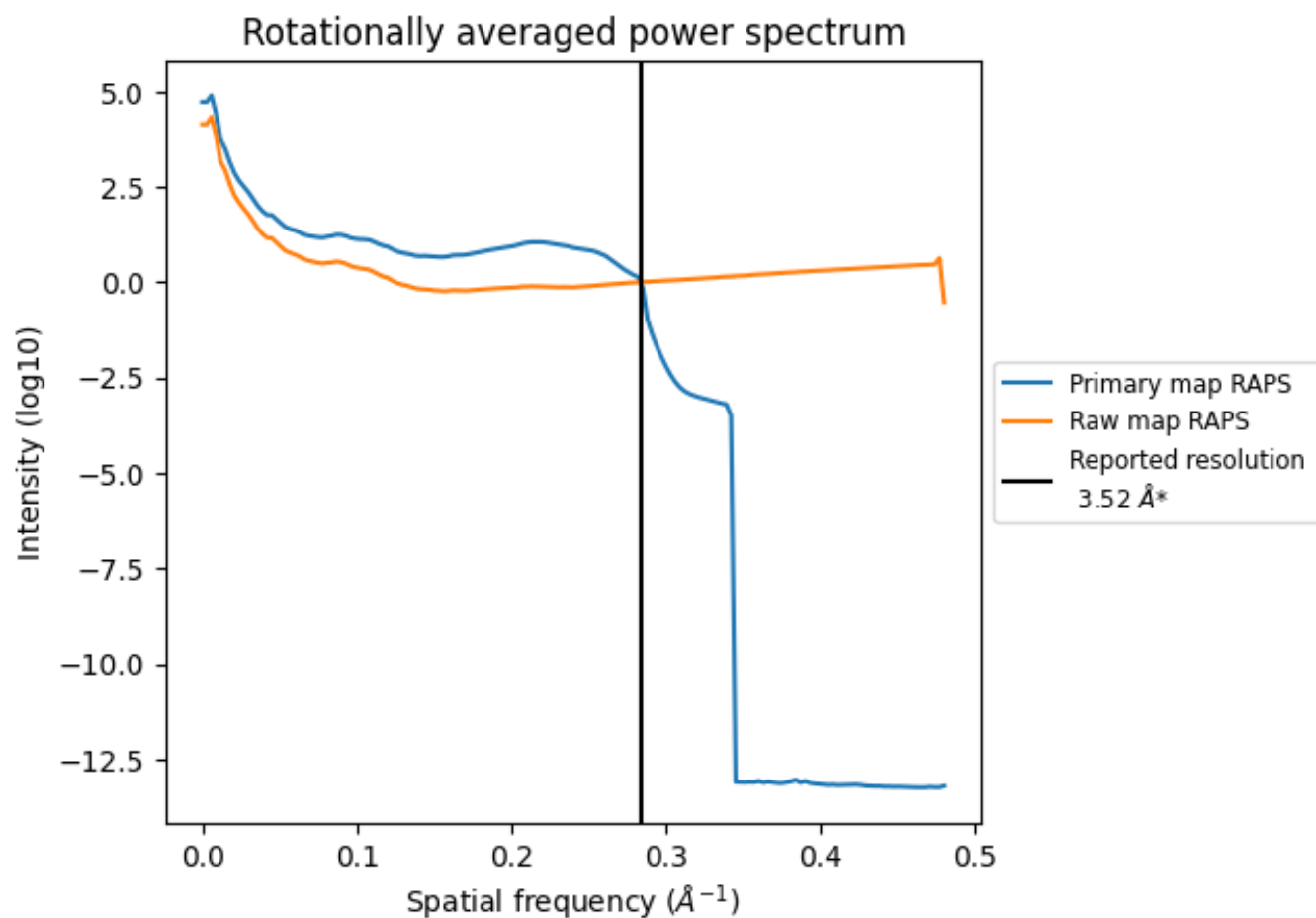
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm^3 ; this corresponds to an approximate mass of 262 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 ⓘ

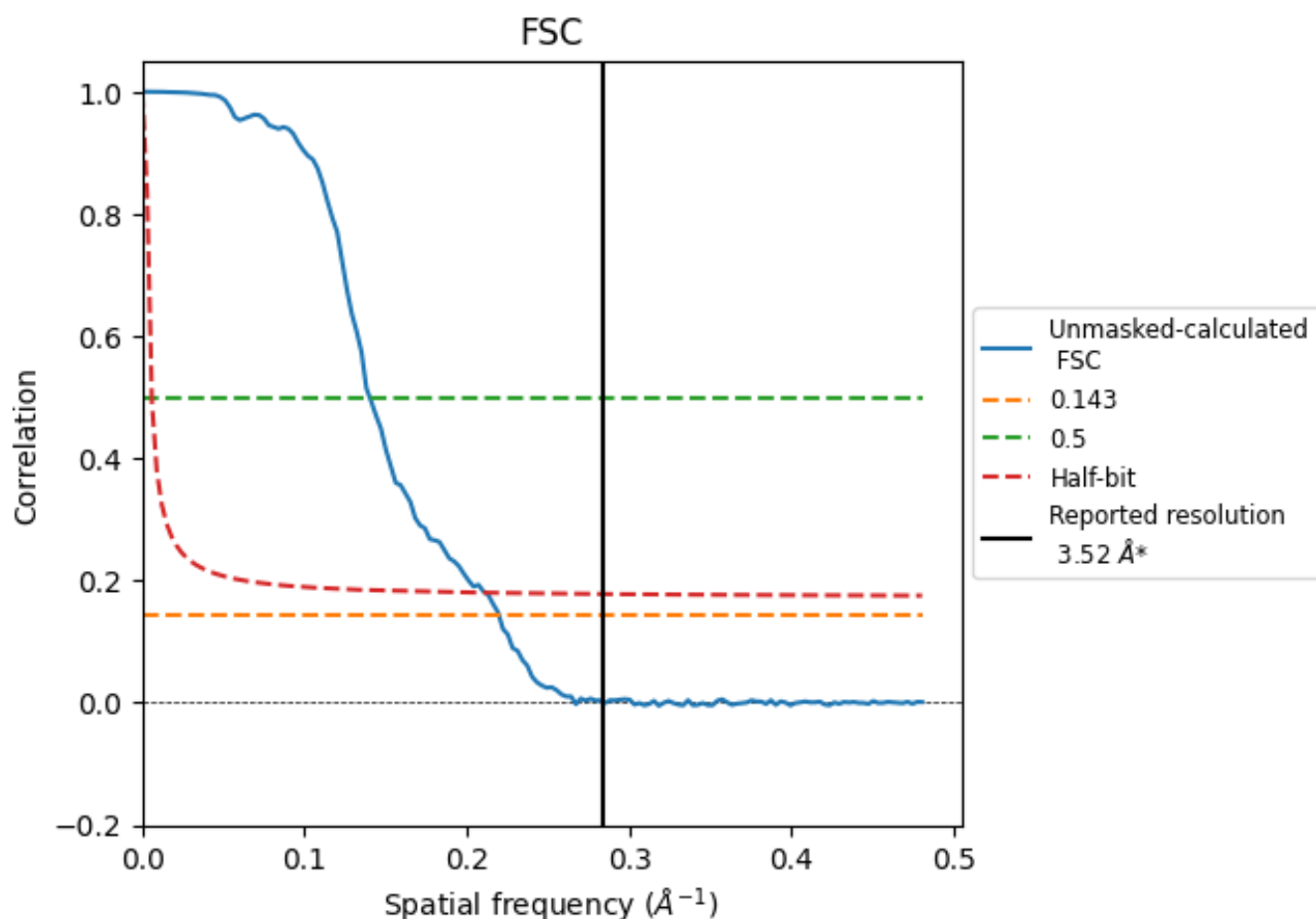


*Reported resolution corresponds to spatial frequency of 0.284 Å⁻¹

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 $0.284 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

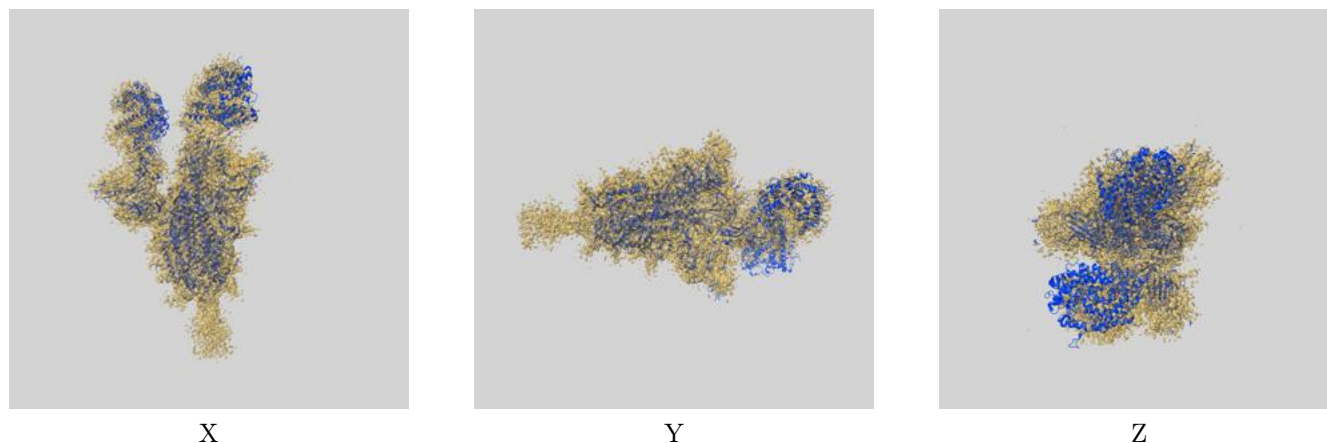
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.52	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.55	7.13	4.73

*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 4.55 differs from the reported value 3.52 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34044 and PDB model 7YR3. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

9.1 Map-model overlay [i](#)



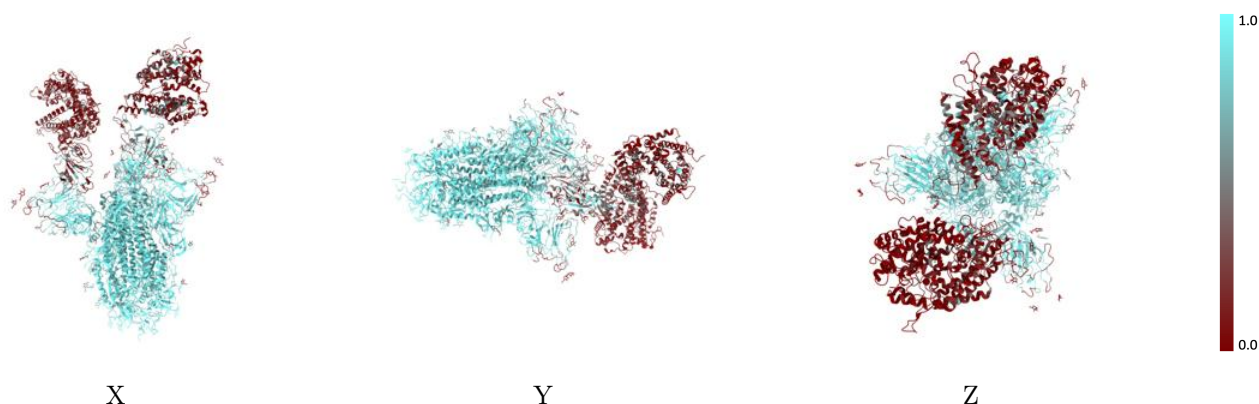
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



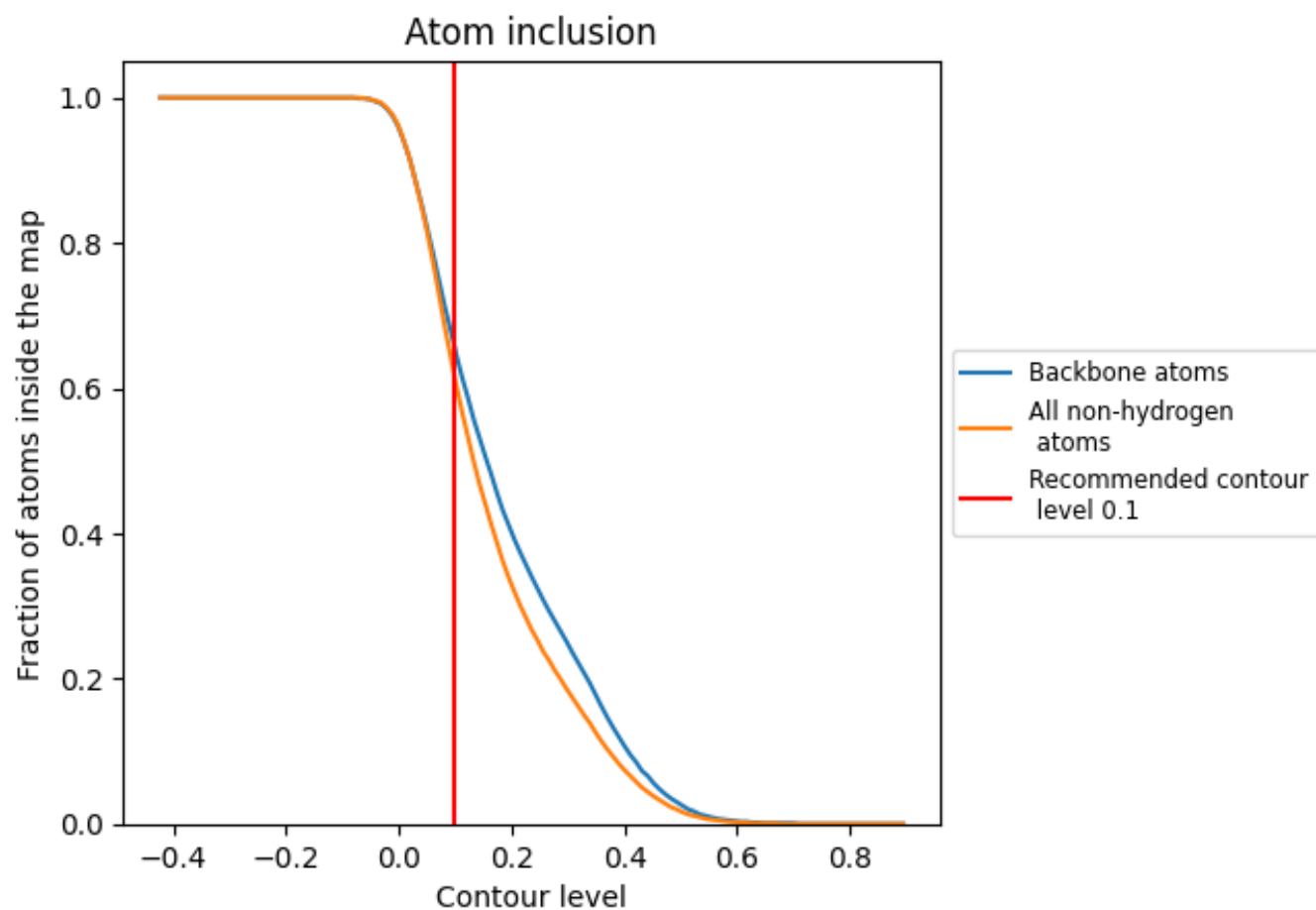
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 61% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6130	0.3140
A	0.8570	0.4270
B	0.7560	0.3810
C	0.8300	0.4090
D	0.0730	0.1000
E	0.7500	0.3650
F	0.7990	0.3860
G	0.1950	0.1130
H	0.6070	0.3760
I	0.8570	0.4830
J	0.6430	0.2910
K	0.6790	0.4300
L	0.8930	0.4500
M	0.5710	0.2810
N	0.6070	0.3400

1.0

0.0

<0.0