



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 07:16 PM UTC

PDB ID : 7UAP / pdb_00007uap
EMDB ID : EMD-26429
Title : Structure of the SARS-CoV-2 S 6P trimer in complex with the neutralizing antibody Fab fragment, C1520
Authors : Barnes, C.O.
Deposited on : 2022-03-13
Resolution : 2.80 Å(reported)
Based on initial model : 7RW2

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

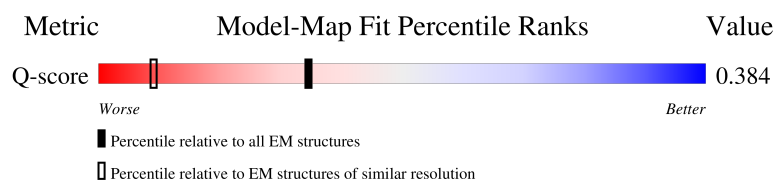
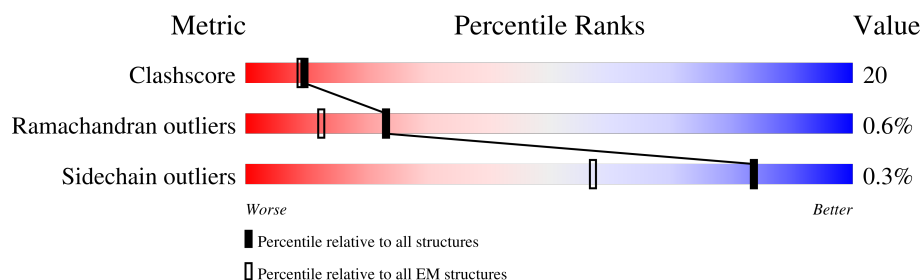
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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.



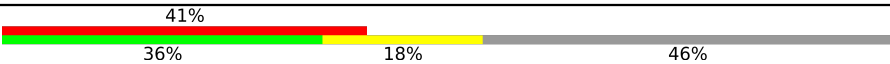
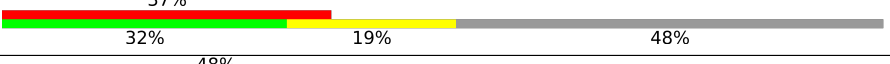
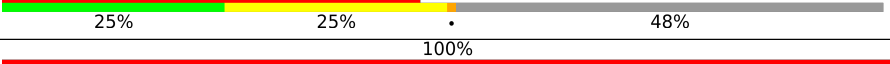
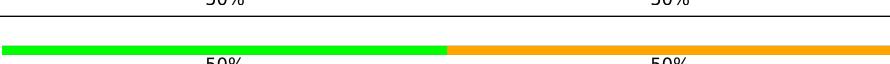
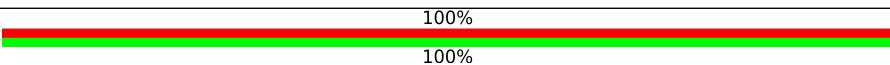
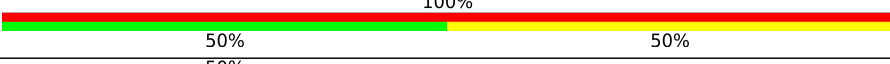
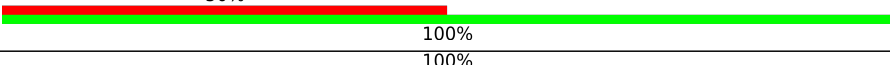
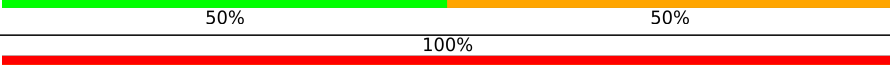
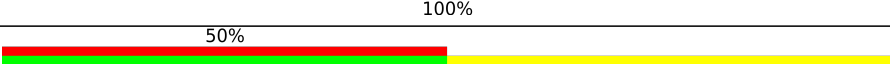
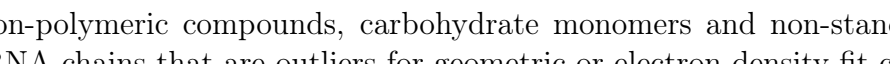
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	A	1256	7% 54% 31% • 14%
1	B	1256	10% 54% 31% • 14%
1	C	1256	14% 53% 31% • 14%
2	H	233	26% 32% 22% 46%

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Mol	Chain	Length	Quality of chain
2	M	233	
2	O	233	
3	L	217	
3	N	217	
3	P	217	
4	D	2	
4	E	2	
4	F	2	
4	G	2	
4	I	2	
4	J	2	
4	K	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	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
5	NAG	B	1301	-	-	X	-
5	NAG	P	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31657 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	A	1081	Total	C	N	O	S	0	0
			8447	5394	1412	1603	38		
1	B	1081	Total	C	N	O	S	0	0
			8447	5394	1412	1603	38		
1	C	1081	Total	C	N	O	S	0	0
			8447	5394	1412	1603	38		

There are 165 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	?	-	ARG	deletion	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1214	SER	-	expression tag	UNP P0DTC2
A	1215	GLY	-	expression tag	UNP P0DTC2
A	1216	ARG	-	expression tag	UNP P0DTC2
A	1217	LEU	-	expression tag	UNP P0DTC2
A	1218	VAL	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	GLY	-	expression tag	UNP P0DTC2
A	1222	SER	-	expression tag	UNP P0DTC2
A	1223	PRO	-	expression tag	UNP P0DTC2
A	1224	GLY	-	expression tag	UNP P0DTC2
A	1225	SER	-	expression tag	UNP P0DTC2
A	1226	GLY	-	expression tag	UNP P0DTC2
A	1227	TYR	-	expression tag	UNP P0DTC2
A	1228	ILE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1229	PRO	-	expression tag	UNP P0DTC2
A	1230	GLU	-	expression tag	UNP P0DTC2
A	1231	ALA	-	expression tag	UNP P0DTC2
A	1232	PRO	-	expression tag	UNP P0DTC2
A	1233	ARG	-	expression tag	UNP P0DTC2
A	1234	ASP	-	expression tag	UNP P0DTC2
A	1235	GLY	-	expression tag	UNP P0DTC2
A	1236	GLN	-	expression tag	UNP P0DTC2
A	1237	ALA	-	expression tag	UNP P0DTC2
A	1238	TYR	-	expression tag	UNP P0DTC2
A	1239	VAL	-	expression tag	UNP P0DTC2
A	1240	ARG	-	expression tag	UNP P0DTC2
A	1241	LYS	-	expression tag	UNP P0DTC2
A	1242	ASP	-	expression tag	UNP P0DTC2
A	1243	GLY	-	expression tag	UNP P0DTC2
A	1244	GLU	-	expression tag	UNP P0DTC2
A	1245	TRP	-	expression tag	UNP P0DTC2
A	1246	VAL	-	expression tag	UNP P0DTC2
A	1247	LEU	-	expression tag	UNP P0DTC2
A	1248	LEU	-	expression tag	UNP P0DTC2
A	1249	SER	-	expression tag	UNP P0DTC2
A	1250	THR	-	expression tag	UNP P0DTC2
A	1251	PHE	-	expression tag	UNP P0DTC2
A	1252	LEU	-	expression tag	UNP P0DTC2
A	1253	GLY	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	HIS	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	?	-	ARG	deletion	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1214	SER	-	expression tag	UNP P0DTC2
B	1215	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1216	ARG	-	expression tag	UNP P0DTC2
B	1217	LEU	-	expression tag	UNP P0DTC2
B	1218	VAL	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	GLY	-	expression tag	UNP P0DTC2
B	1222	SER	-	expression tag	UNP P0DTC2
B	1223	PRO	-	expression tag	UNP P0DTC2
B	1224	GLY	-	expression tag	UNP P0DTC2
B	1225	SER	-	expression tag	UNP P0DTC2
B	1226	GLY	-	expression tag	UNP P0DTC2
B	1227	TYR	-	expression tag	UNP P0DTC2
B	1228	ILE	-	expression tag	UNP P0DTC2
B	1229	PRO	-	expression tag	UNP P0DTC2
B	1230	GLU	-	expression tag	UNP P0DTC2
B	1231	ALA	-	expression tag	UNP P0DTC2
B	1232	PRO	-	expression tag	UNP P0DTC2
B	1233	ARG	-	expression tag	UNP P0DTC2
B	1234	ASP	-	expression tag	UNP P0DTC2
B	1235	GLY	-	expression tag	UNP P0DTC2
B	1236	GLN	-	expression tag	UNP P0DTC2
B	1237	ALA	-	expression tag	UNP P0DTC2
B	1238	TYR	-	expression tag	UNP P0DTC2
B	1239	VAL	-	expression tag	UNP P0DTC2
B	1240	ARG	-	expression tag	UNP P0DTC2
B	1241	LYS	-	expression tag	UNP P0DTC2
B	1242	ASP	-	expression tag	UNP P0DTC2
B	1243	GLY	-	expression tag	UNP P0DTC2
B	1244	GLU	-	expression tag	UNP P0DTC2
B	1245	TRP	-	expression tag	UNP P0DTC2
B	1246	VAL	-	expression tag	UNP P0DTC2
B	1247	LEU	-	expression tag	UNP P0DTC2
B	1248	LEU	-	expression tag	UNP P0DTC2
B	1249	SER	-	expression tag	UNP P0DTC2
B	1250	THR	-	expression tag	UNP P0DTC2
B	1251	PHE	-	expression tag	UNP P0DTC2
B	1252	LEU	-	expression tag	UNP P0DTC2
B	1253	GLY	-	expression tag	UNP P0DTC2
B	1254	HIS	-	expression tag	UNP P0DTC2
B	1255	HIS	-	expression tag	UNP P0DTC2
B	1256	HIS	-	expression tag	UNP P0DTC2
B	1257	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1258	HIS	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	?	-	ARG	deletion	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1214	SER	-	expression tag	UNP P0DTC2
C	1215	GLY	-	expression tag	UNP P0DTC2
C	1216	ARG	-	expression tag	UNP P0DTC2
C	1217	LEU	-	expression tag	UNP P0DTC2
C	1218	VAL	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	GLY	-	expression tag	UNP P0DTC2
C	1222	SER	-	expression tag	UNP P0DTC2
C	1223	PRO	-	expression tag	UNP P0DTC2
C	1224	GLY	-	expression tag	UNP P0DTC2
C	1225	SER	-	expression tag	UNP P0DTC2
C	1226	GLY	-	expression tag	UNP P0DTC2
C	1227	TYR	-	expression tag	UNP P0DTC2
C	1228	ILE	-	expression tag	UNP P0DTC2
C	1229	PRO	-	expression tag	UNP P0DTC2
C	1230	GLU	-	expression tag	UNP P0DTC2
C	1231	ALA	-	expression tag	UNP P0DTC2
C	1232	PRO	-	expression tag	UNP P0DTC2
C	1233	ARG	-	expression tag	UNP P0DTC2
C	1234	ASP	-	expression tag	UNP P0DTC2
C	1235	GLY	-	expression tag	UNP P0DTC2
C	1236	GLN	-	expression tag	UNP P0DTC2
C	1237	ALA	-	expression tag	UNP P0DTC2
C	1238	TYR	-	expression tag	UNP P0DTC2
C	1239	VAL	-	expression tag	UNP P0DTC2
C	1240	ARG	-	expression tag	UNP P0DTC2
C	1241	LYS	-	expression tag	UNP P0DTC2
C	1242	ASP	-	expression tag	UNP P0DTC2
C	1243	GLY	-	expression tag	UNP P0DTC2
C	1244	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1245	TRP	-	expression tag	UNP P0DTC2
C	1246	VAL	-	expression tag	UNP P0DTC2
C	1247	LEU	-	expression tag	UNP P0DTC2
C	1248	LEU	-	expression tag	UNP P0DTC2
C	1249	SER	-	expression tag	UNP P0DTC2
C	1250	THR	-	expression tag	UNP P0DTC2
C	1251	PHE	-	expression tag	UNP P0DTC2
C	1252	LEU	-	expression tag	UNP P0DTC2
C	1253	GLY	-	expression tag	UNP P0DTC2
C	1254	HIS	-	expression tag	UNP P0DTC2
C	1255	HIS	-	expression tag	UNP P0DTC2
C	1256	HIS	-	expression tag	UNP P0DTC2
C	1257	HIS	-	expression tag	UNP P0DTC2
C	1258	HIS	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called C1520 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	126	Total	C	N	O	S	0	0
			997	631	170	191	5		
2	M	126	Total	C	N	O	S	0	0
			997	631	170	191	5		
2	O	126	Total	C	N	O	S	0	0
			997	631	170	191	5		

- Molecule 3 is a protein called C1520 Fab Light Chain.

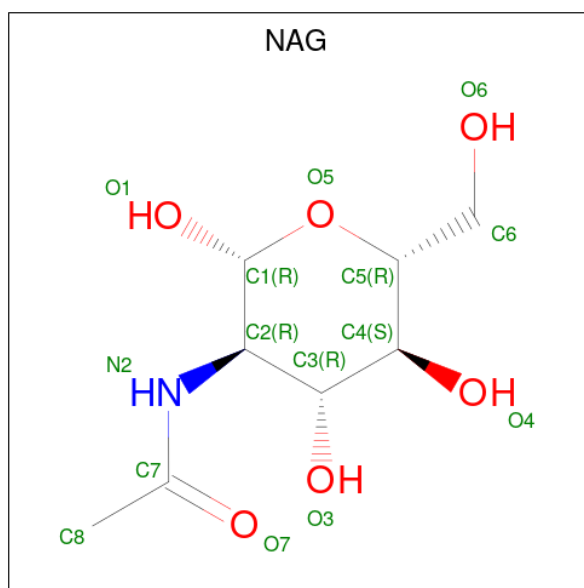
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	112	Total	C	N	O	S	0	0
			833	512	146	172	3		
3	N	112	Total	C	N	O	S	0	0
			833	512	146	172	3		
3	P	112	Total	C	N	O	S	0	0
			833	512	146	172	3		

- Molecule 4 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
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	L	1	Total	C	N	O	0
			14	8	1	5	
5	N	1	Total	C	N	O	0
			14	8	1	5	
5	P	1	Total	C	N	O	0
			14	8	1	5	

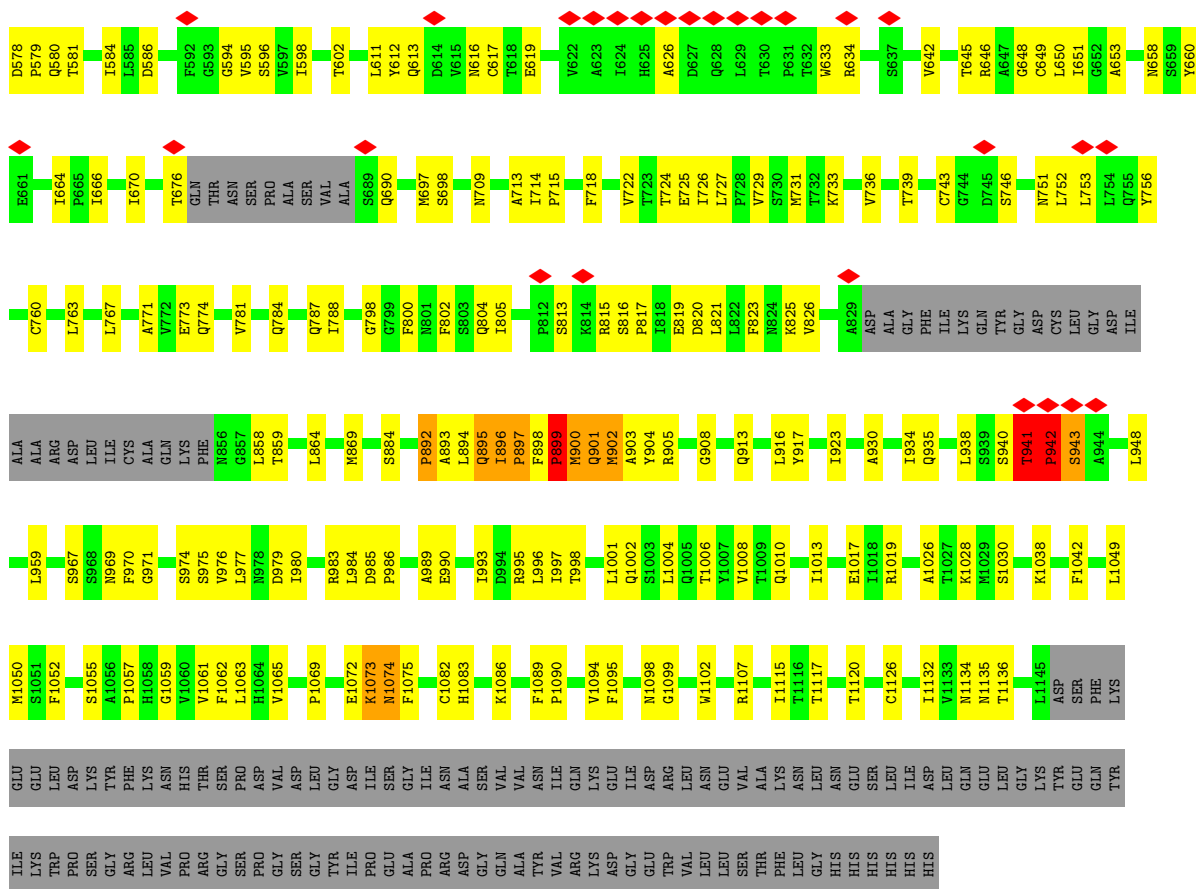
3 Residue-property plots

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.

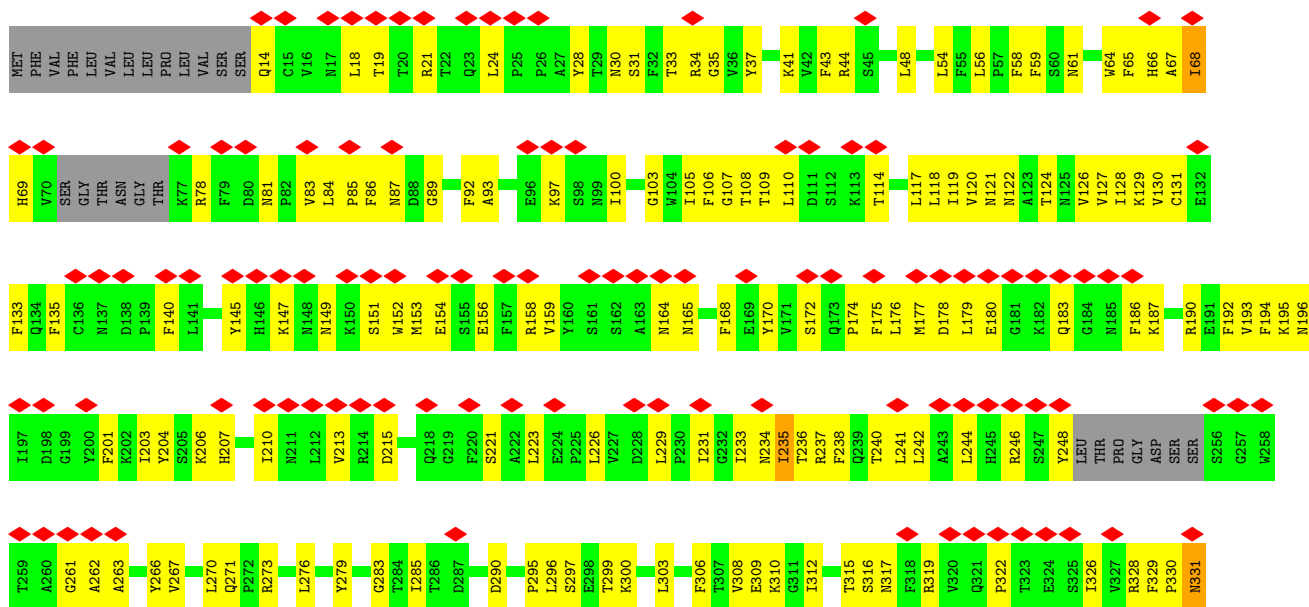
• Molecule 1: Spike glycoprotein





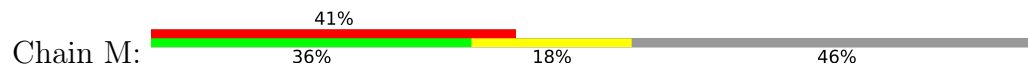


• Molecule 1: Spike glycoprotein



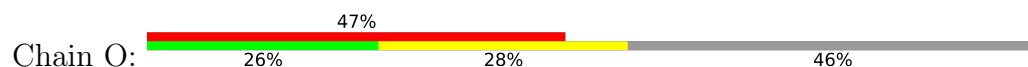
ALA	PRO	SER	SER	SER	LYS	SER	THR	SER	GLY	THR	GLY	THR	THR	ILE	CYS	ALA	ALA	LEU	GLY	CYS	VAL	VAL	LYS	ASP	LYS	THR	TYR	PHE	PRO	GLU	PRO	VAL	VAL	THR	VAL	THR	TRP	SER	ASN	SER	GLY	ALA	LYS	LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	ALA	VAL	GLN	SER	SER	GLY	LEU	TYR	SER	LEU	SER	SER	VAL	VAL	THR	VAL	VAL
PRO	SER	SER	SER	LEU	GLY	THR	GLN	THR	TYR	ILE	CYS	ASN	VAL	VAL	ASN	PRO	LYS	VAL	VAL	ASN	PRO	LYS	SER	ASP	LYS	THR	TYR	PHE	PRO	GLU	PRO	VAL	VAL	THR	VAL	THR	TRP	SER	ASN	SER	GLY	ALA	LYS	LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	ALA	VAL	GLN	SER	SER	GLY	LEU	TYR	SER	LEU	SER	SER	VAL	VAL	THR	VAL	VAL

• Molecule 2: C1520 Fab Heavy Chain



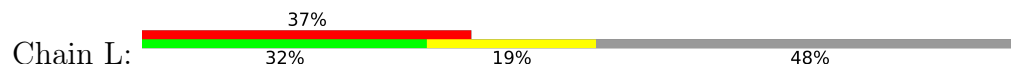
E1	V2	Q3	L4	V5	E6	S7	G8	G9	G10	L11	V12	Q13	P14	G15	G16	S17	L18	R19	L20	A21	C22	V23	A24	S25	G26	F27	T28	F29	S30	I31	Y32	E33	M34	N35	W36	V37	R38	Y39	Q39	A40	P41	G42	K43	G44	L45	E46	W47	V48	S49	Y50	T51	T52	T52A	S53	G54	H55	A56	R57	Y58	N59
A60	D61	S62	V63	K64	G65	R66	F67	T68	I69	D72	N73	S74	K75	N76	Y79	L80	Q81	M82	N82A	S82B	L82C	R83	A84	E85	D86	T87	A88	I89	Y90	Y91	C92	A93	R94	P95	Q96	Y97	H98	Y99	Y100	D101	T102	S103	H106	S107	Y108	G109	F110	D111	I112	W113	Q114	Q115	G116	T117	M118	V119				
T120	V121	S122	SER	ALA	THR	LYS	PRO	SER	VAL	PHE	PRO	LEU	ALA	PRO	SER	SER	LYS	THR	SER	THR	GLY	GLY	THR	ALA	ALA	GLY	CYS	LEU	VAL	LYS	ASP	THR	PHE	PRO	GLU	ARG	VAL	THR	SER	TRP	VAL	SER	LYS	ASP	GLY	ALA	LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	ALA	VAL			

• Molecule 2: C1520 Fab Heavy Chain

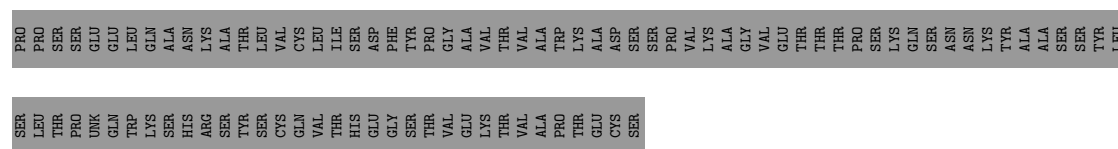


VAL	LEU	GLN	SER	SER	GLY	LEU	LEU	TYR	SER	THR	LYS	SER	GLY	SER	SER	VAL	VAL	THR	THR	PRO	PRO	VAL	LEU	ALA	SER	SER	SER	SER	LEU	GLY	THR	GLN	THR	THR	THR	LYS	VAL	ASP	ASN	PRO	PRO	LEU	SER	ASN	THR	LYS	VAL	PHE	ASP	LYS	ARG	GLU	GLU	PRO	PRO	LYS	SER	CYS	ASP	THR				
V119	T120	V121	S122	SER	ALA	ALA	SER	THR	THR	LYS	GLY	PRO	SER	VAL	VAL	PHE	PRO	PRO	PRO	LEU	ALA	ALA	PRO	SER	PRO	SER	SER	SER	GLY	LYS	SER	GLN	THR	THR	THR	TYR	GLY	THR	THR	ASP	TYR	PHE	PRO	GLU	PRO	VAL	THR	VAL	THR	TRP	ASN	SER	GLY	ALA	LEU	THR	SER	GLY	VAL	HIS	THR	PHE	PRO	ALA
D61	S62	V63	K64	G65	R66	F67	T68	I69	S70	R71	D72	N73	S74	K75	N76	S77	F78	Y79	L80	Q81	M82	N82A	S82B	L82C	R83	A84	E85	D86	T87	A88	I89	Y90	Y91	C92	A93	R94	P95	Q96	Y97	H98	Y99	T102	S103	T104	Y105	H106	S107	Y108	G109	F110	D111	I112	W113	G114	Q115	G116	T117	M118						
E1	V2	Q3	L4	V5	E6	S7	G8	G9	G10	L11	V12	Q13	P14	G15	G16	S17	L18	R19	L20	A21	C22	V23	A24	S25	G26	F27	T28	F29	S30	I31		M34	N35	W36	V37	R38	Q39	A40	P41	G42	K43	G44	L45	E46	W47	V48	S49	Y50	I51	T52	T52A	S53	G54	H55	A56	R57	Y58	N59	A60					

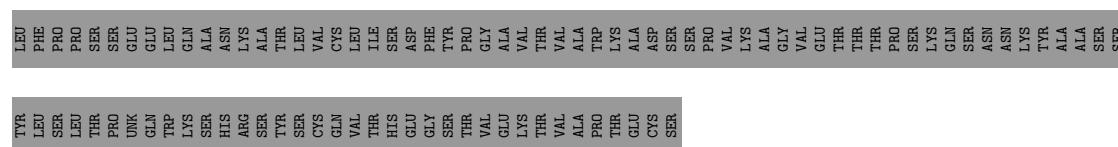
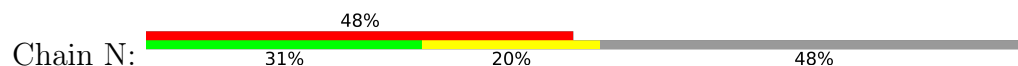
• Molecule 3: C1520 Fab Light Chain



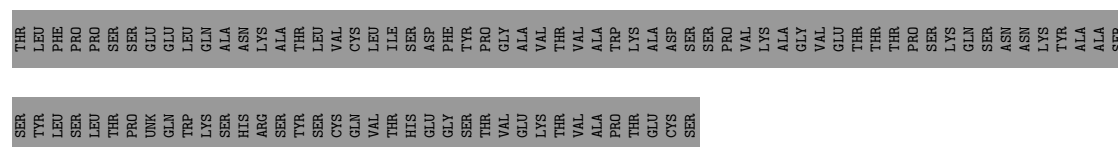
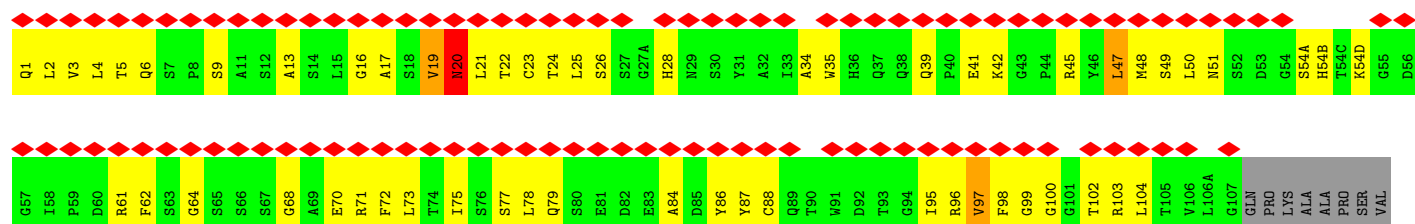
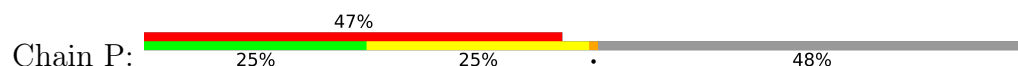
Q1	L2	V3	L4	T5	Q6	S7	P8	S9	A11	S12	A13	S14	L15	G16	A17	S18	V19	N20	L21	T22	C23	T24	L25	S26	H28	N29	S30	Y31	A34	W35	H36	Q37	Q38	Q39	P40	E41	K42	G43	P44	R45	Y46	L47	M48	S49	L50	N51	S52	D53	G54	S54A	H54B	T54C	K54D	G55	D56	G57	I58	
P59	D60	R61	F62	S63	G64	S65	S66	S67	G68	A69	E70	R71	F72	L73	T74	I75	S76	S77	L78	Q79	S80	E81	E82	E83	A84	D85	Y86	Y87	C88	Q89	W90	Y91	D92	I95	R96	V97	F98	G99	G100	G101	T102	R103	L104	T105	S49	V106	L106A	G107	GLN	PRO	LYS	ALA	PRO	SER	VAL	THR	LEU	PHE



• Molecule 3: C1520 Fab Light Chain



• Molecule 3: C1520 Fab Light Chain



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



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





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



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



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



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



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



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





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



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



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



- Molecule 4: 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, C1	Depositor
Number of particles used	524191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.084	Depositor
Minimum map value	-4.131	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.106	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	370.8, 370.8, 370.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	8/8649 (0.1%)	0.77	24/11782 (0.2%)
1	B	0.40	10/8649 (0.1%)	0.74	17/11782 (0.1%)
1	C	0.41	12/8649 (0.1%)	0.78	20/11782 (0.2%)
2	H	0.17	0/1024	0.45	0/1389
2	M	0.17	0/1024	0.46	0/1389
2	O	0.18	0/1024	0.54	0/1389
3	L	0.18	0/850	0.53	0/1153
3	N	0.19	0/850	0.50	0/1153
3	P	0.23	0/850	0.63	1/1153 (0.1%)
All	All	0.37	30/31569 (0.1%)	0.73	62/42972 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
3	P	0	3
All	All	0	5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	897	PRO	C-O	-13.85	1.06	1.23
1	A	897	PRO	C-O	-12.01	1.08	1.23
1	A	902	MET	C-O	-10.13	1.12	1.24
1	C	899	PRO	C-O	-10.09	1.10	1.24
1	C	897	PRO	C-O	-9.87	1.11	1.23
1	A	899	PRO	C-O	-9.85	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	899	PRO	C-O	-9.10	1.12	1.24
1	B	902	MET	C-O	-8.53	1.12	1.24
1	C	900	MET	C-O	-8.08	1.13	1.24
1	C	894	LEU	C-O	-7.55	1.15	1.24
1	C	902	MET	C-O	-7.55	1.14	1.24
1	C	892	PRO	C-O	-6.93	1.15	1.24
1	B	900	MET	C-O	-6.92	1.15	1.24
1	C	901	GLN	C-O	-6.71	1.15	1.24
1	B	942	PRO	N-CD	6.52	1.56	1.47
1	C	942	PRO	CA-C	6.37	1.61	1.52
1	A	901	GLN	C-O	-6.33	1.16	1.24
1	A	900	MET	C-O	-6.30	1.15	1.24
1	B	1073	LYS	C-O	-6.21	1.16	1.23
1	C	898	PHE	C-O	-5.93	1.18	1.24
1	C	942	PRO	N-CD	5.73	1.55	1.47
1	A	892	PRO	N-CD	5.65	1.55	1.47
1	B	896	ILE	C-O	-5.43	1.17	1.24
1	B	901	GLN	C-O	-5.41	1.17	1.24
1	C	893	ALA	CA-CB	-5.38	1.45	1.53
1	B	902	MET	C-N	-5.38	1.26	1.33
1	A	896	ILE	C-O	-5.31	1.17	1.24
1	A	902	MET	C-N	-5.31	1.26	1.34
1	C	896	ILE	C-O	-5.26	1.17	1.24
1	B	892	PRO	N-CD	5.21	1.55	1.47

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	CYS	CA-CB-SG	15.96	151.12	114.40
1	A	897	PRO	N-CA-CB	-15.85	90.00	103.32
1	A	525	CYS	CA-CB-SG	15.29	149.56	114.40
1	C	941	THR	C-N-CD	-12.78	72.58	125.00
1	B	941	THR	C-N-CD	-12.16	75.15	125.00
1	C	899	PRO	N-CA-CB	-10.47	93.01	103.48
1	B	432	CYS	CA-CB-SG	10.20	137.87	114.40
1	A	899	PRO	N-CA-CB	-9.60	93.17	103.25
1	C	432	CYS	CA-CB-SG	9.17	135.49	114.40
1	C	897	PRO	N-CA-CB	-8.81	95.49	103.25
1	C	943	SER	N-CA-C	-8.03	97.41	109.86
1	B	897	PRO	N-CA-CB	-7.64	96.53	103.25
1	C	649	CYS	CA-CB-SG	6.94	130.36	114.40
1	B	902	MET	N-CA-C	-6.52	104.36	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ASN	N-CA-C	6.50	121.05	113.18
1	A	167	THR	N-CA-C	6.48	121.55	112.93
1	A	165	ASN	CA-C-N	-6.46	112.52	122.09
1	A	165	ASN	C-N-CA	-6.46	112.52	122.09
1	A	147	LYS	CA-C-N	6.33	131.40	120.58
1	A	147	LYS	C-N-CA	6.33	131.40	120.58
1	B	1134	ASN	CB-CA-C	-6.29	98.19	109.71
1	B	899	PRO	N-CA-CB	-6.04	96.53	103.30
1	A	895	GLN	O-C-N	-6.04	115.91	122.79
1	A	942	PRO	N-CA-CB	5.98	109.53	103.25
1	A	1082	CYS	CA-CB-SG	5.97	128.14	114.40
3	P	20	ASN	N-CA-CB	5.87	118.94	110.37
1	A	943	SER	CA-C-N	-5.81	110.45	121.54
1	A	943	SER	C-N-CA	-5.81	110.45	121.54
1	B	895	GLN	O-C-N	-5.68	116.31	123.01
1	A	897	PRO	CA-N-CD	5.67	119.94	112.00
1	C	594	GLY	N-CA-C	5.67	126.63	113.18
1	C	901	GLN	CB-CA-C	-5.61	98.94	110.38
1	C	165	ASN	CA-C-N	-5.61	113.80	122.09
1	C	165	ASN	C-N-CA	-5.61	113.80	122.09
1	A	261	GLY	N-CA-C	5.53	122.97	112.62
1	A	525	CYS	CB-CA-C	5.46	121.12	110.30
1	C	899	PRO	N-CD-CG	-5.40	95.10	103.20
1	B	943	SER	N-CA-C	-5.37	102.03	110.36
1	C	67	ALA	CA-C-N	-5.37	116.09	122.11
1	C	67	ALA	C-N-CA	-5.37	116.09	122.11
1	A	1134	ASN	CB-CA-C	-5.35	100.02	109.70
1	C	68	ILE	N-CA-C	5.33	115.32	107.75
1	C	941	THR	N-CA-C	5.32	121.58	109.81
1	B	41	LYS	CA-CB-CG	-5.29	103.51	114.10
1	C	261	GLY	N-CA-C	5.28	122.49	112.62
1	B	261	GLY	N-CA-C	5.25	122.44	112.62
1	C	617	CYS	N-CA-C	5.23	117.89	111.82
1	B	901	GLN	CB-CA-C	-5.23	98.94	109.55
1	C	333	THR	N-CA-C	5.22	116.71	110.44
1	A	1099	GLY	N-CA-C	-5.21	100.84	113.18
1	C	895	GLN	O-C-N	-5.19	116.64	122.97
1	A	891	GLY	C-N-CD	-5.16	103.86	125.00
1	A	897	PRO	N-CD-CG	-5.13	95.50	103.20
1	B	147	LYS	CA-C-N	5.11	127.55	120.29
1	B	147	LYS	C-N-CA	5.11	127.55	120.29
1	A	717	ASN	N-CA-CB	-5.10	102.69	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	GLY	N-CA-C	5.09	125.25	113.18
1	A	898	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	68	ILE	CA-C-N	5.05	131.19	121.54
1	B	68	ILE	C-N-CA	5.05	131.19	121.54
1	B	1134	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	336	CYS	CA-CB-SG	5.01	125.92	114.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	940	SER	Mainchain
1	C	331	ASN	Peptide
3	P	19	VAL	Peptide
3	P	20	ASN	Peptide
3	P	47	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8447	0	8223	316	0
1	B	8447	0	8223	365	0
1	C	8447	0	8220	359	0
2	H	997	0	936	47	0
2	M	997	0	936	35	0
2	O	997	0	936	59	0
3	L	833	0	784	38	0
3	N	833	0	785	33	0
3	P	833	0	785	64	0
4	D	28	0	25	0	0
4	E	28	0	25	2	0
4	F	28	0	25	3	0
4	G	28	0	25	1	0
4	I	28	0	25	0	0
4	J	28	0	25	3	0
4	K	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	1	0
4	T	28	0	25	1	0
4	U	28	0	25	0	0
5	A	154	0	143	9	0
5	B	140	0	130	12	0
5	C	154	0	143	3	0
5	L	14	0	13	0	0
5	N	14	0	13	0	0
5	P	14	0	13	9	0
All	All	31657	0	30583	1235	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1235) 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:940:SER:O	1:B:942:PRO:HD2	1.47	1.14
1:B:892:PRO:HG3	1:C:1072:GLU:OE2	1.54	1.07
1:C:34:ARG:HH22	1:C:221:SER:HB2	1.26	0.98
1:B:941:THR:OG1	1:B:942:PRO:HD3	1.65	0.96
1:C:940:SER:O	1:C:942:PRO:HD2	1.65	0.95
1:B:28:TYR:HB3	5:B:1301:NAG:H3	1.49	0.95
1:B:940:SER:O	1:B:942:PRO:CD	2.14	0.94
1:C:126:VAL:HG23	1:C:174:PRO:HA	1.48	0.94
1:C:941:THR:OG1	1:C:942:PRO:HD3	1.67	0.94
1:A:68:ILE:HG21	1:A:263:ALA:H	1.33	0.93
1:B:126:VAL:HG23	1:B:174:PRO:HA	1.51	0.93
1:B:58:PHE:HD2	1:B:290:ASP:HB2	1.35	0.91
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.04	0.90
1:A:290:ASP:HB3	1:A:293:LEU:HD22	1.55	0.89
1:A:892:PRO:HG3	1:B:1072:GLU:OE1	1.74	0.87
1:A:825:LYS:HZ3	1:A:943:SER:HB3	1.39	0.87
1:A:940:SER:O	1:A:942:PRO:HD2	1.73	0.87
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.55	0.86
1:B:117:LEU:HD21	1:B:119:ILE:HG12	1.57	0.86
1:A:748:GLU:HG2	1:A:751:ASN:HB2	1.58	0.86
1:C:889:GLY:HA3	1:C:1034:LEU:HD12	1.56	0.86
1:B:379:CYS:HA	1:B:432:CYS:HB3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:A:231:ILE:HD12	1.59	0.85
1:B:892:PRO:CG	1:C:1072:GLU:OE2	2.25	0.84
1:B:1102:TRP:HB2	1:B:1135:ASN:HD22	1.39	0.84
1:C:379:CYS:HA	1:C:432:CYS:HB3	1.59	0.83
1:C:34:ARG:HE	1:C:35:GLY:H	1.26	0.83
1:B:68:ILE:HG12	1:B:262:ALA:HA	1.60	0.83
1:B:187:LYS:HZ3	1:B:212:LEU:H	1.25	0.82
2:O:37:VAL:HG13	2:O:45:LEU:HD13	1.62	0.81
1:B:33:THR:HA	1:B:58:PHE:HD1	1.42	0.81
1:C:121:ASN:HD22	1:C:176:LEU:HG	1.46	0.81
1:C:503:VAL:HA	1:C:506:GLN:HE21	1.46	0.81
1:A:1072:GLU:HG2	1:C:894:LEU:HD21	1.60	0.80
3:P:35:TRP:HE3	3:P:86:TYR:HB3	1.46	0.80
3:P:73:LEU:HG	5:P:301:NAG:H82	1.63	0.80
1:C:724:THR:HG23	1:C:934:ILE:HD11	1.64	0.79
3:P:5:THR:HB	3:P:24:THR:HB	1.64	0.78
1:A:804:GLN:O	1:A:817:PRO:HD2	1.84	0.78
1:C:940:SER:O	1:C:942:PRO:CD	2.32	0.77
1:A:752:LEU:HG	1:A:997:ILE:HD11	1.67	0.77
1:B:92:PHE:HE1	1:B:94:SER:HB3	1.50	0.77
2:H:19:ARG:HH22	2:H:81:GLN:HA	1.50	0.77
1:C:1052:PHE:HB2	1:C:1063:LEU:HB2	1.68	0.76
1:A:126:VAL:HB	1:A:174:PRO:HA	1.65	0.76
1:B:61:ASN:HB3	5:B:1301:NAG:H2	1.68	0.76
1:A:825:LYS:NZ	1:A:943:SER:HB3	2.01	0.75
3:P:50:LEU:HD22	3:P:73:LEU:HD11	1.68	0.75
1:A:121:ASN:HD21	1:A:175:PHE:HB2	1.50	0.75
1:C:746:SER:HB2	1:C:977:LEU:HD21	1.65	0.75
1:A:617:CYS:SG	1:A:644:GLN:NE2	2.60	0.74
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.18	0.74
3:L:34:ALA:HB3	3:L:89:GLN:HE21	1.52	0.74
1:A:177:MET:SD	1:A:179:LEU:HB2	2.28	0.74
1:A:616:ASN:HB3	1:A:619:GLU:OE1	1.86	0.74
3:N:85:ASP:HB2	3:N:103:ARG:HH21	1.52	0.73
1:B:983:ARG:HH11	1:C:517:LEU:HB2	1.53	0.73
1:B:613:GLN:HA	1:B:648:GLY:HA3	1.69	0.73
1:C:34:ARG:NH2	1:C:221:SER:HB2	2.03	0.73
1:B:553:THR:HG22	1:B:554:GLU:H	1.53	0.73
1:C:731:MET:HE3	1:C:1018:ILE:HG13	1.69	0.73
1:A:129:LYS:NZ	1:A:169:GLU:OE1	2.21	0.73
1:A:148:ASN:HB2	4:E:1:NAG:H81	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HB	1:C:395:VAL:HG13	1.70	0.73
1:A:1098:ASN:OD1	1:A:1099:GLY:N	2.20	0.73
1:C:69:HIS:HB2	1:C:78:ARG:HH21	1.52	0.73
1:A:197:ILE:HG12	1:A:202:LYS:HZ1	1.54	0.72
1:B:557:LYS:NZ	1:B:586:ASP:OD1	2.22	0.72
1:C:393:THR:OG1	1:C:521:PRO:O	2.07	0.72
1:B:331:ASN:HB3	1:B:580:GLN:HE22	1.54	0.72
1:C:908:GLY:O	1:C:1038:LYS:NZ	2.23	0.72
1:C:190:ARG:HG2	1:C:207:HIS:CD2	2.25	0.72
1:A:613:GLN:HA	1:A:648:GLY:HA3	1.72	0.72
1:B:201:PHE:HB3	1:B:229:LEU:HB2	1.70	0.72
1:B:342:PHE:HB3	5:B:1305:NAG:H83	1.71	0.72
1:C:328:ARG:HH12	1:C:534:VAL:HG23	1.54	0.72
3:P:51:ASN:ND2	3:P:54(A):SER:OG	2.22	0.72
1:B:20:THR:HG21	1:B:77:LYS:HG3	1.71	0.71
2:O:111:ASP:HB3	3:P:103:ARG:HH22	1.55	0.71
1:B:379:CYS:HA	1:B:432:CYS:CB	2.20	0.71
3:P:4:LEU:HD23	3:P:88:CYS:HB3	1.73	0.71
1:B:190:ARG:HG2	1:B:207:HIS:HD2	1.56	0.71
1:A:119:ILE:HD12	1:A:128:ILE:HD12	1.71	0.71
3:P:35:TRP:HB2	3:P:48:MET:HB3	1.73	0.71
3:P:62:PHE:CD1	3:P:75:ILE:HG12	2.25	0.71
1:A:763:LEU:HB2	1:A:1008:VAL:HG21	1.72	0.71
1:C:328:ARG:NH1	1:C:532:ASN:O	2.23	0.71
1:C:626:ALA:HA	1:C:629:LEU:HD13	1.73	0.71
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.72	0.71
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.72	0.71
1:A:128:ILE:HB	1:A:170:TYR:HB3	1.73	0.71
1:C:731:MET:HE1	1:C:1014:ARG:HB3	1.72	0.70
1:C:119:ILE:HD13	1:C:128:ILE:HD12	1.73	0.70
2:O:19:ARG:HH12	2:O:82:MET:H	1.40	0.70
1:B:146:HIS:HB3	4:J:1:NAG:C7	2.22	0.70
3:P:23:CYS:HB2	3:P:35:TRP:CZ2	2.27	0.70
1:B:798:GLY:HA3	1:B:899:PRO:HG3	1.72	0.70
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.23	0.70
1:C:992:GLN:OE1	1:C:995:ARG:NH2	2.25	0.70
1:A:197:ILE:HG12	1:A:202:LYS:NZ	2.06	0.70
1:A:892:PRO:CG	1:B:1072:GLU:OE1	2.39	0.70
1:B:121:ASN:HD22	1:B:176:LEU:HG	1.57	0.70
1:C:676:THR:HA	1:C:690:GLN:HA	1.73	0.70
1:C:310:LYS:HG3	1:C:600:PRO:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:64:GLY:HA3	5:P:301:NAG:H83	1.74	0.69
2:O:95:PRO:HG3	2:O:110:PHE:HE1	1.56	0.69
3:P:6:GLN:NE2	3:P:88:CYS:SG	2.64	0.69
1:C:804:GLN:O	1:C:817:PRO:HD2	1.92	0.69
1:A:383:SER:OG	1:C:988:GLU:OE2	2.11	0.69
1:B:126:VAL:CG2	1:B:174:PRO:HA	2.22	0.69
1:C:577:ARG:HH22	1:C:584:ILE:HA	1.57	0.69
1:C:984:LEU:HB3	1:C:989:ALA:HB2	1.75	0.69
1:C:317:ASN:OD1	1:C:319:ARG:NH1	2.25	0.69
3:P:97:VAL:HG12	3:P:99:GLY:H	1.57	0.69
1:B:1098:ASN:OD1	1:B:1099:GLY:N	2.25	0.69
1:B:190:ARG:HG2	1:B:207:HIS:CD2	2.29	0.68
1:B:372:ALA:HB2	5:B:1305:NAG:H81	1.75	0.68
1:C:100:ILE:HG21	1:C:263:ALA:HB2	1.75	0.68
1:B:895:GLN:NE2	1:C:1074:ASN:OD1	2.27	0.68
2:O:40:ALA:HB3	2:O:43:LYS:HB3	1.75	0.68
1:B:894:LEU:HD11	1:C:715:PRO:HD3	1.76	0.68
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	1.76	0.68
1:C:747:THR:OG1	1:C:748:GLU:OE2	2.12	0.68
2:H:37:VAL:HA	2:H:47:TRP:HA	1.76	0.67
1:A:328:ARG:NH1	1:A:531:THR:O	2.27	0.67
3:N:85:ASP:OD1	3:N:102:THR:N	2.21	0.67
1:B:58:PHE:HZ	1:B:288:ALA:HB3	1.58	0.67
1:B:81:ASN:O	1:B:239:GLN:NE2	2.28	0.67
2:O:52:THR:HG22	2:O:55:HIS:H	1.57	0.67
1:A:903:ALA:HB2	1:A:916:LEU:HD22	1.77	0.67
1:B:722:VAL:HG22	1:B:930:ALA:HB1	1.77	0.67
1:A:1072:GLU:HG2	1:C:894:LEU:CD2	2.25	0.67
1:B:859:THR:OG1	1:C:614:ASP:OD2	2.12	0.67
1:B:917:TYR:HD2	1:C:1089:PHE:HE2	1.43	0.67
1:B:967:SER:O	1:B:975:SER:OG	2.11	0.67
1:B:804:GLN:NE2	1:B:935:GLN:HE21	1.93	0.67
1:A:121:ASN:ND2	1:A:176:LEU:H	1.93	0.66
1:C:379:CYS:HA	1:C:432:CYS:CB	2.24	0.66
1:C:858:LEU:HD13	1:C:959:LEU:HD22	1.76	0.66
1:C:340:GLU:N	1:C:340:GLU:OE1	2.29	0.66
1:A:627:ASP:O	1:A:634:ARG:NH2	2.28	0.66
1:B:277:LEU:HD12	1:B:285:ILE:HG21	1.77	0.66
2:O:87:THR:OG1	2:O:121:VAL:O	2.13	0.66
1:A:562:PHE:HB2	1:C:41:LYS:HE3	1.76	0.66
5:A:1303:NAG:H82	1:B:557:LYS:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:LEU:HD13	1:B:959:LEU:HD22	1.77	0.66
1:C:980:ILE:HD11	1:C:992:GLN:HB3	1.77	0.66
1:A:293:LEU:O	1:A:632:THR:OG1	2.14	0.65
1:A:1072:GLU:CG	1:C:894:LEU:HD21	2.26	0.65
1:A:1090:PRO:O	1:C:913:GLN:NE2	2.28	0.65
1:B:107:GLY:O	1:B:236:THR:N	2.28	0.65
1:C:798:GLY:HA3	1:C:899:PRO:CG	2.26	0.65
1:B:977:LEU:HD13	1:B:996:LEU:HD23	1.78	0.65
1:A:34:ARG:NH2	1:A:191:GLU:OE1	2.29	0.65
1:A:676:THR:HA	1:A:690:GLN:HA	1.79	0.65
1:B:884:SER:OG	1:B:893:ALA:HB1	1.97	0.65
1:A:19:THR:HB	1:A:21:ARG:HG2	1.78	0.65
1:B:389:ASP:HA	1:B:528:LYS:NZ	2.10	0.65
1:A:119:ILE:CD1	1:A:128:ILE:HD12	2.27	0.65
1:A:976:VAL:HG12	1:B:571:ASP:HA	1.78	0.65
1:A:326:ILE:HG12	1:A:539:VAL:HG21	1.79	0.65
1:B:357:ARG:NH1	1:B:396:TYR:OH	2.29	0.65
2:O:75:LYS:NZ	2:O:79:TYR:OH	2.30	0.65
1:B:616:ASN:N	1:B:619:GLU:OE2	2.28	0.65
1:B:28:TYR:HB3	5:B:1301:NAG:HN2	1.62	0.65
2:H:58:TYR:HE1	2:H:69:ILE:H	1.44	0.65
2:O:86:ASP:OD2	2:O:90:TYR:OH	2.15	0.64
1:C:967:SER:O	1:C:975:SER:OG	2.13	0.64
1:B:178:ASP:O	1:B:188:ASN:ND2	2.30	0.64
1:C:384:PRO:HA	1:C:387:LEU:HD23	1.78	0.64
1:C:417:LYS:O	1:C:422:ASN:ND2	2.30	0.64
1:A:630:THR:OG1	1:A:633:TRP:HD1	1.80	0.64
1:B:612:TYR:O	1:B:649:CYS:N	2.26	0.64
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.13	0.64
3:N:85:ASP:HB2	3:N:103:ARG:HE	1.61	0.64
1:B:825:LYS:NZ	1:B:943:SER:OG	2.24	0.64
1:C:175:PHE:HA	1:C:226:LEU:HD21	1.79	0.64
1:B:896:ILE:HG13	1:B:897:PRO:HD2	1.80	0.64
2:O:96:GLN:NE2	2:O:106:HIS:O	2.30	0.64
1:B:28:TYR:CB	5:B:1301:NAG:H3	2.26	0.63
1:B:743:CYS:SG	1:B:752:LEU:HD22	2.38	0.63
1:C:153:MET:HE1	2:O:28:THR:HB	1.80	0.63
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	1.80	0.63
1:C:960:ASN:O	1:C:964:LYS:HD3	1.98	0.63
3:N:48:MET:HE1	3:N:54(C):THR:H	1.62	0.63
1:C:1079:PRO:HD2	1:C:1131:GLY:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:25:LEU:HD12	3:P:71:ARG:HH11	1.64	0.63
1:B:798:GLY:HA3	1:B:899:PRO:CG	2.29	0.63
1:C:14:GLN:O	1:C:158:ARG:HG2	1.99	0.63
1:C:598:ILE:HD13	1:C:650:LEU:HD11	1.81	0.63
1:A:1098:ASN:OD1	4:G:1:NAG:N2	2.31	0.63
1:B:392:PHE:N	1:B:524:VAL:O	2.32	0.63
2:H:15:GLY:N	2:H:82(C):LEU:O	2.32	0.63
1:A:902:MET:SD	1:A:1050:MET:HE1	2.39	0.62
1:B:901:GLN:HG2	1:B:901:GLN:O	1.98	0.62
1:B:739:THR:O	1:B:743:CYS:HB2	1.99	0.62
1:C:246:ARG:HG2	1:C:248:TYR:OH	1.99	0.62
1:B:290:ASP:O	1:B:297:SER:HB2	1.99	0.62
1:C:206:LYS:HB2	1:C:223:LEU:HA	1.80	0.62
1:C:577:ARG:HH22	1:C:584:ILE:HD12	1.63	0.62
3:L:15:LEU:HG	3:L:107:GLY:HA3	1.82	0.62
1:A:749:CYS:O	1:A:753:LEU:HB2	1.99	0.62
2:H:107:SER:O	3:L:91:TRP:NE1	2.32	0.62
3:L:97:VAL:HG12	3:L:99:GLY:H	1.64	0.62
1:B:19:THR:HB	1:B:21:ARG:HG2	1.81	0.62
2:O:5:VAL:HG23	2:O:23:VAL:HB	1.81	0.62
2:O:93:ALA:HB1	2:O:110:PHE:HB3	1.82	0.62
3:P:23:CYS:HB2	3:P:35:TRP:HZ2	1.63	0.62
1:C:309:GLU:HG3	1:C:310:LYS:H	1.64	0.62
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.82	0.61
1:C:328:ARG:NH1	1:C:534:VAL:HG23	2.15	0.61
2:M:31:ILE:HG21	2:M:98:HIS:CE1	2.34	0.61
3:P:96:ARG:O	3:P:98:PHE:N	2.33	0.61
1:A:277:LEU:HD12	1:A:285:ILE:HD13	1.82	0.61
1:A:431:GLY:HA2	1:A:515:PHE:HD2	1.65	0.61
1:C:353:TRP:HZ3	1:C:355:ARG:HE	1.46	0.61
1:A:156:GLU:OE2	1:A:158:ARG:NE	2.33	0.61
1:B:34:ARG:NH2	1:B:217:PRO:O	2.33	0.61
1:A:68:ILE:HG12	1:A:262:ALA:HA	1.81	0.61
1:B:66:HIS:HB2	1:B:264:ALA:HA	1.82	0.61
1:B:289:VAL:HG23	1:B:306:PHE:CE1	2.35	0.61
1:C:773:GLU:OE2	1:C:1019:ARG:NH1	2.24	0.61
1:A:200:TYR:O	1:A:202:LYS:NZ	2.34	0.61
3:P:39:GLN:HG3	3:P:42:LYS:HB2	1.82	0.61
3:L:92:ASP:HB3	3:L:95:ILE:HB	1.81	0.60
1:A:567:ARG:HG3	1:A:573:THR:HA	1.82	0.60
1:B:187:LYS:NZ	1:B:212:LEU:H	1.97	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:58:TYR:HE1	2:M:69:ILE:HG22	1.65	0.60
3:N:15:LEU:HG	3:N:107:GLY:HA3	1.84	0.60
1:B:177:MET:HE1	1:B:179:LEU:HD13	1.82	0.60
1:B:940:SER:C	1:B:942:PRO:HD2	2.22	0.60
1:A:543:PHE:O	1:A:546:LEU:HG	2.01	0.60
1:C:48:LEU:HD12	1:C:276:LEU:HD21	1.82	0.60
1:C:355:ARG:HH11	1:C:396:TYR:HD2	1.49	0.60
2:H:9:GLY:HA2	2:H:119:VAL:HG22	1.83	0.60
1:A:292:ALA:C	1:A:633:TRP:HE1	2.09	0.60
1:C:117:LEU:HD11	1:C:119:ILE:HG12	1.84	0.60
1:A:81:ASN:O	1:A:239:GLN:NE2	2.34	0.60
1:A:735:SER:OG	1:A:859:THR:OG1	2.20	0.60
1:B:948:LEU:HD21	1:B:1059:GLY:HA3	1.84	0.60
1:C:616:ASN:HB3	1:C:619:GLU:OE1	2.01	0.60
3:L:4:LEU:HD22	3:L:100:GLY:H	1.64	0.60
3:P:19:VAL:O	3:P:75:ILE:HG13	2.01	0.60
1:C:83:VAL:HB	1:C:237:ARG:HG2	1.84	0.60
1:C:100:ILE:HG13	1:C:262:ALA:O	2.02	0.60
1:C:718:PHE:CZ	1:C:923:ILE:HD11	2.37	0.60
1:A:14:GLN:O	1:A:158:ARG:HG2	2.01	0.59
1:C:109:THR:OG1	1:C:114:THR:OG1	2.20	0.59
1:A:552:LEU:HD12	1:A:585:LEU:HD13	1.84	0.59
1:A:760:CYS:HA	1:A:763:LEU:HG	1.84	0.59
1:B:497:PHE:CG	1:B:507:PRO:HG3	2.37	0.59
1:B:676:THR:HA	1:B:690:GLN:HA	1.84	0.59
1:C:312:ILE:HD12	1:C:598:ILE:HG22	1.83	0.59
2:H:31:ILE:HB	2:H:99:TYR:HB3	1.84	0.59
2:O:51:ILE:HG21	2:O:71:ARG:HB2	1.84	0.59
1:A:371:SER:HB3	5:A:1305:NAG:H61	1.83	0.59
1:B:121:ASN:ND2	1:B:176:LEU:HG	2.17	0.59
1:C:433:VAL:HG23	1:C:512:VAL:HG22	1.83	0.59
1:B:940:SER:C	1:B:942:PRO:CD	2.74	0.59
2:O:67:PHE:HD1	2:O:82:MET:HE1	1.68	0.59
1:B:21:ARG:NH1	1:B:80:ASP:OD1	2.36	0.59
1:B:69:HIS:HB2	1:B:78:ARG:HH21	1.67	0.59
1:B:148:ASN:HB2	4:J:1:NAG:C7	2.33	0.59
3:N:37:GLN:O	3:N:45:ARG:N	2.30	0.59
3:N:85:ASP:HB2	3:N:103:ARG:NH2	2.17	0.59
1:A:869:MET:HE1	1:B:697:MET:HG2	1.84	0.59
1:C:739:THR:O	1:C:744:GLY:N	2.25	0.59
1:A:497:PHE:CG	1:A:507:PRO:HG3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ASN:OD1	5:A:1308:NAG:N2	2.35	0.59
1:A:948:LEU:HD21	1:A:1059:GLY:HA3	1.85	0.59
1:B:501:ASN:ND2	1:B:505:TYR:O	2.35	0.59
1:B:941:THR:CB	1:B:942:PRO:HD3	2.13	0.59
1:C:140:PHE:HB2	1:C:244:LEU:HD23	1.85	0.59
1:C:462:LYS:HG2	1:C:465:GLU:OE1	2.03	0.59
3:N:6:GLN:NE2	3:N:88:CYS:SG	2.75	0.59
1:A:386:LYS:NZ	1:C:985:ASP:HA	2.18	0.59
1:A:913:GLN:NE2	1:B:1090:PRO:HD2	2.17	0.59
1:B:109:THR:OG1	1:B:114:THR:OG1	2.18	0.59
1:B:502:GLY:O	1:B:506:GLN:HG3	2.03	0.59
1:B:626:ALA:O	1:B:634:ARG:NE	2.36	0.59
1:B:751:ASN:OD1	1:B:752:LEU:N	2.36	0.59
1:C:145:TYR:O	1:C:147:LYS:NZ	2.36	0.59
1:B:1052:PHE:HB2	1:B:1063:LEU:HB2	1.85	0.58
1:C:130:VAL:HG21	1:C:231:ILE:HG23	1.85	0.58
1:C:201:PHE:CE2	1:C:203:ILE:HD11	2.38	0.58
1:C:246:ARG:HG2	1:C:248:TYR:CZ	2.38	0.58
2:H:37:VAL:HG11	2:H:113:TRP:HZ3	1.67	0.58
3:N:85:ASP:CB	3:N:103:ARG:HH21	2.16	0.58
3:N:97:VAL:HG12	3:N:99:GLY:H	1.67	0.58
4:T:1:NAG:H61	4:T:2:NAG:H82	1.84	0.58
1:A:41:LYS:NZ	1:B:562:PHE:HB2	2.18	0.58
3:P:2:LEU:HD22	3:P:97:VAL:HG11	1.84	0.58
1:A:825:LYS:HZ2	1:A:941:THR:H	1.51	0.58
1:B:722:VAL:HG12	1:B:1065:VAL:HB	1.84	0.58
1:C:736:VAL:O	1:C:764:ASN:ND2	2.34	0.58
2:H:47:TRP:HB3	3:L:98:PHE:HE2	1.68	0.58
1:B:433:VAL:HG12	1:B:512:VAL:HG13	1.84	0.58
1:B:559:PHE:HZ	1:B:575:ALA:HB1	1.68	0.58
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.32	0.58
1:C:68:ILE:HD13	1:C:262:ALA:HA	1.84	0.58
2:O:87:THR:HG23	2:O:120:THR:HA	1.86	0.58
3:P:95:ILE:HG22	3:P:97:VAL:H	1.69	0.58
5:P:301:NAG:O7	5:P:301:NAG:O3	2.12	0.58
1:A:384:PRO:HA	1:A:387:LEU:HG	1.84	0.58
1:A:485:GLY:H	1:A:488:CYS:HB2	1.69	0.58
1:A:502:GLY:O	1:A:506:GLN:HG3	2.04	0.58
1:B:27:ALA:O	1:B:64:TRP:HB3	2.03	0.58
1:A:1089:PHE:HE2	1:C:917:TYR:HD2	1.51	0.58
1:B:800:PHE:HE2	1:B:923:ILE:HG22	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:PHE:HB3	1:C:236:THR:HA	1.85	0.58
2:M:82:MET:HE2	2:M:82(C):LEU:HD23	1.84	0.58
1:C:362:VAL:HA	1:C:525:CYS:O	2.03	0.58
3:P:22:THR:OG1	3:P:71:ARG:O	2.22	0.58
1:A:68:ILE:HG21	1:A:263:ALA:N	2.14	0.57
1:B:100:ILE:HG22	1:B:242:LEU:HD22	1.85	0.57
2:O:9:GLY:HA2	2:O:119:VAL:HG22	1.86	0.57
2:O:12:VAL:HG11	2:O:18:LEU:HD11	1.85	0.57
1:A:1141:LEU:HD23	1:A:1145:LEU:HD23	1.87	0.57
1:C:766:ALA:HB1	1:C:1012:LEU:HD21	1.86	0.57
2:M:36:TRP:CD1	2:M:80:LEU:HD13	2.38	0.57
1:C:126:VAL:CG2	1:C:174:PRO:HA	2.27	0.57
1:A:967:SER:O	1:A:975:SER:OG	2.19	0.57
1:C:658:ASN:OD1	1:C:659:SER:N	2.36	0.57
2:H:32:TYR:CZ	2:H:98:HIS:HB3	2.39	0.57
3:P:39:GLN:HA	3:P:84:ALA:HA	1.86	0.57
1:A:277:LEU:HD12	1:A:285:ILE:HG21	1.84	0.57
2:M:4:LEU:HB2	2:M:114:GLY:HA2	1.86	0.57
1:C:109:THR:HA	1:C:237:ARG:HH12	1.70	0.57
3:L:96:ARG:O	3:L:98:PHE:N	2.38	0.57
1:A:826:VAL:HB	1:A:1057:PRO:HG2	1.87	0.57
1:B:612:TYR:HE1	1:B:651:ILE:HD11	1.68	0.57
1:C:798:GLY:HA3	1:C:899:PRO:HG3	1.86	0.57
1:A:711:SER:O	1:C:897:PRO:HD3	2.04	0.57
1:B:26:PRO:HG2	1:B:28:TYR:CE1	2.40	0.57
1:C:92:PHE:HB3	1:C:192:PHE:HB2	1.86	0.57
1:C:948:LEU:HD21	1:C:1059:GLY:HA3	1.85	0.57
2:H:38:ARG:O	2:H:46:GLU:N	2.36	0.57
1:B:578:ASP:OD1	1:B:581:THR:HG22	2.04	0.57
1:B:898:PHE:CZ	1:B:1050:MET:HE1	2.39	0.57
1:C:124:THR:OG1	2:O:52(A):THR:O	2.22	0.57
1:B:566:GLY:HA3	1:B:575:ALA:HB3	1.86	0.56
1:A:571:ASP:HA	1:C:976:VAL:HG12	1.86	0.56
1:B:119:ILE:HD13	1:B:128:ILE:HD12	1.87	0.56
1:B:339:GLY:O	1:B:343:ASN:HB2	2.05	0.56
1:B:869:MET:HE1	1:C:697:MET:HG2	1.87	0.56
1:C:183:GLN:HB2	3:P:28:HIS:CD2	2.40	0.56
1:C:889:GLY:CA	1:C:1034:LEU:HD12	2.31	0.56
1:A:203:ILE:HG22	1:A:226:LEU:HD12	1.88	0.56
1:B:58:PHE:CD2	1:B:290:ASP:HB2	2.27	0.56
1:B:485:GLY:H	1:B:488:CYS:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:THR:HB	2:H:121:VAL:H	1.70	0.56
2:O:16:GLY:O	2:O:82(B):SER:N	2.27	0.56
1:A:41:LYS:HZ2	1:B:562:PHE:HB2	1.70	0.56
1:C:577:ARG:HH12	1:C:584:ILE:HA	1.70	0.56
1:C:707:TYR:CG	1:C:707:TYR:O	2.59	0.56
2:O:80:LEU:O	2:O:82:MET:HG2	2.05	0.56
1:A:173:GLN:HG3	1:A:174:PRO:HD2	1.87	0.56
1:C:106:PHE:HB2	1:C:117:LEU:HD23	1.87	0.56
1:C:196:ASN:ND2	1:C:234:ASN:O	2.39	0.56
1:C:645:THR:OG1	1:C:648:GLY:O	2.14	0.56
1:A:665:PRO:HB3	1:C:864:LEU:HD13	1.88	0.56
1:A:725:GLU:HB3	1:A:1062:PHE:HB2	1.88	0.56
1:B:905:ARG:HD3	1:B:1049:LEU:O	2.05	0.56
2:O:111:ASP:O	3:P:103:ARG:NH2	2.39	0.56
1:C:68:ILE:HG23	1:C:69:HIS:CD2	2.39	0.56
1:C:827:THR:O	1:C:949:GLN:NE2	2.36	0.56
1:C:739:THR:HA	1:C:743:CYS:HB3	1.88	0.56
1:B:68:ILE:HG13	1:B:69:HIS:N	2.20	0.56
1:C:246:ARG:CG	1:C:248:TYR:CZ	2.89	0.56
3:L:25:LEU:HD21	3:L:28:HIS:HB2	1.87	0.56
1:C:392:PHE:N	1:C:524:VAL:O	2.39	0.55
1:B:718:PHE:CZ	1:B:923:ILE:HD11	2.42	0.55
3:N:19:VAL:HG22	3:N:75:ILE:HB	1.87	0.55
1:C:300:LYS:HE2	1:C:306:PHE:HA	1.88	0.55
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.89	0.55
1:B:746:SER:HB2	1:B:977:LEU:HD23	1.88	0.55
1:C:35:GLY:HA3	1:C:56:LEU:HB3	1.87	0.55
5:P:301:NAG:HO3	5:P:301:NAG:C7	2.16	0.55
1:B:804:GLN:O	1:B:817:PRO:HD2	2.07	0.55
2:H:32:TYR:CE1	2:H:98:HIS:HB3	2.42	0.55
2:O:4:LEU:HD21	2:O:34:MET:HE1	1.88	0.55
1:A:290:ASP:O	1:A:297:SER:HB2	2.07	0.55
1:B:984:LEU:O	1:C:386:LYS:NZ	2.35	0.55
1:C:331:ASN:O	1:C:332:ILE:HG23	2.07	0.55
3:N:6:GLN:OE1	3:N:102:THR:HG23	2.07	0.55
3:P:13:ALA:HB3	3:P:17:ALA:HB2	1.88	0.55
1:A:781:VAL:HG22	1:A:1026:ALA:HB2	1.87	0.55
1:C:110:LEU:HB2	1:C:237:ARG:NH2	2.22	0.55
1:C:378:LYS:O	1:C:432:CYS:HB2	2.07	0.55
2:M:75:LYS:O	2:M:75:LYS:HD3	2.07	0.55
3:P:35:TRP:HA	3:P:87:TYR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:HD11	1:A:665:PRO:O	2.08	0.54
1:A:326:ILE:HD12	1:A:532:ASN:O	2.07	0.54
1:A:756:TYR:HB3	1:A:1001:LEU:HD11	1.88	0.54
1:B:106:PHE:CD1	1:B:238:PHE:HB2	2.42	0.54
1:B:244:LEU:HD12	1:B:259:THR:HA	1.89	0.54
1:B:389:ASP:HA	1:B:528:LYS:HZ1	1.70	0.54
3:P:54(B):HIS:CE1	5:P:301:NAG:H3	2.42	0.54
1:B:568:ASP:OD1	1:B:569:ILE:N	2.37	0.54
1:C:97:LYS:O	2:O:105:TYR:OH	2.11	0.54
1:C:201:PHE:HB3	1:C:229:LEU:HB2	1.87	0.54
1:C:1093:GLY:HA2	1:C:1107:ARG:HD2	1.89	0.54
1:B:34:ARG:HG2	1:B:216:LEU:HD12	1.89	0.54
1:B:537:LYS:N	1:B:551:VAL:HG23	2.22	0.54
1:C:798:GLY:HA3	1:C:899:PRO:HG2	1.89	0.54
2:M:40:ALA:HB3	2:M:43:LYS:HB2	1.87	0.54
4:F:1:NAG:H83	4:F:1:NAG:H3	1.89	0.54
1:B:108:THR:HG23	1:B:236:THR:HG22	1.89	0.54
1:B:666:ILE:HG21	1:B:670:ILE:HD11	1.89	0.54
1:B:731:MET:N	1:B:774:GLN:OE1	2.39	0.54
1:C:898:PHE:HB3	1:C:899:PRO:HD3	1.89	0.54
3:L:6:GLN:OE1	3:L:102:THR:OG1	2.24	0.54
2:M:50:TYR:OH	2:M:57:ARG:NH2	2.40	0.54
1:A:177:MET:HE1	1:A:179:LEU:HD13	1.88	0.54
1:A:462:LYS:HB2	1:A:465:GLU:CD	2.33	0.54
1:C:110:LEU:O	1:C:135:PHE:HB2	2.08	0.54
1:C:564:GLN:HA	1:C:577:ARG:CG	2.37	0.54
1:C:814:LYS:HE2	1:C:872:GLN:HG3	1.89	0.54
2:O:36:TRP:NE1	2:O:80:LEU:HB2	2.23	0.54
3:P:20:ASN:OD1	3:P:73:LEU:HB3	2.08	0.54
1:A:205:SER:O	1:A:224:GLU:N	2.41	0.54
1:A:898:PHE:HB3	1:A:899:PRO:HD3	1.89	0.54
1:B:347:PHE:HD2	1:B:401:VAL:HG23	1.72	0.54
1:B:913:GLN:NE2	1:C:1090:PRO:HD2	2.22	0.54
3:P:61:ARG:CZ	3:P:79:GLN:HG3	2.38	0.54
1:A:122:ASN:CG	1:A:123:ALA:H	2.16	0.54
1:A:989:ALA:O	1:A:993:ILE:HG12	2.08	0.54
1:A:1079:PRO:HB3	1:C:917:TYR:CE2	2.43	0.54
1:C:722:VAL:HG12	1:C:1065:VAL:HG22	1.89	0.54
1:B:28:TYR:HB3	5:B:1301:NAG:N2	2.22	0.54
1:B:33:THR:HA	1:B:58:PHE:CD1	2.33	0.54
1:B:110:LEU:HB2	1:B:237:ARG:NH2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:SER:HB3	1:B:980:ILE:HG23	1.90	0.54
1:C:296:LEU:HD13	1:C:608:VAL:HG21	1.90	0.54
1:C:804:GLN:HE22	1:C:935:GLN:HE21	1.55	0.54
2:M:47:TRP:CH2	2:M:57:ARG:HD2	2.43	0.54
3:N:96:ARG:O	3:N:98:PHE:N	2.40	0.54
1:C:1008:VAL:O	1:C:1012:LEU:HG	2.09	0.53
1:A:386:LYS:HZ3	1:C:985:ASP:HA	1.72	0.53
1:B:998:THR:O	1:B:1002:GLN:NE2	2.41	0.53
1:A:44:ARG:HH22	1:B:570:ALA:HB2	1.72	0.53
1:B:311:GLY:HA2	1:B:664:ILE:HG21	1.89	0.53
1:C:625:HIS:O	1:C:628:GLN:HG2	2.09	0.53
3:P:54(B):HIS:CD2	3:P:54(D):LYS:HE3	2.43	0.53
1:C:309:GLU:HG3	1:C:310:LYS:N	2.23	0.53
1:C:577:ARG:NH2	1:C:584:ILE:HA	2.21	0.53
2:O:18:LEU:HD13	2:O:82(C):LEU:HD12	1.90	0.53
2:O:36:TRP:CD1	2:O:80:LEU:HB2	2.43	0.53
3:P:72:PHE:C	3:P:73:LEU:HD12	2.33	0.53
1:C:30:ASN:OD1	1:C:59:PHE:HA	2.08	0.53
1:C:100:ILE:HG22	1:C:242:LEU:HD22	1.90	0.53
1:C:195:LYS:HE2	1:C:204:TYR:HE1	1.73	0.53
1:C:462:LYS:HD3	4:K:1:NAG:H83	1.89	0.53
1:B:819:GLU:OE2	1:B:1055:SER:OG	2.24	0.53
1:C:497:PHE:CG	1:C:507:PRO:HG3	2.44	0.53
1:C:552:LEU:HD13	1:C:585:LEU:HD22	1.90	0.53
2:H:4:LEU:HD23	2:H:24:ALA:HB2	1.90	0.53
3:N:13:ALA:HB3	3:N:19:VAL:HG12	1.90	0.53
3:N:34:ALA:N	3:N:89:GLN:O	2.41	0.53
1:A:417:LYS:O	1:A:422:ASN:ND2	2.41	0.53
1:B:201:PHE:HD2	1:B:229:LEU:HD12	1.74	0.53
1:C:1006:THR:O	1:C:1010:GLN:HG2	2.09	0.53
1:A:121:ASN:HD22	1:A:176:LEU:H	1.57	0.53
1:A:230:PRO:HG3	1:B:396:TYR:OH	2.08	0.53
1:B:746:SER:HB2	1:B:977:LEU:CD2	2.39	0.53
3:N:95:ILE:HG12	3:N:97:VAL:H	1.73	0.53
1:B:34:ARG:NH2	1:B:217:PRO:HG2	2.24	0.52
1:B:616:ASN:O	1:B:617:CYS:HB2	2.09	0.52
2:O:66:ARG:HD2	2:O:83:ARG:HG3	1.91	0.52
1:A:985:ASP:OD2	1:B:383:SER:OG	2.16	0.52
1:C:296:LEU:O	1:C:300:LYS:HG3	2.08	0.52
2:H:29:PHE:HD2	2:H:76:ASN:HD22	1.56	0.52
3:N:36:HIS:O	3:N:87:TYR:N	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:63:VAL:HG22	2:O:66:ARG:H	1.74	0.52
1:A:798:GLY:HA3	1:A:899:PRO:HG3	1.91	0.52
1:B:864:LEU:HD13	1:C:665:PRO:HB3	1.90	0.52
1:C:107:GLY:O	1:C:236:THR:N	2.35	0.52
1:C:121:ASN:ND2	1:C:176:LEU:HG	2.20	0.52
1:A:631:PRO:HA	1:A:634:ARG:HB2	1.92	0.52
1:B:193:VAL:HB	1:B:204:TYR:HB2	1.91	0.52
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.21	0.52
1:C:1076:THR:HB	1:C:1097:SER:HB3	1.92	0.52
1:A:193:VAL:HG13	1:A:270:LEU:HD11	1.89	0.52
1:A:1040:VAL:HG23	1:C:1030:SER:O	2.10	0.52
1:B:781:VAL:HG22	1:B:1026:ALA:HB2	1.91	0.52
1:B:940:SER:O	1:B:942:PRO:HD3	2.06	0.52
1:C:31:SER:HB2	1:C:34:ARG:HB3	1.91	0.52
1:C:193:VAL:HB	1:C:204:TYR:HB2	1.91	0.52
1:C:773:GLU:OE2	1:C:1019:ARG:HD3	2.09	0.52
2:H:38:ARG:N	2:H:46:GLU:O	2.32	0.52
2:M:86:ASP:HB3	2:M:90:TYR:OH	2.10	0.52
1:C:303:LEU:HD12	1:C:308:VAL:HG12	1.91	0.52
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.91	0.52
3:P:50:LEU:HD13	5:P:301:NAG:H81	1.91	0.52
1:A:238:PHE:HZ	1:A:267:VAL:HG11	1.74	0.52
2:O:103:SER:OG	2:O:104:THR:N	2.43	0.52
1:A:922:LEU:HD11	5:A:1308:NAG:H5	1.91	0.52
1:A:1049:LEU:HD21	1:A:1067:TYR:HB2	1.91	0.52
1:B:442:ASP:OD2	1:B:451:TYR:OH	2.27	0.52
1:C:1029:MET:O	1:C:1034:LEU:HD23	2.09	0.52
5:C:1311:NAG:O7	5:C:1311:NAG:O3	2.27	0.52
3:P:61:ARG:HH21	3:P:78:LEU:HA	1.73	0.52
1:A:985:ASP:OD1	1:A:987:PRO:HG2	2.09	0.52
1:C:366:SER:HA	1:C:369:TYR:CZ	2.45	0.52
2:M:41:PRO:HG3	2:M:88:ALA:HB2	1.91	0.52
1:A:299:THR:O	1:A:303:LEU:HG	2.10	0.52
1:A:663:ASP:OD1	1:A:664:ILE:N	2.43	0.52
1:C:804:GLN:NE2	1:C:935:GLN:HE21	2.08	0.52
1:A:1089:PHE:CE2	1:C:917:TYR:HD2	2.29	0.51
1:B:127:VAL:HA	1:B:170:TYR:O	2.10	0.51
1:B:140:PHE:HB2	1:B:244:LEU:HD23	1.91	0.51
2:H:12:VAL:HG21	2:H:16:GLY:HA3	1.92	0.51
2:M:16:GLY:O	2:M:82(B):SER:N	2.44	0.51
3:P:54(B):HIS:HD2	3:P:54(D):LYS:HE3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:SER:HB2	1:A:611:LEU:HB3	1.91	0.51
1:A:822:LEU:HD21	1:A:938:LEU:HD13	1.93	0.51
1:A:825:LYS:NZ	1:A:943:SER:CB	2.73	0.51
1:B:69:HIS:HB2	1:B:78:ARG:NH2	2.24	0.51
1:B:378:LYS:O	1:B:432:CYS:HB2	2.10	0.51
1:A:818:ILE:HD11	1:A:938:LEU:HD12	1.92	0.51
1:B:626:ALA:HB1	1:B:634:ARG:HG2	1.91	0.51
1:B:751:ASN:OD1	1:B:752:LEU:HD12	2.10	0.51
1:C:355:ARG:HD2	1:C:396:TYR:HB3	1.92	0.51
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.92	0.51
1:C:748:GLU:OE2	1:C:748:GLU:N	2.43	0.51
2:O:67:PHE:CD1	2:O:82:MET:HE1	2.46	0.51
1:A:355:ARG:HD3	1:A:396:TYR:HD1	1.76	0.51
1:C:564:GLN:HA	1:C:577:ARG:HG2	1.92	0.51
3:N:35:TRP:HE1	3:N:50:LEU:HD22	1.74	0.51
1:A:110:LEU:O	1:A:135:PHE:HB2	2.10	0.51
1:A:156:GLU:O	1:A:157:PHE:CD1	2.64	0.51
1:A:200:TYR:C	1:A:202:LYS:HZ3	2.19	0.51
1:A:802:PHE:HD1	1:A:805:ILE:HD11	1.75	0.51
1:A:1128:VAL:HG11	1:C:918:GLU:OE1	2.11	0.51
1:C:330:PRO:HG2	1:C:544:ASN:H	1.75	0.51
3:L:54(D):LYS:HD2	3:L:58:ILE:HB	1.91	0.51
3:P:16:GLY:H	3:P:78:LEU:HB3	1.75	0.51
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.75	0.51
1:C:725:GLU:OE2	1:C:1028:LYS:NZ	2.43	0.51
1:A:355:ARG:HD3	1:A:396:TYR:CD1	2.46	0.51
1:A:409:GLN:HA	1:A:414:GLN:HG2	1.93	0.51
1:C:351:TYR:CE1	1:C:452:LEU:HB2	2.46	0.51
3:N:42:LYS:HD2	3:N:43:GLY:H	1.75	0.51
2:O:29:PHE:CE2	2:O:71:ARG:HD2	2.46	0.51
1:A:674:TYR:HD2	1:A:692:ILE:HD13	1.76	0.51
1:B:117:LEU:CD2	1:B:119:ILE:HG12	2.34	0.51
1:B:398:ASP:HB2	1:B:512:VAL:HB	1.93	0.51
1:C:310:LYS:NZ	1:C:663:ASP:OD2	2.26	0.51
1:A:58:PHE:HE1	1:A:288:ALA:O	1.92	0.51
1:A:389:ASP:OD1	1:A:528:LYS:HG3	2.11	0.51
1:A:1094:VAL:HG13	1:A:1107:ARG:HG2	1.92	0.51
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	1.93	0.51
1:B:92:PHE:CE1	1:B:94:SER:HB3	2.40	0.51
1:B:461:LEU:HD22	1:B:465:GLU:HG2	1.92	0.51
1:C:122:ASN:HB2	1:C:154:GLU:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:GLN:OE1	2:H:14:PRO:HD2	2.11	0.51
3:N:85:ASP:HB2	3:N:103:ARG:NE	2.25	0.51
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.92	0.50
1:B:37:TYR:OH	1:B:54:LEU:O	2.22	0.50
1:B:546:LEU:HD11	1:B:573:THR:HG21	1.93	0.50
1:B:917:TYR:CE2	1:C:1079:PRO:HB3	2.45	0.50
1:C:170:TYR:CE2	1:C:172:SER:HB3	2.46	0.50
2:H:5:VAL:O	2:H:23:VAL:N	2.44	0.50
2:O:20:LEU:HG	2:O:82:MET:HG3	1.93	0.50
2:O:88:ALA:HB3	2:O:90:TYR:HE1	1.75	0.50
1:B:457:ARG:NH1	1:B:459:SER:O	2.37	0.50
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.60	0.50
1:C:37:TYR:OH	1:C:54:LEU:O	2.18	0.50
2:M:31:ILE:HG21	2:M:98:HIS:ND1	2.26	0.50
1:C:19:THR:HB	1:C:21:ARG:HG2	1.94	0.50
3:N:62:PHE:HD1	3:N:75:ILE:HG12	1.76	0.50
1:B:119:ILE:HA	1:B:128:ILE:HD12	1.91	0.50
1:C:290:ASP:O	1:C:297:SER:HB2	2.11	0.50
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.22	0.50
3:L:54(B):HIS:NE2	3:L:63:SER:HA	2.27	0.50
3:N:38:GLN:NE2	3:N:39:GLN:O	2.43	0.50
2:O:34:MET:HB2	2:O:78:PHE:CE1	2.46	0.50
1:A:107:GLY:O	1:A:236:THR:N	2.43	0.50
2:M:32:TYR:CG	2:M:94:ARG:HD3	2.46	0.50
1:A:347:PHE:HD2	1:A:401:VAL:HG23	1.76	0.50
1:B:26:PRO:HG2	1:B:28:TYR:HE1	1.76	0.50
1:B:917:TYR:HD2	1:C:1089:PHE:CE2	2.24	0.50
1:C:201:PHE:HD2	1:C:229:LEU:HD12	1.77	0.50
1:C:455:LEU:HD13	1:C:493:GLN:HB2	1.93	0.50
1:C:620:VAL:HG21	1:C:649:CYS:SG	2.51	0.50
2:O:52:THR:HG23	2:O:53:SER:H	1.76	0.50
1:A:36:VAL:HG21	1:A:277:LEU:HD11	1.94	0.50
1:B:19:THR:O	1:B:21:ARG:HD3	2.10	0.50
1:B:195:LYS:HE2	1:B:204:TYR:HE1	1.77	0.50
1:C:822:LEU:HD11	1:C:938:LEU:HD21	1.93	0.50
2:O:18:LEU:O	2:O:19:ARG:HD2	2.11	0.50
1:B:121:ASN:ND2	1:B:175:PHE:HB2	2.27	0.50
1:C:326:ILE:HG13	1:C:539:VAL:HG23	1.94	0.50
1:C:333:THR:HG22	1:C:333:THR:O	2.11	0.50
1:C:395:VAL:O	1:C:396:TYR:HD1	1.95	0.50
1:A:142:GLY:HA3	1:A:156:GLU:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:O	1:A:157:PHE:HD1	1.95	0.50
1:A:353:TRP:HH2	1:A:355:ARG:HH21	1.60	0.50
1:B:577:ARG:HG2	1:B:584:ILE:HD13	1.93	0.50
1:C:485:GLY:H	1:C:488:CYS:HB2	1.76	0.49
2:H:35:ASN:ND2	2:H:95:PRO:HG3	2.27	0.49
1:C:44:ARG:HB2	1:C:279:TYR:CE1	2.47	0.49
3:P:45:ARG:NH1	3:P:47:LEU:HD21	2.27	0.49
1:A:755:GLN:HG2	1:B:969:ASN:OD1	2.12	0.49
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.94	0.49
1:C:295:PRO:HG2	1:C:636:TYR:HD2	1.77	0.49
1:C:338:PHE:HE1	1:C:358:ILE:HG12	1.77	0.49
3:L:20:ASN:OD1	3:L:74:THR:HA	2.13	0.49
1:B:68:ILE:HG13	1:B:69:HIS:H	1.78	0.49
3:P:61:ARG:NE	3:P:77:SER:O	2.45	0.49
1:B:417:LYS:O	1:B:422:ASN:ND2	2.45	0.49
1:B:596:SER:HB2	1:B:611:LEU:HB3	1.95	0.49
1:C:186:PHE:HA	1:C:210:ILE:O	2.12	0.49
1:B:289:VAL:HG11	1:B:300:LYS:HE3	1.94	0.49
1:B:804:GLN:HE22	1:B:935:GLN:HE21	1.58	0.49
1:C:149:ASN:ND2	4:S:1:NAG:O7	2.45	0.49
1:C:752:LEU:HG	1:C:997:ILE:CD1	2.42	0.49
2:H:29:PHE:HD2	2:H:76:ASN:ND2	2.11	0.49
2:O:28:THR:HG23	2:O:31:ILE:HG12	1.94	0.49
1:A:26:PRO:HB2	1:A:63:THR:HG23	1.94	0.49
1:A:457:ARG:NH1	1:A:459:SER:O	2.40	0.49
1:B:329:PHE:HE2	1:B:528:LYS:NZ	2.11	0.49
1:B:611:LEU:HD23	1:B:613:GLN:HE21	1.78	0.49
1:C:658:ASN:ND2	1:C:660:TYR:CE1	2.80	0.49
1:A:282:ASN:ND2	5:A:1303:NAG:C7	2.76	0.49
1:A:292:ALA:O	1:A:633:TRP:NE1	2.31	0.49
1:A:703:ASN:HB2	1:C:787:GLN:OE1	2.13	0.49
1:A:917:TYR:HD2	1:B:1089:PHE:HE2	1.61	0.49
1:B:533:LEU:CD2	1:B:535:LYS:HG3	2.42	0.49
1:B:977:LEU:HD12	1:B:980:ILE:HD11	1.95	0.49
1:B:1082:CYS:HB2	1:B:1132:ILE:HD13	1.95	0.49
1:C:145:TYR:HB2	1:C:152:TRP:NE1	2.27	0.49
1:C:331:ASN:HD22	1:C:580:GLN:HE22	1.60	0.49
1:C:577:ARG:HH12	1:C:584:ILE:CA	2.26	0.49
1:B:108:THR:HA	1:B:236:THR:HG22	1.93	0.49
1:C:393:THR:HG22	1:C:516:GLU:O	2.13	0.49
1:C:902:MET:HE1	1:C:1050:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:24:ALA:HB3	2:H:29:PHE:CE1	2.48	0.49
2:M:58:TYR:CE1	2:M:69:ILE:HG22	2.47	0.49
1:A:186:PHE:HA	1:A:210:ILE:O	2.13	0.49
1:A:230:PRO:HG3	1:B:396:TYR:CZ	2.47	0.49
1:A:326:ILE:HG12	1:A:539:VAL:CG2	2.43	0.49
1:A:330:PRO:HD2	1:A:525:CYS:SG	2.53	0.49
1:B:58:PHE:CZ	1:B:288:ALA:HB3	2.45	0.49
1:B:800:PHE:CE2	1:B:923:ILE:HG22	2.47	0.49
1:C:919:ASN:O	1:C:923:ILE:HG12	2.13	0.49
2:O:95:PRO:HG3	2:O:110:PHE:CE1	2.42	0.49
1:B:206:LYS:HD2	1:B:222:ALA:O	2.13	0.48
1:B:1006:THR:O	1:B:1010:GLN:HG2	2.13	0.48
2:M:98:HIS:HD2	2:M:100:TYR:O	1.95	0.48
3:N:34:ALA:HA	3:N:49:SER:HA	1.94	0.48
1:A:752:LEU:HD11	1:A:993:ILE:HG21	1.95	0.48
1:B:142:GLY:HA2	1:B:244:LEU:O	2.12	0.48
1:B:1074:ASN:H	1:B:1074:ASN:HD22	1.61	0.48
1:C:24:LEU:HD11	1:C:78:ARG:NH1	2.28	0.48
1:C:739:THR:O	1:C:743:CYS:HB3	2.12	0.48
3:P:50:LEU:CD2	3:P:71:ARG:HB3	2.42	0.48
1:B:105:ILE:HG23	1:B:241:LEU:HG	1.95	0.48
1:C:85:PRO:HA	1:C:236:THR:O	2.13	0.48
1:C:663:ASP:OD1	1:C:664:ILE:N	2.46	0.48
1:A:30:ASN:OD1	1:A:59:PHE:HA	2.12	0.48
1:A:1111:GLU:HG2	1:A:1113:GLN:NE2	2.28	0.48
1:B:148:ASN:HB2	4:J:1:NAG:O7	2.12	0.48
1:B:573:THR:HG22	1:B:573:THR:O	2.12	0.48
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.49	0.48
2:H:47:TRP:CZ2	3:L:95:ILE:HA	2.48	0.48
1:A:535:LYS:HA	1:A:552:LEU:HD21	1.94	0.48
1:B:110:LEU:O	1:B:135:PHE:HB2	2.14	0.48
1:B:278:LYS:HB3	1:B:306:PHE:CE2	2.48	0.48
1:B:904:TYR:OH	1:C:1094:VAL:HG22	2.14	0.48
1:A:538:CYS:HB3	1:A:551:VAL:HG22	1.94	0.48
1:B:119:ILE:CD1	1:B:128:ILE:HD12	2.43	0.48
2:M:35:ASN:HB2	2:M:110:PHE:CE1	2.49	0.48
1:A:113:LYS:HZ3	1:B:470:THR:HG1	1.55	0.48
1:C:103:GLY:C	1:C:241:LEU:HB2	2.39	0.48
1:C:196:ASN:HD21	1:C:235:ILE:HB	1.78	0.48
1:A:96:GLU:HG2	1:A:190:ARG:HH12	1.79	0.48
1:A:100:ILE:HB	1:A:263:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:NH1	1:A:396:TYR:OH	2.47	0.48
1:A:802:PHE:CD1	1:A:805:ILE:HD11	2.47	0.48
1:A:816:SER:OG	1:A:819:GLU:HB2	2.14	0.48
1:A:1089:PHE:N	1:A:1121:PHE:O	2.31	0.48
1:B:714:ILE:HD12	1:B:1075:PHE:CD2	2.48	0.48
1:B:725:GLU:OE2	1:B:1028:LYS:HE3	2.13	0.48
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.79	0.48
1:A:63:THR:HG21	1:A:65:PHE:CZ	2.49	0.48
1:A:108:THR:HA	1:A:236:THR:HG22	1.96	0.48
1:A:366:SER:HA	1:A:369:TYR:CZ	2.48	0.48
1:A:736:VAL:HG11	1:A:1004:LEU:HD21	1.96	0.48
1:B:756:TYR:HB3	1:B:1001:LEU:HD11	1.94	0.48
1:C:183:GLN:HB2	3:P:28:HIS:NE2	2.28	0.48
1:C:1049:LEU:HD21	1:C:1067:TYR:HB2	1.96	0.48
3:N:35:TRP:CD1	3:N:73:LEU:HD12	2.49	0.48
1:A:67:ALA:HB1	1:A:80:ASP:H	1.79	0.48
1:B:767:LEU:HD21	1:B:1008:VAL:HG22	1.95	0.48
1:C:332:ILE:HG13	1:C:525:CYS:HB2	1.96	0.48
3:N:29:ASN:OD1	3:N:30:SER:N	2.47	0.48
1:A:17:ASN:OD1	1:A:19:THR:HG23	2.13	0.47
1:A:655:HIS:ND1	1:A:656:VAL:N	2.61	0.47
1:A:943:SER:O	1:A:945:LEU:N	2.45	0.47
1:B:384:PRO:HA	1:B:387:LEU:HG	1.95	0.47
1:B:821:LEU:C	1:B:821:LEU:HD23	2.39	0.47
1:A:365:TYR:HD1	1:A:368:LEU:HD12	1.79	0.47
1:A:815:ARG:HG2	1:A:819:GLU:HB3	1.95	0.47
1:B:61:ASN:CB	5:B:1301:NAG:H2	2.42	0.47
1:B:121:ASN:HD21	1:B:175:PHE:HB2	1.78	0.47
1:B:351:TYR:CE1	1:B:452:LEU:HB2	2.49	0.47
1:C:18:LEU:HD12	1:C:18:LEU:O	2.15	0.47
1:C:398:ASP:HB2	1:C:512:VAL:HB	1.95	0.47
2:M:4:LEU:HD12	2:M:22:CYS:SG	2.53	0.47
1:A:630:THR:OG1	1:A:633:TRP:CD1	2.64	0.47
1:B:131:CYS:HA	1:B:166:CYS:HA	1.96	0.47
1:B:201:PHE:N	1:B:229:LEU:O	2.31	0.47
3:P:68:GLY:O	3:P:71:ARG:NH2	2.47	0.47
1:A:187:LYS:HZ3	1:A:212:LEU:HA	1.80	0.47
1:B:169:GLU:O	1:B:170:TYR:CD1	2.67	0.47
1:B:660:TYR:O	1:B:698:SER:HB2	2.14	0.47
1:C:176:LEU:HD23	1:C:192:PHE:CZ	2.50	0.47
1:A:299:THR:HA	1:A:302:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:GLY:HA3	1:A:899:PRO:CG	2.45	0.47
1:A:916:LEU:HD23	1:A:917:TYR:HD1	1.79	0.47
1:B:645:THR:HG22	1:B:646:ARG:N	2.30	0.47
1:B:718:PHE:HA	1:B:1069:PRO:HA	1.96	0.47
1:B:815:ARG:HA	1:B:819:GLU:OE1	2.15	0.47
1:C:119:ILE:HA	1:C:128:ILE:HD12	1.97	0.47
1:C:131:CYS:HB3	1:C:164:ASN:O	2.14	0.47
1:C:725:GLU:CD	1:C:1028:LYS:HZ3	2.22	0.47
2:H:83:ARG:N	2:H:86:ASP:OD2	2.35	0.47
1:A:18:LEU:O	1:A:18:LEU:HD12	2.15	0.47
1:B:28:TYR:HB3	5:B:1301:NAG:C3	2.32	0.47
1:B:976:VAL:HG13	1:B:979:ASP:H	1.80	0.47
1:C:296:LEU:O	1:C:299:THR:HG22	2.15	0.47
1:C:329:PHE:O	1:C:530:SER:HA	2.14	0.47
2:H:111:ASP:OD1	2:H:112:ILE:N	2.48	0.47
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.95	0.47
2:O:45:LEU:HD12	2:O:46:GLU:N	2.29	0.47
3:P:3:VAL:HG22	3:P:26:SER:HB3	1.96	0.47
3:P:5:THR:O	3:P:23:CYS:HA	2.14	0.47
1:A:1088:HIS:HB3	1:A:1120:THR:CG2	2.44	0.47
1:C:187:LYS:HE2	1:C:210:ILE:HD11	1.97	0.47
1:C:322:PRO:HA	1:C:628:GLN:NE2	2.29	0.47
2:O:66:ARG:HH11	2:O:83:ARG:HD2	1.80	0.47
3:P:20:ASN:HB2	3:P:48:MET:CE	2.45	0.47
1:B:553:THR:HG22	1:B:554:GLU:N	2.27	0.47
1:C:192:PHE:HB3	1:C:194:PHE:CE2	2.49	0.47
1:C:233:ILE:HD12	1:C:235:ILE:HD11	1.97	0.47
2:O:36:TRP:CD1	2:O:78:PHE:HE2	2.33	0.47
1:A:190:ARG:HG2	1:A:207:HIS:CE1	2.50	0.47
1:B:544:ASN:ND2	1:B:579:PRO:HG3	2.30	0.47
1:B:1083:HIS:O	1:B:1086:LYS:HG2	2.15	0.47
1:C:177:MET:O	1:C:190:ARG:NH2	2.46	0.47
1:C:329:PHE:CE2	1:C:528:LYS:HD2	2.50	0.47
1:C:331:ASN:HD22	1:C:580:GLN:NE2	2.12	0.47
1:C:658:ASN:HD21	1:C:660:TYR:HE1	1.63	0.47
3:P:35:TRP:N	3:P:48:MET:O	2.48	0.47
1:A:193:VAL:HB	1:A:204:TYR:HB2	1.97	0.46
1:A:778:THR:HG22	1:A:865:LEU:HD12	1.97	0.46
1:B:989:ALA:O	1:B:993:ILE:HG12	2.16	0.46
1:C:66:HIS:CE1	1:C:68:ILE:O	2.67	0.46
1:C:395:VAL:C	1:C:396:TYR:HD1	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:58:ILE:HG23	3:L:62:PHE:HD2	1.80	0.46
3:P:35:TRP:CG	3:P:48:MET:HG2	2.49	0.46
1:A:317:ASN:OD1	1:A:319:ARG:NH1	2.48	0.46
1:B:983:ARG:NH1	1:C:517:LEU:HB2	2.25	0.46
1:B:1013:ILE:O	1:B:1017:GLU:HG3	2.15	0.46
1:C:733:LYS:HD2	1:C:771:ALA:HB1	1.97	0.46
1:C:905:ARG:NH1	1:C:1050:MET:HG2	2.29	0.46
2:O:27:PHE:CE1	2:O:94:ARG:HD3	2.50	0.46
1:A:746:SER:OG	1:A:977:LEU:HD23	2.15	0.46
1:A:886:TRP:HB3	1:A:905:ARG:NH2	2.29	0.46
1:B:718:PHE:CE1	1:B:923:ILE:HD11	2.50	0.46
1:C:168:PHE:CE2	1:C:170:TYR:HB2	2.49	0.46
2:O:29:PHE:HB2	2:O:76:ASN:OD1	2.15	0.46
3:P:50:LEU:HD23	3:P:71:ARG:HB3	1.97	0.46
1:A:904:TYR:OH	1:B:1094:VAL:HG22	2.16	0.46
1:B:713:ALA:HA	1:B:1073:LYS:O	2.16	0.46
1:C:84:LEU:HB2	1:C:238:PHE:CZ	2.50	0.46
1:C:646:ARG:HB3	1:C:668:ALA:CB	2.45	0.46
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.98	0.46
2:M:36:TRP:CZ3	2:M:90:TYR:HB3	2.50	0.46
3:P:6:GLN:HE22	3:P:88:CYS:N	2.14	0.46
1:A:720:ILE:HD12	1:A:923:ILE:HG23	1.98	0.46
1:A:984:LEU:O	1:B:386:LYS:NZ	2.40	0.46
1:A:986:PRO:O	1:A:990:GLU:HG3	2.15	0.46
1:B:18:LEU:HD12	1:B:18:LEU:O	2.14	0.46
1:C:121:ASN:ND2	1:C:175:PHE:HB2	2.30	0.46
1:C:577:ARG:NH1	1:C:584:ILE:HA	2.30	0.46
2:H:36:TRP:CD2	2:H:80:LEU:HD12	2.51	0.46
2:O:4:LEU:HB2	2:O:114:GLY:HA2	1.98	0.46
3:P:17:ALA:HB3	3:P:78:LEU:HD22	1.98	0.46
1:B:290:ASP:OD2	1:B:293:LEU:HD23	2.15	0.46
1:C:65:PHE:CE2	1:C:84:LEU:HD11	2.51	0.46
1:C:81:ASN:ND2	1:C:240:THR:O	2.43	0.46
1:C:127:VAL:HG12	1:C:129:LYS:CD	2.46	0.46
2:O:29:PHE:HE2	2:O:71:ARG:HD2	1.80	0.46
1:A:38:TYR:HE1	1:A:222:ALA:HB1	1.81	0.46
1:B:389:ASP:HA	1:B:528:LYS:HZ2	1.81	0.46
1:B:1117:THR:HA	1:B:1120:THR:OG1	2.16	0.46
1:C:537:LYS:C	1:C:551:VAL:HG23	2.41	0.46
1:C:770:ILE:O	1:C:774:GLN:HG2	2.15	0.46
1:C:989:ALA:O	1:C:993:ILE:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG12	1:B:171:VAL:HG22	1.97	0.46
3:L:4:LEU:HD23	3:L:6:GLN:CD	2.40	0.46
3:P:21:LEU:HD21	3:P:104:LEU:HD22	1.98	0.46
1:A:134:GLN:O	1:A:160:TYR:HA	2.15	0.46
1:B:985:ASP:N	1:B:985:ASP:OD1	2.49	0.46
2:H:32:TYR:CE1	2:H:94:ARG:HD3	2.51	0.46
3:L:86:TYR:HB2	3:L:102:THR:HB	1.96	0.46
3:P:34:ALA:HA	3:P:49:SER:HA	1.97	0.46
1:A:89:GLY:HA3	1:A:270:LEU:HB2	1.98	0.46
1:A:991:VAL:O	1:A:995:ARG:HG3	2.15	0.46
1:B:105:ILE:HA	1:B:117:LEU:O	2.16	0.46
1:B:722:VAL:HG23	1:B:934:ILE:HG13	1.98	0.46
1:B:802:PHE:CD1	1:B:805:ILE:HD11	2.50	0.46
1:C:108:THR:HA	1:C:236:THR:HG22	1.98	0.46
1:C:127:VAL:O	1:C:128:ILE:HD13	2.16	0.46
1:C:927:PHE:HZ	1:C:1052:PHE:HE2	1.64	0.46
3:N:68:GLY:O	3:N:71:ARG:NH1	2.48	0.46
2:O:2:VAL:HB	2:O:112:ILE:HG21	1.98	0.46
3:P:35:TRP:HB2	3:P:48:MET:CB	2.45	0.46
1:A:187:LYS:HE2	1:A:210:ILE:HD11	1.98	0.45
1:A:645:THR:HG22	1:A:646:ARG:N	2.31	0.45
1:A:915:VAL:O	1:A:919:ASN:ND2	2.49	0.45
1:A:917:TYR:HD2	1:B:1089:PHE:CE2	2.34	0.45
1:B:328:ARG:HH21	1:B:580:GLN:HB2	1.81	0.45
1:C:154:GLU:O	1:C:156:GLU:N	2.43	0.45
1:C:617:CYS:HA	1:C:620:VAL:HG23	1.97	0.45
1:C:1088:HIS:HB3	1:C:1120:THR:CG2	2.46	0.45
3:L:39:GLN:HB2	3:L:42:LYS:HE3	1.99	0.45
2:O:19:ARG:NH1	2:O:82:MET:H	2.11	0.45
1:A:178:ASP:OD2	1:A:180:GLU:HB2	2.17	0.45
1:A:303:LEU:HD21	1:A:308:VAL:HG12	1.98	0.45
1:A:903:ALA:HA	1:A:916:LEU:HD13	1.98	0.45
1:B:146:HIS:O	1:B:150:LYS:HA	2.16	0.45
1:B:816:SER:HB2	1:B:817:PRO:CD	2.47	0.45
1:C:126:VAL:HG11	1:C:175:PHE:CZ	2.51	0.45
1:C:555:SER:HB2	1:C:586:ASP:OD2	2.16	0.45
2:M:18:LEU:HD13	2:M:82(C):LEU:HD12	1.99	0.45
1:A:79:PHE:HE2	1:A:244:LEU:HD21	1.81	0.45
1:A:108:THR:O	1:A:237:ARG:HG3	2.16	0.45
1:C:213:VAL:HG12	1:C:215:ASP:O	2.16	0.45
1:C:279:TYR:CE2	1:C:285:ILE:HG12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.55	0.45
1:C:707:TYR:O	1:C:708:SER:C	2.58	0.45
1:C:777:ASN:O	1:C:781:VAL:HG23	2.17	0.45
1:C:985:ASP:OD1	1:C:985:ASP:N	2.49	0.45
3:N:23:CYS:HB2	3:N:35:TRP:CZ2	2.52	0.45
2:O:92:CYS:O	2:O:114:GLY:N	2.49	0.45
1:A:884:SER:OG	1:A:888:PHE:HB3	2.17	0.45
1:B:187:LYS:HE2	1:B:210:ILE:HG13	1.98	0.45
1:C:30:ASN:OD1	1:C:31:SER:N	2.49	0.45
1:C:34:ARG:HH12	1:C:221:SER:CB	2.29	0.45
3:N:84:ALA:HB3	3:N:86:TYR:HE1	1.81	0.45
1:A:236:THR:HG23	1:A:237:ARG:HG2	1.99	0.45
1:B:28:TYR:CD1	5:B:1301:NAG:H83	2.51	0.45
1:B:567:ARG:HD3	1:B:570:ALA:HA	1.97	0.45
1:C:246:ARG:HG3	1:C:248:TYR:CE2	2.51	0.45
1:A:815:ARG:HD2	1:A:820:ASP:OD1	2.16	0.45
1:B:141:LEU:O	1:B:244:LEU:N	2.39	0.45
1:B:715:PRO:HB3	1:B:1069:PRO:HB2	1.98	0.45
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	1.99	0.45
2:H:110:PHE:HE2	3:L:98:PHE:HZ	1.64	0.45
3:L:63:SER:HB3	3:L:74:THR:OG1	2.16	0.45
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.52	0.45
1:A:546:LEU:HD12	1:A:546:LEU:O	2.17	0.45
2:O:108:TYR:HH	3:P:1:GLN:H3	1.53	0.45
1:A:139:PRO:HB3	1:A:159:VAL:HA	1.99	0.45
1:A:1082:CYS:HB3	1:A:1126:CYS:HB3	1.49	0.45
1:B:658:ASN:ND2	1:B:660:TYR:OH	2.50	0.45
1:A:393:THR:HG22	1:A:516:GLU:O	2.17	0.45
1:A:720:ILE:CD1	1:A:923:ILE:HG23	2.47	0.45
1:A:790:LYS:HE2	1:A:790:LYS:HA	1.98	0.45
1:B:328:ARG:NE	1:B:578:ASP:OD2	2.49	0.45
1:C:901:GLN:O	1:C:901:GLN:HG2	2.17	0.45
2:M:111:ASP:OD1	2:M:112:ILE:N	2.50	0.45
1:A:183:GLN:HE21	3:L:91:TRP:HB2	1.81	0.45
1:B:816:SER:HB2	1:B:817:PRO:HD2	1.99	0.45
1:C:105:ILE:HD11	1:C:241:LEU:CD2	2.47	0.45
1:C:393:THR:HG23	1:C:394:ASN:N	2.32	0.45
2:O:24:ALA:HB1	2:O:27:PHE:CZ	2.52	0.45
1:A:152:TRP:CE3	2:H:31:ILE:HD11	2.53	0.44
1:B:119:ILE:HD13	1:B:128:ILE:HG23	1.99	0.44
1:B:124:THR:OG1	2:M:30:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLN:OE1	1:B:174:PRO:HD2	2.17	0.44
1:B:729:VAL:HG22	1:B:1059:GLY:HA2	1.99	0.44
1:B:821:LEU:HD21	1:B:938:LEU:O	2.16	0.44
2:H:35:ASN:HB2	2:H:110:PHE:CE1	2.52	0.44
2:M:95:PRO:HA	2:M:110:PHE:HA	1.99	0.44
3:N:48:MET:HE1	3:N:54(B):HIS:HA	1.99	0.44
3:P:6:GLN:NE2	3:P:88:CYS:H	2.15	0.44
1:B:278:LYS:HG3	1:B:286:THR:HB	1.99	0.44
1:B:393:THR:HG22	1:B:516:GLU:O	2.17	0.44
1:B:773:GLU:OE2	1:B:1019:ARG:NE	2.32	0.44
1:C:33:THR:HA	1:C:58:PHE:CG	2.52	0.44
1:C:89:GLY:HA3	1:C:270:LEU:HB2	1.98	0.44
1:C:118:LEU:HD23	1:C:118:LEU:O	2.17	0.44
1:C:246:ARG:HG3	1:C:248:TYR:CZ	2.52	0.44
1:C:724:THR:HA	1:C:1062:PHE:O	2.17	0.44
3:N:51:ASN:HD22	3:N:54(A):SER:HB2	1.82	0.44
1:A:102:ARG:HA	1:A:102:ARG:HD3	1.83	0.44
1:B:372:ALA:CB	5:B:1305:NAG:H81	2.43	0.44
1:B:533:LEU:HD21	1:B:535:LYS:HG3	2.00	0.44
1:C:238:PHE:HZ	1:C:267:VAL:HG11	1.83	0.44
3:P:6:GLN:OE1	3:P:102:THR:OG1	2.33	0.44
1:A:38:TYR:CE1	1:A:222:ALA:HB1	2.52	0.44
1:A:118:LEU:HD23	1:A:118:LEU:O	2.18	0.44
1:A:551:VAL:N	1:A:588:THR:O	2.51	0.44
1:B:41:LYS:HD2	1:B:42:VAL:N	2.33	0.44
1:B:784:GLN:HE21	1:B:784:GLN:HB2	1.58	0.44
1:C:395:VAL:HA	1:C:514:SER:O	2.18	0.44
1:C:765:ARG:HE	1:C:765:ARG:HB2	1.63	0.44
2:H:47:TRP:HB3	3:L:98:PHE:CE2	2.52	0.44
3:L:47:LEU:C	3:L:48:MET:HG3	2.43	0.44
1:B:81:ASN:ND2	1:B:240:THR:O	2.40	0.44
1:B:133:PHE:HB3	1:B:160:TYR:HB2	1.99	0.44
1:B:722:VAL:HG12	1:B:1065:VAL:CB	2.48	0.44
1:C:718:PHE:CE1	1:C:923:ILE:HD11	2.52	0.44
2:H:69:ILE:HD12	2:H:80:LEU:HA	1.99	0.44
1:A:37:TYR:HB3	1:A:223:LEU:HB2	1.98	0.44
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.99	0.44
1:B:34:ARG:HH21	1:B:217:PRO:HG2	1.81	0.44
1:C:655:HIS:HA	1:C:694:ALA:O	2.18	0.44
1:C:718:PHE:HZ	1:C:923:ILE:HD11	1.81	0.44
2:H:94:ARG:HD2	2:H:95:PRO:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:6:GLN:HE22	3:P:88:CYS:H	1.66	0.44
1:A:230:PRO:HB2	1:B:355:ARG:HD3	2.00	0.44
1:B:169:GLU:O	1:B:170:TYR:HD1	2.00	0.44
1:B:328:ARG:NH2	1:B:580:GLN:HB2	2.33	0.44
1:B:612:TYR:HB2	1:B:649:CYS:HB3	1.99	0.44
1:B:722:VAL:HG23	1:B:934:ILE:CG1	2.48	0.44
2:O:44:GLY:HA3	3:P:72:PHE:CE2	2.53	0.44
3:P:41:GLU:HB3	3:P:42:LYS:HZ2	1.82	0.44
3:P:87:TYR:HA	3:P:100:GLY:O	2.18	0.44
1:A:146:HIS:O	1:A:150:LYS:HA	2.18	0.44
1:B:34:ARG:HD3	1:B:34:ARG:HA	1.61	0.44
1:B:565:PHE:CD1	1:B:576:VAL:HG23	2.53	0.44
1:B:1050:MET:HB2	1:B:1065:VAL:CG1	2.47	0.44
1:C:120:VAL:O	1:C:126:VAL:HG13	2.18	0.44
1:C:1038:LYS:HE2	1:C:1038:LYS:HA	2.00	0.44
1:A:574:ASP:OD1	1:A:575:ALA:N	2.51	0.44
1:B:118:LEU:O	1:B:118:LEU:HD23	2.18	0.44
1:C:66:HIS:ND1	1:C:68:ILE:HG22	2.33	0.44
1:C:131:CYS:HB2	1:C:133:PHE:CE1	2.53	0.44
1:C:819:GLU:O	1:C:823:PHE:HD1	2.00	0.44
1:A:109:THR:OG1	1:A:114:THR:OG1	2.35	0.43
1:A:731:MET:HG2	1:A:774:GLN:OE1	2.18	0.43
1:A:800:PHE:HE2	1:A:923:ILE:HG22	1.81	0.43
1:B:528:LYS:HZ3	1:B:528:LYS:HB2	1.82	0.43
1:C:800:PHE:HE2	1:C:923:ILE:HG22	1.82	0.43
1:C:826:VAL:HB	1:C:1057:PRO:HG2	1.99	0.43
2:H:5:VAL:HG23	2:H:115:GLN:HE22	1.84	0.43
1:A:39:PRO:HG3	1:A:51:THR:HG21	2.00	0.43
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.83	0.43
1:A:165:ASN:OD1	5:A:1302:NAG:N2	2.51	0.43
1:B:308:VAL:HG22	1:B:602:THR:HG23	2.00	0.43
1:B:1095:PHE:CE1	1:B:1115:ILE:HD12	2.53	0.43
1:C:580:GLN:OE1	5:C:1304:NAG:H82	2.18	0.43
3:L:25:LEU:HD23	3:L:26:SER:O	2.17	0.43
2:M:47:TRP:HH2	2:M:57:ARG:HD2	1.80	0.43
1:A:106:PHE:HB2	1:A:117:LEU:HD23	2.01	0.43
1:A:801:ASN:OD1	5:A:1309:NAG:O5	2.36	0.43
1:B:535:LYS:NZ	1:B:554:GLU:HB2	2.34	0.43
1:B:787:GLN:OE1	1:C:703:ASN:HB2	2.18	0.43
1:B:1107:ARG:H	1:B:1107:ARG:HD2	1.82	0.43
1:C:64:TRP:CZ3	1:C:266:TYR:CE1	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:ALA:HB3	1:C:266:TYR:HD2	1.84	0.43
1:C:299:THR:O	1:C:303:LEU:HG	2.18	0.43
1:C:784:GLN:NE2	1:C:1026:ALA:O	2.51	0.43
1:C:1028:LYS:HB2	1:C:1028:LYS:HE3	1.80	0.43
2:H:64:LYS:HB2	2:H:83:ARG:NH1	2.32	0.43
2:H:69:ILE:HD11	2:H:78:PHE:CZ	2.54	0.43
2:M:47:TRP:HE1	2:M:50:TYR:HB3	1.83	0.43
1:A:234:ASN:HB3	4:F:1:NAG:O5	2.18	0.43
1:A:592:PHE:HZ	1:A:612:TYR:HD2	1.67	0.43
1:A:722:VAL:HG22	1:A:1065:VAL:HB	2.01	0.43
1:A:927:PHE:HZ	1:A:1052:PHE:HE2	1.64	0.43
1:C:577:ARG:NH2	1:C:584:ILE:HD12	2.31	0.43
2:H:4:LEU:HD11	2:H:94:ARG:HB2	1.99	0.43
3:L:23:CYS:HB2	3:L:35:TRP:CZ2	2.54	0.43
1:B:535:LYS:NZ	1:B:554:GLU:OE1	2.47	0.43
1:B:1030:SER:O	1:C:1040:VAL:HG23	2.17	0.43
1:C:271:GLN:HG3	1:C:273:ARG:HG2	2.01	0.43
1:C:718:PHE:HA	1:C:1069:PRO:HA	2.00	0.43
1:A:32:PHE:HB3	1:A:218:GLN:CD	2.43	0.43
1:A:675:GLN:HB3	1:A:693:ILE:HD13	1.99	0.43
1:A:1045:LYS:HA	1:A:1045:LYS:HD3	1.76	0.43
1:C:940:SER:C	1:C:942:PRO:CD	2.91	0.43
1:C:1080:ALA:O	1:C:1081:ILE:HD13	2.18	0.43
1:A:66:HIS:O	1:A:66:HIS:CG	2.72	0.43
1:A:282:ASN:HD22	5:A:1303:NAG:C7	2.30	0.43
1:B:106:PHE:HA	1:B:238:PHE:HA	2.00	0.43
1:B:170:TYR:CD2	1:B:229:LEU:HD22	2.54	0.43
1:C:802:PHE:O	1:C:806:LEU:HB2	2.19	0.43
1:A:108:THR:HG23	1:A:236:THR:HG22	2.01	0.43
1:A:205:SER:HB3	1:A:226:LEU:HD11	2.00	0.43
1:A:298:GLU:HG2	1:A:315:THR:HB	2.01	0.43
1:B:79:PHE:CE2	1:B:244:LEU:HD21	2.54	0.43
1:B:788:ILE:HD11	1:C:699:LEU:HG	2.00	0.43
1:B:1004:LEU:O	1:B:1008:VAL:HG23	2.19	0.43
1:C:109:THR:HA	1:C:237:ARG:NH1	2.32	0.43
2:O:3:GLN:C	2:O:4:LEU:HD12	2.44	0.43
1:A:290:ASP:HB3	1:A:293:LEU:CD2	2.36	0.43
1:A:433:VAL:HG22	1:A:512:VAL:HG13	2.00	0.43
1:A:603:ASN:OD1	1:A:604:THR:N	2.52	0.43
1:A:900:MET:HB3	1:A:900:MET:HE3	1.47	0.43
1:B:86:PHE:HB3	1:B:236:THR:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:800:PHE:CE2	1:C:923:ILE:HG22	2.53	0.43
1:C:972:ALA:HA	1:C:992:GLN:NE2	2.33	0.43
3:L:20:ASN:OD1	3:L:74:THR:HG22	2.19	0.43
2:M:57:ARG:HD3	3:N:94:GLY:HA2	2.01	0.43
2:M:86:ASP:HB2	2:M:121:VAL:HG11	2.01	0.43
1:A:80:ASP:OD2	1:A:82:PRO:HD3	2.19	0.43
1:A:183:GLN:NE2	3:L:91:TRP:HB2	2.34	0.43
1:A:730:SER:O	1:A:1058:HIS:HB3	2.18	0.43
1:B:68:ILE:O	1:B:78:ARG:NH2	2.52	0.43
1:B:182:LYS:HG3	3:N:93:THR:OG1	2.19	0.43
1:B:347:PHE:CD2	1:B:509:ARG:HG2	2.53	0.43
1:B:986:PRO:O	1:B:990:GLU:HG3	2.19	0.43
1:C:34:ARG:HE	1:C:35:GLY:N	2.03	0.43
1:C:119:ILE:HD13	1:C:128:ILE:CD1	2.46	0.43
1:A:41:LYS:HD3	1:B:520:ALA:HB2	2.01	0.42
1:A:149:ASN:HB2	4:E:1:NAG:H83	2.01	0.42
1:A:208:THR:HA	1:A:209:PRO:HD3	1.92	0.42
1:A:362:VAL:HA	1:A:525:CYS:O	2.19	0.42
1:A:887:THR:HG21	1:A:894:LEU:HD12	1.99	0.42
1:B:175:PHE:O	1:B:177:MET:N	2.46	0.42
1:B:337:PRO:HG3	1:B:356:LYS:HZ1	1.84	0.42
1:B:343:ASN:OD1	5:B:1305:NAG:H2	2.19	0.42
1:B:821:LEU:HD13	1:B:935:GLN:OE1	2.19	0.42
1:C:865:LEU:HD23	1:C:865:LEU:HA	1.88	0.42
1:C:903:ALA:HB2	1:C:916:LEU:HD22	2.01	0.42
1:A:92:PHE:HB3	1:A:192:PHE:HB2	2.01	0.42
1:A:206:LYS:HB2	1:A:223:LEU:HA	2.01	0.42
1:A:229:LEU:HA	1:A:230:PRO:HD3	1.89	0.42
1:A:420:ASP:OD1	1:A:421:TYR:N	2.52	0.42
1:A:442:ASP:O	1:A:448:ASN:ND2	2.32	0.42
1:A:748:GLU:O	1:A:752:LEU:HD13	2.19	0.42
1:A:914:ASN:ND2	1:A:1111:GLU:OE2	2.45	0.42
1:B:193:VAL:HG23	1:B:223:LEU:HD22	2.01	0.42
1:B:650:LEU:HD21	1:B:653:ALA:HB3	2.00	0.42
1:B:894:LEU:HD21	1:C:1072:GLU:HG2	2.01	0.42
1:B:1095:PHE:HE1	1:B:1115:ILE:HD12	1.84	0.42
1:C:315:THR:HG22	1:C:316:SER:O	2.18	0.42
1:C:552:LEU:HA	1:C:586:ASP:O	2.19	0.42
1:C:1081:ILE:O	1:C:1088:HIS:N	2.47	0.42
2:H:98:HIS:NE2	2:H:100:TYR:O	2.52	0.42
3:P:24:THR:HG23	3:P:70:GLU:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:O	1:A:299:THR:HG22	2.18	0.42
1:A:328:ARG:HB2	1:A:543:PHE:HD1	1.83	0.42
1:A:1095:PHE:HE1	1:A:1115:ILE:HD12	1.83	0.42
1:B:154:GLU:O	1:B:156:GLU:N	2.44	0.42
1:B:331:ASN:HB3	1:B:580:GLN:NE2	2.29	0.42
1:B:724:THR:HA	1:B:1062:PHE:O	2.19	0.42
1:B:903:ALA:HA	1:B:916:LEU:HD13	2.02	0.42
3:L:6:GLN:HG2	3:L:22:THR:O	2.19	0.42
1:B:176:LEU:HD23	1:B:192:PHE:CZ	2.54	0.42
1:B:202:LYS:HE3	1:B:202:LYS:HB3	1.88	0.42
1:C:85:PRO:O	1:C:238:PHE:HE1	2.01	0.42
2:H:108:TYR:C	3:L:91:TRP:HE1	2.27	0.42
2:M:17:SER:C	2:M:18:LEU:HD12	2.44	0.42
1:A:107:GLY:C	1:A:235:ILE:HA	2.44	0.42
1:B:246:ARG:HG2	1:B:248:TYR:CZ	2.55	0.42
1:B:328:ARG:NH2	1:B:578:ASP:OD1	2.51	0.42
1:B:752:LEU:HG	1:B:997:ILE:CD1	2.49	0.42
1:C:403:ARG:NH1	1:C:406:GLU:OE2	2.52	0.42
3:P:64:GLY:HA3	5:P:301:NAG:C8	2.48	0.42
1:A:117:LEU:HD11	1:A:119:ILE:CD1	2.49	0.42
1:A:664:ILE:HA	1:A:665:PRO:HD3	1.87	0.42
1:A:976:VAL:HG23	1:A:979:ASP:H	1.83	0.42
1:A:1097:SER:HB2	1:A:1102:TRP:CD2	2.54	0.42
1:B:666:ILE:HB	1:B:670:ILE:HG13	2.01	0.42
1:B:736:VAL:HG22	1:B:858:LEU:CD2	2.48	0.42
1:C:804:GLN:NE2	1:C:935:GLN:HG2	2.34	0.42
1:C:993:ILE:HG22	1:C:997:ILE:HD11	2.02	0.42
1:C:1088:HIS:HB3	1:C:1120:THR:HG21	2.02	0.42
2:H:34:MET:O	2:H:50:TYR:HB2	2.19	0.42
2:O:17:SER:C	2:O:18:LEU:HD12	2.45	0.42
1:A:241:LEU:HD23	1:A:241:LEU:HA	1.90	0.42
1:A:274:THR:O	1:A:291:CYS:HB2	2.19	0.42
1:A:1019:ARG:NH2	1:B:1017:GLU:HG2	2.35	0.42
1:B:94:SER:O	1:B:95:THR:C	2.62	0.42
1:B:195:LYS:HE2	1:B:204:TYR:CE1	2.53	0.42
1:B:395:VAL:HA	1:B:514:SER:O	2.20	0.42
1:B:715:PRO:CB	1:B:1069:PRO:HB2	2.50	0.42
1:B:819:GLU:O	1:B:823:PHE:HD1	2.03	0.42
1:C:337:PRO:HB2	1:C:340:GLU:HB2	2.01	0.42
1:C:543:PHE:HD2	1:C:576:VAL:HG11	1.85	0.42
1:C:617:CYS:HB2	1:C:649:CYS:HB3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:GLU:O	2:H:95:PRO:HD2	2.20	0.42
1:A:31:SER:HA	1:A:216:LEU:HB2	2.01	0.42
1:A:224:GLU:HA	1:A:225:PRO:HD2	1.93	0.42
1:B:213:VAL:HG12	1:B:215:ASP:O	2.19	0.42
1:B:390:LEU:HD22	1:B:517:LEU:HD12	2.00	0.42
3:L:61:ARG:NH2	3:L:78:LEU:HA	2.34	0.42
3:L:104:LEU:HG	3:L:106:VAL:HG23	2.02	0.42
1:A:334:ASN:O	1:A:362:VAL:HG12	2.20	0.42
1:A:390:LEU:HD11	1:C:983:ARG:HB3	2.02	0.42
1:A:763:LEU:HD22	1:A:1004:LEU:HB3	2.02	0.42
1:B:393:THR:OG1	1:B:521:PRO:O	2.23	0.42
1:C:343:ASN:ND2	5:C:1305:NAG:C7	2.79	0.42
1:A:43:PHE:CZ	1:A:283:GLY:HA3	2.55	0.42
1:A:393:THR:HG23	1:A:394:ASN:N	2.35	0.42
1:A:571:ASP:CB	1:C:967:SER:HA	2.49	0.42
1:B:170:TYR:HD2	1:B:229:LEU:HD22	1.85	0.42
1:B:760:CYS:HA	1:B:763:LEU:HD12	2.02	0.42
1:B:903:ALA:HB2	1:B:916:LEU:HD22	2.01	0.42
1:C:319:ARG:HH11	1:C:595:VAL:CG1	2.33	0.42
1:C:748:GLU:HB3	1:C:751:ASN:HB2	2.02	0.42
2:M:14:PRO:HA	2:M:83:ARG:HA	2.02	0.42
1:A:557:LYS:HD2	1:A:559:PHE:HE1	1.85	0.41
1:A:898:PHE:O	1:A:899:PRO:C	2.61	0.41
1:A:943:SER:OG	1:A:945:LEU:HD12	2.20	0.41
1:B:535:LYS:HZ1	1:B:554:GLU:HB2	1.85	0.41
1:B:826:VAL:HB	1:B:1057:PRO:HG2	2.01	0.41
1:C:121:ASN:HD21	1:C:175:PHE:HB2	1.84	0.41
2:M:14:PRO:HA	2:M:82(C):LEU:O	2.20	0.41
1:A:741:TYR:CE2	1:A:1004:LEU:HG	2.54	0.41
1:A:903:ALA:HB1	1:A:913:GLN:HB2	2.02	0.41
1:B:393:THR:HG23	1:B:394:ASN:N	2.35	0.41
1:B:970:PHE:HD2	1:B:996:LEU:HD12	1.85	0.41
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.56	0.41
1:C:353:TRP:HH2	1:C:355:ARG:HH21	1.66	0.41
1:C:885:GLY:HA2	1:C:901:GLN:CD	2.45	0.41
1:C:1075:PHE:HB3	1:C:1096:VAL:HG13	2.02	0.41
1:A:114:THR:O	1:A:132:GLU:HG2	2.19	0.41
1:A:337:PRO:O	1:A:341:VAL:HG23	2.19	0.41
1:A:347:PHE:CD2	1:A:401:VAL:HG23	2.54	0.41
1:B:278:LYS:HD2	1:B:306:PHE:CD1	2.55	0.41
1:B:393:THR:HA	1:B:522:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.02	0.41
1:C:303:LEU:HD12	1:C:308:VAL:CG1	2.50	0.41
1:C:944:ALA:O	1:C:945:LEU:HD22	2.19	0.41
1:C:1134:ASN:OD1	1:C:1134:ASN:O	2.38	0.41
2:H:108:TYR:HB2	3:L:91:TRP:CD1	2.54	0.41
3:N:23:CYS:HB2	3:N:35:TRP:CH2	2.56	0.41
2:O:43:LYS:HG3	2:O:44:GLY:N	2.36	0.41
3:P:9:SER:HA	3:P:104:LEU:HD12	2.01	0.41
1:A:406:GLU:HA	1:A:409:GLN:HG3	2.01	0.41
1:B:144:TYR:CZ	1:B:246:ARG:HD3	2.55	0.41
1:B:199:GLY:O	1:B:230:PRO:HA	2.20	0.41
1:B:544:ASN:HD21	1:B:579:PRO:HG3	1.85	0.41
1:C:950:ASP:O	1:C:954:GLN:HG3	2.21	0.41
3:L:4:LEU:HD21	3:L:88:CYS:HB3	2.03	0.41
1:A:79:PHE:CE2	1:A:244:LEU:HD21	2.56	0.41
1:A:391:CYS:HB3	1:A:525:CYS:HB2	1.38	0.41
1:A:592:PHE:HE1	1:A:624:ILE:HG22	1.86	0.41
1:B:295:PRO:HG3	1:B:633:TRP:CH2	2.55	0.41
1:B:319:ARG:NH1	1:B:595:VAL:HG21	2.35	0.41
1:B:442:ASP:OD1	1:B:509:ARG:NE	2.53	0.41
1:C:159:VAL:HG11	1:C:241:LEU:HD21	2.01	0.41
1:C:238:PHE:CZ	1:C:267:VAL:HG11	2.56	0.41
2:M:33:GLU:HB2	2:M:52:THR:HA	2.01	0.41
2:M:35:ASN:HB2	2:M:110:PHE:HE1	1.83	0.41
1:A:741:TYR:CE1	1:A:966:LEU:HD13	2.55	0.41
1:B:329:PHE:HE2	1:B:528:LYS:HZ3	1.69	0.41
1:B:462:LYS:HG2	4:F:1:NAG:O7	2.19	0.41
1:C:30:ASN:HD21	1:C:59:PHE:HD1	1.69	0.41
1:C:558:LYS:HD3	1:C:558:LYS:N	2.36	0.41
1:C:731:MET:N	1:C:774:GLN:OE1	2.54	0.41
1:C:1030:SER:O	1:C:1034:LEU:HB2	2.20	0.41
2:H:110:PHE:HE2	3:L:98:PHE:CZ	2.39	0.41
2:O:95:PRO:HB3	2:O:108:TYR:HA	2.02	0.41
1:A:330:PRO:HD2	1:A:391:CYS:SG	2.61	0.41
1:B:159:VAL:HG23	1:B:160:TYR:HD2	1.85	0.41
1:B:1038:LYS:HE2	1:B:1038:LYS:HA	2.02	0.41
1:A:94:SER:O	1:A:95:THR:C	2.62	0.41
1:A:282:ASN:ND2	5:A:1303:NAG:O7	2.54	0.41
1:A:699:LEU:HG	1:C:788:ILE:HG13	2.01	0.41
1:B:244:LEU:HD12	1:B:260:ALA:N	2.35	0.41
1:C:33:THR:HA	1:C:58:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1028:LYS:HD3	1:C:1032:CYS:SG	2.61	0.41
3:P:62:PHE:HD2	5:P:301:NAG:H61	1.84	0.41
1:A:173:GLN:HG3	1:A:174:PRO:CD	2.48	0.41
1:A:808:ASP:HA	1:A:809:PRO:HD3	1.94	0.41
1:B:34:ARG:NH1	1:B:221:SER:OG	2.54	0.41
1:B:152:TRP:CE3	2:M:98:HIS:CE1	3.09	0.41
1:B:567:ARG:O	1:B:567:ARG:HG3	2.21	0.41
1:B:642:VAL:HA	1:B:651:ILE:HG22	2.03	0.41
1:B:815:ARG:HB2	1:B:820:ASP:OD1	2.21	0.41
1:C:28:TYR:HB3	1:C:61:ASN:HB2	2.02	0.41
1:C:233:ILE:CD1	1:C:235:ILE:HD11	2.51	0.41
1:C:404:GLY:HA2	1:C:508:TYR:CD1	2.55	0.41
1:C:454:ARG:HE	1:C:491:PRO:HB2	1.86	0.41
3:L:76:SER:C	3:L:77:SER:HG	2.29	0.41
2:M:102:THR:O	2:M:103:SER:OG	2.32	0.41
2:O:18:LEU:C	2:O:19:ARG:HD2	2.46	0.41
3:P:62:PHE:HD2	5:P:301:NAG:C6	2.34	0.41
1:A:102:ARG:HH12	2:H:100:TYR:HE2	1.69	0.41
1:A:370:ASN:OD1	1:B:455:LEU:HD21	2.21	0.41
1:A:1088:HIS:HB3	1:A:1120:THR:HG21	2.02	0.41
1:B:100:ILE:HG13	1:B:262:ALA:O	2.21	0.41
1:B:813:SER:HB3	1:B:815:ARG:HG3	2.03	0.41
3:P:45:ARG:HH12	3:P:47:LEU:HD21	1.86	0.41
1:A:83:VAL:CG1	1:A:237:ARG:HB3	2.51	0.40
1:A:198:ASP:OD1	1:B:463:PRO:HB2	2.21	0.40
1:A:406:GLU:HB3	1:A:418:ILE:HG13	2.02	0.40
1:A:960:ASN:HA	1:A:963:VAL:HG22	2.02	0.40
1:B:109:THR:O	1:B:237:ARG:NH2	2.51	0.40
1:B:129:LYS:HA	1:B:168:PHE:O	2.21	0.40
1:C:120:VAL:HG12	1:C:127:VAL:O	2.22	0.40
1:C:149:ASN:C	1:C:151:SER:H	2.29	0.40
1:C:384:PRO:HA	1:C:387:LEU:CD2	2.47	0.40
1:C:649:CYS:SG	1:C:651:ILE:HD11	2.61	0.40
1:C:927:PHE:HE2	1:C:1065:VAL:HG21	1.86	0.40
1:A:141:LEU:O	1:A:243:ALA:HA	2.21	0.40
1:B:85:PRO:HA	1:B:236:THR:O	2.21	0.40
1:B:403:ARG:HG2	1:B:504:GLY:O	2.22	0.40
1:B:753:LEU:HD23	1:B:753:LEU:HA	1.81	0.40
1:B:902:MET:SD	1:B:1050:MET:HE3	2.61	0.40
1:C:1095:PHE:HE1	1:C:1115:ILE:HD12	1.86	0.40
1:B:33:THR:CA	1:B:58:PHE:HD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ILE:HD13	1:B:598:ILE:HG12	2.03	0.40
1:B:733:LYS:HD2	1:B:771:ALA:HB1	2.04	0.40
1:C:178:ASP:C	1:C:180:GLU:H	2.28	0.40
1:C:984:LEU:HD22	1:C:988:GLU:HG2	2.03	0.40
1:C:1095:PHE:CE1	1:C:1115:ILE:HD12	2.56	0.40
2:H:14:PRO:HA	2:H:83:ARG:HA	2.03	0.40
2:H:56:ALA:O	2:H:57:ARG:NE	2.55	0.40
2:O:36:TRP:CD1	2:O:78:PHE:CE2	3.09	0.40
2:O:51:ILE:HG23	2:O:54:GLY:HA2	2.02	0.40
1:A:83:VAL:HG22	1:A:239:GLN:OE1	2.21	0.40
1:A:298:GLU:HB2	1:A:633:TRP:HH2	1.86	0.40
1:A:551:VAL:HG23	1:A:590:CYS:HA	2.02	0.40
1:A:660:TYR:O	1:A:698:SER:HB2	2.22	0.40
1:A:865:LEU:HD23	1:A:865:LEU:HA	1.86	0.40
1:C:329:PHE:CD2	1:C:528:LYS:HD2	2.57	0.40
1:C:366:SER:HA	1:C:369:TYR:CE2	2.57	0.40
1:C:888:PHE:CZ	1:C:1034:LEU:HD13	2.56	0.40
3:L:35:TRP:CG	3:L:73:LEU:HD12	2.56	0.40
2:M:19:ARG:HD2	2:M:19:ARG:HA	1.92	0.40
1:A:984:LEU:HB3	1:A:989:ALA:HB2	2.03	0.40
1:B:352:ALA:HB2	1:B:468:ILE:HG22	2.04	0.40
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.87	0.40
1:C:458:LYS:H	1:C:458:LYS:HG3	1.76	0.40
3:L:2:LEU:HD22	3:L:25:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1071/1256 (85%)	994 (93%)	71 (7%)	6 (1%)	21 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1071/1256 (85%)	999 (93%)	64 (6%)	8 (1%)	18	47
1	C	1071/1256 (85%)	1001 (94%)	65 (6%)	5 (0%)	24	55
2	H	124/233 (53%)	111 (90%)	13 (10%)	0	100	100
2	M	124/233 (53%)	105 (85%)	19 (15%)	0	100	100
2	O	124/233 (53%)	108 (87%)	16 (13%)	0	100	100
3	L	110/217 (51%)	99 (90%)	10 (9%)	1 (1%)	14	41
3	N	110/217 (51%)	103 (94%)	6 (6%)	1 (1%)	14	41
3	P	110/217 (51%)	96 (87%)	13 (12%)	1 (1%)	14	41
All	All	3915/5118 (76%)	3616 (92%)	277 (7%)	22 (1%)	23	51

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	892	PRO
1	A	941	THR
1	B	69	HIS
1	B	198	ASP
1	B	941	THR
1	B	942	PRO
1	C	941	THR
1	C	942	PRO
1	A	69	HIS
1	A	87	ASN
1	A	199	GLY
1	A	235	ILE
1	B	235	ILE
3	L	97	VAL
3	N	97	VAL
3	P	97	VAL
1	B	709	ASN
1	C	87	ASN
1	C	235	ILE
1	B	178	ASP
1	B	260	ALA
1	C	179	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	943/1096 (86%)	940 (100%)	3 (0%)	86	95
1	B	943/1096 (86%)	940 (100%)	3 (0%)	86	95
1	C	943/1096 (86%)	939 (100%)	4 (0%)	84	94
2	H	105/198 (53%)	105 (100%)	0	100	100
2	M	105/198 (53%)	105 (100%)	0	100	100
2	O	105/198 (53%)	105 (100%)	0	100	100
3	L	91/182 (50%)	91 (100%)	0	100	100
3	N	91/182 (50%)	91 (100%)	0	100	100
3	P	91/182 (50%)	91 (100%)	0	100	100
All	All	3417/4428 (77%)	3407 (100%)	10 (0%)	84	95

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	897	PRO
1	A	899	PRO
1	A	900	MET
1	B	899	PRO
1	B	900	MET
1	B	1074	ASN
1	C	895	GLN
1	C	896	ILE
1	C	899	PRO
1	C	900	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	207	HIS
1	A	334	ASN

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Mol	Chain	Res	Type
1	A	360	ASN
1	A	439	ASN
1	A	613	GLN
1	A	703	ASN
1	A	1002	GLN
1	A	1101	HIS
1	B	69	HIS
1	B	121	ASN
1	B	125	ASN
1	B	188	ASN
1	B	207	HIS
1	B	271	GLN
1	B	360	ASN
1	B	439	ASN
1	B	481	ASN
1	B	658	ASN
1	B	784	GLN
1	B	804	GLN
1	B	901	GLN
1	B	913	GLN
1	B	935	GLN
1	B	1002	GLN
1	B	1074	ASN
1	C	69	HIS
1	C	115	GLN
1	C	121	ASN
1	C	271	GLN
1	C	439	ASN
1	C	481	ASN
1	C	542	ASN
1	C	556	ASN
1	C	580	GLN
1	C	628	GLN
1	C	762	GLN
1	C	779	GLN
1	C	804	GLN
1	C	913	GLN
3	L	89	GLN
2	M	98	HIS
2	O	81	GLN
2	O	82(A)	ASN
2	O	96	GLN

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Mol	Chain	Res	Type
3	P	54(B)	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

24 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$
4	NAG	D	1	1,4	14,14,15	0.99	1 (7%)	17,19,21	1.01	1 (5%)
4	NAG	D	2	4	14,14,15	0.18	0	17,19,21	0.40	0
4	NAG	E	1	1,4	14,14,15	0.21	0	17,19,21	0.51	0
4	NAG	E	2	4	14,14,15	0.41	0	17,19,21	0.38	0
4	NAG	F	1	1,4	14,14,15	0.83	1 (7%)	17,19,21	1.61	3 (17%)
4	NAG	F	2	4	14,14,15	0.31	0	17,19,21	0.50	0
4	NAG	G	1	1,4	14,14,15	0.43	0	17,19,21	0.75	1 (5%)
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.47	0
4	NAG	I	1	1,4	14,14,15	0.58	0	17,19,21	0.74	0
4	NAG	I	2	4	14,14,15	0.36	0	17,19,21	0.62	0
4	NAG	J	1	1,4	14,14,15	1.01	2 (14%)	17,19,21	1.78	3 (17%)
4	NAG	J	2	4	14,14,15	0.30	0	17,19,21	0.60	1 (5%)
4	NAG	K	1	1,4	14,14,15	0.18	0	17,19,21	0.48	0
4	NAG	K	2	4	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	Q	1	1,4	14,14,15	0.37	0	17,19,21	0.61	0
4	NAG	Q	2	4	14,14,15	0.33	0	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	R	1	1,4	14,14,15	0.56	0	17,19,21	1.02	1 (5%)
4	NAG	R	2	4	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	S	1	1,4	14,14,15	0.63	1 (7%)	17,19,21	1.15	2 (11%)
4	NAG	S	2	4	14,14,15	0.33	0	17,19,21	0.48	0
4	NAG	T	1	1,4	14,14,15	0.92	1 (7%)	17,19,21	0.96	1 (5%)
4	NAG	T	2	4	14,14,15	0.29	0	17,19,21	0.63	1 (5%)
4	NAG	U	1	1,4	14,14,15	1.03	2 (14%)	17,19,21	0.86	1 (5%)
4	NAG	U	2	4	14,14,15	0.29	0	17,19,21	0.38	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	D	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	D	2	4	-	3/6/23/26	0/1/1/1
4	NAG	E	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	5/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	3/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	3/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	U	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	NAG	O5-C1	-3.55	1.37	1.43
4	T	1	NAG	O5-C1	-3.09	1.38	1.43
4	J	1	NAG	C1-C2	2.65	1.56	1.52
4	J	1	NAG	O5-C1	2.62	1.48	1.43
4	U	1	NAG	C1-C2	2.55	1.55	1.52
4	U	1	NAG	O5-C1	-2.45	1.39	1.43
4	F	1	NAG	C1-C2	2.31	1.55	1.52
4	S	1	NAG	C1-C2	2.20	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	1	NAG	C1-O5-C5	5.05	118.96	112.19
4	F	1	NAG	C2-N2-C7	4.41	128.81	122.90
4	J	1	NAG	C2-N2-C7	3.69	127.84	122.90
4	F	1	NAG	C1-O5-C5	3.61	117.02	112.19
4	S	1	NAG	C1-O5-C5	3.05	116.28	112.19
4	J	1	NAG	C1-C2-N2	2.91	115.02	110.43
4	S	1	NAG	C2-N2-C7	2.69	126.51	122.90
4	D	1	NAG	O4-C4-C3	-2.43	104.64	110.38
4	F	1	NAG	C1-C2-N2	2.41	114.22	110.43
4	U	1	NAG	C4-C3-C2	2.27	114.35	111.02
4	T	1	NAG	C3-C4-C5	2.27	114.34	110.23
4	R	1	NAG	C3-C4-C5	2.22	114.25	110.23
4	G	1	NAG	C1-O5-C5	2.14	115.06	112.19
4	T	2	NAG	C1-O5-C5	2.09	114.99	112.19
4	J	2	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	J	1	NAG	C1-C2-N2-C7
4	S	1	NAG	C1-C2-N2-C7
4	I	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	I	2	NAG	C4-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	U	1	NAG	O5-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	U	2	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	U	2	NAG	O5-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	E	1	NAG	C8-C7-N2-C2
4	E	1	NAG	O7-C7-N2-C2
4	F	1	NAG	C8-C7-N2-C2
4	F	1	NAG	O7-C7-N2-C2
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	J	2	NAG	C4-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6
4	R	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6

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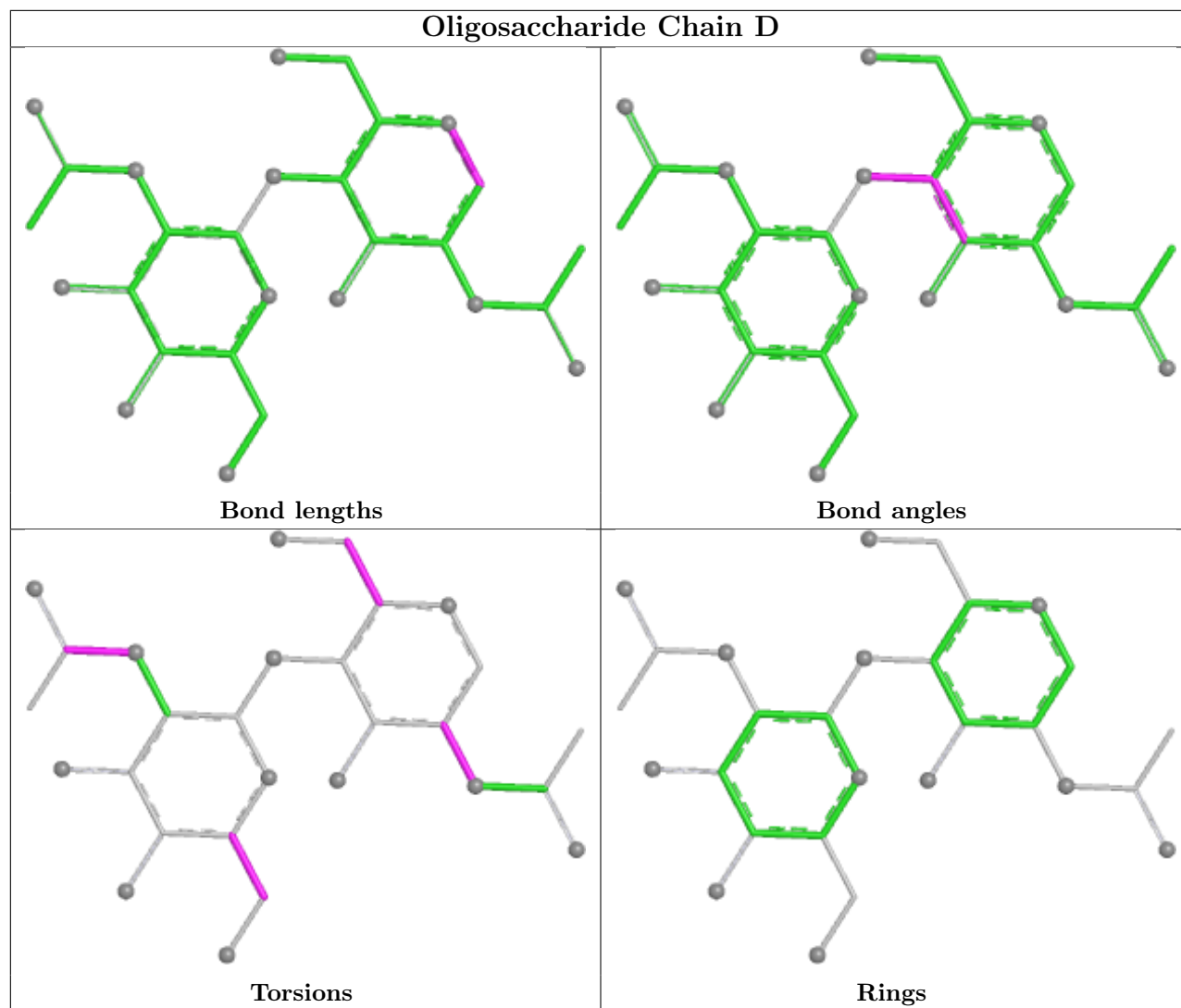
Mol	Chain	Res	Type	Atoms
4	J	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C1-C2-N2-C7
4	I	1	NAG	C1-C2-N2-C7
4	K	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C3-C2-N2-C7
4	I	2	NAG	C3-C2-N2-C7
4	Q	2	NAG	C3-C2-N2-C7
4	R	1	NAG	C3-C2-N2-C7
4	D	2	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	F	1	NAG	C1-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7
4	Q	2	NAG	C1-C2-N2-C7
4	U	2	NAG	C1-C2-N2-C7
4	D	1	NAG	C3-C2-N2-C7
4	F	1	NAG	C3-C2-N2-C7
4	Q	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6

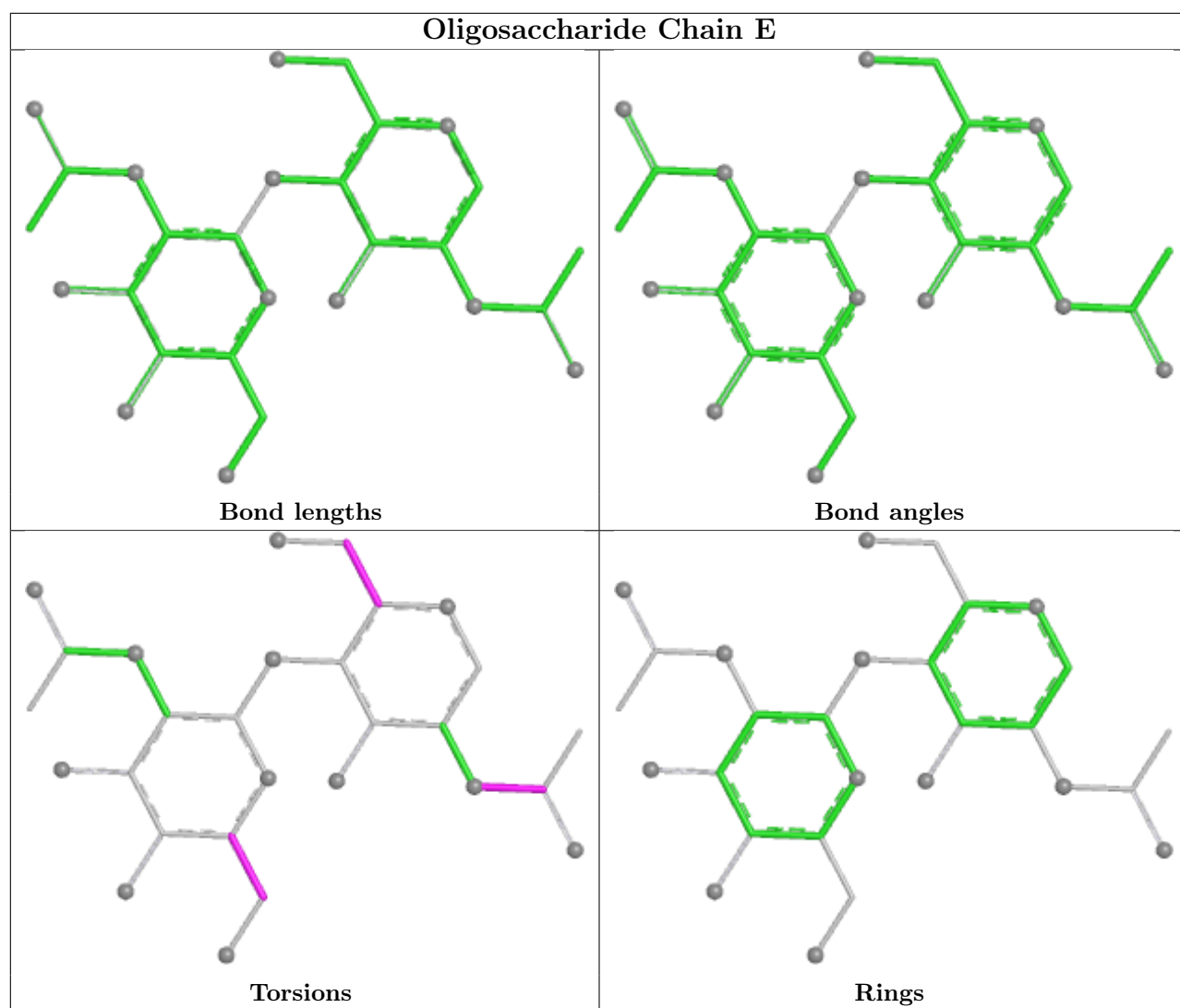
There are no ring outliers.

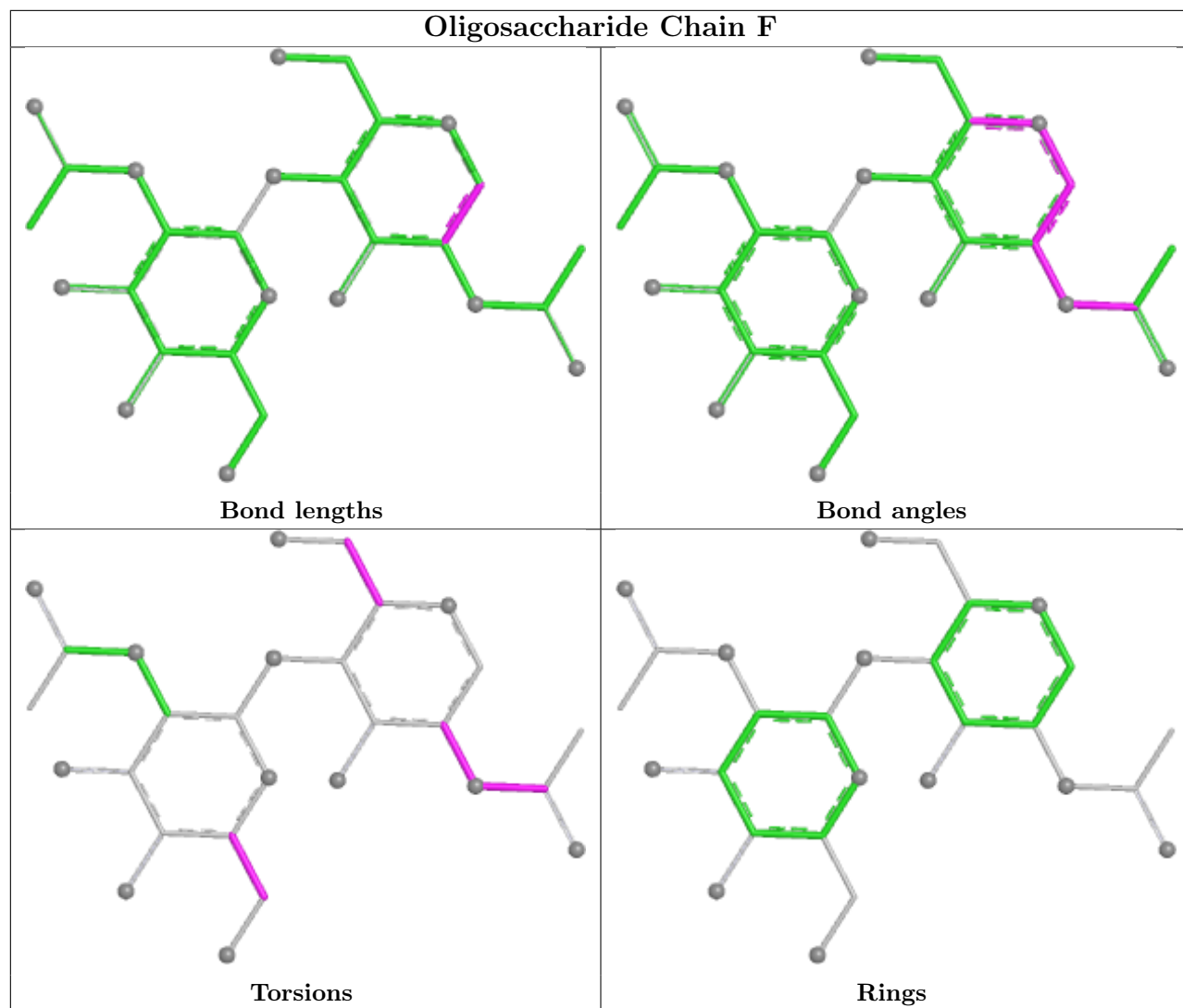
8 monomers are involved in 12 short contacts:

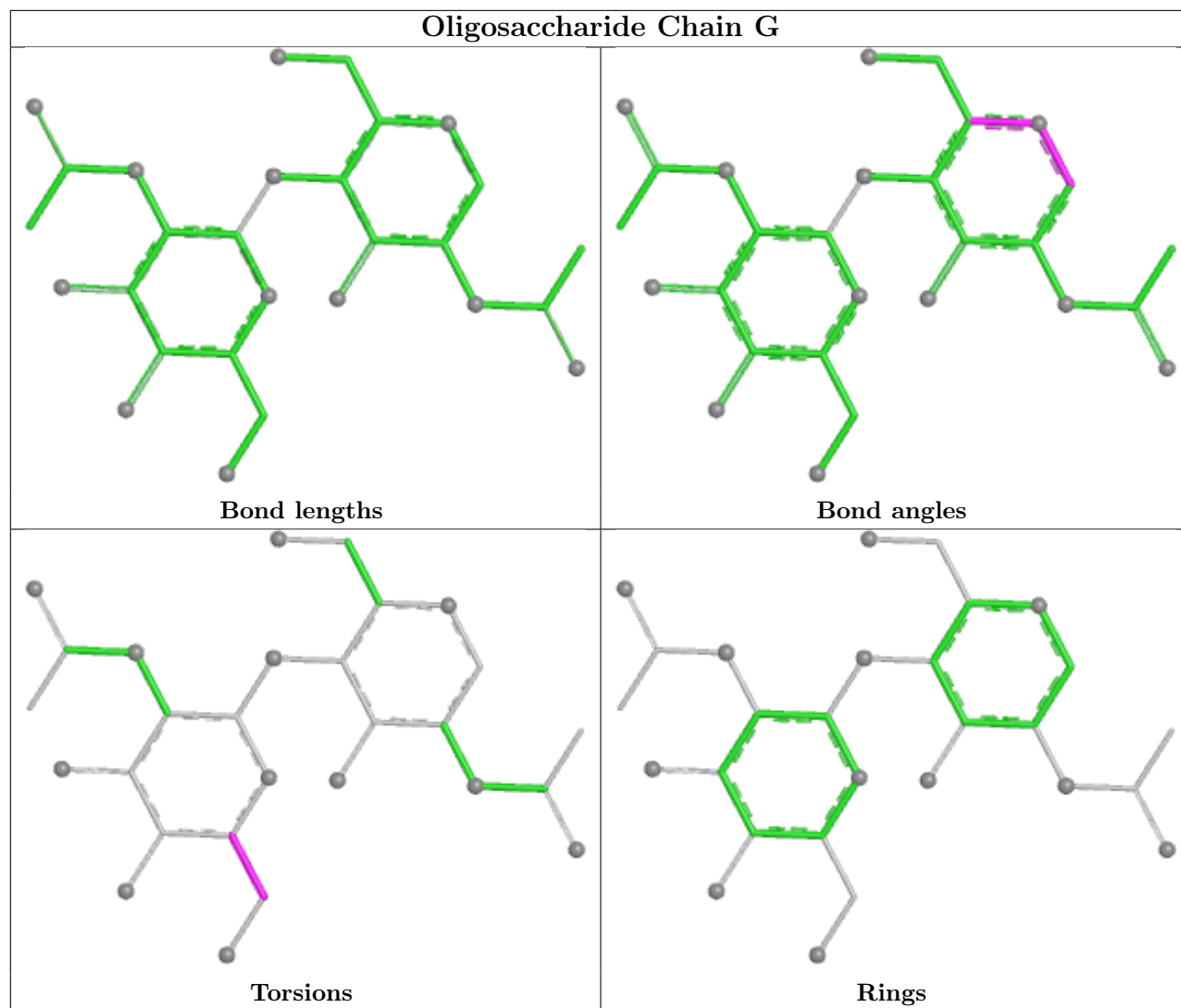
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1	NAG	2	0
4	S	1	NAG	1	0
4	T	1	NAG	1	0
4	K	1	NAG	1	0
4	J	1	NAG	3	0
4	T	2	NAG	1	0
4	F	1	NAG	3	0
4	G	1	NAG	1	0

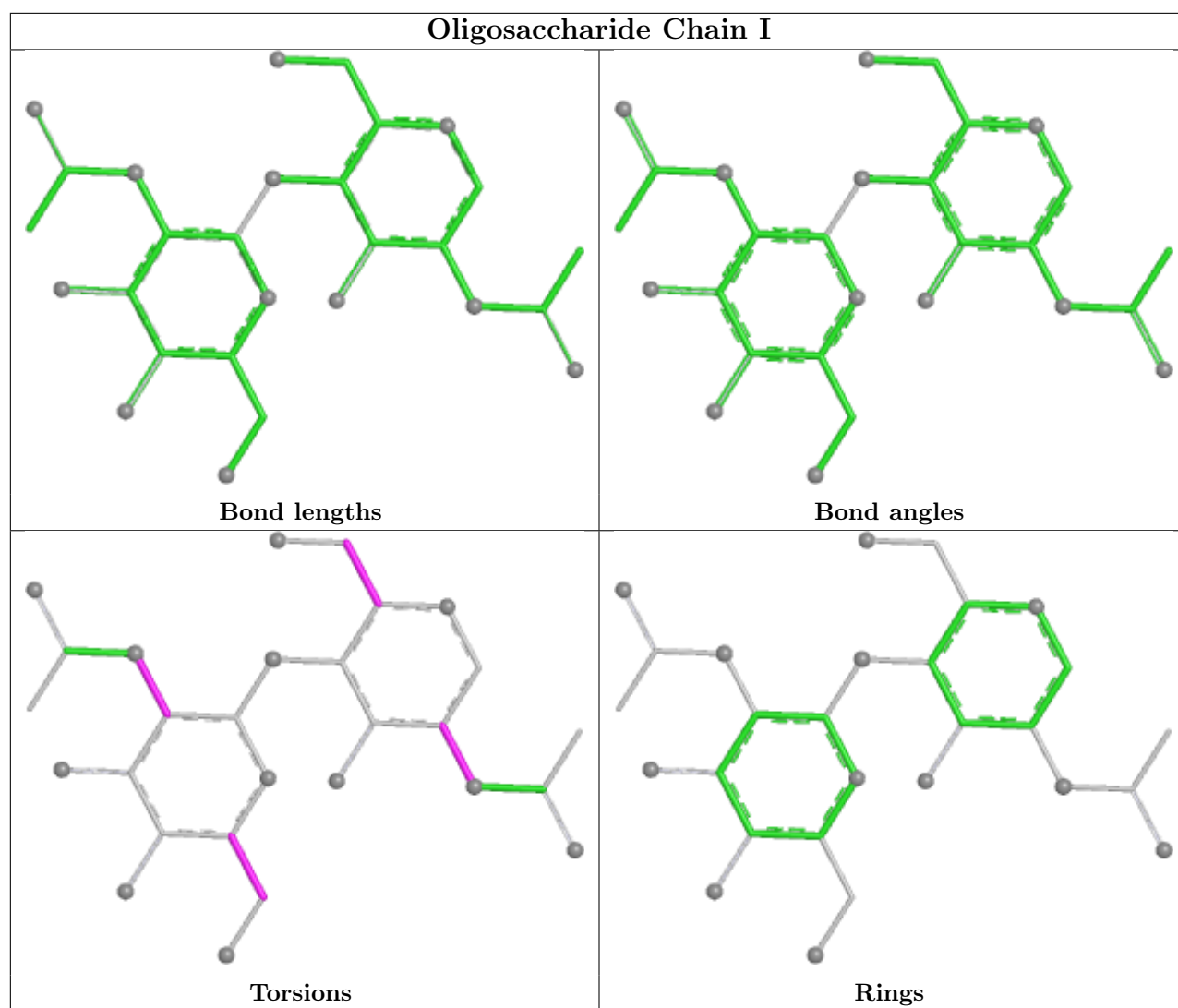
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

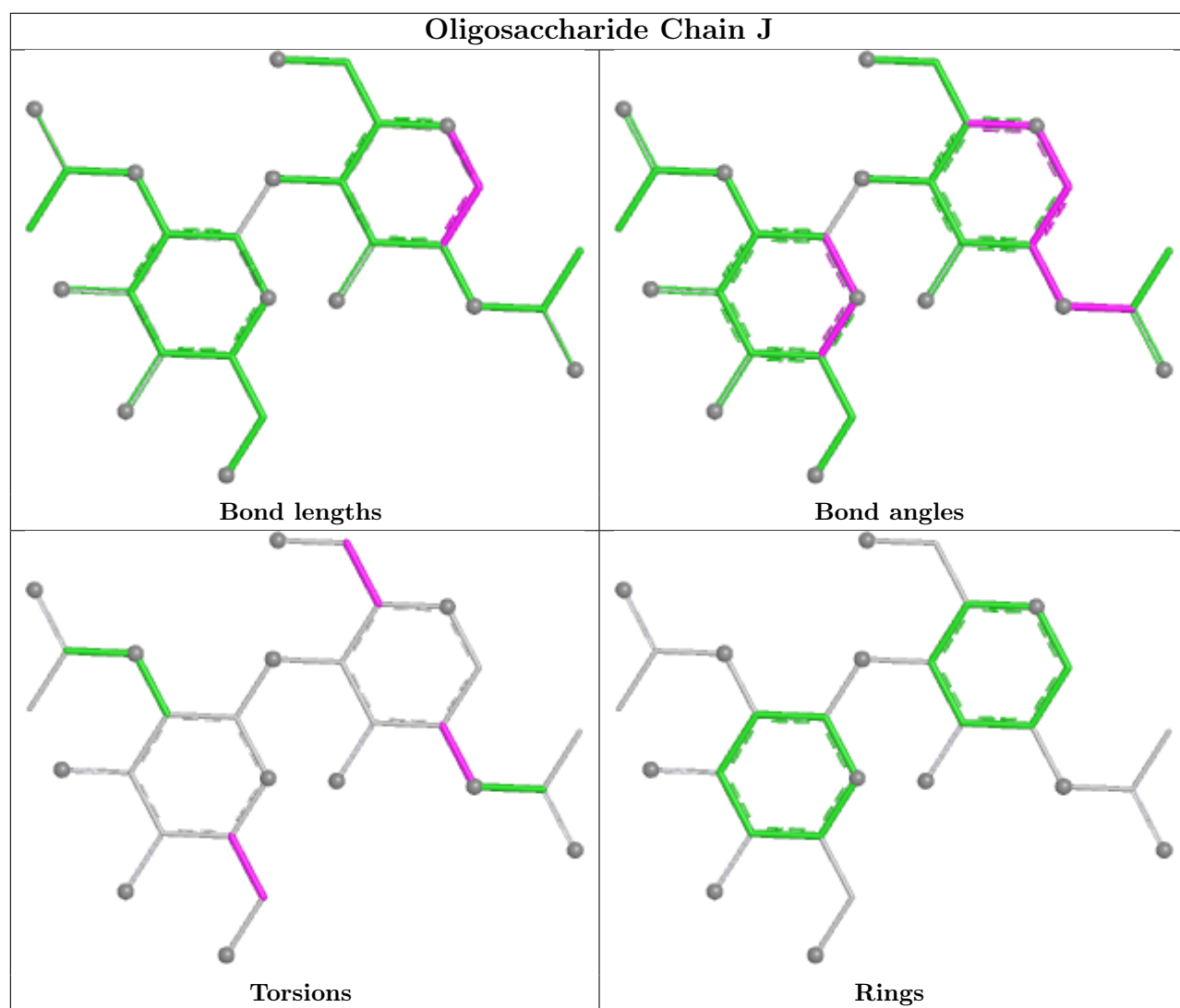


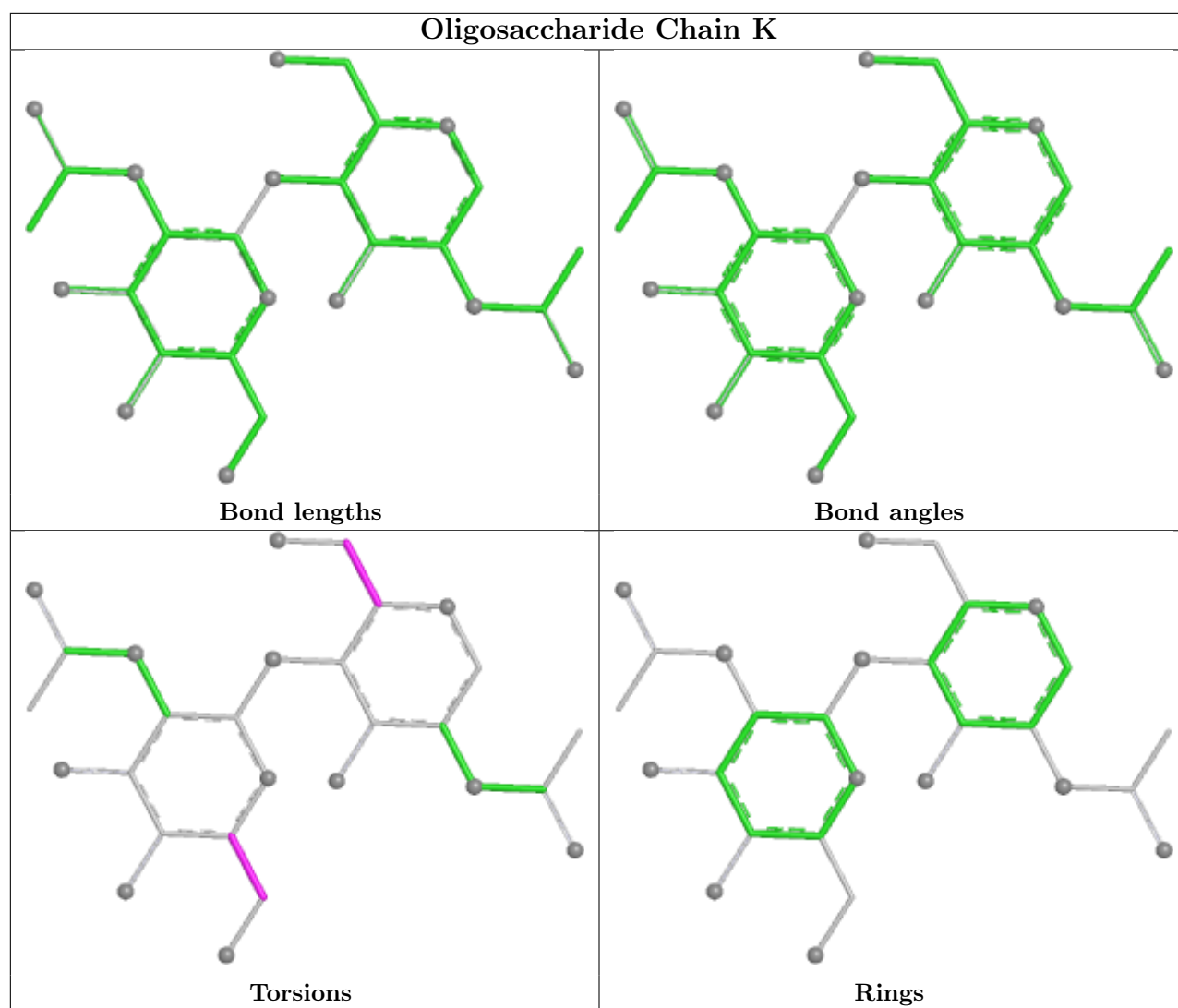


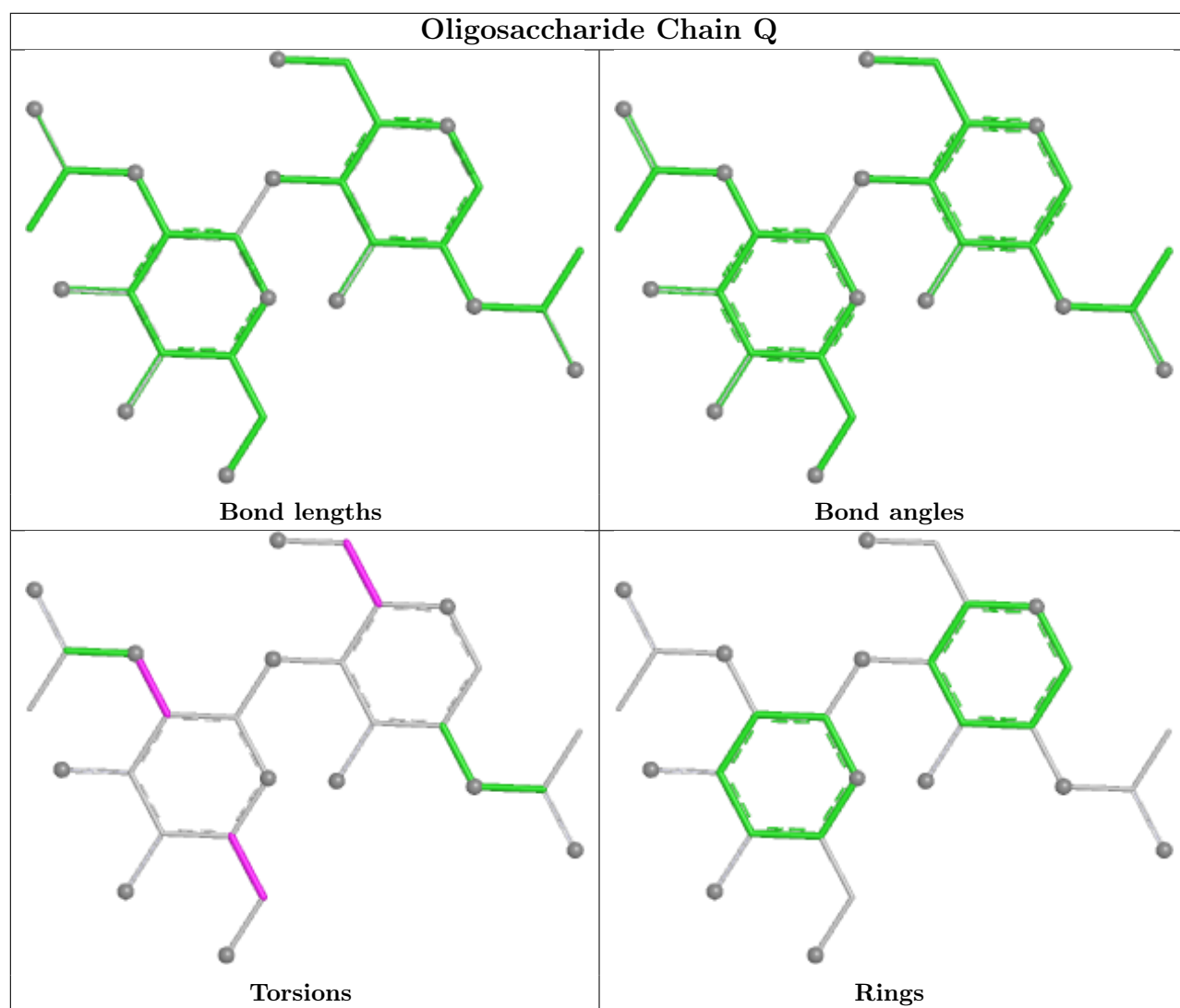


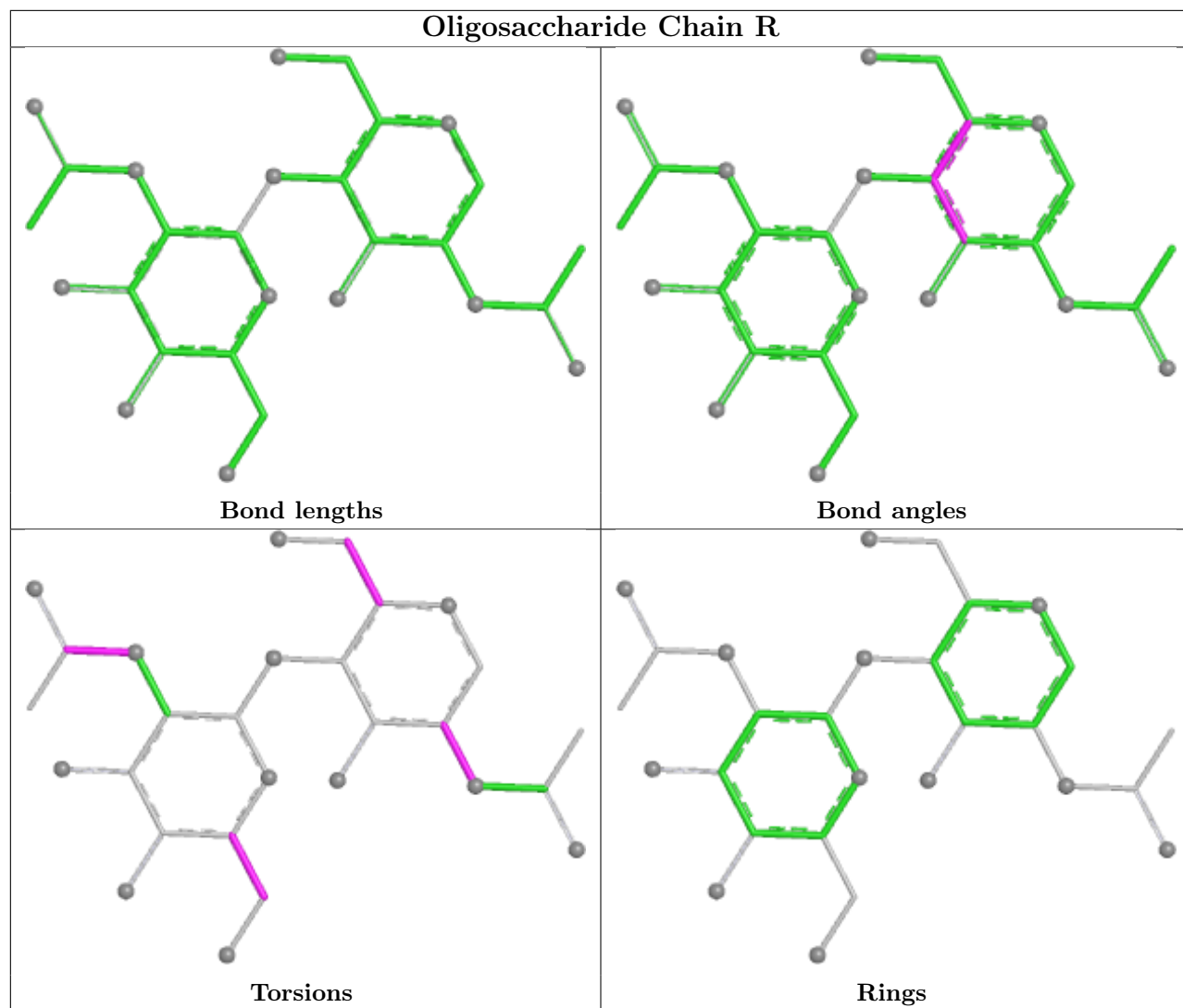


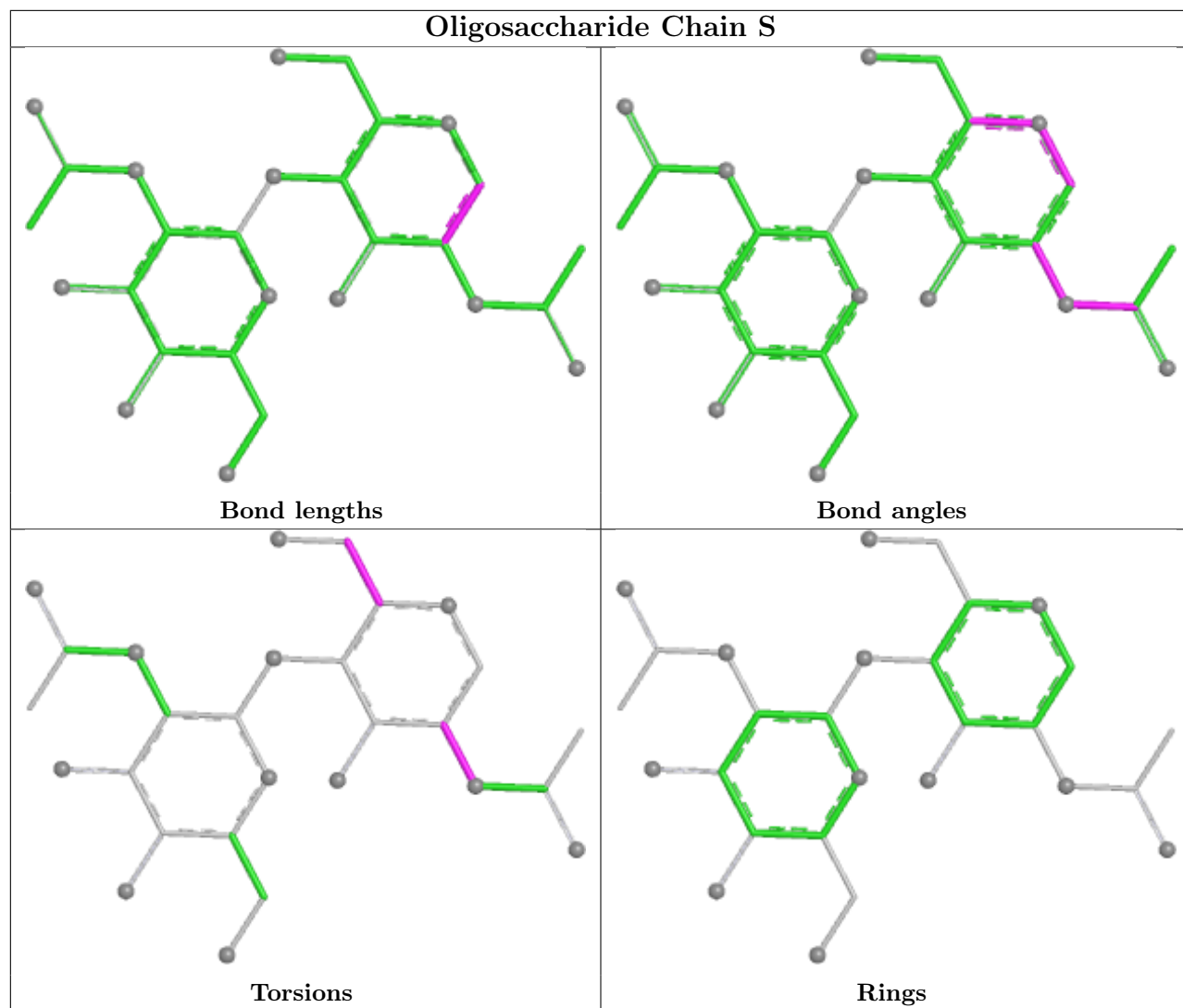


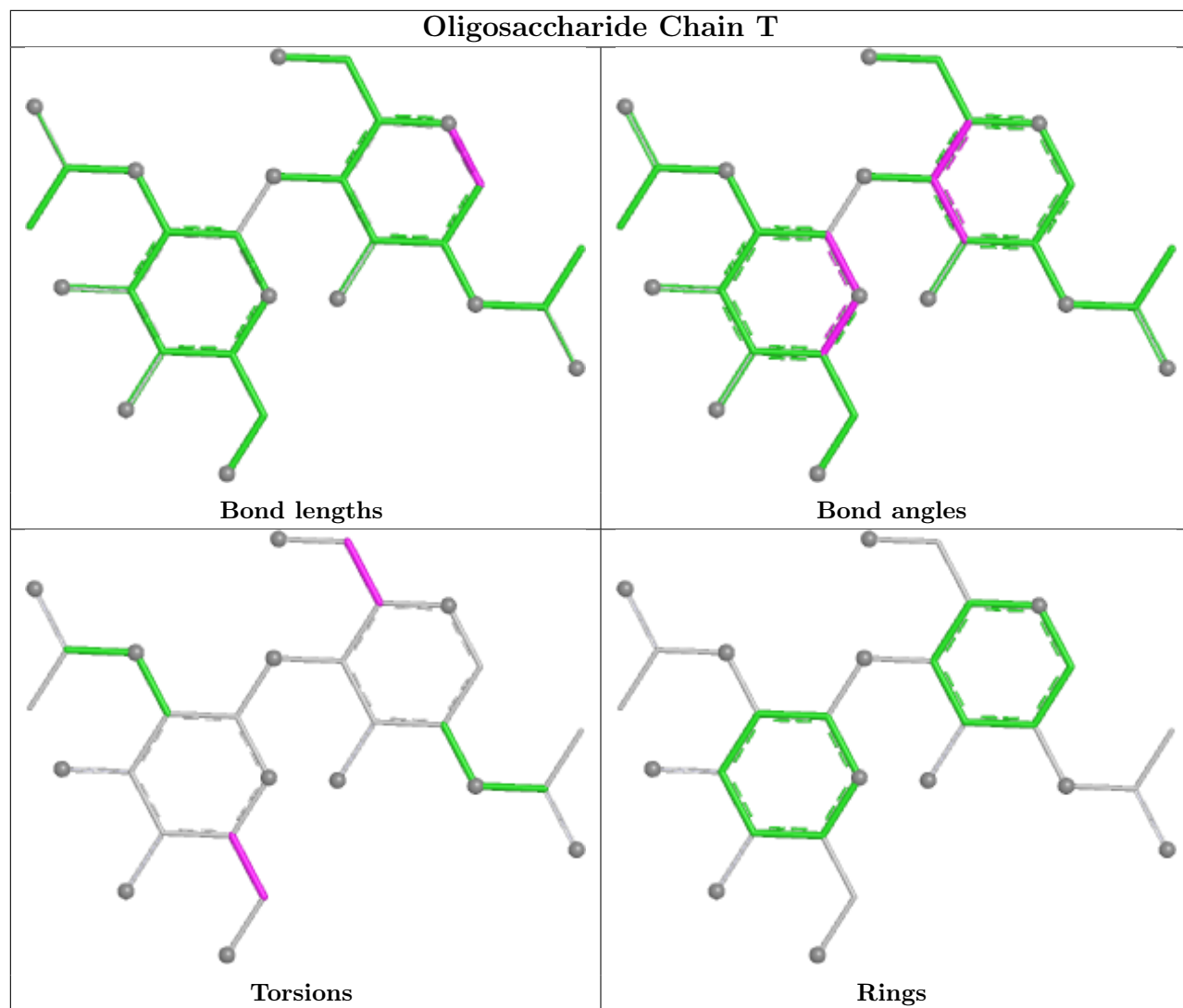


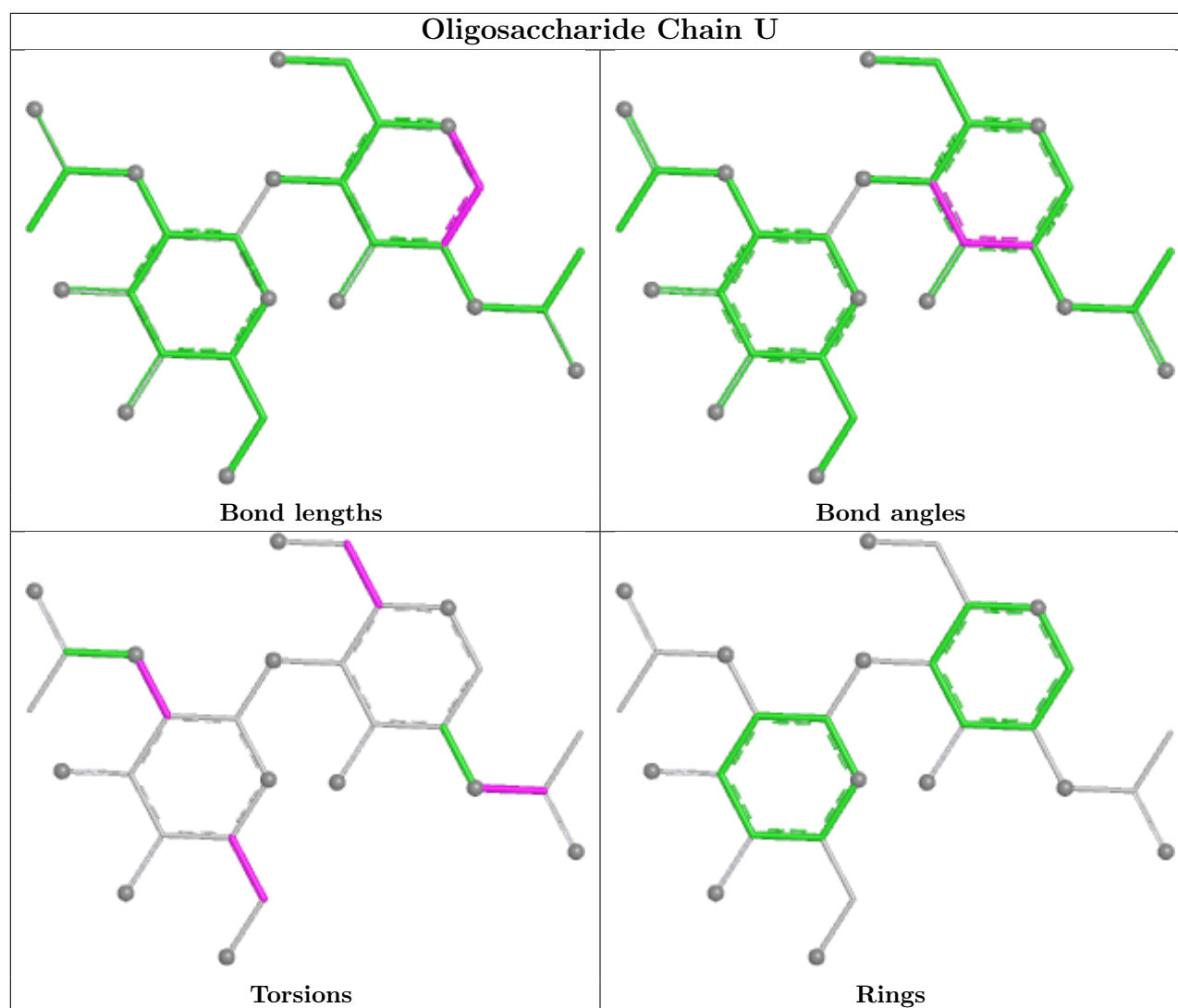












5.6 Ligand geometry [i](#)

35 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1311	1	14,14,15	0.31	0	17,19,21	0.47	0
5	NAG	B	1303	1	14,14,15	0.75	1 (7%)	17,19,21	1.02	1 (5%)
5	NAG	C	1307	1	14,14,15	0.23	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	1304	1	14,14,15	0.54	0	17,19,21	0.86	1 (5%)
5	NAG	A	1301	1	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	A	1306	1	14,14,15	0.38	0	17,19,21	0.68	1 (5%)
5	NAG	B	1305	1	14,14,15	0.60	0	17,19,21	0.78	1 (5%)
5	NAG	L	301	3	14,14,15	0.49	0	17,19,21	0.86	0
5	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.39	0
5	NAG	B	1306	1	14,14,15	0.31	0	17,19,21	0.53	0
5	NAG	C	1301	1	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	C	1308	1	14,14,15	0.21	0	17,19,21	0.52	0
5	NAG	A	1303	1	14,14,15	0.80	1 (7%)	17,19,21	1.07	1 (5%)
5	NAG	C	1303	1	14,14,15	0.31	0	17,19,21	0.50	0
5	NAG	C	1302	1	14,14,15	0.23	0	17,19,21	0.33	0
5	NAG	P	301	3	14,14,15	1.25	2 (14%)	17,19,21	0.91	1 (5%)
5	NAG	C	1310	1	14,14,15	0.23	0	17,19,21	0.51	0
5	NAG	A	1305	1	14,14,15	0.26	0	17,19,21	0.68	1 (5%)
5	NAG	A	1304	1	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	B	1304	1	14,14,15	0.90	1 (7%)	17,19,21	1.18	1 (5%)
5	NAG	C	1305	1	14,14,15	0.73	1 (7%)	17,19,21	0.73	0
5	NAG	A	1307	1	14,14,15	0.35	0	17,19,21	0.36	0
5	NAG	B	1309	1	14,14,15	0.29	0	17,19,21	0.59	0
5	NAG	C	1311	1	14,14,15	0.53	0	17,19,21	0.65	0
5	NAG	A	1309	1	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
5	NAG	C	1306	1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	C	1309	1	14,14,15	0.28	0	17,19,21	0.45	0
5	NAG	A	1302	1	14,14,15	0.29	0	17,19,21	0.51	0
5	NAG	A	1310	1	14,14,15	0.19	0	17,19,21	0.50	0
5	NAG	A	1308	1	14,14,15	0.62	1 (7%)	17,19,21	0.64	0
5	NAG	B	1301	1	14,14,15	0.72	1 (7%)	17,19,21	0.88	1 (5%)
5	NAG	B	1302	1	14,14,15	0.23	0	17,19,21	0.37	0
5	NAG	N	301	3	14,14,15	0.46	0	17,19,21	0.56	0
5	NAG	B	1310	1	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	B	1308	1	14,14,15	0.94	1 (7%)	17,19,21	1.41	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1311	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1303	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1306	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	L	301	3	-	1/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	P	301	3	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	N	301	3	-	0/6/23/26	0/1/1/1
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	301	NAG	C1-C2	3.76	1.57	1.52
5	B	1308	NAG	O5-C1	3.39	1.49	1.43
5	B	1304	NAG	O5-C1	3.12	1.48	1.43
5	A	1303	NAG	O5-C1	-2.72	1.39	1.43
5	B	1301	NAG	O5-C1	2.45	1.47	1.43
5	P	301	NAG	O5-C1	2.30	1.47	1.43
5	C	1305	NAG	O5-C1	-2.21	1.40	1.43
5	B	1303	NAG	O5-C1	2.20	1.47	1.43
5	A	1308	NAG	C1-C2	2.17	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1308	NAG	C1-O5-C5	5.59	119.67	112.19
5	B	1304	NAG	C1-O5-C5	4.65	118.41	112.19
5	B	1303	NAG	C1-O5-C5	3.74	117.20	112.19
5	B	1301	NAG	C1-O5-C5	3.31	116.62	112.19
5	A	1309	NAG	C1-O5-C5	3.13	116.39	112.19
5	C	1304	NAG	C1-O5-C5	3.13	116.38	112.19
5	A	1303	NAG	C2-N2-C7	2.68	126.49	122.90
5	P	301	NAG	C1-O5-C5	2.63	115.70	112.19
5	B	1305	NAG	C1-O5-C5	2.46	115.49	112.19
5	A	1305	NAG	C1-O5-C5	2.20	115.13	112.19
5	A	1306	NAG	C1-O5-C5	2.14	115.06	112.19

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1303	NAG	C1-C2-N2-C7
5	B	1303	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	B	1303	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	C	1309	NAG	C4-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	B	1309	NAG	C4-C5-C6-O6
5	A	1303	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	C	1302	NAG	O5-C5-C6-O6
5	A	1311	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	C	1306	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1303	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	A	1306	NAG	O5-C5-C6-O6
5	A	1307	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	A	1303	NAG	C4-C5-C6-O6
5	B	1302	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	C	1303	NAG	C4-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
5	C	1306	NAG	C4-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	A	1311	NAG	C4-C5-C6-O6
5	P	301	NAG	O5-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
5	A	1306	NAG	C4-C5-C6-O6
5	A	1307	NAG	C4-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	B	1306	NAG	C4-C5-C6-O6
5	P	301	NAG	C3-C2-N2-C7
5	B	1301	NAG	O5-C5-C6-O6
5	B	1309	NAG	C1-C2-N2-C7
5	C	1303	NAG	C1-C2-N2-C7
5	C	1305	NAG	C1-C2-N2-C7
5	C	1311	NAG	C1-C2-N2-C7
5	B	1306	NAG	O5-C5-C6-O6
5	A	1306	NAG	C3-C2-N2-C7
5	B	1303	NAG	C3-C2-N2-C7
5	B	1305	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	C	1305	NAG	C3-C2-N2-C7
5	C	1311	NAG	C3-C2-N2-C7
5	L	301	NAG	O5-C5-C6-O6
5	A	1306	NAG	C1-C2-N2-C7
5	B	1303	NAG	C1-C2-N2-C7
5	B	1305	NAG	C1-C2-N2-C7
5	B	1309	NAG	C3-C2-N2-C7
5	C	1303	NAG	C3-C2-N2-C7
5	B	1307	NAG	C4-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1304	NAG	1	0
5	B	1305	NAG	4	0
5	A	1303	NAG	4	0
5	P	301	NAG	9	0
5	A	1305	NAG	1	0
5	C	1305	NAG	1	0
5	C	1311	NAG	1	0
5	A	1309	NAG	1	0
5	A	1302	NAG	1	0
5	A	1308	NAG	2	0
5	B	1301	NAG	8	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.

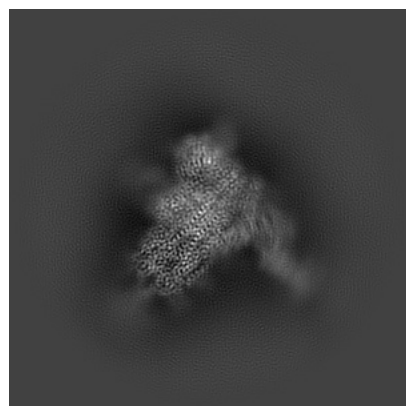
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26429. These allow visual inspection of the internal detail of the map and identification of artifacts.

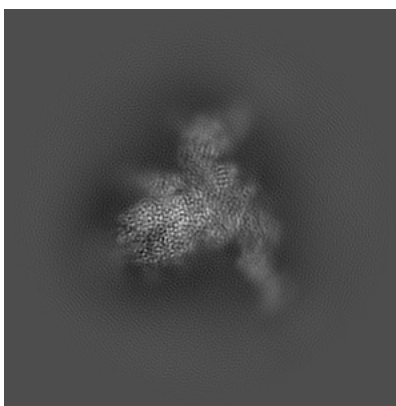
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

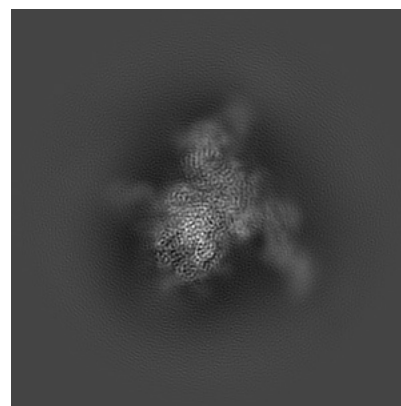
6.1.1 Primary map



X

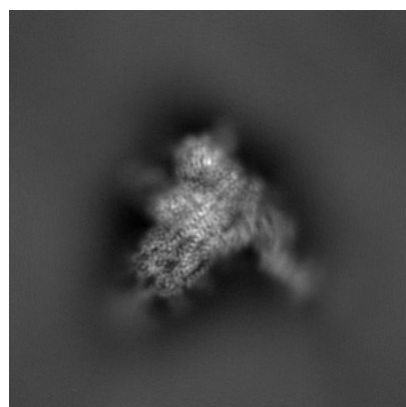


Y

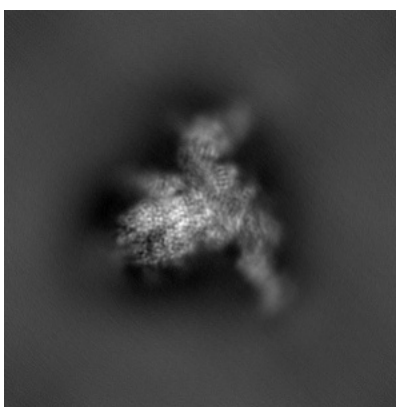


Z

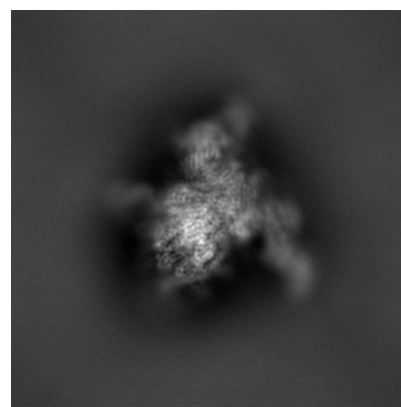
6.1.2 Raw map



X



Y

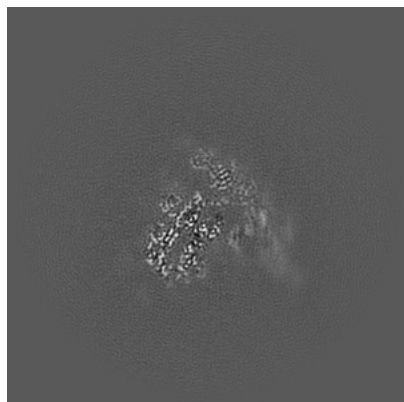


Z

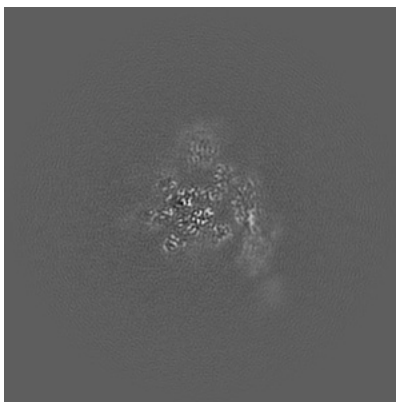
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

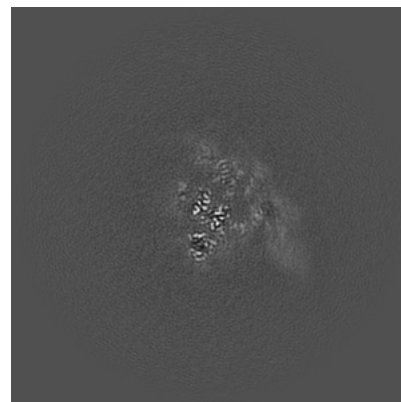
6.2.1 Primary map



X Index: 180

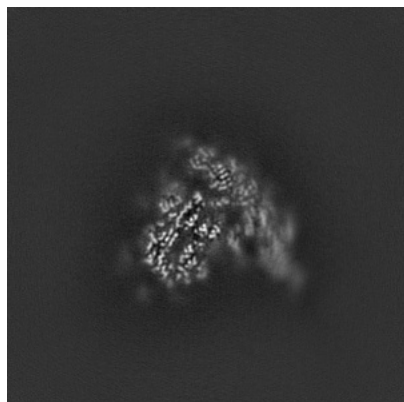


Y Index: 180

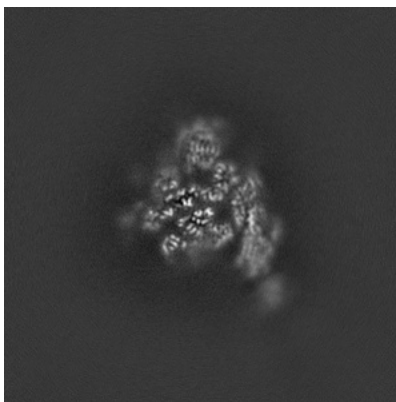


Z Index: 180

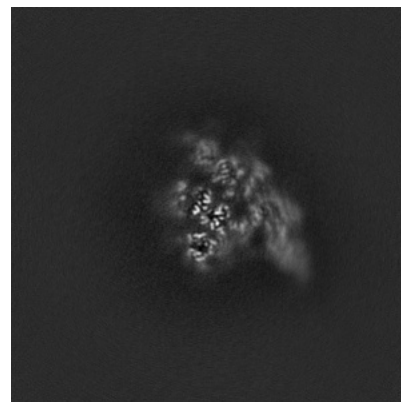
6.2.2 Raw map



X Index: 180



Y Index: 180

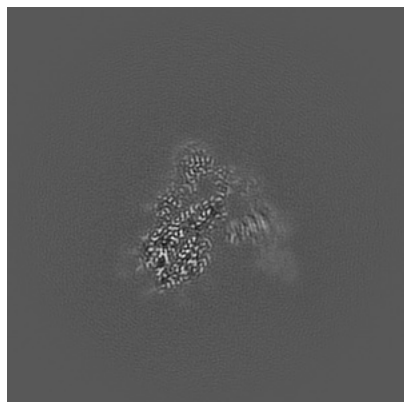


Z Index: 180

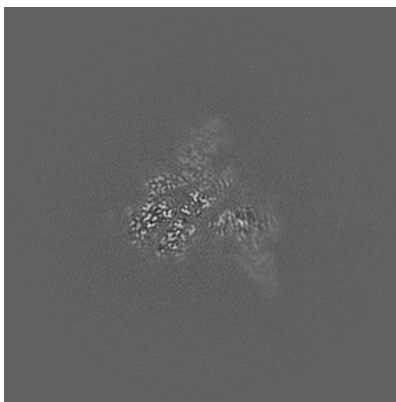
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

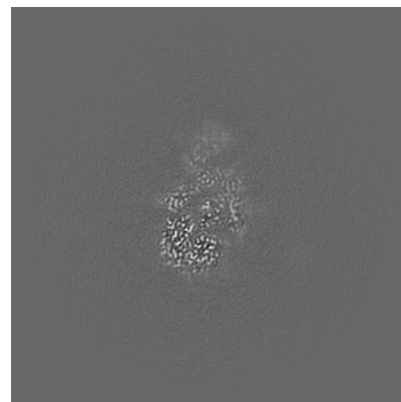
6.3.1 Primary map



X Index: 172

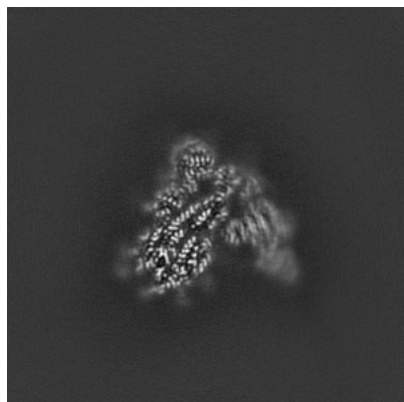


Y Index: 164

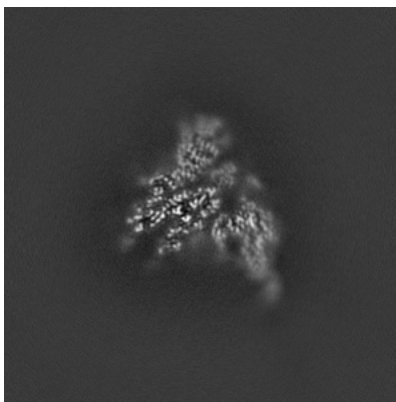


Z Index: 150

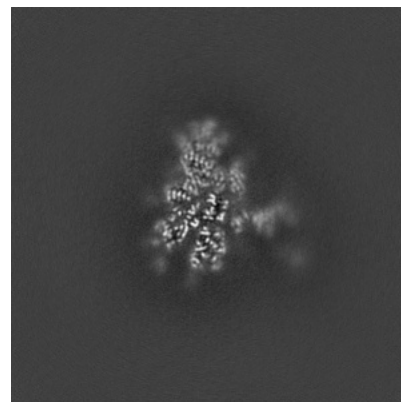
6.3.2 Raw map



X Index: 172



Y Index: 170

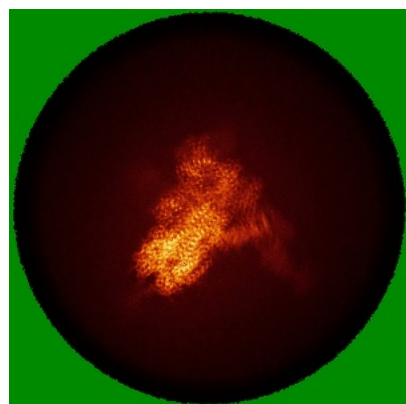


Z Index: 158

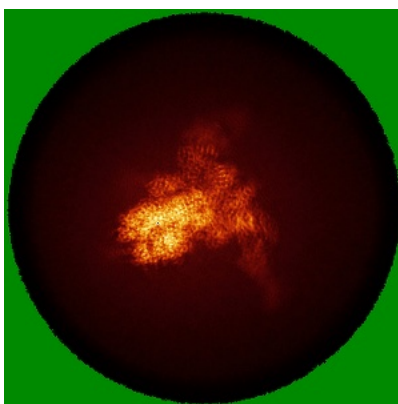
The images above show the largest variance slices of the map in three orthogonal directions.

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

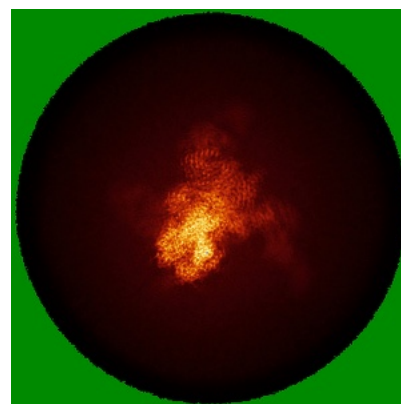
6.4.1 Primary map



X

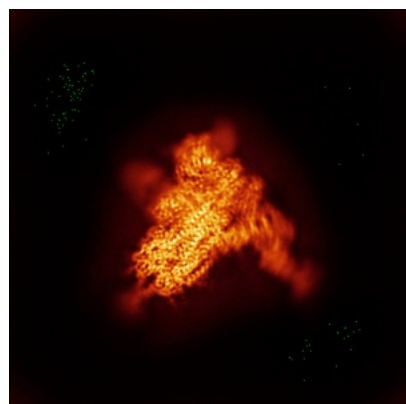


Y

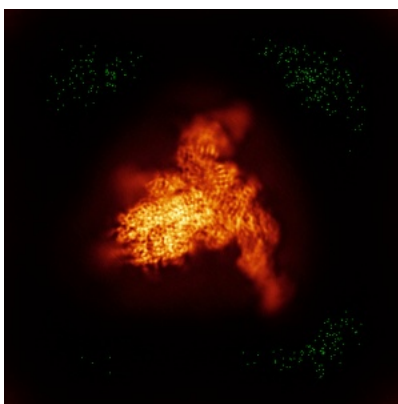


Z

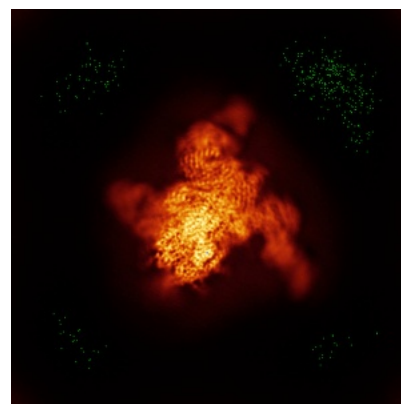
6.4.2 Raw map



X



Y

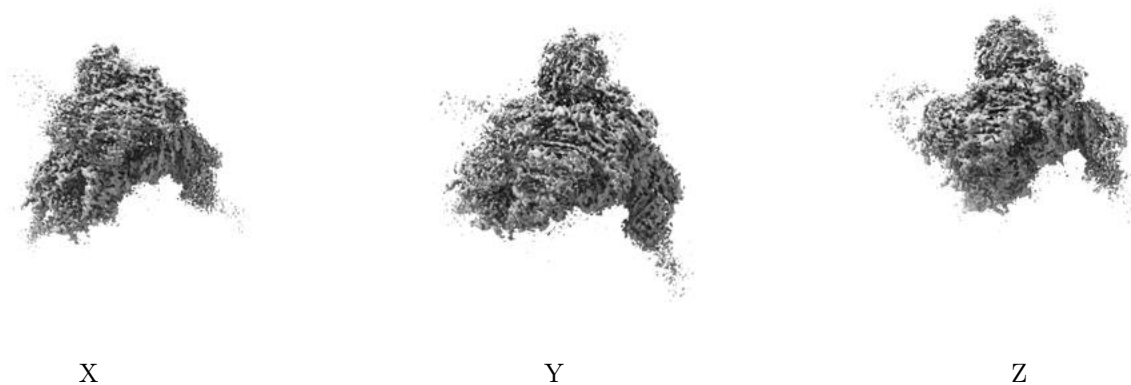


Z

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

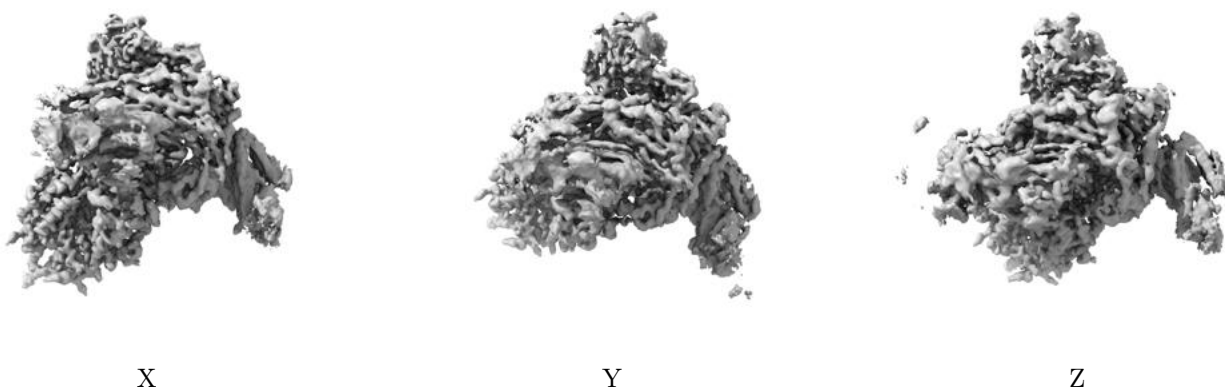
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. 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.

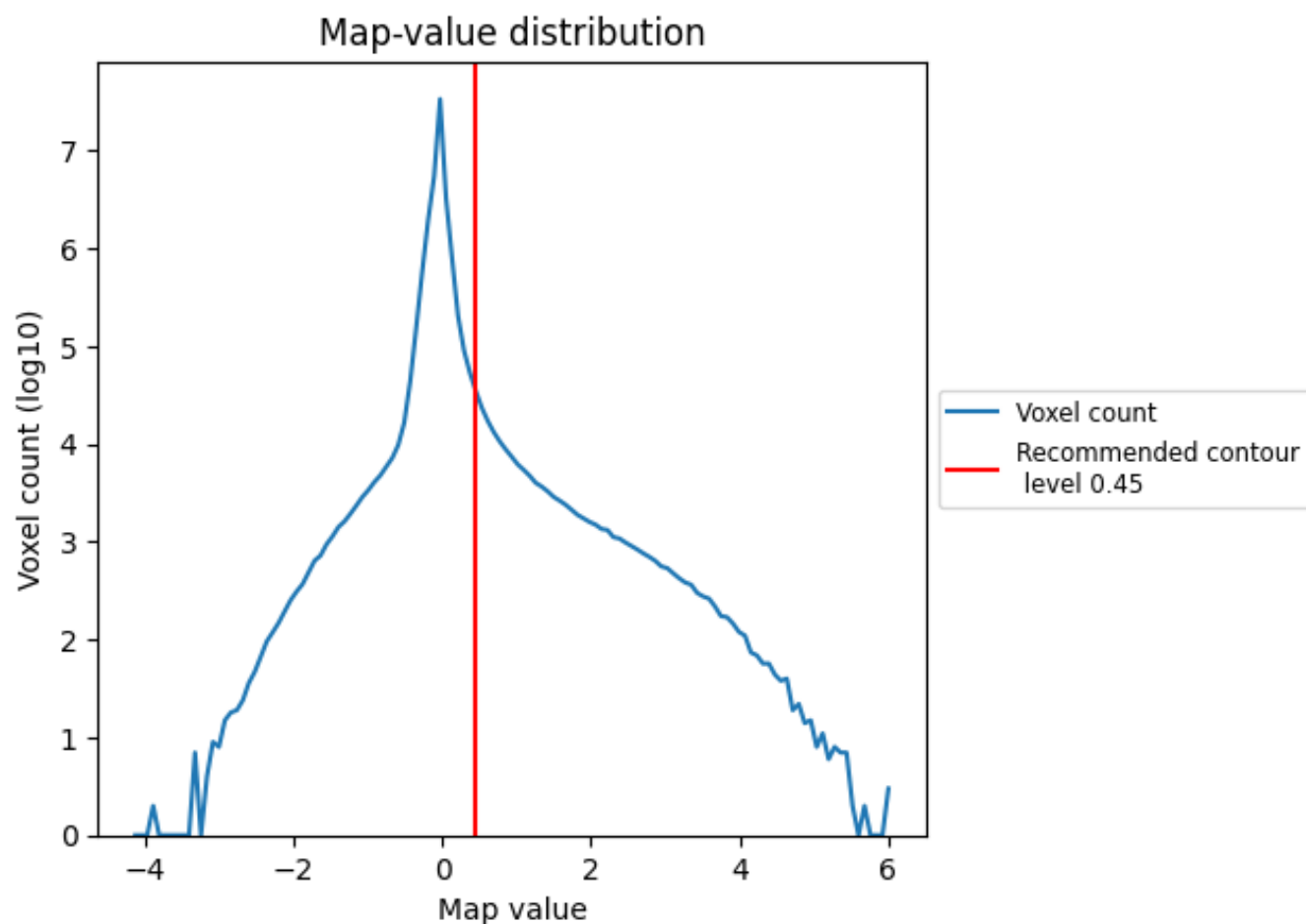
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

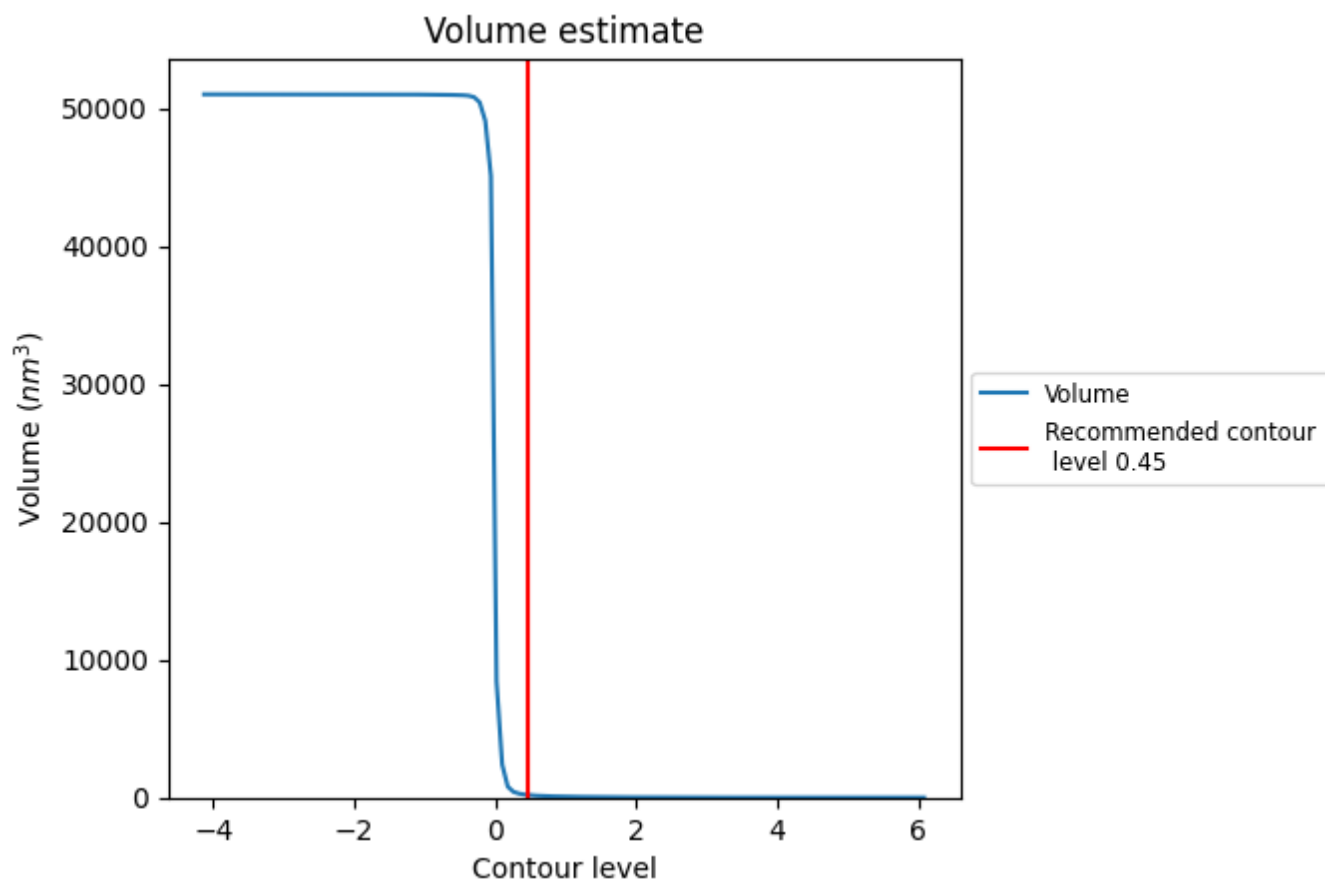
This section contains the results of statistical analysis of the map.

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.

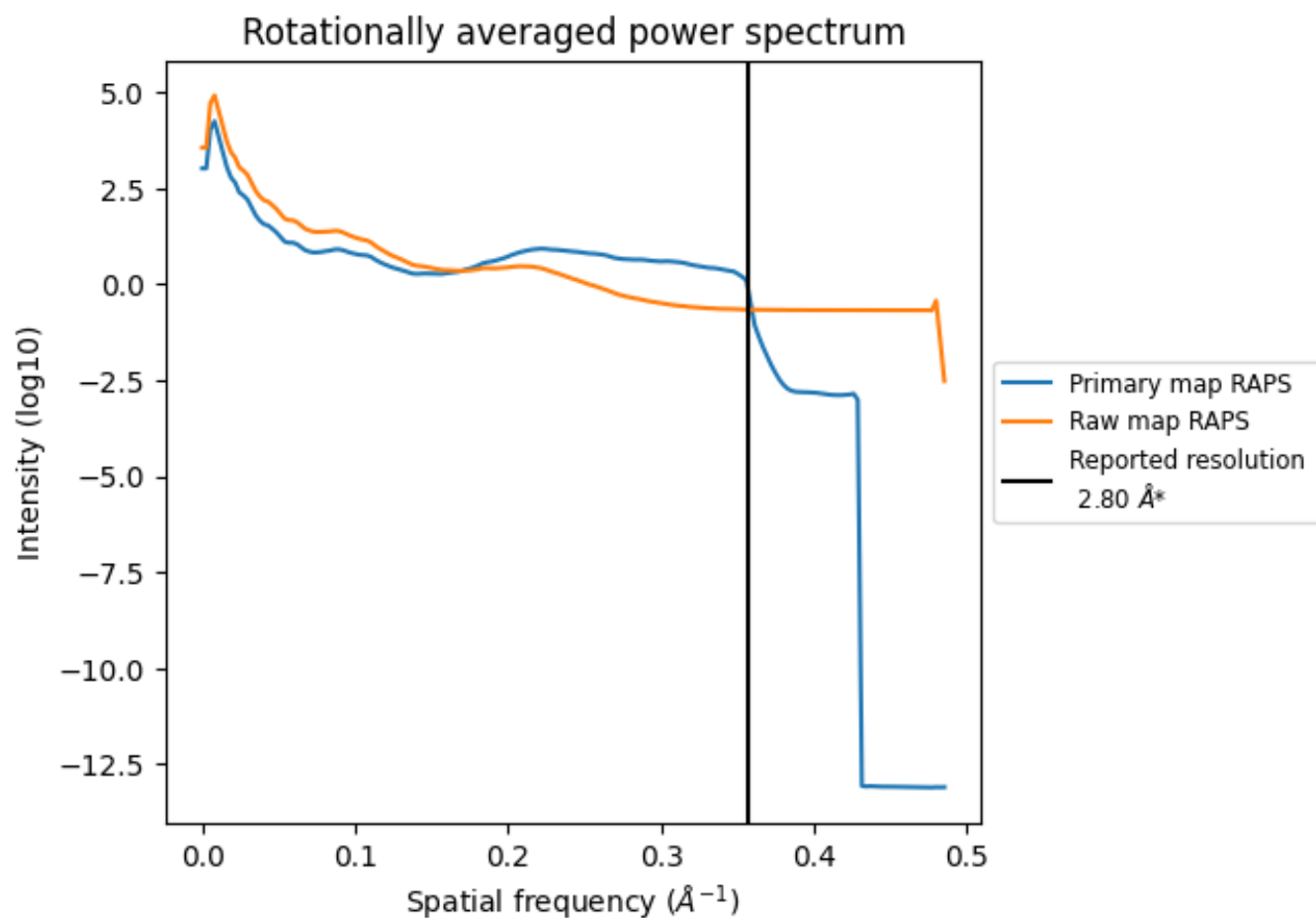
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 195 nm³; this corresponds to an approximate mass of 176 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 ⓘ

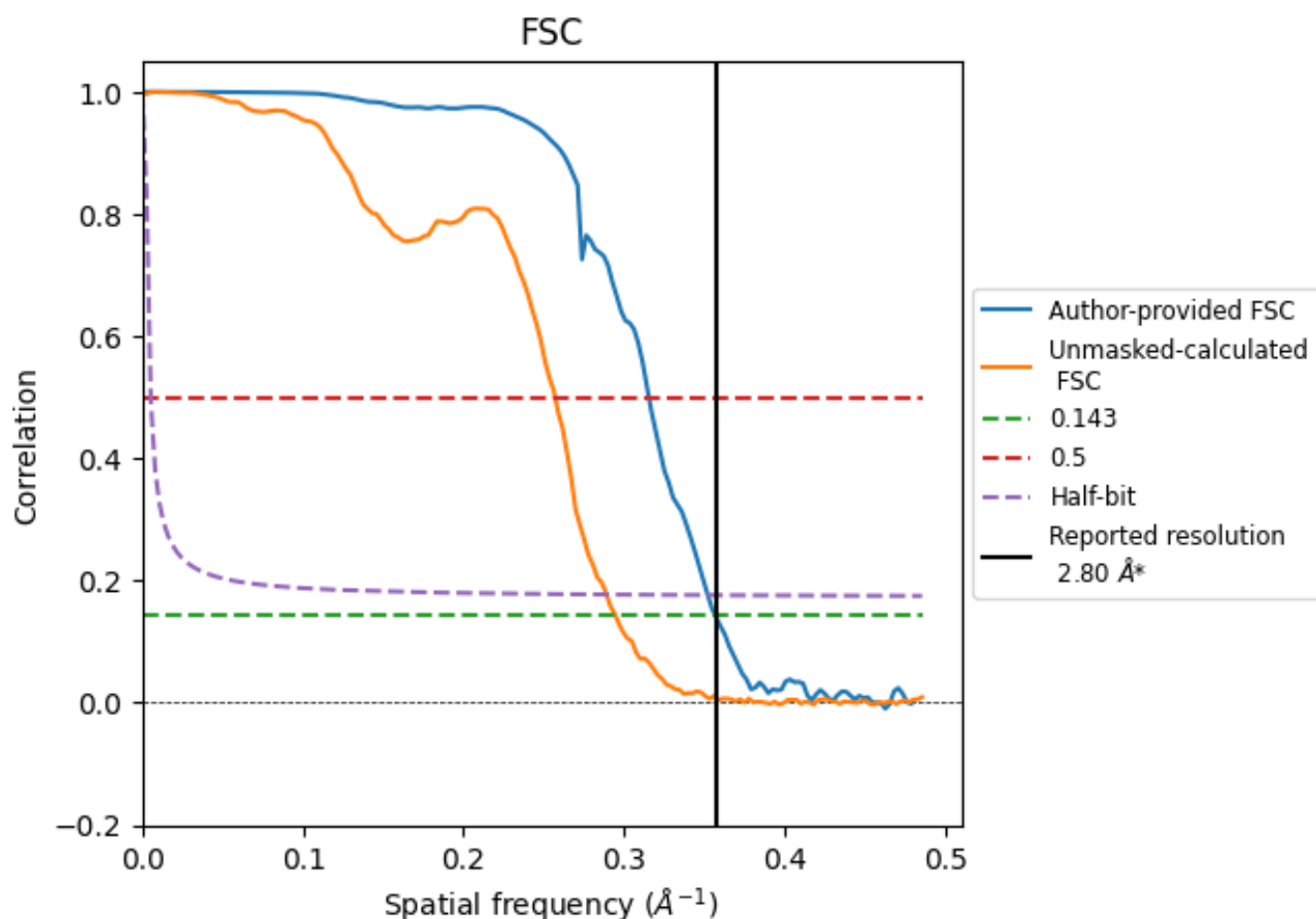


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

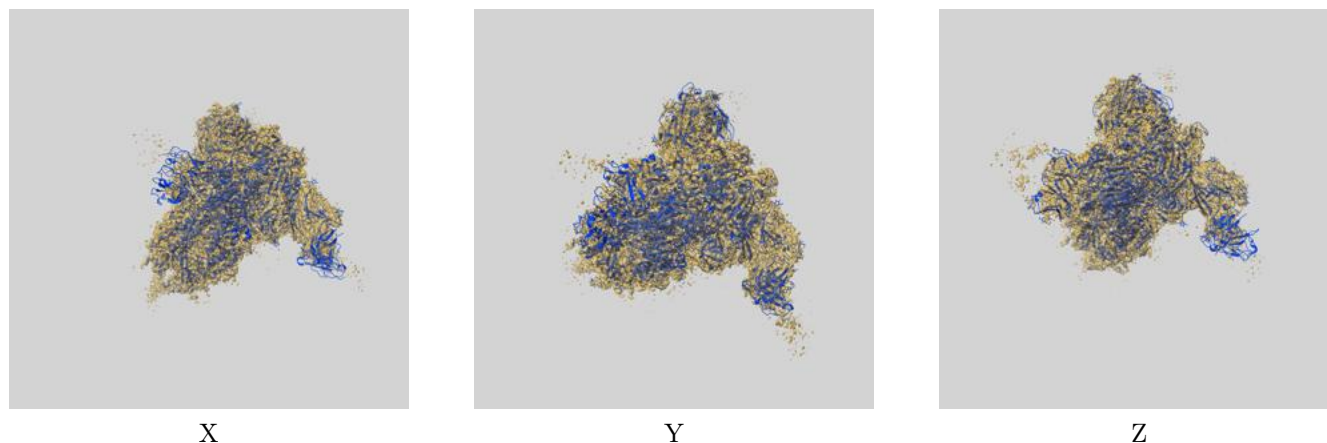
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.17	2.84
Unmasked-calculated*	3.40	3.89	3.46

*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 3.40 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

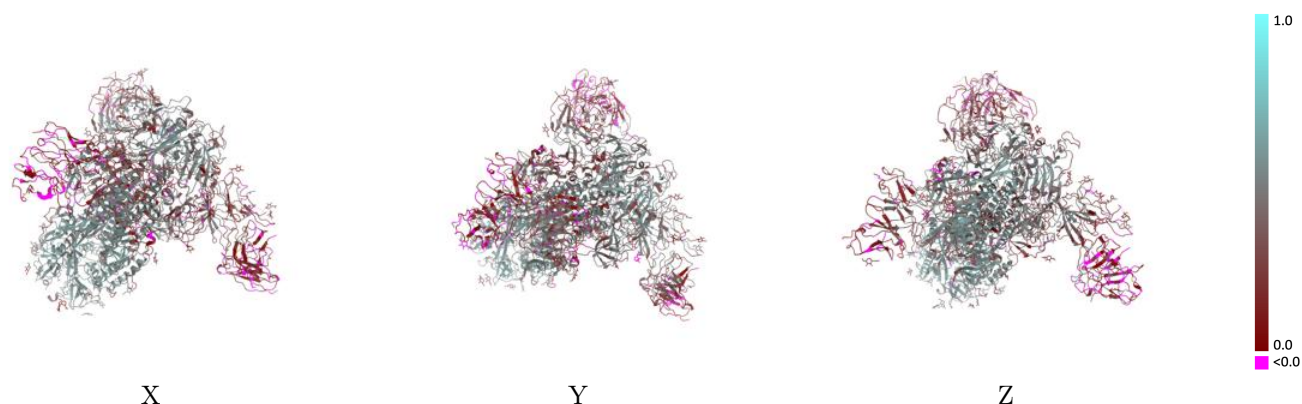
This section contains information regarding the fit between EMDB map EMD-26429 and PDB model 7UAP. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



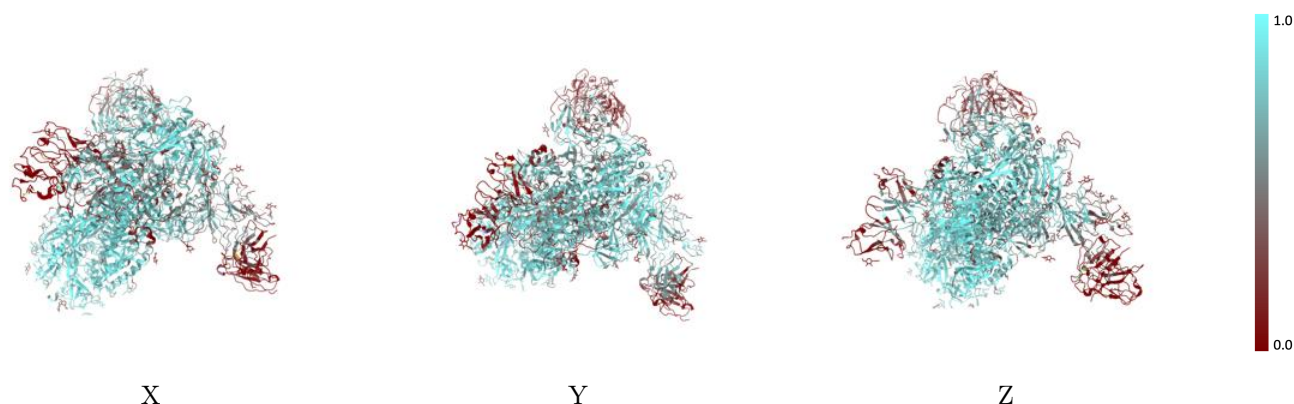
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



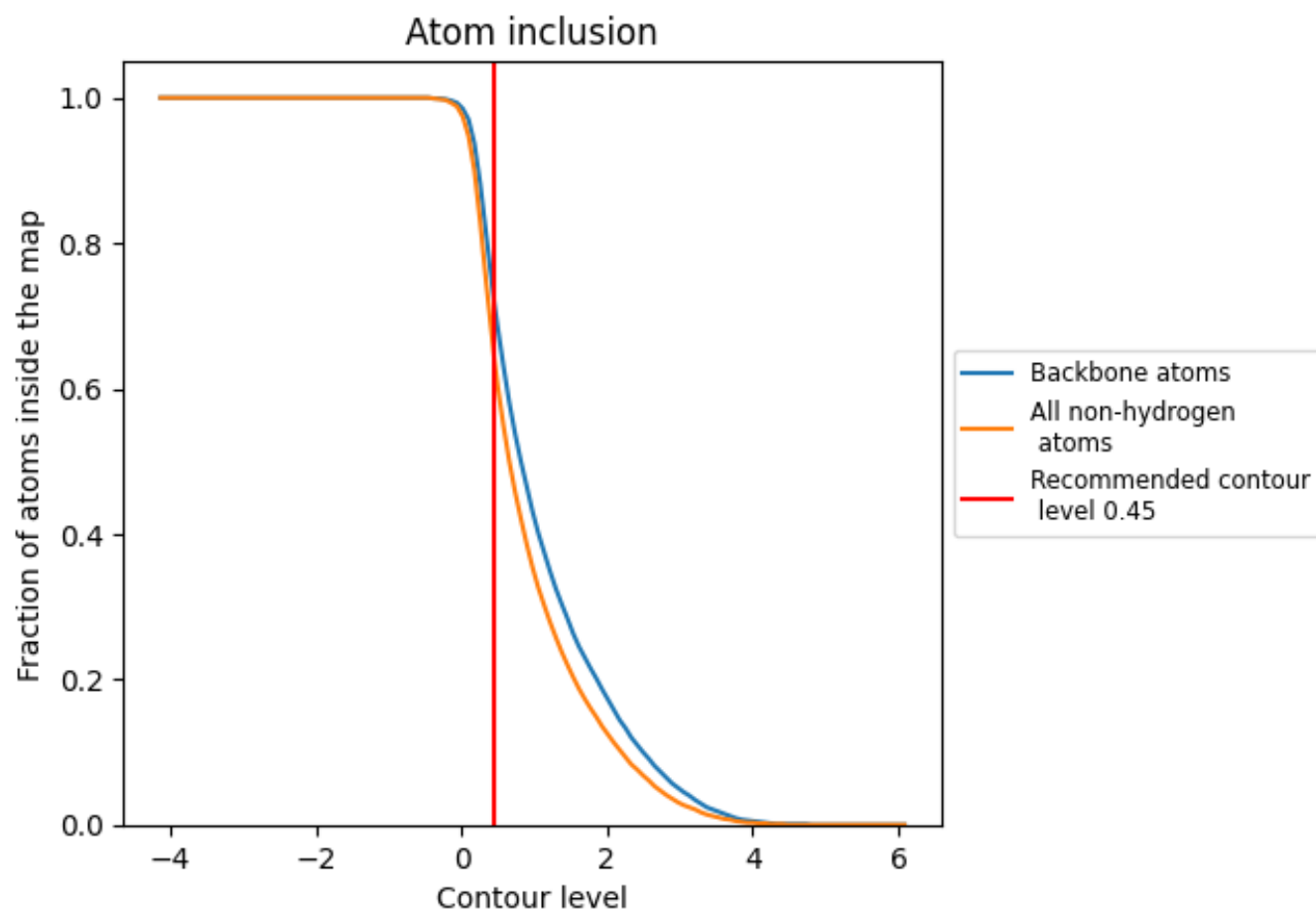
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 64% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6420	 0.3840
A	 0.7730	 0.4580
B	 0.7490	 0.4330
C	 0.6970	 0.4150
D	 0.3570	 0.1660
E	 0.3930	 0.2630
F	 0.4290	 0.2580
G	 0.6070	 0.3270
H	 0.4460	 0.2890
I	 0.1430	 0.1410
J	 0.2140	 0.2990
K	 0.2140	 0.1780
L	 0.2520	 0.1740
M	 0.2240	 0.1360
N	 0.0810	 0.1110
O	 0.1340	 0.1210
P	 0.0470	 0.0590
Q	 0.5360	 0.2130
R	 0.1430	 0.1720
S	 0.2860	 0.2550
T	 0.2140	 0.1750
U	 0.3210	 0.0770

