



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:33 PM UTC

PDB ID : 7R4I / pdb_00007r4i
EMDB ID : EMD-14313
Title : The SARS-CoV-2 spike in complex with the 2.15 neutralizing nanobody
Authors : Casasnovas, J.M.; Melero, R.; Arranz, R.; Fernandez, L.A.
Deposited on : 2022-02-08
Resolution : 3.20 Å (reported)
Based on initial models : 6ZXN, 6DBA

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

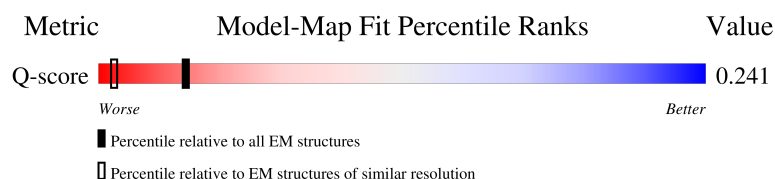
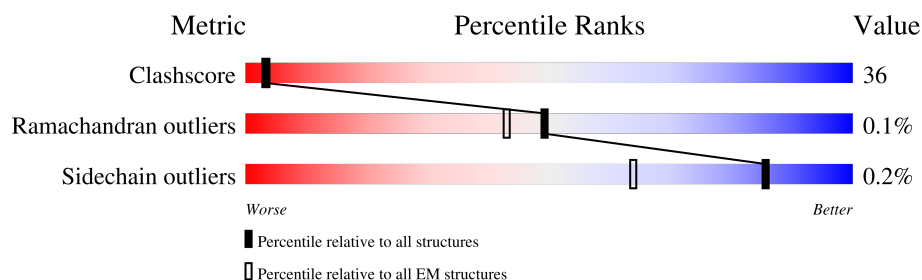
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	1264	
1	B	1264	
1	C	1264	
2	D	130	

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Mol	Chain	Length	Quality of chain
2	E	130	12%13%82%
3	F	2	50%50%
3	G	2	50%100%
3	H	2	50%50%
3	I	2	50%100%
3	J	2	100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 52010 atoms, of which 24685 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	1057	Total	C	H	N	O	S	2	0
			16320	5278	8045	1380	1579	38		
1	B	1056	Total	C	H	N	O	S	3	0
			16302	5277	8034	1380	1573	38		
1	C	1060	Total	C	H	N	O	S	1	0
			16361	5292	8069	1382	1580	38		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	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	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	SER	-	expression tag	UNP P0DTC2
A	1213	GLY	-	expression tag	UNP P0DTC2
A	1214	TYR	-	expression tag	UNP P0DTC2
A	1215	ILE	-	expression tag	UNP P0DTC2
A	1216	PRO	-	expression tag	UNP P0DTC2
A	1217	GLU	-	expression tag	UNP P0DTC2
A	1218	ALA	-	expression tag	UNP P0DTC2
A	1219	PRO	-	expression tag	UNP P0DTC2
A	1220	ARG	-	expression tag	UNP P0DTC2
A	1221	ASP	-	expression tag	UNP P0DTC2
A	1222	GLY	-	expression tag	UNP P0DTC2
A	1223	GLN	-	expression tag	UNP P0DTC2
A	1224	ALA	-	expression tag	UNP P0DTC2
A	1225	TYR	-	expression tag	UNP P0DTC2
A	1226	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1227	ARG	-	expression tag	UNP P0DTC2
A	1228	LYS	-	expression tag	UNP P0DTC2
A	1229	ASP	-	expression tag	UNP P0DTC2
A	1230	GLY	-	expression tag	UNP P0DTC2
A	1231	GLU	-	expression tag	UNP P0DTC2
A	1232	TRP	-	expression tag	UNP P0DTC2
A	1233	VAL	-	expression tag	UNP P0DTC2
A	1234	LEU	-	expression tag	UNP P0DTC2
A	1235	LEU	-	expression tag	UNP P0DTC2
A	1236	SER	-	expression tag	UNP P0DTC2
A	1237	THR	-	expression tag	UNP P0DTC2
A	1238	PHE	-	expression tag	UNP P0DTC2
A	1239	LEU	-	expression tag	UNP P0DTC2
A	1240	GLY	-	expression tag	UNP P0DTC2
A	1241	THR	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	ASN	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	TYR	-	expression tag	UNP P0DTC2
A	1246	PHE	-	expression tag	UNP P0DTC2
A	1247	GLN	-	expression tag	UNP P0DTC2
A	1248	GLY	-	expression tag	UNP P0DTC2
A	1249	ASP	-	expression tag	UNP P0DTC2
A	1250	TYR	-	expression tag	UNP P0DTC2
A	1251	LYS	-	expression tag	UNP P0DTC2
A	1252	ASP	-	expression tag	UNP P0DTC2
A	1253	ASP	-	expression tag	UNP P0DTC2
A	1254	ASP	-	expression tag	UNP P0DTC2
A	1255	ASP	-	expression tag	UNP P0DTC2
A	1256	LYS	-	expression tag	UNP P0DTC2
A	1257	GLY	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2
A	1259	HIS	-	expression tag	UNP P0DTC2
A	1260	HIS	-	expression tag	UNP P0DTC2
A	1261	HIS	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	HIS	-	expression tag	UNP P0DTC2
A	1264	HIS	-	expression tag	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1209	GLY	-	expression tag	UNP P0DTC2
B	1210	SER	-	expression tag	UNP P0DTC2
B	1211	GLY	-	expression tag	UNP P0DTC2
B	1212	SER	-	expression tag	UNP P0DTC2
B	1213	GLY	-	expression tag	UNP P0DTC2
B	1214	TYR	-	expression tag	UNP P0DTC2
B	1215	ILE	-	expression tag	UNP P0DTC2
B	1216	PRO	-	expression tag	UNP P0DTC2
B	1217	GLU	-	expression tag	UNP P0DTC2
B	1218	ALA	-	expression tag	UNP P0DTC2
B	1219	PRO	-	expression tag	UNP P0DTC2
B	1220	ARG	-	expression tag	UNP P0DTC2
B	1221	ASP	-	expression tag	UNP P0DTC2
B	1222	GLY	-	expression tag	UNP P0DTC2
B	1223	GLN	-	expression tag	UNP P0DTC2
B	1224	ALA	-	expression tag	UNP P0DTC2
B	1225	TYR	-	expression tag	UNP P0DTC2
B	1226	VAL	-	expression tag	UNP P0DTC2
B	1227	ARG	-	expression tag	UNP P0DTC2
B	1228	LYS	-	expression tag	UNP P0DTC2
B	1229	ASP	-	expression tag	UNP P0DTC2
B	1230	GLY	-	expression tag	UNP P0DTC2
B	1231	GLU	-	expression tag	UNP P0DTC2
B	1232	TRP	-	expression tag	UNP P0DTC2
B	1233	VAL	-	expression tag	UNP P0DTC2
B	1234	LEU	-	expression tag	UNP P0DTC2
B	1235	LEU	-	expression tag	UNP P0DTC2
B	1236	SER	-	expression tag	UNP P0DTC2
B	1237	THR	-	expression tag	UNP P0DTC2
B	1238	PHE	-	expression tag	UNP P0DTC2
B	1239	LEU	-	expression tag	UNP P0DTC2
B	1240	GLY	-	expression tag	UNP P0DTC2
B	1241	THR	-	expression tag	UNP P0DTC2
B	1242	GLU	-	expression tag	UNP P0DTC2
B	1243	ASN	-	expression tag	UNP P0DTC2
B	1244	LEU	-	expression tag	UNP P0DTC2
B	1245	TYR	-	expression tag	UNP P0DTC2
B	1246	PHE	-	expression tag	UNP P0DTC2
B	1247	GLN	-	expression tag	UNP P0DTC2
B	1248	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1249	ASP	-	expression tag	UNP P0DTC2
B	1250	TYR	-	expression tag	UNP P0DTC2
B	1251	LYS	-	expression tag	UNP P0DTC2
B	1252	ASP	-	expression tag	UNP P0DTC2
B	1253	ASP	-	expression tag	UNP P0DTC2
B	1254	ASP	-	expression tag	UNP P0DTC2
B	1255	ASP	-	expression tag	UNP P0DTC2
B	1256	LYS	-	expression tag	UNP P0DTC2
B	1257	GLY	-	expression tag	UNP P0DTC2
B	1258	SER	-	expression tag	UNP P0DTC2
B	1259	HIS	-	expression tag	UNP P0DTC2
B	1260	HIS	-	expression tag	UNP P0DTC2
B	1261	HIS	-	expression tag	UNP P0DTC2
B	1262	HIS	-	expression tag	UNP P0DTC2
B	1263	HIS	-	expression tag	UNP P0DTC2
B	1264	HIS	-	expression tag	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	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	1209	GLY	-	expression tag	UNP P0DTC2
C	1210	SER	-	expression tag	UNP P0DTC2
C	1211	GLY	-	expression tag	UNP P0DTC2
C	1212	SER	-	expression tag	UNP P0DTC2
C	1213	GLY	-	expression tag	UNP P0DTC2
C	1214	TYR	-	expression tag	UNP P0DTC2
C	1215	ILE	-	expression tag	UNP P0DTC2
C	1216	PRO	-	expression tag	UNP P0DTC2
C	1217	GLU	-	expression tag	UNP P0DTC2
C	1218	ALA	-	expression tag	UNP P0DTC2
C	1219	PRO	-	expression tag	UNP P0DTC2
C	1220	ARG	-	expression tag	UNP P0DTC2
C	1221	ASP	-	expression tag	UNP P0DTC2
C	1222	GLY	-	expression tag	UNP P0DTC2
C	1223	GLN	-	expression tag	UNP P0DTC2
C	1224	ALA	-	expression tag	UNP P0DTC2
C	1225	TYR	-	expression tag	UNP P0DTC2
C	1226	VAL	-	expression tag	UNP P0DTC2
C	1227	ARG	-	expression tag	UNP P0DTC2
C	1228	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1229	ASP	-	expression tag	UNP P0DTC2
C	1230	GLY	-	expression tag	UNP P0DTC2
C	1231	GLU	-	expression tag	UNP P0DTC2
C	1232	TRP	-	expression tag	UNP P0DTC2
C	1233	VAL	-	expression tag	UNP P0DTC2
C	1234	LEU	-	expression tag	UNP P0DTC2
C	1235	LEU	-	expression tag	UNP P0DTC2
C	1236	SER	-	expression tag	UNP P0DTC2
C	1237	THR	-	expression tag	UNP P0DTC2
C	1238	PHE	-	expression tag	UNP P0DTC2
C	1239	LEU	-	expression tag	UNP P0DTC2
C	1240	GLY	-	expression tag	UNP P0DTC2
C	1241	THR	-	expression tag	UNP P0DTC2
C	1242	GLU	-	expression tag	UNP P0DTC2
C	1243	ASN	-	expression tag	UNP P0DTC2
C	1244	LEU	-	expression tag	UNP P0DTC2
C	1245	TYR	-	expression tag	UNP P0DTC2
C	1246	PHE	-	expression tag	UNP P0DTC2
C	1247	GLN	-	expression tag	UNP P0DTC2
C	1248	GLY	-	expression tag	UNP P0DTC2
C	1249	ASP	-	expression tag	UNP P0DTC2
C	1250	TYR	-	expression tag	UNP P0DTC2
C	1251	LYS	-	expression tag	UNP P0DTC2
C	1252	ASP	-	expression tag	UNP P0DTC2
C	1253	ASP	-	expression tag	UNP P0DTC2
C	1254	ASP	-	expression tag	UNP P0DTC2
C	1255	ASP	-	expression tag	UNP P0DTC2
C	1256	LYS	-	expression tag	UNP P0DTC2
C	1257	GLY	-	expression tag	UNP P0DTC2
C	1258	SER	-	expression tag	UNP P0DTC2
C	1259	HIS	-	expression tag	UNP P0DTC2
C	1260	HIS	-	expression tag	UNP P0DTC2
C	1261	HIS	-	expression tag	UNP P0DTC2
C	1262	HIS	-	expression tag	UNP P0DTC2
C	1263	HIS	-	expression tag	UNP P0DTC2
C	1264	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Camel-derived nanobody 2.15.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	125	Total	C	N	O	S	0	0
			944	589	164	186	5		

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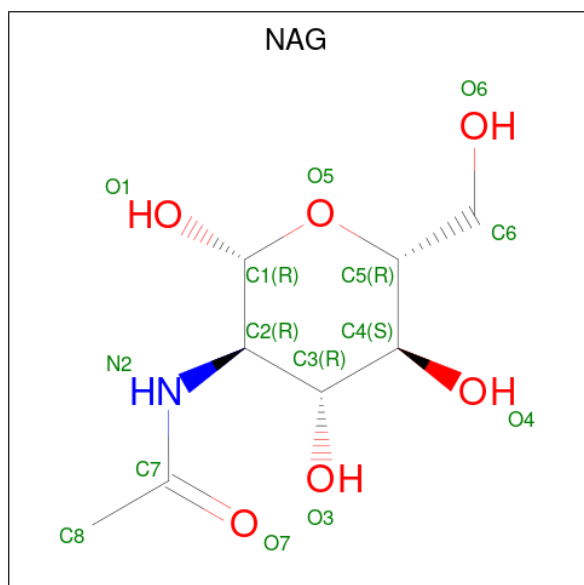
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	125	Total	C	N	O	S	0	0
			944	589	164	186	5		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	G	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	H	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	I	2	Total	C	H	N	O	0	0
			53	16	25	2	10		
3	J	2	Total	C	H	N	O	0	0
			53	16	25	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	A	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	

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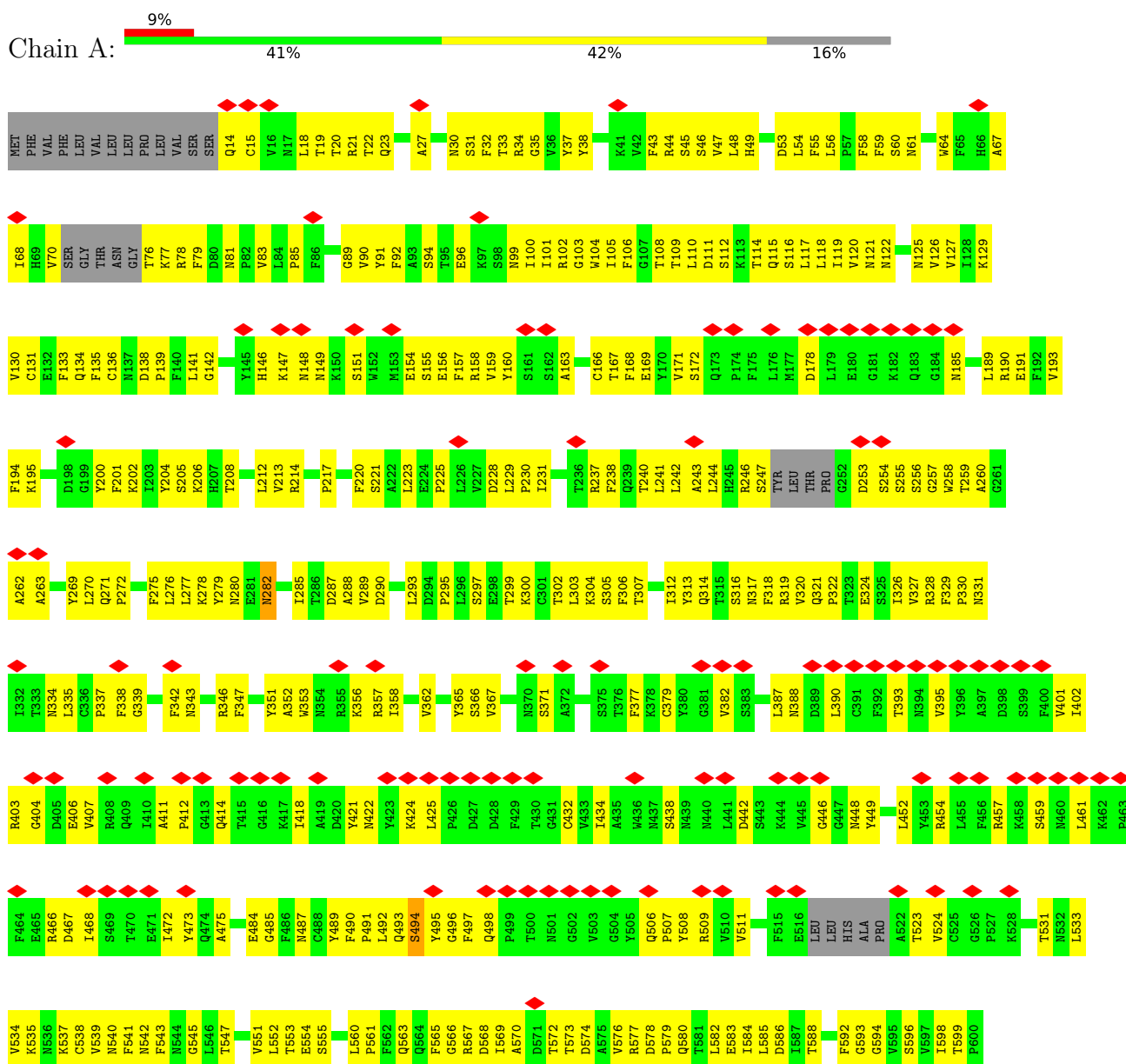
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Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	B	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			26	8	12	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	1	Total	C	H	N	O	0
			27	8	13	1	5	
4	C	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.

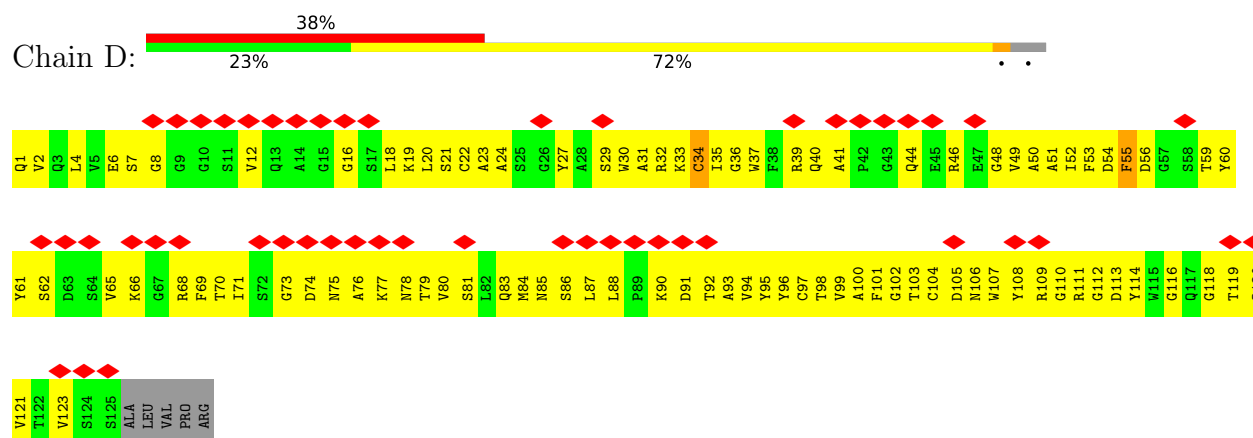
• Molecule 1: Spike glycoprotein



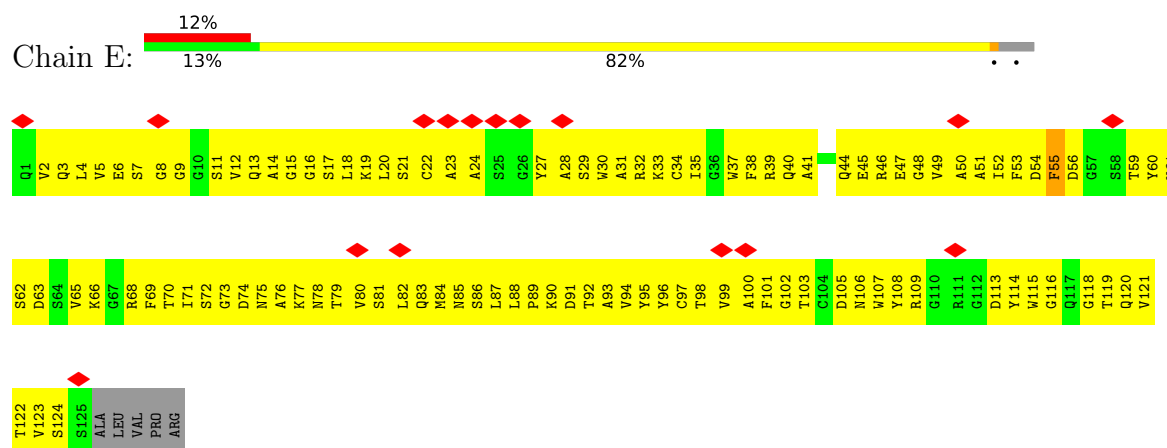


GLY	T1100	R1000	T909	LYS	M740	TRP	G548	P479	T415	R346	E281	H207	Q134
ASP	H1101	L1001	G910	GLN	Y741	ARG	T549	C480	I418	F347	M282	T208	F135
TYR	W1102	L1004	V911	TYR	I742	VAL	G550	N481	I419	A348	G283	P209	C136
LYS	E1111	L1008	T912	GLY	C743	TRP	V551	G482	A419	S349	T284	I210	M137
ASP	E1111	V1008	G913	ASP	L752	THR	E554	G482	D420	V350	T286	L212	F140
LEU	T1116	L1012	E917	LEU	L753	GLY	S555	E484	Y421	Y351	D287	R214	L141
ASP	T1117	L1015	E918	ASP	L754	SER	N556	G485	N422	W353	V289	D215	G142
GLY	V1128	A1015	N919	ILE	Q755	THR	K557	F486	Y423	D290	V289	D215	V143
LEU	A1016	A1016	N919	ALA	F759		D568	G486	K424	N354	C291	P217	V144
ILE	Q920	A1016	Q920	ALA	F759		D568	G486	K424	N354	C291	P217	V144
ASP	R921	E1017	E918	ALA	F759		D568	G486	K424	N354	C291	P217	V144
LEU	L1018	E1017	E918	ALA	F759		D568	G486	K424	N354	C291	P217	V144
HIS	Y1138	R1019	L922	ARG	Q762		A570	C488	L425	R355	A292	L229	K147
HIS	D1139	R1019	L922	ARG	Q762		A570	C488	L425	R355	A292	L229	K147
HIS	Q1142	A1022	A924	LEU	N764		D571	Y489	P426	R357	P295	L231	N148
GLY	P1143	M1023	N925	ILE	R765		R577	F490	D428	N360	L296	G232	K150
LEU	M1023	M1023	Q926	CYS	A766		R577	F490	D428	N360	L296	G232	K150
LYS	L1024	L1024	Q926	ALA	A766		R577	F490	D428	N360	L296	G232	K150
TYR	A1025	F927	E927	ALA	A766		R577	F490	D428	N360	L296	G232	K150
GLU	A1026	N928	N928	GLN	G769		P579	L492	G431	C361	E296	N234	M153
GLN	S929	LYS	L770	GLN	Q493		Q580	L492	G431	C361	E296	N234	M153
ASP	A930	F855	G669	LYS	Q493		S494	L492	G431	C361	E296	N234	M153
GLY	I931	F855	G669	LYS	Q493		S494	L492	G431	C361	E296	N234	M153
SER	M1029	P862	V674	THR	E773		E583	T500	W436	D364	T302	Q239	V159
GLY	S1030	P863	V674	THR	Q774		E583	T500	W436	D364	T302	Q239	V159
LEU	E1031	P863	V674	THR	Q774		E583	T500	W436	D364	T302	Q239	V159
GLY	C1032	L865	V674	THR	Q774		E583	T500	W436	D364	T302	Q239	V159
TYR	R1039	D867	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ILE	P1040	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
PRO	D1041	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ASN	F1042	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
HIS	C1043	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
THR	L1049	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ASP	M1050	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLY	S1051	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLN	F1052	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ALA	P1053	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
TYR	P1053	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
VAL	Q1054	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ARG	S1055	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
LYS	A1056	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ASP	P1057	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLY	H1058	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLY	G1059	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
TRP	V1060	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ILE	V1061	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
VAL	F1062	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
LEU	S1063	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
VAL	H1064	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
THR	T1077	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
PHE	A989	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
LEU	E990	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLY	V991	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ILE	Q992	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLN	F1079	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
LYS	A1080	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
THR	F1089	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLU	S1097	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
ASN	N1098	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
GLN	G1099	E863	V781	ASN	N777		E583	T500	W436	D364	T302	Q239	V159
TRP	T998	G999											
PHE	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
ASP	T998	G999											
TYR	T998	G999											
LEU	T998	G999											
ASP	T998	G999											
PHE	T998	G999											
GLN	T998	G999											
TRP	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
ASP	T998	G999											
TYR	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
TRP	T998	G999											
LEU	T998	G999											
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ASN	T998	G999											
GLN	T998	G999											
TRP	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
TRP	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
TRP	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
TRP	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
TRP	T998	G999											
LEU	T998	G999											
ASN	T998	G999											
GLN	T998	G999											
TRP	T998												

- Molecule 2: Camel-derived nanobody 2.15



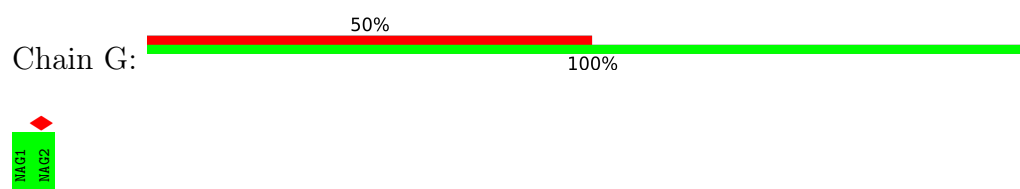
- Molecule 2: Camel-derived nanobody 2.15



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



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



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

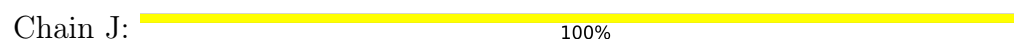




- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.973	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	420.66, 420.66, 420.66	wwPDB
Map dimensions	492, 492, 492	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.855, 0.855, 0.855	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	0.50	1/8472 (0.0%)	0.57	5/11525 (0.0%)
1	B	0.52	1/8469 (0.0%)	0.57	5/11521 (0.0%)
1	C	0.38	0/8490	0.55	3/11550 (0.0%)
2	D	1.82	6/965 (0.6%)	0.55	0/1306
2	E	1.83	6/965 (0.6%)	0.60	0/1306
All	All	0.66	14/27361 (0.1%)	0.56	13/37208 (0.0%)

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
All	All	0	2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	494	SER	CA-CB	29.75	1.98	1.53
1	A	494	SER	CA-CB	29.61	1.98	1.53
2	E	55	PHE	CD1-CE1	28.77	2.25	1.38
2	D	55	PHE	CD2-CE2	27.55	2.21	1.38
2	E	55	PHE	CE2-CZ	25.37	2.14	1.38
2	E	55	PHE	CD2-CE2	25.22	2.14	1.38
2	D	55	PHE	CE1-CZ	24.89	2.13	1.38
2	D	55	PHE	CD1-CE1	24.71	2.12	1.38
2	D	55	PHE	CE2-CZ	24.47	2.12	1.38
2	E	55	PHE	CE1-CZ	22.29	2.05	1.38
2	E	55	PHE	CG-CD2	17.72	1.76	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	55	PHE	CG-CD2	17.34	1.75	1.38
2	E	55	PHE	CG-CD1	16.87	1.74	1.38
2	D	55	PHE	CG-CD1	16.61	1.73	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	SER	CA-CB-OG	10.32	131.74	111.10
1	A	494	SER	CA-CB-OG	9.29	129.68	111.10
1	B	494	SER	CB-CA-C	8.50	124.27	110.16
1	C	942	PRO	CA-N-CD	-8.49	100.12	112.00
1	B	942	PRO	CA-N-CD	-8.44	100.18	112.00
1	A	942	PRO	CA-N-CD	-8.41	100.23	112.00
1	A	494	SER	N-CA-C	-8.25	95.79	109.07
1	B	494	SER	N-CA-C	-7.72	95.82	108.41
1	A	494	SER	CB-CA-C	7.39	122.50	109.72
1	A	494	SER	N-CA-CB	7.34	122.10	110.57
1	B	494	SER	N-CA-CB	6.19	120.31	110.65
1	C	478	THR	OG1-CB-CG2	5.51	120.32	109.30
1	C	478	THR	CA-CB-CG2	5.00	119.01	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	811	LYS	Peptide
1	C	812	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8275	8045	8048	527	0
1	B	8268	8034	8055	529	0
1	C	8292	8069	8075	410	0
2	D	944	0	887	263	0
2	E	944	0	887	375	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	25	25	1	0
3	G	28	25	25	0	0
3	H	28	25	25	3	0
3	I	28	25	25	2	0
3	J	28	25	25	1	0
4	A	196	181	182	8	0
4	B	182	167	169	13	0
4	C	84	64	78	5	0
All	All	27325	24685	26506	1958	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 36.

All (1958) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:PHE:CD2	2:D:55:PHE:CG	1.75	1.68
2:E:55:PHE:CD2	2:E:55:PHE:CG	1.76	1.65
1:A:494:SER:HB2	2:D:55:PHE:CD1	1.48	1.46
1:B:494:SER:HA	2:E:55:PHE:CZ	1.48	1.44
2:E:55:PHE:CZ	2:E:55:PHE:CE1	2.05	1.43
1:B:494:SER:CA	1:B:494:SER:CB	1.98	1.42
1:A:494:SER:HA	2:D:55:PHE:CE2	1.54	1.41
1:A:494:SER:CB	1:A:494:SER:CA	1.98	1.40
1:B:494:SER:HB3	2:E:55:PHE:CD2	1.57	1.40
1:B:494:SER:HB2	2:E:55:PHE:CE2	1.56	1.39
2:D:55:PHE:CE2	2:D:55:PHE:CZ	2.12	1.38
1:B:494:SER:HB3	2:E:55:PHE:CG	1.59	1.38
2:D:55:PHE:CD1	2:D:55:PHE:CE1	2.12	1.37
1:A:494:SER:HB3	2:D:55:PHE:CE1	1.60	1.36
2:E:55:PHE:CD2	2:E:55:PHE:CE2	2.14	1.36
1:A:494:SER:CB	2:D:55:PHE:CE1	2.09	1.35
1:B:494:SER:CB	2:E:55:PHE:CE1	2.10	1.35
2:D:55:PHE:CZ	2:D:55:PHE:CE1	2.13	1.35
2:E:55:PHE:CZ	2:E:55:PHE:CE2	2.14	1.35
1:A:494:SER:CB	2:D:55:PHE:CE2	2.10	1.35
1:B:494:SER:CB	2:E:55:PHE:CD1	2.09	1.33
1:A:494:SER:CB	2:D:55:PHE:CD2	2.14	1.31
1:A:494:SER:HB3	2:D:55:PHE:CZ	1.65	1.30
1:B:494:SER:CB	2:E:55:PHE:CZ	2.15	1.29
1:A:494:SER:CB	2:D:55:PHE:CZ	2.14	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:SER:CB	2:E:55:PHE:CE2	2.13	1.29
1:B:494:SER:CB	2:E:55:PHE:CD2	2.17	1.27
1:A:494:SER:CB	2:D:55:PHE:CD1	2.17	1.26
2:D:55:PHE:CD2	2:D:55:PHE:CE2	2.21	1.26
2:E:55:PHE:CE1	2:E:55:PHE:CD1	2.25	1.25
1:A:494:SER:HB2	2:D:55:PHE:CG	1.71	1.24
1:A:494:SER:HA	2:D:55:PHE:CZ	1.71	1.24
1:A:494:SER:CA	2:D:55:PHE:CE2	2.21	1.22
1:B:494:SER:CB	2:E:55:PHE:CG	2.23	1.21
1:A:494:SER:CB	2:D:55:PHE:CG	2.25	1.20
1:B:494:SER:CA	2:E:55:PHE:CE1	2.28	1.16
1:B:494:SER:CA	2:E:55:PHE:CZ	2.29	1.16
1:A:494:SER:CA	2:D:55:PHE:CZ	2.27	1.16
1:B:494:SER:CA	2:E:55:PHE:CE2	2.31	1.14
1:B:494:SER:OG	2:E:55:PHE:CE1	2.01	1.12
1:B:494:SER:HB2	2:E:55:PHE:CZ	1.80	1.12
2:E:65:VAL:HG13	2:E:69:PHE:HB2	1.13	1.12
2:D:99:VAL:HB	2:D:114:TYR:HB2	1.28	1.11
2:E:94:VAL:HA	2:E:120:GLN:HA	1.32	1.09
2:E:92:THR:HA	2:E:122:THR:HA	1.24	1.09
1:A:494:SER:C	2:D:55:PHE:CE1	2.31	1.08
1:A:494:SER:CA	2:D:55:PHE:CD2	2.37	1.07
2:D:40:GLN:HG3	2:D:46:ARG:HB3	1.33	1.07
1:B:494:SER:N	2:E:55:PHE:CD2	2.23	1.07
2:E:99:VAL:HB	2:E:114:TYR:HB2	1.25	1.06
1:A:494:SER:CA	2:D:55:PHE:CE1	2.39	1.06
1:B:353:TRP:O	1:B:466:ARG:NH1	1.89	1.05
1:A:494:SER:OG	2:D:55:PHE:CE2	2.09	1.05
2:D:84:MET:HE1	2:D:121:VAL:HG11	1.37	1.05
2:E:18:LEU:HB3	2:E:84:MET:HB2	1.35	1.04
2:D:53:PHE:HB3	2:D:56:ASP:HB2	1.35	1.04
1:B:494:SER:CA	2:E:55:PHE:CD1	2.40	1.03
2:D:33:LYS:O	2:D:54:ASP:N	1.90	1.03
1:A:494:SER:N	2:D:55:PHE:CD2	2.27	1.02
2:E:17:SER:HA	2:E:85:ASN:HA	1.42	1.01
1:A:253:ASP:O	1:A:257:GLY:N	1.93	1.00
2:E:16:GLY:H	2:E:87:LEU:HB2	1.23	1.00
1:A:494:SER:OG	2:D:55:PHE:CD2	2.15	0.98
1:B:494:SER:CA	2:E:55:PHE:CD2	2.46	0.98
2:E:33:LYS:O	2:E:54:ASP:N	1.96	0.98
1:B:494:SER:C	2:E:55:PHE:CD1	2.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:ARG:HG2	2:D:53:PHE:HE1	1.25	0.98
2:D:39:ARG:HD3	2:D:49:VAL:HG22	1.43	0.97
1:A:494:SER:CA	2:D:55:PHE:CD1	2.48	0.96
1:B:53:ASP:OD2	1:B:195:LYS:NZ	1.98	0.96
2:E:4:LEU:HD21	2:E:99:VAL:HG23	1.46	0.95
2:D:41:ALA:HB3	2:D:44:GLN:HG2	1.47	0.95
1:B:393:THR:OG1	1:B:521:PRO:O	1.82	0.95
1:B:494:SER:HA	2:E:55:PHE:CE2	2.01	0.94
2:E:65:VAL:HA	2:E:69:PHE:HD1	1.32	0.94
2:D:49:VAL:HG13	2:D:65:VAL:HG21	1.49	0.93
1:A:414:GLN:O	1:A:424:LYS:NZ	2.02	0.93
1:B:494:SER:CA	2:E:55:PHE:CG	2.52	0.92
2:E:38:PHE:HD1	2:E:98:THR:HG21	1.32	0.92
1:A:70:VAL:HG11	1:A:76:THR:HG21	1.52	0.92
1:C:969:ASN:OD1	1:C:975:SER:N	2.03	0.92
2:D:52:ILE:HD11	2:D:80:VAL:HG12	1.52	0.91
1:B:290:ASP:OD1	1:B:291:CYS:N	2.04	0.91
1:C:618:THR:OG1	1:C:619:GLU:OE1	1.89	0.91
2:E:89:PRO:O	2:E:92:THR:HG23	1.71	0.91
1:B:494:SER:OG	2:E:55:PHE:CD1	2.24	0.91
1:A:494:SER:CA	2:D:55:PHE:CG	2.54	0.90
1:A:747:THR:O	1:A:751:ASN:ND2	2.03	0.90
1:B:416:GLY:O	1:B:420:ASP:N	2.04	0.90
1:B:494:SER:C	2:E:55:PHE:CE1	2.49	0.90
2:E:6:GLU:HG2	2:E:97:CYS:SG	2.11	0.90
2:E:120:GLN:HE21	2:E:122:THR:HG23	1.36	0.89
1:A:106:PHE:O	1:A:116:SER:OG	1.90	0.89
2:E:51:ALA:HB3	2:E:60:TYR:HB3	1.53	0.89
1:C:21:ARG:O	1:C:23:GLN:NE2	2.04	0.89
1:B:37:TYR:OH	1:B:195:LYS:NZ	2.06	0.89
1:B:144:TYR:N	1:B:155:SER:OG	2.06	0.88
1:B:14:GLN:O	1:B:158:ARG:NH1	2.06	0.88
1:A:147:LYS:NZ	1:A:247:SER:O	2.06	0.88
2:D:4:LEU:HD21	2:D:35:ILE:HD11	1.53	0.88
1:A:618:THR:OG1	1:A:619:GLU:OE1	1.91	0.88
2:E:71:ILE:HG22	2:E:82:LEU:HB2	1.56	0.88
1:B:21:ARG:NE	1:B:79:PHE:O	2.06	0.87
1:A:37:TYR:OH	1:A:54:LEU:O	1.92	0.86
1:A:494:SER:N	2:D:55:PHE:CG	2.44	0.86
2:E:74:ASP:O	2:E:78:ASN:N	2.08	0.86
2:E:51:ALA:O	2:E:59:THR:OG1	1.92	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASN:O	1:A:102:ARG:NE	2.08	0.86
1:A:109:THR:HG1	1:A:114:THR:HG1	1.01	0.86
2:E:71:ILE:HG23	2:E:82:LEU:HD13	1.58	0.85
2:E:72:SER:O	2:E:81:SER:N	2.08	0.85
2:E:84:MET:HB3	2:E:87:LEU:HD21	1.58	0.85
1:A:473:TYR:N	1:A:489:TYR:O	2.09	0.85
1:B:707:TYR:OH	1:C:897:PRO:O	1.94	0.84
1:B:391:CYS:HB2	1:B:525:CYS:HA	1.59	0.84
2:E:40:GLN:HB2	2:E:46:ARG:HG2	1.58	0.84
1:C:912:THR:OG1	1:C:914:ASN:OD1	1.95	0.84
2:D:32:ARG:HG2	2:D:53:PHE:CE1	2.12	0.84
2:E:51:ALA:O	2:E:60:TYR:N	2.09	0.84
1:A:96:GLU:OE1	1:A:100:ILE:N	2.11	0.84
1:B:490:PHE:O	2:E:31:ALA:HB2	1.76	0.84
1:C:77:LYS:NZ	1:C:258:TRP:O	2.10	0.83
1:C:246:ARG:NH2	1:C:254:SER:O	2.10	0.83
2:D:2:VAL:HG11	2:D:99:VAL:HG11	1.60	0.83
2:E:17:SER:HB3	2:E:85:ASN:HD22	1.44	0.83
2:E:120:GLN:NE2	2:E:122:THR:HG23	1.92	0.83
2:D:33:LYS:H	2:D:54:ASP:HB2	1.42	0.83
2:E:12:VAL:O	2:E:124:SER:N	2.12	0.83
1:A:452:LEU:HD13	2:D:55:PHE:CE2	2.14	0.82
2:D:61:TYR:OH	2:D:71:ILE:N	2.12	0.82
1:A:112:SER:OG	1:A:134:GLN:OE1	1.95	0.82
1:A:30:ASN:OD1	1:A:31:SER:N	2.12	0.82
1:A:737:ASP:OD1	1:C:317:ASN:ND2	2.11	0.82
1:C:106:PHE:O	1:C:116:SER:OG	1.97	0.82
2:E:84:MET:HA	2:E:84:MET:HE2	1.59	0.82
1:B:343:ASN:OD1	4:B:1306:NAG:N2	2.13	0.82
1:C:99:ASN:O	1:C:102:ARG:NE	2.13	0.82
1:A:484:GLU:OE2	2:D:33:LYS:NZ	2.13	0.82
1:B:954:GLN:O	1:B:1014:ARG:NH1	2.11	0.82
1:B:124:THR:HG23	4:B:1301:NAG:H83	1.62	0.81
1:C:290:ASP:OD2	1:C:293:LEU:N	2.13	0.81
2:D:109:ARG:HH21	2:D:112:GLY:H	1.26	0.81
1:A:89:GLY:O	1:A:270:LEU:N	2.13	0.81
1:C:805:ILE:HD12	1:C:878:LEU:HD11	1.61	0.81
1:A:55:PHE:N	1:A:271:GLN:O	2.14	0.81
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.62	0.81
2:D:7:SER:OG	2:D:21:SER:OG	1.96	0.81
1:A:193:VAL:HG23	1:A:223:LEU:HD12	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:GLN:O	1:B:615:VAL:HG23	1.81	0.81
2:D:32:ARG:NH1	2:D:102:GLY:O	2.13	0.81
2:D:68:ARG:HE	2:D:86:SER:HB2	1.45	0.81
1:B:120:VAL:O	1:B:127:VAL:N	2.12	0.81
2:E:90:LYS:HE2	2:E:90:LYS:HA	1.61	0.81
1:B:170:TYR:HH	1:B:172:SER:HG	0.94	0.81
2:E:4:LEU:HB3	2:E:97:CYS:HB3	1.62	0.81
2:E:14:ALA:HB1	2:E:89:PRO:HD3	1.62	0.81
2:E:95:TYR:CD2	2:E:121:VAL:HB	2.15	0.81
1:A:67:ALA:N	1:A:263:ALA:O	2.14	0.80
1:A:457:ARG:NH1	1:A:459[A]:SER:O	2.15	0.80
1:B:480:CYS:O	1:B:482:GLY:N	2.15	0.80
2:E:18:LEU:O	2:E:84:MET:N	2.13	0.80
1:A:393:THR:O	1:A:523:THR:OG1	2.00	0.80
1:B:323:THR:OG1	1:B:324:GLU:OE2	1.99	0.80
2:E:4:LEU:CD2	2:E:99:VAL:HG23	2.12	0.80
1:C:30:ASN:OD1	1:C:31:SER:N	2.15	0.80
1:B:492:LEU:O	2:E:31:ALA:HB1	1.81	0.80
2:D:84:MET:CE	2:D:121:VAL:HG11	2.12	0.80
1:A:570:ALA:HB1	1:B:963:VAL:HG11	1.63	0.80
1:B:1006:THR:O	1:B:1010:GLN:NE2	2.15	0.80
1:B:598:ILE:HB	1:B:609:ALA:HB3	1.64	0.79
1:C:328:ARG:NH2	1:C:580:GLN:OE1	2.15	0.79
2:D:32:ARG:HB2	2:D:54:ASP:O	1.81	0.79
1:C:709:ASN:ND2	4:C:1306:NAG:O7	2.16	0.79
1:A:457:ARG:NH1	1:A:459[B]:SER:O	2.15	0.79
2:E:52:ILE:HA	2:E:59:THR:HA	1.65	0.79
2:E:72:SER:N	2:E:81:SER:O	2.16	0.79
1:A:568:ASP:OD1	1:A:569:ILE:HD12	1.82	0.79
2:E:16:GLY:O	2:E:86:SER:N	2.17	0.78
2:D:65:VAL:HG13	2:D:69:PHE:HB2	1.65	0.78
2:E:48:GLY:O	2:E:62:SER:HB2	1.82	0.78
1:B:792:PRO:O	1:B:795:LYS:NZ	2.16	0.78
2:E:45:GLU:HG3	2:E:46:ARG:H	1.47	0.78
1:B:494:SER:HA	2:E:55:PHE:CE1	2.16	0.78
2:D:99:VAL:CB	2:D:114:TYR:HB2	2.09	0.78
1:A:67:ALA:HB1	1:A:260:ALA:HB1	1.66	0.78
2:E:77:LYS:HA	2:E:77:LYS:HE3	1.66	0.78
1:C:1018:ILE:O	1:C:1022:ALA:N	2.17	0.77
2:E:88:LEU:HD12	2:E:89:PRO:HD2	1.66	0.77
1:B:31:SER:O	1:B:59:PHE:N	2.16	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:GLN:HA	2:E:46:ARG:HA	1.67	0.77
2:E:94:VAL:CA	2:E:120:GLN:HA	2.12	0.77
2:D:106:ASN:HB2	2:D:109:ARG:HH22	1.49	0.77
2:E:23:ALA:HA	2:E:79:THR:HA	1.66	0.77
1:C:66:HIS:N	1:C:80:ASP:OD2	2.18	0.77
1:B:39:PRO:HG3	1:B:51:THR:HG21	1.67	0.77
1:B:406:GLU:O	1:B:409:GLN:N	2.17	0.77
2:E:16:GLY:N	2:E:87:LEU:HB2	1.99	0.77
1:A:122:ASN:OD1	1:A:125:ASN:N	2.16	0.77
2:E:5:VAL:HG22	2:E:23:ALA:O	1.85	0.77
2:D:12:VAL:HG11	2:D:87:LEU:HD13	1.65	0.76
1:B:103:GLY:O	1:B:241:LEU:N	2.18	0.76
4:B:1302:NAG:O3	4:B:1302:NAG:O7	2.03	0.76
2:E:49:VAL:O	2:E:62:SER:N	2.19	0.76
1:C:112:SER:OG	1:C:134:GLN:OE1	2.03	0.76
1:C:619:GLU:OE1	1:C:619:GLU:N	2.19	0.76
2:E:49:VAL:CG1	2:E:65:VAL:HG21	2.16	0.76
1:A:22:THR:O	1:A:78:ARG:NH2	2.18	0.76
1:A:287:ASP:OD2	1:A:288:ALA:N	2.19	0.76
1:B:31:SER:N	1:B:60:SER:O	2.19	0.76
1:A:494:SER:HA	1:A:494:SER:CB	2.13	0.76
1:A:77:LYS:HZ1	1:A:259:THR:HG23	1.51	0.75
1:B:280:ASN:OD1	1:B:284:THR:N	2.19	0.75
1:B:473:TYR:N	1:B:489:TYR:O	2.18	0.75
2:D:4:LEU:HD13	2:D:22:CYS:SG	2.27	0.75
1:B:354:ASN:OD1	1:B:399:SER:OG	2.03	0.75
1:B:484:GLU:HG3	2:E:102:GLY:HA3	1.68	0.75
2:E:87:LEU:O	2:E:123:VAL:HG11	1.87	0.75
2:E:91:ASP:HB2	2:E:123:VAL:CG2	2.17	0.75
1:B:437:ASN:OD1	1:B:439:ASN:N	2.20	0.75
2:E:90:LYS:O	2:E:90:LYS:HD3	1.85	0.75
1:B:747:THR:O	1:B:751:ASN:ND2	2.19	0.75
4:B:1304:NAG:H83	4:B:1304:NAG:H3	1.69	0.74
2:D:61:TYR:CZ	2:D:71:ILE:HG22	2.23	0.74
1:A:30:ASN:OD1	1:A:60:SER:N	2.20	0.74
1:C:409:GLN:OE1	1:C:409:GLN:N	2.20	0.74
1:A:253:ASP:O	1:A:256:SER:N	2.19	0.74
1:B:118:LEU:HD21	1:B:120:VAL:HB	1.69	0.74
1:B:802:PHE:HD1	1:B:805:ILE:HD11	1.52	0.74
1:B:963:VAL:O	1:B:966:LEU:N	2.21	0.74
2:E:7:SER:OG	2:E:21:SER:HB2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:GLY:O	1:B:506:GLN:N	2.21	0.74
2:E:39:ARG:NH1	2:E:41:ALA:HB2	2.03	0.74
1:C:455:LEU:HD11	1:C:493:GLN:HB2	1.69	0.74
2:D:74:ASP:O	2:D:78:ASN:N	2.21	0.74
2:D:52:ILE:HG22	2:D:59:THR:HG23	1.70	0.73
1:B:494:SER:HA	1:B:494:SER:CB	2.13	0.73
1:B:349:SER:OG	1:B:452:LEU:O	2.05	0.73
1:C:332:ILE:HG23	1:C:333:THR:H	1.52	0.73
1:A:402:ILE:HD11	1:A:407:VAL:HG12	1.68	0.73
1:A:494:SER:HB2	2:D:55:PHE:CE1	2.20	0.73
2:D:34:CYS:C	2:D:100:ALA:HB3	2.13	0.73
2:E:41:ALA:HB3	2:E:44:GLN:HB3	1.69	0.73
1:A:1047:TYR:HH	1:B:886:TRP:CD1	2.07	0.73
2:D:35:ILE:HG23	2:D:80:VAL:HG11	1.68	0.73
1:B:969:ASN:ND2	1:B:975:SER:OG	2.21	0.73
1:C:568:ASP:OD1	1:C:569:ILE:N	2.22	0.73
2:D:35:ILE:CG2	2:D:80:VAL:HG11	2.19	0.73
1:A:112:SER:N	1:A:133:PHE:O	2.21	0.72
1:C:393:THR:O	1:C:523:THR:OG1	2.04	0.72
1:A:189:LEU:N	1:A:208:THR:O	2.22	0.72
2:D:100:ALA:CB	2:D:107:TRP:HB2	2.19	0.72
1:A:142:GLY:O	1:A:155:SER:OG	2.07	0.72
1:C:495:TYR:O	1:C:505:TYR:OH	2.07	0.72
2:E:38:PHE:CD1	2:E:98:THR:HG21	2.22	0.72
2:D:61:TYR:HB2	2:D:66:LYS:CE	2.18	0.72
1:C:30:ASN:OD1	1:C:32:PHE:N	2.23	0.72
2:D:4:LEU:CD2	2:D:35:ILE:HD11	2.20	0.72
1:C:96:GLU:OE1	1:C:100:ILE:N	2.23	0.72
2:E:65:VAL:HA	2:E:69:PHE:CD1	2.21	0.72
2:E:61:TYR:CZ	2:E:71:ILE:HG12	2.25	0.72
1:A:55:PHE:O	1:A:271:GLN:N	2.19	0.72
1:A:494:SER:C	2:D:55:PHE:CD1	2.67	0.71
2:E:6:GLU:HB3	2:E:119:THR:CG2	2.19	0.71
2:E:14:ALA:N	2:E:124:SER:O	2.23	0.71
2:E:88:LEU:CD1	2:E:89:PRO:HD2	2.20	0.71
1:A:438:SER:O	1:A:442:ASP:N	2.23	0.71
1:A:1141:LEU:O	1:A:1145:LEU:N	2.22	0.71
1:B:83:VAL:HG12	1:B:239:GLN:HB3	1.73	0.71
2:E:33:LYS:HD2	2:E:101:PHE:C	2.14	0.71
1:A:578:ASP:OD1	1:A:583:GLU:N	2.23	0.71
1:B:49:HIS:O	1:B:276:LEU:HD12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:VAL:HB	2:D:114:TYR:CB	2.13	0.71
2:E:24:ALA:O	2:E:78:ASN:HB3	1.90	0.71
1:A:787:GLN:OE1	1:C:703:ASN:ND2	2.24	0.71
2:E:37:TRP:CD1	2:E:97:CYS:HA	2.26	0.71
1:C:578:ASP:OD1	1:C:583:GLU:N	2.23	0.71
2:E:91:ASP:O	2:E:123:VAL:N	2.23	0.71
1:B:436:TRP:O	1:B:509:ARG:N	2.22	0.71
1:C:282:ASN:OD1	4:C:1301:NAG:N2	2.23	0.71
2:E:89:PRO:HA	2:E:123:VAL:HG12	1.71	0.71
2:E:11:SER:HA	2:E:122:THR:O	1.91	0.71
1:A:568:ASP:OD1	1:A:569:ILE:N	2.23	0.71
1:B:195:LYS:O	1:B:202:LYS:N	2.23	0.71
2:D:33:LYS:HD3	2:D:101:PHE:HA	1.72	0.71
2:D:71:ILE:HA	2:D:81:SER:O	1.90	0.71
1:A:351:TYR:CZ	1:A:492:LEU:HD22	2.26	0.70
1:B:452:LEU:HG	1:B:492:LEU:HD23	1.73	0.70
2:E:17:SER:CB	2:E:85:ASN:HD22	2.03	0.70
2:E:41:ALA:N	2:E:44:GLN:O	2.21	0.70
2:E:107:TRP:HE3	2:E:108:TYR:HD1	1.37	0.70
1:B:533:LEU:HD11	1:B:585:LEU:HD11	1.73	0.70
1:C:14:GLN:OE1	1:C:15:CYS:N	2.24	0.70
1:A:20:THR:HG22	1:A:20:THR:O	1.91	0.70
2:E:20:LEU:HD13	2:E:84:MET:HG3	1.72	0.70
2:D:34:CYS:CB	2:D:100:ALA:HB3	2.21	0.70
2:E:69:PHE:CD2	2:E:84:MET:HA	2.27	0.70
1:B:229:LEU:CB	1:B:231:ILE:HD11	2.22	0.70
2:E:98:THR:HB	2:E:113:ASP:OD1	1.91	0.70
1:C:781:VAL:HG22	1:C:1026:ALA:HB2	1.74	0.70
2:E:89:PRO:HA	2:E:123:VAL:CG1	2.22	0.70
1:B:229:LEU:HB3	1:B:231:ILE:HD11	1.74	0.70
1:B:780:GLU:O	1:B:784:GLN:NE2	2.25	0.70
1:B:872:GLN:O	1:B:875:SER:OG	2.09	0.70
2:D:48:GLY:O	2:D:62:SER:HB3	1.92	0.70
2:E:39:ARG:C	2:E:46:ARG:HA	2.17	0.70
1:A:154:GLU:OE2	1:A:156:GLU:N	2.25	0.69
1:C:391:CYS:HB2	1:C:525:CYS:HA	1.75	0.69
1:C:971:GLY:O	1:C:995:ARG:NH2	2.25	0.69
2:D:40:GLN:HG3	2:D:46:ARG:CB	2.16	0.69
2:D:40:GLN:CG	2:D:46:ARG:HB3	2.17	0.69
1:C:406:GLU:HB3	1:C:418:ILE:HG21	1.72	0.69
1:B:280:ASN:O	1:B:283:GLY:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:LEU:HB3	2:E:97:CYS:CB	2.22	0.69
2:E:68:ARG:HD2	2:E:86:SER:HB2	1.75	0.69
1:C:98:SER:OG	1:C:180:GLU:O	2.02	0.69
2:E:95:TYR:HD2	2:E:121:VAL:HB	1.56	0.69
1:C:332:ILE:O	1:C:334:ASN:N	2.25	0.69
2:E:73:GLY:CA	2:E:80:VAL:HA	2.23	0.69
1:A:167:THR:O	1:C:357:ARG:NH2	2.26	0.69
2:D:94:VAL:HA	2:D:120:GLN:HA	1.75	0.69
1:B:691:SER:OG	1:B:692:ILE:N	2.20	0.68
1:A:103:GLY:O	1:A:241:LEU:N	2.24	0.68
2:D:36:GLY:O	2:D:98:THR:N	2.26	0.68
2:E:22:CYS:O	2:E:80:VAL:HG12	1.92	0.68
2:E:73:GLY:HA3	2:E:80:VAL:HA	1.75	0.68
2:D:4:LEU:HD12	2:D:99:VAL:HG23	1.76	0.68
2:D:53:PHE:CD2	2:D:104:CYS:HB2	2.29	0.68
2:D:110:GLY:HA2	2:D:113:ASP:OD2	1.93	0.68
1:B:84:LEU:N	1:B:238:PHE:O	2.25	0.68
2:D:4:LEU:HB3	2:D:22:CYS:SG	2.34	0.68
1:A:49:HIS:O	1:A:276:LEU:HD12	1.93	0.68
1:A:616:ASN:ND2	4:A:1308:NAG:O7	2.27	0.68
1:B:193:VAL:HG23	1:B:223:LEU:HD12	1.76	0.68
1:B:816:SER:O	1:B:819:GLU:N	2.26	0.68
1:C:995:ARG:O	1:C:998:THR:N	2.27	0.68
2:E:5:VAL:CG2	2:E:23:ALA:HB3	2.23	0.68
2:E:34:CYS:O	2:E:100:ALA:HB3	1.94	0.68
1:A:282:ASN:OD1	1:A:282:ASN:N	2.20	0.68
1:B:93:ALA:HB1	1:B:189:LEU:HD11	1.75	0.68
1:B:124:THR:HG23	4:B:1301:NAG:C8	2.24	0.68
1:A:31:SER:N	1:A:60:SER:O	2.26	0.68
1:C:354:ASN:ND2	1:C:399:SER:O	2.26	0.68
1:C:395:VAL:HG23	1:C:524:VAL:HG11	1.75	0.68
2:E:18:LEU:CB	2:E:84:MET:HB2	2.19	0.68
1:B:495:TYR:N	2:E:55:PHE:CE1	2.62	0.68
1:B:1050:MET:HE2	1:B:1052:PHE:CZ	2.29	0.68
1:C:986:PRO:O	1:C:990:GLU:N	2.27	0.68
2:D:39:ARG:CD	2:D:49:VAL:HG22	2.22	0.68
1:A:472:ILE:HG23	1:A:489:TYR:C	2.19	0.67
1:B:30:ASN:OD1	1:B:31:SER:N	2.27	0.67
2:D:20:LEU:HD12	2:D:95:TYR:HD2	1.58	0.67
2:E:2:VAL:HB	2:E:114:TYR:CD2	2.29	0.67
1:B:310:LYS:NZ	1:B:663:ASP:OD1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ASN:OD1	1:B:642:VAL:N	2.26	0.67
2:D:2:VAL:HG12	2:D:99:VAL:HG21	1.76	0.67
1:C:105:ILE:HG23	1:C:241:LEU:HD21	1.76	0.67
1:C:924:ALA:O	1:C:928:ASN:ND2	2.27	0.67
1:B:345:THR:O	1:B:509:ARG:NH2	2.27	0.67
1:B:520:ALA:HB1	1:C:41:LYS:HD2	1.76	0.67
1:B:605:SER:OG	1:B:606:ASN:N	2.28	0.67
2:D:94:VAL:HG23	2:D:119:THR:C	2.19	0.67
1:C:816:SER:OG	1:C:1054:GLN:OE1	2.09	0.67
2:E:12:VAL:HG23	2:E:123:VAL:HG22	1.76	0.67
1:A:660:TYR:O	1:A:698:SER:N	2.27	0.67
1:C:110:LEU:O	1:C:135:PHE:N	2.28	0.67
2:E:17:SER:CA	2:E:85:ASN:HA	2.21	0.67
2:E:18:LEU:HD12	2:E:19:LYS:H	1.57	0.67
2:E:68:ARG:O	2:E:85:ASN:HB2	1.94	0.67
1:B:364:ASP:O	1:B:367:VAL:HG22	1.96	0.66
2:E:6:GLU:HB3	2:E:119:THR:HG23	1.76	0.66
2:E:8:GLY:HA3	2:E:20:LEU:HG	1.78	0.66
1:A:46:SER:N	1:A:280:ASN:O	2.28	0.66
1:A:786:LYS:NZ	1:C:699:LEU:O	2.28	0.66
1:A:492:LEU:O	2:D:31:ALA:HB1	1.95	0.66
1:B:118:LEU:HD23	1:B:118:LEU:C	2.20	0.66
1:B:474:GLN:NE2	1:B:480:CYS:SG	2.68	0.66
1:B:782:PHE:CE1	1:B:1029:MET:HE1	2.30	0.66
2:D:100:ALA:HB2	2:D:107:TRP:CD1	2.30	0.66
2:D:68:ARG:CZ	2:D:88:LEU:HG	2.24	0.66
1:B:339:GLY:O	1:B:343:ASN:N	2.29	0.66
1:B:569:ILE:H	1:B:569:ILE:HD12	1.60	0.66
2:D:12:VAL:CG1	2:D:87:LEU:HD13	2.25	0.66
2:D:33:LYS:HB2	2:D:54:ASP:OD2	1.94	0.66
1:B:494:SER:N	2:E:55:PHE:CE2	2.64	0.66
1:B:1022:ALA:O	1:B:1026:ALA:N	2.28	0.66
1:C:31:SER:OG	1:C:60:SER:N	2.27	0.66
1:C:144:TYR:N	1:C:153:MET:O	2.23	0.66
1:B:610:VAL:O	1:B:650:LEU:HD12	1.94	0.66
1:C:405:ASP:N	1:C:504:GLY:O	2.29	0.66
1:C:644:GLN:NE2	1:C:648:GLY:O	2.28	0.66
2:E:4:LEU:CG	2:E:99:VAL:HG23	2.26	0.66
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.31	0.66
1:B:1022:ALA:O	1:B:1025:ALA:N	2.29	0.66
2:E:40:GLN:CA	2:E:46:ARG:HA	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:61:TYR:OH	2:E:71:ILE:N	2.27	0.66
1:A:466:ARG:HE	1:A:468:ILE:HD11	1.61	0.66
1:B:393:THR:O	1:B:523:THR:OG1	2.14	0.66
2:E:63:ASP:HA	2:E:66:LYS:CD	2.26	0.65
1:A:1056:ALA:HB1	1:A:1057:PRO:HD2	1.78	0.65
1:A:971:GLY:N	1:B:755:GLN:OE1	2.28	0.65
2:E:37:TRP:HZ3	2:E:71:ILE:HG22	1.61	0.65
2:E:39:ARG:HE	2:E:93:ALA:HB3	1.61	0.65
1:A:496:GLY:N	2:D:55:PHE:HE1	1.94	0.65
1:B:494:SER:N	2:E:55:PHE:CG	2.65	0.65
1:B:1123:SER:OG	1:C:918:GLU:OE2	2.15	0.65
1:C:578:ASP:O	1:C:582:LEU:N	2.30	0.65
1:C:914:ASN:ND2	1:C:1111:GLU:OE2	2.28	0.65
1:C:96:GLU:OE1	1:C:101:ILE:N	2.25	0.65
1:B:328:ARG:NH1	1:B:531:THR:O	2.27	0.65
1:B:490:PHE:C	2:E:31:ALA:HB2	2.21	0.65
1:C:328:ARG:NE	1:C:531:THR:O	2.30	0.65
1:C:1008:VAL:O	1:C:1012:LEU:N	2.30	0.65
2:D:34:CYS:HB3	2:D:100:ALA:HB3	1.79	0.65
2:E:9:GLY:HA2	2:E:121:VAL:HG22	1.79	0.65
2:E:33:LYS:HD2	2:E:102:GLY:N	2.12	0.65
2:E:39:ARG:O	2:E:39:ARG:HD3	1.98	0.64
1:B:518:LEU:HD23	1:B:518:LEU:H	1.61	0.64
1:A:353:TRP:O	1:A:466:ARG:NH2	2.30	0.64
2:E:6:GLU:OE1	2:E:119:THR:N	2.29	0.64
2:E:65:VAL:HG22	2:E:69:PHE:CD1	2.31	0.64
1:A:45:SER:OG	1:A:280:ASN:O	2.15	0.64
1:A:329:PHE:O	1:A:580:GLN:NE2	2.31	0.64
2:D:68:ARG:NE	2:D:86:SER:HB2	2.11	0.64
2:E:21:SER:HA	2:E:80:VAL:O	1.97	0.64
1:A:318:PHE:N	1:A:593:GLY:O	2.31	0.64
1:B:91:TYR:N	1:B:268:GLY:O	2.29	0.64
1:B:543:PHE:HB3	1:B:576:VAL:HG21	1.78	0.64
1:B:866:THR:HG23	1:B:869:MET:HE2	1.78	0.64
1:C:332:ILE:HD11	1:C:362:VAL:HG11	1.78	0.64
2:E:14:ALA:HA	2:E:123:VAL:CG1	2.28	0.64
1:A:118:LEU:C	1:A:118:LEU:HD12	2.22	0.64
1:C:210:ILE:HG22	1:C:211:ASN:H	1.63	0.64
2:E:45:GLU:HG3	2:E:46:ARG:N	2.11	0.64
2:E:96:TYR:HB3	2:E:115:TRP:HE3	1.63	0.64
1:A:108:THR:O	1:A:237:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:ILE:CG2	2:D:59:THR:HG23	2.28	0.64
2:E:39:ARG:HH21	2:E:93:ALA:HB2	1.63	0.64
1:B:457:ARG:NH1	1:B:459[A]:SER:OG	2.31	0.63
2:D:100:ALA:HB2	2:D:107:TRP:HB2	1.80	0.63
2:E:14:ALA:HB2	2:E:89:PRO:HB3	1.79	0.63
1:B:437:ASN:OD1	1:B:438:SER:N	2.31	0.63
1:B:977:LEU:O	1:B:980:ILE:N	2.30	0.63
2:E:20:LEU:HD13	2:E:84:MET:CG	2.28	0.63
1:A:935:GLN:O	1:A:939:SER:N	2.31	0.63
2:E:38:PHE:HA	2:E:49:VAL:HG23	1.79	0.63
1:A:553:THR:O	1:A:586:ASP:N	2.31	0.63
1:B:1050:MET:HE2	1:B:1052:PHE:CE1	2.33	0.63
1:C:909:ILE:HD13	1:C:1049:LEU:HD21	1.81	0.63
2:D:55:PHE:H	2:D:75:ASN:ND2	1.96	0.63
2:D:71:ILE:HD12	2:D:81:SER:O	1.99	0.63
1:C:118:LEU:HD13	1:C:120:VAL:HG23	1.80	0.63
1:C:124:THR:OG1	3:H:1:NAG:N2	2.32	0.63
1:A:157:PHE:CE2	1:A:159:VAL:HG22	2.33	0.63
1:B:351:TYR:OH	1:B:452:LEU:HD23	1.99	0.63
2:E:22:CYS:HB3	2:E:80:VAL:CG1	2.28	0.63
2:D:6:GLU:OE2	2:D:37:TRP:NE1	2.32	0.63
1:A:467:ASP:O	1:A:468:ILE:HD13	1.98	0.62
1:B:37:TYR:OH	1:B:54:LEU:O	2.09	0.62
2:D:51:ALA:HB2	2:D:107:TRP:CZ2	2.34	0.62
2:E:4:LEU:CD2	2:E:97:CYS:HB3	2.29	0.62
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.81	0.62
1:C:500:THR:O	1:C:500:THR:HG22	2.00	0.62
2:E:37:TRP:CZ3	2:E:82:LEU:HB2	2.34	0.62
2:E:40:GLN:NE2	2:E:41:ALA:O	2.33	0.62
1:A:1000:ARG:O	1:A:1003:SER:N	2.33	0.62
1:B:448:ASN:OD1	1:B:450:ASN:ND2	2.32	0.62
1:C:46:SER:N	1:C:280:ASN:O	2.32	0.62
2:D:4:LEU:HD21	2:D:35:ILE:CD1	2.29	0.62
1:A:605:SER:OG	1:A:606:ASN:N	2.33	0.62
1:A:193:VAL:CG2	1:A:223:LEU:HD12	2.28	0.62
2:E:92:THR:CA	2:E:122:THR:HA	2.16	0.62
1:A:22:THR:OG1	1:A:78:ARG:NH2	2.32	0.62
1:B:338:PHE:O	1:B:341:VAL:N	2.29	0.62
2:E:51:ALA:CB	2:E:60:TYR:HB3	2.25	0.62
1:A:619:GLU:OE1	1:A:619:GLU:N	2.33	0.62
2:D:92:THR:O	2:D:92:THR:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:GLU:OE1	2:E:119:THR:HG23	2.00	0.62
1:A:56:LEU:HD22	1:A:91:TYR:HD2	1.65	0.62
2:D:65:VAL:HG13	2:D:69:PHE:CB	2.29	0.62
2:E:50:ALA:HB1	2:E:60:TYR:O	2.00	0.62
2:E:71:ILE:HA	2:E:82:LEU:HA	1.81	0.62
1:A:367:VAL:O	1:A:371:SER:OG	2.17	0.62
1:B:287:ASP:OD1	1:B:288:ALA:N	2.33	0.62
1:B:1056:ALA:HB1	1:B:1057:PRO:CD	2.30	0.62
1:C:1056:ALA:HB3	1:C:1059:GLY:O	1.99	0.62
2:D:4:LEU:HB3	2:D:97:CYS:SG	2.39	0.62
1:A:299:THR:HG23	1:A:300:LYS:N	2.15	0.61
1:A:537:LYS:H	1:A:551:VAL:HG23	1.65	0.61
1:C:199:GLY:O	1:C:232:GLY:N	2.27	0.61
1:C:898:PHE:CZ	1:C:1050:MET:HE1	2.35	0.61
1:C:540:ASN:HA	1:C:549:THR:HG22	1.82	0.61
2:E:16:GLY:O	2:E:87:LEU:HG	2.00	0.61
2:E:94:VAL:HG23	2:E:120:GLN:N	2.15	0.61
1:B:417:LYS:O	1:B:421:TYR:N	2.33	0.61
1:C:76:THR:OG1	1:C:77:LYS:N	2.31	0.61
1:C:921:LYS:O	1:C:924:ALA:N	2.33	0.61
1:A:131:CYS:HA	1:A:166:CYS:HB3	1.83	0.61
1:A:490:PHE:HD2	2:D:31:ALA:HB3	1.65	0.61
1:C:118:LEU:HD13	1:C:120:VAL:CG2	2.31	0.61
1:B:926:GLN:O	1:B:930:ALA:N	2.33	0.61
2:D:52:ILE:HD11	2:D:80:VAL:CG1	2.29	0.61
2:E:20:LEU:O	2:E:81:SER:HA	2.01	0.61
2:E:41:ALA:HB3	2:E:44:GLN:H	1.65	0.61
2:E:45:GLU:CG	2:E:46:ARG:H	2.13	0.61
2:E:106:ASN:HA	2:E:109:ARG:HH21	1.64	0.61
1:C:926:GLN:O	1:C:930:ALA:N	2.34	0.61
2:D:12:VAL:HG11	2:D:87:LEU:CD1	2.31	0.61
2:D:68:ARG:NE	2:D:88:LEU:HG	2.15	0.61
2:E:12:VAL:HB	2:E:87:LEU:HD13	1.82	0.61
2:E:33:LYS:H	2:E:54:ASP:HB3	1.65	0.61
1:A:1031:GLU:OE1	1:C:1039:ARG:NE	2.30	0.61
2:D:19:LYS:NZ	2:D:21:SER:HB3	2.15	0.61
2:D:94:VAL:HG13	2:D:96:TYR:CE2	2.35	0.61
2:E:4:LEU:HD23	2:E:97:CYS:HB3	1.81	0.61
1:B:38:TYR:OH	1:B:285:ILE:N	2.30	0.61
1:B:615:VAL:O	1:B:644:GLN:NE2	2.34	0.61
1:B:717:ASN:HD21	4:B:1310:NAG:C7	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ASN:OD1	1:C:125:ASN:N	2.29	0.61
2:D:106:ASN:HA	2:D:109:ARG:HH12	1.66	0.61
1:A:253:ASP:OD2	1:A:256:SER:N	2.34	0.60
1:A:495:TYR:N	2:D:55:PHE:CE1	2.68	0.60
1:A:572:THR:HG23	1:A:572:THR:O	2.00	0.60
1:A:979:ASP:O	1:A:982:SER:N	2.32	0.60
1:B:349:SER:O	1:B:353:TRP:N	2.34	0.60
2:D:1:GLN:OE1	2:D:114:TYR:OH	2.17	0.60
2:E:69:PHE:HD2	2:E:84:MET:HA	1.65	0.60
2:E:107:TRP:CE3	2:E:108:TYR:HD1	2.18	0.60
1:A:300:LYS:O	1:A:304:LYS:N	2.33	0.60
1:B:116:SER:N	1:B:131:CYS:O	2.26	0.60
2:E:40:GLN:HA	2:E:45:GLU:C	2.26	0.60
2:E:91:ASP:HB2	2:E:123:VAL:HG21	1.82	0.60
1:A:753:LEU:HD12	1:A:754:LEU:N	2.16	0.60
1:B:126:VAL:HG23	1:B:175:PHE:HE2	1.66	0.60
1:B:398:ASP:O	1:B:512:VAL:N	2.26	0.60
1:B:494:SER:O	2:E:55:PHE:CD1	2.52	0.60
1:A:1071:GLN:NE2	4:A:1311:NAG:O7	2.31	0.60
1:A:763:LEU:HD13	1:A:1004:LEU:HD23	1.83	0.60
1:C:455:LEU:N	1:C:491:PRO:O	2.28	0.60
2:E:18:LEU:HB3	2:E:84:MET:CB	2.22	0.60
2:E:39:ARG:H	2:E:47:GLU:H	1.48	0.60
2:E:50:ALA:CB	2:E:71:ILE:HD13	2.30	0.60
1:A:931:ILE:O	1:A:934:ILE:N	2.31	0.60
1:A:1047:TYR:HH	1:B:886:TRP:HD1	1.47	0.60
2:D:33:LYS:HB3	2:D:101:PHE:C	2.26	0.60
1:A:299:THR:O	1:A:302:THR:N	2.35	0.60
2:E:92:THR:HG22	2:E:123:VAL:N	2.15	0.60
1:A:21:ARG:O	1:A:23:GLN:NE2	2.35	0.60
1:A:1056:ALA:HB1	1:A:1057:PRO:CD	2.32	0.60
1:A:1094:VAL:HG11	1:B:904:TYR:OH	2.02	0.60
1:B:93:ALA:HA	1:B:191:GLU:HA	1.84	0.60
2:D:100:ALA:HB1	2:D:107:TRP:HB2	1.84	0.60
1:A:1056:ALA:HB3	1:A:1059:GLY:O	2.02	0.59
1:A:592:PHE:CD1	1:B:740:MET:HE1	2.38	0.59
2:D:20:LEU:HD13	2:D:119:THR:HG21	1.85	0.59
1:A:746:SER:OG	1:A:748:GLU:OE2	2.20	0.59
1:A:1048:HIS:CD2	1:A:1051:SER:HG	2.20	0.59
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.31	0.59
1:B:100:ILE:O	1:B:243:ALA:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:N	1:B:563:GLN:OE1	2.36	0.59
1:A:70:VAL:HG21	1:A:76:THR:HB	1.84	0.59
1:B:276:LEU:HD23	1:B:306:PHE:HE1	1.66	0.59
2:D:16:GLY:C	2:D:87:LEU:HD12	2.27	0.59
2:D:65:VAL:CG1	2:D:69:PHE:HB2	2.30	0.59
2:E:74:ASP:OD2	2:E:77:LYS:HG2	2.02	0.59
1:B:85:PRO:HA	1:B:237:ARG:HA	1.84	0.59
1:B:753:LEU:HD11	1:B:1001:LEU:HD11	1.84	0.59
1:C:282:ASN:HB2	1:C:284:THR:HG22	1.84	0.59
2:D:51:ALA:HB3	2:D:60:TYR:HD2	1.67	0.59
2:E:15:GLY:HA2	2:E:86:SER:O	2.03	0.59
1:A:999:GLY:O	1:A:1003:SER:N	2.34	0.59
1:B:102:ARG:N	1:B:241:LEU:O	2.27	0.59
1:B:336:CYS:O	1:B:338:PHE:N	2.36	0.59
1:A:568:ASP:N	1:A:574:ASP:OD1	2.35	0.59
1:B:76:THR:OG1	1:B:77:LYS:N	2.36	0.59
1:B:391:CYS:CB	1:B:525:CYS:HA	2.32	0.59
1:B:572:THR:HG23	1:B:572:THR:O	2.02	0.59
1:C:31:SER:HG	1:C:60:SER:H	1.51	0.59
2:D:68:ARG:HB3	2:D:85:ASN:O	2.03	0.59
1:B:914:ASN:OD1	1:B:915:VAL:HG23	2.03	0.58
1:C:189:LEU:HD22	1:C:217:PRO:HG2	1.85	0.58
1:C:1050:MET:HE2	1:C:1052:PHE:CE2	2.38	0.58
2:E:91:ASP:HB2	2:E:123:VAL:HG23	1.84	0.58
1:B:400:PHE:CZ	1:B:510:VAL:HG11	2.38	0.58
1:C:942:PRO:HD2	1:C:942:PRO:O	2.02	0.58
2:E:17:SER:HA	2:E:84:MET:O	2.03	0.58
1:C:391:CYS:CB	1:C:525:CYS:HA	2.32	0.58
2:E:22:CYS:O	2:E:80:VAL:N	2.35	0.58
2:E:4:LEU:HD13	2:E:115:TRP:O	2.03	0.58
2:E:93:ALA:O	2:E:121:VAL:N	2.32	0.58
1:A:484:GLU:OE1	2:D:102:GLY:HA3	2.03	0.58
2:E:34:CYS:HA	2:E:52:ILE:O	2.03	0.58
1:C:212:LEU:HD12	1:C:213:VAL:N	2.19	0.58
1:A:904:TYR:O	1:A:907:ASN:N	2.36	0.58
1:B:274:THR:HG23	1:B:274:THR:O	2.03	0.58
1:B:489:TYR:CD1	2:E:30:TRP:HB2	2.39	0.58
1:B:493:GLN:NE2	2:E:75:ASN:OD1	2.36	0.58
2:E:70:THR:O	2:E:82:LEU:HA	2.04	0.58
2:E:94:VAL:HA	2:E:120:GLN:CA	2.21	0.58
1:A:743:CYS:SG	1:A:753:LEU:HD23	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:SER:O	1:C:47:VAL:HG23	2.03	0.58
1:A:722:VAL:HG23	1:A:930:ALA:HB1	1.86	0.58
1:C:84:LEU:O	1:C:238:PHE:N	2.31	0.58
2:D:53:PHE:HD2	2:D:104:CYS:HB2	1.67	0.58
1:A:193:VAL:N	1:A:204:TYR:O	2.37	0.58
2:E:82:LEU:O	2:E:84:MET:HE3	2.04	0.58
1:C:743:CYS:SG	1:C:753:LEU:HD23	2.44	0.57
2:E:41:ALA:HB3	2:E:44:GLN:CB	2.33	0.57
2:E:84:MET:HB3	2:E:87:LEU:CD2	2.30	0.57
1:A:570:ALA:CB	1:B:963:VAL:HG11	2.34	0.57
1:C:210:ILE:HG22	1:C:211:ASN:N	2.19	0.57
2:E:12:VAL:CG2	2:E:87:LEU:HD13	2.34	0.57
1:A:594:GLY:N	1:A:613:GLN:OE1	2.37	0.57
1:B:20:THR:O	1:B:20:THR:HG22	2.04	0.57
1:B:452:LEU:CD1	2:E:55:PHE:HE2	2.17	0.57
2:D:39:ARG:NH1	2:D:48:GLY:O	2.37	0.57
2:E:39:ARG:O	2:E:46:ARG:HA	2.05	0.57
1:A:493:GLN:NE2	2:D:75:ASN:HB3	2.20	0.57
1:A:859:THR:OG1	1:A:860:VAL:N	2.37	0.57
1:B:191:GLU:O	1:B:205:SER:OG	2.17	0.57
1:B:559:PHE:O	1:B:560:LEU:HD12	2.04	0.57
1:C:216:LEU:HD23	1:C:216:LEU:C	2.30	0.57
1:C:327:VAL:O	1:C:531:THR:N	2.33	0.57
1:C:330:PRO:HA	1:C:579:PRO:HB2	1.84	0.57
1:C:586:ASP:OD1	1:C:587:ILE:N	2.37	0.57
2:E:65:VAL:CG1	2:E:82:LEU:HD11	2.34	0.57
1:A:255:SER:O	1:A:258:TRP:NE1	2.38	0.57
1:A:974:SER:OG	1:A:975:SER:N	2.35	0.57
1:B:253:ASP:O	1:B:257:GLY:N	2.29	0.57
2:D:94:VAL:HG23	2:D:120:GLN:N	2.20	0.57
2:E:39:ARG:HG3	2:E:95:TYR:CZ	2.40	0.57
2:E:61:TYR:CE2	2:E:70:THR:HA	2.39	0.57
1:C:784:GLN:NE2	1:C:1030:SER:OG	2.37	0.57
2:D:53:PHE:HZ	2:D:102:GLY:O	1.88	0.57
2:E:38:PHE:HB2	2:E:115:TRP:CZ3	2.40	0.57
2:E:69:PHE:CD2	2:E:84:MET:HE2	2.40	0.57
1:C:752:LEU:O	1:C:755:GLN:N	2.31	0.57
2:D:27:TYR:CE2	2:D:29:SER:HB3	2.40	0.57
2:E:63:ASP:C	2:E:66:LYS:HG2	2.30	0.57
1:A:305:SER:OG	1:A:307:THR:O	2.15	0.57
1:B:231:ILE:HG22	1:B:233:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:LYS:HG2	2:D:102:GLY:HA2	1.87	0.57
1:C:63:THR:HG21	1:C:65:PHE:CE2	2.40	0.57
2:D:49:VAL:O	2:D:62:SER:N	2.37	0.57
2:D:71:ILE:HD12	2:D:81:SER:C	2.29	0.57
2:E:16:GLY:O	2:E:87:LEU:N	2.38	0.57
1:B:691:SER:HG	1:B:692:ILE:H	1.50	0.56
2:D:49:VAL:CG1	2:D:65:VAL:HG11	2.34	0.56
1:A:70:VAL:HG21	1:A:76:THR:CB	2.36	0.56
1:A:699:LEU:HD22	1:B:873:TYR:OH	2.03	0.56
1:C:774:GLN:O	1:C:777:ASN:N	2.38	0.56
2:E:94:VAL:N	2:E:120:GLN:OE1	2.38	0.56
1:A:276:LEU:C	1:A:277:LEU:HD12	2.30	0.56
1:A:496:GLY:N	2:D:55:PHE:CE1	2.72	0.56
1:A:551:VAL:C	1:A:552:LEU:HD12	2.31	0.56
1:A:871:ALA:O	1:A:874:THR:OG1	2.23	0.56
1:A:936:ASP:O	1:A:940:SER:OG	2.19	0.56
1:B:140:PHE:N	1:B:158:ARG:O	2.34	0.56
1:C:17:ASN:OD1	1:C:137:ASN:ND2	2.38	0.56
2:E:2:VAL:HB	2:E:114:TYR:CE2	2.40	0.56
2:E:39:ARG:HB2	2:E:95:TYR:CE1	2.40	0.56
2:E:68:ARG:HB2	2:E:86:SER:HB2	1.86	0.56
2:E:68:ARG:NE	2:E:88:LEU:HB2	2.21	0.56
2:E:94:VAL:HG13	2:E:96:TYR:CE2	2.40	0.56
1:A:446:GLY:O	1:A:449:TYR:OH	2.21	0.56
1:A:664:ILE:O	1:A:672:ALA:N	2.39	0.56
2:D:93:ALA:O	2:D:121:VAL:N	2.36	0.56
2:E:40:GLN:HA	2:E:46:ARG:CA	2.34	0.56
1:A:739:THR:O	1:A:742:ILE:N	2.38	0.56
1:A:773:GLU:OE2	1:A:1019:ARG:NH2	2.31	0.56
1:B:436:TRP:N	1:B:509:ARG:O	2.33	0.56
1:B:437:ASN:HA	1:B:508:TYR:CD1	2.40	0.56
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.86	0.56
2:E:37:TRP:CZ3	2:E:71:ILE:HG22	2.39	0.56
1:A:212:LEU:HD12	1:A:213:VAL:N	2.20	0.56
1:A:490:PHE:CD2	2:D:32:ARG:HD2	2.40	0.56
1:C:316:SER:OG	1:C:317:ASN:N	2.39	0.56
2:D:52:ILE:CG2	2:D:71:ILE:HG23	2.36	0.56
2:E:53:PHE:HD1	2:E:56:ASP:HB2	1.69	0.56
1:B:105:ILE:HG23	1:B:117:LEU:O	2.05	0.56
2:E:39:ARG:HH12	2:E:41:ALA:HB2	1.70	0.56
1:A:106:PHE:O	1:A:117:LEU:N	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:819:GLU:O	1:A:822:LEU:N	2.39	0.56
1:B:569:ILE:O	1:B:572:THR:HG22	2.06	0.56
1:B:574:ASP:HA	1:B:587:ILE:HB	1.88	0.56
2:D:4:LEU:HD23	2:D:24:ALA:N	2.21	0.56
1:A:560:LEU:O	1:A:577:ARG:NH1	2.37	0.56
1:C:615:VAL:HG12	1:C:616:ASN:N	2.21	0.56
2:E:38:PHE:HA	2:E:47:GLU:O	2.06	0.56
2:E:49:VAL:HG13	2:E:65:VAL:HG21	1.87	0.56
1:B:493:GLN:C	2:E:55:PHE:CE2	2.85	0.55
1:B:599:THR:HG22	1:B:608:VAL:HG12	1.88	0.55
1:C:276:LEU:HD23	1:C:306:PHE:HE1	1.71	0.55
1:C:332:ILE:CD1	1:C:362:VAL:HG11	2.36	0.55
1:C:880:GLY:O	1:C:884:SER:N	2.34	0.55
1:C:898:PHE:HZ	1:C:1050:MET:HE1	1.70	0.55
2:D:4:LEU:HD22	2:D:22:CYS:SG	2.46	0.55
2:E:35:ILE:O	2:E:52:ILE:HG22	2.06	0.55
2:E:97:CYS:O	2:E:115:TRP:HA	2.06	0.55
1:A:118:LEU:HD13	1:A:120:VAL:HG23	1.87	0.55
1:A:387:LEU:HD23	1:A:390:LEU:HD12	1.88	0.55
1:A:490:PHE:O	2:D:31:ALA:HB2	2.06	0.55
1:A:736:VAL:HG13	1:A:858:LEU:HD23	1.88	0.55
1:A:1025:ALA:O	1:A:1028:LYS:N	2.37	0.55
2:E:37:TRP:CZ2	2:E:80:VAL:HG13	2.41	0.55
1:A:138:ASP:N	1:A:139:PRO:CD	2.70	0.55
1:B:356:LYS:O	1:B:397:ALA:N	2.34	0.55
1:B:707:TYR:CD1	1:B:708:SER:N	2.74	0.55
2:E:4:LEU:CB	2:E:97:CYS:HB3	2.35	0.55
1:A:115:GLN:CD	1:A:130:VAL:HG12	2.31	0.55
1:A:146:HIS:ND1	1:A:151:SER:O	2.31	0.55
1:C:408:ARG:O	1:C:414:GLN:NE2	2.40	0.55
2:D:37:TRP:HA	2:D:96:TYR:O	2.06	0.55
2:E:40:GLN:N	2:E:46:ARG:HA	2.22	0.55
1:A:76:THR:OG1	1:A:77:LYS:N	2.39	0.55
1:A:713:ALA:HB2	1:B:895:GLN:CD	2.31	0.55
1:C:216:LEU:HD23	1:C:217:PRO:O	2.06	0.55
2:D:68:ARG:O	2:D:85:ASN:HB3	2.06	0.55
2:E:12:VAL:CB	2:E:87:LEU:HD13	2.36	0.55
2:D:34:CYS:SG	2:D:53:PHE:HD2	2.30	0.55
2:D:37:TRP:CH2	2:D:80:VAL:HG23	2.42	0.55
1:A:858:LEU:HD12	1:A:963:VAL:CG2	2.37	0.55
1:A:963:VAL:CG1	1:C:570:ALA:HB2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ASN:ND2	1:B:211:ASN:O	2.40	0.55
1:C:534:VAL:HG22	1:C:535:LYS:H	1.71	0.55
2:D:20:LEU:HD13	2:D:119:THR:CG2	2.37	0.55
2:D:109:ARG:HB3	2:D:109:ARG:NH1	2.22	0.55
2:E:69:PHE:HA	2:E:83:GLN:O	2.07	0.55
1:A:47:VAL:HG12	1:A:48:LEU:N	2.22	0.55
1:A:253:ASP:N	1:A:256:SER:OG	2.40	0.55
1:A:269:TYR:O	1:A:271:GLN:NE2	2.40	0.55
1:A:496:GLY:CA	2:D:55:PHE:HE1	2.19	0.55
2:D:49:VAL:HG12	2:D:65:VAL:HG11	1.87	0.55
1:A:494:SER:O	2:D:55:PHE:CD1	2.59	0.55
1:B:645:THR:OG1	1:B:647:ALA:N	2.30	0.55
1:B:825:LYS:NZ	1:B:941:THR:O	2.33	0.55
1:A:14:GLN:O	1:A:158:ARG:NH1	2.40	0.54
2:D:68:ARG:HH21	2:D:87:LEU:N	2.05	0.54
1:A:858:LEU:HD12	1:A:963:VAL:HG23	1.89	0.54
1:B:46:SER:N	1:B:279:TYR:O	2.40	0.54
1:B:452:LEU:HA	2:E:55:PHE:CZ	2.42	0.54
1:C:341:VAL:HG22	1:C:356:LYS:HE3	1.88	0.54
2:D:68:ARG:HD2	2:D:88:LEU:HD21	1.88	0.54
2:E:63:ASP:HA	2:E:66:LYS:HD2	1.89	0.54
2:D:62:SER:OG	2:D:65:VAL:HB	2.07	0.54
2:E:50:ALA:HB1	2:E:71:ILE:HD13	1.88	0.54
1:A:748:GLU:OE2	1:A:748:GLU:N	2.36	0.54
1:B:185:ASN:ND2	1:B:212:LEU:O	2.40	0.54
2:E:88:LEU:CG	2:E:89:PRO:HD2	2.37	0.54
1:B:132:GLU:OE1	1:B:165:ASN:ND2	2.41	0.54
1:B:520:ALA:HB3	1:B:521:PRO:CD	2.38	0.54
1:C:362:VAL:HG13	1:C:526:GLY:O	2.07	0.54
2:D:34:CYS:HA	2:D:53:PHE:HA	1.89	0.54
2:E:55:PHE:CD2	2:E:55:PHE:CB	2.78	0.54
1:A:220:PHE:CD2	1:A:221:SER:N	2.76	0.54
1:A:466:ARG:NE	1:A:468:ILE:HD11	2.23	0.54
1:A:936:ASP:O	1:A:940:SER:N	2.36	0.54
2:D:6:GLU:HG2	2:D:97:CYS:SG	2.48	0.54
2:E:63:ASP:O	2:E:66:LYS:HG2	2.07	0.54
2:E:70:THR:O	2:E:83:GLN:N	2.33	0.54
1:A:159:VAL:HG23	1:A:160:TYR:N	2.22	0.54
1:A:542:ASN:HB2	1:A:547:THR:HG22	1.89	0.54
1:C:973:ILE:HG13	1:C:974:SER:N	2.23	0.54
2:D:103:THR:HB	2:D:105:ASP:OD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:VAL:O	2:E:22:CYS:HA	2.07	0.54
1:A:193:VAL:HG23	1:A:223:LEU:CD1	2.35	0.54
1:B:435:ALA:HA	1:B:509:ARG:O	2.07	0.54
2:D:76:ALA:HB3	2:D:77:LYS:NZ	2.22	0.54
2:E:95:TYR:CE2	2:E:121:VAL:HB	2.43	0.54
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.42	0.54
1:B:699:LEU:HD22	1:C:873:TYR:CZ	2.43	0.54
1:C:51:THR:HG23	1:C:51:THR:O	2.07	0.54
1:C:124:THR:HG23	3:H:1:NAG:H83	1.89	0.54
1:C:526:GLY:O	1:C:528:LYS:N	2.41	0.54
1:C:868:GLU:OE1	1:C:868:GLU:N	2.40	0.54
2:D:20:LEU:HD12	2:D:95:TYR:CD2	2.41	0.54
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.38	0.54
1:B:406:GLU:OE1	1:B:409:GLN:NE2	2.41	0.54
1:A:105:ILE:HA	1:A:117:LEU:O	2.08	0.53
1:A:307:THR:HG1	1:A:602:THR:HG1	1.55	0.53
1:A:493:GLN:C	2:D:55:PHE:CD2	2.86	0.53
1:A:645:THR:O	1:A:647:ALA:N	2.41	0.53
1:B:34:ARG:O	1:B:56:LEU:HD23	2.07	0.53
1:B:437:ASN:HA	1:B:508:TYR:HA	1.90	0.53
1:B:897:PRO:O	1:B:901:GLN:HG3	2.08	0.53
1:B:991:VAL:O	1:B:994:ASP:N	2.40	0.53
1:C:336:CYS:SG	1:C:524:VAL:HG23	2.47	0.53
2:D:19:LYS:HZ3	2:D:21:SER:HB3	1.74	0.53
2:D:20:LEU:HG	2:D:84:MET:SD	2.48	0.53
2:E:22:CYS:HB2	2:E:37:TRP:CZ2	2.43	0.53
1:B:81:ASN:N	1:B:82:PRO:CD	2.71	0.53
1:C:405:ASP:O	1:C:408:ARG:NH2	2.42	0.53
2:D:69:PHE:CE1	2:D:84:MET:HG2	2.43	0.53
2:D:109:ARG:HE	2:D:111:ARG:HB3	1.72	0.53
2:E:29:SER:O	2:E:31:ALA:HA	2.08	0.53
2:E:40:GLN:HG2	2:E:45:GLU:HA	1.90	0.53
1:C:318:PHE:N	1:C:593:GLY:O	2.37	0.53
1:C:821:LEU:HD22	1:C:939:SER:HA	1.90	0.53
1:B:42:VAL:HG12	1:B:43:PHE:N	2.23	0.53
1:B:276:LEU:O	1:B:288:ALA:HB1	2.08	0.53
1:C:29:THR:HG23	1:C:62:VAL:CG2	2.39	0.53
1:C:1023:ASN:O	1:C:1026:ALA:N	2.40	0.53
2:D:70:THR:HG22	2:D:83:GLN:HB3	1.89	0.53
2:D:109:ARG:HE	2:D:111:ARG:CB	2.21	0.53
2:E:37:TRP:CH2	2:E:80:VAL:HG13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLY:O	1:B:419:ALA:N	2.42	0.53
1:C:216:LEU:HD23	1:C:217:PRO:N	2.23	0.53
1:A:327:VAL:O	1:A:531:THR:N	2.41	0.53
1:A:995:ARG:O	1:A:998:THR:N	2.41	0.53
2:E:46:ARG:HD2	2:E:115:TRP:CH2	2.44	0.53
1:A:30:ASN:HA	1:A:61:ASN:HA	1.91	0.53
1:A:277:LEU:HD12	1:A:277:LEU:N	2.23	0.53
1:B:418:ILE:HG23	1:B:422:ASN:HB2	1.91	0.53
1:B:1056:ALA:HB1	1:B:1057:PRO:HD2	1.90	0.53
1:C:766:ALA:O	1:C:769:GLY:N	2.42	0.53
1:A:312:ILE:HG23	1:A:313:TYR:N	2.24	0.53
1:B:107:GLY:N	1:B:235:ILE:HG23	2.24	0.53
1:B:138:ASP:N	1:B:139:PRO:HD3	2.23	0.53
2:D:61:TYR:HB2	2:D:66:LYS:HD3	1.89	0.53
2:D:110:GLY:O	2:D:113:ASP:HB2	2.09	0.53
2:E:17:SER:HB3	2:E:85:ASN:ND2	2.19	0.53
1:B:351:TYR:CZ	1:B:452:LEU:HD23	2.44	0.53
1:B:866:THR:HG1	1:B:869:MET:H	1.55	0.53
1:C:83:VAL:HG11	1:C:237:ARG:NH1	2.24	0.53
1:C:422:ASN:OD1	1:C:454:ARG:N	2.42	0.53
1:C:569:ILE:H	1:C:569:ILE:HD12	1.73	0.53
2:D:4:LEU:HD11	2:D:35:ILE:CD1	2.39	0.53
2:D:24:ALA:HB3	2:D:27:TYR:CE1	2.43	0.53
2:D:51:ALA:HB2	2:D:107:TRP:CH2	2.44	0.53
2:E:12:VAL:HG21	2:E:87:LEU:HD13	1.90	0.53
2:E:95:TYR:O	2:E:119:THR:N	2.42	0.53
1:C:402:ILE:O	1:C:508:TYR:N	2.32	0.53
1:C:970:PHE:CD1	1:C:999:GLY:HA3	2.44	0.53
2:E:55:PHE:CG	2:E:55:PHE:O	2.62	0.53
1:A:484:GLU:CD	2:D:102:GLY:HA3	2.34	0.52
1:B:205:SER:OG	1:B:206:LYS:N	2.41	0.52
1:C:611:LEU:HD12	1:C:612:TYR:N	2.24	0.52
2:E:8:GLY:HA3	2:E:20:LEU:CG	2.39	0.52
2:E:12:VAL:CG2	2:E:123:VAL:HG22	2.39	0.52
1:A:1002:GLN:O	1:A:1006:THR:OG1	2.27	0.52
1:B:23:GLN:OE1	1:B:23:GLN:N	2.43	0.52
1:B:111:ASP:HA	1:B:134:GLN:HA	1.92	0.52
1:B:569:ILE:HD12	1:B:569:ILE:N	2.24	0.52
1:C:213:VAL:HG13	1:C:214:ARG:N	2.25	0.52
1:C:327:VAL:HG22	1:C:542:ASN:HB3	1.90	0.52
2:E:33:LYS:N	2:E:54:ASP:HB3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.91	0.52
1:C:240:THR:O	1:C:241:LEU:HD23	2.09	0.52
1:A:692:ILE:HG22	1:A:693:ILE:N	2.24	0.52
1:B:587:ILE:HG22	1:B:588:THR:N	2.25	0.52
1:C:29:THR:HG23	1:C:62:VAL:HG23	1.91	0.52
2:D:61:TYR:HB2	2:D:66:LYS:HE2	1.92	0.52
1:B:121:ASN:ND2	1:B:177:MET:SD	2.82	0.52
1:B:452:LEU:HD12	2:E:55:PHE:HE2	1.75	0.52
2:E:34:CYS:HA	2:E:53:PHE:HA	1.90	0.52
2:E:51:ALA:O	2:E:71:ILE:HD11	2.09	0.52
1:A:81:ASN:HA	1:A:240:THR:HG22	1.90	0.52
1:A:111:ASP:O	1:A:112:SER:OG	2.27	0.52
1:A:1125:ASN:C	1:A:1125:ASN:OD1	2.52	0.52
2:D:69:PHE:HE1	2:D:95:TYR:HE2	1.55	0.52
2:E:88:LEU:HG	2:E:89:PRO:HD2	1.92	0.52
2:E:91:ASP:O	2:E:123:VAL:HG23	2.08	0.52
1:A:449:TYR:OH	2:D:73:GLY:O	2.27	0.52
1:A:712:ILE:HB	1:A:1077:THR:CG2	2.40	0.52
1:A:1090:PRO:HG3	1:A:1095:PHE:CE2	2.44	0.52
1:B:31:SER:OG	1:B:56:LEU:HD21	2.10	0.52
1:B:129:LYS:HE2	1:B:166:CYS:SG	2.50	0.52
1:B:193:VAL:HG23	1:B:223:LEU:CD1	2.40	0.52
1:B:1104:VAL:HG12	1:B:1105:THR:N	2.24	0.52
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.91	0.52
2:E:8:GLY:HA3	2:E:20:LEU:CD1	2.40	0.52
2:E:19:LYS:HD2	2:E:19:LYS:O	2.09	0.52
2:E:19:LYS:HG2	2:E:81:SER:HB2	1.92	0.52
1:B:133:PHE:HB3	1:B:160:TYR:HB2	1.92	0.52
1:B:615:VAL:HG12	1:B:616:ASN:N	2.25	0.52
1:C:85:PRO:HA	1:C:237:ARG:HA	1.92	0.52
1:C:287:ASP:OD2	1:C:288:ALA:N	2.43	0.52
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.28	0.52
1:A:551:VAL:HG22	1:A:552:LEU:N	2.25	0.52
1:B:367:VAL:HG23	1:B:368:LEU:H	1.75	0.52
1:C:739:THR:O	1:C:743:CYS:N	2.34	0.52
1:C:1022:ALA:O	1:C:1025:ALA:N	2.43	0.52
2:D:24:ALA:O	2:D:78:ASN:HB3	2.10	0.52
1:B:149:ASN:HD21	4:B:1302:NAG:C1	2.23	0.52
1:B:331:ASN:O	1:B:331:ASN:ND2	2.43	0.52
1:B:472:ILE:HG22	1:B:474:GLN:OE1	2.10	0.52
1:B:534:VAL:HG12	1:B:535:LYS:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:LEU:HD23	1:C:425:LEU:H	1.75	0.52
2:D:4:LEU:HD11	2:D:35:ILE:HD11	1.92	0.52
2:D:22:CYS:O	2:D:80:VAL:HG22	2.10	0.52
2:D:60:TYR:HB3	2:D:108:TYR:OH	2.10	0.52
2:E:23:ALA:HB1	2:E:78:ASN:O	2.10	0.52
2:E:39:ARG:HG3	2:E:95:TYR:CE1	2.45	0.52
1:A:561:PRO:O	1:A:577:ARG:NH2	2.41	0.51
1:B:229:LEU:HB2	1:B:231:ILE:HD11	1.92	0.51
1:B:367:VAL:HG23	1:B:368:LEU:N	2.26	0.51
1:C:213:VAL:HG13	1:C:214:ARG:H	1.75	0.51
2:E:12:VAL:HG23	2:E:123:VAL:HA	1.92	0.51
1:A:319:ARG:HD3	1:B:740:MET:HE3	1.92	0.51
1:C:1001:LEU:O	1:C:1004:LEU:N	2.40	0.51
2:E:95:TYR:N	2:E:119:THR:O	2.31	0.51
1:B:390:LEU:O	1:B:391:CYS:HB3	2.10	0.51
1:B:569:ILE:HG22	1:B:570:ALA:N	2.25	0.51
1:B:983:ARG:C	1:B:984:LEU:HD22	2.35	0.51
1:C:103:GLY:O	1:C:241:LEU:N	2.42	0.51
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.44	0.51
2:E:51:ALA:HB3	2:E:60:TYR:CB	2.33	0.51
1:B:763:LEU:HD13	1:B:1004:LEU:HD23	1.93	0.51
1:B:1074:ASN:OD1	4:B:1311:NAG:N2	2.43	0.51
2:E:27:TYR:HE1	2:E:78:ASN:OD1	1.93	0.51
2:E:74:ASP:OD1	2:E:76:ALA:N	2.43	0.51
1:C:205:SER:OG	1:C:206:LYS:N	2.43	0.51
2:D:37:TRP:CD1	2:D:95:TYR:HB3	2.46	0.51
2:D:61:TYR:HB2	2:D:66:LYS:CD	2.40	0.51
2:E:63:ASP:N	2:E:63:ASP:OD1	2.41	0.51
2:E:107:TRP:HE3	2:E:108:TYR:CD1	2.24	0.51
1:A:551:VAL:O	1:A:552:LEU:HD12	2.09	0.51
1:B:394:ASN:ND2	1:C:200:TYR:OH	2.43	0.51
1:B:1008:VAL:O	1:B:1012:LEU:N	2.40	0.51
1:B:1081:ILE:HG22	1:B:1082:CYS:N	2.26	0.51
1:C:100:ILE:HG21	1:C:263:ALA:CB	2.41	0.51
2:D:107:TRP:HA	2:D:113:ASP:OD2	2.11	0.51
2:E:41:ALA:HB3	2:E:44:GLN:N	2.26	0.51
1:B:1094:VAL:HG11	1:C:904:TYR:OH	2.11	0.51
1:C:603:ASN:OD1	4:C:1302:NAG:N2	2.44	0.51
2:D:61:TYR:HD2	2:D:66:LYS:HZ3	1.59	0.51
2:E:5:VAL:O	2:E:5:VAL:HG23	2.11	0.51
1:A:496:GLY:O	1:A:498:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:VAL:O	1:B:707:TYR:N	2.44	0.51
1:C:70:VAL:HG21	1:C:76:THR:OG1	2.11	0.51
1:C:296:LEU:HB2	1:C:608:VAL:HG21	1.91	0.51
2:D:96:TYR:CD1	2:D:118:GLY:HA3	2.45	0.51
2:E:53:PHE:HD1	2:E:56:ASP:CB	2.23	0.51
2:E:82:LEU:HG	2:E:84:MET:CE	2.40	0.51
3:J:1:NAG:O4	3:J:2:NAG:O7	2.29	0.51
1:A:352:ALA:O	1:A:466:ARG:NH1	2.43	0.51
1:A:540:ASN:OD1	1:A:541:PHE:N	2.44	0.51
1:A:712:ILE:HB	1:A:1077:THR:HG21	1.92	0.51
1:B:119:ILE:HG23	1:B:128:ILE:HG12	1.92	0.51
1:B:316:SER:OG	1:B:317:ASN:N	2.43	0.51
1:B:440:ASN:N	1:B:440:ASN:OD1	2.43	0.51
1:C:94:SER:HB2	1:C:190:ARG:HB2	1.93	0.51
1:C:253:ASP:N	1:C:256:SER:OG	2.40	0.51
1:C:315:THR:OG1	1:C:316:SER:N	2.44	0.51
1:C:534:VAL:HG22	1:C:535:LYS:N	2.25	0.51
1:C:1016:ALA:O	1:C:1019:ARG:N	2.44	0.51
2:D:109:ARG:HB3	2:D:109:ARG:CZ	2.40	0.51
2:E:65:VAL:HG13	2:E:82:LEU:HD11	1.93	0.51
1:B:117:LEU:HD23	1:B:118:LEU:N	2.27	0.51
2:E:50:ALA:CB	2:E:61:TYR:HA	2.41	0.51
1:A:130:VAL:HG21	1:A:231:ILE:HG22	1.93	0.50
1:A:577:ARG:HA	1:A:584:ILE:HA	1.94	0.50
1:C:332:ILE:HG23	1:C:333:THR:N	2.25	0.50
1:A:366:SER:OG	1:A:388:ASN:OD1	2.26	0.50
1:A:963:VAL:HG11	1:C:570:ALA:HB2	1.93	0.50
1:B:520:ALA:HB3	1:B:521:PRO:HD3	1.93	0.50
1:B:749:CYS:O	1:B:752:LEU:N	2.33	0.50
1:C:54:LEU:HD23	1:C:271:GLN:C	2.35	0.50
2:D:62:SER:O	2:D:66:LYS:HB2	2.10	0.50
2:E:63:ASP:HA	2:E:66:LYS:CE	2.41	0.50
1:A:755:GLN:NE2	1:C:969:ASN:HB2	2.26	0.50
1:B:748:GLU:OE2	1:B:748:GLU:N	2.32	0.50
1:C:187:LYS:NZ	1:C:210:ILE:O	2.43	0.50
1:A:35:GLY:HA3	1:A:56:LEU:HB3	1.94	0.50
1:A:290:ASP:OD2	1:A:293:LEU:N	2.44	0.50
1:A:542:ASN:OD1	1:A:545:GLY:N	2.44	0.50
1:B:22:THR:HG23	1:B:76:THR:HA	1.92	0.50
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.94	0.50
1:B:983:ARG:O	1:B:984:LEU:HD22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1049:LEU:HD12	1:B:1065:VAL:HG12	1.93	0.50
1:C:171:VAL:HG12	1:C:172:SER:N	2.26	0.50
1:A:70:VAL:CG1	1:A:76:THR:HG21	2.35	0.50
2:D:74:ASP:HB3	2:D:77:LYS:HG2	1.93	0.50
1:A:489:TYR:HB3	2:D:30:TRP:O	2.12	0.50
1:C:124:THR:O	1:C:175:PHE:N	2.42	0.50
1:C:144:TYR:O	1:C:153:MET:N	2.45	0.50
1:C:273:ARG:HE	1:C:292:ALA:HB3	1.75	0.50
2:E:41:ALA:HB3	2:E:44:GLN:CA	2.41	0.50
1:A:253:ASP:O	1:A:254:SER:C	2.55	0.50
1:A:327:VAL:C	1:A:531:THR:HG1	2.16	0.50
1:B:154:GLU:OE2	1:B:156:GLU:N	2.45	0.50
2:E:2:VAL:HG11	2:E:99:VAL:HG11	1.92	0.50
2:E:35:ILE:HG23	2:E:52:ILE:CG2	2.42	0.50
1:A:613:GLN:NE2	1:B:859:THR:HG21	2.27	0.50
1:B:94:SER:O	1:B:189:LEU:HA	2.12	0.50
1:B:725:GLU:OE2	1:B:1064:HIS:NE2	2.42	0.50
1:C:382:VAL:CG2	1:C:387:LEU:HD21	2.42	0.50
1:A:44:ARG:NH2	1:A:49:HIS:ND1	2.60	0.50
1:B:912:THR:HG23	1:B:1106:GLN:OE1	2.12	0.50
1:C:906:PHE:CD1	1:C:1049:LEU:HD22	2.47	0.50
2:E:34:CYS:SG	2:E:53:PHE:HD2	2.34	0.50
2:E:41:ALA:CB	2:E:44:GLN:HB3	2.39	0.50
2:E:83:GLN:HB3	2:E:85:ASN:OD1	2.12	0.50
1:A:452:LEU:HA	2:D:55:PHE:CE2	2.47	0.49
1:A:578:ASP:OD1	1:A:582:LEU:N	2.45	0.49
1:A:1087:ALA:HB2	1:A:1125:ASN:O	2.11	0.49
2:E:18:LEU:CD1	2:E:19:LYS:H	2.24	0.49
1:A:596:SER:HB2	1:A:611:LEU:HD23	1.94	0.49
1:B:393:THR:HA	1:B:523:THR:H	1.77	0.49
1:B:878:LEU:O	1:B:882:ILE:HG23	2.12	0.49
1:C:380:TYR:N	1:C:431:GLY:O	2.43	0.49
1:C:692:ILE:HG22	1:C:693:ILE:N	2.27	0.49
2:E:13:GLN:HE22	2:E:15:GLY:C	2.21	0.49
2:E:99:VAL:CB	2:E:114:TYR:HB2	2.18	0.49
1:A:402:ILE:HD12	1:A:406:GLU:HB2	1.94	0.49
1:C:877:LEU:HD13	1:C:1029:MET:SD	2.52	0.49
2:E:45:GLU:OE2	2:E:46:ARG:HG3	2.11	0.49
2:E:94:VAL:HG23	2:E:119:THR:C	2.36	0.49
2:E:100:ALA:CB	2:E:107:TRP:HB2	2.42	0.49
1:A:18:LEU:HD22	1:A:258:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PHE:CE2	1:A:552:LEU:HD21	2.46	0.49
1:C:118:LEU:O	1:C:118:LEU:HD12	2.13	0.49
2:D:19:LYS:C	2:D:19:LYS:HD3	2.36	0.49
2:E:35:ILE:N	2:E:52:ILE:O	2.44	0.49
1:A:131:CYS:HA	1:A:166:CYS:CB	2.42	0.49
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.92	0.49
1:C:58:PHE:HB3	1:C:59:PHE:HD1	1.78	0.49
1:C:294:ASP:O	1:C:297:SER:N	2.43	0.49
1:C:299:THR:HG21	1:C:597:VAL:HG11	1.93	0.49
2:D:29:SER:O	2:D:31:ALA:HA	2.12	0.49
2:D:46:ARG:NH2	2:D:110:GLY:HA3	2.28	0.49
2:D:51:ALA:HB2	2:D:107:TRP:CE2	2.48	0.49
2:E:38:PHE:HD1	2:E:98:THR:CG2	2.15	0.49
2:E:72:SER:OG	2:E:83:GLN:OE1	2.29	0.49
2:E:74:ASP:OD1	2:E:76:ALA:HB3	2.11	0.49
1:A:213:VAL:HG13	1:A:214:ARG:N	2.28	0.49
1:A:334:ASN:O	1:A:362:VAL:HG12	2.13	0.49
1:A:914:ASN:ND2	1:A:1111:GLU:OE1	2.46	0.49
1:B:213:VAL:HG13	1:B:214:ARG:N	2.28	0.49
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.46	0.49
1:C:341:VAL:HG13	1:C:356:LYS:HE3	1.93	0.49
1:C:517:LEU:HD23	1:C:517:LEU:C	2.37	0.49
2:D:2:VAL:HB	2:D:114:TYR:CG	2.47	0.49
2:E:5:VAL:HG21	2:E:23:ALA:HB3	1.92	0.49
1:A:56:LEU:HD22	1:A:91:TYR:CD2	2.47	0.49
1:A:382:VAL:CG2	1:A:387:LEU:HD21	2.43	0.49
1:B:120:VAL:N	1:B:127:VAL:O	2.24	0.49
1:B:142:GLY:HA2	1:B:244:LEU:H	1.78	0.49
1:B:402:ILE:HG12	1:B:510:VAL:HG21	1.95	0.49
2:D:18:LEU:HD22	2:D:84:MET:SD	2.53	0.49
2:D:40:GLN:OE1	2:D:96:TYR:CD2	2.66	0.49
2:E:14:ALA:HB1	2:E:89:PRO:CD	2.39	0.49
1:B:227:VAL:HG22	1:B:229:LEU:HG	1.95	0.49
2:E:22:CYS:HB3	2:E:80:VAL:HG12	1.94	0.49
2:E:40:GLN:CB	2:E:46:ARG:HG2	2.37	0.49
2:E:88:LEU:C	2:E:123:VAL:HG11	2.38	0.49
2:E:97:CYS:HB2	2:E:116:GLY:HA3	1.94	0.49
1:A:537:LYS:N	1:A:551:VAL:HG23	2.27	0.49
1:A:539:VAL:HG12	1:A:540:ASN:O	2.13	0.49
1:A:569:ILE:HD12	1:A:569:ILE:H	1.77	0.49
1:B:563:GLN:O	1:B:577:ARG:NE	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:GLN:C	2:E:4:LEU:HD12	2.38	0.49
2:E:62:SER:O	2:E:66:LYS:N	2.37	0.49
2:E:109:ARG:HH11	2:E:109:ARG:HG3	1.77	0.49
1:A:121:ASN:HA	1:A:126:VAL:HA	1.94	0.49
1:A:171:VAL:HG12	1:A:172:SER:O	2.12	0.49
1:A:402:ILE:O	1:A:507:PRO:HA	2.12	0.49
1:A:555:SER:OG	1:A:584:ILE:HG22	2.13	0.49
1:B:259:THR:HG22	1:B:260:ALA:N	2.28	0.49
1:B:411:ALA:HB3	1:B:414:GLN:HB2	1.95	0.49
1:B:515:PHE:O	1:B:517:LEU:N	2.40	0.49
1:B:736:VAL:HG12	1:B:737:ASP:N	2.27	0.49
1:C:332:ILE:HD11	1:C:362:VAL:CG1	2.43	0.49
2:D:61:TYR:OH	2:D:71:ILE:HG22	2.13	0.49
1:A:118:LEU:HD12	1:A:119:ILE:N	2.28	0.48
1:B:83:VAL:HG23	1:B:83:VAL:O	2.13	0.48
1:B:92:PHE:CE1	1:B:265:TYR:HB2	2.48	0.48
1:C:540:ASN:CA	1:C:549:THR:HG22	2.43	0.48
1:C:569:ILE:O	1:C:570:ALA:HB3	2.12	0.48
2:D:8:GLY:O	2:D:18:LEU:HD21	2.13	0.48
2:E:71:ILE:HA	2:E:81:SER:O	2.12	0.48
1:B:143:VAL:HG13	1:B:153:MET:O	2.13	0.48
1:B:961:THR:O	1:B:961:THR:HG22	2.13	0.48
1:B:1130:ILE:HD12	1:C:920:GLN:OE1	2.13	0.48
1:C:297:SER:HA	1:C:300:LYS:HB2	1.94	0.48
1:C:763:LEU:HD13	1:C:1004:LEU:HD23	1.95	0.48
2:D:18:LEU:HD23	2:D:18:LEU:C	2.38	0.48
2:D:40:GLN:OE1	2:D:96:TYR:HD2	1.97	0.48
2:D:65:VAL:HG13	2:D:69:PHE:CG	2.48	0.48
1:A:34:ARG:O	1:A:56:LEU:HD23	2.13	0.48
1:A:538:CYS:C	1:A:539:VAL:HG23	2.38	0.48
1:A:1091:ARG:NE	1:A:1118:ASP:O	2.42	0.48
1:B:244:LEU:HD13	1:B:258:TRP:HB2	1.95	0.48
1:C:404:GLY:O	1:C:408:ARG:NH1	2.46	0.48
1:C:606:ASN:O	1:C:608:VAL:HG23	2.13	0.48
1:C:898:PHE:HA	1:C:901:GLN:HB3	1.94	0.48
2:D:52:ILE:HG23	2:D:71:ILE:HG23	1.94	0.48
1:A:555:SER:HB3	1:A:586:ASP:N	2.28	0.48
1:A:986:PRO:N	1:A:987:PRO:HD2	2.27	0.48
2:E:40:GLN:HA	2:E:45:GLU:O	2.13	0.48
2:E:68:ARG:HG3	2:E:69:PHE:CZ	2.49	0.48
1:A:491:PRO:C	2:D:31:ALA:HB2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TYR:HA	1:B:229:LEU:O	2.13	0.48
1:B:227:VAL:CG2	1:B:229:LEU:HD21	2.42	0.48
1:B:976:VAL:HG13	1:B:976:VAL:O	2.13	0.48
2:D:55:PHE:H	2:D:75:ASN:HD21	1.60	0.48
2:D:94:VAL:HG13	2:D:94:VAL:O	2.13	0.48
1:A:452:LEU:HD13	2:D:55:PHE:HE2	1.74	0.48
1:A:607:GLN:C	1:A:608:VAL:HG23	2.39	0.48
1:B:406:GLU:O	1:B:409:GLN:HB2	2.13	0.48
1:C:427:ASP:OD2	1:C:428:ASP:N	2.47	0.48
1:C:1043:CYS:C	1:C:1064:HIS:CD2	2.91	0.48
1:B:29:THR:O	1:B:62:VAL:N	2.35	0.48
1:B:93:ALA:HA	1:B:190:ARG:O	2.13	0.48
1:B:120:VAL:CG1	1:B:121:ASN:N	2.76	0.48
1:B:399:SER:HA	1:B:511:VAL:HA	1.96	0.48
1:B:576:VAL:HG22	1:B:577:ARG:N	2.28	0.48
1:A:338:PHE:O	1:A:342:PHE:N	2.44	0.48
1:A:864:LEU:HD13	1:C:665:PRO:HB2	1.95	0.48
1:A:1116:THR:HG22	1:A:1117:THR:N	2.29	0.48
1:B:81:ASN:N	1:B:82:PRO:HD3	2.29	0.48
1:B:713:ALA:HB2	1:C:895:GLN:CD	2.38	0.48
1:C:242:LEU:HD23	1:C:242:LEU:H	1.79	0.48
2:D:23:ALA:HB2	2:D:79:THR:OG1	2.14	0.48
1:A:880:GLY:O	1:A:884:SER:N	2.46	0.48
1:C:605:SER:OG	1:C:606:ASN:N	2.47	0.48
1:A:94:SER:OG	1:A:190:ARG:HB2	2.14	0.48
1:A:489:TYR:CB	2:D:30:TRP:HD1	2.27	0.48
1:A:977:LEU:HD11	1:A:993:ILE:CD1	2.44	0.48
1:B:39:PRO:CG	1:B:51:THR:HG21	2.42	0.48
1:B:362:VAL:HA	1:B:525:CYS:O	2.14	0.48
1:C:880:GLY:O	1:C:885:GLY:N	2.45	0.48
2:D:69:PHE:HA	2:D:83:GLN:O	2.13	0.48
1:A:566:GLY:HA2	1:B:43:PHE:H	1.79	0.47
1:A:1019:ARG:O	1:A:1022:ALA:N	2.38	0.47
1:B:64:TRP:HH2	1:B:214:ARG:HB2	1.79	0.47
1:B:205:SER:N	1:B:224:GLU:O	2.42	0.47
2:D:61:TYR:HB2	2:D:66:LYS:NZ	2.29	0.47
2:E:55:PHE:HB2	2:E:75:ASN:OD1	2.14	0.47
2:E:65:VAL:HG11	2:E:82:LEU:HD21	1.96	0.47
2:E:88:LEU:N	2:E:91:ASP:OD2	2.47	0.47
1:A:246:ARG:NE	1:A:257:GLY:O	2.47	0.47
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:802:PHE:O	1:B:803:SER:C	2.57	0.47
1:C:244:LEU:C	1:C:244:LEU:HD12	2.39	0.47
2:E:53:PHE:O	2:E:56:ASP:N	2.47	0.47
1:A:34:ARG:NH2	1:A:217:PRO:HG2	2.30	0.47
1:A:49:HIS:C	1:A:276:LEU:HD12	2.38	0.47
1:A:755:GLN:HE22	1:C:971:GLY:H	1.61	0.47
1:A:988:GLU:HA	1:A:991:VAL:HG12	1.96	0.47
1:B:584:ILE:HG22	1:B:585:LEU:H	1.77	0.47
1:C:99:ASN:O	1:C:102:ARG:CZ	2.61	0.47
2:D:33:LYS:HD3	2:D:101:PHE:CA	2.41	0.47
1:A:99:ASN:O	1:A:102:ARG:CZ	2.62	0.47
1:A:103:GLY:C	1:A:104:TRP:CE3	2.92	0.47
1:A:402:ILE:HD11	1:A:407:VAL:CG1	2.43	0.47
1:A:454:ARG:HA	1:A:492:LEU:HB3	1.96	0.47
1:B:156:GLU:HG3	1:B:158:ARG:HG2	1.96	0.47
1:B:245:HIS:HB2	1:B:259:THR:HB	1.97	0.47
1:B:452:LEU:HD11	1:B:492:LEU:HB3	1.95	0.47
1:B:869:MET:O	1:B:872:GLN:N	2.41	0.47
1:B:882:ILE:HB	1:B:898:PHE:CZ	2.49	0.47
1:B:1137:VAL:HG12	1:B:1138:TYR:N	2.30	0.47
1:C:301:CYS:O	1:C:304:LYS:N	2.44	0.47
1:C:766:ALA:HB1	1:C:1012:LEU:HD21	1.96	0.47
1:C:1012:LEU:O	1:C:1015:ALA:HB3	2.14	0.47
2:E:84:MET:HA	2:E:84:MET:CE	2.40	0.47
1:A:569:ILE:HG22	1:A:570:ALA:N	2.30	0.47
1:A:873:TYR:CE1	1:C:699:LEU:HD22	2.49	0.47
1:B:112:SER:N	1:B:133:PHE:O	2.48	0.47
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.97	0.47
1:C:554:GLU:HA	1:C:585:LEU:HD23	1.96	0.47
1:C:691:SER:OG	1:C:692:ILE:N	2.36	0.47
2:D:33:LYS:HD3	2:D:102:GLY:N	2.30	0.47
2:E:32:ARG:HB2	2:E:54:ASP:O	2.14	0.47
1:A:120:VAL:O	1:A:127:VAL:N	2.47	0.47
1:A:205:SER:OG	1:A:206:LYS:N	2.48	0.47
1:A:316:SER:OG	1:A:317:ASN:N	2.39	0.47
1:C:444:LYS:HD3	1:C:445:VAL:N	2.30	0.47
2:E:90:LYS:HA	2:E:90:LYS:CE	2.36	0.47
2:E:103:THR:HB	2:E:106:ASN:HD22	1.79	0.47
1:A:195:LYS:HB2	1:A:202:LYS:HB2	1.96	0.47
1:A:346:ARG:NE	1:A:347:PHE:O	2.48	0.47
1:A:449:TYR:O	1:A:494:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:THR:HG22	1:A:720:ILE:N	2.29	0.47
1:A:774:GLN:O	1:A:777:ASN:N	2.47	0.47
1:A:1080:ALA:O	1:A:1081:ILE:HD13	2.15	0.47
1:A:1097:SER:HB3	1:A:1102:TRP:CD2	2.50	0.47
1:B:43:PHE:CD1	1:B:44:ARG:N	2.82	0.47
1:B:115:GLN:NE2	1:B:167:THR:OG1	2.48	0.47
1:B:118:LEU:HD21	1:B:120:VAL:CB	2.43	0.47
1:B:314:GLN:NE2	1:B:316:SER:O	2.48	0.47
1:B:356:LYS:N	1:B:397:ALA:O	2.46	0.47
1:B:1046:GLY:HA2	1:C:890:ALA:HB1	1.96	0.47
1:C:29:THR:OG1	1:C:30:ASN:N	2.46	0.47
1:C:34:ARG:O	1:C:56:LEU:HD23	2.14	0.47
1:C:54:LEU:HD23	1:C:272:PRO:N	2.30	0.47
1:C:379:CYS:HA	1:C:432:CYS:HA	1.96	0.47
1:C:539:VAL:HG12	1:C:540:ASN:N	2.29	0.47
1:C:643:PHE:CE1	1:C:655:HIS:ND1	2.83	0.47
1:C:772:VAL:HG23	1:C:773:GLU:N	2.28	0.47
2:D:34:CYS:CB	2:D:100:ALA:CB	2.90	0.47
2:D:34:CYS:HB3	2:D:100:ALA:CB	2.45	0.47
2:E:2:VAL:HG12	2:E:99:VAL:HG21	1.96	0.47
1:A:330:PRO:HA	1:A:579:PRO:HB2	1.95	0.47
1:B:120:VAL:HG12	1:B:121:ASN:N	2.29	0.47
1:C:156:GLU:OE2	1:C:246:ARG:NH1	2.40	0.47
1:C:555:SER:HB3	1:C:586:ASP:HB2	1.97	0.47
1:C:902:MET:HE1	1:C:1050:MET:SD	2.53	0.47
1:C:911:VAL:HG12	1:C:912:THR:N	2.29	0.47
2:D:61:TYR:OH	2:D:70:THR:HA	2.14	0.47
2:D:61:TYR:HB2	2:D:66:LYS:HZ3	1.79	0.47
1:A:149:ASN:O	1:A:151:SER:OG	2.20	0.47
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.79	0.47
1:B:62:VAL:HG21	1:B:216:LEU:HD22	1.97	0.47
1:B:124:THR:OG1	4:B:1301:NAG:N2	2.43	0.47
1:B:367:VAL:O	1:B:371:SER:N	2.44	0.47
1:C:1056:ALA:HB1	1:C:1057:PRO:CD	2.45	0.47
2:D:52:ILE:HG23	2:D:71:ILE:CG2	2.45	0.47
2:E:68:ARG:HE	2:E:88:LEU:H	1.61	0.47
1:A:18:LEU:HD23	1:A:255:SER:HA	1.97	0.47
1:B:84:LEU:O	1:B:238:PHE:N	2.37	0.47
1:B:186:PHE:HB3	1:B:210:ILE:HD11	1.96	0.47
1:B:327:VAL:HG22	1:B:542:ASN:HB3	1.97	0.47
1:B:570:ALA:HB2	1:C:963:VAL:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ILE:O	1:B:901:GLN:NE2	2.48	0.47
1:B:1027:THR:O	1:B:1031:GLU:N	2.47	0.47
4:B:1304:NAG:H3	4:B:1304:NAG:C8	2.41	0.47
2:D:119:THR:HG23	2:D:119:THR:O	2.13	0.47
2:E:30:TRP:CD1	2:E:30:TRP:O	2.68	0.47
2:E:50:ALA:HB3	2:E:71:ILE:HD13	1.96	0.47
2:E:105:ASP:OD2	2:E:109:ARG:NH2	2.39	0.47
1:A:38:TYR:CD1	1:A:285:ILE:HD12	2.50	0.46
1:A:136:CYS:C	1:A:139:PRO:HD3	2.40	0.46
1:A:442:ASP:OD1	1:A:509:ARG:NH2	2.48	0.46
1:B:491:PRO:C	1:B:492:LEU:HD12	2.39	0.46
1:B:898:PHE:C	1:B:900:MET:N	2.73	0.46
1:B:1133:VAL:HG12	1:B:1134:ASN:N	2.29	0.46
1:C:800:PHE:HB2	1:C:802:PHE:CE2	2.50	0.46
1:C:1098:ASN:CG	1:C:1099:GLY:H	2.23	0.46
2:E:82:LEU:HG	2:E:84:MET:HE3	1.96	0.46
2:E:100:ALA:HB2	2:E:107:TRP:HB2	1.97	0.46
1:A:118:LEU:HD12	1:A:119:ILE:CA	2.45	0.46
1:A:905:ARG:HD3	1:A:1049:LEU:O	2.16	0.46
1:A:1109:PHE:CD2	1:A:1110:TYR:N	2.83	0.46
1:B:449:TYR:HA	1:B:494:SER:HG	1.79	0.46
1:B:914:ASN:OD1	1:B:915:VAL:N	2.49	0.46
1:B:1128:VAL:HG23	1:B:1129:VAL:N	2.29	0.46
1:C:946:GLY:O	1:C:947:LYS:C	2.58	0.46
1:C:1056:ALA:HB3	1:C:1059:GLY:C	2.41	0.46
2:E:68:ARG:CZ	2:E:88:LEU:HB2	2.45	0.46
1:A:133:PHE:CE2	1:A:163:ALA:HB2	2.50	0.46
1:A:452:LEU:HD22	2:D:55:PHE:HE2	1.81	0.46
1:B:312:ILE:C	1:B:313:TYR:CD2	2.94	0.46
1:B:576:VAL:HG22	1:B:577:ARG:H	1.79	0.46
1:C:103:GLY:C	1:C:241:LEU:HB2	2.40	0.46
1:C:692:ILE:CG2	1:C:693:ILE:N	2.77	0.46
2:E:119:THR:O	2:E:121:VAL:HG23	2.15	0.46
1:A:106:PHE:CD1	1:A:238:PHE:CB	2.97	0.46
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.97	0.46
1:A:991:VAL:HG13	1:A:992:GLN:N	2.30	0.46
1:B:435:ALA:HB2	1:B:510:VAL:HG13	1.97	0.46
1:B:615:VAL:CG1	1:B:616:ASN:N	2.78	0.46
1:B:692:ILE:CG2	1:B:693:ILE:N	2.78	0.46
1:B:1104:VAL:CG1	1:B:1105:THR:N	2.77	0.46
1:C:134:GLN:HB3	1:C:162:SER:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PHE:HB3	1:A:277:LEU:HD11	1.97	0.46
1:A:1110:TYR:CD1	1:A:1112:PRO:HD3	2.51	0.46
1:B:19:THR:O	1:B:20:THR:HB	2.16	0.46
1:B:140:PHE:O	1:B:158:ARG:O	2.33	0.46
1:B:483:VAL:O	1:B:483:VAL:HG23	2.16	0.46
1:C:269:TYR:O	1:C:271:GLN:NE2	2.47	0.46
1:C:733:LYS:NZ	1:C:862:PRO:O	2.45	0.46
1:C:781:VAL:HG22	1:C:1026:ALA:CB	2.44	0.46
2:E:53:PHE:CD1	2:E:56:ASP:HB2	2.48	0.46
2:E:68:ARG:HG3	2:E:69:PHE:CE1	2.51	0.46
1:A:412:PRO:HA	1:A:425:LEU:HD11	1.97	0.46
1:A:551:VAL:N	1:A:588:THR:O	2.46	0.46
1:A:728:PRO:HD2	1:A:1021:SER:OG	2.15	0.46
4:B:1302:NAG:HO3	4:B:1302:NAG:C7	2.19	0.46
1:C:100:ILE:HG21	1:C:263:ALA:HB2	1.97	0.46
1:C:175:PHE:C	1:C:176:LEU:HD22	2.41	0.46
1:C:206:LYS:HG3	1:C:208:THR:HG23	1.98	0.46
1:C:931:ILE:O	1:C:934:ILE:N	2.37	0.46
1:A:20:THR:O	1:A:20:THR:CG2	2.61	0.46
1:A:612:TYR:O	1:A:649:CYS:N	2.39	0.46
1:A:817:PHE:HE1	1:A:821:LEU:HD11	1.81	0.46
1:A:912:THR:OG1	1:A:1106:GLN:NE2	2.49	0.46
1:A:986:PRO:O	1:A:990:GLU:N	2.49	0.46
1:B:132:GLU:OE1	1:B:165:ASN:N	2.46	0.46
1:B:203:ILE:HB	1:B:227:VAL:HG12	1.98	0.46
1:B:559:PHE:C	1:B:560:LEU:HD12	2.41	0.46
1:C:18:LEU:HD23	1:C:255:SER:HA	1.98	0.46
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.51	0.46
2:D:55:PHE:CD2	2:D:55:PHE:CB	2.80	0.46
1:C:1128:VAL:HG13	1:C:1129:VAL:N	2.29	0.46
2:D:53:PHE:HD1	2:D:56:ASP:OD1	1.99	0.46
2:E:33:LYS:CD	2:E:102:GLY:HA2	2.46	0.46
1:A:719:THR:O	1:A:720:ILE:HD13	2.15	0.46
1:B:101:ILE:HA	1:B:242:LEU:HA	1.98	0.46
2:E:80:VAL:HG22	2:E:81:SER:N	2.30	0.46
1:A:31:SER:C	1:A:32:PHE:CD2	2.94	0.46
1:A:751:ASN:HA	1:A:754:LEU:HD21	1.96	0.46
1:A:1029:MET:SD	1:A:1033:VAL:HG21	2.56	0.46
1:B:210:ILE:HD12	1:B:212:LEU:HG	1.98	0.46
1:B:245:HIS:HB2	1:B:259:THR:CB	2.46	0.46
1:B:426:PRO:HG2	1:B:429:PHE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:CG	1:C:44:ARG:N	2.84	0.46
1:C:131:CYS:HA	1:C:166:CYS:CB	2.45	0.46
1:C:542:ASN:CG	1:C:547:THR:HG22	2.40	0.46
1:C:802:PHE:O	1:C:803:SER:C	2.59	0.46
2:E:8:GLY:O	2:E:20:LEU:HD11	2.15	0.46
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.98	0.45
1:A:322:PRO:HA	1:A:538:CYS:O	2.16	0.45
1:A:328:ARG:O	1:A:579:PRO:HG2	2.16	0.45
1:B:110:LEU:HD12	1:B:110:LEU:N	2.31	0.45
1:B:227:VAL:CG2	1:B:229:LEU:CD2	2.95	0.45
1:B:375:SER:OG	1:B:376:THR:N	2.48	0.45
1:B:390:LEU:HD11	1:C:983:ARG:HG2	1.98	0.45
1:B:435:ALA:HB1	1:B:510:VAL:HG22	1.99	0.45
1:B:1107:ARG:NH1	1:C:904:TYR:CD1	2.84	0.45
1:C:189:LEU:HD11	1:C:191:GLU:OE1	2.16	0.45
1:C:822:LEU:HD23	1:C:945:LEU:HD21	1.98	0.45
2:D:52:ILE:HG13	2:D:52:ILE:O	2.15	0.45
2:E:35:ILE:HG23	2:E:52:ILE:HG22	1.96	0.45
1:A:138:ASP:N	1:A:139:PRO:HD3	2.31	0.45
1:A:457:ARG:NH2	1:A:467:ASP:OD1	2.49	0.45
1:A:570:ALA:HB1	1:B:963:VAL:CG1	2.39	0.45
1:A:800:PHE:N	1:A:800:PHE:CD1	2.83	0.45
1:B:178:ASP:N	1:B:178:ASP:OD2	2.49	0.45
1:B:204:TYR:HA	1:B:224:GLU:O	2.17	0.45
1:B:667:GLY:O	1:B:669:GLY:N	2.49	0.45
1:B:976:VAL:HG13	1:B:979:ASP:HB3	1.98	0.45
2:D:69:PHE:CZ	2:D:84:MET:HA	2.51	0.45
1:A:85:PRO:HA	1:A:237:ARG:HA	1.98	0.45
1:A:101:ILE:HA	1:A:242:LEU:CB	2.46	0.45
1:A:129:LYS:HE3	1:A:169:GLU:HG2	1.99	0.45
1:A:185:ASN:ND2	1:A:212:LEU:O	2.44	0.45
1:A:204:TYR:HA	1:A:225:PRO:HA	1.98	0.45
1:A:324:GLU:O	1:A:326:ILE:HG23	2.16	0.45
1:B:321:GLN:NE2	1:B:322:PRO:O	2.49	0.45
1:B:435:ALA:HA	1:B:510:VAL:HA	1.98	0.45
1:B:705:VAL:HB	1:C:883:THR:HG21	1.98	0.45
1:B:882:ILE:O	1:B:898:PHE:CZ	2.69	0.45
1:C:382:VAL:HG21	1:C:387:LEU:HD21	1.98	0.45
2:E:109:ARG:HG3	2:E:109:ARG:NH1	2.31	0.45
1:A:1076:THR:HG22	1:A:1077:THR:N	2.31	0.45
1:B:54:LEU:HD23	1:B:272:PRO:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:PHE:CG	1:B:430:THR:N	2.85	0.45
1:B:453:TYR:CD1	1:B:493:GLN:O	2.70	0.45
1:B:472:ILE:HG23	1:B:489:TYR:C	2.41	0.45
1:B:921:LYS:O	1:B:924:ALA:N	2.50	0.45
1:B:995:ARG:NH2	1:C:994:ASP:OD1	2.50	0.45
1:C:77:LYS:O	1:C:78:ARG:C	2.60	0.45
1:C:557:LYS:HB2	1:C:584:ILE:HG21	1.99	0.45
1:C:762:GLN:O	1:C:765:ARG:N	2.45	0.45
2:D:68:ARG:NH2	2:D:69:PHE:HE2	2.14	0.45
2:D:99:VAL:O	2:D:113:ASP:HA	2.16	0.45
2:E:4:LEU:HD11	2:E:99:VAL:HG23	1.98	0.45
1:A:19:THR:O	1:A:258:TRP:CZ2	2.69	0.45
1:A:159:VAL:CG2	1:A:160:TYR:HD1	2.30	0.45
1:B:21:ARG:O	1:B:23:GLN:NE2	2.50	0.45
1:C:42:VAL:HG12	1:C:43:PHE:N	2.31	0.45
2:D:106:ASN:OD1	2:D:107:TRP:N	2.50	0.45
1:A:489:TYR:HD1	2:D:33:LYS:HZ1	1.65	0.45
1:B:132:GLU:O	1:B:163:ALA:HA	2.16	0.45
1:B:193:VAL:O	1:B:203:ILE:HA	2.17	0.45
1:B:811:LYS:HG3	1:B:811:LYS:O	2.16	0.45
1:B:1013:ILE:O	1:B:1016:ALA:N	2.35	0.45
2:D:100:ALA:HA	2:D:113:ASP:OD1	2.16	0.45
1:A:110:LEU:O	1:A:135:PHE:HB2	2.16	0.45
1:A:869:MET:HE1	1:C:669:GLY:HA2	1.98	0.45
1:B:195:LYS:HB2	1:B:202:LYS:HB2	1.99	0.45
1:B:797:PHE:CD1	1:B:898:PHE:CE2	3.05	0.45
1:B:986:PRO:O	1:B:988:GLU:N	2.49	0.45
1:B:1097:SER:HB3	1:B:1102:TRP:CE2	2.51	0.45
1:C:294:ASP:O	1:C:296:LEU:N	2.49	0.45
1:C:551:VAL:O	1:C:551:VAL:HG13	2.17	0.45
1:C:802:PHE:O	1:C:804:GLN:N	2.50	0.45
2:D:2:VAL:CG1	2:D:99:VAL:HG21	2.46	0.45
2:E:8:GLY:CA	2:E:20:LEU:HG	2.46	0.45
2:E:88:LEU:HD12	2:E:89:PRO:CD	2.42	0.45
1:A:90:VAL:HG22	1:A:269:TYR:HA	1.99	0.45
1:A:379:CYS:HA	1:A:432:CYS:HA	1.98	0.45
1:A:485:GLY:O	2:D:101:PHE:HZ	1.99	0.45
1:A:995:ARG:O	1:A:996:LEU:C	2.58	0.45
1:B:156:GLU:CG	1:B:158:ARG:HG2	2.47	0.45
1:B:1089:PHE:N	1:B:1121:PHE:O	2.43	0.45
1:C:64:TRP:CD1	1:C:65:PHE:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1078:ALA:HB3	1:C:1102:TRP:CH2	2.52	0.45
2:D:33:LYS:HG2	2:D:102:GLY:CA	2.46	0.45
2:D:76:ALA:HB3	2:D:77:LYS:HZ2	1.81	0.45
2:E:44:GLN:CD	2:E:45:GLU:H	2.24	0.45
1:A:31:SER:O	1:A:59:PHE:HA	2.16	0.45
1:B:379:CYS:HB2	1:B:384:PRO:HD3	1.99	0.45
1:B:393:THR:HB	1:B:518:LEU:CD1	2.46	0.45
1:B:416:GLY:O	1:B:417:LYS:C	2.60	0.45
1:B:568:ASP:OD2	1:B:572:THR:HG23	2.16	0.45
1:B:654:GLU:O	1:B:694:ALA:N	2.48	0.45
1:B:660:TYR:O	1:B:698:SER:OG	2.29	0.45
1:B:898:PHE:O	1:B:900:MET:N	2.50	0.45
1:B:931:ILE:O	1:B:934:ILE:N	2.35	0.45
1:C:128:ILE:O	1:C:170:TYR:N	2.48	0.45
1:C:327:VAL:HG13	1:C:542:ASN:HB3	1.98	0.45
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.31	0.45
1:B:157:PHE:CE2	1:B:160:TYR:HE1	2.35	0.45
1:C:303:LEU:HD21	1:C:313:TYR:CD2	2.52	0.45
1:C:339:GLY:O	1:C:343:ASN:N	2.50	0.45
1:A:67:ALA:O	1:A:262:ALA:HA	2.16	0.44
1:A:68:ILE:O	1:A:77:LYS:HA	2.16	0.44
1:A:79:PHE:CE2	1:A:260:ALA:HB2	2.52	0.44
1:A:105:ILE:HG23	1:A:241:LEU:HD21	1.99	0.44
1:A:339:GLY:O	1:A:343:ASN:N	2.43	0.44
1:A:511:VAL:O	1:A:511:VAL:HG23	2.17	0.44
1:A:565:PHE:HB3	1:A:576:VAL:HG23	1.98	0.44
1:A:800:PHE:CE2	1:A:898:PHE:CE2	3.05	0.44
1:A:822:LEU:HD21	1:A:938:LEU:HD13	1.99	0.44
1:B:584:ILE:HG22	1:B:585:LEU:N	2.33	0.44
1:C:189:LEU:HB3	1:C:208:THR:O	2.17	0.44
1:C:395:VAL:CG2	1:C:524:VAL:HG11	2.47	0.44
1:A:554:GLU:OE2	1:A:555:SER:N	2.50	0.44
1:A:800:PHE:CE2	1:A:898:PHE:HE2	2.35	0.44
1:B:97:LYS:HE3	1:B:262:ALA:HB3	1.99	0.44
1:B:338:PHE:HE2	1:B:363:ALA:HB1	1.81	0.44
1:B:531:THR:HG22	1:B:532:ASN:H	1.81	0.44
1:B:977:LEU:O	1:B:978:ASN:C	2.60	0.44
1:C:16:VAL:HA	3:I:1:NAG:H81	1.98	0.44
1:C:140:PHE:C	1:C:141:LEU:HD12	2.42	0.44
1:C:212:LEU:HD12	1:C:212:LEU:C	2.40	0.44
1:C:294:ASP:O	1:C:295:PRO:C	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:CYS:HB2	1:C:524:VAL:O	2.17	0.44
1:C:404:GLY:N	1:C:506:GLN:O	2.49	0.44
1:C:577:ARG:HA	1:C:583:GLU:O	2.16	0.44
1:C:778:THR:O	1:C:778:THR:HG22	2.17	0.44
1:C:921:LYS:O	1:C:922:LEU:C	2.59	0.44
1:C:1116:THR:HG22	1:C:1117:THR:N	2.31	0.44
2:D:12:VAL:O	2:D:123:VAL:HA	2.17	0.44
2:D:30:TRP:HA	2:D:31:ALA:HA	1.59	0.44
2:D:50:ALA:HB2	2:D:61:TYR:CD1	2.52	0.44
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.99	0.44
1:A:1121:PHE:HD1	1:A:1122:VAL:N	2.15	0.44
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.52	0.44
1:B:473:TYR:O	1:B:489:TYR:N	2.48	0.44
1:C:433:VAL:HG23	1:C:512:VAL:HG22	1.98	0.44
1:C:452:LEU:HB3	1:C:492:LEU:HD12	2.00	0.44
1:C:1097:SER:HB3	1:C:1102:TRP:CE2	2.52	0.44
1:A:19:THR:O	1:A:20:THR:HB	2.17	0.44
1:A:44:ARG:HB3	1:A:47:VAL:HG21	1.99	0.44
1:A:115:GLN:NE2	1:A:130:VAL:HG12	2.32	0.44
1:A:934:ILE:O	1:A:937:SER:OG	2.24	0.44
1:A:1010:GLN:OE1	1:B:1012:LEU:HD11	2.17	0.44
1:B:32:PHE:CD2	1:B:32:PHE:N	2.85	0.44
1:B:119:ILE:HG12	1:B:128:ILE:HG23	1.98	0.44
1:B:454:ARG:HA	1:B:492:LEU:HA	1.99	0.44
1:C:62:VAL:HB	1:C:267:VAL:O	2.18	0.44
1:C:143:VAL:HG12	1:C:144:TYR:N	2.32	0.44
1:C:707:TYR:CD2	1:C:708:SER:N	2.86	0.44
1:C:800:PHE:CE1	1:C:924:ALA:HA	2.53	0.44
2:D:96:TYR:HD1	2:D:116:GLY:O	2.00	0.44
2:E:4:LEU:HD11	2:E:99:VAL:CG2	2.48	0.44
2:E:90:LYS:HE2	2:E:90:LYS:CA	2.37	0.44
1:A:178:ASP:N	1:A:178:ASP:OD1	2.49	0.44
1:A:567:ARG:HG2	1:A:573:THR:N	2.32	0.44
1:C:303:LEU:HD11	1:C:313:TYR:CD2	2.53	0.44
1:C:329:PHE:O	1:C:580:GLN:CG	2.66	0.44
1:C:656:VAL:HG23	1:C:695:TYR:HB3	1.99	0.44
2:E:98:THR:HG22	2:E:115:TRP:CZ3	2.52	0.44
1:A:83:VAL:O	1:A:83:VAL:HG23	2.18	0.44
1:A:617:CYS:O	1:A:620:VAL:HG13	2.17	0.44
1:B:18:LEU:HD22	1:B:140:PHE:CZ	2.52	0.44
1:B:76:THR:C	1:B:78:ARG:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:GLY:HA3	1:C:43:PHE:HB3	2.00	0.44
1:B:720:ILE:HG22	1:B:721:SER:N	2.33	0.44
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.44	0.44
1:C:323:THR:N	1:C:538:CYS:O	2.50	0.44
1:C:363:ALA:N	1:C:525:CYS:O	2.34	0.44
2:D:41:ALA:HB3	2:D:44:GLN:CG	2.33	0.44
2:E:4:LEU:HD21	2:E:99:VAL:N	2.32	0.44
2:E:38:PHE:HB3	2:E:46:ARG:HB3	2.00	0.44
2:E:94:VAL:CB	2:E:120:GLN:HA	2.48	0.44
1:A:130:VAL:O	1:A:166:CYS:HB2	2.17	0.44
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.99	0.44
1:C:111:ASP:HB2	1:C:113:LYS:NZ	2.33	0.44
2:D:16:GLY:O	2:D:87:LEU:HD12	2.17	0.44
2:D:18:LEU:HD23	2:D:19:LYS:N	2.33	0.44
2:E:23:ALA:HB2	2:E:79:THR:CB	2.47	0.44
2:E:32:ARG:HG2	2:E:53:PHE:CZ	2.53	0.44
1:A:490:PHE:CD2	2:D:31:ALA:HB3	2.49	0.44
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	2.00	0.44
1:B:282:ASN:OD1	4:B:1304:NAG:H2	2.18	0.44
1:B:320:VAL:HG12	1:B:321:GLN:N	2.33	0.44
1:B:802:PHE:O	1:B:804:GLN:N	2.51	0.44
1:C:20:THR:O	1:C:20:THR:HG22	2.17	0.44
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.32	0.44
2:E:6:GLU:CD	2:E:118:GLY:H	2.26	0.44
1:B:567:ARG:NH2	1:B:571:ASP:OD1	2.51	0.44
1:C:1100:THR:HG1	1:C:1101:HIS:HD1	1.65	0.44
1:A:44:ARG:HB2	1:A:279:TYR:CD2	2.52	0.43
1:A:753:LEU:HD13	1:A:760:CYS:SG	2.58	0.43
1:B:349:SER:O	1:B:352:ALA:N	2.46	0.43
1:B:358:ILE:HG22	1:B:361:CYS:SG	2.58	0.43
1:B:761:THR:O	1:B:762:GLN:C	2.62	0.43
1:C:103:GLY:N	1:C:241:LEU:O	2.47	0.43
1:C:124:THR:CG2	3:H:1:NAG:H83	2.48	0.43
1:C:323:THR:O	1:C:324:GLU:C	2.60	0.43
1:C:811:LYS:N	1:C:812:PRO:CD	2.81	0.43
2:D:4:LEU:CD1	2:D:35:ILE:HD11	2.48	0.43
2:E:17:SER:HA	2:E:85:ASN:CA	2.31	0.43
2:E:63:ASP:CA	2:E:66:LYS:HG2	2.48	0.43
1:A:148:ASN:OD1	1:A:149:ASN:N	2.47	0.43
1:A:335:LEU:N	1:A:335:LEU:HD12	2.33	0.43
1:A:977:LEU:O	1:A:978:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:TRP:HA	1:B:240:THR:HA	1.99	0.43
1:B:240:THR:HG23	1:B:242:LEU:CD1	2.47	0.43
1:B:518:LEU:O	1:B:518:LEU:HG	2.18	0.43
1:B:712:ILE:HB	1:B:1077:THR:CG2	2.48	0.43
2:E:53:PHE:HB3	2:E:56:ASP:HB2	1.99	0.43
2:E:98:THR:HG22	2:E:115:TRP:CE3	2.53	0.43
1:A:67:ALA:O	1:A:263:ALA:N	2.33	0.43
1:A:337:PRO:HD2	1:A:358:ILE:HG23	2.00	0.43
1:A:473:TYR:O	1:A:489:TYR:N	2.43	0.43
1:A:1082:CYS:SG	1:A:1132:ILE:HD13	2.58	0.43
1:B:705:VAL:CG1	1:C:895:GLN:HB3	2.48	0.43
1:B:800:PHE:N	1:B:800:PHE:CD1	2.84	0.43
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.51	0.43
1:C:312:ILE:C	1:C:313:TYR:CD1	2.96	0.43
1:C:555:SER:OG	1:C:584:ILE:HG22	2.19	0.43
1:C:581:THR:HG23	1:C:583:GLU:HG3	1.99	0.43
1:C:737:ASP:O	1:C:738:CYS:C	2.61	0.43
1:C:812:PRO:O	1:C:813:SER:HB3	2.17	0.43
1:C:986:PRO:N	1:C:987:PRO:HD2	2.33	0.43
1:A:498:GLN:NE2	2:D:74:ASP:OD1	2.51	0.43
1:A:716:THR:HG22	1:A:1110:TYR:HD2	1.84	0.43
1:B:42:VAL:HG12	1:B:43:PHE:H	1.83	0.43
1:B:94:SER:N	1:B:190:ARG:O	2.47	0.43
1:B:118:LEU:HD23	1:B:119:ILE:N	2.32	0.43
1:B:212:LEU:HD12	1:B:213:VAL:N	2.33	0.43
1:B:297:SER:O	1:B:300:LYS:N	2.51	0.43
1:B:878:LEU:O	1:B:882:ILE:HG12	2.18	0.43
1:C:47:VAL:HG12	1:C:48:LEU:N	2.33	0.43
1:C:65:PHE:HB2	1:C:265:TYR:CE1	2.53	0.43
1:C:103:GLY:HA2	1:C:104:TRP:CE3	2.53	0.43
1:C:117:LEU:HD12	1:C:118:LEU:H	1.83	0.43
1:C:619:GLU:C	1:C:620:VAL:HG13	2.44	0.43
1:C:819:GLU:O	1:C:823:PHE:N	2.50	0.43
2:D:18:LEU:O	2:D:84:MET:HB2	2.17	0.43
1:A:91:TYR:CD1	1:A:92:PHE:N	2.87	0.43
1:A:146:HIS:HD1	1:A:151:SER:C	2.21	0.43
1:A:533:LEU:HD21	1:A:585:LEU:HD11	1.99	0.43
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	2.01	0.43
1:B:143:VAL:N	1:B:244:LEU:O	2.44	0.43
1:B:1133:VAL:CG1	1:B:1134:ASN:N	2.81	0.43
1:C:906:PHE:CE1	1:C:1049:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:22:CYS:HB2	2:E:37:TRP:HZ2	1.84	0.43
2:E:69:PHE:CB	2:E:82:LEU:HD11	2.48	0.43
1:A:103:GLY:N	1:A:241:LEU:O	2.50	0.43
1:A:494:SER:C	2:D:55:PHE:CZ	2.93	0.43
1:A:784:GLN:NE2	1:A:1030:SER:OG	2.51	0.43
1:B:18:LEU:HD22	1:B:140:PHE:CE1	2.54	0.43
1:B:51:THR:O	1:B:51:THR:HG23	2.17	0.43
1:C:105:ILE:O	1:C:105:ILE:HG13	2.18	0.43
1:A:130:VAL:HB	1:A:168:PHE:HB3	2.01	0.43
1:A:365:TYR:CD1	1:A:387:LEU:HB3	2.53	0.43
1:A:777:ASN:O	1:A:781:VAL:HG23	2.19	0.43
1:A:855:PHE:N	1:A:858:LEU:O	2.52	0.43
1:B:281:GLU:OE1	1:B:281:GLU:HA	2.18	0.43
1:B:602:THR:O	1:B:604:THR:N	2.52	0.43
1:C:118:LEU:HD12	1:C:118:LEU:C	2.44	0.43
1:A:715:PRO:O	1:A:1110:TYR:HB2	2.18	0.43
1:A:752:LEU:O	1:A:755:GLN:N	2.41	0.43
1:A:874:THR:O	1:A:875:SER:C	2.62	0.43
1:A:1129:VAL:HG12	1:A:1130:ILE:N	2.34	0.43
1:B:83:VAL:HG12	1:B:239:GLN:OE1	2.19	0.43
1:B:201:PHE:O	1:B:228:ASP:HA	2.18	0.43
1:B:274:THR:HG23	1:B:291:CYS:HB2	2.01	0.43
1:B:452:LEU:HD13	2:E:55:PHE:HE2	1.84	0.43
1:C:110:LEU:O	1:C:135:PHE:HB2	2.18	0.43
1:C:332:ILE:C	1:C:334:ASN:H	2.26	0.43
1:C:1060:VAL:HG22	1:C:1061:VAL:N	2.33	0.43
1:A:421:TYR:C	1:A:461:LEU:HD11	2.44	0.43
1:A:657:ASN:CB	4:A:1309:NAG:O5	2.66	0.43
1:A:770:ILE:HG23	1:A:1015:ALA:HB1	1.99	0.43
1:B:391:CYS:C	1:B:392:PHE:CD2	2.97	0.43
1:B:473:TYR:HB3	1:B:489:TYR:HB2	2.00	0.43
1:C:709:ASN:ND2	4:C:1306:NAG:C7	2.80	0.43
1:C:759:PHE:O	1:C:762:GLN:N	2.52	0.43
1:C:942:PRO:O	1:C:942:PRO:CD	2.66	0.43
1:C:985:ASP:HB2	1:C:986:PRO:CD	2.49	0.43
2:D:4:LEU:HD11	2:D:35:ILE:HG13	2.01	0.43
2:E:17:SER:CB	2:E:85:ASN:HA	2.49	0.43
1:A:320:VAL:HG12	1:A:321:GLN:N	2.33	0.43
1:A:449:TYR:HD1	2:D:55:PHE:CE1	2.37	0.43
1:A:599:THR:HG22	1:A:601:GLY:H	1.84	0.43
1:B:118:LEU:HG	1:B:120:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG23	1:B:175:PHE:CE2	2.50	0.43
1:B:128:ILE:HB	1:B:170:TYR:HB3	2.01	0.43
1:B:874:THR:O	1:B:875:SER:C	2.61	0.43
1:B:969:ASN:HB2	1:C:755:GLN:NE2	2.34	0.43
1:C:529:LYS:HD3	1:C:530:SER:N	2.33	0.43
1:C:811:LYS:HD2	1:C:813:SER:H	1.83	0.43
2:E:96:TYR:CD1	2:E:118:GLY:HA3	2.54	0.43
1:A:347:PHE:HB2	1:A:401:VAL:HG23	2.00	0.42
1:A:407:VAL:HG11	1:A:508:TYR:CD2	2.53	0.42
1:A:467:ASP:C	1:A:468:ILE:HD13	2.43	0.42
1:A:858:LEU:CD1	1:A:963:VAL:HG23	2.48	0.42
1:B:391:CYS:HB2	1:B:525:CYS:CA	2.39	0.42
1:B:438:SER:O	1:B:441:LEU:N	2.47	0.42
1:B:531:THR:HG22	1:B:532:ASN:N	2.34	0.42
2:E:96:TYR:HB3	2:E:115:TRP:CE3	2.48	0.42
1:A:33:THR:HA	1:A:58:PHE:CD1	2.54	0.42
1:A:105:ILE:C	1:A:106:PHE:HD1	2.27	0.42
1:A:115:GLN:NE2	1:A:130:VAL:O	2.52	0.42
1:A:295:PRO:C	1:A:297:SER:N	2.77	0.42
1:A:449:TYR:HA	2:D:55:PHE:CE1	2.54	0.42
1:A:897:PRO:O	1:A:898:PHE:HB3	2.19	0.42
1:B:596:SER:HB2	1:B:611:LEU:HD23	2.01	0.42
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.54	0.42
1:C:454:ARG:HA	1:C:492:LEU:HA	2.01	0.42
1:C:524:VAL:O	1:C:524:VAL:HG13	2.18	0.42
2:E:40:GLN:HB2	2:E:46:ARG:CG	2.38	0.42
1:A:551:VAL:HG22	1:A:552:LEU:H	1.83	0.42
1:A:789:TYR:HB2	1:A:879:ALA:HB3	2.01	0.42
1:A:1031:GLU:OE1	1:C:1039:ARG:NH2	2.50	0.42
1:A:1087:ALA:HB2	1:A:1125:ASN:C	2.45	0.42
1:C:169:GLU:N	1:C:169:GLU:OE1	2.53	0.42
1:C:642:VAL:HG12	1:C:643:PHE:N	2.34	0.42
2:E:16:GLY:C	2:E:87:LEU:HG	2.44	0.42
1:A:191:GLU:N	1:A:191:GLU:OE2	2.52	0.42
1:A:484:GLU:OE2	2:D:102:GLY:HA3	2.18	0.42
1:A:772:VAL:HG23	1:A:773:GLU:N	2.34	0.42
1:B:133:PHE:HD1	1:B:163:ALA:HB2	1.84	0.42
1:B:449:TYR:HA	1:B:494:SER:OG	2.19	0.42
1:B:520:ALA:CB	1:B:521:PRO:HD3	2.50	0.42
1:B:900:MET:O	1:B:903:ALA:N	2.52	0.42
1:C:39:PRO:HG3	1:C:51:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:969:ASN:OD1	1:C:974:SER:C	2.62	0.42
2:E:68:ARG:HB2	2:E:86:SER:CB	2.48	0.42
1:A:240:THR:O	1:A:241:LEU:HD23	2.20	0.42
1:A:280:ASN:C	1:A:282:ASN:O	2.62	0.42
1:A:404:GLY:N	1:A:506:GLN:O	2.52	0.42
1:B:24:LEU:HD23	1:B:25:PRO:O	2.19	0.42
1:B:56:LEU:HD12	1:B:57:PRO:N	2.34	0.42
1:B:358:ILE:HD12	1:B:397:ALA:HB2	2.01	0.42
1:B:361:CYS:SG	1:B:524:VAL:HG23	2.60	0.42
1:B:569:ILE:O	1:B:570:ALA:HB3	2.20	0.42
1:B:1039:ARG:HD2	1:C:1031:GLU:CD	2.44	0.42
1:B:1114:ILE:O	1:B:1119:ASN:ND2	2.51	0.42
1:C:105:ILE:CG2	1:C:241:LEU:HD21	2.47	0.42
1:C:988:GLU:O	1:C:991:VAL:HG12	2.20	0.42
2:E:29:SER:HB3	2:E:31:ALA:O	2.19	0.42
2:E:73:GLY:HA2	2:E:80:VAL:HA	2.01	0.42
1:A:48:LEU:HD13	1:A:277:LEU:O	2.19	0.42
1:A:141:LEU:O	1:A:244:LEU:HG	2.19	0.42
1:A:303:LEU:HD11	1:A:313:TYR:CD2	2.54	0.42
1:A:377:PHE:CD1	1:A:434:ILE:HD12	2.54	0.42
1:A:418:ILE:HD13	1:A:422:ASN:HD22	1.84	0.42
1:A:592:PHE:CG	1:B:740:MET:HE1	2.54	0.42
1:A:805:ILE:HD12	1:A:878:LEU:HD11	2.01	0.42
1:A:986:PRO:O	1:A:987:PRO:C	2.63	0.42
1:B:43:PHE:CD1	1:B:43:PHE:C	2.97	0.42
1:B:333:THR:HG22	1:B:333:THR:O	2.18	0.42
1:B:973:ILE:N	1:B:992:GLN:OE1	2.46	0.42
1:C:800:PHE:CE2	1:C:898:PHE:HE2	2.38	0.42
1:C:818:ILE:O	1:C:819:GLU:C	2.62	0.42
2:E:69:PHE:HB2	2:E:82:LEU:HD11	2.02	0.42
1:A:126:VAL:HG23	1:A:172:SER:HB2	2.00	0.42
1:A:314:GLN:NE2	1:A:316:SER:O	2.52	0.42
1:A:920:GLN:O	1:A:924:ALA:N	2.50	0.42
1:B:171:VAL:HG13	1:B:171:VAL:O	2.19	0.42
1:B:187:LYS:O	1:B:210:ILE:N	2.34	0.42
1:B:345:THR:OG1	1:B:346:ARG:N	2.53	0.42
1:B:968:SER:O	1:B:970:PHE:HD2	2.03	0.42
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.49	0.42
1:C:332:ILE:CG2	1:C:333:THR:H	2.26	0.42
1:C:455:LEU:HD11	1:C:493:GLN:CB	2.45	0.42
1:C:492:LEU:HD23	1:C:492:LEU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1028:LYS:O	1:C:1032:CYS:N	2.49	0.42
2:D:101:PHE:HB2	2:D:106:ASN:HD21	1.85	0.42
1:A:49:HIS:O	1:A:276:LEU:HA	2.19	0.42
1:A:452:LEU:HD13	2:D:55:PHE:CD2	2.54	0.42
1:A:534:VAL:HG22	1:A:535:LYS:N	2.35	0.42
1:A:872:GLN:O	1:A:873:TYR:C	2.63	0.42
1:B:1104:VAL:HG23	1:B:1115:ILE:HG12	2.01	0.42
1:C:328:ARG:O	1:C:579:PRO:HG2	2.19	0.42
1:C:481:ASN:O	1:C:481:ASN:ND2	2.53	0.42
1:C:781:VAL:CG2	1:C:1026:ALA:HB2	2.46	0.42
1:C:963:VAL:HG12	1:C:963:VAL:O	2.19	0.42
2:D:69:PHE:CE1	2:D:84:MET:HA	2.54	0.42
2:D:99:VAL:O	2:D:99:VAL:HG12	2.20	0.42
2:E:74:ASP:CG	2:E:77:LYS:H	2.28	0.42
1:A:358:ILE:HB	1:A:395:VAL:HB	2.02	0.42
1:A:524:VAL:O	1:A:524:VAL:HG13	2.20	0.42
1:A:753:LEU:HD12	1:A:753:LEU:C	2.44	0.42
1:B:106:PHE:HD1	1:B:238:PHE:HB2	1.85	0.42
1:B:206:LYS:HD2	1:B:207:HIS:H	1.85	0.42
1:B:411:ALA:HB3	1:B:414:GLN:CB	2.49	0.42
1:B:520:ALA:CB	1:B:521:PRO:CD	2.98	0.42
1:B:665:PRO:HB2	1:C:864:LEU:HD13	2.02	0.42
1:B:746:SER:O	1:B:749:CYS:N	2.50	0.42
1:B:1079:PRO:HB3	1:C:917:TYR:CE1	2.55	0.42
1:C:58:PHE:HB2	1:C:293:LEU:HD22	2.01	0.42
1:A:200:TYR:HA	1:A:229:LEU:O	2.20	0.42
1:A:289:VAL:O	1:A:289:VAL:HG23	2.19	0.42
1:A:985:ASP:C	1:A:987:PRO:HD2	2.45	0.42
1:A:1027:THR:O	1:A:1027:THR:HG22	2.19	0.42
1:A:1030:SER:HB3	1:C:1041:ASP:HB2	2.02	0.42
1:B:54:LEU:HD13	1:B:88:ASP:O	2.20	0.42
1:B:133:PHE:HB3	1:B:160:TYR:CB	2.50	0.42
1:B:357:ARG:NH2	1:B:394:ASN:HD22	2.18	0.42
1:B:367:VAL:HG23	1:B:368:LEU:CD1	2.50	0.42
1:B:406:GLU:O	1:B:407:VAL:C	2.62	0.42
1:B:874:THR:O	1:B:877:LEU:N	2.53	0.42
1:B:1139:ASP:C	1:B:1139:ASP:OD1	2.63	0.42
1:C:36:VAL:HG12	1:C:37:TYR:N	2.34	0.42
1:C:44:ARG:NH2	1:C:49:HIS:ND1	2.68	0.42
1:C:201:PHE:N	1:C:229:LEU:O	2.53	0.42
1:C:351:TYR:O	1:C:466:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1022:ALA:O	1:C:1026:ALA:N	2.52	0.42
2:D:105:ASP:OD2	2:D:105:ASP:N	2.53	0.42
2:E:23:ALA:HB2	2:E:79:THR:HB	2.02	0.42
1:A:79:PHE:CZ	1:A:244:LEU:HB3	2.54	0.41
1:A:159:VAL:CG2	1:A:160:TYR:N	2.83	0.41
1:A:406:GLU:HG2	1:A:418:ILE:CG1	2.49	0.41
1:A:468:ILE:HG22	1:A:468:ILE:O	2.20	0.41
1:A:492:LEU:C	2:D:31:ALA:HB1	2.45	0.41
1:A:959:LEU:O	1:A:962:LEU:N	2.48	0.41
1:B:56:LEU:HD12	1:B:57:PRO:HD2	2.01	0.41
1:B:110:LEU:O	1:B:135:PHE:N	2.53	0.41
1:B:118:LEU:N	1:B:129:LYS:O	2.53	0.41
1:B:160:TYR:CE2	1:B:162:SER:HA	2.55	0.41
1:B:187:LYS:HA	1:B:210:ILE:O	2.20	0.41
1:B:383:SER:O	1:B:384:PRO:C	2.63	0.41
1:B:566:GLY:HA2	1:C:43:PHE:H	1.85	0.41
1:B:866:THR:O	1:B:870:ILE:HD12	2.20	0.41
1:C:98:SER:HB3	1:C:100:ILE:HD11	2.01	0.41
1:C:101:ILE:C	1:C:102:ARG:HD3	2.45	0.41
1:C:355:ARG:HG3	1:C:398:ASP:OD1	2.20	0.41
1:C:753:LEU:HD12	1:C:753:LEU:C	2.45	0.41
2:D:40:GLN:N	2:D:40:GLN:CD	2.78	0.41
2:D:90:LYS:C	2:D:90:LYS:HD3	2.45	0.41
2:E:33:LYS:HD2	2:E:102:GLY:CA	2.50	0.41
2:E:86:SER:O	2:E:87:LEU:C	2.62	0.41
1:A:99:ASN:O	1:A:102:ARG:NH2	2.53	0.41
1:A:278:LYS:HB2	1:A:306:PHE:CE2	2.54	0.41
1:A:749:CYS:O	1:A:752:LEU:N	2.40	0.41
1:A:905:ARG:HD3	1:A:1050:MET:HB3	2.02	0.41
1:A:1121:PHE:CD1	1:A:1121:PHE:C	2.97	0.41
1:B:46:SER:H	1:B:280:ASN:C	2.28	0.41
1:B:313:TYR:O	1:B:596:SER:HA	2.20	0.41
1:B:451:TYR:C	2:E:55:PHE:HZ	2.28	0.41
1:B:484:GLU:CG	2:E:102:GLY:HA3	2.43	0.41
1:B:493:GLN:OE1	1:B:493:GLN:HA	2.20	0.41
1:B:516:GLU:O	1:B:517:LEU:C	2.63	0.41
1:B:557:LYS:HD3	1:C:43:PHE:CZ	2.55	0.41
1:B:811:LYS:N	1:B:812:PRO:CD	2.83	0.41
1:B:1008:VAL:O	1:B:1012:LEU:HG	2.20	0.41
1:C:159:VAL:CG2	1:C:160:TYR:HD1	2.33	0.41
1:C:198:ASP:C	1:C:200:TYR:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:HD23	2:D:23:ALA:C	2.45	0.41
2:D:68:ARG:NH1	2:D:91:ASP:OD2	2.53	0.41
2:E:38:PHE:CA	2:E:49:VAL:HG23	2.49	0.41
2:E:39:ARG:NH2	2:E:93:ALA:HB2	2.32	0.41
2:E:49:VAL:HG12	2:E:65:VAL:HG21	1.98	0.41
1:B:336:CYS:HA	1:B:361:CYS:HB2	2.01	0.41
1:C:49:HIS:CD2	1:C:50:SER:N	2.88	0.41
1:C:49:HIS:C	1:C:276:LEU:HD12	2.46	0.41
1:C:85:PRO:HB2	1:C:87:ASN:OD1	2.20	0.41
1:C:211:ASN:N	1:C:211:ASN:OD1	2.53	0.41
2:E:34:CYS:SG	2:E:53:PHE:HA	2.61	0.41
3:I:1:NAG:H62	3:I:2:NAG:H82	2.02	0.41
1:A:22:THR:OG1	1:A:78:ARG:NH1	2.52	0.41
1:A:560:LEU:HB3	1:A:561:PRO:CD	2.51	0.41
1:A:572:THR:O	1:A:573:THR:C	2.64	0.41
1:A:616:ASN:ND2	4:A:1308:NAG:C7	2.83	0.41
1:A:1062:PHE:HB3	1:A:1064:HIS:CE1	2.55	0.41
1:B:31:SER:O	1:B:59:PHE:CA	2.67	0.41
1:B:143:VAL:HG12	1:B:152:TRP:HE3	1.86	0.41
1:B:475:ALA:HB3	1:B:489:TYR:HE2	1.85	0.41
1:B:617:CYS:HB3	1:B:649:CYS:HB3	1.90	0.41
1:C:195:LYS:O	1:C:201:PHE:HA	2.21	0.41
1:C:866:THR:C	1:C:868:GLU:N	2.78	0.41
1:C:973:ILE:HG13	1:C:974:SER:H	1.85	0.41
4:C:1301:NAG:O7	4:C:1301:NAG:O3	2.31	0.41
2:E:29:SER:C	2:E:31:ALA:HA	2.45	0.41
2:E:68:ARG:NH2	2:E:88:LEU:HB3	2.35	0.41
1:A:15:CYS:HA	1:A:158:ARG:HB3	2.02	0.41
1:A:421:TYR:O	1:A:461:LEU:HD11	2.20	0.41
1:A:569:ILE:HG22	1:A:570:ALA:H	1.83	0.41
1:A:709:ASN:ND2	4:A:1310:NAG:O7	2.53	0.41
1:A:755:GLN:OE1	1:C:971:GLY:N	2.54	0.41
1:B:170:TYR:CD2	1:B:170:TYR:C	2.97	0.41
1:B:517:LEU:HD11	1:C:983:ARG:NH1	2.35	0.41
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.83	0.41
1:C:104:TRP:CA	1:C:241:LEU:HG	2.50	0.41
1:C:295:PRO:O	1:C:296:LEU:C	2.62	0.41
1:C:393:THR:HA	1:C:523:THR:H	1.86	0.41
1:C:1080:ALA:HB2	1:C:1089:PHE:CE1	2.55	0.41
2:D:36:GLY:C	2:D:98:THR:HB	2.45	0.41
2:E:28:ALA:O	2:E:29:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:62:SER:O	2:E:66:LYS:HG2	2.21	0.41
2:E:71:ILE:CG2	2:E:82:LEU:HD13	2.39	0.41
1:A:299:THR:O	1:A:300:LYS:C	2.63	0.41
1:A:475:ALA:H	1:A:487:ASN:C	2.28	0.41
1:A:563:GLN:NE2	1:B:43:PHE:HA	2.36	0.41
1:A:988:GLU:C	1:A:990:GLU:N	2.77	0.41
1:B:554:GLU:OE1	1:B:555:SER:N	2.53	0.41
1:B:1076:THR:HG22	1:B:1077:THR:N	2.36	0.41
1:C:200:TYR:HA	1:C:230:PRO:HA	2.03	0.41
1:C:342:PHE:HD1	1:C:436:TRP:CH2	2.39	0.41
1:C:805:ILE:CD1	1:C:878:LEU:HD11	2.41	0.41
1:C:897:PRO:O	1:C:898:PHE:CB	2.69	0.41
2:E:32:ARG:HD3	2:E:32:ARG:N	2.34	0.41
2:E:94:VAL:HG13	2:E:96:TYR:CZ	2.54	0.41
1:A:85:PRO:HA	1:A:237:ARG:HG2	2.03	0.41
1:A:89:GLY:HA2	1:A:194:PHE:O	2.20	0.41
1:A:111:ASP:HA	1:A:134:GLN:HA	2.01	0.41
1:A:312:ILE:O	1:A:313:TYR:CG	2.74	0.41
1:A:403:ARG:CG	1:A:406:GLU:OE1	2.69	0.41
1:A:569:ILE:O	1:A:572:THR:HG22	2.20	0.41
1:A:817:PHE:CE1	1:A:821:LEU:HD11	2.56	0.41
1:B:115:GLN:OE1	1:B:115:GLN:HA	2.20	0.41
1:B:200:TYR:HB3	1:B:228:ASP:OD2	2.20	0.41
1:B:394:ASN:C	1:B:394:ASN:OD1	2.62	0.41
1:B:453:TYR:O	1:B:493:GLN:N	2.51	0.41
1:B:659:SER:HB3	1:B:698:SER:HB3	2.02	0.41
1:B:660:TYR:N	1:B:698:SER:OG	2.53	0.41
4:B:1307:NAG:O7	4:B:1307:NAG:H3	2.21	0.41
1:C:527:PRO:O	1:C:529:LYS:HE2	2.21	0.41
1:C:611:LEU:HD12	1:C:612:TYR:H	1.86	0.41
2:E:32:ARG:HG2	2:E:32:ARG:O	2.20	0.41
2:E:71:ILE:HG22	2:E:82:LEU:CB	2.40	0.41
3:F:1:NAG:C1	3:F:1:NAG:H83	2.51	0.41
1:A:45:SER:O	1:A:47:VAL:HG23	2.20	0.41
1:A:104:TRP:HA	1:A:240:THR:HA	2.01	0.41
1:A:356:LYS:HG2	1:A:357:ARG:N	2.36	0.41
1:A:645:THR:C	1:A:647:ALA:N	2.79	0.41
1:A:795:LYS:HA	1:A:797:PHE:CE2	2.56	0.41
1:B:58:PHE:HB2	1:B:293:LEU:HD22	2.03	0.41
1:B:134:GLN:O	1:B:160:TYR:HA	2.20	0.41
1:B:985:ASP:O	1:B:986:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:VAL:HG23	1:C:160:TYR:HD1	1.86	0.41
1:C:329:PHE:CB	1:C:528:LYS:HB3	2.51	0.41
1:C:551:VAL:HG13	1:C:588:THR:HB	2.01	0.41
1:C:821:LEU:HD13	1:C:939:SER:OG	2.21	0.41
2:D:41:ALA:CB	2:D:44:GLN:HG2	2.35	0.41
2:E:9:GLY:HA3	2:E:119:THR:HB	2.02	0.41
2:E:63:ASP:HA	2:E:66:LYS:HG2	2.02	0.41
1:A:53:ASP:O	1:A:272:PRO:HA	2.19	0.41
1:A:448:ASN:N	1:A:497:PHE:O	2.51	0.41
1:A:495:TYR:N	2:D:55:PHE:CZ	2.88	0.41
1:A:768:THR:O	1:A:771:ALA:N	2.54	0.41
1:A:902:MET:HE1	1:A:1050:MET:SD	2.61	0.41
1:A:920:GLN:O	1:A:923:ILE:N	2.54	0.41
1:A:979:ASP:O	1:A:980:ILE:C	2.64	0.41
1:A:1053:PRO:O	1:A:1054:GLN:HG2	2.21	0.41
1:A:1098:ASN:OD1	1:A:1099:GLY:N	2.48	0.41
1:B:104:TRP:CD1	1:B:240:THR:HA	2.56	0.41
1:B:271:GLN:HB3	1:B:272:PRO:CD	2.51	0.41
1:B:400:PHE:O	1:B:510:VAL:N	2.48	0.41
1:B:434:ILE:O	1:B:511:VAL:N	2.32	0.41
1:B:778:THR:HG22	1:B:778:THR:O	2.20	0.41
1:C:58:PHE:HB3	1:C:59:PHE:CD1	2.55	0.41
1:C:539:VAL:O	1:C:549:THR:HA	2.20	0.41
1:C:569:ILE:O	1:C:570:ALA:CB	2.69	0.41
1:C:1138:TYR:CD1	1:C:1139:ASP:N	2.89	0.41
2:E:4:LEU:HD12	2:E:4:LEU:N	2.36	0.41
2:E:8:GLY:HA3	2:E:20:LEU:HD12	2.01	0.41
2:E:59:THR:HG21	2:E:61:TYR:HE1	1.85	0.41
1:A:406:GLU:HB3	1:A:418:ILE:HG13	2.02	0.41
1:A:418:ILE:HA	1:A:422:ASN:HB2	2.02	0.41
1:A:551:VAL:HG12	1:A:588:THR:HB	2.02	0.41
1:A:811:LYS:O	1:A:811:LYS:HD3	2.21	0.41
1:A:922:LEU:HD11	4:A:1311:NAG:H5	2.03	0.41
1:A:954:GLN:O	1:A:957:GLN:N	2.54	0.41
1:A:1007:TYR:CD2	1:A:1007:TYR:C	2.99	0.41
1:A:1089:PHE:HZ	1:A:1129:VAL:HG21	1.86	0.41
1:B:30:ASN:HB3	1:B:32:PHE:HE2	1.85	0.41
1:B:77:LYS:O	1:B:78:ARG:C	2.63	0.41
1:B:244:LEU:HB2	1:B:259:THR:O	2.21	0.41
1:B:280:ASN:O	1:B:281:GLU:C	2.62	0.41
1:B:374:PHE:HD1	1:B:436:TRP:CB	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ALA:CB	1:B:510:VAL:HG22	2.50	0.41
1:B:642:VAL:HG12	1:B:643:PHE:N	2.36	0.41
1:C:453:TYR:OH	1:C:493:GLN:NE2	2.54	0.41
1:C:539:VAL:CG1	1:C:540:ASN:N	2.84	0.41
1:C:712:ILE:HB	1:C:1077:THR:HG21	2.03	0.41
2:E:38:PHE:HB2	2:E:115:TRP:HZ3	1.85	0.41
2:E:106:ASN:CA	2:E:109:ARG:HH21	2.32	0.41
1:A:141:LEU:HB2	1:A:243:ALA:HA	2.02	0.40
1:A:299:THR:CG2	1:A:300:LYS:N	2.83	0.40
1:A:800:PHE:HB2	1:A:802:PHE:CE2	2.56	0.40
1:A:1121:PHE:CD1	1:A:1122:VAL:N	2.89	0.40
1:B:44:ARG:NH2	1:B:49:HIS:CE1	2.89	0.40
1:B:93:ALA:CA	1:B:190:ARG:O	2.69	0.40
1:B:428:ASP:OD2	1:B:428:ASP:N	2.54	0.40
1:B:503:VAL:HG13	1:B:508:TYR:OH	2.21	0.40
1:B:587:ILE:CG2	1:B:588:THR:N	2.83	0.40
1:B:990:GLU:O	1:B:993:ILE:HB	2.21	0.40
1:C:38:TYR:CE1	1:C:285:ILE:HG13	2.56	0.40
1:C:110:LEU:HB3	1:C:135:PHE:HB2	2.03	0.40
1:C:234:ASN:O	1:C:234:ASN:CG	2.64	0.40
1:C:246:ARG:HE	1:C:258:TRP:HB3	1.85	0.40
1:C:741:TYR:HE1	1:C:962:LEU:HG	1.86	0.40
1:C:994:ASP:O	1:C:998:THR:HG23	2.22	0.40
1:C:1062:PHE:HB3	1:C:1064:HIS:CE1	2.56	0.40
2:D:53:PHE:CE2	2:D:104:CYS:HB2	2.55	0.40
1:A:43:PHE:O	1:A:44:ARG:HG3	2.21	0.40
1:A:130:VAL:CG2	1:A:168:PHE:HB3	2.51	0.40
1:A:212:LEU:HD12	1:A:212:LEU:C	2.45	0.40
1:A:411:ALA:HB3	1:A:414:GLN:CD	2.47	0.40
1:A:1142:GLN:HA	1:A:1145:LEU:HD12	2.03	0.40
1:B:168:PHE:CD2	1:B:169:GLU:N	2.90	0.40
1:B:227:VAL:CG2	1:B:229:LEU:HG	2.51	0.40
1:B:749:CYS:O	1:B:750:SER:C	2.64	0.40
1:B:1048:HIS:CG	1:B:1049:LEU:N	2.89	0.40
1:C:453:TYR:CE2	1:C:455:LEU:HD21	2.56	0.40
1:C:529:LYS:HE2	1:C:529:LYS:HA	2.03	0.40
2:D:34:CYS:CA	2:D:100:ALA:HB3	2.50	0.40
2:D:37:TRP:HZ3	2:D:71:ILE:HD11	1.87	0.40
2:D:68:ARG:HD3	2:D:88:LEU:HD11	2.03	0.40
2:E:4:LEU:CD1	2:E:99:VAL:HG23	2.51	0.40
2:E:19:LYS:HD2	2:E:19:LYS:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:ARG:O	2:E:85:ASN:O	2.39	0.40
2:E:70:THR:C	2:E:82:LEU:HD12	2.46	0.40
2:E:98:THR:HA	2:E:114:TYR:O	2.21	0.40
1:A:201:PHE:O	1:A:228:ASP:HA	2.20	0.40
1:A:201:PHE:O	1:A:229:LEU:N	2.44	0.40
1:A:1012:LEU:O	1:A:1016:ALA:N	2.54	0.40
1:A:1060:VAL:HG22	1:A:1061:VAL:N	2.37	0.40
1:A:1100:THR:OG1	1:A:1101:HIS:ND1	2.55	0.40
1:B:19:THR:O	1:B:20:THR:CB	2.69	0.40
1:B:379:CYS:SG	1:B:384:PRO:HB3	2.61	0.40
1:B:402:ILE:HD11	1:B:407:VAL:HA	2.04	0.40
1:B:490:PHE:CD1	1:B:491:PRO:HD3	2.56	0.40
1:C:106:PHE:HE2	1:C:201:PHE:HZ	1.70	0.40
1:C:874:THR:O	1:C:875:SER:C	2.63	0.40
2:D:4:LEU:HD12	2:D:99:VAL:CG2	2.50	0.40
2:D:84:MET:HE1	2:D:121:VAL:CG1	2.28	0.40
2:E:40:GLN:HA	2:E:46:ARG:N	2.36	0.40
1:A:168:PHE:CE1	1:A:230:PRO:HD2	2.57	0.40
1:A:656:VAL:HG22	1:A:694:ALA:O	2.22	0.40
1:A:665:PRO:HA	1:A:671:CYS:SG	2.60	0.40
1:A:739:THR:HG1	1:A:740:MET:H	1.70	0.40
1:A:794:ILE:O	1:A:794:ILE:HG13	2.21	0.40
1:A:860:VAL:HG12	1:A:861:LEU:N	2.36	0.40
1:A:921:LYS:O	1:A:924:ALA:N	2.54	0.40
1:A:1101:HIS:CE1	4:A:1313:NAG:H5	2.56	0.40
1:B:363:ALA:HB3	1:B:365:TYR:CE2	2.56	0.40
1:C:27:ALA:C	1:C:28:TYR:CD1	2.99	0.40
1:C:140:PHE:O	1:C:141:LEU:HD12	2.21	0.40
1:C:210:ILE:CG2	1:C:211:ASN:H	2.33	0.40
1:C:309:GLU:O	1:C:310:LYS:C	2.64	0.40
1:C:328:ARG:HA	1:C:530:SER:HB3	2.04	0.40
1:C:329:PHE:O	1:C:330:PRO:C	2.63	0.40
1:C:992:GLN:OE1	1:C:995:ARG:NH2	2.55	0.40
2:D:4:LEU:CD1	2:D:99:VAL:HG23	2.48	0.40
1:A:85:PRO:HA	1:A:237:ARG:CB	2.51	0.40
1:A:122:ASN:OD1	1:A:122:ASN:C	2.64	0.40
1:A:280:ASN:O	1:A:282:ASN:O	2.39	0.40
1:A:709:ASN:ND2	4:A:1310:NAG:C7	2.84	0.40
1:A:752:LEU:O	1:A:755:GLN:CB	2.69	0.40
1:A:819:GLU:O	1:A:820:ASP:C	2.65	0.40
1:A:924:ALA:C	1:A:926:GLN:N	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:CG2	1:B:76:THR:HA	2.51	0.40
1:B:36:VAL:O	1:B:36:VAL:HG13	2.22	0.40
1:B:392:PHE:CD2	1:B:392:PHE:N	2.89	0.40
1:C:887:THR:HG1	1:C:894:LEU:H	1.68	0.40
2:D:34:CYS:SG	2:D:53:PHE:CD2	3.12	0.40
2:E:6:GLU:OE1	2:E:118:GLY:C	2.64	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	1042/1264 (82%)	914 (88%)	128 (12%)	0	100	100
1	B	1043/1264 (82%)	896 (86%)	146 (14%)	1 (0%)	48	79
1	C	1045/1264 (83%)	906 (87%)	138 (13%)	1 (0%)	48	79
2	D	123/130 (95%)	111 (90%)	12 (10%)	0	100	100
2	E	123/130 (95%)	107 (87%)	16 (13%)	0	100	100
All	All	3376/4052 (83%)	2934 (87%)	440 (13%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	THR
1	B	942	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	927/1100 (84%)	925 (100%)	2 (0%)	87	89
1	B	926/1100 (84%)	925 (100%)	1 (0%)	88	91
1	C	929/1100 (84%)	928 (100%)	1 (0%)	88	91
2	D	97/101 (96%)	96 (99%)	1 (1%)	68	80
2	E	97/101 (96%)	97 (100%)	0	100	100
All	All	2976/3502 (85%)	2971 (100%)	5 (0%)	85	89

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

Mol	Chain	Res	Type
1	A	282	ASN
1	A	331	ASN
1	B	331	ASN
1	C	61	ASN
2	D	34	CYS

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

Mol	Chain	Res	Type
1	A	69	HIS
1	A	137	ASN
1	A	164	ASN
1	A	207	HIS
1	A	321	GLN
1	A	343	ASN
1	A	450	ASN
1	A	493	GLN
1	A	498	GLN
1	A	532	ASN
1	A	606	ASN
1	A	655	HIS
1	A	751	ASN
1	A	784	GLN
1	A	1106	GLN
1	B	49	HIS
1	B	115	GLN
1	B	164	ASN

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Mol	Chain	Res	Type
1	B	165	ASN
1	B	245	HIS
1	B	331	ASN
1	B	394	ASN
1	B	409	GLN
1	B	422	ASN
1	B	448	ASN
1	B	450	ASN
1	B	498	GLN
1	B	655	HIS
1	B	658	ASN
1	B	703	ASN
1	B	717	ASN
1	B	751	ASN
1	B	935	GLN
1	B	969	ASN
1	B	978	ASN
1	B	1010	GLN
1	B	1135	ASN
1	C	23	GLN
1	C	99	ASN
1	C	185	ASN
1	C	207	HIS
1	C	280	ASN
1	C	317	ASN
1	C	321	GLN
1	C	388	ASN
1	C	414	GLN
1	C	493	GLN
1	C	607	GLN
1	C	784	GLN
1	C	1064	HIS
1	C	1071	GLN
1	C	1083	HIS
2	D	75	ASN
2	E	13	GLN
2	E	83	GLN
2	E	85	ASN
2	E	106	ASN

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 ⓘ

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	1	3	14,14,15	0.35	0	17,19,21	0.46	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.42	0
3	NAG	G	1	3	14,14,15	0.24	0	17,19,21	0.49	0
3	NAG	G	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	NAG	H	1	1,3	14,14,15	0.43	0	17,19,21	0.57	0
3	NAG	H	2	3	14,14,15	0.22	0	17,19,21	0.50	0
3	NAG	I	1	1,3	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	I	2	3	14,14,15	0.20	0	17,19,21	0.36	0
3	NAG	J	1	1,3	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	J	2	3	14,14,15	0.22	0	17,19,21	0.40	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

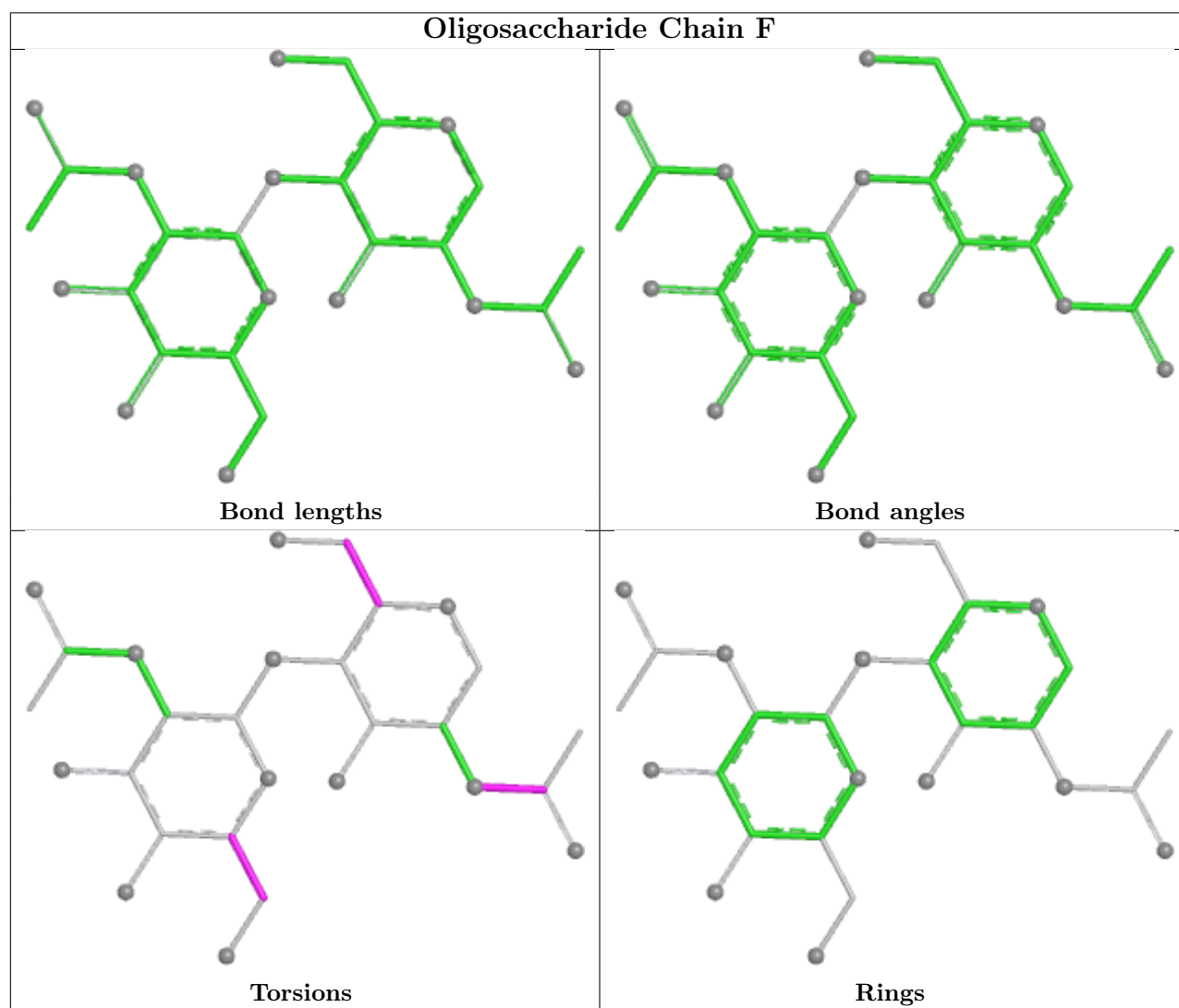
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	G	1	NAG	C8-C7-N2-C2
3	G	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	J	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	J	2	NAG	C1-C2-N2-C7

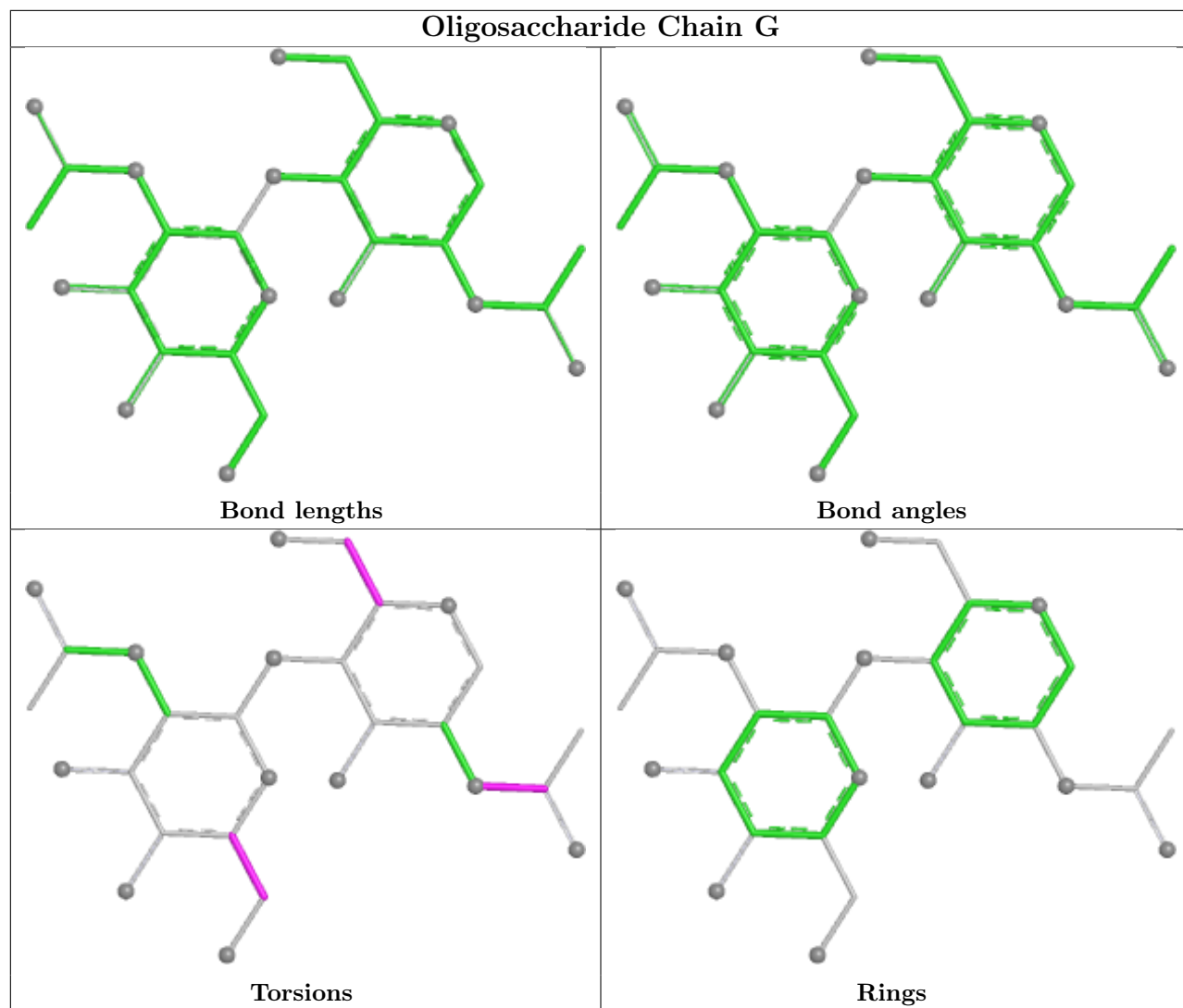
There are no ring outliers.

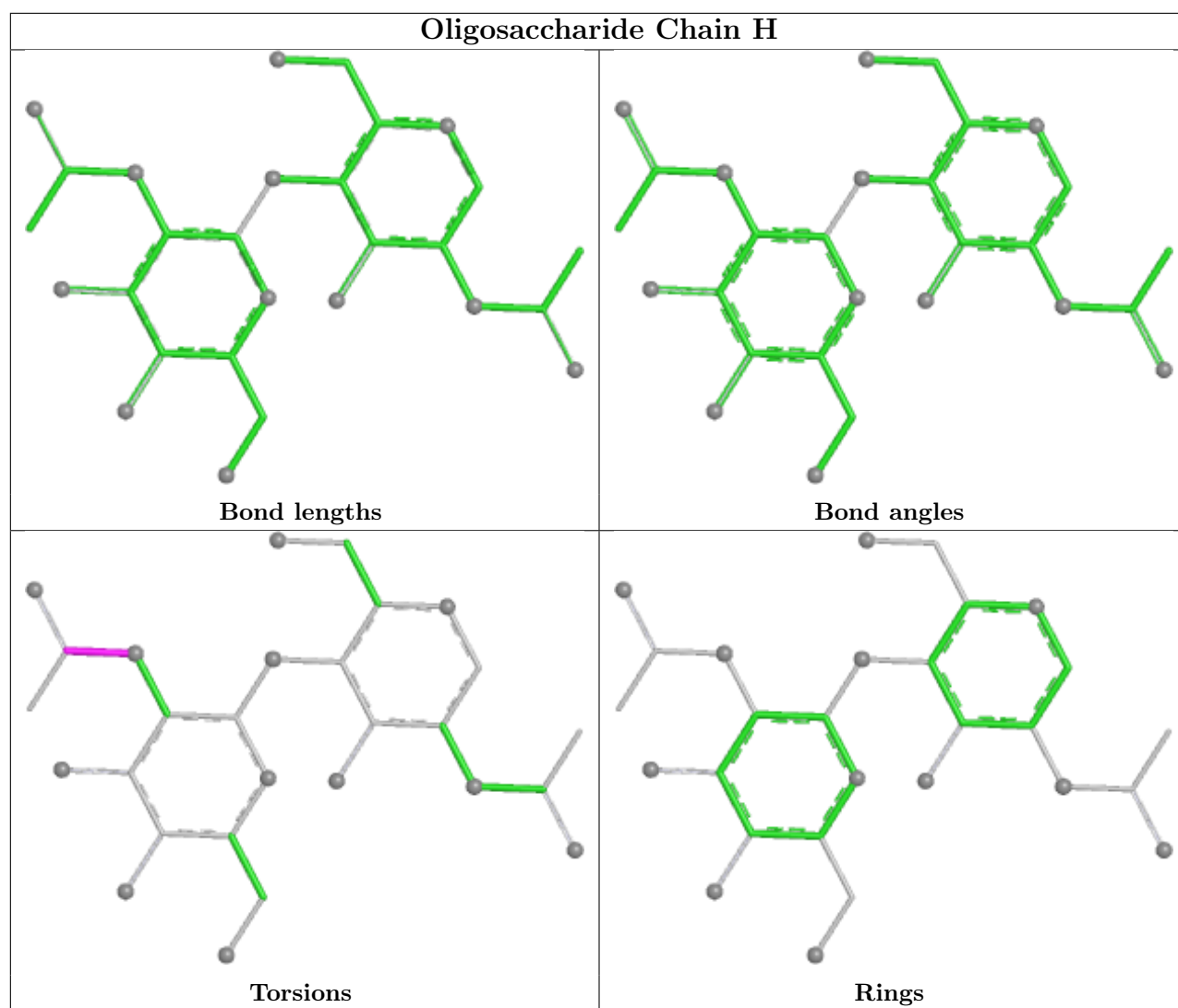
6 monomers are involved in 7 short contacts:

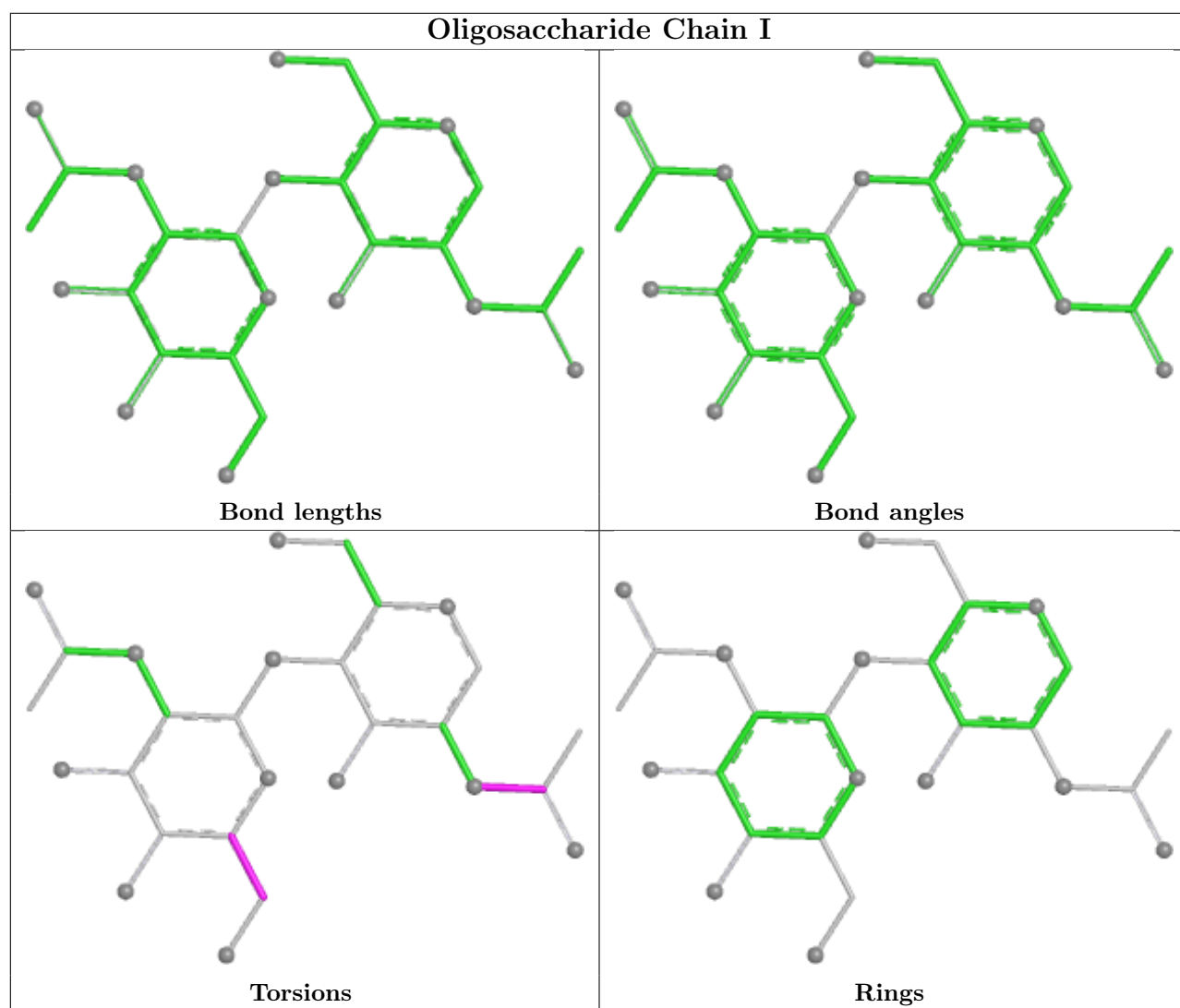
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2	NAG	1	0
3	F	1	NAG	1	0
3	I	1	NAG	2	0
3	H	1	NAG	3	0
3	J	2	NAG	1	0
3	J	1	NAG	1	0

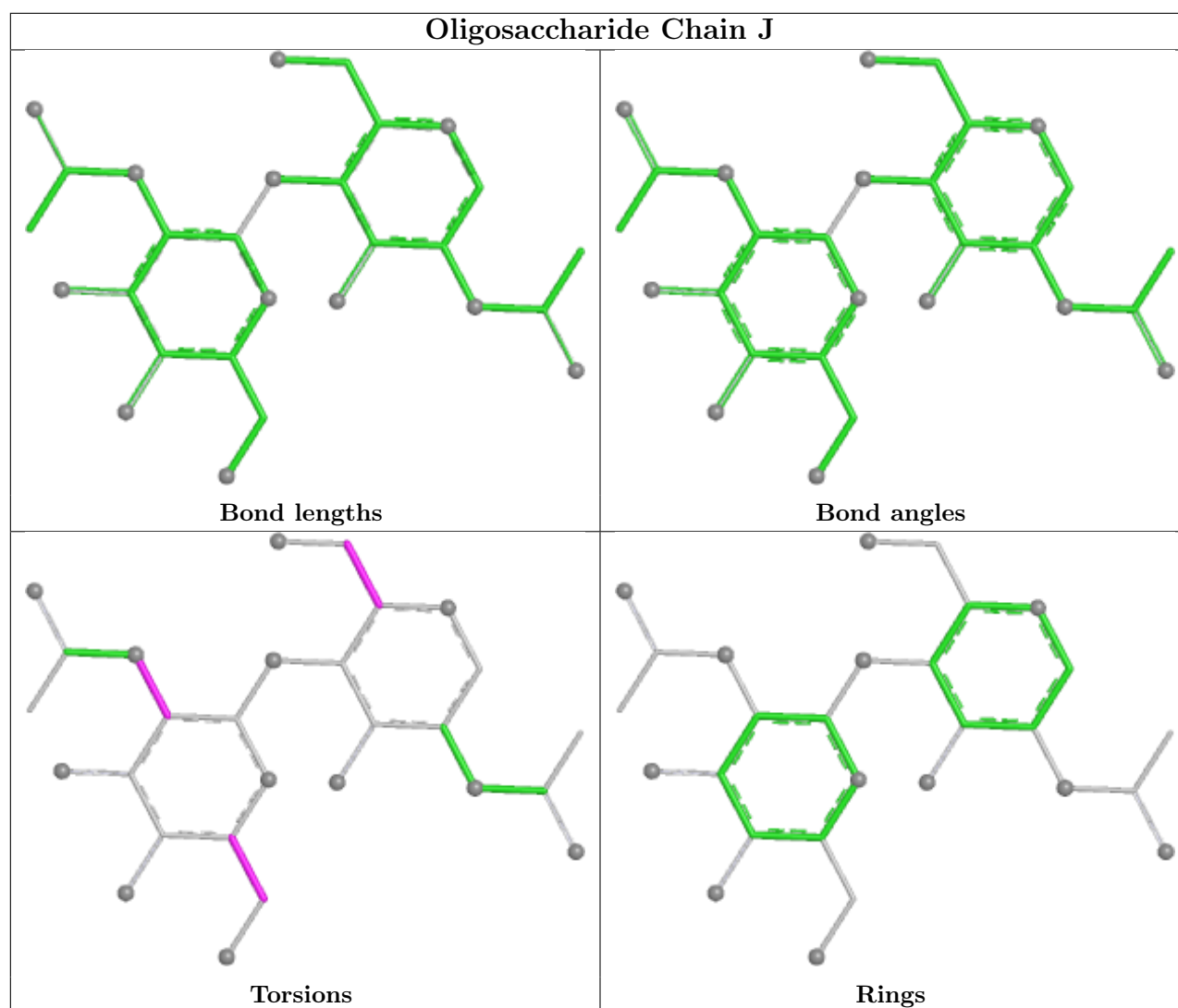
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
4	NAG	B	1308	1	14,14,15	0.17	0	17,19,21	0.59	0
4	NAG	C	1302	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	A	1312	-	14,14,15	0.21	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1301	1	14,14,15	0.32	0	17,19,21	0.44	0
4	NAG	B	1313	1	14,14,15	0.17	0	17,19,21	0.51	0
4	NAG	A	1314	1	14,14,15	0.24	0	17,19,21	0.64	1 (5%)
4	NAG	B	1304	1	14,14,15	0.19	0	17,19,21	0.93	1 (5%)
4	NAG	B	1303	-	14,14,15	0.19	0	17,19,21	0.54	0
4	NAG	B	1305	-	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	A	1313	1	14,14,15	0.16	0	17,19,21	0.62	1 (5%)
4	NAG	C	1306	1	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	A	1307	1	14,14,15	0.48	0	17,19,21	0.85	1 (5%)
4	NAG	B	1301	1	14,14,15	0.50	0	17,19,21	0.72	0
4	NAG	A	1308	1	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	B	1312	1	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	B	1311	1	14,14,15	0.26	0	17,19,21	0.54	0
4	NAG	B	1310	-	14,14,15	0.26	0	17,19,21	0.52	0
4	NAG	C	1304	-	14,14,15	0.26	0	17,19,21	0.47	0
4	NAG	B	1302	-	14,14,15	0.21	0	17,19,21	0.47	0
4	NAG	C	1305	1	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	A	1310	1	14,14,15	0.25	0	17,19,21	0.37	0
4	NAG	A	1311	1	14,14,15	0.37	0	17,19,21	0.53	0
4	NAG	A	1306	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	B	1307	1	14,14,15	0.57	0	17,19,21	0.74	1 (5%)
4	NAG	A	1302	-	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	B	1309	1	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	C	1303	1	14,14,15	0.17	0	17,19,21	0.44	0
4	NAG	A	1304	1	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	B	1306	-	14,14,15	0.28	0	17,19,21	0.55	0
4	NAG	A	1303	-	14,14,15	0.35	0	17,19,21	0.37	0
4	NAG	A	1305	-	14,14,15	0.17	0	17,19,21	0.49	0
4	NAG	A	1301	-	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	A	1309	1	14,14,15	0.32	0	17,19,21	0.55	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	B	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1312	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1303	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1313	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1312	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1310	-	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	-	-	3/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1311	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1302	-	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1303	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1305	-	-	3/6/23/26	0/1/1/1
4	NAG	A	1301	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1307	NAG	C1-O5-C5	3.08	116.32	112.19
4	B	1304	NAG	C2-N2-C7	2.81	126.67	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1307	NAG	C1-O5-C5	2.56	115.61	112.19
4	A	1314	NAG	C1-O5-C5	2.10	115.00	112.19
4	A	1313	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1307	NAG	C1-C2-N2-C7
4	B	1306	NAG	C3-C2-N2-C7
4	B	1310	NAG	C1-C2-N2-C7
4	B	1313	NAG	O5-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1311	NAG	O5-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1311	NAG	O5-C5-C6-O6
4	A	1314	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	A	1312	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	A	1311	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	C	1304	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	B	1313	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1311	NAG	C4-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	A	1312	NAG	C4-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	C	1304	NAG	C4-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	B	1309	NAG	C4-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	A	1314	NAG	C4-C5-C6-O6
4	A	1302	NAG	C8-C7-N2-C2
4	A	1302	NAG	O7-C7-N2-C2
4	B	1303	NAG	C8-C7-N2-C2
4	B	1303	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	1304	NAG	C8-C7-N2-C2
4	B	1304	NAG	O7-C7-N2-C2
4	B	1308	NAG	C8-C7-N2-C2
4	B	1308	NAG	O7-C7-N2-C2
4	C	1305	NAG	C8-C7-N2-C2
4	C	1305	NAG	O7-C7-N2-C2
4	B	1301	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	B	1302	NAG	O5-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	B	1302	NAG	C3-C2-N2-C7
4	B	1305	NAG	C3-C2-N2-C7
4	C	1306	NAG	C3-C2-N2-C7
4	A	1309	NAG	C4-C5-C6-O6
4	A	1305	NAG	C4-C5-C6-O6
4	B	1305	NAG	C1-C2-N2-C7
4	C	1306	NAG	C1-C2-N2-C7
4	A	1305	NAG	O5-C5-C6-O6
4	B	1304	NAG	C3-C2-N2-C7
4	B	1307	NAG	C3-C2-N2-C7
4	B	1312	NAG	C3-C2-N2-C7
4	C	1301	NAG	C3-C2-N2-C7
4	C	1303	NAG	C3-C2-N2-C7
4	A	1309	NAG	O5-C5-C6-O6
4	B	1302	NAG	C4-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	A	1308	NAG	C1-C2-N2-C7
4	A	1313	NAG	C1-C2-N2-C7
4	B	1304	NAG	C1-C2-N2-C7
4	B	1312	NAG	C1-C2-N2-C7
4	C	1303	NAG	C1-C2-N2-C7
4	A	1303	NAG	C3-C2-N2-C7
4	A	1305	NAG	C3-C2-N2-C7
4	A	1308	NAG	C3-C2-N2-C7
4	B	1310	NAG	C3-C2-N2-C7

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1302	NAG	1	0
4	C	1301	NAG	2	0
4	B	1304	NAG	3	0
4	A	1313	NAG	1	0
4	C	1306	NAG	2	0
4	B	1301	NAG	3	0
4	A	1308	NAG	2	0
4	B	1311	NAG	1	0
4	B	1310	NAG	1	0
4	B	1302	NAG	3	0
4	A	1310	NAG	2	0
4	A	1311	NAG	2	0
4	B	1307	NAG	1	0
4	B	1306	NAG	1	0
4	A	1309	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	C	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	528:LYS	C	529:LYS	N	5.56
1	A	458:LYS	C	459[B]:SER	N	3.08
1	A	458:LYS	C	459[A]:SER	N	3.03
1	B	481:ASN	C	482:GLY	N	2.95

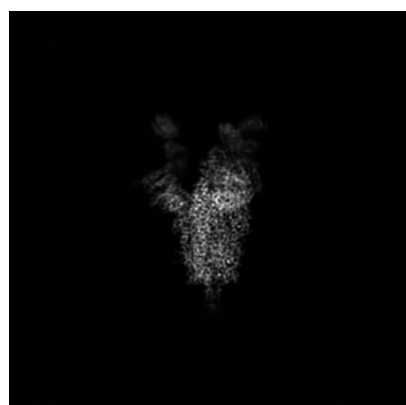
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14313. These allow visual inspection of the internal detail of the map and identification of artifacts.

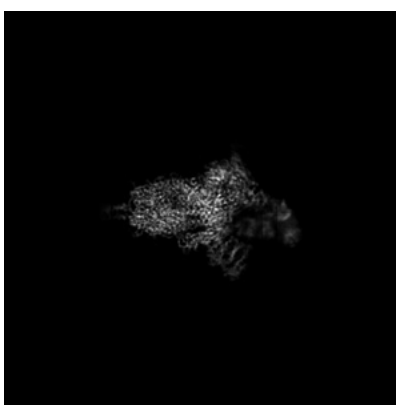
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

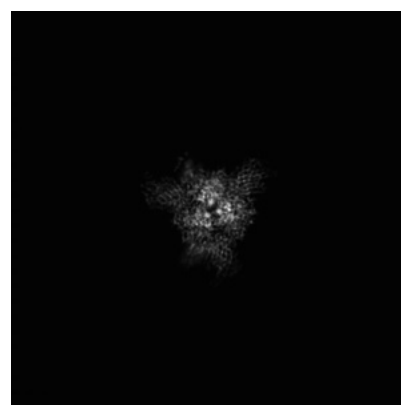
6.1.1 Primary map



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: 246



Y Index: 246



Z Index: 246

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: 243



Y Index: 240

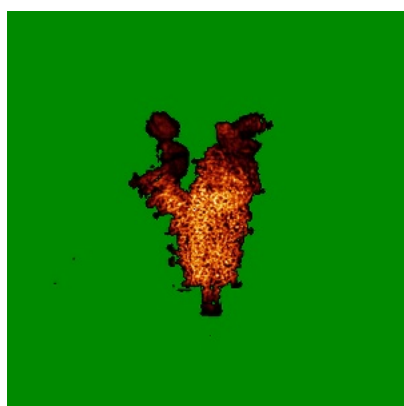


Z Index: 253

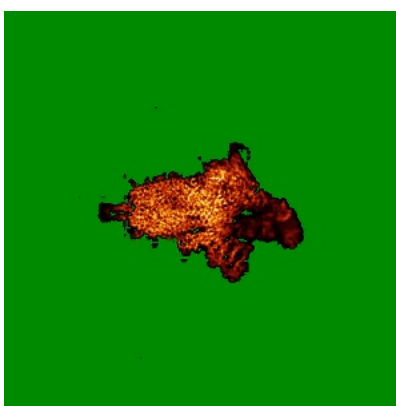
The images above show the largest variance slices of the map in three orthogonal directions.

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

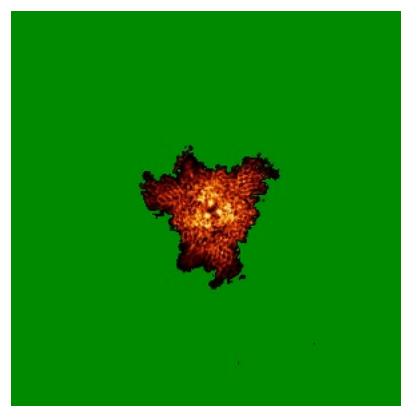
6.4.1 Primary map



X



Y

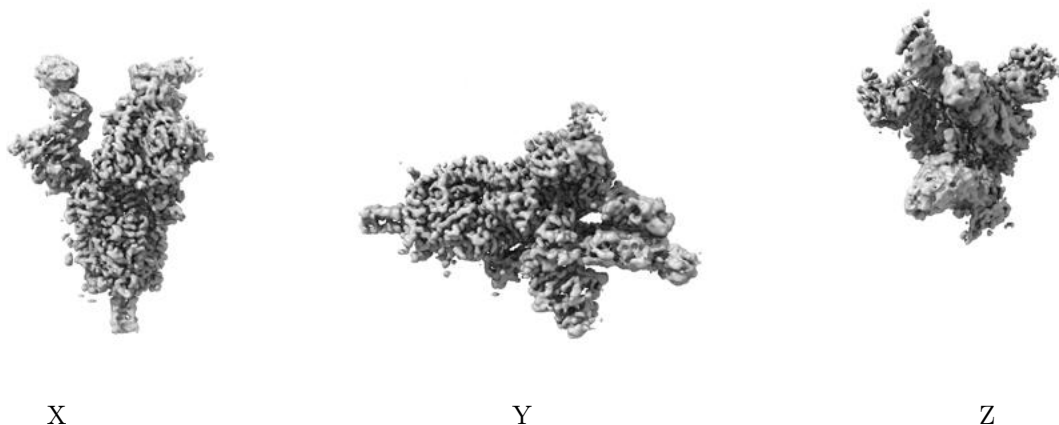


Z

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 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

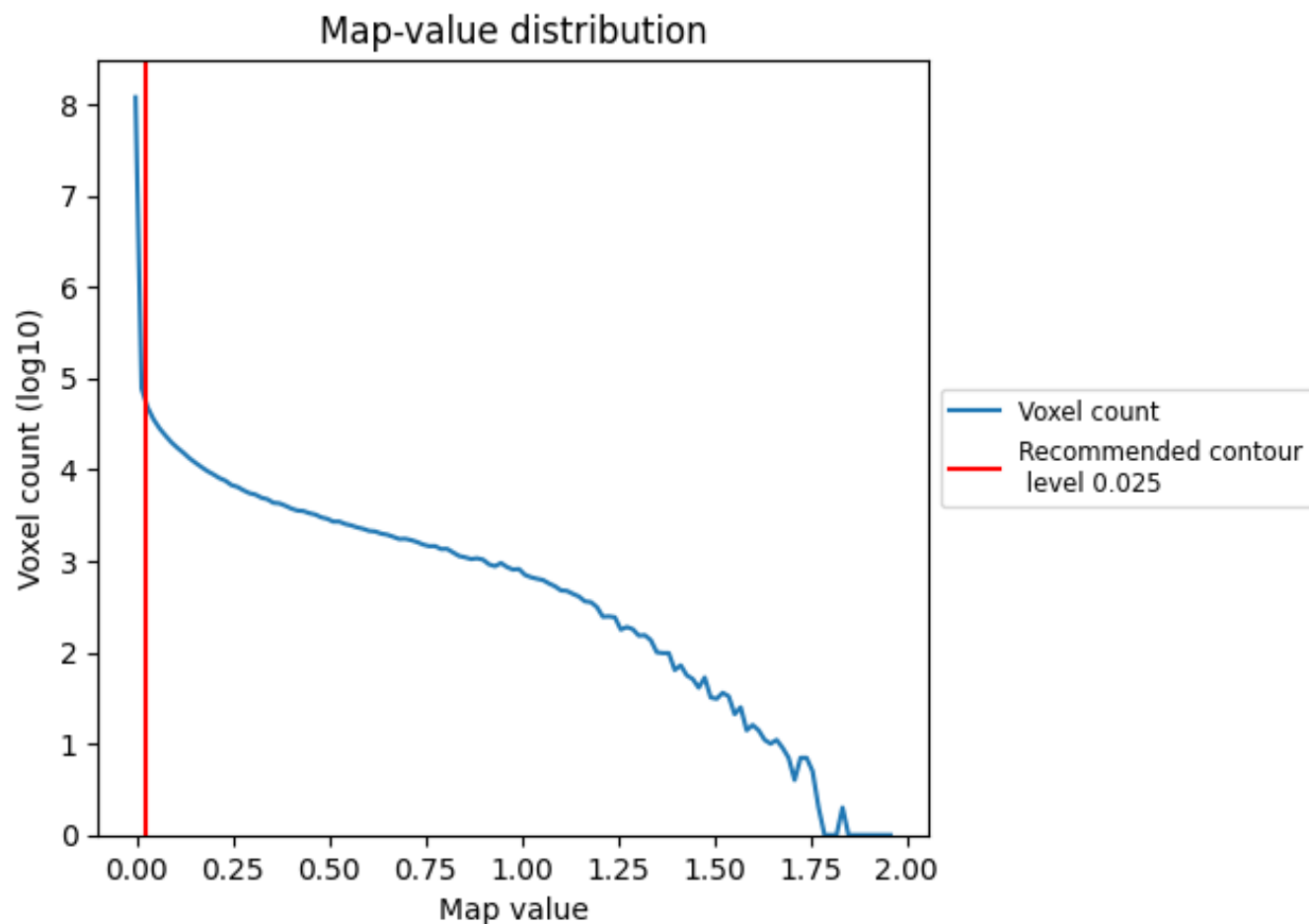
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

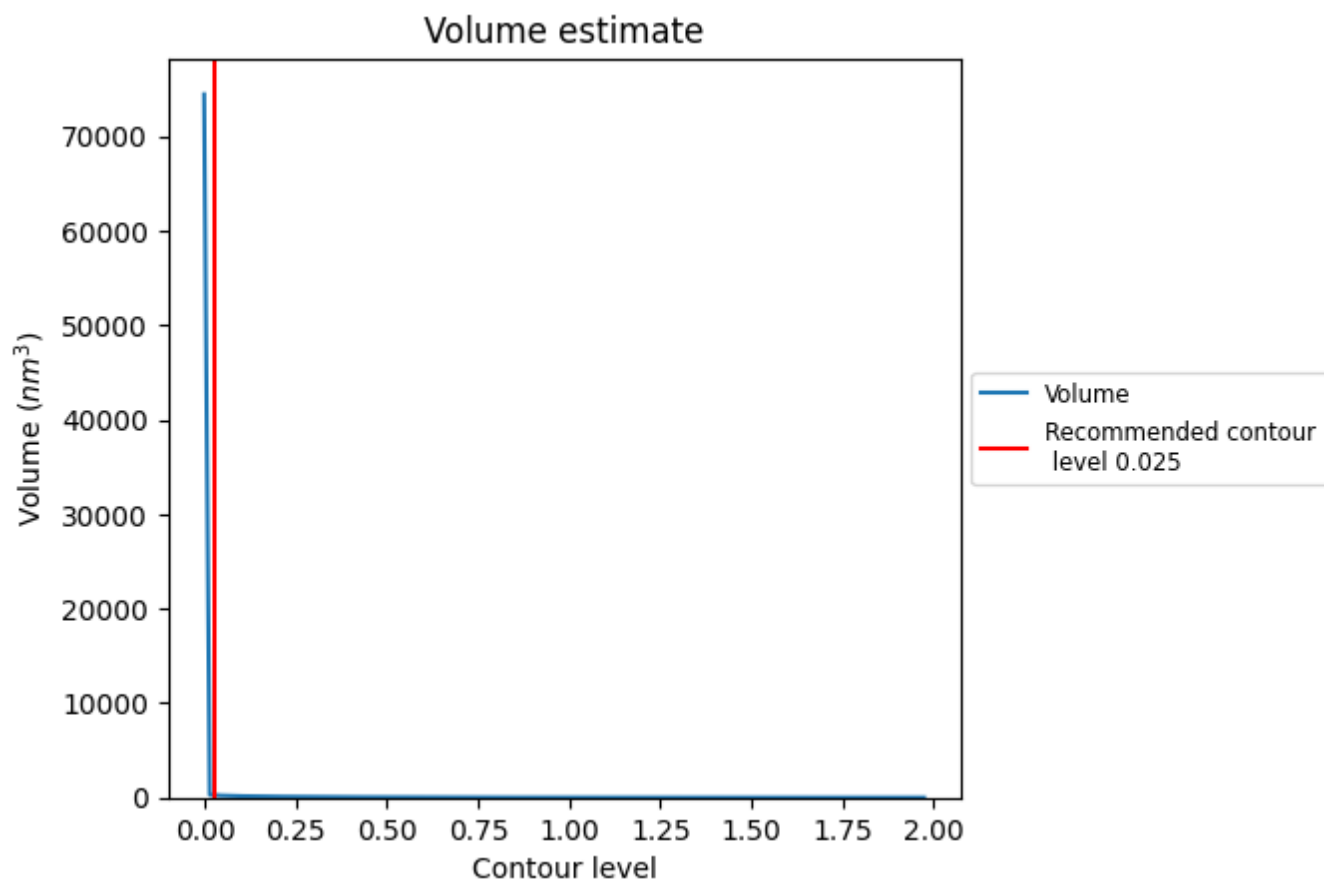
This section contains the results of statistical analysis of the map.

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.

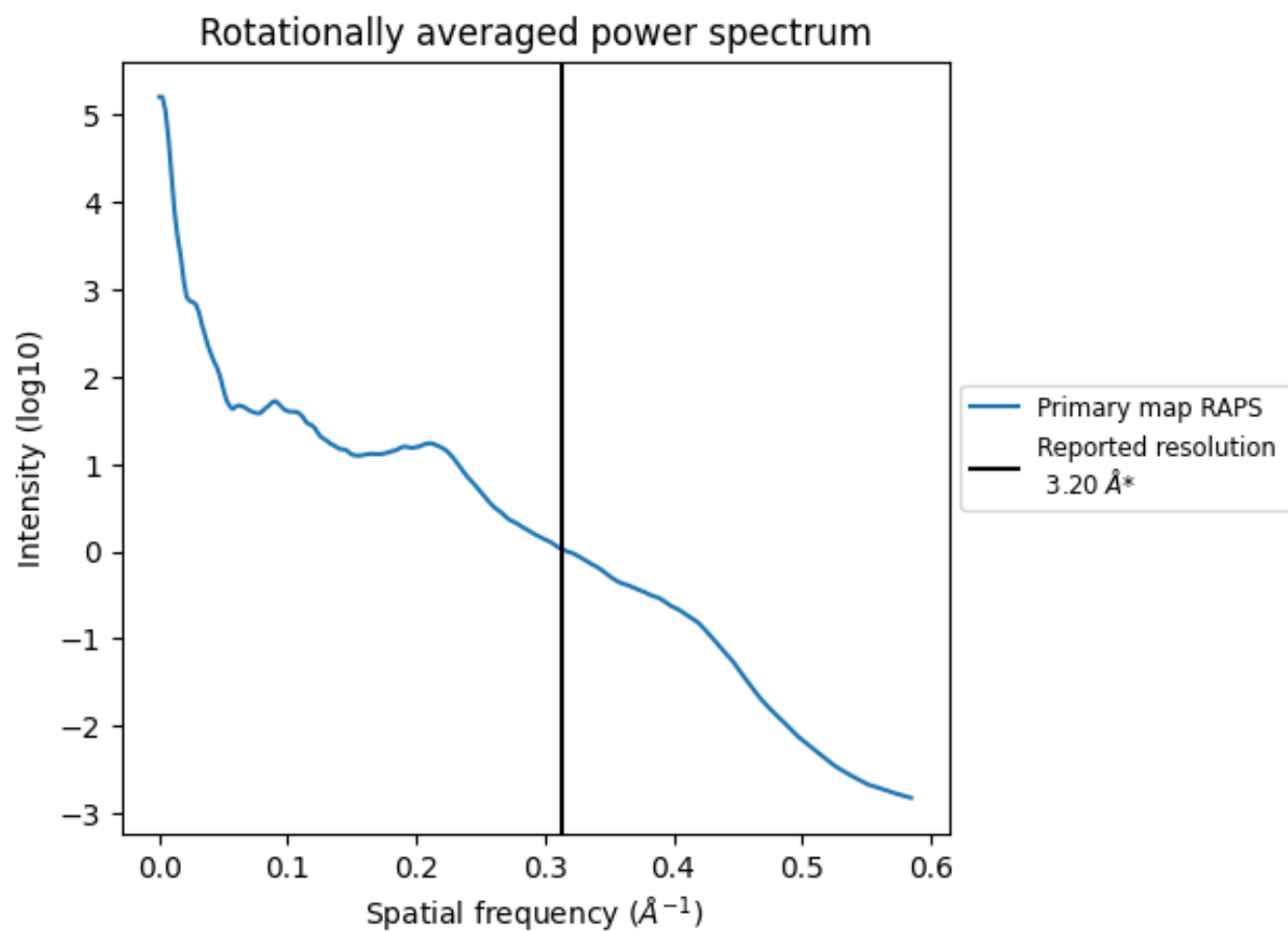
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm^3 ; this corresponds to an approximate mass of 234 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 ⓘ

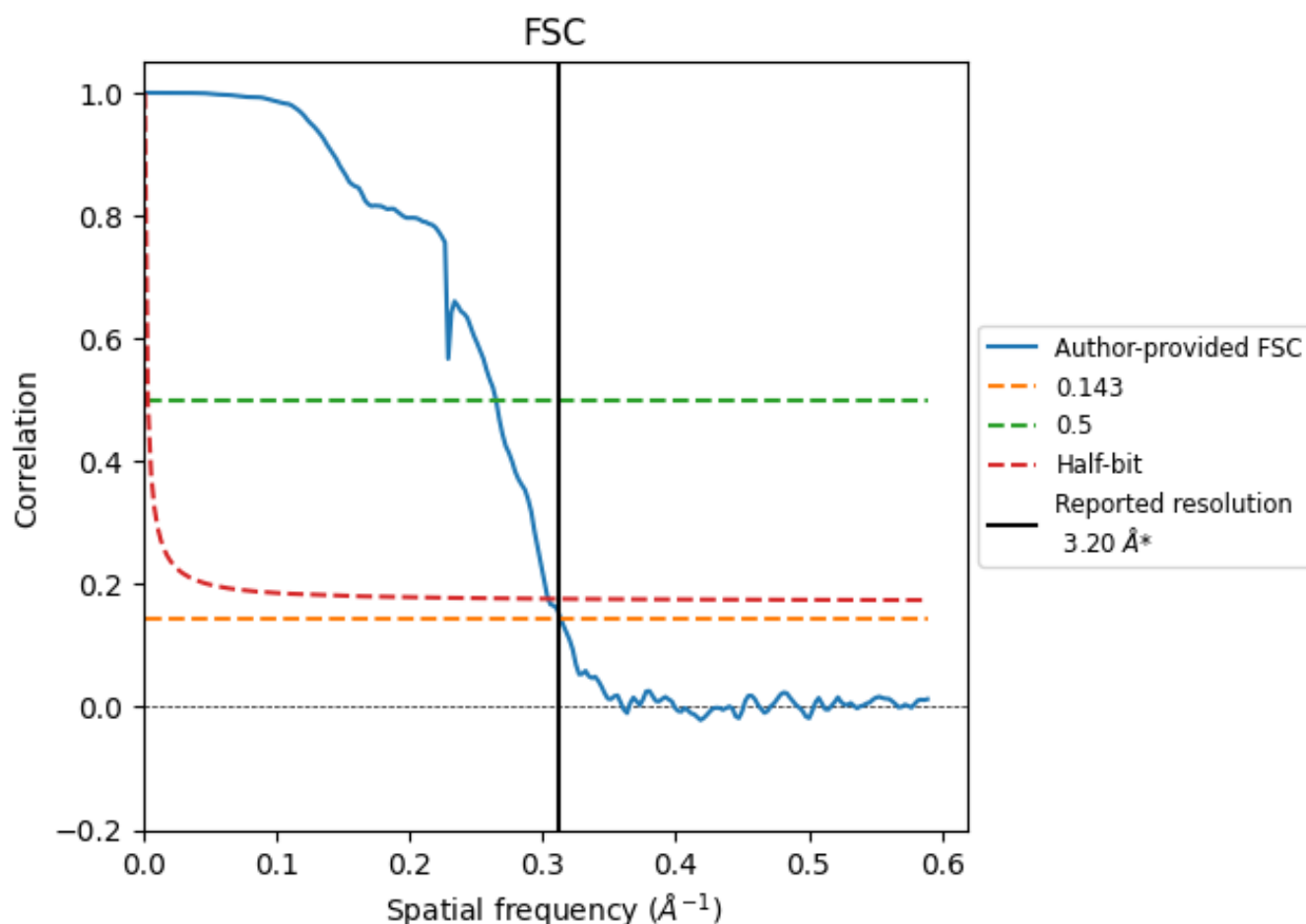


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

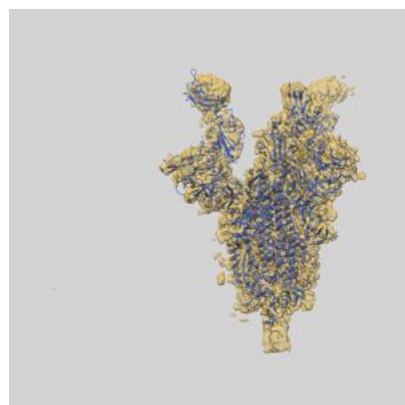
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.77	3.29
Unmasked-calculated*	-	-	-

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

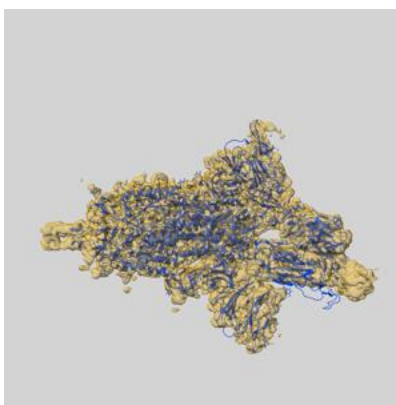
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14313 and PDB model 7R4I. Per-residue inclusion information can be found in section 3 on page 12.

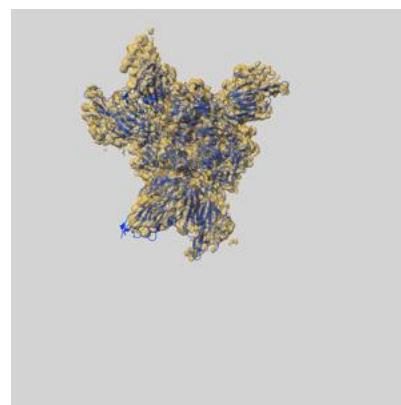
9.1 Map-model overlay [i](#)



X



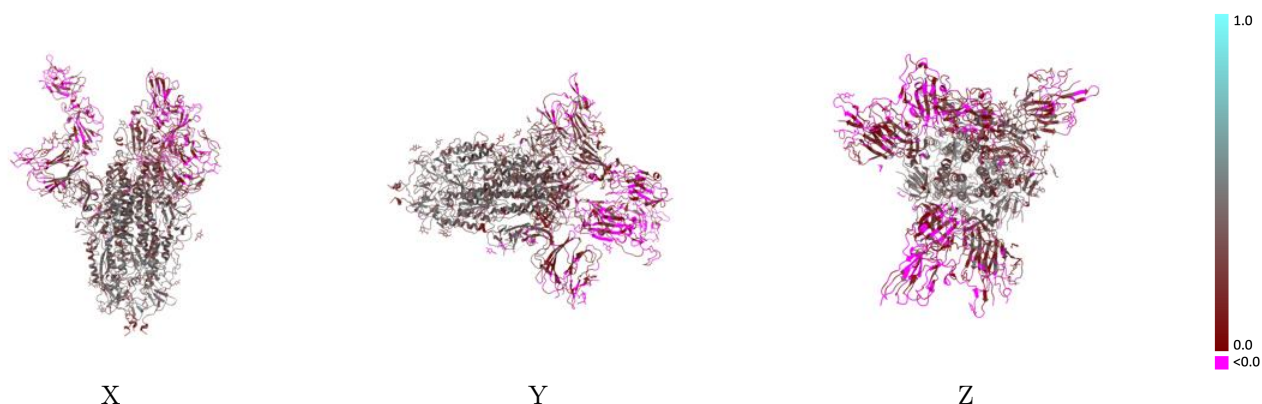
Y



Z

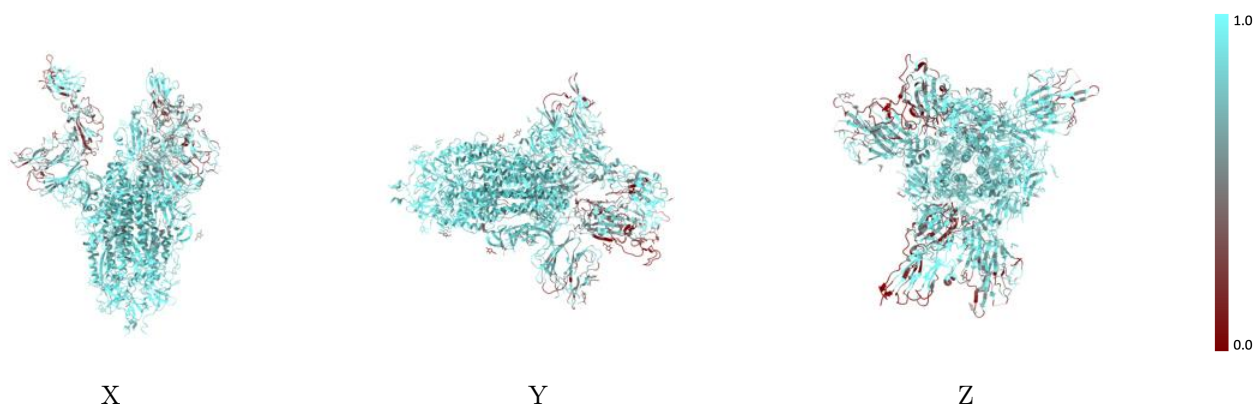
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



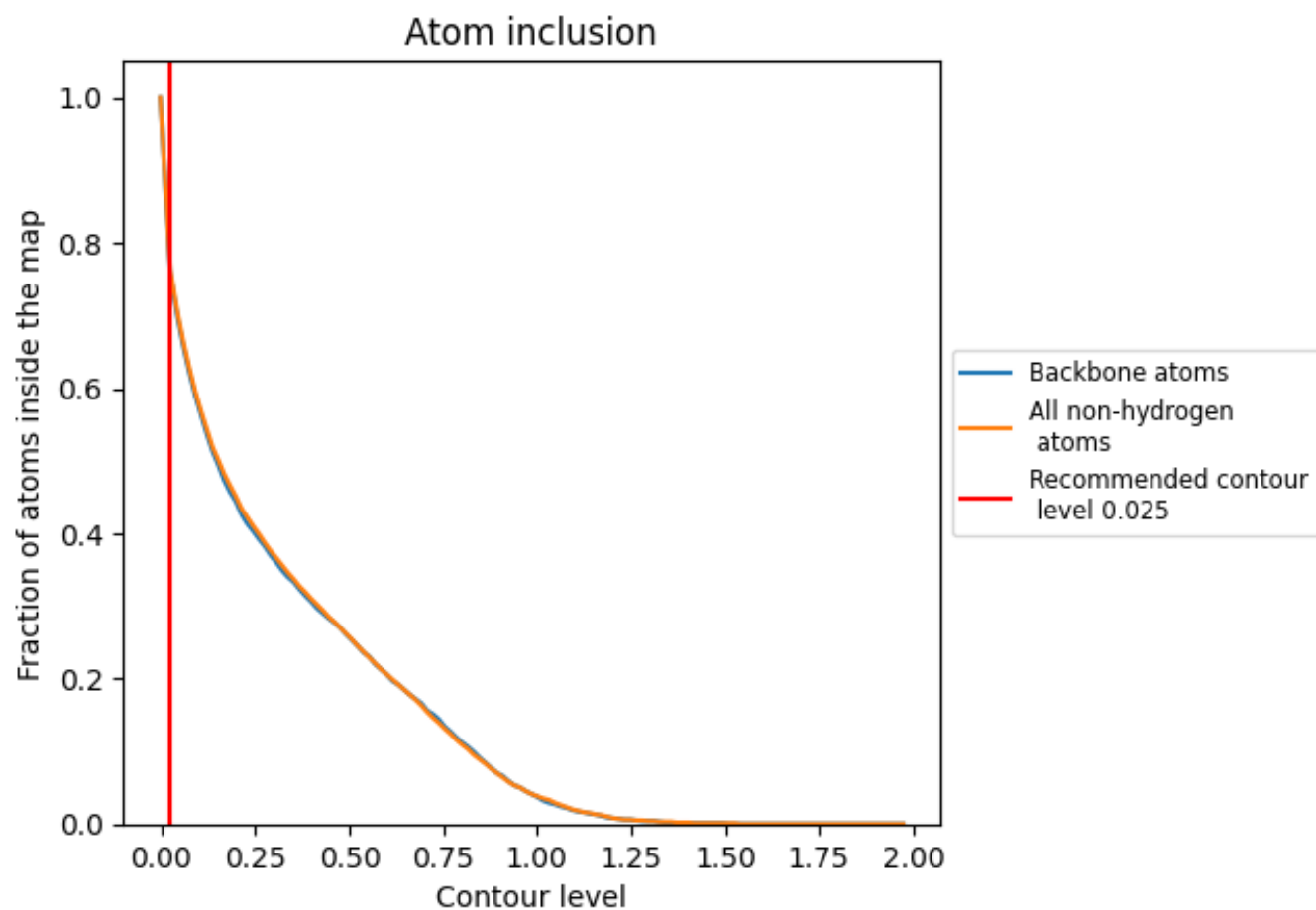
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7630	 0.2410
A	 0.7650	 0.2390
B	 0.8160	 0.2810
C	 0.7520	 0.2540
D	 0.5980	 -0.0080
E	 0.7360	 0.0460
F	 0.6070	 0.0780
G	 0.4640	 0.1390
H	 0.5000	 0.0780
I	 0.6790	 0.1490
J	 0.6430	 0.1650

