



## Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 11:17 AM UTC

PDB ID : 7O7R / pdb\_00007o7r  
EMDB ID : EMD-12754  
Title : (h-alpha2M)4 plasmin-activated I state  
Authors : Luque, D.; Goulas, T.; Mata, C.P.; Mendes, S.R.; Gomis-Ruth, F.X.; Caston, J.R.  
Deposited on : 2021-04-13  
Resolution : 3.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

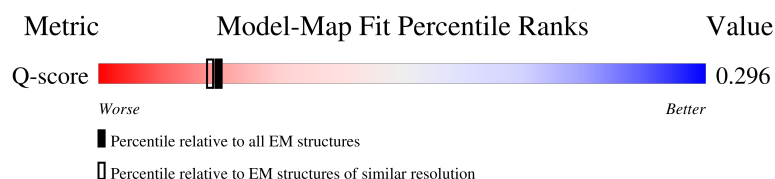
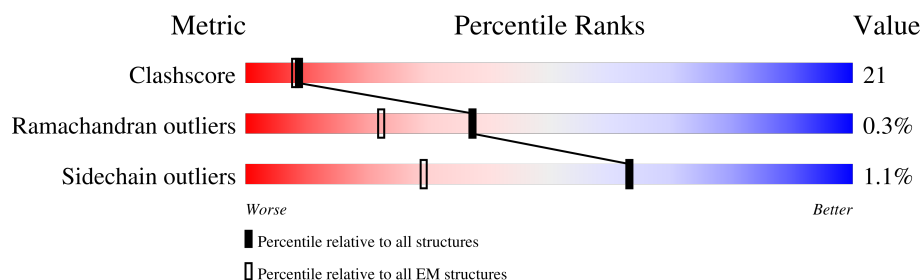
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 3.90 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	8855 ( 3.40 - 4.40 )

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  $\geq 3$ , 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	1474	<div> <div>13%</div> <div>53%</div> <div>34%</div> <div>13%</div> </div>
1	B	1474	<div> <div>9%</div> <div>49%</div> <div>37%</div> <div>13%</div> </div>
1	C	1474	<div> <div>12%</div> <div>52%</div> <div>35%</div> <div>13%</div> </div>
1	D	1474	<div> <div>10%</div> <div>51%</div> <div>35%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	2	
2	G	2	
2	I	2	
2	K	2	
3	F	3	
3	H	3	
3	J	3	
3	L	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	H	1	-	-	X	-

## 2 Entry composition [i](#)

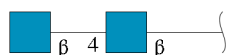
There are 4 unique types of molecules in this entry. The entry contains 40530 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-2-macroglobulin.

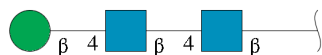
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0
			10023	6375	1681	1924	43		
1	B	1278	Total	C	N	O	S	0	0
			9968	6336	1674	1915	43		
1	C	1285	Total	C	N	O	S	0	0
			10023	6375	1681	1924	43		
1	D	1278	Total	C	N	O	S	0	0
			9968	6336	1674	1915	43		

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



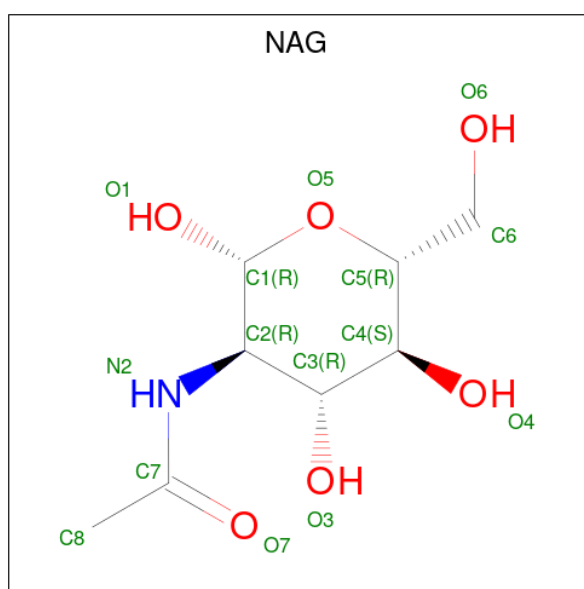
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		

- 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	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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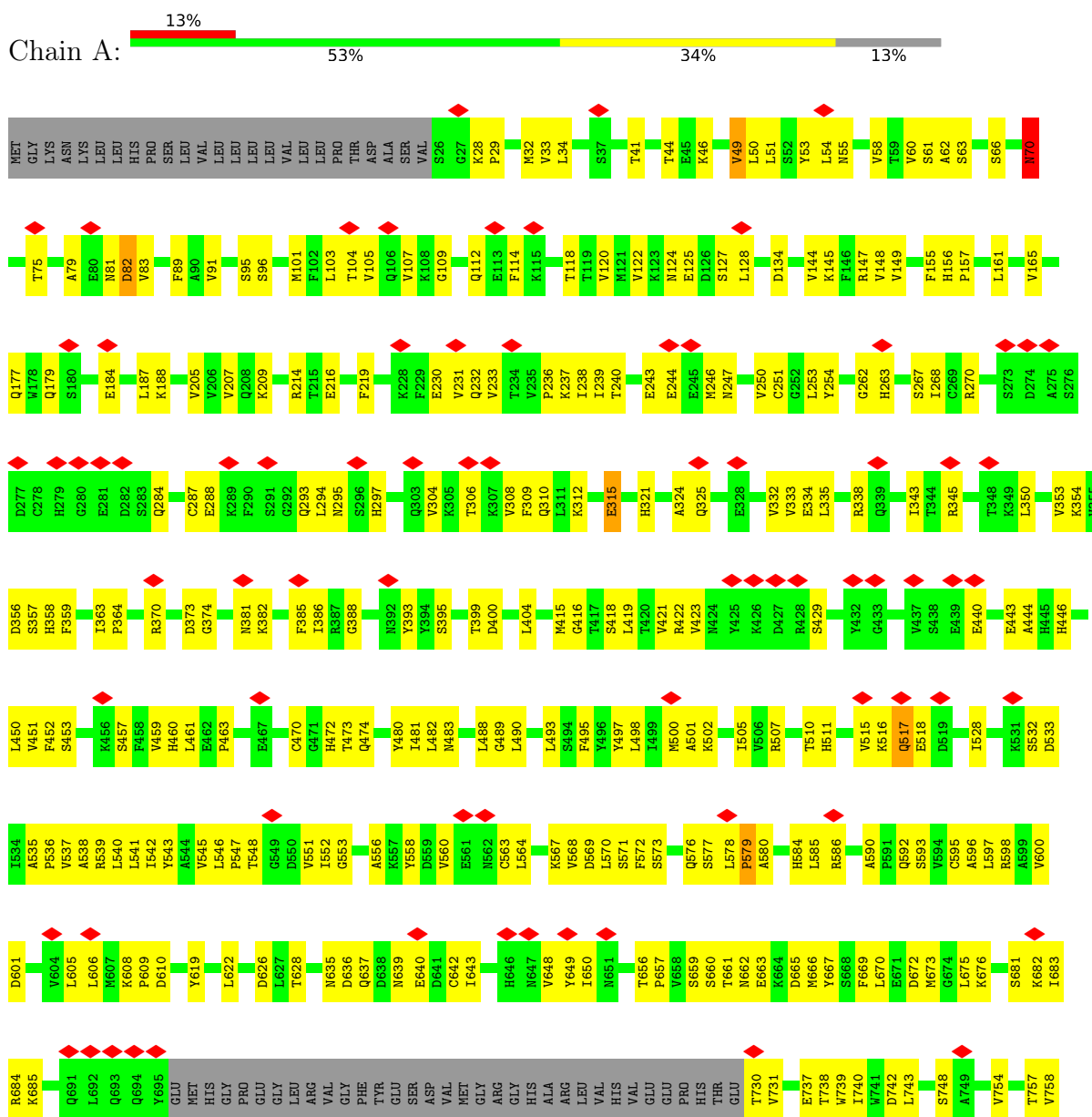
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

### 3 Residue-property plots

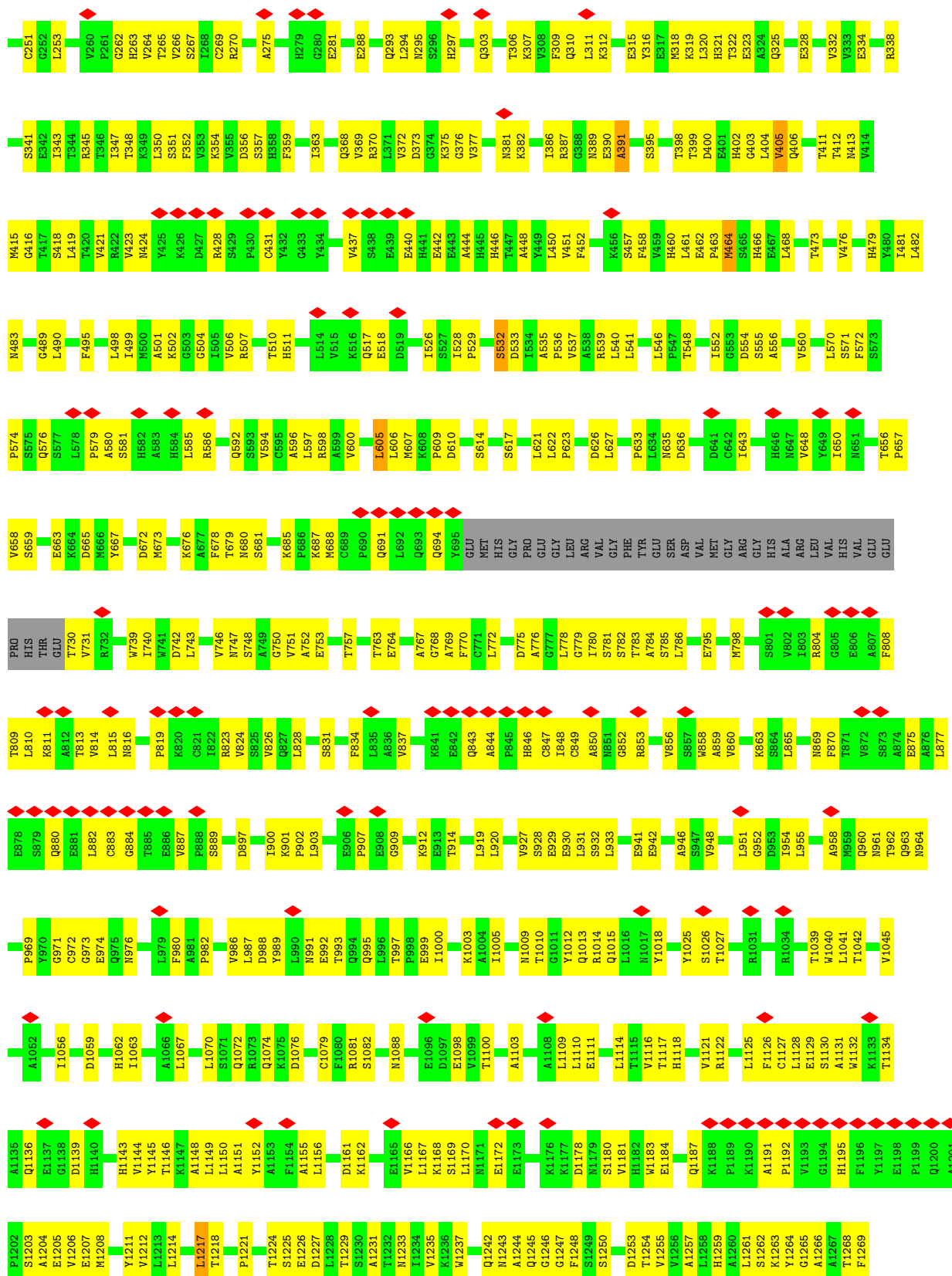
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

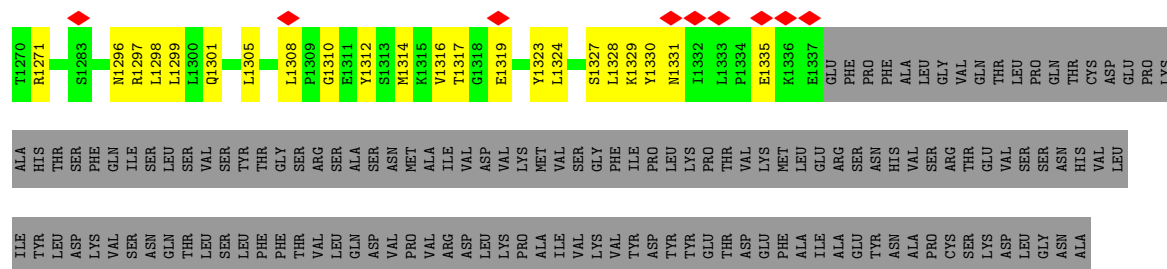
#### • Molecule 1: Alpha-2-macroglobulin



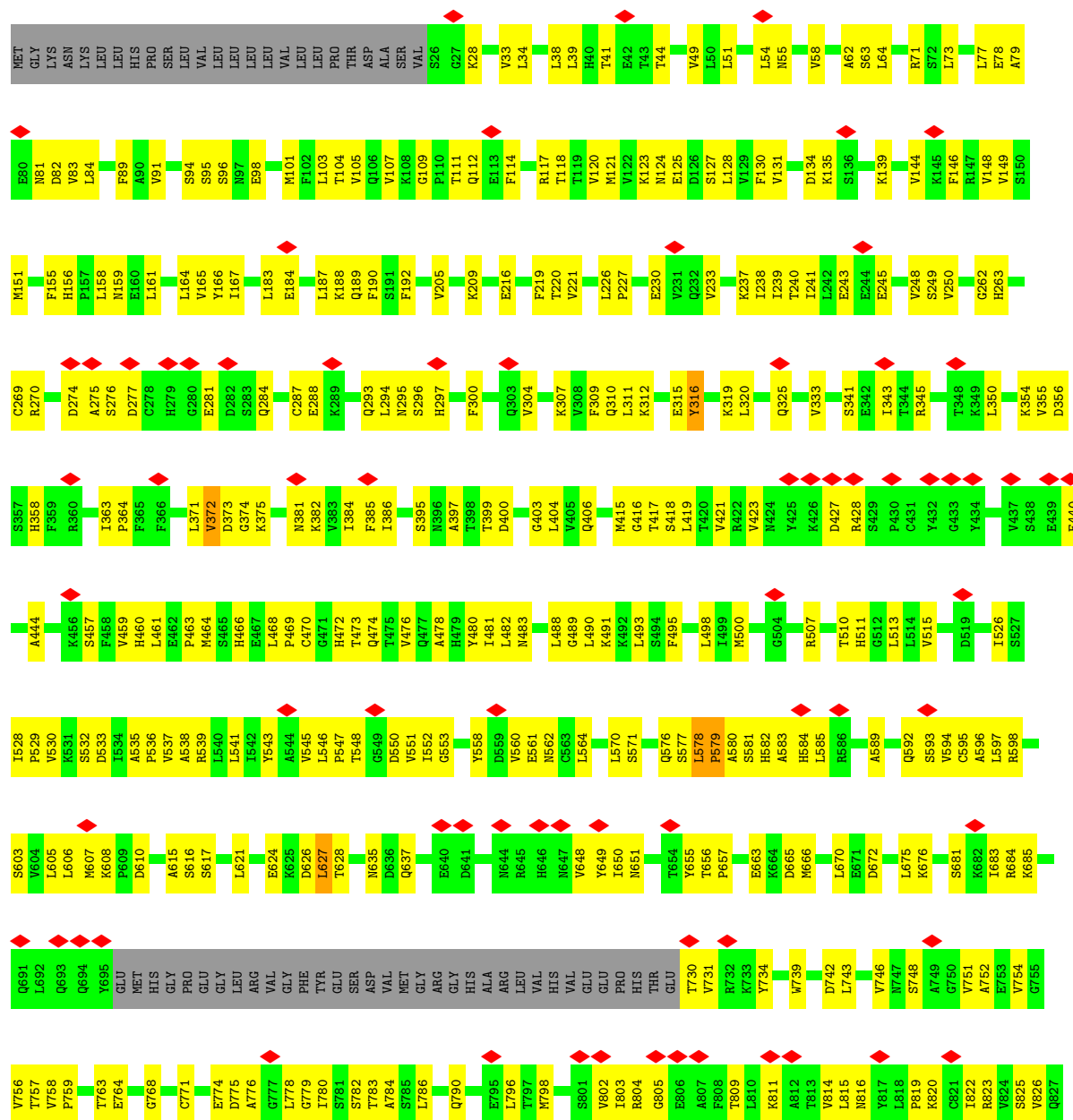








# • Molecule 1: Alpha-2-macroglobulin





VAL	T1232	L1156	L1067	V978	L903	A836	E753	Q693	E612	D533	L450	V369
SER	M1233	L1162	I1068	L979	L904	V837	V756	Q694	L613	I534	L451	V369
GLY	I1234	K1162	S1071	E906	E906	P838	T757	Y695	S614	A535	V451	D373
ILE	Y1235	E1165	Q1072	P907	P907	V839	D760	GLU	S617	P536	S453	
PRO	M1237	V1166	R1073	E908	E908	E840	T761	HIS	L621	V537	K456	N381
LEU	I1238	L1167	Q1074	E992	E909	K841	I762	GLY	P623	A538	V457	K382
LYS	T1239	K1168	D1076	Q994	L910	E842	T763	PRO	L622	L540	F458	V383
PRO	K1240	L1168	D1077	Q995	E911	E843	E764	GLY	L541	L541	V459	I384
THR	Q1241	L1168	G1078	Q995	E911	E844	E765	LEU	P631	I542	H460	F385
VAL	Q1242	E1172	T997	L996	K912	E845		ARG	G832	V545	L461	I386
LYS	N1243	E1173	M1088	P998	E913	P844	G768	VAL	P633	L546	E462	K387
ALA	A1244	D1178	M1089	P998	T915	H846	A769	GLY	D636	P547	M464	G388
GLU	G1247	N1179	V1095	I1000	F916	E847	F770	PHE	Q637	T548	S465	Y393
ARG	T1251	S1180	E1096	K1001	N917	E848	C771	TYR	D638	V551	H466	S395
SER	G1252	E1096	D1097	K1003	S918	A850	L778	GLU	C642	I552	E467	N396
ASN	D1253	D1097	T1100	A1004	L919	E852	G779	ASP	H645	G553	L468	A397
VAL	T1254	E1184	I1101	I1005	L920	G852	I780	VAL	N647	D554	P469	T399
SER	V1255	Q1187	S1102	L1008	V927	R853	S781	MET	H645	S555	T473	D400
ARG	H1259	K1188	A1103	N1009	S928	Q854	T782	GLY	N647	D569	T473	T411
GLN	S1262	P1189	Y1104	T1010	E929	T783	V648	ARG	Q474	L570	Q474	T412
VAL	K1263	K1190	I1105	G1011	E930	A784	A784	GLY	Y649	Y558	V476	M415
SER	G1264	A1191	T1106	Y1012	L931	S785	S785	HIS	I650	D559	V476	L417
THR	G1265	P1192	Q1013	S932	L933	S857	L786	ALA	N651	V560		L419
CYS	T1268	A1193	R1014	N938	V939	A859	A788	LEU	T654	V568	L481	L420
VAL	F1269	G1194	Q1015	Q1015	V940	F789	Q790	HIS	Y655	L570	L482	V421
LEU	T1270	H1195	L1016	L1016	E941	F791	P791	THR	Y657	S571	T486	M415
LYS	R1271	F1196	N1017	N1017	E942	S864	L796	GLU	P657	Q576	L490	G416
ALA	T1272	Y1197	Y1025	Y1025	S943	L865	T797	PRO	V658	S577	L490	T417
SER	G1273	E1198	S1026	S1026	S944	L865	L797	HIS	S659	L578	F495	S418
THR	P1200	P1199	T1027	T1027	A944	R869	M798	THR	S660	A580		L419
GLN	Q1200	Q1200	E1030	E1030	R945	T870	M798	GLU	N662	L585	L498	T420
ASN	A1201	F1126	R1031	R1031	S947	V872	L803	VAL	E663	L585	I505	R422
THR	C1127	C1127	Y1032	Y1032	Y948	S873	R804	THR	K654	M500	V506	V422
LEU	L1128	L1128	G1033	G1033	S949	A874	G805	GLU	D665	A501	K502	M424
SER	E1129	E1129	R1034	R1034	V960	E875	E806	GLU	F669	R586	I505	Y425
VAL	S1130	S1130	M1035	M1035	L951	A876	A807	THR	M673	A589	K426	Y425
LEU	A1131	A1131	Q1036	Q1036	L955	L877	F808	GLU	G674	A590	K426	K426
SER	T1134	T1134	N1038	N1038	G956	E878	T809	GLU	L675	P591	D427	D427
VAL	E1137	E1137	T1039	T1039	S957	S879	L810	THR	K676	Q592	R428	R428
GLN	H1140	H1140	M1040	M1040	A958	Q880	K811	GLU	A677	S593	S429	S429
ASP	V1144	V1144	T1042	T1042	Q960	E881	A812	GLU	F678	V594	P430	P430
PRO	M1313	M1313	L1041	L1041	N961	L882	N816	VAL	T679	C595	C431	C431
VAL	M1314	M1314	K1047	K1047	T962	C883	L818	GLU	N880	A596	Y432	Y432
ARG	K1315	K1315	T1046	T1046	Q963	C884	P819	VAL	S881	R598	G433	G433
ASP	V1316	V1316	I1056	I1056	N964	T885	P819	GLU	K685	V604	Y434	Y434
LEU	T1317	T1317	D1059	D1059	Q967	E886	R823	GLU	K687	L605	Q435	Q435
LYS	T1224	T1224	H1062	H1062	V968	V887	V824	VAL	M688	K608	V437	V437
VAL	S1225	S1225	I1063	I1063	P969	P888	E750	GLU	C689	P609	S438	S438
PRO	Q1325	Q1325	Y1152	Y1152	G973	S889	L828	VAL	Q691	D610	E439	E439
ALA			A1066	A1066	E974	V890	L835	THR	L692	A511	E440	E440
MET						P891	L835	THR	L692		E443	E443
						R695					A444	A444

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

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



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



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



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



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



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





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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	121437	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38.7	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.081	Depositor
Minimum map value	-0.002	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size ( $\text{\AA}$ )	336.64, 336.64, 336.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.052, 1.052, 1.052	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.60	0/10247	0.76	2/13921 (0.0%)
1	B	0.67	3/10189 (0.0%)	0.81	10/13842 (0.1%)
1	C	0.68	3/10247 (0.0%)	0.80	5/13921 (0.0%)
1	D	0.68	4/10189 (0.0%)	0.80	9/13842 (0.1%)
All	All	0.66	10/40872 (0.0%)	0.79	26/55526 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	902	PRO	N-CA	22.76	1.70	1.47
1	B	29	PRO	N-CA	18.84	1.71	1.47
1	D	29	PRO	N-CA	18.55	1.71	1.47
1	D	168	GLN	C-N	-10.66	1.16	1.33
1	C	967	GLN	C-N	-8.26	1.21	1.33
1	B	168	GLN	C-N	-6.70	1.20	1.33
1	D	475	THR	C-N	-6.02	1.25	1.33
1	D	28	LYS	C-N	5.19	1.46	1.33
1	B	28	LYS	C-N	5.18	1.46	1.33
1	C	901	LYS	C-N	5.09	1.45	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	LYS	CA-C-N	15.13	138.75	119.84
1	B	28	LYS	C-N-CA	15.13	138.75	119.84
1	D	28	LYS	CA-C-N	15.02	138.61	119.84
1	D	28	LYS	C-N-CA	15.02	138.61	119.84
1	C	901	LYS	CA-C-N	14.79	140.01	120.79
1	C	901	LYS	C-N-CA	14.79	140.01	120.79
1	C	902	PRO	CA-N-CD	-9.65	98.49	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	PRO	CA-N-CD	-7.97	100.84	112.00
1	D	29	PRO	CA-N-CD	-7.89	100.96	112.00
1	B	991	ASN	CA-CB-CG	-7.56	105.04	112.60
1	B	991	ASN	CB-CA-C	7.38	123.89	109.72
1	B	991	ASN	OD1-CG-ND2	6.79	129.39	122.60
1	B	391	ALA	N-CA-C	-6.77	105.03	113.28
1	A	70	ASN	N-CA-CB	6.67	121.91	111.56
1	D	735	PHE	CA-C-N	6.57	128.06	119.84
1	D	735	PHE	C-N-CA	6.57	128.06	119.84
1	D	761	THR	CB-CA-C	6.38	120.63	111.82
1	B	1246	GLY	N-CA-C	-6.05	105.44	111.85
1	B	235	VAL	N-CA-C	-5.78	104.45	109.19
1	B	53	TYR	CB-CA-C	5.78	121.91	110.42
1	D	951	LEU	N-CA-C	5.61	115.25	107.73
1	C	316	TYR	CA-C-N	5.58	130.89	120.95
1	C	316	TYR	C-N-CA	5.58	130.89	120.95
1	D	951	LEU	CA-C-N	5.28	125.24	121.65
1	D	951	LEU	C-N-CA	5.28	125.24	121.65
1	A	184	GLU	N-CA-C	-5.06	107.18	113.55

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10023	0	9917	407	0
1	B	9968	0	9866	425	0
1	C	10023	0	9917	421	0
1	D	9968	0	9866	415	0
2	E	28	0	25	1	0
2	G	28	0	25	0	0
2	I	28	0	25	3	0
2	K	28	0	25	1	0
3	F	39	0	34	6	0
3	H	39	0	34	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	39	0	34	5	0
3	L	39	0	34	4	0
4	A	70	0	65	13	0
4	B	70	0	65	1	0
4	C	70	0	65	5	0
4	D	70	0	65	5	0
All	All	40530	0	40062	1694	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 21.

All (1694) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:PRO:N	1:D:29:PRO:CA	1.71	1.46
1:C:902:PRO:N	1:C:902:PRO:CA	1.70	1.46
1:B:29:PRO:N	1:B:29:PRO:CA	1.71	1.39
1:C:871:THR:HG22	1:C:900:ILE:HG23	1.15	1.10
4:A:2001:NAG:H3	4:A:2001:NAG:H83	1.34	1.08
3:L:2:NAG:H83	3:L:2:NAG:H3	1.36	1.07
3:F:2:NAG:H83	3:F:2:NAG:H3	1.36	1.06
3:J:2:NAG:H3	3:J:2:NAG:H83	1.34	1.05
1:D:944:ALA:HB1	1:D:1328:LEU:HD11	1.39	1.04
1:A:535:ALA:HB3	1:A:537:VAL:HG12	1.41	1.03
1:B:1271:ARG:NH2	3:H:2:NAG:HN2	1.59	1.01
1:C:871:THR:CG2	1:C:900:ILE:HG23	1.91	1.00
3:H:2:NAG:H3	3:H:2:NAG:H83	1.38	0.99
4:D:2001:NAG:H3	4:D:2001:NAG:H83	1.46	0.97
1:A:579:PRO:HA	1:A:757:THR:HG21	1.49	0.94
1:C:871:THR:HG22	1:C:900:ILE:CG2	1.98	0.93
1:A:517:GLN:HG3	1:A:518:GLU:HG2	1.51	0.92
1:B:29:PRO:HA	1:B:53:TYR:HB2	1.53	0.90
4:A:2003:NAG:H3	4:A:2003:NAG:H83	1.52	0.89
1:B:657:PRO:O	1:C:656:THR:OG1	1.91	0.89
1:A:730:THR:N	1:A:898:THR:HG1	1.70	0.89
1:C:570:LEU:HD11	1:C:585:LEU:HD21	1.55	0.89
1:B:730:THR:HG23	1:B:731:VAL:HG13	1.58	0.85
1:D:967:GLN:HB2	1:D:979:LEU:HD12	1.58	0.84
1:D:1125:LEU:HD23	1:D:1128:LEU:HD12	1.60	0.84
1:A:656:THR:OG1	1:D:657:PRO:O	1.96	0.83
1:B:238:ILE:O	1:B:375:LYS:NZ	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:THR:HG22	1:C:91:VAL:HG11	1.61	0.83
1:C:350:LEU:HD11	1:C:444:ALA:HB2	1.61	0.82
1:A:127:SER:O	1:A:209:LYS:NZ	2.13	0.82
1:C:992:GLU:OE2	1:C:1266:ALA:HB2	1.80	0.81
1:B:127:SER:O	1:B:209:LYS:NZ	2.14	0.81
4:C:2003:NAG:H83	4:C:2003:NAG:H3	1.63	0.81
3:J:1:NAG:H3	3:J:2:NAG:H82	1.62	0.81
1:B:656:THR:OG1	1:C:657:PRO:O	1.99	0.80
1:D:127:SER:O	1:D:209:LYS:NZ	2.13	0.80
1:D:295:ASN:ND2	1:D:297:HIS:O	2.15	0.79
1:B:992:GLU:OE2	3:H:1:NAG:N2	2.15	0.79
1:D:360:ARG:NH2	1:D:459:VAL:O	2.15	0.79
1:D:233:VAL:O	1:D:338:ARG:NH2	2.16	0.78
1:B:598:ARG:NH2	1:B:610:ASP:OD2	2.17	0.78
1:A:1185:ARG:O	1:A:1187:GLN:NE2	2.17	0.78
1:B:955:LEU:HD23	1:B:958:ALA:HB3	1.65	0.78
1:C:1281:GLN:O	1:C:1313:SER:OG	2.00	0.78
1:C:295:ASN:ND2	1:C:297:HIS:O	2.17	0.78
1:A:96:SER:O	1:A:124:ASN:ND2	2.16	0.77
1:B:989:TYR:O	1:B:993:THR:OG1	2.02	0.77
1:D:400:ASP:OD1	1:D:404:LEU:N	2.17	0.77
1:A:637:GLN:O	1:A:684:ARG:NH1	2.17	0.77
1:C:96:SER:O	1:C:124:ASN:ND2	2.17	0.77
1:A:51:LEU:O	1:A:82:ASP:N	2.17	0.77
4:C:2003:NAG:H3	4:C:2003:NAG:C8	2.15	0.77
1:D:994:GLN:CD	1:D:1271:ARG:HD2	2.09	0.77
1:D:1224:THR:OG1	1:D:1227:ASP:OD1	2.02	0.76
1:C:238:ILE:O	1:C:375:LYS:NZ	2.14	0.76
1:D:823:ARG:NH1	1:D:824:VAL:O	2.18	0.76
1:D:938:ASN:ND2	1:D:1335:GLU:OE2	2.19	0.76
1:A:177:GLN:NE2	1:A:179:GLN:OE1	2.18	0.76
1:B:262:GLY:O	1:B:293:GLN:NE2	2.19	0.76
1:A:41:THR:HG22	1:A:91:VAL:HG11	1.67	0.76
1:D:1180:SER:OG	1:D:1233:ASN:O	2.03	0.76
1:A:580:ALA:O	1:A:757:THR:OG1	2.03	0.76
1:A:648:VAL:HG21	1:D:656:THR:HG21	1.66	0.75
1:B:233:VAL:O	1:B:338:ARG:NH2	2.19	0.75
1:A:507:ARG:NH2	1:A:532:SER:O	2.19	0.75
1:B:174:ARG:NH1	1:B:177:GLN:OE1	2.19	0.75
1:B:328:GLU:OE2	1:B:853:ARG:NH2	2.19	0.75
1:C:960:GLN:NE2	1:C:1244:ALA:O	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:LYS:NZ	1:A:1211:TYR:OH	2.20	0.75
1:A:914:THR:N	1:A:1328:LEU:O	2.20	0.75
1:B:243:GLU:O	1:B:306:THR:OG1	2.05	0.75
4:A:2001:NAG:H3	4:A:2001:NAG:C8	2.14	0.75
1:B:386:ILE:N	1:B:395:SER:O	2.20	0.75
1:C:307:LYS:O	1:C:310:GLN:NE2	2.20	0.75
1:C:41:THR:OG1	1:C:125:GLU:OE1	2.04	0.74
1:C:1242:GLN:NE2	1:C:1243:ASN:O	2.19	0.74
1:A:730:THR:HG23	1:A:731:VAL:HG13	1.68	0.74
1:C:227:PRO:O	1:C:603:SER:OG	2.03	0.74
1:D:243:GLU:O	1:D:306:THR:OG1	2.03	0.74
1:A:325:GLN:HA	1:A:332:VAL:HG22	1.69	0.74
1:C:81:ASN:ND2	1:C:82:ASP:OD2	2.20	0.74
1:C:570:LEU:HD21	1:C:585:LEU:HD11	1.67	0.74
1:D:51:LEU:O	1:D:82:ASP:N	2.19	0.74
1:D:931:LEU:HD23	1:D:933:LEU:HD11	1.70	0.74
1:B:555:SER:OG	1:B:556:ALA:N	2.18	0.74
1:C:205:VAL:HG23	1:C:219:PHE:CE1	2.22	0.74
1:D:1036:GLN:NE2	1:D:1037:GLY:O	2.21	0.74
1:C:663:GLU:O	1:C:685:LYS:NZ	2.20	0.74
1:C:1232:THR:OG1	1:C:1264:TYR:OH	2.04	0.74
1:B:1039:THR:O	1:B:1042:THR:OG1	2.05	0.74
1:D:1301:GLN:OE1	1:D:1301:GLN:N	2.21	0.73
1:B:1250:SER:O	1:B:1254:THR:OG1	2.03	0.73
1:A:1232:THR:OG1	1:A:1264:TYR:OH	2.06	0.73
3:J:2:NAG:H62	3:J:3:BMA:H2	1.69	0.73
1:D:384:ILE:HD12	1:D:421:VAL:HG11	1.69	0.73
1:B:96:SER:O	1:B:124:ASN:ND2	2.21	0.73
1:D:917:ASN:ND2	1:D:1233:ASN:OD1	2.21	0.73
1:A:284:GLN:NE2	1:A:287:CYS:SG	2.62	0.73
1:D:961:ASN:OD1	1:D:1247:GLY:N	2.22	0.73
3:H:1:NAG:H82	3:H:1:NAG:C1	2.19	0.73
4:A:2003:NAG:H3	4:A:2003:NAG:C8	2.18	0.73
1:D:227:PRO:O	1:D:228:LYS:NZ	2.21	0.73
1:B:177:GLN:NE2	1:B:179:GLN:OE1	2.21	0.72
1:B:691:GLN:O	1:B:694:GLN:NE2	2.22	0.72
1:C:415:MET:SD	1:C:416:GLY:N	2.62	0.72
1:A:385:PHE:C	1:A:421:VAL:HG13	2.13	0.72
1:A:415:MET:SD	1:A:416:GLY:N	2.63	0.72
1:C:598:ARG:O	1:C:768:GLY:N	2.22	0.72
1:B:363:ILE:O	1:B:411:THR:OG1	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ILE:HG22	1:C:341:SER:HB3	1.71	0.72
1:B:415:MET:SD	1:B:416:GLY:N	2.63	0.72
1:B:993:THR:O	1:B:995:GLN:NE2	2.21	0.72
1:B:1184:GLU:OE1	1:B:1187:GLN:NE2	2.22	0.72
1:A:400:ASP:OD1	1:A:404:LEU:N	2.21	0.72
1:B:636:ASP:O	1:D:1072:GLN:NE2	2.22	0.72
1:D:691:GLN:O	1:D:694:GLN:NE2	2.23	0.72
1:A:608:LYS:NZ	1:A:609:PRO:O	2.18	0.72
1:B:1203:SER:OG	1:B:1205:GLU:OE1	2.06	0.72
1:D:239:ILE:HG22	1:D:341:SER:HB3	1.72	0.72
1:D:464:MET:SD	1:D:466:HIS:NE2	2.63	0.72
1:A:81:ASN:ND2	1:A:82:ASP:OD2	2.23	0.71
1:C:270:ARG:NH1	1:C:309:PHE:O	2.23	0.71
1:B:345:ARG:O	1:B:440:GLU:N	2.22	0.71
1:D:415:MET:SD	1:D:416:GLY:N	2.62	0.71
1:A:563:CYS:O	1:A:619:TYR:OH	2.07	0.71
1:A:795:GLU:O	1:A:813:THR:N	2.22	0.71
1:D:791:PRO:O	1:D:817:TYR:N	2.23	0.71
1:D:1059:ASP:OD2	1:D:1062:HIS:ND1	2.23	0.71
1:C:650:ILE:HG22	1:C:650:ILE:O	1.90	0.71
3:H:1:NAG:H3	3:H:1:NAG:H83	1.72	0.71
1:C:44:THR:OG1	1:C:89:PHE:O	2.09	0.71
1:C:507:ARG:NH2	1:C:532:SER:O	2.22	0.71
1:A:538:ALA:HB3	1:A:558:TYR:HB2	1.72	0.71
1:B:464:MET:SD	1:B:466:HIS:NE2	2.64	0.71
4:A:2003:NAG:H82	4:A:2003:NAG:C1	2.19	0.71
1:D:421:VAL:H	1:D:444:ALA:HB3	1.54	0.71
1:A:157:PRO:HG3	1:A:772:LEU:HD22	1.71	0.70
1:B:969:PRO:O	1:B:1014:ARG:NH1	2.23	0.70
1:A:44:THR:OG1	1:A:89:PHE:O	2.06	0.70
1:A:270:ARG:NH1	1:A:309:PHE:O	2.24	0.70
1:A:592:GLN:OE1	1:A:748:SER:OG	2.10	0.70
1:A:1125:LEU:HA	1:A:1128:LEU:HD12	1.72	0.70
1:B:1262:SER:O	1:B:1266:ALA:N	2.24	0.70
3:L:2:NAG:H3	3:L:2:NAG:C8	2.13	0.70
1:D:270:ARG:NH1	1:D:309:PHE:O	2.25	0.70
1:D:1129:GLU:OE1	1:D:1162:LYS:NZ	2.23	0.70
1:A:497:TYR:HB3	1:A:542:ILE:HD12	1.74	0.70
1:B:270:ARG:NH1	1:B:309:PHE:O	2.24	0.70
1:B:1259:HIS:O	1:B:1262:SER:OG	2.07	0.70
1:C:118:THR:OG1	1:C:676:LYS:NZ	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:NH2	1:A:672:ASP:O	2.25	0.70
1:A:598:ARG:NH2	1:A:610:ASP:OD2	2.24	0.70
1:A:999:GLU:N	1:A:999:GLU:OE2	2.25	0.70
1:C:964:ASN:ND2	1:C:1245:GLN:O	2.25	0.70
1:C:1231:ALA:O	1:C:1235:VAL:HG23	1.92	0.70
1:D:255:THR:HB	1:D:762:ILE:HG13	1.72	0.70
1:A:577:SER:HA	1:A:788:ALA:HB1	1.72	0.70
1:A:804:ARG:NE	1:A:863:LYS:O	2.25	0.70
1:B:1100:THR:HG22	1:B:1146:THR:HG22	1.74	0.70
1:C:400:ASP:OD1	1:C:404:LEU:N	2.25	0.70
1:D:592:GLN:OE1	1:D:748:SER:OG	2.10	0.70
1:D:1039:THR:O	1:D:1042:THR:OG1	2.06	0.70
1:D:1152:TYR:CZ	1:D:1214:LEU:HD22	2.27	0.70
1:B:400:ASP:OD1	1:B:404:LEU:N	2.24	0.69
1:A:1180:SER:OG	1:A:1233:ASN:O	2.08	0.69
1:C:354:LYS:NZ	1:C:463:PRO:O	2.25	0.69
1:C:959:MET:SD	1:C:995:GLN:NE2	2.65	0.69
1:C:648:VAL:HB	1:C:656:THR:HG23	1.73	0.69
1:D:96:SER:O	1:D:124:ASN:ND2	2.25	0.69
1:D:1242:GLN:NE2	1:D:1243:ASN:O	2.24	0.69
1:C:545:VAL:HA	1:C:551:VAL:HG23	1.74	0.69
1:A:233:VAL:HG12	1:A:250:VAL:HA	1.75	0.69
1:D:495:PHE:N	1:D:511:HIS:O	2.26	0.69
1:A:381:ASN:N	1:A:399:THR:OG1	2.25	0.69
1:B:295:ASN:ND2	1:B:297:HIS:O	2.26	0.69
1:B:576:GLN:OE1	1:B:576:GLN:N	2.26	0.69
1:D:402:HIS:HB2	1:D:404:LEU:HD12	1.73	0.69
1:A:570:LEU:HD22	1:A:784:ALA:HB2	1.74	0.69
1:A:959:MET:O	1:A:962:THR:OG1	2.11	0.69
1:B:270:ARG:NH2	1:B:315:GLU:O	2.25	0.69
1:B:596:ALA:N	1:B:770:PHE:O	2.25	0.69
1:B:598:ARG:O	1:B:768:GLY:N	2.26	0.69
1:B:1072:GLN:NE2	1:D:636:ASP:O	2.25	0.69
1:D:585:LEU:N	1:D:753:GLU:O	2.25	0.69
1:B:205:VAL:HG23	1:B:219:PHE:CE1	2.28	0.69
1:B:747:ASN:OD1	1:B:750:GLY:N	2.26	0.69
1:B:929:GLU:O	1:B:1314:MET:N	2.26	0.69
1:D:205:VAL:HG23	1:D:219:PHE:CE1	2.28	0.69
1:D:109:GLY:N	1:D:112:GLN:O	2.26	0.68
1:C:929:GLU:O	1:C:1314:MET:N	2.26	0.68
1:A:1301:GLN:OE1	1:A:1301:GLN:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1098:GLU:OE1	1:C:1098:GLU:N	2.26	0.68
1:D:177:GLN:NE2	1:D:179:GLN:OE1	2.26	0.68
1:C:999:GLU:N	1:C:999:GLU:OE2	2.26	0.68
1:A:457:SER:OG	1:A:483:ASN:N	2.27	0.68
1:B:1111:GLU:OE2	1:B:1152:TYR:OH	2.09	0.68
1:B:159:ASN:OD1	1:B:186:GLY:N	2.27	0.68
1:C:107:VAL:N	1:C:114:PHE:O	2.26	0.68
1:A:1304:SER:O	1:A:1305:LEU:HD23	1.94	0.68
1:D:56:GLU:N	1:D:56:GLU:OE2	2.26	0.68
1:C:363:ILE:HD12	1:C:364:PRO:HD2	1.74	0.67
1:C:598:ARG:NH2	1:C:610:ASP:OD2	2.26	0.67
1:D:955:LEU:HB2	1:D:1298:LEU:HD13	1.75	0.67
1:B:1059:ASP:OD2	1:B:1062:HIS:ND1	2.28	0.67
1:C:734:TYR:HB3	1:C:758:VAL:HG23	1.76	0.67
1:C:854:GLN:NE2	1:C:855:THR:O	2.27	0.67
1:B:931:LEU:HG	1:B:933:LEU:HD21	1.76	0.67
1:C:262:GLY:O	1:C:293:GLN:NE2	2.27	0.67
1:D:596:ALA:N	1:D:770:PHE:O	2.27	0.67
1:A:516:LYS:HD3	1:A:516:LYS:C	2.19	0.67
1:C:382:LYS:N	1:C:399:THR:OG1	2.28	0.67
1:A:295:ASN:ND2	1:A:297:HIS:O	2.27	0.67
1:D:77:LEU:CD2	1:D:79:ALA:HB2	2.25	0.67
1:D:957:SER:OG	1:D:960:GLN:NE2	2.27	0.67
1:A:517:GLN:NE2	1:A:517:GLN:HA	2.08	0.66
1:D:576:GLN:CG	1:D:580:ALA:HB3	2.25	0.66
3:F:1:NAG:H3	3:F:2:NAG:H82	1.77	0.66
1:A:315:GLU:HA	1:A:315:GLU:OE1	1.94	0.66
1:B:536:PRO:O	1:B:560:VAL:N	2.28	0.66
1:C:288:GLU:OE1	1:C:288:GLU:N	2.27	0.66
1:C:1152:TYR:CE2	1:C:1214:LEU:HD13	2.30	0.66
1:A:628:THR:OG1	1:A:672:ASP:OD1	2.12	0.66
1:B:869:ASN:OD1	1:B:902:PRO:HB3	1.96	0.66
1:D:663:GLU:O	1:D:685:LYS:NZ	2.28	0.66
1:B:235:VAL:HG23	1:B:248:VAL:HG22	1.78	0.66
1:D:293:GLN:NE2	1:D:294:LEU:O	2.28	0.66
1:A:979:LEU:O	1:A:983:ASN:ND2	2.28	0.66
1:C:650:ILE:HG12	1:C:656:THR:HG22	1.76	0.66
1:D:139:LYS:NZ	1:D:224:PHE:O	2.21	0.66
1:B:955:LEU:HB2	1:B:1298:LEU:HD13	1.77	0.66
1:C:570:LEU:CD1	1:C:585:LEU:HD21	2.25	0.66
1:B:823:ARG:NH1	1:B:824:VAL:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:LEU:O	1:B:920:LEU:HD23	1.96	0.66
1:D:73:LEU:HD12	1:D:91:VAL:HG22	1.77	0.66
1:B:30:GLN:H	1:B:53:TYR:HD2	1.43	0.66
1:D:994:GLN:NE2	1:D:1271:ARG:HD2	2.11	0.66
1:A:101:MET:O	1:A:120:VAL:N	2.29	0.65
1:B:381:ASN:N	1:B:399:THR:OG1	2.29	0.65
1:B:964:ASN:ND2	1:B:1245:GLN:O	2.29	0.65
1:D:381:ASN:N	1:D:399:THR:OG1	2.28	0.65
1:D:386:ILE:N	1:D:395:SER:O	2.28	0.65
3:L:1:NAG:C1	3:L:1:NAG:H82	2.26	0.65
1:A:58:VAL:HG22	1:A:109:GLY:CA	2.26	0.65
1:D:49:VAL:O	1:D:84:LEU:HD12	1.96	0.65
1:A:590:ALA:O	1:A:593:SER:OG	2.14	0.65
1:C:1039:THR:O	1:C:1042:THR:OG1	2.13	0.65
1:D:614:SER:O	1:D:617:SER:OG	2.10	0.65
1:A:579:PRO:HA	1:A:757:THR:CG2	2.25	0.65
1:B:877:LEU:O	1:B:889:SER:OG	2.12	0.65
1:B:1211:TYR:HA	1:B:1214:LEU:HD12	1.78	0.65
1:C:589:ALA:HB3	1:C:746:VAL:HG21	1.79	0.65
1:D:941:GLU:OE1	1:D:942:GLU:N	2.28	0.65
1:A:1183:TRP:CZ3	1:A:1212:VAL:HG11	2.32	0.65
1:D:232:GLN:OE1	1:D:233:VAL:N	2.30	0.65
1:D:914:THR:N	1:D:1328:LEU:O	2.30	0.65
1:C:1139:ASP:O	1:C:1143:HIS:NE2	2.30	0.64
1:D:351:SER:OG	1:D:352:PHE:O	2.15	0.64
1:A:46:LYS:O	1:A:505:ILE:HD12	1.97	0.64
1:A:1102:SER:HA	1:A:1105:ILE:HD12	1.79	0.64
1:B:648:VAL:HG21	1:B:657:PRO:HA	1.79	0.64
1:B:973:GLY:O	1:B:1015:GLN:NE2	2.30	0.64
1:B:1206:VAL:HG22	1:B:1237:TRP:CH2	2.32	0.64
1:C:237:LYS:O	1:C:238:ILE:HD13	1.97	0.64
1:D:418:SER:C	1:D:419:LEU:HD12	2.22	0.64
1:A:28:LYS:N	1:A:547:PRO:O	2.31	0.64
1:A:354:LYS:NZ	1:A:463:PRO:O	2.27	0.64
1:A:803:ILE:HG22	1:A:805:GLY:H	1.60	0.64
1:C:649:TYR:CG	1:C:649:TYR:O	2.50	0.64
1:D:763:THR:OG1	1:D:764:GLU:N	2.26	0.64
1:A:58:VAL:HG22	1:A:109:GLY:HA2	1.79	0.64
1:A:984:ILE:HA	1:A:987:LEU:HD12	1.78	0.64
1:C:1125:LEU:HA	1:C:1128:LEU:HD12	1.78	0.64
1:A:60:VAL:HG23	1:A:107:VAL:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LEU:HD23	1:A:571:SER:N	2.11	0.64
1:B:763:THR:OG1	1:B:764:GLU:OE1	2.13	0.64
1:B:1242:GLN:NE2	1:B:1243:ASN:O	2.30	0.64
1:D:912:LYS:N	1:D:1330:TYR:O	2.30	0.64
1:D:382:LYS:N	1:D:399:THR:OG1	2.30	0.64
1:D:598:ARG:NH2	1:D:610:ASP:OD2	2.30	0.64
1:D:1269:PHE:HE1	1:D:1271:ARG:HG2	1.63	0.64
1:B:156:HIS:NE2	1:B:775:ASP:O	2.30	0.64
1:C:1301:GLN:OE1	1:C:1301:GLN:N	2.31	0.64
1:D:232:GLN:N	1:D:251:CYS:O	2.30	0.64
1:D:1120:VAL:O	1:D:1124:ALA:N	2.30	0.64
1:B:269:CYS:N	1:B:319:LYS:O	2.30	0.64
1:B:999:GLU:N	1:B:999:GLU:OE2	2.31	0.64
1:A:125:GLU:N	1:A:125:GLU:OE1	2.31	0.64
1:A:246:MET:N	1:A:304:VAL:O	2.31	0.64
1:A:955:LEU:HB2	1:A:1298:LEU:HD22	1.80	0.64
1:B:663:GLU:O	1:B:685:LYS:NZ	2.31	0.64
1:B:1335:GLU:N	1:B:1335:GLU:OE1	2.31	0.64
1:C:1100:THR:CG2	1:C:1146:THR:HG22	2.28	0.64
1:A:101:MET:N	1:A:120:VAL:O	2.30	0.63
1:B:288:GLU:N	1:B:288:GLU:OE1	2.31	0.63
1:C:730:THR:HG23	1:C:731:VAL:HG13	1.80	0.63
1:C:742:ASP:N	1:C:742:ASP:OD1	2.31	0.63
1:D:648:VAL:HG21	1:D:657:PRO:HA	1.80	0.63
1:B:387:ARG:O	1:B:389:ASN:ND2	2.32	0.63
1:C:385:PHE:HE1	4:C:2004:NAG:H82	1.63	0.63
1:A:500:MET:SD	1:A:675:LEU:HD23	2.39	0.63
1:A:1327:SER:OG	1:A:1328:LEU:N	2.30	0.63
1:B:941:GLU:OE1	1:B:942:GLU:N	2.31	0.63
1:D:596:ALA:C	1:D:597:LEU:HD12	2.23	0.63
1:D:969:PRO:O	1:D:1014:ARG:NH1	2.30	0.63
1:A:657:PRO:O	1:D:656:THR:OG1	2.16	0.63
1:B:1081:ARG:NH1	1:D:638:ASP:OD2	2.31	0.63
1:C:578:LEU:O	1:C:580:ALA:N	2.32	0.63
1:C:828:LEU:HB3	1:C:872:VAL:HG12	1.81	0.63
1:D:1205:GLU:HG2	1:D:1206:VAL:HG23	1.80	0.63
1:A:230:GLU:HB3	1:A:253:LEU:HD11	1.79	0.63
1:D:239:ILE:HG23	1:D:343:ILE:HG13	1.80	0.63
1:C:386:ILE:N	1:C:395:SER:O	2.30	0.63
1:D:747:ASN:OD1	1:D:750:GLY:N	2.31	0.63
1:D:919:LEU:HD23	1:D:920:LEU:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:OG1	1:A:676:LYS:NZ	2.27	0.62
1:A:596:ALA:C	1:A:597:LEU:HD12	2.24	0.62
1:A:635:ASN:OD1	1:C:1072:GLN:NE2	2.31	0.62
1:A:1231:ALA:O	1:A:1235:VAL:HG23	1.99	0.62
1:D:1264:TYR:CE1	1:D:1268:THR:HG21	2.34	0.62
1:B:354:LYS:NZ	1:B:463:PRO:O	2.32	0.62
1:D:354:LYS:NZ	1:D:463:PRO:O	2.30	0.62
1:D:459:VAL:HG23	1:D:552:ILE:CD1	2.29	0.62
1:A:473:THR:OG1	1:A:474:GLN:N	2.32	0.62
1:A:605:LEU:HD12	1:A:608:LYS:O	1.99	0.62
1:B:570:LEU:HD22	1:B:784:ALA:CB	2.28	0.62
1:B:1271:ARG:NH2	3:H:2:NAG:N2	2.40	0.62
1:C:739:TRP:NE1	1:C:756:VAL:O	2.31	0.62
1:C:865:LEU:HD12	1:C:905:VAL:HG13	1.80	0.62
1:C:1111:GLU:OE1	1:C:1152:TYR:OH	2.12	0.62
1:B:622:LEU:HD23	1:B:623:PRO:N	2.14	0.62
1:C:270:ARG:NH2	1:C:315:GLU:HB2	2.13	0.62
1:D:993:THR:O	1:D:995:GLN:NE2	2.32	0.62
1:C:384:ILE:HD12	1:C:421:VAL:HG11	1.80	0.62
1:B:739:TRP:O	1:B:740:ILE:HD13	1.99	0.62
1:C:1102:SER:HA	1:C:1105:ILE:HD12	1.80	0.62
1:D:535:ALA:HB1	1:D:536:PRO:HD2	1.81	0.62
1:D:1168:LYS:O	1:D:1172:GLU:N	2.31	0.62
1:B:592:GLN:OE1	1:B:748:SER:OG	2.17	0.62
1:A:51:LEU:HG	1:A:79:ALA:HB1	1.82	0.62
1:A:473:THR:OG1	1:A:528:ILE:O	2.14	0.62
1:D:881:GLU:HG3	1:D:887:VAL:HG12	1.81	0.62
1:A:957:SER:OG	1:A:960:GLN:NE2	2.33	0.62
1:C:919:LEU:HD23	1:C:920:LEU:N	2.15	0.62
1:D:576:GLN:HG2	1:D:580:ALA:HB3	1.82	0.62
1:B:767:ALA:HB3	1:B:784:ALA:HB3	1.80	0.62
1:C:1113:PRO:O	1:C:1114:LEU:HD23	1.99	0.62
1:D:54:LEU:HG	4:D:2001:NAG:H82	1.81	0.62
1:D:1110:LEU:HD13	1:D:1156:LEU:CB	2.30	0.62
1:A:128:LEU:HD13	1:A:622:LEU:HA	1.81	0.61
1:A:660:SER:OG	1:A:661:THR:N	2.32	0.61
1:B:237:LYS:O	1:B:238:ILE:HD13	2.00	0.61
1:B:742:ASP:OD1	1:B:742:ASP:N	2.31	0.61
1:B:1039:THR:O	1:B:1042:THR:N	2.33	0.61
1:D:916:PHE:CB	1:D:931:LEU:HD21	2.29	0.61
2:I:2:NAG:O3	2:I:2:NAG:O7	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:THR:HG23	1:B:764:GLU:O	2.00	0.61
1:B:920:LEU:HD22	1:B:927:VAL:HG11	1.81	0.61
1:C:381:ASN:N	1:C:399:THR:OG1	2.32	0.61
1:D:1039:THR:O	1:D:1042:THR:N	2.33	0.61
1:B:1067:LEU:HD11	1:B:1109:LEU:HD11	1.82	0.61
1:D:1100:THR:HG22	1:D:1146:THR:HG22	1.83	0.61
1:B:402:HIS:HB2	1:B:404:LEU:HD12	1.82	0.61
1:B:546:LEU:HB2	1:B:548:THR:HG22	1.81	0.61
1:B:679:THR:HG22	1:B:681:SER:H	1.65	0.61
1:B:883:CYS:SG	1:B:884:GLY:N	2.74	0.61
1:B:418:SER:C	1:B:419:LEU:HD12	2.26	0.61
1:B:554:ASP:OD1	1:B:555:SER:N	2.34	0.61
1:B:1139:ASP:O	1:B:1143:HIS:NE2	2.34	0.61
1:C:167:ILE:HG12	1:C:205:VAL:HG22	1.83	0.61
1:D:495:PHE:O	1:D:510:THR:OG1	2.15	0.61
1:D:1130:SER:O	1:D:1134:THR:HG23	2.01	0.61
1:A:1100:THR:CG2	1:A:1146:THR:HG22	2.31	0.61
1:B:1118:HIS:HB3	1:B:1121:VAL:HG12	1.83	0.61
1:C:58:VAL:HG22	1:C:109:GLY:HA2	1.83	0.61
1:C:920:LEU:HD22	1:C:927:VAL:HG11	1.81	0.61
1:A:41:THR:HG22	1:A:91:VAL:CG1	2.30	0.61
1:B:169:ASP:N	1:B:173:ASN:O	2.32	0.61
1:B:382:LYS:N	1:B:399:THR:OG1	2.32	0.61
1:C:931:LEU:HG	1:C:933:LEU:HD21	1.82	0.61
1:A:545:VAL:HA	1:A:551:VAL:HG23	1.81	0.61
1:A:546:LEU:HB2	1:A:548:THR:HG22	1.82	0.61
1:A:933:LEU:O	1:A:1310:GLY:N	2.33	0.61
1:D:578:LEU:N	1:D:789:PHE:O	2.34	0.61
1:B:585:LEU:N	1:B:753:GLU:O	2.32	0.60
1:C:51:LEU:O	1:C:82:ASP:N	2.33	0.60
1:C:158:LEU:HD12	1:C:159:ASN:H	1.65	0.60
1:C:578:LEU:HD11	1:C:790:GLN:HG3	1.81	0.60
1:C:969:PRO:O	1:C:1014:ARG:NH1	2.33	0.60
1:B:481:ILE:C	1:B:482:LEU:HD12	2.26	0.60
1:C:125:GLU:OE1	1:C:125:GLU:N	2.34	0.60
1:A:112:GLN:OE1	1:A:112:GLN:HA	2.00	0.60
1:A:473:THR:HG1	1:A:528:ILE:C	2.06	0.60
1:A:962:THR:O	1:A:966:LEU:HD11	2.00	0.60
1:B:55:ASN:HB3	1:B:110:PRO:HD2	1.82	0.60
1:B:1327:SER:OG	1:B:1328:LEU:N	2.33	0.60
1:D:121:MET:HE1	1:D:633:PRO:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:VAL:HG22	1:D:751:VAL:HB	1.81	0.60
1:A:1264:TYR:CE1	1:A:1268:THR:HG21	2.37	0.60
4:C:2003:NAG:C1	4:C:2003:NAG:H82	2.32	0.60
1:C:269:CYS:N	1:C:319:LYS:O	2.34	0.60
1:D:29:PRO:N	1:D:29:PRO:C	2.58	0.60
1:A:989:TYR:CE1	1:A:993:THR:HG21	2.36	0.60
1:B:988:ASP:O	1:B:992:GLU:N	2.31	0.60
3:F:2:NAG:H3	3:F:2:NAG:C8	2.16	0.60
1:A:819:PRO:HA	1:A:850:ALA:HB2	1.84	0.60
4:A:2002:NAG:O7	4:A:2002:NAG:H3	2.00	0.60
1:B:275:ALA:HB1	1:B:281:GLU:HB3	1.84	0.60
1:B:779:GLY:C	1:B:780:ILE:HD12	2.27	0.60
1:D:507:ARG:NH1	1:D:529:PRO:O	2.35	0.60
1:B:767:ALA:CB	1:B:784:ALA:HB3	2.32	0.60
1:B:763:THR:OG1	1:B:764:GLU:N	2.33	0.60
1:A:916:PHE:CZ	1:A:933:LEU:HD22	2.37	0.60
1:B:948:VAL:HG12	1:B:1305:LEU:HD11	1.85	0.59
1:B:1132:TRP:O	1:B:1136:GLN:N	2.35	0.59
1:C:918:SER:OG	1:C:919:LEU:N	2.35	0.59
1:D:363:ILE:O	1:D:411:THR:OG1	2.13	0.59
1:D:930:GLU:OE1	1:D:1312:TYR:N	2.34	0.59
1:A:63:SER:OG	1:A:104:THR:O	2.12	0.59
1:A:356:ASP:OD1	1:A:358:HIS:N	2.34	0.59
1:A:451:VAL:HG22	1:A:452:PHE:O	2.02	0.59
1:A:1098:GLU:OE1	1:A:1098:GLU:N	2.33	0.59
1:B:1271:ARG:NH2	3:H:1:NAG:O3	2.35	0.59
1:C:428:ARG:NH2	1:C:440:GLU:OE2	2.35	0.59
1:C:974:GLU:O	1:C:978:VAL:HG23	2.03	0.59
1:B:1129:GLU:OE1	1:B:1162:LYS:NZ	2.35	0.59
1:D:232:GLN:O	1:D:251:CYS:N	2.33	0.59
1:D:1224:THR:OG1	1:D:1226:GLU:N	2.36	0.59
1:B:136:SER:OG	1:B:609:PRO:O	2.18	0.59
1:B:183:LEU:HD22	1:B:187:LEU:C	2.27	0.59
1:C:675:LEU:HD12	1:C:676:LYS:N	2.17	0.59
1:B:920:LEU:HD12	1:B:1316:VAL:HG21	1.84	0.59
1:C:804:ARG:HD3	1:C:865:LEU:HD13	1.85	0.59
1:C:914:THR:O	1:C:1328:LEU:N	2.33	0.59
1:A:385:PHE:O	1:A:421:VAL:HG13	2.01	0.59
1:B:1125:LEU:HA	1:B:1128:LEU:HD12	1.84	0.59
4:B:2002:NAG:H3	4:B:2002:NAG:O7	2.01	0.59
1:C:284:GLN:NE2	1:C:287:CYS:SG	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:GLN:NE2	1:D:517:GLN:O	2.36	0.59
1:A:974:GLU:O	1:A:978:VAL:HG23	2.01	0.59
1:A:1059:ASP:OD2	1:A:1062:HIS:ND1	2.35	0.59
1:B:517:GLN:O	1:B:517:GLN:NE2	2.35	0.59
1:D:545:VAL:HG23	1:D:551:VAL:HB	1.85	0.59
3:H:1:NAG:H3	3:H:1:NAG:C8	2.32	0.59
1:A:386:ILE:N	1:A:395:SER:O	2.31	0.59
1:A:517:GLN:HA	1:A:517:GLN:HE21	1.68	0.59
1:B:189:GLN:N	1:B:189:GLN:OE1	2.36	0.59
1:C:315:GLU:OE1	1:C:315:GLU:HA	2.01	0.59
1:D:500:MET:CE	1:D:675:LEU:HD23	2.33	0.59
1:A:216:GLU:N	1:A:216:GLU:OE2	2.36	0.59
1:B:814:VAL:C	1:B:815:LEU:HD12	2.27	0.59
1:D:1226:GLU:N	1:D:1226:GLU:OE1	2.36	0.59
1:A:1113:PRO:O	1:A:1114:LEU:HD23	2.03	0.59
1:A:1279:THR:HG23	1:A:1289:LYS:HG2	1.85	0.59
1:D:1039:THR:OG1	1:D:1040:TRP:N	2.33	0.59
1:C:637:GLN:O	1:C:684:ARG:NH1	2.36	0.58
1:C:1250:SER:OG	1:C:1253:ASP:OD1	2.15	0.58
1:D:270:ARG:NH2	1:D:315:GLU:O	2.36	0.58
1:D:1217:LEU:HD21	1:D:1231:ALA:HB1	1.85	0.58
1:A:576:GLN:NE2	1:A:580:ALA:O	2.36	0.58
1:A:960:GLN:OE1	1:A:960:GLN:N	2.35	0.58
1:B:451:VAL:HG22	1:B:452:PHE:O	2.04	0.58
1:B:230:GLU:HB2	1:B:606:LEU:HD21	1.83	0.58
1:B:539:ARG:NH1	1:B:672:ASP:O	2.36	0.58
1:B:607:MET:O	1:B:607:MET:HE3	2.03	0.58
1:C:596:ALA:C	1:C:597:LEU:HD12	2.28	0.58
1:D:730:THR:HG23	1:D:731:VAL:HG13	1.85	0.58
1:B:798:MET:HE3	1:B:903:LEU:HB3	1.86	0.58
1:C:627:LEU:HD12	1:C:628:THR:N	2.18	0.58
1:C:822:ILE:HG23	1:C:887:VAL:CG2	2.34	0.58
1:D:1203:SER:OG	1:D:1205:GLU:OE1	2.20	0.58
1:B:1005:ILE:O	1:B:1009:ASN:ND2	2.35	0.58
1:D:973:GLY:O	1:D:1015:GLN:NE2	2.36	0.58
1:B:359:PHE:CZ	1:B:450:LEU:HD23	2.38	0.58
1:D:739:TRP:O	1:D:740:ILE:HD13	2.04	0.58
1:D:1184:GLU:OE1	1:D:1187:GLN:NE2	2.36	0.58
1:C:33:VAL:C	1:C:34:LEU:HD12	2.29	0.58
1:C:649:TYR:HA	1:C:655:TYR:CE1	2.39	0.58
1:D:95:SER:OG	1:D:96:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:VAL:HG23	1:D:248:VAL:HG22	1.85	0.58
1:D:500:MET:HE1	1:D:675:LEU:HD23	1.85	0.58
1:A:730:THR:N	1:A:898:THR:OG1	2.34	0.58
1:B:155:PHE:HB3	1:B:778:LEU:HD22	1.86	0.58
1:B:579:PRO:HB3	1:B:731:VAL:HG12	1.86	0.58
1:B:785:SER:C	1:B:786:LEU:HD12	2.27	0.58
1:C:134:ASP:OD2	1:C:135:LYS:NZ	2.36	0.58
1:D:459:VAL:HG23	1:D:552:ILE:HD12	1.85	0.58
1:D:622:LEU:HD23	1:D:623:PRO:N	2.18	0.58
1:A:237:LYS:O	1:A:238:ILE:HD13	2.03	0.58
1:B:1180:SER:OG	1:B:1233:ASN:O	2.11	0.57
1:D:570:LEU:HD21	1:D:585:LEU:HD11	1.84	0.57
1:A:600:VAL:HG22	1:A:601:ASP:C	2.28	0.57
1:A:1262:SER:OG	1:A:1263:LYS:N	2.34	0.57
1:B:232:GLN:N	1:B:251:CYS:O	2.37	0.57
3:H:2:NAG:H3	3:H:2:NAG:C8	2.14	0.57
1:A:742:ASP:C	1:A:743:LEU:HD12	2.28	0.57
1:A:793:PHE:CE2	1:A:815:LEU:HD13	2.39	0.57
1:A:964:ASN:ND2	1:A:1245:GLN:O	2.38	0.57
1:C:948:VAL:HG13	1:C:1305:LEU:HD11	1.86	0.57
1:D:30:GLN:HB2	1:D:53:TYR:CD2	2.39	0.57
1:C:49:VAL:O	1:C:84:LEU:HD12	2.04	0.57
1:C:418:SER:C	1:C:419:LEU:HD12	2.28	0.57
1:C:1206:VAL:O	1:C:1209:THR:OG1	2.16	0.57
1:D:779:GLY:C	1:D:780:ILE:HD12	2.29	0.57
1:A:916:PHE:N	1:A:1326:THR:O	2.36	0.57
1:B:167:ILE:HG12	1:B:205:VAL:HG22	1.84	0.57
1:C:38:LEU:HD22	1:C:624:GLU:OE2	2.05	0.57
1:C:95:SER:OG	1:C:96:SER:N	2.37	0.57
1:C:293:GLN:NE2	1:C:294:LEU:O	2.38	0.57
1:C:345:ARG:O	1:C:440:GLU:N	2.36	0.57
1:D:495:PHE:O	1:D:511:HIS:N	2.37	0.57
1:C:681:SER:OG	1:C:683:ILE:HD11	2.04	0.57
1:C:948:VAL:CG1	1:C:1305:LEU:HD11	2.35	0.57
1:D:244:GLU:N	1:D:244:GLU:OE2	2.38	0.57
1:D:1100:THR:CG2	1:D:1146:THR:HG22	2.34	0.57
1:B:400:ASP:OD1	1:B:403:GLY:N	2.37	0.57
1:C:41:THR:HG22	1:C:91:VAL:CG1	2.33	0.57
1:C:156:HIS:ND1	1:C:774:GLU:O	2.37	0.57
1:D:34:LEU:HD22	1:D:498:LEU:HD11	1.87	0.57
1:D:164:LEU:HD12	1:D:165:VAL:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:LEU:CB	1:A:548:THR:HG22	2.35	0.57
1:B:535:ALA:HB3	1:B:537:VAL:O	2.04	0.57
1:D:685:LYS:O	1:D:687:LYS:N	2.37	0.57
1:D:1251:THR:O	1:D:1255:VAL:HG23	2.05	0.57
1:A:33:VAL:C	1:A:34:LEU:HD12	2.30	0.57
1:D:502:LYS:CG	1:D:535:ALA:HB2	2.35	0.57
1:D:891:PRO:O	1:D:895:ARG:NH2	2.38	0.57
1:A:187:LEU:HD12	1:A:188:LYS:CA	2.35	0.57
1:B:999:GLU:O	1:B:1003:LYS:N	2.35	0.57
1:B:1039:THR:OG1	1:B:1040:TRP:N	2.37	0.57
1:D:384:ILE:HD12	1:D:421:VAL:CG1	2.35	0.57
1:B:914:THR:N	1:B:1328:LEU:O	2.37	0.56
1:B:1152:TYR:CE2	1:B:1214:LEU:HD13	2.40	0.56
1:D:819:PRO:HA	1:D:850:ALA:HB2	1.85	0.56
3:F:2:NAG:H83	3:F:2:NAG:C3	2.19	0.56
1:A:742:ASP:HA	1:A:743:LEU:HD12	1.87	0.56
1:D:1206:VAL:HG22	1:D:1237:TRP:CH2	2.40	0.56
1:A:1025:TYR:CD2	1:A:1042:THR:HG22	2.40	0.56
1:B:356:ASP:O	1:B:446:HIS:NE2	2.38	0.56
1:B:431:CYS:O	1:B:437:VAL:HG11	2.05	0.56
1:B:914:THR:C	1:B:1327:SER:HG	2.09	0.56
1:B:1074:GLN:OE1	1:D:117:ARG:NH2	2.37	0.56
1:B:1152:TYR:CD2	1:B:1214:LEU:HD13	2.40	0.56
1:C:101:MET:O	1:C:120:VAL:N	2.37	0.56
1:C:481:ILE:C	1:C:482:LEU:HD12	2.31	0.56
1:C:582:HIS:HD2	1:C:754:VAL:HG11	1.70	0.56
1:C:828:LEU:HD13	1:C:872:VAL:HG12	1.86	0.56
1:D:476:VAL:N	1:D:526:ILE:O	2.38	0.56
1:D:954:ILE:HG23	1:D:955:LEU:HG	1.87	0.56
1:C:979:LEU:O	1:C:983:ASN:ND2	2.37	0.56
1:D:101:MET:N	1:D:120:VAL:O	2.32	0.56
1:D:359:PHE:CE2	1:D:450:LEU:HD23	2.41	0.56
1:B:1100:THR:CG2	1:B:1146:THR:HG22	2.36	0.56
1:D:262:GLY:O	1:D:293:GLN:NE2	2.36	0.56
1:B:1110:LEU:HD13	1:B:1156:LEU:CB	2.36	0.56
1:C:579:PRO:HA	1:C:757:THR:CG2	2.35	0.56
1:C:1227:ASP:OD1	1:C:1227:ASP:N	2.37	0.56
1:D:345:ARG:O	1:D:440:GLU:N	2.38	0.56
1:C:583:ALA:C	1:C:754:VAL:HG13	2.31	0.56
1:C:648:VAL:HB	1:C:656:THR:CG2	2.36	0.56
1:C:1185:ARG:O	1:C:1187:GLN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ILE:O	1:D:311:LEU:HD12	2.06	0.56
1:A:459:VAL:HG23	1:A:552:ILE:HD12	1.87	0.56
1:C:71:ARG:HH21	1:C:73:LEU:HD21	1.71	0.56
1:C:262:GLY:O	1:C:294:LEU:N	2.38	0.56
1:C:532:SER:OG	1:C:533:ASP:N	2.36	0.56
1:C:920:LEU:HD22	1:C:927:VAL:CG1	2.35	0.56
1:D:785:SER:C	1:D:786:LEU:HD12	2.31	0.56
1:A:570:LEU:HD21	1:A:585:LEU:HD11	1.88	0.56
1:A:661:THR:OG1	1:A:662:ASN:N	2.38	0.56
1:A:954:ILE:HG23	1:A:955:LEU:HG	1.87	0.56
1:C:58:VAL:HG22	1:C:109:GLY:CA	2.35	0.56
1:C:128:LEU:HD11	1:C:155:PHE:HE1	1.71	0.56
1:B:350:LEU:N	1:B:442:GLU:OE1	2.39	0.56
1:B:808:PHE:N	1:B:860:VAL:O	2.38	0.56
1:B:974:GLU:OE2	1:B:1027:THR:OG1	2.16	0.56
1:C:62:ALA:HA	1:C:105:VAL:HG22	1.87	0.56
1:C:491:LYS:O	1:C:515:VAL:HG22	2.05	0.56
1:D:1253:ASP:OD1	1:D:1254:THR:N	2.38	0.56
1:A:498:LEU:HD12	1:A:541:LEU:HD21	1.87	0.55
1:A:532:SER:OG	1:A:533:ASP:N	2.38	0.55
1:A:681:SER:OG	1:A:682:LYS:N	2.38	0.55
1:C:459:VAL:HG23	1:C:552:ILE:HD12	1.88	0.55
1:C:1025:TYR:CE2	1:C:1045:VAL:HG11	2.41	0.55
1:A:308:VAL:O	1:A:310:GLN:NE2	2.38	0.55
1:A:585:LEU:HD23	1:A:586:ARG:N	2.20	0.55
1:B:972:CYS:SG	1:B:974:GLU:N	2.79	0.55
1:C:1039:THR:OG1	1:C:1040:TRP:N	2.37	0.55
1:D:1217:LEU:HD21	1:D:1231:ALA:CB	2.36	0.55
1:A:268:ILE:HG23	1:A:288:GLU:HB2	1.88	0.55
1:B:143:THR:HG22	1:B:193:PRO:HA	1.88	0.55
1:C:822:ILE:HG21	1:C:876:ALA:HB1	1.89	0.55
1:D:481:ILE:C	1:D:482:LEU:HD12	2.31	0.55
1:D:535:ALA:HB3	1:D:537:VAL:O	2.06	0.55
1:A:388:GLY:N	1:A:393:TYR:O	2.39	0.55
1:A:453:SER:OG	1:A:457:SER:O	2.20	0.55
1:A:1051:GLN:O	1:A:1054:ALA:HB3	2.05	0.55
1:B:233:VAL:HG13	1:B:338:ARG:CZ	2.36	0.55
1:B:428:ARG:NH2	1:B:440:GLU:OE2	2.39	0.55
1:C:189:GLN:OE1	1:C:189:GLN:N	2.38	0.55
1:D:808:PHE:CZ	1:D:860:VAL:HG13	2.42	0.55
1:A:878:GLU:OE2	1:A:879:SER:OG	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:ALA:O	1:B:1235:VAL:HG23	2.06	0.55
1:C:553:GLY:HA3	1:C:666:MET:HE1	1.88	0.55
1:D:421:VAL:N	1:D:444:ALA:HB3	2.21	0.55
1:D:1103:ALA:HB3	1:D:1149:LEU:HD23	1.88	0.55
1:A:58:VAL:C	1:A:79:ALA:HB3	2.31	0.55
1:A:1178:ASP:OD1	1:A:1179:ASN:N	2.40	0.55
1:B:458:PHE:HA	1:B:552:ILE:HD13	1.88	0.55
1:C:333:VAL:CG1	1:C:607:MET:HE1	2.36	0.55
1:A:310:GLN:O	1:A:312:LYS:N	2.40	0.55
1:B:539:ARG:HB3	1:B:673:MET:HE1	1.88	0.55
1:B:826:VAL:HG11	1:B:856:VAL:HG21	1.89	0.55
1:B:1131:ALA:O	1:B:1134:THR:OG1	2.25	0.55
1:D:174:ARG:CZ	1:D:1298:LEU:HD23	2.36	0.55
1:B:919:LEU:HD23	1:B:920:LEU:N	2.22	0.55
1:C:1178:ASP:OD1	1:C:1179:ASN:N	2.39	0.55
1:C:1211:TYR:HA	1:C:1214:LEU:HD12	1.87	0.55
1:D:837:VAL:N	1:D:859:ALA:O	2.40	0.55
1:C:473:THR:HG22	1:C:529:PRO:HA	1.89	0.55
1:C:1253:ASP:OD1	1:C:1253:ASP:N	2.40	0.55
1:D:954:ILE:HG22	1:D:1297:ARG:NH2	2.21	0.55
1:D:733:LYS:HZ3	1:D:736:PRO:HG3	1.70	0.55
1:D:1206:VAL:HG22	1:D:1237:TRP:CZ3	2.42	0.55
3:J:2:NAG:H83	3:J:2:NAG:C3	2.20	0.55
1:A:60:VAL:HG23	1:A:107:VAL:HG22	1.89	0.54
1:B:570:LEU:HD22	1:B:784:ALA:HB2	1.87	0.54
1:B:579:PRO:O	1:B:581:SER:N	2.41	0.54
1:B:1079:CYS:N	1:B:1127:CYS:SG	2.80	0.54
1:B:1152:TYR:HE1	1:B:1218:THR:HG21	1.71	0.54
1:C:187:LEU:HD12	1:C:188:LYS:N	2.22	0.54
1:C:274:ASP:OD1	1:D:436:TRP:NE1	2.39	0.54
1:D:269:CYS:N	1:D:319:LYS:O	2.39	0.54
1:D:585:LEU:HD23	1:D:586:ARG:N	2.22	0.54
2:E:1:NAG:H3	2:E:1:NAG:O7	2.07	0.54
1:A:538:ALA:HB2	1:A:560:VAL:CG2	2.38	0.54
1:C:546:LEU:CB	1:C:548:THR:HG22	2.38	0.54
1:D:1110:LEU:HD13	1:D:1156:LEU:HB3	1.89	0.54
1:D:1335:GLU:OE1	1:D:1335:GLU:N	2.40	0.54
1:B:33:VAL:HG12	1:B:49:VAL:HG23	1.89	0.54
1:B:971:GLY:O	1:B:1018:TYR:OH	2.15	0.54
1:C:498:LEU:HD12	1:C:541:LEU:HD21	1.89	0.54
1:C:1225:SER:O	1:C:1229:THR:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:946:ALA:N	1:D:1305:LEU:O	2.38	0.54
1:A:41:THR:OG1	1:A:125:GLU:OE1	2.25	0.54
1:A:386:ILE:HA	1:A:421:VAL:HG22	1.88	0.54
1:A:1022:ASP:OD1	1:A:1023:GLY:N	2.40	0.54
1:B:412:THR:N	1:B:413:ASN:OD1	2.39	0.54
1:C:546:LEU:HB2	1:C:548:THR:HG22	1.89	0.54
1:A:422:ARG:NH2	1:A:443:GLU:OE1	2.41	0.54
1:B:31:TYR:OH	1:B:680:ASN:ND2	2.41	0.54
1:D:1262:SER:O	1:D:1265:GLY:N	2.39	0.54
1:A:564:LEU:O	1:A:567:LYS:NZ	2.28	0.54
1:B:819:PRO:HA	1:B:850:ALA:HB2	1.89	0.54
1:C:545:VAL:CA	1:C:551:VAL:HG23	2.37	0.54
1:D:159:ASN:OD1	1:D:186:GLY:N	2.41	0.54
1:B:30:GLN:O	1:B:52:SER:N	2.41	0.54
1:B:80:GLU:N	1:B:80:GLU:OE1	2.41	0.54
1:B:130:PHE:O	1:B:149:VAL:N	2.41	0.54
1:B:742:ASP:C	1:B:743:LEU:HD12	2.33	0.54
1:C:822:ILE:HD13	1:C:889:SER:HB2	1.89	0.54
1:D:31:TYR:OH	1:D:680:ASN:ND2	2.41	0.54
1:B:241:ILE:HG22	1:B:242:LEU:HD22	1.90	0.54
1:B:118:THR:HG21	1:B:676:LYS:HD3	1.89	0.54
1:C:127:SER:O	1:C:209:LYS:NZ	2.41	0.54
1:D:240:THR:C	1:D:343:ILE:HG23	2.32	0.54
1:C:742:ASP:O	1:C:743:LEU:HD12	2.07	0.54
1:C:1022:ASP:OD1	1:C:1023:GLY:N	2.41	0.54
1:D:30:GLN:HB2	1:D:53:TYR:HD2	1.73	0.54
1:D:239:ILE:HG22	1:D:341:SER:CB	2.38	0.54
1:D:263:HIS:O	1:D:325:GLN:N	2.41	0.54
1:A:601:ASP:OD2	1:A:761:THR:OG1	2.26	0.53
1:B:580:ALA:O	1:B:757:THR:OG1	2.20	0.53
1:A:161:LEU:HD23	1:A:161:LEU:H	1.71	0.53
1:B:225:VAL:HG13	1:B:227:PRO:HD3	1.90	0.53
1:B:730:THR:HG22	1:B:897:ASP:HA	1.90	0.53
1:B:1328:LEU:HD12	1:B:1329:LYS:H	1.74	0.53
1:C:489:GLY:C	1:C:490:LEU:HD12	2.33	0.53
1:D:918:SER:OG	1:D:919:LEU:N	2.41	0.53
1:D:1179:ASN:O	1:D:1233:ASN:ND2	2.41	0.53
1:A:263:HIS:ND1	1:A:293:GLN:OE1	2.42	0.53
1:A:578:LEU:O	1:A:580:ALA:N	2.41	0.53
1:C:779:GLY:C	1:C:780:ILE:HD12	2.33	0.53
1:D:347:ILE:HG22	1:D:348:THR:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ILE:C	1:A:482:LEU:HD12	2.33	0.53
1:A:495:PHE:O	1:A:511:HIS:N	2.41	0.53
1:B:310:GLN:O	1:B:312:LYS:N	2.41	0.53
1:D:1227:ASP:OD1	1:D:1227:ASP:N	2.42	0.53
1:A:502:LYS:HE3	1:A:535:ALA:HB2	1.89	0.53
1:B:132:GLN:O	1:B:147:ARG:N	2.37	0.53
1:C:270:ARG:CZ	1:C:315:GLU:HB2	2.38	0.53
1:C:980:PHE:O	1:C:983:ASN:ND2	2.40	0.53
1:D:214:ARG:NH2	1:D:959:MET:SD	2.82	0.53
1:D:974:GLU:HG3	1:D:1027:THR:HG23	1.90	0.53
1:A:939:VAL:HG12	1:A:1332:ILE:HG22	1.90	0.53
1:D:118:THR:HG21	1:D:676:LYS:HD2	1.90	0.53
1:B:626:ASP:OD1	1:B:627:LEU:N	2.42	0.53
1:A:1025:TYR:CE2	1:A:1045:VAL:HG11	2.43	0.53
1:A:1206:VAL:HG13	1:A:1238:ILE:CD1	2.39	0.53
1:B:782:SER:OG	1:B:783:THR:N	2.40	0.53
1:B:932:SER:O	1:B:933:LEU:HD23	2.09	0.53
1:C:820:LYS:HD3	1:C:822:ILE:HD11	1.91	0.53
1:D:948:VAL:HG12	1:D:1305:LEU:HD11	1.91	0.53
1:B:1205:GLU:HG2	1:B:1206:VAL:HG23	1.91	0.53
1:C:577:SER:O	1:C:578:LEU:HB2	2.09	0.53
1:D:423:VAL:HG13	1:D:424:ASN:ND2	2.24	0.53
1:A:382:LYS:N	1:A:399:THR:OG1	2.40	0.53
1:A:931:LEU:CD1	1:A:933:LEU:HD21	2.39	0.53
1:B:457:SER:OG	1:B:483:ASN:N	2.40	0.53
1:C:648:VAL:HG12	1:C:648:VAL:O	2.07	0.53
1:C:949:SER:N	1:C:1325:GLN:O	2.42	0.53
1:D:42:GLU:N	1:D:91:VAL:O	2.42	0.53
1:D:62:ALA:HA	1:D:105:VAL:HG22	1.89	0.53
1:D:384:ILE:N	1:D:397:ALA:O	2.40	0.53
1:A:932:SER:O	1:A:933:LEU:HD23	2.09	0.52
1:A:948:VAL:CG1	1:A:1305:LEU:HD11	2.40	0.52
1:C:276:SER:OG	1:C:281:GLU:OE2	2.26	0.52
1:D:949:SER:N	1:D:1325:GLN:O	2.42	0.52
1:A:739:TRP:O	1:A:740:ILE:HD13	2.09	0.52
1:D:164:LEU:HD12	1:D:165:VAL:N	2.24	0.52
1:D:333:VAL:HG12	1:D:334:GLU:H	1.74	0.52
1:D:782:SER:OG	1:D:783:THR:N	2.32	0.52
3:H:1:NAG:C1	3:H:1:NAG:C8	2.86	0.52
1:A:70:ASN:HD22	1:A:70:ASN:N	2.08	0.52
1:A:418:SER:C	1:A:419:LEU:HD12	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLY:O	1:A:490:LEU:HD12	2.09	0.52
1:B:235:VAL:HB	1:B:248:VAL:HG13	1.91	0.52
1:B:1226:GLU:OE1	1:B:1226:GLU:N	2.41	0.52
1:D:351:SER:OG	1:D:352:PHE:N	2.40	0.52
1:B:614:SER:O	1:B:617:SER:OG	2.25	0.52
1:B:617:SER:O	1:B:621:LEU:HD13	2.09	0.52
1:B:650:ILE:HG21	1:B:656:THR:HG22	1.91	0.52
1:C:539:ARG:NH2	1:C:672:ASP:O	2.43	0.52
1:D:796:LEU:HD13	1:D:798:MET:SD	2.50	0.52
1:D:869:ASN:OD1	1:D:902:PRO:HB3	2.08	0.52
1:A:81:ASN:O	1:A:83:VAL:HG23	2.10	0.52
1:A:763:THR:OG1	1:A:764:GLU:N	2.43	0.52
1:A:1152:TYR:CE2	1:A:1214:LEU:HD13	2.45	0.52
1:B:648:VAL:HG13	1:B:658:VAL:HG13	1.92	0.52
1:B:831:SER:HG	1:B:834:PHE:HE1	1.56	0.52
1:B:952:GLY:HA3	1:B:1297:ARG:HH12	1.74	0.52
1:C:985:TYR:CE2	1:C:1255:VAL:HG13	2.44	0.52
1:C:1293:ASP:OD1	1:C:1294:ASN:N	2.43	0.52
1:D:579:PRO:O	1:D:581:SER:N	2.42	0.52
1:C:1206:VAL:O	1:C:1209:THR:N	2.41	0.52
1:C:1319:GLU:OE1	1:C:1319:GLU:N	2.42	0.52
1:D:568:VAL:HG23	1:D:589:ALA:HB2	1.92	0.52
1:B:38:LEU:HD23	1:B:39:LEU:N	2.25	0.52
1:B:648:VAL:HG13	1:B:658:VAL:CG1	2.40	0.52
1:B:795:GLU:O	1:B:813:THR:N	2.40	0.52
1:C:803:ILE:HG22	1:C:805:GLY:H	1.75	0.52
1:C:1148:ALA:O	1:C:1151:ALA:HB3	2.09	0.52
1:D:739:TRP:NE1	1:D:756:VAL:O	2.39	0.52
1:D:939:VAL:HG22	1:D:940:VAL:H	1.75	0.52
1:D:1025:TYR:HB2	1:D:1042:THR:HG22	1.91	0.52
4:A:2003:NAG:C8	4:A:2003:NAG:C1	2.86	0.52
1:C:538:ALA:HB3	1:C:558:TYR:HB2	1.91	0.52
1:C:814:VAL:C	1:C:815:LEU:HD12	2.35	0.52
1:D:486:THR:HG21	1:D:490:LEU:O	2.09	0.52
1:D:742:ASP:N	1:D:742:ASP:OD1	2.41	0.52
1:A:543:TYR:HD2	1:A:551:VAL:HG21	1.75	0.52
1:A:972:CYS:O	1:A:976:ASN:N	2.39	0.52
1:A:1142:SER:O	1:A:1144:VAL:HG22	2.09	0.52
1:B:824:VAL:HG23	1:B:875:GLU:C	2.35	0.52
1:D:596:ALA:N	1:D:597:LEU:HD12	2.25	0.52
1:B:495:PHE:N	1:B:511:HIS:O	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1166:VAL:O	1:B:1169:SER:OG	2.20	0.52
1:D:33:VAL:HG12	1:D:49:VAL:HG23	1.92	0.51
1:D:241:ILE:N	1:D:343:ILE:HG23	2.24	0.51
1:D:517:GLN:NE2	1:D:518:GLU:OE2	2.41	0.51
1:A:134:ASP:N	1:A:145:LYS:O	2.44	0.51
1:A:356:ASP:O	1:A:446:HIS:NE2	2.43	0.51
1:A:954:ILE:HG22	1:A:1297:ARG:HH21	1.74	0.51
1:B:49:VAL:O	1:B:84:LEU:HD12	2.09	0.51
1:B:507:ARG:NH1	1:B:529:PRO:O	2.43	0.51
1:C:230:GLU:CG	1:C:606:LEU:HD21	2.40	0.51
1:C:763:THR:OG1	1:C:764:GLU:N	2.42	0.51
1:D:580:ALA:O	1:D:757:THR:OG1	2.23	0.51
1:B:570:LEU:HD21	1:B:585:LEU:HD11	1.92	0.51
1:B:678:PHE:O	1:B:679:THR:OG1	2.25	0.51
1:B:912:LYS:N	1:B:1330:TYR:O	2.40	0.51
1:C:1142:SER:O	1:C:1144:VAL:HG22	2.10	0.51
1:D:1063:ILE:O	1:D:1067:LEU:N	2.43	0.51
1:A:919:LEU:HD23	1:A:920:LEU:N	2.25	0.51
1:B:1224:THR:OG1	1:B:1227:ASP:OD1	2.21	0.51
1:C:418:SER:N	1:C:419:LEU:HD12	2.25	0.51
1:D:1068:ILE:O	1:D:1071:SER:OG	2.19	0.51
1:B:635:ASN:OD1	1:B:636:ASP:N	2.42	0.51
1:D:999:GLU:O	1:D:1003:LYS:N	2.42	0.51
1:D:1126:PHE:O	1:D:1130:SER:OG	2.19	0.51
1:A:95:SER:OG	1:A:96:SER:N	2.43	0.51
1:B:1255:VAL:O	1:B:1255:VAL:CG1	2.57	0.51
1:C:562:ASN:ND2	1:C:616:SER:OG	2.44	0.51
1:C:650:ILE:HG12	1:C:656:THR:CG2	2.40	0.51
1:C:919:LEU:O	1:C:920:LEU:HD23	2.10	0.51
1:C:990:LEU:O	1:C:994:GLN:N	2.44	0.51
1:D:128:LEU:HD13	1:D:622:LEU:HA	1.92	0.51
1:D:554:ASP:OD1	1:D:555:SER:N	2.44	0.51
1:B:415:MET:HA	1:B:450:LEU:HD21	1.92	0.51
1:B:1067:LEU:HD12	1:B:1070:LEU:HD12	1.92	0.51
1:B:1117:THR:O	1:B:1122:ARG:NH1	2.44	0.51
1:C:992:GLU:CD	1:C:1266:ALA:HB2	2.35	0.51
1:D:489:GLY:O	1:D:490:LEU:HD23	2.10	0.51
1:D:570:LEU:HD22	1:D:784:ALA:HB2	1.93	0.51
3:J:2:NAG:H3	3:J:2:NAG:C8	2.13	0.51
1:A:782:SER:OG	1:A:783:THR:N	2.34	0.51
4:A:2001:NAG:H82	4:A:2001:NAG:C1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:VAL:O	1:B:859:ALA:N	2.43	0.51
1:A:1148:ALA:O	1:A:1151:ALA:HB3	2.11	0.51
1:B:51:LEU:O	1:B:82:ASP:N	2.40	0.51
1:B:321:HIS:ND1	1:B:334:GLU:OE2	2.42	0.51
1:B:571:SER:O	1:B:586:ARG:N	2.41	0.51
1:B:643:ILE:HD12	1:B:688:MET:HA	1.92	0.51
1:B:914:THR:O	1:B:914:THR:OG1	2.29	0.51
1:C:350:LEU:HD11	1:C:444:ALA:CB	2.37	0.51
1:D:1077:ASN:OD1	1:D:1078:GLY:N	2.43	0.51
1:D:1213:LEU:O	1:D:1217:LEU:HD23	2.11	0.51
1:A:58:VAL:HG22	1:A:109:GLY:HA3	1.93	0.51
1:A:147:ARG:HH12	1:A:743:LEU:HD11	1.75	0.51
1:A:246:MET:O	1:A:304:VAL:N	2.33	0.51
1:A:541:LEU:HD12	1:A:670:LEU:HD11	1.91	0.51
1:A:563:CYS:C	1:A:564:LEU:HD22	2.36	0.51
1:B:928:SER:OG	1:B:929:GLU:N	2.43	0.51
1:C:828:LEU:CB	1:C:872:VAL:HG12	2.41	0.51
1:D:570:LEU:HD11	1:D:585:LEU:HD21	1.93	0.51
1:D:1146:THR:O	1:D:1150:LEU:HD23	2.10	0.51
4:D:2002:NAG:H3	4:D:2002:NAG:O7	2.11	0.51
1:A:834:PHE:CD2	1:A:860:VAL:HG23	2.46	0.50
1:B:372:VAL:HG12	1:B:373:ASP:N	2.26	0.50
1:C:489:GLY:O	1:C:490:LEU:HD12	2.11	0.50
1:C:551:VAL:HG22	1:C:552:ILE:O	2.11	0.50
1:D:187:LEU:HD12	1:D:188:LYS:N	2.26	0.50
1:D:570:LEU:HD23	1:D:571:SER:N	2.26	0.50
1:D:1110:LEU:HD13	1:D:1156:LEU:HB2	1.93	0.50
1:B:351:SER:OG	1:B:352:PHE:O	2.28	0.50
1:B:1204:ALA:HB1	1:B:1207:GLU:OE2	2.12	0.50
1:C:579:PRO:HG3	1:C:759:PRO:HA	1.93	0.50
1:C:834:PHE:HE2	1:C:836:ALA:HB2	1.77	0.50
1:C:992:GLU:OE2	1:C:1266:ALA:CB	2.57	0.50
1:D:660:SER:OG	1:D:661:THR:N	2.43	0.50
1:D:960:GLN:OE1	1:D:960:GLN:N	2.44	0.50
1:A:345:ARG:O	1:A:440:GLU:N	2.44	0.50
1:A:983:ASN:HB2	1:A:1008:LEU:HD21	1.92	0.50
1:B:843:GLN:NE2	1:B:844:ALA:O	2.44	0.50
1:C:148:VAL:HG22	1:C:149:VAL:H	1.76	0.50
1:C:553:GLY:CA	1:C:666:MET:HE1	2.40	0.50
1:C:899:VAL:HG12	1:C:901:LYS:HG2	1.93	0.50
1:C:1022:ASP:OD1	1:C:1024:SER:N	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1025:TYR:CD2	1:C:1042:THR:HG22	2.46	0.50
1:C:1146:THR:O	1:C:1150:LEU:HD23	2.12	0.50
1:B:187:LEU:HD12	1:B:188:LYS:N	2.27	0.50
1:C:809:THR:OG1	1:C:857:SER:OG	2.10	0.50
1:D:604:VAL:O	1:D:608:LYS:N	2.44	0.50
1:A:63:SER:O	1:A:103:LEU:HD12	2.10	0.50
1:A:553:GLY:HA3	1:A:666:MET:HE1	1.92	0.50
1:B:101:MET:N	1:B:120:VAL:O	2.40	0.50
1:B:596:ALA:C	1:B:597:LEU:HD12	2.36	0.50
1:D:134:ASP:OD2	1:D:738:THR:OG1	2.28	0.50
1:D:679:THR:HG22	1:D:681:SER:H	1.76	0.50
1:D:1012:TYR:OH	1:D:1059:ASP:OD1	2.30	0.50
1:A:214:ARG:HH22	1:A:959:MET:HE3	1.77	0.50
1:A:779:GLY:C	1:A:780:ILE:HD12	2.37	0.50
1:C:576:GLN:OE1	1:C:580:ALA:HB3	2.11	0.50
1:C:1144:VAL:HG23	1:C:1145:TYR:N	2.26	0.50
1:A:965:LEU:HD11	1:A:1247:GLY:HA3	1.93	0.50
1:B:350:LEU:HD11	1:B:444:ALA:HB2	1.94	0.50
1:B:1261:LEU:O	1:B:1265:GLY:N	2.41	0.50
1:C:576:GLN:NE2	1:C:757:THR:HG21	2.27	0.50
1:C:825:SER:O	1:C:825:SER:OG	2.25	0.50
1:C:1299:LEU:HD23	1:C:1301:GLN:NE2	2.26	0.50
1:D:324:ALA:O	1:D:332:VAL:HG12	2.12	0.50
1:D:675:LEU:HD12	1:D:676:LYS:N	2.26	0.50
1:A:948:VAL:HG13	1:A:1305:LEU:HD11	1.93	0.50
1:A:965:LEU:HD11	1:A:1246:GLY:C	2.36	0.50
1:A:1185:ARG:HH12	1:A:1201:ALA:HB1	1.76	0.50
1:B:135:LYS:N	1:B:138:TYR:OH	2.39	0.50
1:B:165:VAL:HG13	1:B:207:VAL:HG22	1.93	0.50
1:D:458:PHE:HA	1:D:552:ILE:HD13	1.93	0.50
1:C:775:ASP:OD1	1:C:776:ALA:N	2.44	0.50
1:D:1002:SER:HA	1:D:1005:ILE:HD12	1.93	0.50
1:D:1026:SER:OG	1:D:1027:THR:N	2.44	0.50
1:A:61:SER:OG	1:A:75:THR:O	2.25	0.49
1:A:385:PHE:HE1	4:A:2004:NAG:H82	1.77	0.49
1:C:1148:ALA:HA	1:C:1170:LEU:HD11	1.94	0.49
1:D:944:ALA:HB2	1:D:1330:TYR:HB3	1.93	0.49
1:D:955:LEU:HD23	1:D:958:ALA:HB3	1.93	0.49
1:A:187:LEU:HD12	1:A:188:LYS:N	2.26	0.49
1:A:639:ASN:OD1	1:A:640:GLU:N	2.44	0.49
4:A:2001:NAG:H83	4:A:2001:NAG:C3	2.21	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:PHE:O	1:B:510:THR:OG1	2.22	0.49
1:B:535:ALA:HB1	1:B:536:PRO:HD2	1.94	0.49
1:C:958:ALA:O	1:C:962:THR:OG1	2.22	0.49
1:D:38:LEU:HD23	1:D:39:LEU:N	2.27	0.49
1:A:370:ARG:HE	1:A:404:LEU:HD21	1.76	0.49
1:A:737:GLU:O	1:A:738:THR:OG1	2.28	0.49
1:B:1041:LEU:O	1:B:1045:VAL:HG12	2.12	0.49
1:C:96:SER:OG	1:C:98:GLU:O	2.23	0.49
1:D:369:VAL:O	1:D:405:VAL:N	2.39	0.49
1:A:32:MET:O	1:A:50:LEU:N	2.44	0.49
1:B:837:VAL:N	1:B:859:ALA:O	2.45	0.49
1:B:1125:LEU:HD23	1:B:1128:LEU:HD12	1.94	0.49
1:C:121:MET:HE2	1:C:123:LYS:HE3	1.94	0.49
1:C:363:ILE:HD12	1:C:364:PRO:CD	2.42	0.49
1:C:579:PRO:HA	1:C:757:THR:HG22	1.93	0.49
1:D:761:THR:HG23	1:D:765:TRP:CZ2	2.47	0.49
1:D:1152:TYR:OH	1:D:1214:LEU:HD22	2.12	0.49
4:D:2001:NAG:H3	4:D:2001:NAG:C8	2.22	0.49
1:A:165:VAL:HG13	1:A:207:VAL:HG12	1.94	0.49
1:A:820:LYS:HD3	1:A:822:ILE:HD11	1.95	0.49
1:A:918:SER:OG	1:A:919:LEU:N	2.45	0.49
1:A:1019:LYS:NZ	1:A:1020:HIS:O	2.25	0.49
1:B:804:ARG:CD	1:B:865:LEU:HD13	2.42	0.49
1:B:1264:TYR:CZ	1:B:1268:THR:HG21	2.47	0.49
1:D:578:LEU:HD22	1:D:790:GLN:HB2	1.93	0.49
1:D:964:ASN:ND2	1:D:1244:ALA:O	2.42	0.49
1:A:954:ILE:HG12	1:A:993:THR:HG22	1.94	0.49
1:A:1005:ILE:HG21	1:C:1057:PHE:CD2	2.48	0.49
1:B:870:PHE:N	1:B:901:LYS:O	2.45	0.49
1:C:500:MET:HE1	1:C:675:LEU:HD23	1.95	0.49
1:C:593:SER:OG	1:C:594:VAL:N	2.43	0.49
1:D:541:LEU:HB3	1:D:673:MET:HE3	1.94	0.49
1:A:930:GLU:OE2	1:A:1312:TYR:N	2.44	0.49
1:B:510:THR:OG1	1:B:511:HIS:N	2.45	0.49
1:B:952:GLY:HA3	1:B:1297:ARG:NH1	2.27	0.49
1:B:1208:MET:O	1:B:1212:VAL:N	2.37	0.49
1:C:1180:SER:OG	1:C:1181:VAL:N	2.44	0.49
1:A:540:LEU:HB3	1:A:556:ALA:HB3	1.95	0.49
1:A:563:CYS:CA	1:A:564:LEU:HD22	2.43	0.49
1:A:598:ARG:O	1:A:768:GLY:N	2.45	0.49
1:A:1272:THR:O	1:A:1274:LYS:NZ	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:VAL:HG11	1:B:294:LEU:HD13	1.95	0.49
1:B:1166:VAL:O	1:B:1169:SER:N	2.46	0.49
1:D:908:GLU:O	1:D:1331:ASN:ND2	2.45	0.49
1:A:156:HIS:ND1	1:A:774:GLU:O	2.46	0.49
1:A:232:GLN:NE2	1:A:335:LEU:HD13	2.28	0.49
1:B:464:MET:O	1:B:466:HIS:N	2.46	0.49
1:B:600:VAL:HG11	1:B:605:LEU:HD23	1.94	0.49
1:D:903:LEU:HD12	1:D:904:LEU:O	2.12	0.49
1:D:1102:SER:O	1:D:1106:THR:HG22	2.12	0.49
1:A:60:VAL:HG23	1:A:107:VAL:HG23	1.93	0.49
1:A:62:ALA:HA	1:A:105:VAL:HG22	1.93	0.49
1:A:359:PHE:CZ	1:A:450:LEU:HD23	2.48	0.49
1:A:382:LYS:NZ	1:A:423:VAL:HG21	2.27	0.49
1:A:648:VAL:HB	1:A:656:THR:O	2.13	0.49
1:A:661:THR:HG21	1:D:654:THR:HG22	1.93	0.49
1:C:371:LEU:N	1:C:403:GLY:O	2.45	0.49
1:C:595:CYS:HA	1:C:771:CYS:HA	1.95	0.49
1:D:539:ARG:HB3	1:D:673:MET:HE1	1.95	0.49
1:D:1152:TYR:CE2	1:D:1214:LEU:HD13	2.48	0.49
2:I:1:NAG:H3	2:I:1:NAG:O7	2.13	0.49
1:B:1301:GLN:N	1:B:1301:GLN:OE1	2.45	0.48
1:C:123:LYS:O	1:C:125:GLU:N	2.46	0.48
1:D:373:ASP:OD1	1:D:373:ASP:N	2.46	0.48
1:D:763:THR:OG1	1:D:764:GLU:OE1	2.31	0.48
1:A:263:HIS:O	1:A:325:GLN:N	2.46	0.48
1:A:493:LEU:HD11	1:A:545:VAL:O	2.13	0.48
1:A:1242:GLN:NE2	1:A:1243:ASN:O	2.46	0.48
1:B:153:GLU:O	1:B:502:LYS:NZ	2.46	0.48
1:B:389:ASN:C	1:B:391:ALA:H	2.21	0.48
1:D:578:LEU:HA	1:D:788:ALA:HB1	1.95	0.48
3:L:1:NAG:O4	3:L:1:NAG:O6	2.29	0.48
1:A:357:SER:OG	1:A:358:HIS:ND1	2.41	0.48
1:A:1072:GLN:NE2	1:C:635:ASN:OD1	2.43	0.48
1:B:1026:SER:OG	1:B:1027:THR:N	2.46	0.48
1:C:28:LYS:N	1:C:547:PRO:O	2.46	0.48
1:C:233:VAL:HG12	1:C:250:VAL:HA	1.95	0.48
1:C:500:MET:HE1	1:C:675:LEU:CD2	2.42	0.48
1:D:307:LYS:O	1:D:310:GLN:NE2	2.45	0.48
1:D:746:VAL:HG12	1:D:747:ASN:O	2.13	0.48
1:A:822:ILE:HG22	1:A:823:ARG:O	2.13	0.48
1:D:808:PHE:CE2	1:D:860:VAL:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:883:CYS:SG	1:D:884:GLY:N	2.86	0.48
1:C:581:SER:HB2	1:C:756:VAL:HG13	1.96	0.48
1:D:55:ASN:HB3	1:D:110:PRO:HD2	1.96	0.48
1:D:916:PHE:HB3	1:D:931:LEU:HD21	1.94	0.48
1:A:760:ASP:CG	1:A:899:VAL:HG22	2.39	0.48
1:A:974:GLU:HG3	1:A:1027:THR:HG22	1.94	0.48
1:B:264:VAL:CG1	1:B:294:LEU:HD13	2.44	0.48
1:B:372:VAL:HG11	1:B:376:GLY:HA2	1.95	0.48
1:B:1248:PHE:HD1	1:B:1254:THR:HG23	1.78	0.48
1:C:373:ASP:OD1	1:C:374:GLY:N	2.46	0.48
1:C:1257:ALA:O	1:C:1261:LEU:HD12	2.13	0.48
1:D:1148:ALA:O	1:D:1151:ALA:HB3	2.14	0.48
1:B:31:TYR:HB2	1:B:51:LEU:HD23	1.95	0.48
1:B:55:ASN:HB3	1:B:110:PRO:CD	2.43	0.48
1:B:461:LEU:N	1:B:461:LEU:HD12	2.29	0.48
1:C:155:PHE:HB3	1:C:778:LEU:CD2	2.43	0.48
1:C:576:GLN:NE2	1:C:576:GLN:O	2.46	0.48
1:A:1187:GLN:O	1:A:1188:LYS:NZ	2.25	0.48
1:B:665:ASP:OD1	1:B:667:TYR:N	2.45	0.48
1:C:996:LEU:HD11	1:C:1001:LYS:HD2	1.95	0.48
1:A:155:PHE:HB3	1:A:778:LEU:HD22	1.96	0.48
1:B:29:PRO:N	1:B:29:PRO:C	2.63	0.48
1:B:476:VAL:HB	1:B:526:ILE:HG23	1.96	0.48
1:B:775:ASP:OD1	1:B:776:ALA:N	2.47	0.48
1:B:1076:ASP:OD1	1:B:1076:ASP:N	2.47	0.48
1:C:400:ASP:OD1	1:C:403:GLY:N	2.46	0.48
1:D:1004:ALA:O	1:D:1008:LEU:N	2.45	0.48
1:D:1047:LYS:NZ	1:D:1211:TYR:OH	2.47	0.48
1:C:161:LEU:H	1:C:161:LEU:HD23	1.79	0.48
1:C:457:SER:OG	1:C:483:ASN:N	2.42	0.48
1:C:798:MET:HE3	1:C:903:LEU:HD23	1.96	0.48
1:D:665:ASP:O	1:D:669:PHE:N	2.42	0.48
1:D:931:LEU:HG	1:D:933:LEU:HD21	1.95	0.48
1:D:1167:LEU:HD12	1:D:1168:LYS:N	2.29	0.48
1:A:666:MET:CG	1:A:683:ILE:HG23	2.44	0.47
1:A:1183:TRP:CH2	1:A:1212:VAL:HG11	2.49	0.47
1:B:489:GLY:O	1:B:490:LEU:HD23	2.13	0.47
1:B:828:LEU:HD12	1:B:870:PHE:CZ	2.49	0.47
1:C:109:GLY:N	1:C:112:GLN:O	2.44	0.47
1:C:742:ASP:C	1:C:743:LEU:HD12	2.39	0.47
1:C:1264:TYR:CE1	1:C:1268:THR:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASN:HB3	1:D:110:PRO:CD	2.44	0.47
1:D:546:LEU:HB2	1:D:548:THR:HG22	1.96	0.47
1:D:1131:ALA:O	1:D:1134:THR:OG1	2.31	0.47
1:B:942:GLU:HA	1:B:1308:LEU:HD11	1.96	0.47
1:B:960:GLN:NE2	1:B:1244:ALA:O	2.47	0.47
1:B:1316:VAL:HG12	1:B:1317:THR:N	2.29	0.47
1:C:77:LEU:HD12	1:C:78:GLU:N	2.29	0.47
1:C:319:LYS:C	1:C:320:LEU:HD12	2.39	0.47
1:C:535:ALA:HB3	1:C:537:VAL:CG1	2.44	0.47
1:C:592:GLN:OE1	1:C:748:SER:OG	2.09	0.47
1:C:861:THR:HG22	1:C:862:PRO:HD2	1.96	0.47
1:D:733:LYS:NZ	1:D:736:PRO:HG3	2.29	0.47
1:A:489:GLY:C	1:A:490:LEU:HD12	2.39	0.47
1:B:517:GLN:NE2	1:B:518:GLU:OE2	2.46	0.47
1:B:597:LEU:HD13	1:B:743:LEU:HA	1.97	0.47
1:D:1183:TRP:HB3	1:D:1208:MET:HE1	1.96	0.47
1:A:66:SER:CA	1:A:101:MET:HE1	2.45	0.47
1:A:470:CYS:O	1:A:472:HIS:ND1	2.47	0.47
1:B:369:VAL:O	1:B:405:VAL:N	2.42	0.47
1:C:58:VAL:C	1:C:79:ALA:HB3	2.40	0.47
1:C:778:LEU:HD23	1:C:778:LEU:H	1.79	0.47
1:C:932:SER:OG	1:C:1310:GLY:O	2.31	0.47
1:D:578:LEU:HD11	1:D:760:ASP:HA	1.96	0.47
1:A:205:VAL:HG23	1:A:219:PHE:CZ	2.50	0.47
1:A:742:ASP:CA	1:A:743:LEU:HD12	2.44	0.47
1:A:887:VAL:O	1:A:887:VAL:HG13	2.15	0.47
1:B:164:LEU:HD21	1:B:166:TYR:CD2	2.49	0.47
1:B:476:VAL:N	1:B:526:ILE:O	2.45	0.47
1:B:1144:VAL:HG23	1:B:1145:TYR:N	2.30	0.47
1:C:849:CYS:O	1:C:852:GLY:N	2.45	0.47
1:D:816:ASN:O	1:D:851:ASN:N	2.47	0.47
1:A:1210:SER:OG	1:A:1256:VAL:HG23	2.14	0.47
1:B:1146:THR:O	1:B:1150:LEU:HD23	2.14	0.47
1:C:939:VAL:HG12	1:C:1332:ILE:HG22	1.96	0.47
1:C:1019:LYS:NZ	1:C:1020:HIS:O	2.37	0.47
1:C:1036:GLN:NE2	1:C:1037:GLY:O	2.47	0.47
1:A:128:LEU:HD13	1:A:622:LEU:CA	2.43	0.47
1:B:954:ILE:HG21	1:B:1269:PHE:CD1	2.50	0.47
1:C:164:LEU:HD21	1:C:166:TYR:CD2	2.49	0.47
1:C:277:ASP:OD2	1:D:434:TYR:OH	2.21	0.47
1:C:495:PHE:O	1:C:511:HIS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:LEU:HD21	1:C:585:LEU:CD1	2.42	0.47
1:C:597:LEU:HD13	1:C:743:LEU:HA	1.96	0.47
1:C:948:VAL:HG13	1:C:1305:LEU:HD21	1.95	0.47
1:C:976:ASN:ND2	1:C:1015:GLN:OE1	2.48	0.47
1:D:174:ARG:NH2	1:D:1298:LEU:HD23	2.30	0.47
1:D:310:GLN:O	1:D:312:LYS:N	2.47	0.47
1:D:763:THR:HG23	1:D:764:GLU:O	2.13	0.47
1:D:1259:HIS:O	1:D:1262:SER:OG	2.32	0.47
1:A:965:LEU:HD11	1:A:1247:GLY:CA	2.45	0.47
1:B:390:GLU:OE1	1:B:390:GLU:HA	2.15	0.47
1:C:240:THR:O	1:C:311:LEU:HD12	2.14	0.47
1:C:263:HIS:O	1:C:325:GLN:N	2.48	0.47
1:C:564:LEU:HD21	1:C:615:ALA:HB1	1.97	0.47
1:C:816:ASN:O	1:C:851:ASN:N	2.48	0.47
1:C:1184:GLU:OE1	1:C:1184:GLU:N	2.47	0.47
1:C:1204:ALA:O	1:C:1208:MET:HE3	2.15	0.47
1:D:510:THR:OG1	1:D:511:HIS:N	2.47	0.47
1:D:849:CYS:O	1:D:852:GLY:N	2.44	0.47
1:A:239:ILE:HD11	1:A:243:GLU:HB3	1.95	0.47
1:A:353:VAL:HG23	1:A:354:LYS:H	1.79	0.47
1:B:982:PRO:O	1:B:986:VAL:HG12	2.15	0.47
1:B:1116:VAL:HA	1:B:1121:VAL:HG11	1.97	0.47
1:B:1257:ALA:C	1:B:1261:LEU:HD12	2.40	0.47
1:D:241:ILE:O	1:D:243:GLU:N	2.47	0.47
1:D:502:LYS:HG2	1:D:535:ALA:HB2	1.96	0.47
1:A:415:MET:HA	1:A:450:LEU:HD21	1.97	0.47
1:A:955:LEU:CB	1:A:1298:LEU:HD22	2.44	0.47
1:B:152:ASP:OD1	1:B:152:ASP:N	2.48	0.47
1:B:319:LYS:C	1:B:320:LEU:HD12	2.40	0.47
1:C:1051:GLN:O	1:C:1054:ALA:HB3	2.14	0.47
2:I:1:NAG:H62	2:I:2:NAG:HN2	1.80	0.47
1:A:459:VAL:HG12	1:A:460:HIS:N	2.29	0.46
1:A:635:ASN:OD1	1:A:636:ASP:N	2.46	0.46
1:A:1025:TYR:HD2	1:A:1042:THR:HG22	1.80	0.46
1:B:540:LEU:O	1:B:556:ALA:N	2.48	0.46
1:B:865:LEU:HD11	1:B:907:PRO:HD3	1.97	0.46
1:B:1178:ASP:OD1	1:B:1178:ASP:N	2.46	0.46
1:C:94:SER:OG	1:C:124:ASN:ND2	2.48	0.46
4:C:2005:NAG:O7	4:C:2005:NAG:O3	2.30	0.46
1:D:1005:ILE:O	1:D:1009:ASN:ND2	2.43	0.46
1:D:1228:LEU:O	1:D:1232:THR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:SER:N	1:A:104:THR:O	2.42	0.46
1:A:914:THR:O	1:A:1328:LEU:N	2.46	0.46
1:B:498:LEU:HD12	1:B:541:LEU:HD21	1.97	0.46
1:D:121:MET:HE2	1:D:631:PRO:HB2	1.96	0.46
1:D:359:PHE:CZ	1:D:450:LEU:HD23	2.50	0.46
1:D:1316:VAL:HG12	1:D:1317:THR:N	2.29	0.46
1:A:516:LYS:O	1:A:517:GLN:C	2.58	0.46
1:A:785:SER:O	1:A:785:SER:OG	2.26	0.46
1:A:809:THR:HG21	1:A:811:LYS:HE3	1.97	0.46
1:B:685:LYS:O	1:B:687:LYS:N	2.47	0.46
1:C:510:THR:OG1	1:C:511:HIS:N	2.46	0.46
1:C:819:PRO:HA	1:C:850:ALA:HB2	1.96	0.46
1:D:118:THR:HG21	1:D:676:LYS:CD	2.45	0.46
1:D:578:LEU:HB3	1:D:579:PRO:HD3	1.96	0.46
1:D:1231:ALA:O	1:D:1235:VAL:HG23	2.16	0.46
1:A:356:ASP:OD1	1:A:357:SER:N	2.48	0.46
1:B:130:PHE:CE1	1:B:149:VAL:HG11	2.50	0.46
1:B:656:THR:HG21	1:C:648:VAL:HG11	1.97	0.46
1:C:104:THR:HG23	1:C:117:ARG:HB3	1.97	0.46
1:C:665:ASP:OD2	1:C:685:LYS:N	2.48	0.46
1:A:642:CYS:SG	1:A:643:ILE:N	2.88	0.46
1:A:824:VAL:HG22	1:A:874:ALA:HB1	1.98	0.46
1:A:1181:VAL:HG23	1:A:1234:ILE:CG2	2.46	0.46
1:A:1333:LEU:HD13	1:A:1336:LYS:CE	2.44	0.46
1:B:118:THR:HG21	1:B:676:LYS:CD	2.45	0.46
1:B:126:ASP:N	1:B:126:ASP:OD1	2.48	0.46
1:B:1152:TYR:O	1:B:1155:ALA:HB3	2.15	0.46
1:B:1168:LYS:O	1:B:1172:GLU:N	2.48	0.46
1:C:822:ILE:HG12	1:C:887:VAL:HG23	1.98	0.46
1:C:1113:PRO:C	1:C:1114:LEU:HD23	2.40	0.46
1:C:1144:VAL:HG23	1:C:1145:TYR:H	1.81	0.46
1:C:1180:SER:OG	1:C:1233:ASN:O	2.27	0.46
1:D:605:LEU:HD12	1:D:608:LYS:O	2.16	0.46
1:A:354:LYS:HZ3	1:A:463:PRO:C	2.19	0.46
1:A:834:PHE:HD2	1:A:860:VAL:HG23	1.79	0.46
1:C:77:LEU:HD12	1:C:78:GLU:H	1.79	0.46
1:C:550:ASP:OD1	1:C:551:VAL:N	2.42	0.46
1:D:239:ILE:HG23	1:D:343:ILE:CG1	2.46	0.46
1:D:1125:LEU:HA	1:D:1128:LEU:HD12	1.97	0.46
1:A:33:VAL:HG12	1:A:49:VAL:HB	1.97	0.46
1:A:205:VAL:HG23	1:A:219:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LYS:O	1:B:341:SER:OG	2.32	0.46
1:B:266:VAL:HG23	1:B:322:THR:HB	1.97	0.46
1:B:423:VAL:HG13	1:B:424:ASN:ND2	2.30	0.46
1:B:594:VAL:O	1:B:772:LEU:N	2.45	0.46
1:B:869:ASN:HA	1:B:902:PRO:HA	1.98	0.46
1:C:130:PHE:CZ	1:C:149:VAL:HG21	2.51	0.46
1:C:183:LEU:HD22	1:C:187:LEU:C	2.40	0.46
1:C:576:GLN:O	1:C:576:GLN:CD	2.59	0.46
1:C:1187:GLN:O	1:C:1188:LYS:NZ	2.25	0.46
1:D:237:LYS:O	1:D:238:ILE:HD13	2.15	0.46
1:D:386:ILE:HA	1:D:421:VAL:HG13	1.98	0.46
1:A:363:ILE:HD12	1:A:364:PRO:HD2	1.98	0.46
1:A:948:VAL:HG13	1:A:1305:LEU:HD21	1.97	0.46
1:A:1146:THR:O	1:A:1150:LEU:HD23	2.15	0.46
1:B:56:GLU:O	1:B:58:VAL:N	2.49	0.46
1:B:778:LEU:HD23	1:B:778:LEU:H	1.80	0.46
1:C:146:PHE:O	1:C:190:PHE:N	2.45	0.46
1:C:570:LEU:HD23	1:C:571:SER:N	2.31	0.46
1:C:809:THR:HG21	1:C:811:LYS:HE2	1.97	0.46
1:C:916:PHE:CG	1:C:931:LEU:HD21	2.51	0.46
1:C:1177:LYS:N	1:C:1180:SER:O	2.45	0.46
1:D:871:THR:HG23	1:D:900:ILE:HG12	1.98	0.46
1:A:373:ASP:OD1	1:A:374:GLY:N	2.49	0.46
1:A:578:LEU:O	1:A:579:PRO:C	2.59	0.46
1:A:1211:TYR:HA	1:A:1214:LEU:HD12	1.97	0.46
1:A:1227:ASP:OD1	1:A:1227:ASP:N	2.47	0.46
1:A:1293:ASP:N	1:A:1296:ASN:OD1	2.47	0.46
1:B:570:LEU:HD23	1:B:571:SER:N	2.30	0.46
1:B:954:ILE:HG21	1:B:1269:PHE:CE1	2.51	0.46
1:B:1063:ILE:O	1:B:1067:LEU:N	2.48	0.46
1:B:1103:ALA:HB3	1:B:1149:LEU:HD23	1.98	0.46
1:C:1144:VAL:HG21	1:C:1185:ARG:HA	1.98	0.46
1:D:804:ARG:NH2	1:D:863:LYS:O	2.47	0.46
1:B:955:LEU:HD21	1:B:995:GLN:CD	2.40	0.46
1:B:958:ALA:O	1:B:962:THR:HG21	2.16	0.46
1:B:1323:TYR:C	1:B:1324:LEU:HD12	2.41	0.46
1:C:582:HIS:CD2	1:C:754:VAL:HG11	2.49	0.46
1:C:1118:HIS:HB3	1:C:1121:VAL:HG22	1.98	0.46
1:D:595:CYS:HB3	1:D:597:LEU:HD11	1.98	0.46
1:A:233:VAL:HG12	1:A:250:VAL:CA	2.43	0.45
1:C:164:LEU:HD12	1:C:165:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLU:N	1:C:216:GLU:OE2	2.49	0.45
1:D:1211:TYR:HA	1:D:1214:LEU:HD12	1.97	0.45
1:C:159:ASN:ND2	1:C:184:GLU:O	2.47	0.45
1:C:488:LEU:HD12	1:C:489:GLY:N	2.31	0.45
1:C:823:ARG:HH21	1:C:844:ALA:HB1	1.81	0.45
1:D:1121:VAL:HG22	1:D:1125:LEU:HD11	1.98	0.45
1:A:233:VAL:HG23	1:A:338:ARG:HH22	1.81	0.45
1:B:137:ILE:HG22	1:B:220:THR:HB	1.97	0.45
1:C:249:SER:OG	1:C:250:VAL:N	2.49	0.45
1:D:411:THR:OG1	1:D:411:THR:O	2.35	0.45
1:D:837:VAL:O	1:D:859:ALA:N	2.47	0.45
1:D:889:SER:O	1:D:889:SER:OG	2.33	0.45
1:D:903:LEU:HD12	1:D:904:LEU:N	2.31	0.45
1:A:429:SER:O	1:B:1195:HIS:NE2	2.48	0.45
1:A:650:ILE:HG12	1:A:656:THR:HG22	1.98	0.45
1:B:952:GLY:C	1:B:1297:ARG:HH12	2.24	0.45
1:C:144:VAL:HG12	1:C:192:PHE:HB3	1.98	0.45
1:C:310:GLN:O	1:C:312:LYS:N	2.49	0.45
1:C:947:SER:N	1:C:1305:LEU:HD12	2.32	0.45
1:C:1323:TYR:C	1:C:1324:LEU:HD12	2.42	0.45
1:D:577:SER:OG	1:D:578:LEU:N	2.50	0.45
1:D:875:GLU:N	1:D:875:GLU:OE1	2.50	0.45
1:A:103:LEU:HD12	1:A:104:THR:H	1.80	0.45
1:A:666:MET:HG3	1:A:683:ILE:HG23	1.99	0.45
1:A:880:GLN:H	1:A:887:VAL:HG11	1.82	0.45
1:A:1253:ASP:OD1	1:A:1253:ASP:N	2.50	0.45
1:C:63:SER:O	1:C:103:LEU:HD12	2.17	0.45
1:C:877:LEU:O	1:C:887:VAL:HG22	2.15	0.45
1:C:1210:SER:OG	1:C:1211:TYR:N	2.49	0.45
1:D:55:ASN:HB3	1:D:110:PRO:CG	2.46	0.45
1:A:1039:THR:OG1	1:A:1040:TRP:N	2.50	0.45
1:A:1137:GLU:OE1	1:A:1137:GLU:N	2.50	0.45
1:B:1225:SER:O	1:B:1229:THR:HG23	2.17	0.45
1:C:81:ASN:O	1:C:83:VAL:HG23	2.16	0.45
1:C:128:LEU:HD11	1:C:155:PHE:CE1	2.51	0.45
1:C:249:SER:OG	1:C:300:PHE:O	2.35	0.45
1:C:535:ALA:HB3	1:C:537:VAL:HG12	1.97	0.45
1:C:887:VAL:O	1:C:887:VAL:HG13	2.16	0.45
1:C:1152:TYR:O	1:C:1155:ALA:HB3	2.16	0.45
1:D:415:MET:HA	1:D:450:LEU:HD21	1.99	0.45
1:D:536:PRO:O	1:D:560:VAL:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:CA	1:A:343:ILE:HG23	2.47	0.45
1:C:151:MET:SD	1:C:778:LEU:HD22	2.57	0.45
1:C:796:LEU:HD13	1:C:798:MET:HG2	1.97	0.45
1:C:997:THR:CG2	1:C:1000:ILE:HG22	2.47	0.45
1:D:233:VAL:HA	1:D:250:VAL:HA	1.99	0.45
1:A:517:GLN:HE21	1:A:517:GLN:CA	2.26	0.45
1:A:665:ASP:O	1:A:669:PHE:N	2.48	0.45
1:B:164:LEU:HD12	1:B:165:VAL:N	2.32	0.45
1:B:816:ASN:ND2	1:B:848:ILE:O	2.47	0.45
1:C:804:ARG:CD	1:C:865:LEU:HD13	2.46	0.45
1:D:1137:GLU:N	1:D:1137:GLU:OE2	2.50	0.45
1:A:570:LEU:HD21	1:A:585:LEU:CD1	2.46	0.45
1:A:1129:GLU:OE1	1:A:1162:LYS:NZ	2.49	0.45
1:B:462:GLU:OE1	1:B:479:HIS:NE2	2.50	0.45
1:B:1217:LEU:HD21	1:B:1231:ALA:HB1	1.99	0.45
1:D:325:GLN:HA	1:D:332:VAL:HG12	1.99	0.45
1:D:1281:GLN:O	1:D:1313:SER:N	2.45	0.45
1:A:536:PRO:HA	1:A:560:VAL:HB	1.99	0.45
1:B:499:ILE:HD11	1:B:528:ILE:HD13	1.97	0.45
1:B:1167:LEU:HD12	1:B:1168:LYS:N	2.32	0.45
1:D:53:TYR:CE1	1:D:547:PRO:HG3	2.52	0.45
1:D:233:VAL:HG23	1:D:250:VAL:HG22	1.97	0.45
1:D:351:SER:O	1:D:369:VAL:HG13	2.17	0.45
1:D:1144:VAL:HG11	1:D:1184:GLU:O	2.17	0.45
1:A:66:SER:N	1:A:101:MET:HE1	2.31	0.44
1:A:165:VAL:HG22	1:A:207:VAL:HG12	1.99	0.44
1:A:584:HIS:CD2	1:A:754:VAL:HG22	2.52	0.44
1:A:663:GLU:O	1:A:685:LYS:NZ	2.50	0.44
1:A:1086:LEU:HD12	1:A:1087:LEU:C	2.42	0.44
1:A:1202:PRO:O	1:A:1203:SER:OG	2.27	0.44
1:A:1312:TYR:O	1:A:1314:MET:HE1	2.16	0.44
1:B:244:GLU:OE1	1:B:244:GLU:N	2.45	0.44
1:D:733:LYS:HE2	1:D:901:LYS:HE3	1.99	0.44
1:D:910:LEU:HD23	1:D:911:GLU:O	2.17	0.44
1:D:939:VAL:HG23	1:D:1331:ASN:O	2.17	0.44
4:A:2001:NAG:C8	4:A:2001:NAG:C1	2.95	0.44
1:B:266:VAL:HG22	1:B:267:SER:N	2.32	0.44
1:B:546:LEU:CB	1:B:548:THR:HG22	2.46	0.44
1:C:464:MET:HE2	1:C:466:HIS:CE1	2.52	0.44
1:C:1100:THR:HG22	1:C:1146:THR:HG22	1.98	0.44
1:D:60:VAL:HG23	1:D:107:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:ILE:HG22	1:D:220:THR:HG1	1.82	0.44
1:D:735:PHE:O	1:D:735:PHE:CD1	2.70	0.44
1:D:959:MET:O	1:D:962:THR:OG1	2.35	0.44
1:D:1269:PHE:CE1	1:D:1271:ARG:HG2	2.49	0.44
1:A:762:ILE:HG13	1:A:762:ILE:O	2.17	0.44
1:A:981:ALA:O	1:A:984:ILE:HD12	2.17	0.44
1:B:1127:CYS:O	1:B:1131:ALA:N	2.43	0.44
1:C:491:LYS:O	1:C:515:VAL:N	2.40	0.44
1:D:545:VAL:C	1:D:546:LEU:HD23	2.43	0.44
1:D:598:ARG:O	1:D:768:GLY:N	2.40	0.44
1:A:240:THR:HA	1:A:343:ILE:HG23	1.98	0.44
1:A:516:LYS:HD3	1:A:517:GLN:N	2.32	0.44
1:A:665:ASP:OD1	1:A:667:TYR:N	2.50	0.44
1:B:42:GLU:N	1:B:91:VAL:O	2.49	0.44
1:B:226:LEU:O	1:B:228:LYS:NZ	2.49	0.44
1:B:1110:LEU:HD13	1:B:1156:LEU:HB2	1.99	0.44
1:C:469:PRO:O	1:C:530:VAL:HG11	2.17	0.44
1:C:1205:GLU:OE1	1:C:1205:GLU:N	2.45	0.44
1:D:58:VAL:HG22	1:D:59:THR:N	2.32	0.44
1:D:63:SER:N	1:D:104:THR:O	2.43	0.44
1:D:388:GLY:N	1:D:393:TYR:O	2.51	0.44
1:D:929:GLU:O	1:D:1314:MET:N	2.50	0.44
1:A:584:HIS:NE2	1:A:754:VAL:HG22	2.33	0.44
1:B:997:THR:CG2	1:B:1000:ILE:HG22	2.47	0.44
1:C:461:LEU:HD11	1:C:478:ALA:HB1	2.00	0.44
1:C:470:CYS:O	1:C:472:HIS:ND1	2.48	0.44
1:C:584:HIS:CG	1:C:754:VAL:HG22	2.52	0.44
1:C:606:LEU:O	1:C:606:LEU:HD23	2.18	0.44
1:C:982:PRO:O	1:C:986:VAL:HG23	2.17	0.44
1:D:33:VAL:O	1:D:677:ALA:HB1	2.18	0.44
1:D:38:LEU:HD23	1:D:40:HIS:N	2.33	0.44
1:D:842:GLU:OE2	1:D:842:GLU:N	2.48	0.44
1:A:1076:ASP:OD1	1:A:1077:ASN:N	2.50	0.44
1:B:1161:ASP:OD1	1:B:1162:LYS:N	2.50	0.44
1:C:593:SER:HG	1:C:594:VAL:H	1.65	0.44
1:C:826:VAL:HG23	1:C:874:ALA:HB2	1.99	0.44
1:C:955:LEU:HB2	1:C:1298:LEU:HD13	1.99	0.44
1:D:137:ILE:HG22	1:D:220:THR:OG1	2.18	0.44
1:D:230:GLU:HB3	1:D:253:LEU:HD21	1.99	0.44
1:D:798:MET:HE3	1:D:903:LEU:HB3	1.98	0.44
1:D:1206:VAL:HG13	1:D:1237:TRP:HZ3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HA	1:A:53:TYR:HB2	1.99	0.44
1:A:501:ALA:HB1	1:A:537:VAL:CG1	2.48	0.44
1:B:809:THR:HG21	1:B:811:LYS:HE3	1.98	0.44
1:C:648:VAL:O	1:C:648:VAL:CG1	2.65	0.44
1:C:782:SER:OG	1:C:783:THR:N	2.38	0.44
1:D:648:VAL:HG13	1:D:658:VAL:HG13	2.00	0.44
3:F:1:NAG:H3	3:F:2:NAG:C8	2.48	0.44
1:A:1203:SER:OG	1:A:1205:GLU:OE1	2.34	0.44
1:B:1180:SER:OG	1:B:1181:VAL:N	2.48	0.44
1:B:1250:SER:OG	1:B:1253:ASP:OD1	2.26	0.44
1:C:128:LEU:HD21	1:C:151:MET:HB3	2.00	0.44
1:C:230:GLU:HG3	1:C:606:LEU:HD21	1.98	0.44
1:C:992:GLU:HA	1:C:992:GLU:OE1	2.18	0.44
1:C:1142:SER:OG	1:C:1146:THR:OG1	2.09	0.44
1:D:590:ALA:O	1:D:593:SER:OG	2.22	0.44
1:D:949:SER:OG	1:D:1325:GLN:N	2.50	0.44
1:A:230:GLU:HB2	1:A:606:LEU:HD21	1.98	0.44
1:A:460:HIS:C	1:A:461:LEU:HD12	2.43	0.44
1:B:58:VAL:HG22	1:B:59:THR:N	2.33	0.44
1:B:94:SER:OG	1:B:96:SER:O	2.36	0.44
1:B:1217:LEU:CD2	1:B:1231:ALA:HB1	2.48	0.44
1:C:476:VAL:HB	1:C:526:ILE:HG22	2.00	0.44
1:D:50:LEU:HD23	1:D:50:LEU:C	2.43	0.44
1:D:354:LYS:HZ3	1:D:463:PRO:C	2.24	0.44
1:D:1012:TYR:CZ	1:D:1016:LEU:HD11	2.52	0.44
1:A:421:VAL:H	1:A:444:ALA:HB3	1.82	0.43
1:A:1086:LEU:HD12	1:A:1087:LEU:N	2.33	0.43
1:A:1299:LEU:HD23	1:A:1301:GLN:NE2	2.33	0.43
1:B:1271:ARG:NH1	3:H:1:NAG:O3	2.49	0.43
1:C:417:THR:OG1	1:C:419:LEU:HD11	2.18	0.43
1:C:464:MET:SD	1:C:474:GLN:NE2	2.91	0.43
1:C:1076:ASP:OD1	1:C:1077:ASN:N	2.51	0.43
1:D:453:SER:OG	1:D:456:LYS:N	2.51	0.43
1:D:823:ARG:HD2	1:D:877:LEU:HD22	1.99	0.43
1:A:103:LEU:HD12	1:A:104:THR:N	2.32	0.43
1:A:538:ALA:HB2	1:A:560:VAL:HG23	1.99	0.43
1:A:570:LEU:HD21	1:A:585:LEU:CG	2.47	0.43
1:B:30:GLN:N	1:B:53:TYR:HD2	2.13	0.43
1:B:101:MET:O	1:B:120:VAL:N	2.44	0.43
1:B:954:ILE:HG23	1:B:955:LEU:HG	2.00	0.43
1:B:1088:ASN:OD1	1:B:1088:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:PRO:HA	1:C:560:VAL:HB	2.01	0.43
1:C:1107:ILE:HG21	1:C:1149:LEU:HD11	2.01	0.43
1:C:1208:MET:O	1:C:1212:VAL:HG23	2.18	0.43
1:D:155:PHE:HB3	1:D:778:LEU:CD2	2.49	0.43
1:A:480:TYR:HB2	1:A:482:LEU:HD11	1.99	0.43
1:A:510:THR:OG1	1:A:511:HIS:N	2.50	0.43
1:A:1074:GLN:OE1	1:A:1075:LYS:N	2.47	0.43
1:A:1213:LEU:HD23	1:A:1260:ALA:HB1	2.01	0.43
1:B:849:CYS:O	1:B:852:GLY:N	2.44	0.43
1:B:887:VAL:HG13	1:B:887:VAL:O	2.18	0.43
1:B:930:GLU:OE1	1:B:1312:TYR:N	2.51	0.43
1:C:128:LEU:H	1:C:128:LEU:HD23	1.83	0.43
1:C:461:LEU:HD11	1:C:478:ALA:CB	2.48	0.43
1:C:1248:PHE:CD1	1:C:1254:THR:HG23	2.53	0.43
1:A:244:GLU:C	1:A:306:THR:HG22	2.43	0.43
1:A:576:GLN:CD	1:A:580:ALA:HB3	2.43	0.43
4:A:2005:NAG:O7	4:A:2005:NAG:O3	2.29	0.43
1:B:52:SER:HA	1:B:82:ASP:H	1.83	0.43
1:B:230:GLU:HB3	1:B:253:LEU:HD21	1.99	0.43
1:B:1206:VAL:HG22	1:B:1237:TRP:HH2	1.81	0.43
1:B:1262:SER:OG	1:B:1263:LYS:N	2.51	0.43
1:C:275:ALA:HB1	1:C:281:GLU:HB3	2.00	0.43
1:C:355:VAL:HG13	1:C:355:VAL:O	2.18	0.43
1:C:870:PHE:N	1:C:901:LYS:O	2.50	0.43
1:D:66:SER:HB3	1:D:71:ARG:HB2	1.99	0.43
1:A:262:GLY:O	1:A:294:LEU:N	2.50	0.43
1:A:595:CYS:HA	1:A:771:CYS:HA	2.01	0.43
1:A:802:VAL:HG23	1:A:905:VAL:HG23	2.01	0.43
1:A:984:ILE:HG13	1:A:1008:LEU:HD11	2.00	0.43
1:A:1227:ASP:OD1	1:A:1228:LEU:N	2.51	0.43
1:B:121:MET:HE1	1:B:633:PRO:HG2	2.01	0.43
1:B:1271:ARG:HH22	3:H:1:NAG:C4	2.30	0.43
1:C:459:VAL:HG12	1:C:460:HIS:N	2.33	0.43
1:D:173:ASN:OD1	1:D:173:ASN:N	2.52	0.43
1:D:476:VAL:HB	1:D:526:ILE:HG23	2.00	0.43
1:D:570:LEU:HD23	1:D:571:SER:CA	2.48	0.43
1:D:916:PHE:CZ	1:D:933:LEU:HD22	2.54	0.43
1:D:927:VAL:HG12	1:D:928:SER:N	2.33	0.43
1:D:1232:THR:HG21	1:D:1323:TYR:CD1	2.52	0.43
1:A:232:GLN:O	1:A:251:CYS:N	2.41	0.43
1:A:488:LEU:HD12	1:A:489:GLY:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:LEU:HD11	1:A:1247:GLY:N	2.33	0.43
1:A:1039:THR:O	1:A:1042:THR:OG1	2.28	0.43
1:B:1025:TYR:HE2	1:B:1045:VAL:HG21	1.83	0.43
1:D:348:THR:CG2	1:D:423:VAL:HG11	2.49	0.43
1:D:772:LEU:HD23	1:D:778:LEU:HA	2.00	0.43
1:D:804:ARG:NE	1:D:863:LYS:O	2.48	0.43
3:H:1:NAG:C8	3:H:1:NAG:C3	2.96	0.43
1:C:384:ILE:N	1:C:397:ALA:O	2.44	0.43
1:D:1118:HIS:HB3	1:D:1121:VAL:HG12	2.00	0.43
1:A:596:ALA:O	1:A:770:PHE:N	2.52	0.43
1:A:907:PRO:O	1:A:1331:ASN:ND2	2.51	0.43
1:A:1248:PHE:HD1	1:A:1254:THR:HG23	1.84	0.43
1:B:370:ARG:HB3	1:B:404:LEU:HD23	2.01	0.43
1:B:804:ARG:NH2	1:B:863:LYS:O	2.51	0.43
1:C:296:SER:OG	1:C:851:ASN:ND2	2.52	0.43
1:C:311:LEU:HD23	1:C:311:LEU:H	1.84	0.43
1:C:316:TYR:N	1:C:316:TYR:CD1	2.87	0.43
1:C:564:LEU:HD22	1:C:564:LEU:N	2.34	0.43
1:C:576:GLN:CD	1:C:576:GLN:C	2.87	0.43
1:C:605:LEU:HD12	1:C:608:LYS:O	2.18	0.43
1:C:822:ILE:HG22	1:C:823:ARG:O	2.18	0.43
1:C:916:PHE:N	1:C:1326:THR:O	2.49	0.43
1:C:1176:LYS:HA	1:C:1181:VAL:HG12	2.00	0.43
1:C:1185:ARG:N	1:C:1208:MET:HE1	2.33	0.43
1:D:570:LEU:CD1	1:D:585:LEU:HD21	2.48	0.43
1:A:350:LEU:C	1:A:350:LEU:HD12	2.44	0.43
1:B:933:LEU:O	1:B:1310:GLY:N	2.50	0.43
1:C:243:GLU:HB2	1:C:311:LEU:HD11	2.01	0.43
1:C:427:ASP:OD1	1:C:428:ARG:N	2.51	0.43
1:C:570:LEU:HD22	1:C:784:ALA:HB2	2.01	0.43
1:C:751:VAL:HG22	1:C:752:ALA:N	2.33	0.43
1:D:56:GLU:O	1:D:58:VAL:N	2.51	0.43
1:D:506:VAL:HG21	1:D:533:ASP:O	2.19	0.43
1:D:551:VAL:HG22	1:D:552:ILE:N	2.34	0.43
1:A:757:THR:HG22	1:A:758:VAL:H	1.84	0.43
1:A:974:GLU:CG	1:A:1027:THR:HG22	2.49	0.43
1:A:1144:VAL:HG21	1:A:1185:ARG:HA	2.00	0.43
1:B:38:LEU:HD21	1:B:40:HIS:CD2	2.53	0.43
1:B:952:GLY:CA	1:B:1297:ARG:HH12	2.32	0.43
1:C:468:LEU:HD12	1:C:469:PRO:HD2	2.01	0.43
1:C:1107:ILE:HD11	1:C:1152:TYR:CG	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1205:GLU:HG2	1:C:1206:VAL:HG23	2.01	0.43
1:C:1250:SER:O	1:C:1254:THR:OG1	2.24	0.43
1:D:101:MET:O	1:D:120:VAL:N	2.49	0.43
1:D:642:CYS:SG	1:D:689:CYS:N	2.84	0.43
1:D:1124:ALA:O	1:D:1127:CYS:N	2.52	0.43
1:A:568:VAL:HG22	1:A:569:ASP:N	2.34	0.42
1:A:659:SER:N	1:D:656:THR:OG1	2.52	0.42
1:A:1002:SER:HA	1:A:1005:ILE:HD12	2.01	0.42
1:B:159:ASN:ND2	1:B:184:GLU:O	2.46	0.42
1:B:241:ILE:O	1:B:243:GLU:N	2.52	0.42
1:B:1025:TYR:CD2	1:B:1045:VAL:HG11	2.54	0.42
1:C:493:LEU:O	1:C:513:LEU:N	2.48	0.42
1:C:617:SER:O	1:C:621:LEU:HD13	2.18	0.42
1:C:1296:ASN:HB2	1:C:1299:LEU:HD22	2.01	0.42
1:D:33:VAL:CG1	1:D:49:VAL:HG23	2.48	0.42
1:D:648:VAL:CG1	1:D:658:VAL:HG13	2.49	0.42
1:D:816:ASN:ND2	1:D:848:ILE:O	2.46	0.42
1:A:516:LYS:HZ3	1:A:517:GLN:HB3	1.84	0.42
1:A:1036:GLN:NE2	1:A:1037:GLY:O	2.52	0.42
1:B:1319:GLU:OE1	1:B:1319:GLU:N	2.52	0.42
1:C:130:PHE:CE2	1:C:149:VAL:HG21	2.54	0.42
1:C:873:SER:OG	1:C:898:THR:HG23	2.19	0.42
1:C:985:TYR:CD2	1:C:1255:VAL:HG13	2.54	0.42
1:C:1163:ARG:HE	1:C:1164:LYS:HG3	1.84	0.42
1:D:498:LEU:HD12	1:D:541:LEU:HD21	2.01	0.42
1:D:854:GLN:OE1	1:D:855:THR:N	2.52	0.42
1:D:948:VAL:HG22	1:D:949:SER:N	2.35	0.42
1:A:148:VAL:HG22	1:A:149:VAL:H	1.84	0.42
1:A:1299:LEU:HD23	1:A:1301:GLN:CD	2.44	0.42
1:B:418:SER:N	1:B:419:LEU:HD12	2.34	0.42
1:C:421:VAL:O	1:C:444:ALA:HB3	2.19	0.42
1:C:1328:LEU:HD23	1:C:1329:LYS:N	2.35	0.42
1:D:912:LYS:O	1:D:1330:TYR:N	2.43	0.42
1:D:1217:LEU:CD2	1:D:1217:LEU:N	2.82	0.42
1:A:1176:LYS:HB2	1:A:1181:VAL:HG12	2.00	0.42
1:B:38:LEU:HD23	1:B:40:HIS:N	2.33	0.42
1:B:961:ASN:OD1	1:B:1247:GLY:N	2.46	0.42
1:C:406:GLN:OE1	1:C:406:GLN:N	2.52	0.42
1:C:1248:PHE:HD1	1:C:1254:THR:HG23	1.84	0.42
1:D:158:LEU:HD12	1:D:159:ASN:N	2.34	0.42
1:D:782:SER:HG	1:D:783:THR:H	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:837:VAL:HG12	1:D:838:PRO:O	2.18	0.42
1:A:760:ASP:OD1	1:A:899:VAL:HG22	2.19	0.42
1:A:1248:PHE:CD1	1:A:1254:THR:HG23	2.55	0.42
1:B:33:VAL:C	1:B:34:LEU:HD12	2.44	0.42
1:B:740:ILE:HG22	1:B:742:ASP:OD1	2.20	0.42
1:B:1152:TYR:O	1:B:1155:ALA:N	2.53	0.42
1:C:241:ILE:HD13	1:C:343:ILE:HG22	2.02	0.42
1:C:626:ASP:OD1	1:C:627:LEU:N	2.52	0.42
1:C:828:LEU:CD1	1:C:872:VAL:HG12	2.50	0.42
1:D:38:LEU:HD21	1:D:40:HIS:CD2	2.54	0.42
1:A:60:VAL:HG22	1:A:61:SER:N	2.35	0.42
1:A:988:ASP:HA	1:A:1055:TYR:OH	2.20	0.42
1:A:1175:VAL:HG21	1:A:1184:GLU:OE1	2.19	0.42
1:B:532:SER:OG	1:B:533:ASP:N	2.52	0.42
1:C:536:PRO:O	1:C:560:VAL:N	2.47	0.42
1:C:1086:LEU:HD12	1:C:1087:LEU:N	2.35	0.42
1:C:1238:ILE:HG21	1:C:1261:LEU:HD11	2.00	0.42
1:D:253:LEU:HD12	1:D:254:TYR:N	2.34	0.42
1:D:804:ARG:HD2	1:D:865:LEU:HD13	2.02	0.42
1:D:917:ASN:OD1	1:D:917:ASN:N	2.50	0.42
1:D:1088:ASN:OD1	1:D:1088:ASN:N	2.51	0.42
1:A:107:VAL:N	1:A:114:PHE:O	2.52	0.42
1:A:911:GLU:OE1	1:A:1330:TYR:N	2.52	0.42
1:B:173:ASN:OD1	1:B:173:ASN:N	2.51	0.42
1:B:946:ALA:O	1:B:1305:LEU:N	2.51	0.42
1:C:343:ILE:H	1:C:343:ILE:HD12	1.84	0.42
1:C:650:ILE:O	1:C:650:ILE:CG2	2.61	0.42
1:C:911:GLU:OE2	1:C:943:SER:OG	2.32	0.42
1:D:1328:LEU:HD12	1:D:1329:LYS:H	1.84	0.42
3:F:2:NAG:C8	3:F:2:NAG:C1	2.97	0.42
1:A:649:TYR:O	1:A:649:TYR:CG	2.72	0.42
1:B:265:THR:HG22	1:B:266:VAL:N	2.35	0.42
1:B:974:GLU:HG3	1:B:1027:THR:HG23	2.01	0.42
1:B:1148:ALA:O	1:B:1151:ALA:HB3	2.19	0.42
1:C:101:MET:N	1:C:120:VAL:O	2.45	0.42
1:C:989:TYR:O	1:C:993:THR:OG1	2.26	0.42
1:D:997:THR:CG2	1:D:1000:ILE:HG22	2.49	0.42
1:A:1314:MET:N	1:A:1314:MET:SD	2.92	0.42
1:B:270:ARG:NE	1:B:316:TYR:O	2.52	0.42
1:B:460:HIS:C	1:B:461:LEU:HD12	2.45	0.42
1:B:927:VAL:HG12	1:B:928:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1227:ASP:OD1	1:B:1227:ASP:N	2.52	0.42
1:C:58:VAL:O	1:C:79:ALA:HB3	2.20	0.42
1:C:64:LEU:HD23	1:C:73:LEU:HG	2.02	0.42
1:C:248:VAL:HG12	1:C:249:SER:N	2.35	0.42
1:C:356:ASP:OD1	1:C:358:HIS:N	2.45	0.42
1:C:576:GLN:O	1:C:576:GLN:CG	2.67	0.42
1:C:786:LEU:N	1:C:786:LEU:HD12	2.35	0.42
1:C:927:VAL:HG12	1:C:928:SER:N	2.35	0.42
1:C:1025:TYR:HD2	1:C:1042:THR:HG22	1.84	0.42
1:C:1327:SER:HG	1:C:1328:LEU:H	1.66	0.42
1:D:916:PHE:N	1:D:1326:THR:O	2.50	0.42
1:D:1105:ILE:O	1:D:1108:ALA:N	2.53	0.42
1:A:539:ARG:NE	1:A:673:MET:O	2.48	0.42
1:A:1214:LEU:O	1:A:1218:THR:N	2.45	0.42
1:B:241:ILE:O	1:B:311:LEU:HD12	2.20	0.42
1:C:311:LEU:HB2	1:C:343:ILE:HG21	2.01	0.42
1:C:372:VAL:HG12	1:C:373:ASP:H	1.85	0.42
1:C:779:GLY:HA2	1:C:780:ILE:HD12	2.01	0.42
1:D:451:VAL:HG22	1:D:452:PHE:O	2.18	0.42
1:D:506:VAL:HG21	1:D:533:ASP:C	2.45	0.42
1:D:617:SER:O	1:D:621:LEU:HD13	2.20	0.42
1:A:553:GLY:CA	1:A:666:MET:HE1	2.50	0.41
1:A:570:LEU:HD11	1:A:585:LEU:HD21	2.02	0.41
1:A:1152:TYR:O	1:A:1155:ALA:HB3	2.20	0.41
1:B:164:LEU:HD21	1:B:166:TYR:HD2	1.84	0.41
1:B:1082:SER:N	1:B:1098:GLU:OE2	2.53	0.41
1:B:1110:LEU:HD13	1:B:1156:LEU:HB3	2.01	0.41
1:B:1296:ASN:HB2	1:B:1299:LEU:HD22	2.02	0.41
1:C:802:VAL:HG23	1:C:905:VAL:HG23	2.02	0.41
1:D:321:HIS:ND1	1:D:334:GLU:OE2	2.48	0.41
1:D:469:PRO:O	1:D:530:VAL:HG11	2.20	0.41
1:D:974:GLU:O	1:D:978:VAL:HG23	2.19	0.41
1:D:1207:GLU:O	1:D:1210:SER:OG	2.38	0.41
1:A:267:SER:N	1:A:321:HIS:O	2.51	0.41
1:A:885:THR:OG1	1:A:886:GLU:OE2	2.31	0.41
1:B:237:LYS:HA	1:B:338:ARG:HG3	2.02	0.41
1:B:570:LEU:CD1	1:B:585:LEU:HD21	2.50	0.41
1:B:1010:THR:O	1:B:1013:GLN:N	2.51	0.41
1:B:1012:TYR:OH	1:B:1059:ASP:OD1	2.38	0.41
1:C:480:TYR:HB2	1:C:482:LEU:HD11	2.03	0.41
1:C:491:LYS:HA	1:C:515:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:955:LEU:HD21	1:D:995:GLN:OE1	2.20	0.41
1:D:1076:ASP:OD1	1:D:1076:ASP:N	2.52	0.41
1:A:333:VAL:HG12	1:A:334:GLU:H	1.84	0.41
1:B:109:GLY:N	1:B:112:GLN:O	2.52	0.41
1:B:1144:VAL:O	1:B:1148:ALA:N	2.50	0.41
1:B:1170:LEU:O	1:B:1183:TRP:NE1	2.49	0.41
1:C:560:VAL:HG12	1:C:561:GLU:N	2.34	0.41
1:C:579:PRO:CG	1:C:759:PRO:HB3	2.50	0.41
1:D:1067:LEU:HD11	1:D:1109:LEU:HD11	2.01	0.41
1:D:1178:ASP:OD1	1:D:1178:ASP:N	2.52	0.41
1:A:233:VAL:HG23	1:A:338:ARG:NH2	2.35	0.41
1:A:254:TYR:OH	1:A:853:ARG:NH1	2.53	0.41
1:A:965:LEU:HD21	1:A:1246:GLY:HA3	2.03	0.41
1:A:1120:VAL:HG13	1:C:117:ARG:HH22	1.85	0.41
1:A:1281:GLN:O	1:A:1313:SER:N	2.52	0.41
1:A:1304:SER:C	1:A:1305:LEU:HD23	2.45	0.41
1:B:227:PRO:O	1:B:228:LYS:NZ	2.43	0.41
1:B:622:LEU:HD23	1:B:623:PRO:O	2.21	0.41
1:B:650:ILE:O	1:B:650:ILE:HG22	2.20	0.41
1:B:751:VAL:HG22	1:B:752:ALA:N	2.35	0.41
1:B:976:ASN:O	1:B:980:PHE:N	2.50	0.41
1:C:38:LEU:HD23	1:C:39:LEU:N	2.35	0.41
1:C:538:ALA:O	1:C:558:TYR:N	2.53	0.41
1:C:1157:ALA:HB3	1:C:1159:ASN:H	1.85	0.41
1:D:1239:THR:HG23	1:D:1240:LYS:N	2.35	0.41
1:A:62:ALA:HB1	1:A:103:LEU:HD11	2.02	0.41
1:A:237:LYS:C	1:A:238:ILE:HD13	2.46	0.41
1:A:997:THR:CG2	1:A:1000:ILE:HG22	2.51	0.41
1:A:1279:THR:C	1:A:1280:ILE:HD13	2.45	0.41
1:B:61:SER:N	1:B:106:GLN:O	2.48	0.41
1:B:205:VAL:C	1:B:206:VAL:HG23	2.45	0.41
1:B:372:VAL:HG13	1:B:377:VAL:C	2.45	0.41
1:B:909:GLY:O	1:B:1331:ASN:ND2	2.54	0.41
1:C:164:LEU:HD21	1:C:166:TYR:HD2	1.85	0.41
1:C:460:HIS:C	1:C:461:LEU:HD12	2.45	0.41
1:C:543:TYR:HD2	1:C:551:VAL:HG21	1.85	0.41
1:C:595:CYS:HB2	1:C:597:LEU:HD11	2.02	0.41
1:C:822:ILE:HG23	1:C:887:VAL:HG23	2.02	0.41
1:D:333:VAL:HG12	1:D:334:GLU:N	2.34	0.41
1:D:744:VAL:HG12	1:D:745:VAL:N	2.36	0.41
1:A:101:MET:HG3	1:A:122:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG12	1:A:324:ALA:HB3	2.02	0.41
1:A:353:VAL:HG23	1:A:354:LYS:N	2.36	0.41
1:A:813:THR:HA	1:A:855:THR:HG23	2.03	0.41
1:A:881:GLU:CD	1:A:887:VAL:HG12	2.45	0.41
1:A:1046:LEU:HD11	1:A:1063:ILE:HB	2.02	0.41
1:B:303:GLN:O	1:B:303:GLN:CD	2.64	0.41
1:B:769:ALA:HB3	1:B:781:SER:HB3	2.02	0.41
1:B:1126:PHE:O	1:B:1130:SER:OG	2.21	0.41
1:B:1262:SER:O	1:B:1265:GLY:N	2.54	0.41
1:C:1161:ASP:OD1	1:C:1161:ASP:N	2.54	0.41
1:D:250:VAL:O	1:D:300:PHE:N	2.54	0.41
1:D:255:THR:CB	1:D:762:ILE:HG13	2.45	0.41
1:D:385:PHE:CE1	4:D:2004:NAG:H82	2.56	0.41
1:D:1076:ASP:OD1	1:D:1077:ASN:N	2.52	0.41
1:A:570:LEU:HD23	1:A:571:SER:CA	2.51	0.41
1:A:572:PHE:HD2	1:A:573:SER:O	2.04	0.41
1:A:792:PHE:CE1	1:A:824:VAL:HG21	2.55	0.41
1:B:323:GLU:N	1:B:323:GLU:OE2	2.54	0.41
1:B:846:HIS:ND1	1:B:847:CYS:SG	2.91	0.41
1:C:1183:TRP:CZ3	1:C:1212:VAL:HG11	2.55	0.41
1:D:1010:THR:O	1:D:1013:GLN:N	2.53	0.41
1:A:33:VAL:HG12	1:A:49:VAL:CB	2.50	0.41
1:A:626:ASP:OD1	1:A:626:ASP:N	2.47	0.41
1:A:637:GLN:HB2	1:A:676:LYS:HZ3	1.86	0.41
1:A:826:VAL:HA	1:A:874:ALA:HB2	2.02	0.41
1:A:982:PRO:O	1:A:986:VAL:HG23	2.21	0.41
1:A:1225:SER:O	1:A:1229:THR:HG23	2.21	0.41
1:A:1251:THR:O	1:A:1255:VAL:HG23	2.21	0.41
1:A:1283:SER:OG	1:A:1284:GLY:N	2.54	0.41
4:A:2001:NAG:C8	4:A:2001:NAG:C3	2.85	0.41
1:B:357:SER:C	1:B:448:ALA:HB1	2.46	0.41
1:B:742:ASP:O	1:B:743:LEU:HD12	2.21	0.41
1:C:541:LEU:CD1	1:C:670:LEU:HD11	2.51	0.41
1:D:1208:MET:O	1:D:1212:VAL:N	2.48	0.41
1:A:70:ASN:C	1:A:70:ASN:ND2	2.74	0.41
1:A:545:VAL:HG22	1:A:546:LEU:N	2.36	0.41
1:A:821:CYS:SG	1:A:849:CYS:N	2.94	0.41
1:A:916:PHE:CE2	1:A:933:LEU:HD22	2.54	0.41
1:B:572:PHE:CE2	1:B:574:PRO:HA	2.56	0.41
1:B:659:SER:OG	1:C:655:TYR:O	2.36	0.41
1:B:810:LEU:N	1:B:858:TRP:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:GLN:O	1:B:882:LEU:N	2.52	0.41
1:B:986:VAL:HG13	1:B:987:LEU:N	2.36	0.41
1:C:158:LEU:HD12	1:C:159:ASN:N	2.32	0.41
1:C:248:VAL:CG2	1:C:304:VAL:HG22	2.51	0.41
1:C:635:ASN:OD1	1:C:635:ASN:N	2.54	0.41
1:D:461:LEU:HD21	1:D:542:ILE:HG22	2.01	0.41
1:D:502:LYS:HG3	1:D:535:ALA:HB2	2.03	0.41
1:D:828:LEU:HD13	1:D:858:TRP:CE2	2.55	0.41
2:K:2:NAG:O7	2:K:2:NAG:O3	2.34	0.41
1:A:333:VAL:HG12	1:A:334:GLU:N	2.36	0.41
1:A:954:ILE:HG22	1:A:1297:ARG:NH2	2.35	0.41
1:B:306:THR:OG1	1:B:311:LEU:HD11	2.20	0.41
1:B:962:THR:OG1	1:B:963:GLN:N	2.54	0.41
1:B:1253:ASP:OD1	1:B:1253:ASP:N	2.54	0.41
1:C:1189:PRO:HB2	1:C:1193:VAL:HG11	2.02	0.41
1:D:387:ARG:HB2	1:D:420:THR:HG23	2.02	0.41
1:D:412:THR:O	1:D:412:THR:OG1	2.38	0.41
1:A:236:PRO:HD2	1:A:247:ASN:O	2.21	0.40
1:A:493:LEU:HB2	1:A:515:VAL:HG11	2.04	0.40
1:A:1103:ALA:HB1	1:A:1149:LEU:HG	2.03	0.40
1:B:146:PHE:CE1	1:B:190:PHE:HB2	2.56	0.40
1:B:165:VAL:HG13	1:B:207:VAL:CG2	2.51	0.40
1:B:262:GLY:O	1:B:294:LEU:N	2.50	0.40
1:B:318:MET:HG3	1:B:343:ILE:HD11	2.03	0.40
1:B:325:GLN:HA	1:B:332:VAL:HG12	2.04	0.40
1:B:421:VAL:H	1:B:444:ALA:HB3	1.86	0.40
1:B:1067:LEU:HD11	1:B:1109:LEU:CD1	2.49	0.40
1:C:139:LYS:NZ	1:C:226:LEU:HD21	2.36	0.40
1:C:220:THR:HG22	1:C:221:VAL:N	2.37	0.40
1:C:382:LYS:NZ	1:C:423:VAL:HG21	2.36	0.40
1:C:998:PRO:HA	1:C:1001:LYS:HB3	2.03	0.40
1:C:1184:GLU:C	1:C:1208:MET:HE1	2.45	0.40
1:D:1278:VAL:CG1	1:D:1280:ILE:HD11	2.51	0.40
1:A:571:SER:O	1:A:586:ARG:N	2.50	0.40
1:A:780:ILE:HD12	1:A:780:ILE:N	2.36	0.40
1:B:263:HIS:O	1:B:325:GLN:N	2.48	0.40
1:B:307:LYS:O	1:B:310:GLN:NE2	2.54	0.40
1:B:501:ALA:N	1:B:504:GLY:O	2.41	0.40
1:B:576:GLN:HE21	1:B:757:THR:HG23	1.86	0.40
1:B:1191:ALA:HB1	1:B:1192:PRO:HD2	2.03	0.40
1:D:1095:VAL:HG13	1:D:1097:ASP:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:ARG:N	1:A:768:GLY:O	2.51	0.40
1:A:870:PHE:CE2	1:A:903:LEU:HD21	2.57	0.40
1:A:946:ALA:HB3	1:A:1305:LEU:HB2	2.02	0.40
1:A:1235:VAL:HG21	1:A:1264:TYR:CE2	2.56	0.40
1:B:73:LEU:HD11	1:B:92:PRO:HD2	2.03	0.40
1:B:117:ARG:NH2	1:D:1074:GLN:OE1	2.49	0.40
1:B:347:ILE:HG22	1:B:348:THR:N	2.36	0.40
1:B:368:GLN:OE1	1:B:406:GLN:NE2	2.49	0.40
1:C:474:GLN:O	1:C:528:ILE:N	2.53	0.40
1:C:538:ALA:HB2	1:C:560:VAL:CG2	2.51	0.40
1:D:46:LYS:O	1:D:505:ILE:HD12	2.20	0.40
1:D:360:ARG:NH2	1:D:554:ASP:OD2	2.52	0.40
1:A:370:ARG:NE	1:A:404:LEU:HD21	2.35	0.40
1:A:551:VAL:HG22	1:A:552:ILE:N	2.36	0.40
1:A:1185:ARG:O	1:A:1187:GLN:N	2.54	0.40
1:B:570:LEU:HD11	1:B:585:LEU:HD21	2.02	0.40
1:B:930:GLU:OE1	1:B:931:LEU:N	2.54	0.40
1:B:1264:TYR:CE2	1:B:1268:THR:HG21	2.56	0.40
1:C:930:GLU:OE2	1:C:1312:TYR:N	2.54	0.40
1:D:249:SER:OG	1:D:300:PHE:O	2.30	0.40
1:D:538:ALA:HB3	1:D:558:TYR:HB2	2.03	0.40
1:D:570:LEU:HD22	1:D:784:ALA:CB	2.51	0.40
1:A:822:ILE:HG23	1:A:887:VAL:HG23	2.02	0.40
1:B:398:THR:OG1	1:B:399:THR:N	2.54	0.40
1:B:931:LEU:CG	1:B:933:LEU:HD21	2.49	0.40
1:B:1110:LEU:HD23	1:B:1114:LEU:HB2	2.04	0.40
1:D:266:VAL:HG22	1:D:267:SER:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	1281/1474 (87%)	1025 (80%)	250 (20%)	6 (0%)	24	59
1	B	1274/1474 (86%)	1057 (83%)	214 (17%)	3 (0%)	43	74
1	C	1281/1474 (87%)	1036 (81%)	239 (19%)	6 (0%)	24	59
1	D	1274/1474 (86%)	1041 (82%)	231 (18%)	2 (0%)	43	74
All	All	5110/5896 (87%)	4159 (81%)	934 (18%)	17 (0%)	37	69

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	PRO
1	C	579	PRO
1	C	651	ASN
1	D	53	TYR
1	A	54	LEU
1	A	517	GLN
1	B	53	TYR
1	C	54	LEU
1	D	1219	ALA
1	A	82	ASP
1	A	936	PRO
1	C	578	LEU
1	C	1221	PRO
1	A	1221	PRO
1	B	532	SER
1	B	1221	PRO
1	C	936	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1120/1290 (87%)	1111 (99%)	9 (1%)	73	77
1	B	1115/1290 (86%)	1099 (99%)	16 (1%)	59	71
1	C	1120/1290 (87%)	1111 (99%)	9 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	1115/1290 (86%)	1101 (99%)	14 (1%)	61	71
All	All	4470/5160 (87%)	4422 (99%)	48 (1%)	63	74

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	55	ASN
1	A	70	ASN
1	A	144	VAL
1	A	315	GLU
1	A	948	VAL
1	A	1167	LEU
1	A	1308	LEU
1	A	1316	VAL
1	B	89	PHE
1	B	107	VAL
1	B	112	GLN
1	B	137	ILE
1	B	245	GLU
1	B	405	VAL
1	B	464	MET
1	B	468	LEU
1	B	473	THR
1	B	506	VAL
1	B	605	LEU
1	B	746	VAL
1	B	900	ILE
1	B	951	LEU
1	B	1056	ILE
1	B	1217	LEU
1	C	55	ASN
1	C	111	THR
1	C	131	VAL
1	C	245	GLU
1	C	372	VAL
1	C	627	LEU
1	C	900	ILE
1	C	996	LEU
1	C	1218	THR
1	D	54	LEU
1	D	107	VAL

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Mol	Chain	Res	Type
1	D	332	VAL
1	D	396	ASN
1	D	464	MET
1	D	473	THR
1	D	486	THR
1	D	515	VAL
1	D	621	LEU
1	D	735	PHE
1	D	763	THR
1	D	992	GLU
1	D	1056	ILE
1	D	1214	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	97	ASN
1	A	177	GLN
1	A	217	HIS
1	A	232	GLN
1	A	303	GLN
1	A	361	GLN
1	A	474	GLN
1	A	511	HIS
1	A	517	GLN
1	A	523	HIS
1	A	963	GLN
1	A	964	ASN
1	A	1017	ASN
1	A	1187	GLN
1	A	1252	GLN
1	B	85	HIS
1	B	293	GLN
1	B	310	GLN
1	B	327	GLN
1	B	424	ASN
1	B	474	GLN
1	B	511	HIS
1	B	562	ASN
1	B	582	HIS
1	B	651	ASN

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Mol	Chain	Res	Type
1	B	960	GLN
1	B	1159	ASN
1	B	1187	GLN
1	C	142	GLN
1	C	177	GLN
1	C	232	GLN
1	C	302	GLN
1	C	303	GLN
1	C	361	GLN
1	C	389	ASN
1	C	474	GLN
1	C	511	HIS
1	C	517	GLN
1	C	576	GLN
1	C	662	ASN
1	C	790	GLN
1	C	851	ASN
1	C	960	GLN
1	C	1242	GLN
1	C	1259	HIS
1	D	112	GLN
1	D	310	GLN
1	D	389	ASN
1	D	424	ASN
1	D	474	GLN
1	D	662	ASN
1	D	917	ASN
1	D	967	GLN
1	D	994	GLN
1	D	1038	ASN
1	D	1051	GLN
1	D	1072	GLN
1	D	1159	ASN
1	D	1187	GLN
1	D	1233	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 ⓘ

20 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	$\# Z  > 2$
2	NAG	E	1	2,1	14,14,15	0.27	0	17,19,21	0.75	1 (5%)
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	0.65	0
3	NAG	F	2	3	14,14,15	0.34	0	17,19,21	0.60	0
3	BMA	F	3	3	11,11,12	0.25	0	15,15,17	0.47	0
2	NAG	G	1	2,1	14,14,15	0.30	0	17,19,21	0.69	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.60	0
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	1.40	2 (11%)
3	NAG	H	2	3	14,14,15	0.34	0	17,19,21	0.57	0
3	BMA	H	3	3	11,11,12	0.24	0	15,15,17	0.51	0
2	NAG	I	1	2,1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	J	1	1,3	14,14,15	0.31	0	17,19,21	0.63	0
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	0.66	0
3	BMA	J	3	3	11,11,12	0.26	0	15,15,17	0.49	0
2	NAG	K	1	2,1	14,14,15	0.32	0	17,19,21	0.80	0
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	L	1	1,3	14,14,15	0.49	0	17,19,21	1.42	2 (11%)
3	NAG	L	2	3	14,14,15	0.36	0	17,19,21	0.70	0
3	BMA	L	3	3	11,11,12	0.25	0	15,15,17	0.52	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
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	5/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	5/6/23/26	0/1/1/1
3	NAG	L	2	3	-	5/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	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(°)
3	L	1	NAG	O5-C1-C2	4.36	118.04	111.29
3	H	1	NAG	C1-O5-C5	3.87	117.37	112.19
3	H	1	NAG	O5-C1-C2	3.08	116.05	111.29
3	L	1	NAG	C1-O5-C5	2.36	115.34	112.19
2	E	1	NAG	C4-C3-C2	-2.07	107.98	111.02

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	I	2	NAG	C3-C2-N2-C7
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C3-C2-N2-C7
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C1-C2-N2-C7
3	H	1	NAG	C8-C7-N2-C2
3	H	1	NAG	O7-C7-N2-C2
3	H	2	NAG	C3-C2-N2-C7
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	J	1	NAG	O7-C7-N2-C2
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	L	1	NAG	C1-C2-N2-C7
3	L	1	NAG	C8-C7-N2-C2
3	L	1	NAG	O7-C7-N2-C2
3	L	2	NAG	C3-C2-N2-C7
3	L	2	NAG	C8-C7-N2-C2
3	L	2	NAG	O7-C7-N2-C2
3	L	1	NAG	C4-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C8-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O7-C7-N2-C2
3	L	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C3-C2-N2-C7
2	K	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6

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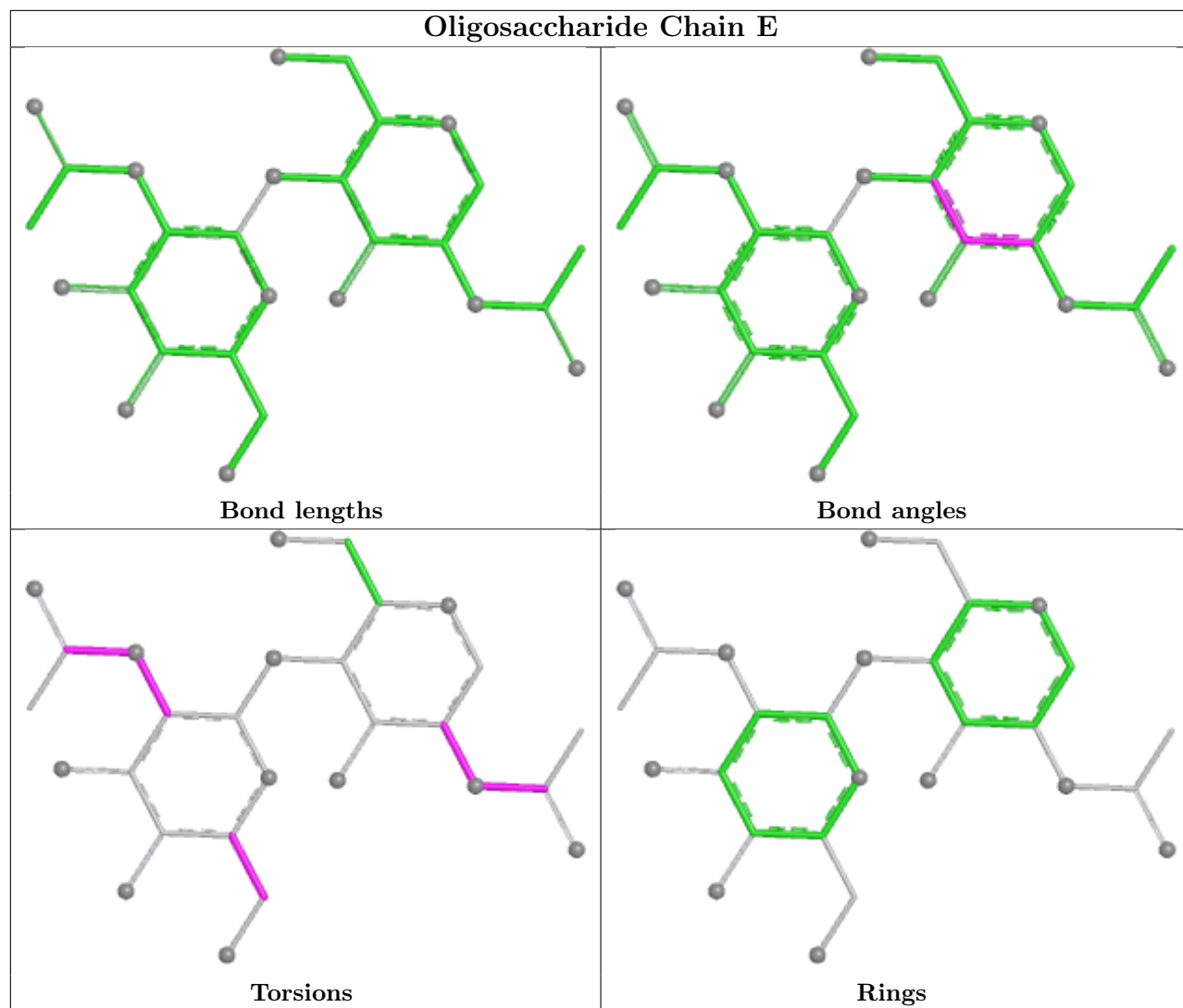
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O5-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	K	1	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	K	1	NAG	O5-C5-C6-O6

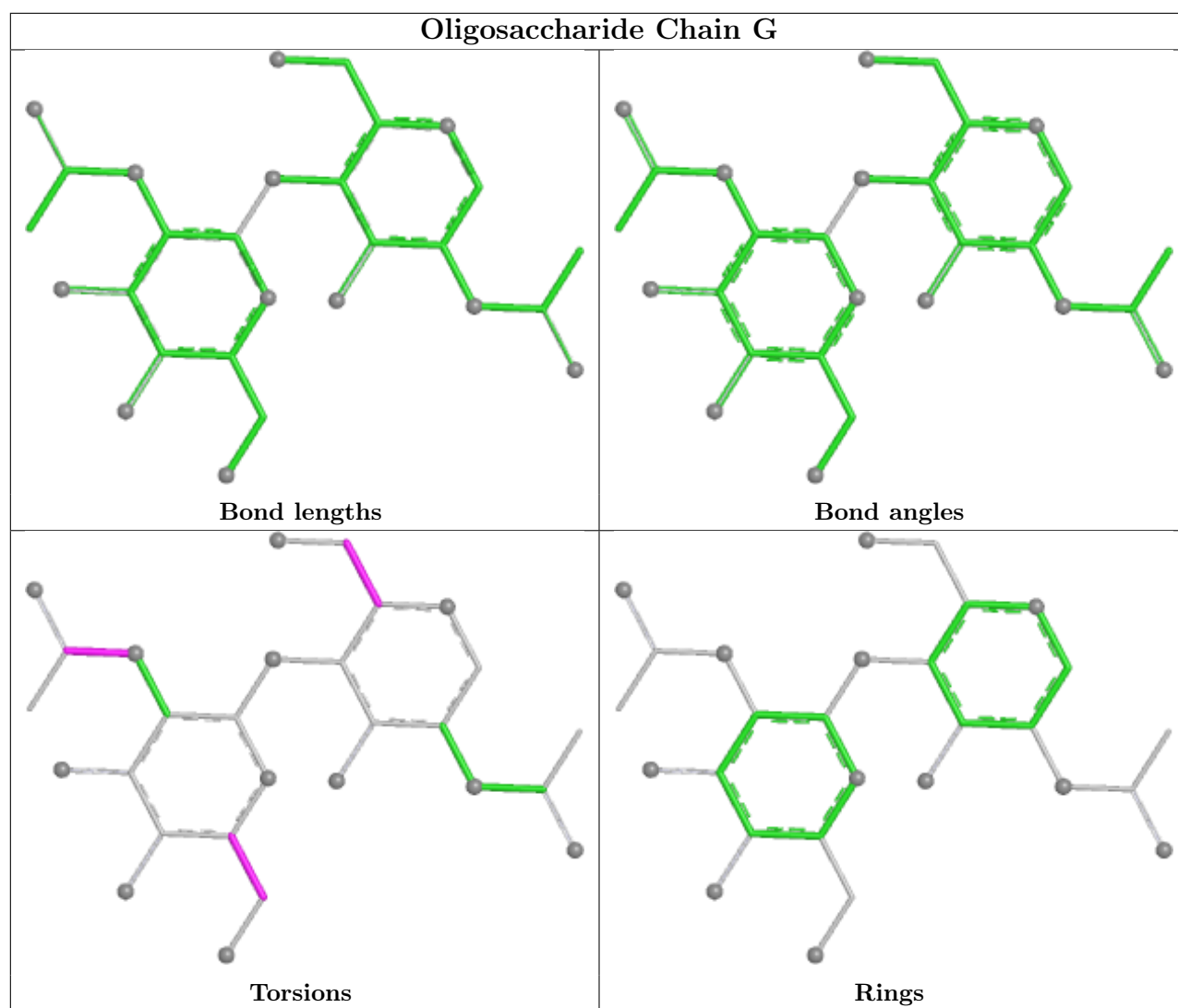
There are no ring outliers.

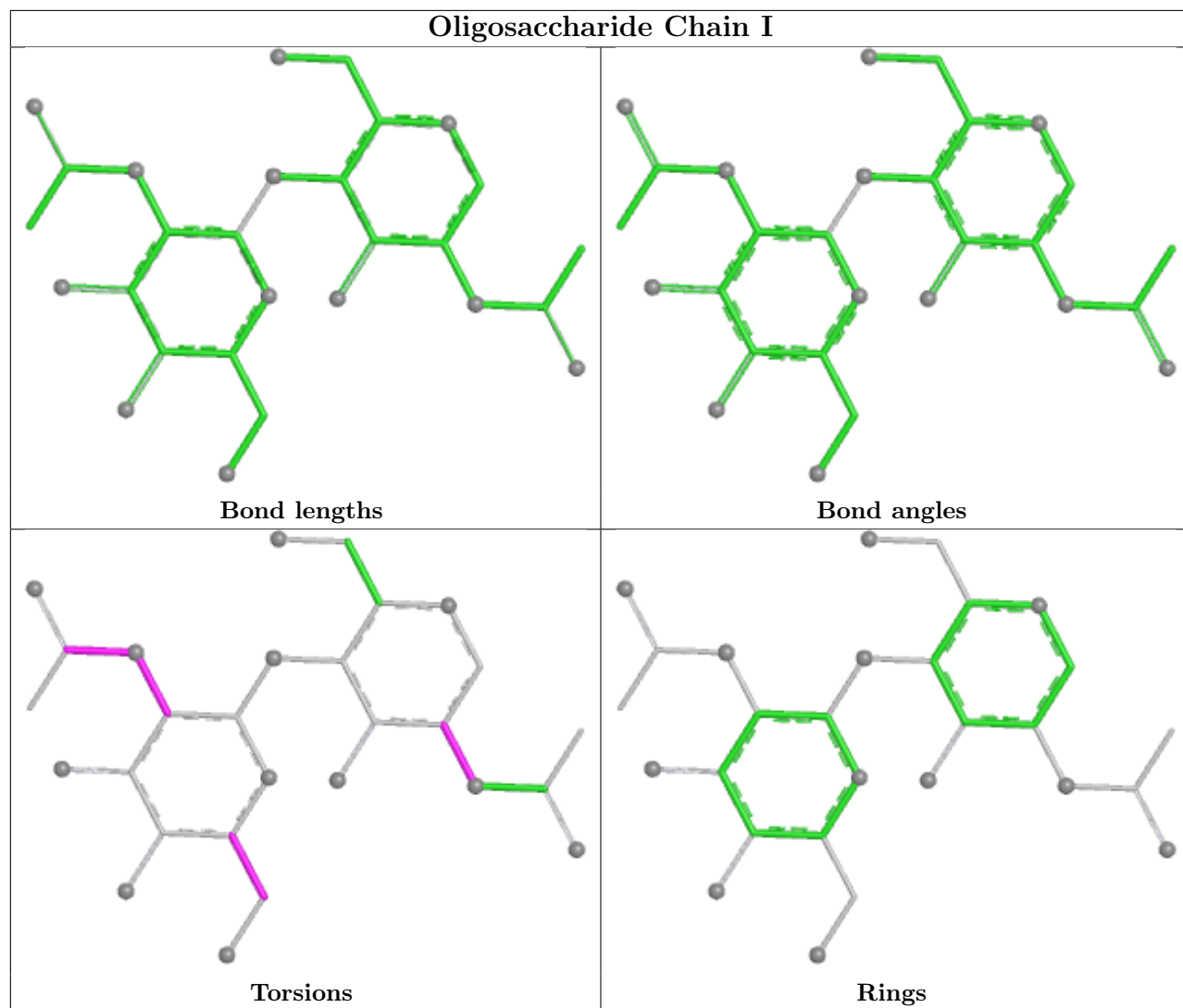
13 monomers are involved in 33 short contacts:

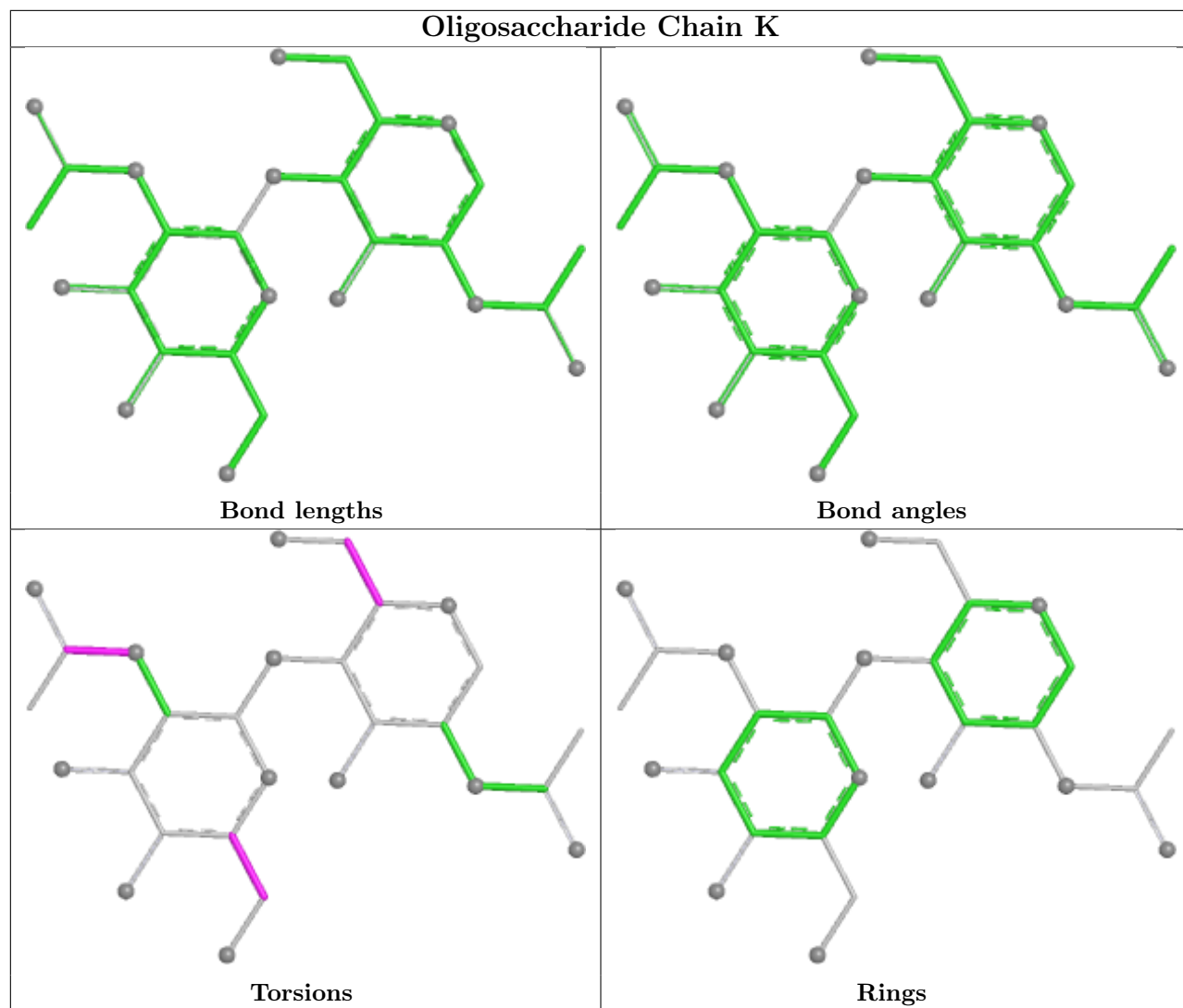
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	6	0
2	K	2	NAG	1	0
2	I	1	NAG	2	0
3	J	3	BMA	1	0
2	E	1	NAG	1	0
3	L	2	NAG	2	0
3	L	1	NAG	2	0
3	H	1	NAG	9	0
2	I	2	NAG	2	0
3	J	2	NAG	5	0
3	F	1	NAG	2	0
3	H	2	NAG	4	0
3	J	1	NAG	1	0

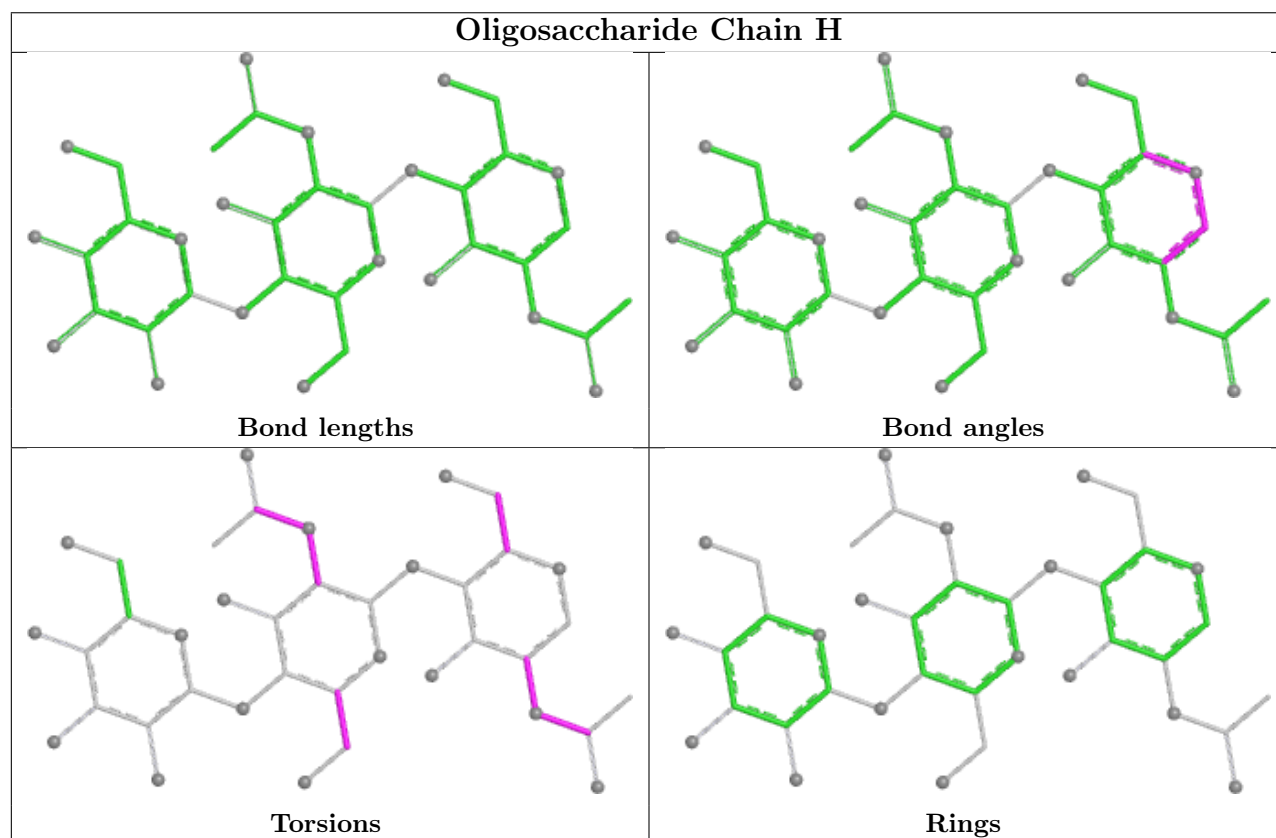
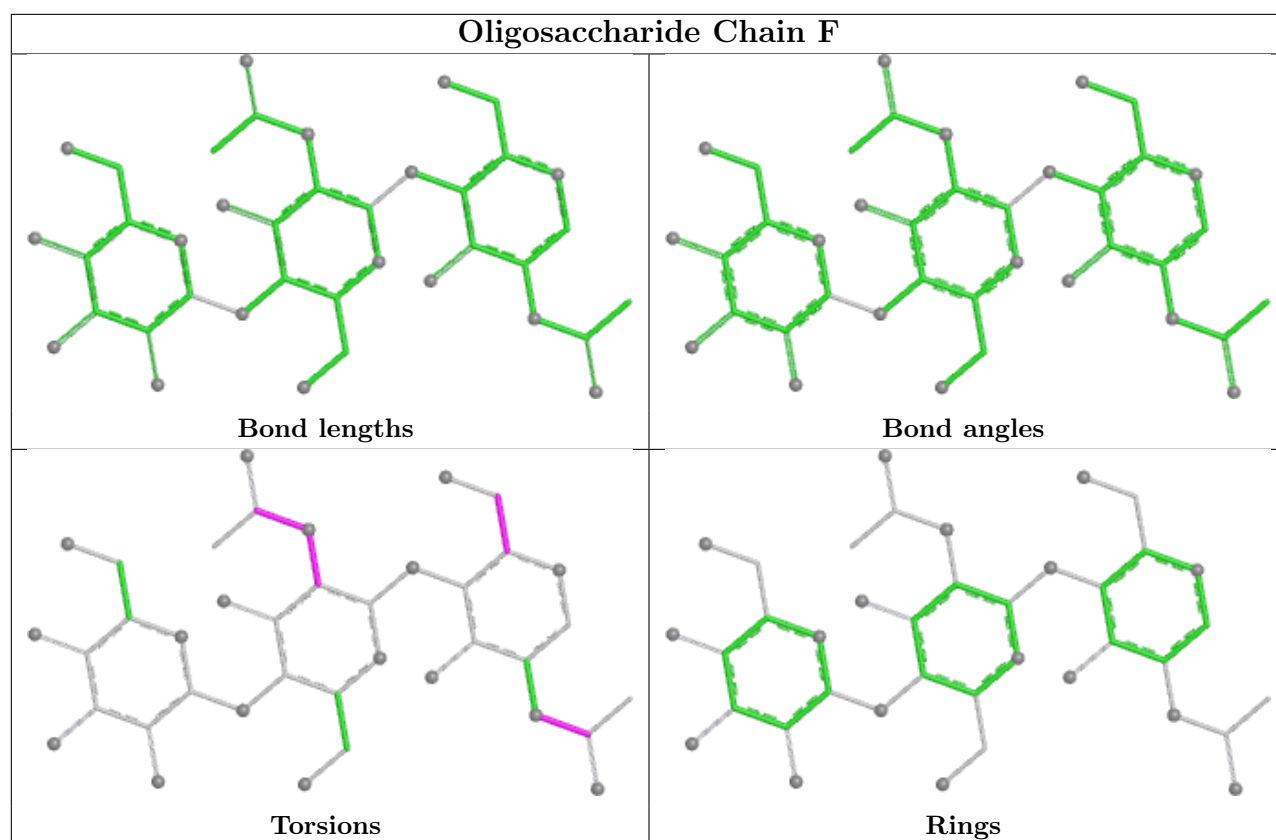
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



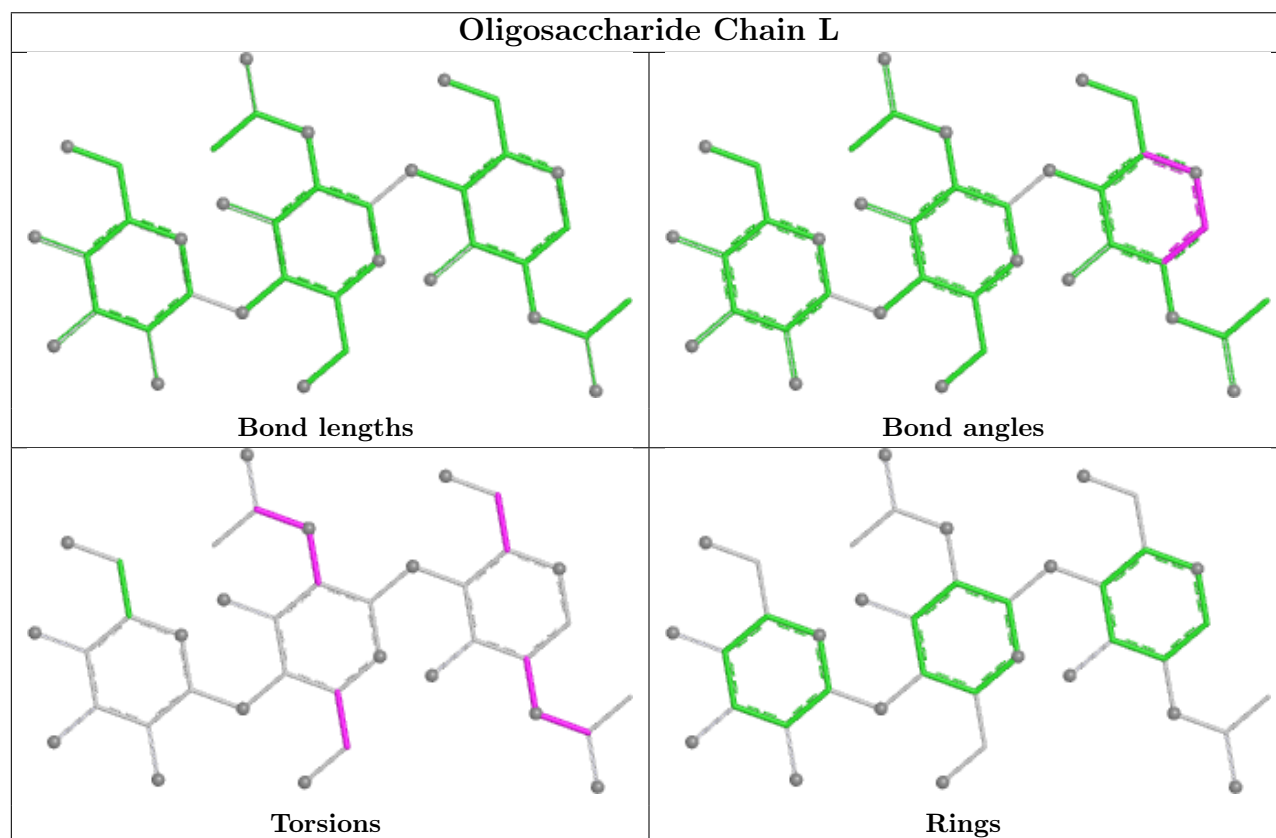
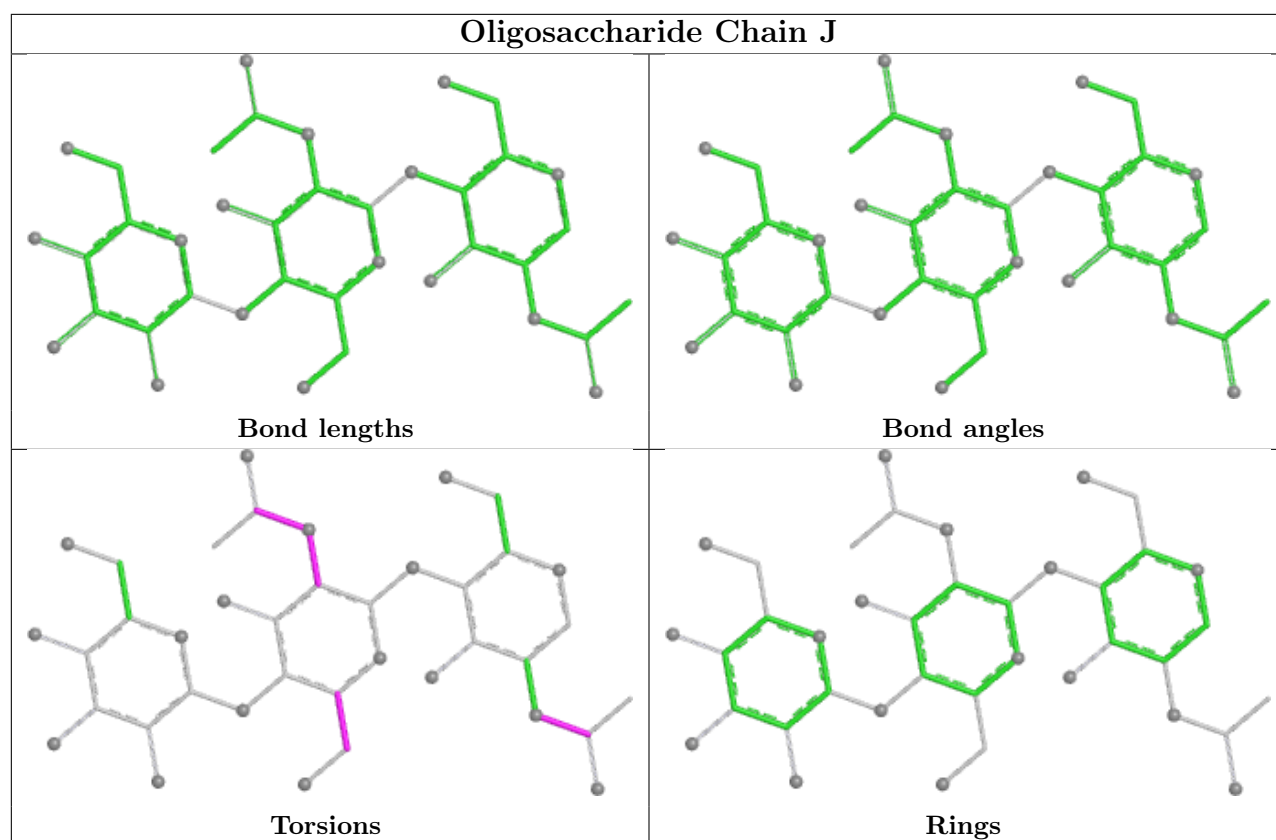












## 5.6 Ligand geometry

20 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	2005	1	14,14,15	0.30	0	17,19,21	0.55	0
4	NAG	A	2001	1	14,14,15	0.69	0	17,19,21	0.85	0
4	NAG	B	2001	1	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	C	2001	1	14,14,15	1.14	1 (7%)	17,19,21	1.82	5 (29%)
4	NAG	B	2002	1	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	D	2003	1	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	D	2004	1	14,14,15	0.50	0	17,19,21	1.41	3 (17%)
4	NAG	A	2005	1	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	A	2003	1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	C	2002	1	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	A	2004	1	14,14,15	0.28	0	17,19,21	0.65	0
4	NAG	D	2001	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	B	2004	1	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	C	2004	1	14,14,15	0.29	0	17,19,21	0.74	1 (5%)
4	NAG	D	2002	1	14,14,15	0.34	0	17,19,21	0.58	0
4	NAG	C	2003	1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	B	2003	1	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	A	2002	1	14,14,15	0.31	0	17,19,21	0.58	0
4	NAG	D	2005	1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	C	2005	1	14,14,15	0.29	0	17,19,21	0.65	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	2005	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	5/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2001	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	1/6/23/26	0/1/1/1
4	NAG	D	2003	1	-	3/6/23/26	0/1/1/1
4	NAG	D	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2001	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	D	2005	1	-	3/6/23/26	0/1/1/1
4	NAG	C	2005	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2001	NAG	O4-C4	2.81	1.49	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	NAG	C1-O5-C5	3.84	117.34	112.19
4	D	2004	NAG	C1-O5-C5	3.59	116.99	112.19
4	C	2001	NAG	C4-C3-C2	3.41	116.02	111.02
4	C	2001	NAG	C3-C4-C5	-3.10	104.61	110.23
4	C	2001	NAG	O4-C4-C5	2.86	116.36	109.32
4	D	2004	NAG	O5-C1-C2	-2.85	106.88	111.29
4	D	2004	NAG	C3-C4-C5	-2.54	105.63	110.23
4	C	2001	NAG	O4-C4-C3	2.37	115.95	110.38
4	C	2004	NAG	O5-C1-C2	-2.01	108.18	111.29

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2003	NAG	C1-C2-N2-C7
4	A	2003	NAG	C8-C7-N2-C2
4	B	2001	NAG	C3-C2-N2-C7
4	B	2002	NAG	C3-C2-N2-C7
4	B	2003	NAG	C1-C2-N2-C7
4	B	2005	NAG	C8-C7-N2-C2
4	B	2005	NAG	O7-C7-N2-C2
4	C	2002	NAG	C1-C2-N2-C7
4	C	2003	NAG	C1-C2-N2-C7
4	C	2003	NAG	C8-C7-N2-C2
4	C	2003	NAG	O7-C7-N2-C2
4	D	2001	NAG	C3-C2-N2-C7
4	D	2001	NAG	C8-C7-N2-C2
4	D	2001	NAG	O7-C7-N2-C2
4	D	2003	NAG	C1-C2-N2-C7
4	D	2005	NAG	C8-C7-N2-C2
4	D	2005	NAG	O7-C7-N2-C2
4	C	2001	NAG	C4-C5-C6-O6
4	A	2003	NAG	O7-C7-N2-C2
4	B	2001	NAG	C8-C7-N2-C2
4	B	2001	NAG	O7-C7-N2-C2
4	C	2004	NAG	O5-C5-C6-O6
4	A	2002	NAG	O5-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	C	2005	NAG	O5-C5-C6-O6
4	C	2001	NAG	O5-C5-C6-O6
4	A	2001	NAG	C4-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6
4	B	2004	NAG	C4-C5-C6-O6
4	A	2004	NAG	C4-C5-C6-O6
4	A	2001	NAG	C8-C7-N2-C2
4	A	2001	NAG	O7-C7-N2-C2
4	A	2001	NAG	O5-C5-C6-O6
4	A	2004	NAG	O5-C5-C6-O6
4	A	2002	NAG	C4-C5-C6-O6
4	A	2004	NAG	C8-C7-N2-C2
4	D	2002	NAG	C4-C5-C6-O6
4	C	2005	NAG	C4-C5-C6-O6
4	C	2002	NAG	O5-C5-C6-O6
4	B	2005	NAG	O5-C5-C6-O6
4	A	2005	NAG	O5-C5-C6-O6
4	D	2005	NAG	O5-C5-C6-O6
4	A	2002	NAG	C3-C2-N2-C7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	D	2002	NAG	C3-C2-N2-C7
4	A	2004	NAG	O7-C7-N2-C2
4	D	2002	NAG	O5-C5-C6-O6
4	A	2001	NAG	C3-C2-N2-C7
4	A	2005	NAG	C3-C2-N2-C7
4	C	2001	NAG	C3-C2-N2-C7
4	D	2003	NAG	O5-C5-C6-O6
4	B	2001	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	C	2001	NAG	C1-C2-N2-C7
4	A	2003	NAG	C3-C2-N2-C7
4	B	2003	NAG	C3-C2-N2-C7
4	C	2002	NAG	C3-C2-N2-C7
4	C	2005	NAG	C3-C2-N2-C7
4	D	2003	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	NAG	6	0
4	B	2002	NAG	1	0
4	D	2004	NAG	1	0
4	A	2005	NAG	1	0
4	A	2003	NAG	4	0
4	A	2004	NAG	1	0
4	D	2001	NAG	3	0
4	C	2004	NAG	1	0
4	D	2002	NAG	1	0
4	C	2003	NAG	3	0
4	A	2002	NAG	1	0
4	C	2005	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	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	168:GLN	C	169:ASP	N	1.16

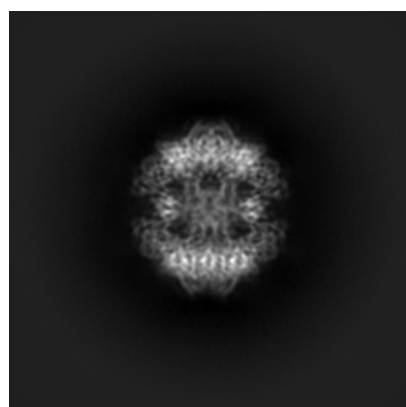
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12754. These allow visual inspection of the internal detail of the map and identification of artifacts.

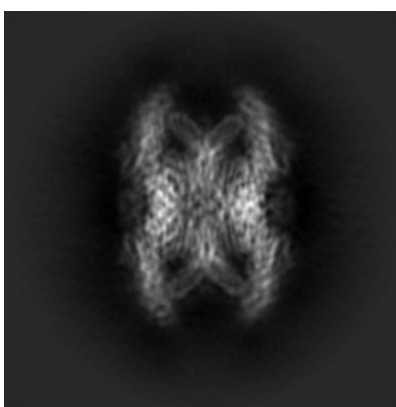
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

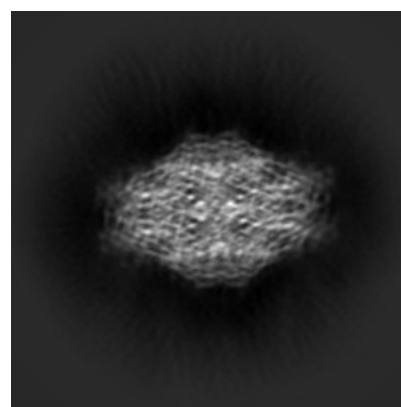
#### 6.1.1 Primary map



X



Y

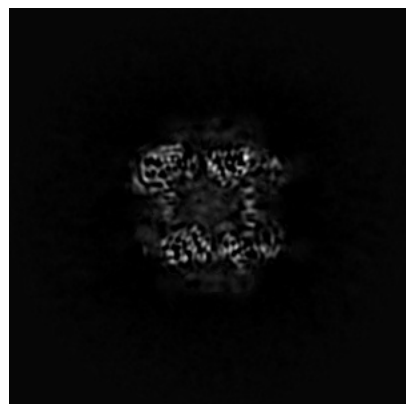


Z

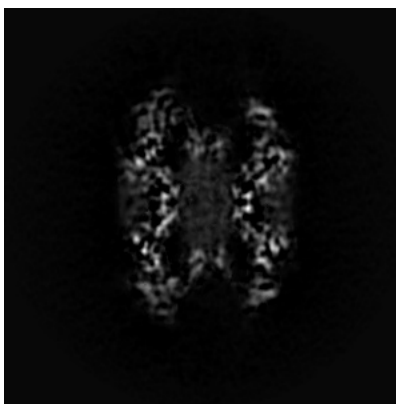
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

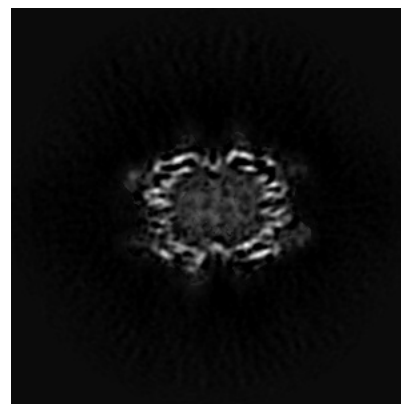
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

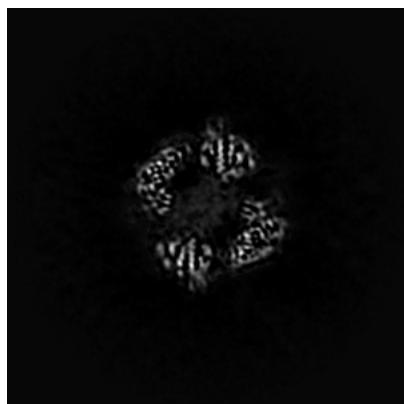


Z Index: 160

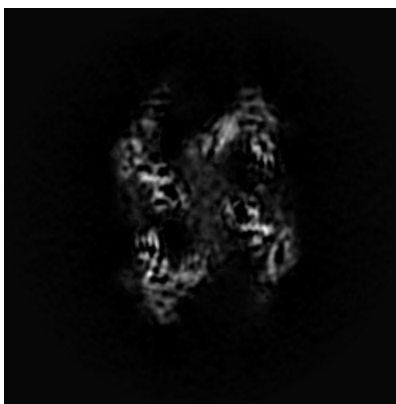
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

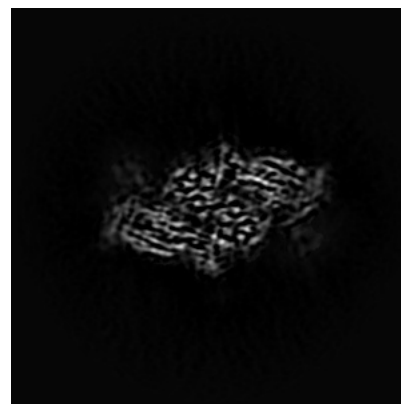
### 6.3.1 Primary map



X Index: 144



Y Index: 171



Z Index: 202

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

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

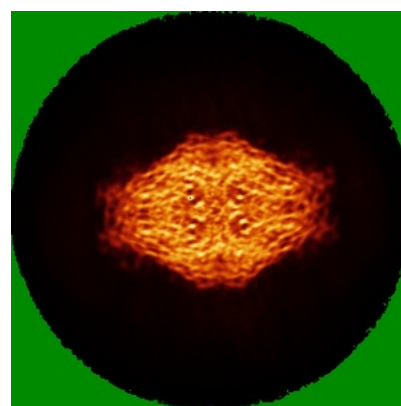
### 6.4.1 Primary map



X



Y



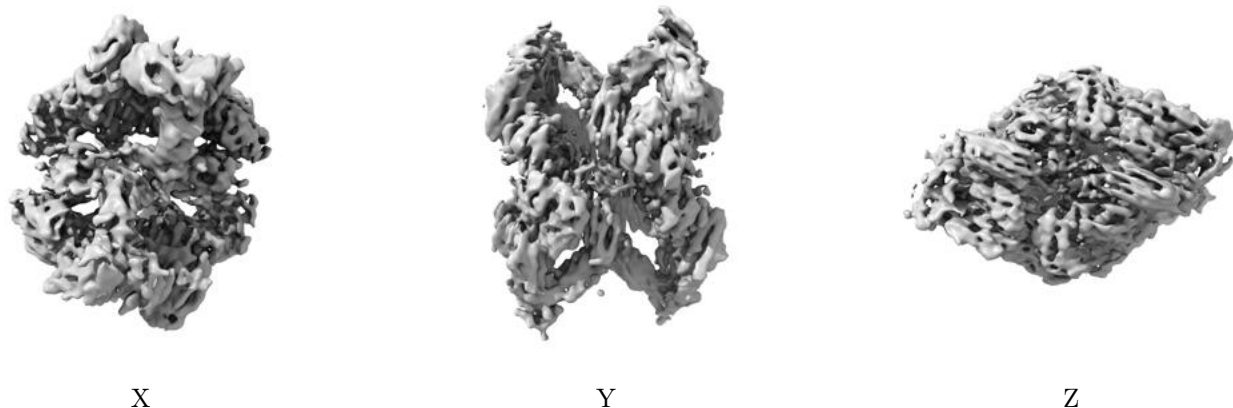
Z

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

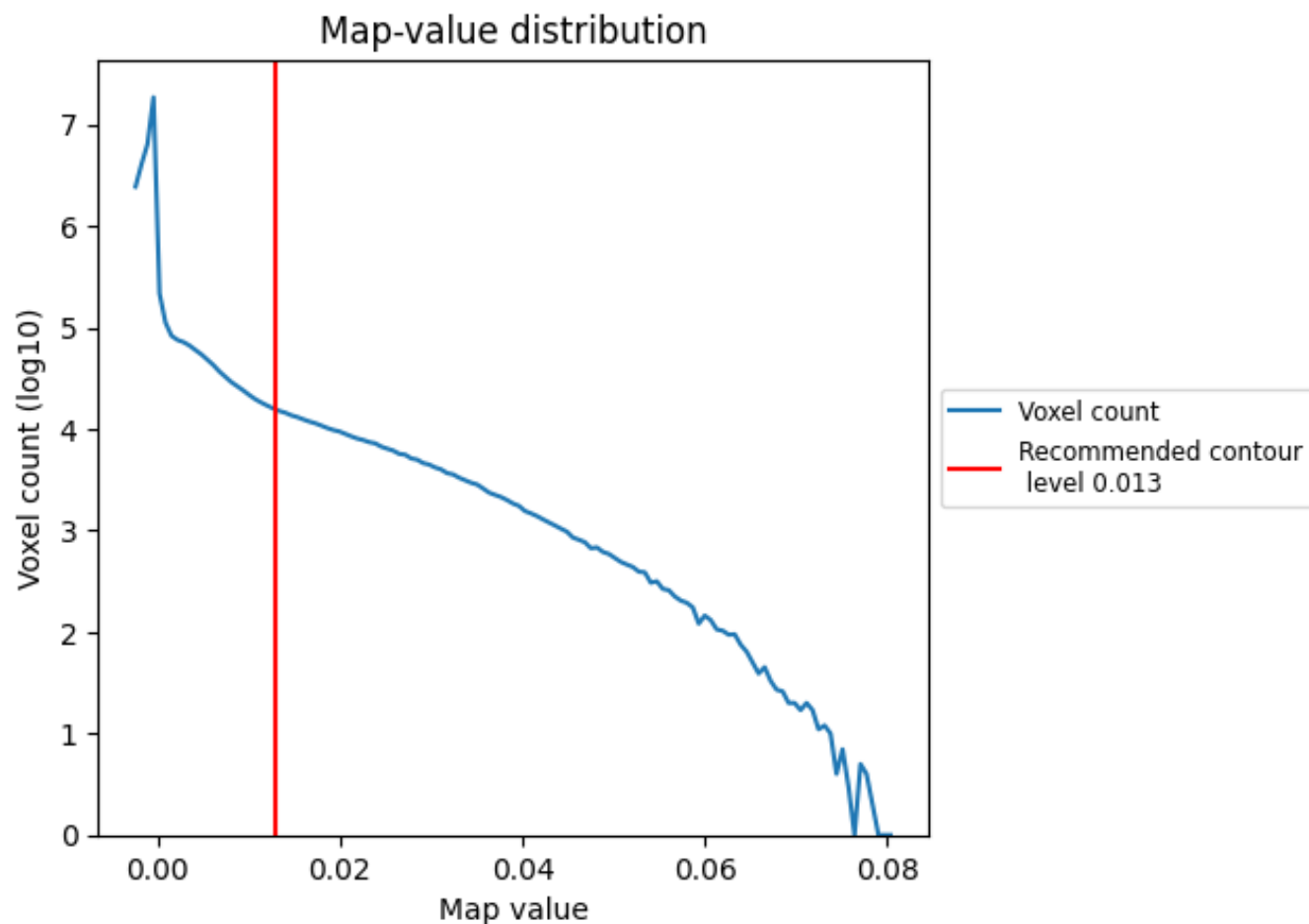
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

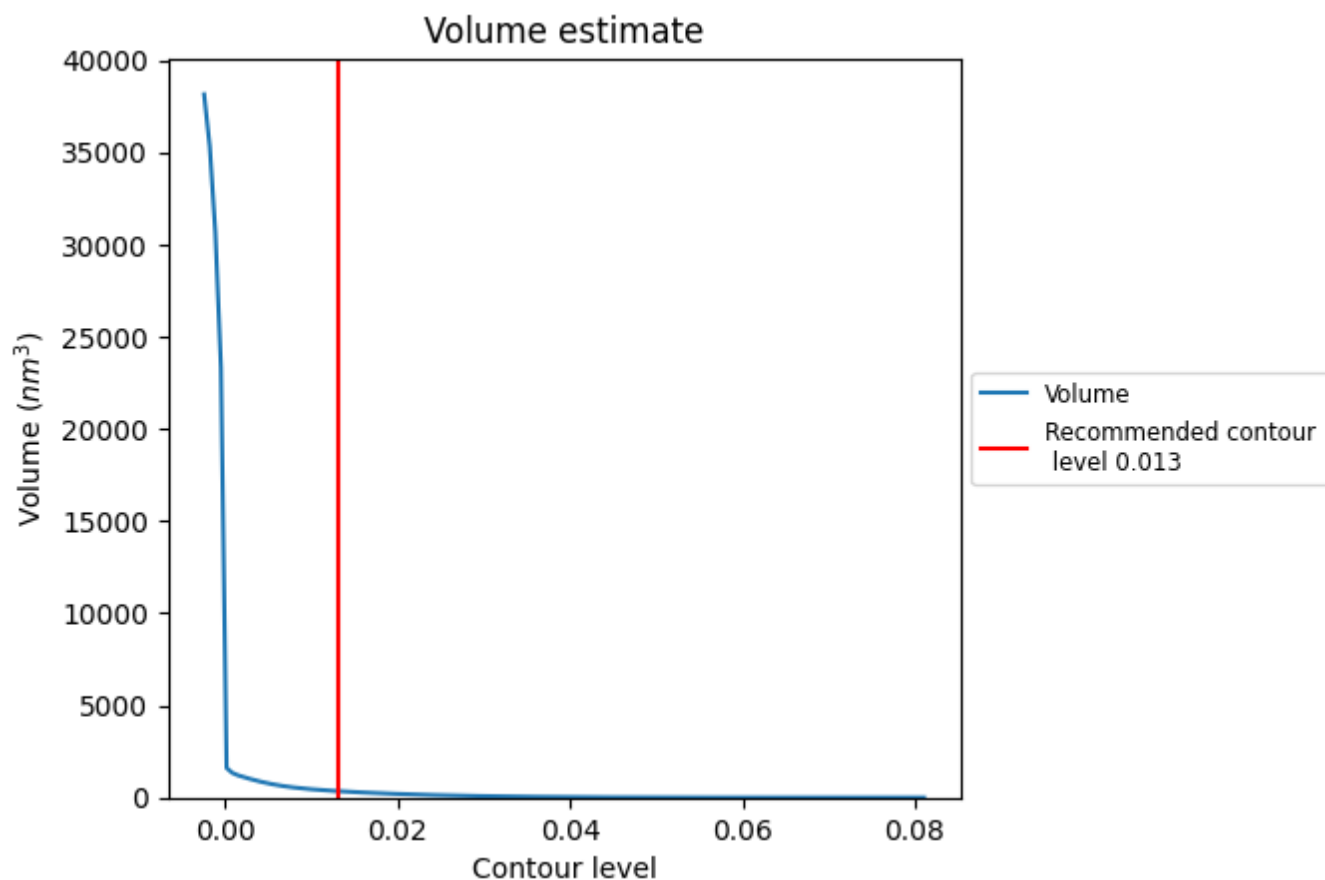
This section contains the results of statistical analysis of the map.

### 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.

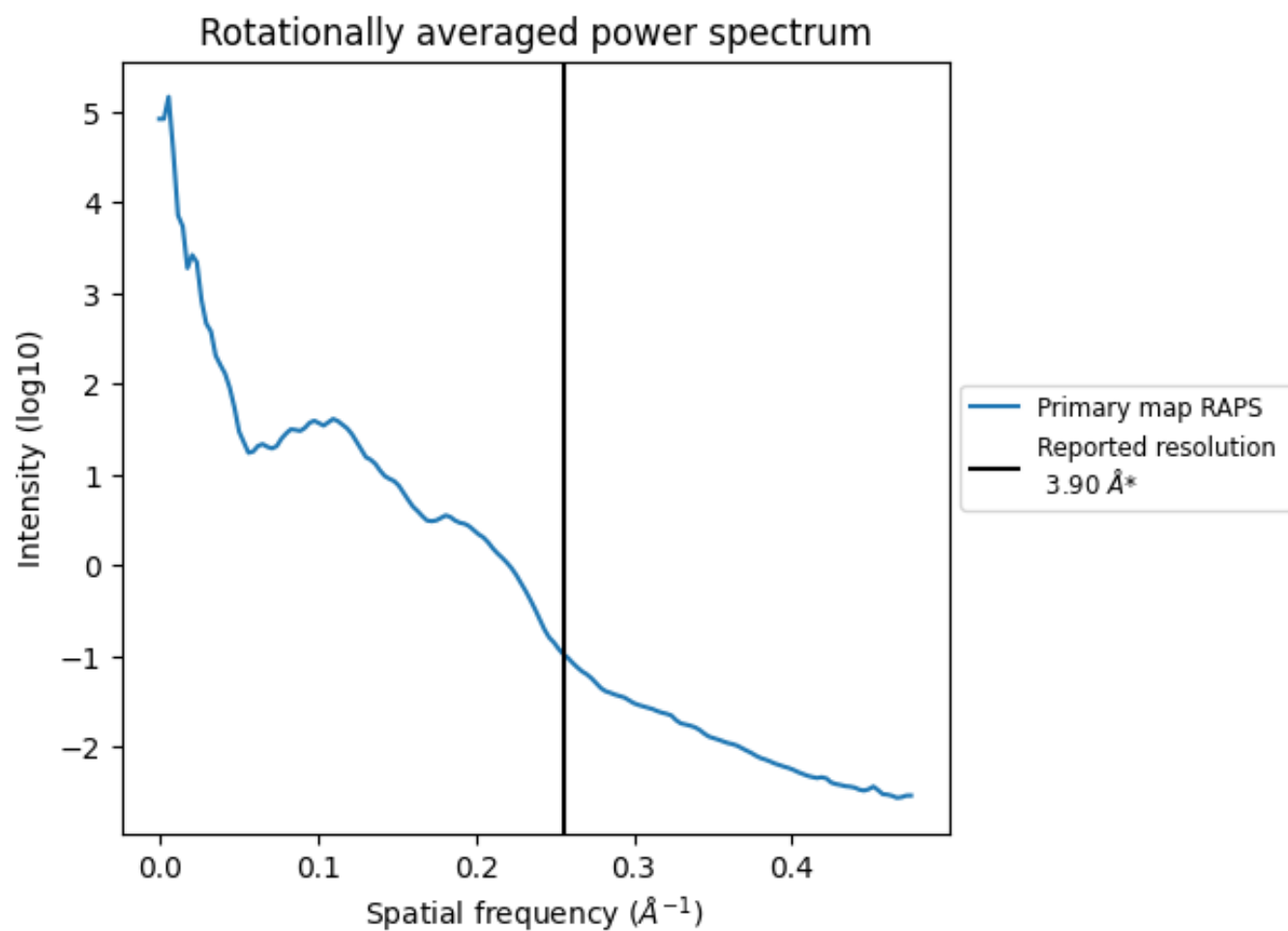
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm<sup>3</sup>; this corresponds to an approximate mass of 317 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 0.256  $\text{\AA}^{-1}$

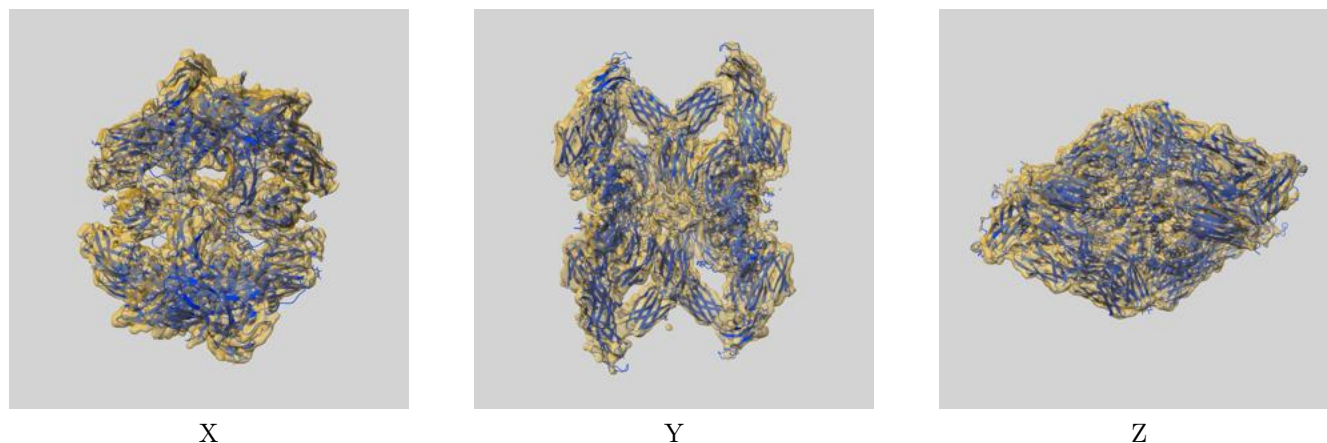
## 8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

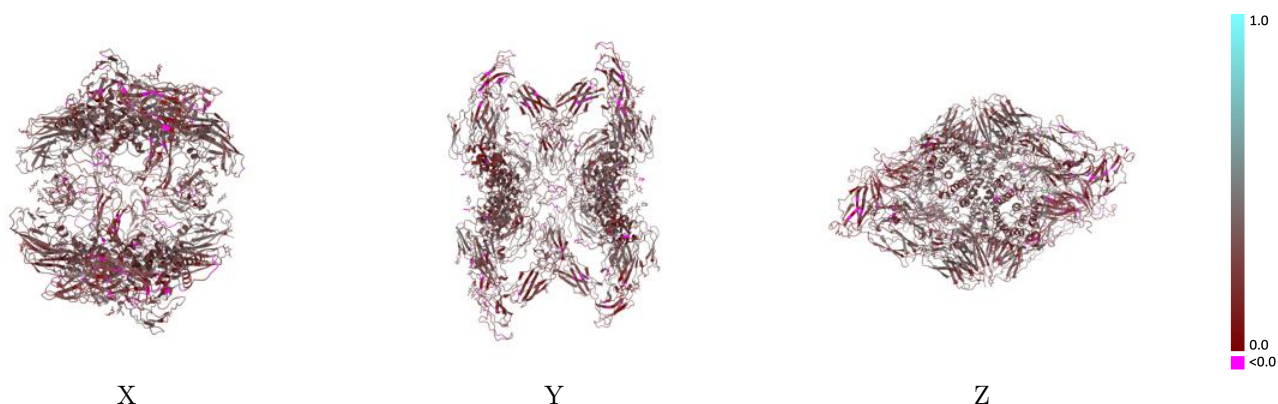
This section contains information regarding the fit between EMDB map EMD-12754 and PDB model 7O7R. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



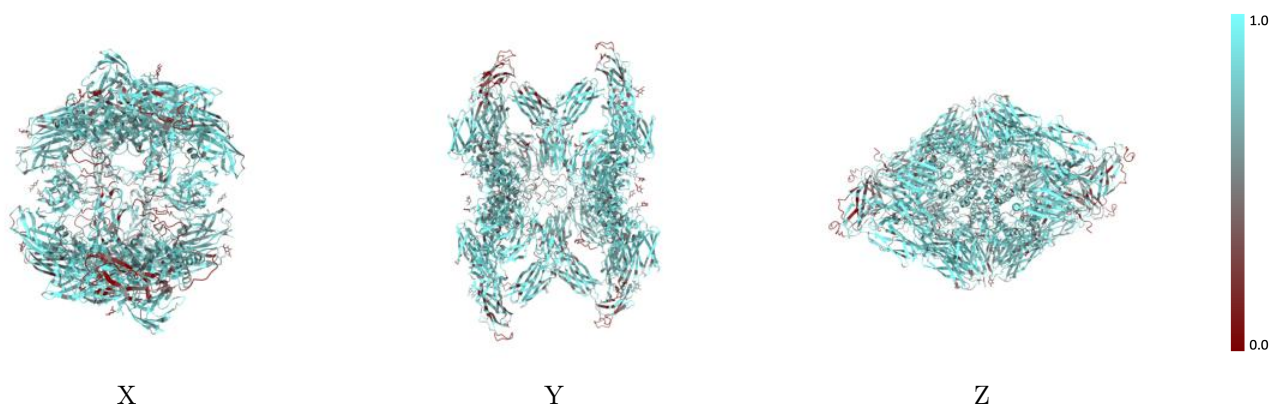
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



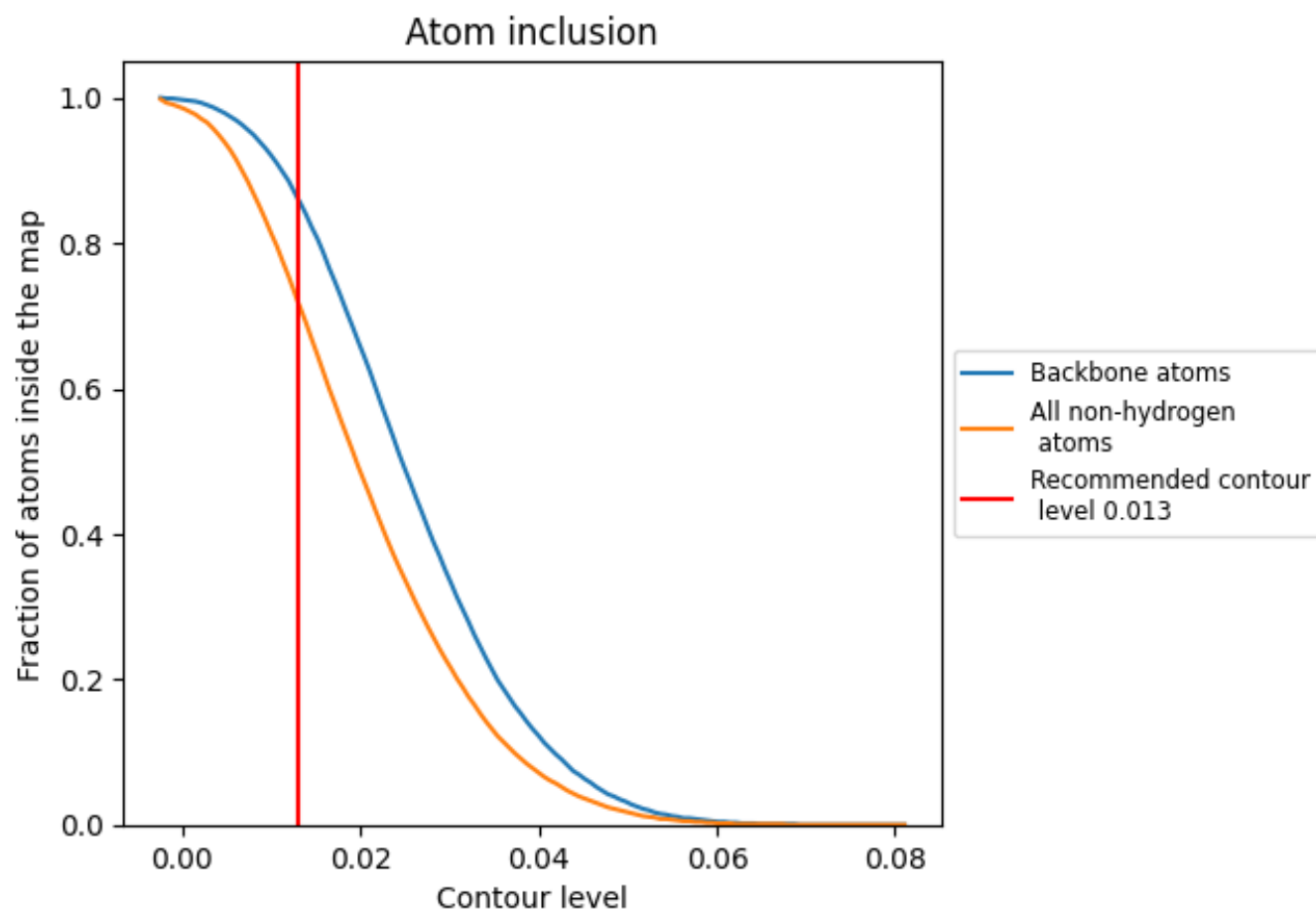
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7180	<div></div> 0.2960
A	<div></div> 0.6940	<div></div> 0.2900
B	<div></div> 0.7400	<div></div> 0.3030
C	<div></div> 0.7100	<div></div> 0.2870
D	<div></div> 0.7350	<div></div> 0.3060
E	<div></div> 0.5000	<div></div> 0.2430
F	<div></div> 0.5130	<div></div> 0.1480
G	<div></div> 0.3930	<div></div> 0.1770
H	<div></div> 0.5380	<div></div> 0.1800
I	<div></div> 0.7140	<div></div> 0.3220
J	<div></div> 0.5380	<div></div> 0.1360
K	<div></div> 0.4640	<div></div> 0.2000
L	<div></div> 0.4620	<div></div> 0.2800

1.0

0.0

<0.0