



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 07:02 PM UTC

PDB ID : 5GJV / pdb_00005gjb
EMDB ID : EMD-9513
Title : Structure of the mammalian voltage-gated calcium channel Cav1.1 complex at near atomic resolution
Authors : Wu, J.P.; Yan, Z.; Li, Z.Q.; Zhou, Q.; Yan, N.
Deposited on : 2016-07-02
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

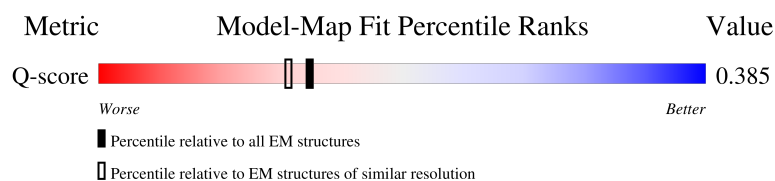
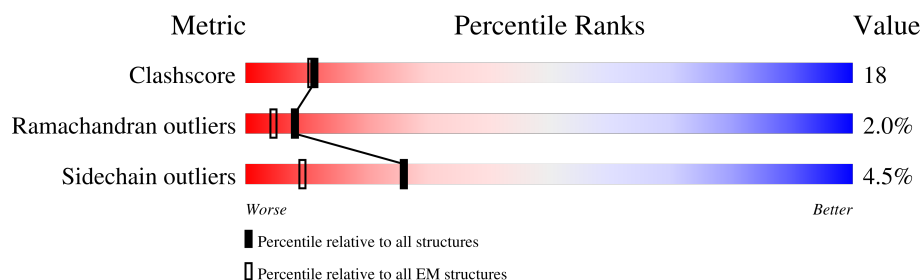
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



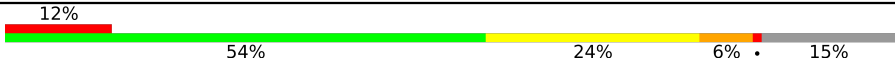
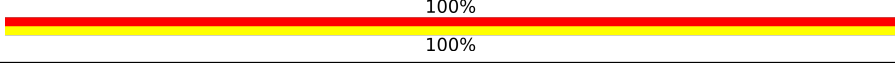
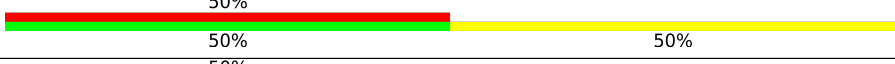
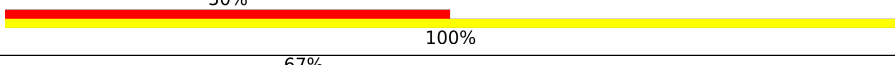
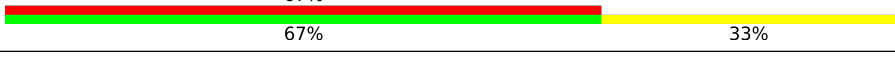
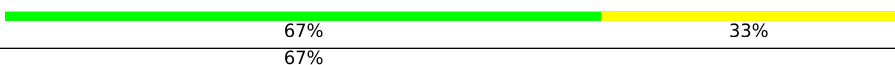
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	1873	
2	B	106	
3	C	199	
4	E	222	

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Mol	Chain	Length	Quality of chain
5	F	1106	
6	D	2	
6	G	2	
6	J	2	
6	K	2	
7	H	3	
7	I	3	
8	L	3	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21904 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1276	Total	C	N	O	S	4	0
			10183	6699	1673	1742	69		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	100	Total	C	N	O	S	0	0
			710	455	125	129	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP P19517
B	70	LEU	-	expression tag	UNP P19517
B	71	GLU	-	expression tag	UNP P19517
B	72	VAL	-	expression tag	UNP P19517
B	73	LEU	-	expression tag	UNP P19517
B	74	PHE	-	expression tag	UNP P19517
B	75	GLN	-	expression tag	UNP P19517
B	76	GLY	-	expression tag	UNP P19517
B	77	PRO	-	expression tag	UNP P19517
B	78	HIS	-	expression tag	UNP P19517
B	79	MET	-	expression tag	UNP P19517

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	178	Total	C	N	O	S	0	0
			1367	876	232	254	5		

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	166	Total	C	N	O	S	0	0
			1304	860	213	213	18		

- Molecule 5 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	942	Total	C	N	O	S	1	0
			7567	4809	1277	1451	30		

There is a discrepancy between the modelled and reference sequences:

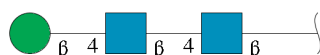
Chain	Residue	Modelled	Actual	Comment	Reference
F	1075	ETA	GLY	conflict	UNP P13806

- Molecule 6 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
6	D	2	Total	C	N	O	0	0
			28	16	2	10		
6	G	2	Total	C	N	O	0	0
			28	16	2	10		
6	J	2	Total	C	N	O	0	0
			28	16	2	10		
6	K	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 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.



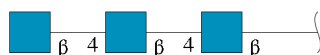
Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	3	Total	C	N	O	0	0
			39	22	2	15		

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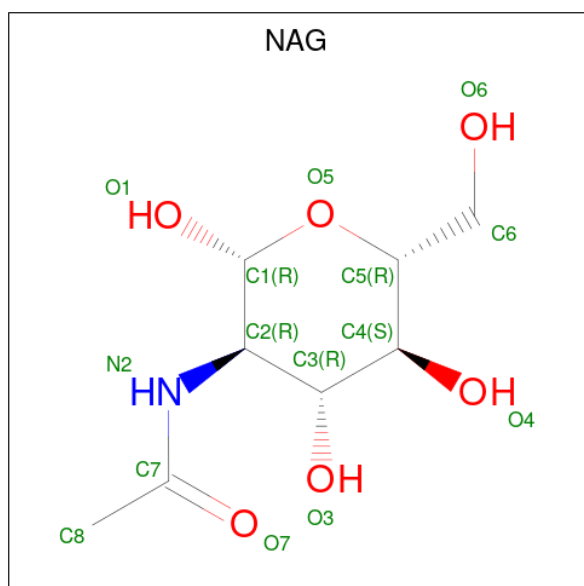
Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
8	L	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



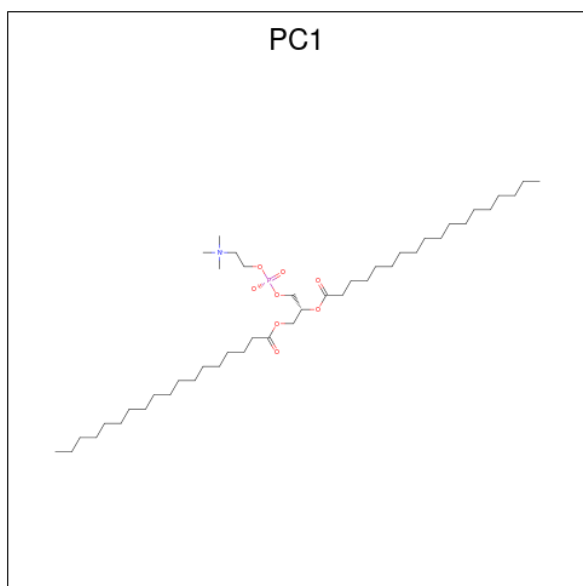
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
10	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
10	A	1	Total	C	N	O	P	0
			42	32	1	8	1	
10	A	1	Total	C	N	O	P	0
			38	28	1	8	1	
10	A	1	Total	C				0
			18	18				
10	A	1	Total	C				0
			12	12				
10	A	1	Total	C				0
			12	12				

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Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 15 15	0
10	A	1	Total C 18 18	0
10	A	1	Total C N O P 48 38 1 8 1	0
10	A	1	Total C N O P 45 35 1 8 1	0
10	A	1	Total C 18 18	0
10	A	1	Total C 14 14	0
10	A	1	Total C N O P 48 38 1 8 1	0

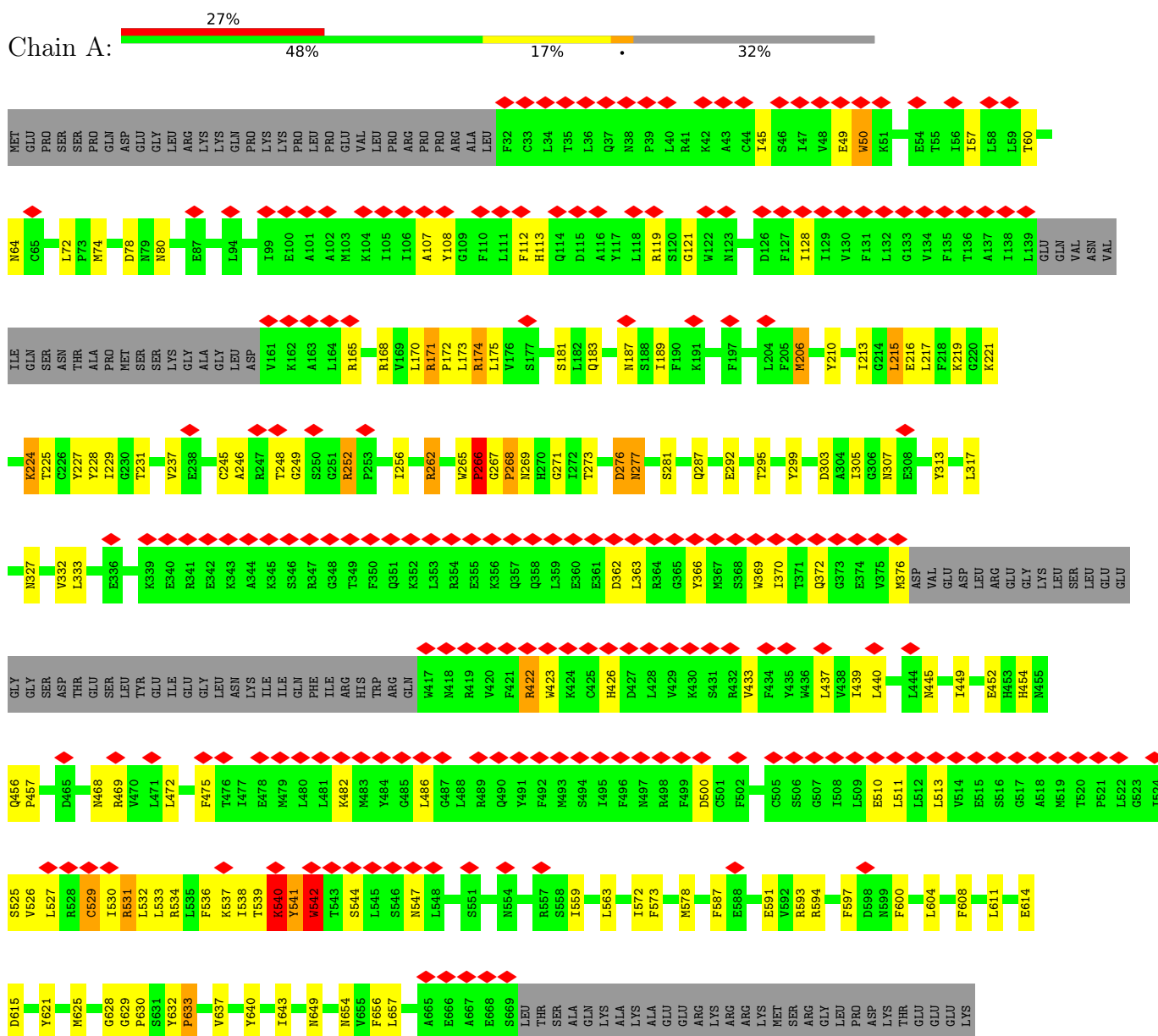
- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
11	A	2	Total Ca 2 2	0
11	F	1	Total Ca 1 1	0

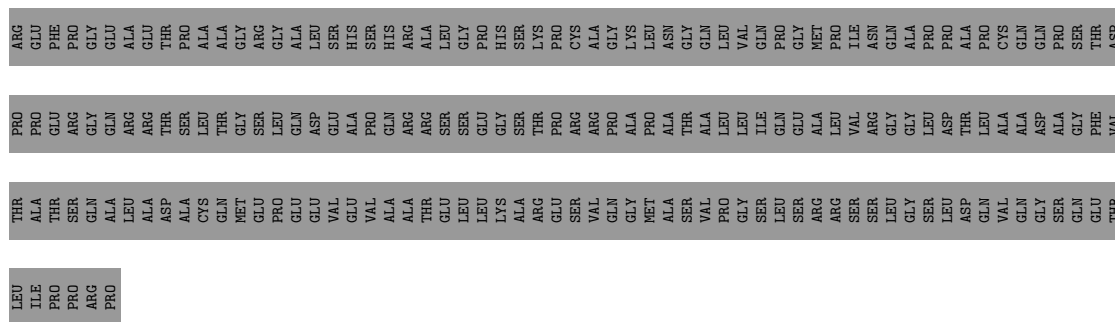
3 Residue-property plots

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.

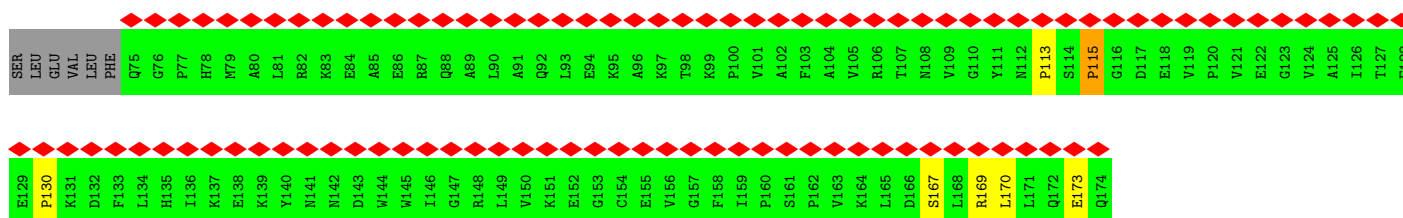
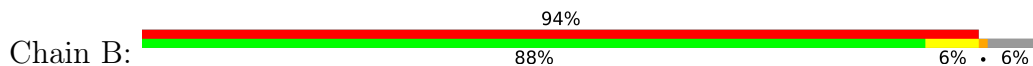
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S



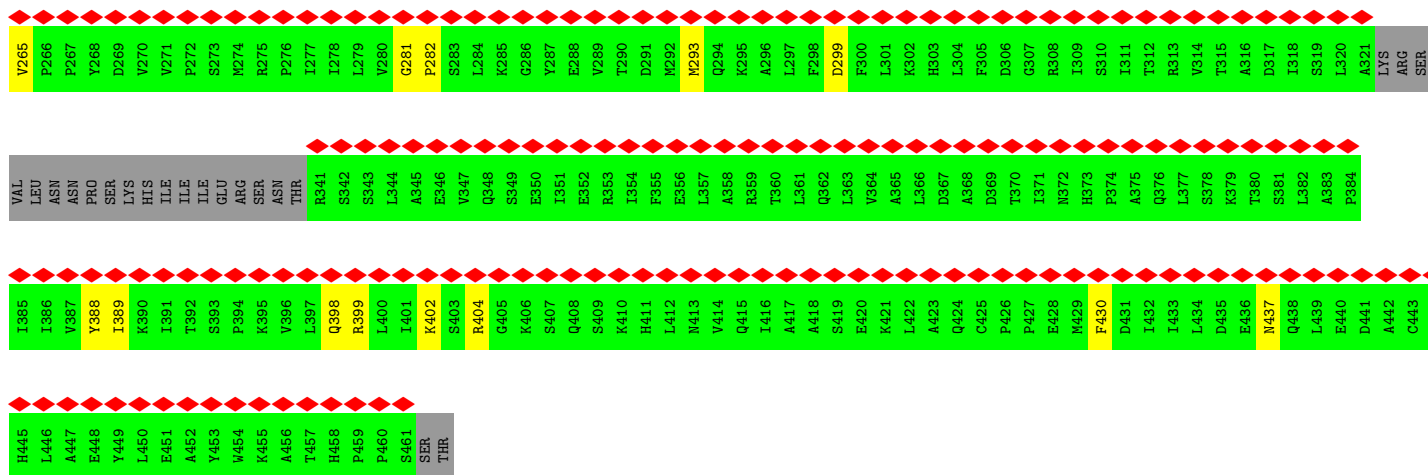
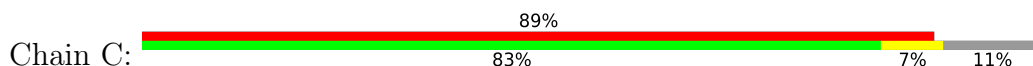
LEU	GLN	PRO	Q1508	R1447	T1388	N1303	VAL	HI139	Q1071	Y875	M883	P821	SER
PHE	PHE	ILE	V1509	L1448	R1389	N1304	ASP	Q1142	G1072	K976	C884	I822	VAL
ALA	ALA	ARG	I1510	V1449	M1305	F1306	PRO	S1143	E1073	D977	L885	A824	MET
GLU	GLU	THR	P1511	G1450	W1391	Q1311	GLU	E1144	T1074	Q882	GLU	E826	LYS
ILE	ILE	THR	P1512	M1451	S1392	Q1311	SER	E1145	E1075	R886	SER		LEU
MET	MET	SER	I1513	M1452	I1393	L1315	ALA	HI148	Y1076	R987	THR		GLN
GLY	GLY	GLY	G1514	M1453	L1394	R1318			K1077	Q888	ILE		LEU
ASP	ASP	LEU	D1515	P1454	G1395	T1321	I1229	D1151	N1078	Q889	SER		GLN
THR	THR	THR		M1455	P1396	E1322	I1230	I1152	C1079	Q890	LYS		LEU
VAL	VAL	ALA		N1456	HI397	E1323	S1231	I1153	N1078	Q891	LYS		GLY
PRO	PRO	GLU		S1457	HI398	A1324	A1233	L1154	C1079	H992	VAL		GLY
VAL	VAL	GLU		D1458	L1399	W1325	F1235	F1157	D1082	H993	ALA		ILE
GLY	GLY	LEU		T1459	D1401	E1326	L1237	T1158	K1083	H994	VAL		PRO
LEU	LEU	GLU		G1459	E1401	Q1327	F1238	I1159	N1084	H996	ALA		GLY
GLU	GLU	GLU		T1460	F1402	I1328	R1239	I1160	Q1085	H997	PRO		GLY
ASP	ASP	ARG		V1461	K1403	L1329	V1240	I1160	R1086	D998	THR		THR
PHE	PHE	ALA		T1462	A1404	L1330		E1164	Q1087	D999	ALA		ALA
PRO	PRO	VAL		F1463	I1405	C1331	I1244	M1165		H998	GLU		THR
GLN	GLN	VAL		N1464	W1406	S1332	L1247	I1166		R900	THR		THR
ALA	ALA	ALA		A1465	A1407	Y1334	S1248	L1167		V901	LEU		LYS
THR	THR	MET		T1466	E1408	G1335	R1249	L1167		I902	VAL		LYS
ASN	ASN	GLU		L1467	Y1409	K1336	A1250	L1170		P904	ASP		ASP
LEU	LEU	ARG			D1410	L1337	A1251	L1170		L905	GLY		GLY
ALA	ALA	ILE		L1470	P1411	C1338	E1251	K1173		R906	SER		SER
ALA	ALA	LYS		V1471	E1412	D1339		A1174		I907	LYS		ASN
ARG	ARG	PHE		L1472	A1413	P1340	R1254	R1175		I908	VAL		VAL
ASN	ASN	ARG		T1473	K1414	E1341	T1255	R1175		N909	ASN		ASN
THR	THR	LYS		A1474	S1342	G1342		D1180		R910	VAL		VAL
GLY	GLY	ARG		L1475	D1343	D1343	W1258	G1192		A911	GLY		GLY
ASN	ASN	GLN		K1476	Y1344	Y1344	F1260	G1192		K912	THR		THR
ALA	ALA	GLY		I1477	A1345	P1346	I1261	I1195		R915	PRO		PRO
ASN	ASN	PHE		T1478	G1347	G1347	K1262	D1196		H916	TYR		TYR
GLN	GLN	GLY		T1479	E1348	E1348	K1263	L1199		T853	PRO		PRO
VAL	VAL	VAL		A1480	E1349	E1349	F1264	S1200		T795	ALA		ALA
THR	THR	ALA		D1421	Y1350	T1351	Q1265	E1201		Q855	ASP		ASP
GLY	GLY	PHE		V1422	T1354	N1355	A1266	I1202		F857	PHE		PHE
ASN	ASN	LEU		V1423	T1354	N1355	L1267	I1202		L858	PRO		PRO
SER	SER	LEU		F1483	N1355	N1355	I1274	Q1108		H859	GLY		GLY
THR	THR	GLU		E1484	Y1358	Y1358	V1275	Y1109		R861	ASP		ASP
VAL	VAL	THR		Q1485	Y1359	Y1359	M1276	T1204		S862	GLY		GLY
ASN	ASN	ASN		R1427	Y1360	Y1360		Q1110		N930	ASP		ASP
ILE	ILE	LEU		A1486	F1370	F1370	Y1281	Y1113		F942	GLY		GLY
GLN	GLN	LEU		N1487	F1370	F1370	M1286	T1116		I945	PRO		PRO
ALA	ALA	ALA		E1488	F1376	F1376	K1291	S1117		M1056	GLY		GLY
PRO	PRO	PRO		E1489	V1377	V1377	I1292	S1118		M1057	ILE		ILE
MET	MET	VAL		L1490	Y1377	Y1377	A1293	Y1119		F1060	PRO		PRO
PHE	PHE	VAL		R1491	P1432	P1432	L1294	F1120		F954	VAL		VAL
SER	SER	ALA		L1492	L1433	L1433	L1295	S956		F955	SER		SER
ASN	ASN	ASN		A1492	G1434	G1434	V1295	C1121		C957	THR		THR
VAL	VAL	ASN		I1493	F1435	F1435	D1296	Y1122		N958	ARG		ARG
HIS	HIS	GLN		I1494	G1436	G1436	Q1299	L1123		D959	PRO		PRO
GLY	GLY	GLU		K1495	K1437	K1437	R1302	F1125		T964	ARG		ARG
ALA	ALA	ALA		K1496	I1497	I1497		A1126		E965	ALA		ALA
GLY	GLY	PRO		I1497	W1498	W1498		L1127		R969	PRO		PRO
MET	MET	VAL		K1499	P1440	P1440		T1132		V974	VAL		VAL
THR	THR	THR		R1500	R1442	R1442		I1133			SER		SER
ASN	ASN	THR		T1501	V1443	V1443		C1134			THR		THR
GLN	GLN	THR		M1503	M1503	M1503		Q1138			GLY		GLY
ASN	ASN	GLY		K1504	C1445	C1445					THR		THR
CYS	CYS	PRO		L1505	L1505	L1505					ARG		ARG
GLY	GLY	PRO		D1507	D1507	D1507					PRO		PRO



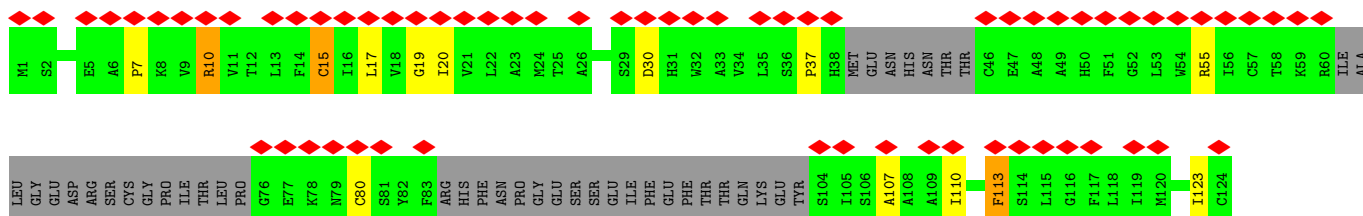
- Molecule 2: Voltage-dependent L-type calcium channel subunit beta-1

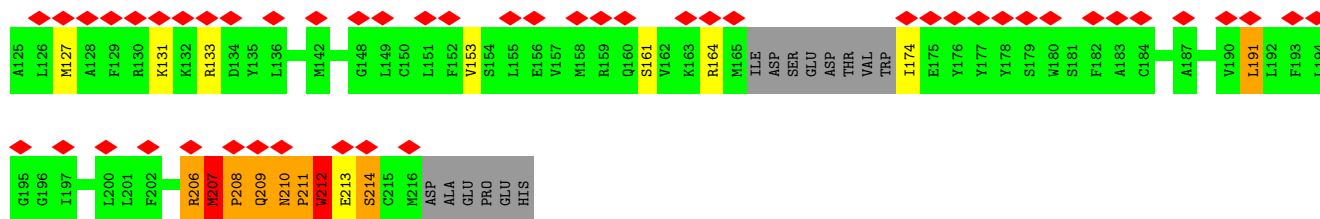


- Molecule 3: Voltage-dependent L-type calcium channel subunit beta-1

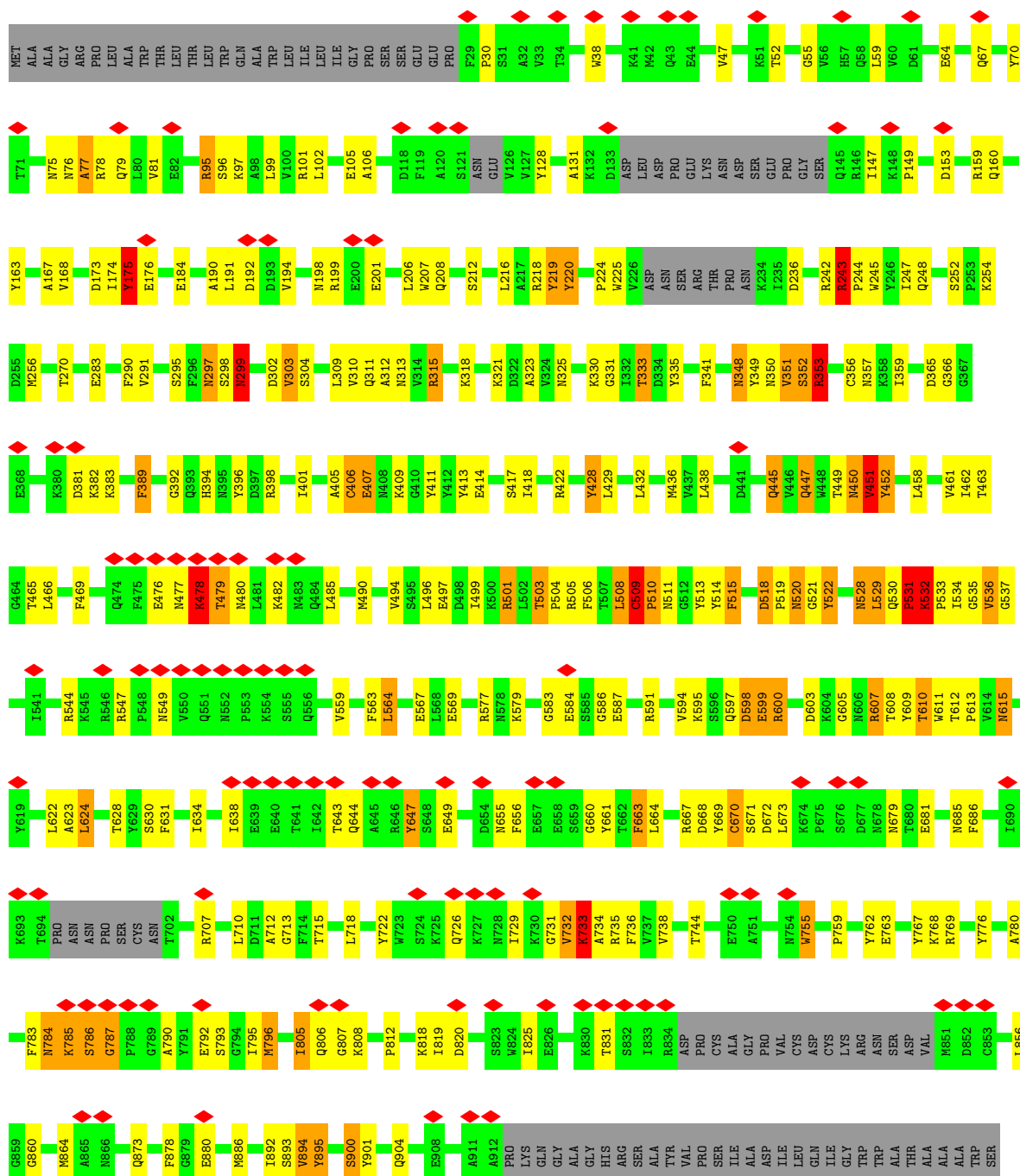


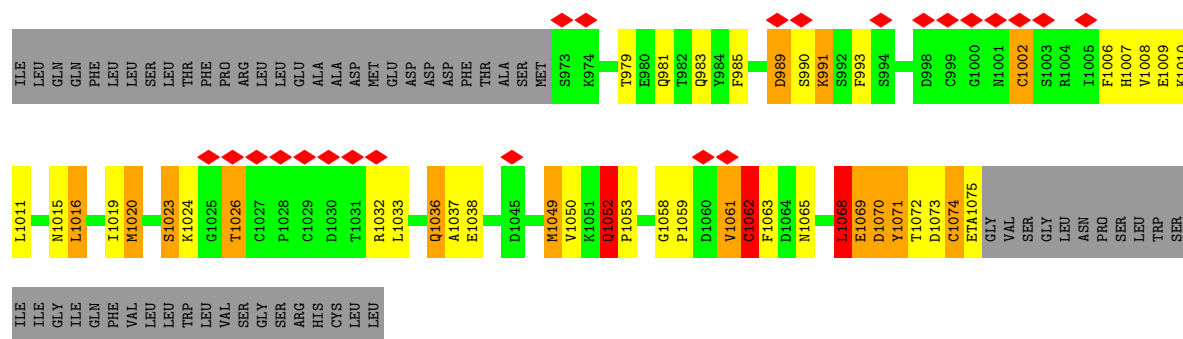
- Molecule 4: Voltage-dependent calcium channel gamma-1 subunit





• Molecule 5: Voltage-dependent calcium channel subunit alpha-2/delta-1





- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  67% 33%



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  33% 67% 67%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	527833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1.3	Depositor
Maximum defocus (nm)	2.9	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.294	Depositor
Minimum map value	-0.187	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CA, PC1, ETA, 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	0.56	3/10431 (0.0%)	0.91	28/14157 (0.2%)
2	B	0.49	0/723	0.91	3/979 (0.3%)
3	C	0.48	0/1394	0.70	0/1892
4	E	0.37	2/1336 (0.1%)	0.71	5/1802 (0.3%)
5	F	0.69	15/7721 (0.2%)	1.07	75/10463 (0.7%)
All	All	0.59	20/21605 (0.1%)	0.95	111/29293 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
3	C	0	2
5	F	0	14
All	All	0	27

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	C-O	24.09	1.48	1.24
5	F	647	TYR	C-N	17.13	1.57	1.34
5	F	312	ALA	C-O	10.61	1.37	1.23
5	F	1062	CYS	C-O	-9.31	1.12	1.24
1	A	540	LYS	CA-C	7.41	1.63	1.52
1	A	171	ARG	C-N	7.08	1.42	1.34
5	F	503	THR	C-N	6.87	1.40	1.33
5	F	405	ALA	C-N	6.05	1.42	1.33
5	F	607	ARG	C-N	5.83	1.43	1.33
5	F	504	PRO	N-CD	5.57	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1053	PRO	N-CD	5.44	1.55	1.47
5	F	533	PRO	N-CD	5.36	1.55	1.47
5	F	244	PRO	N-CD	5.34	1.55	1.47
5	F	510	PRO	N-CD	5.33	1.55	1.47
5	F	1059	PRO	N-CD	5.27	1.55	1.47
4	E	208	PRO	N-CD	5.26	1.55	1.47
5	F	531	PRO	N-CD	5.12	1.54	1.47
5	F	780	ALA	C-N	-5.10	1.27	1.33
5	F	673	LEU	C-N	-5.09	1.26	1.33
4	E	211	PRO	N-CD	5.07	1.54	1.47

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	518	ASP	CB-CA-C	-14.41	88.55	108.87
5	F	445	GLN	CB-CA-C	11.05	129.57	110.45
1	A	540	LYS	N-CA-C	-11.04	98.91	112.38
5	F	175	TYR	N-CA-C	10.55	133.27	110.80
5	F	607	ARG	N-CA-C	-10.33	91.56	108.41
5	F	469	PHE	CB-CA-C	-10.32	91.12	109.71
1	A	171	ARG	CA-C-N	-10.26	109.20	119.87
1	A	171	ARG	C-N-CA	-10.26	109.20	119.87
2	B	130	PRO	N-CA-CB	8.99	111.17	103.35
1	A	171	ARG	O-C-N	8.95	129.12	120.71
5	F	607	ARG	CA-C-N	8.90	135.22	122.85
5	F	607	ARG	C-N-CA	8.90	135.22	122.85
5	F	406	CYS	O-C-N	-8.85	109.52	122.43
5	F	535	GLY	N-CA-C	8.82	122.98	111.70
1	A	1417	ILE	CB-CA-C	8.69	125.53	111.29
1	A	1461	VAL	CB-CA-C	8.57	123.32	111.49
1	A	633	PRO	CB-CA-C	8.19	123.64	111.68
1	A	957	CYS	CB-CA-C	-8.10	95.67	109.51
5	F	663	PHE	CB-CA-C	-8.05	95.12	109.70
5	F	609	TYR	CB-CA-C	7.99	126.17	109.79
2	B	113	PRO	N-CA-CB	7.91	110.70	103.34
5	F	1002	CYS	N-CA-C	-7.76	95.87	109.06
2	B	115	PRO	N-CA-CB	7.64	111.41	103.23
5	F	216	LEU	CB-CA-C	-7.55	96.61	109.83
5	F	664	LEU	CB-CA-C	-7.35	98.90	110.74
5	F	624	LEU	CB-CA-C	-7.34	99.25	110.26
5	F	254	LYS	CB-CA-C	-7.34	98.84	110.14
5	F	783	PHE	CA-C-N	7.25	135.38	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	783	PHE	C-N-CA	7.25	135.38	121.54
5	F	522	TYR	CB-CA-C	-7.15	96.79	110.24
5	F	254	LYS	N-CA-C	7.01	119.90	108.26
5	F	735	ARG	CB-CA-C	-6.97	97.73	109.65
5	F	1002	CYS	CB-CA-C	6.93	123.45	109.38
1	A	1341	GLU	N-CA-C	-6.89	106.07	114.75
5	F	445	GLN	N-CA-C	-6.85	100.32	110.46
1	A	181	SER	CB-CA-C	6.82	123.99	110.42
5	F	405	ALA	O-C-N	-6.81	113.37	122.23
1	A	281	SER	N-CA-C	-6.81	103.94	111.36
5	F	219	TYR	N-CA-C	6.76	119.50	107.80
5	F	522	TYR	CA-C-N	6.72	131.53	123.19
5	F	522	TYR	C-N-CA	6.72	131.53	123.19
5	F	518	ASP	N-CA-C	6.71	118.52	110.07
1	A	281	SER	CB-CA-C	6.65	122.16	110.85
5	F	1006	PHE	CB-CA-C	-6.62	98.31	109.50
5	F	784	ASN	CA-C-N	6.61	134.16	121.54
5	F	784	ASN	C-N-CA	6.61	134.16	121.54
5	F	663	PHE	N-CA-C	6.60	119.92	108.76
5	F	603	ASP	CB-CA-C	-6.54	98.72	110.36
4	E	214	SER	N-CA-C	6.49	118.50	109.15
5	F	735	ARG	N-CA-C	6.45	119.82	110.28
1	A	267	GLY	N-CA-C	6.42	119.71	112.00
1	A	1174	ALA	N-CA-C	6.41	124.46	110.80
1	A	452	GLU	N-CA-C	6.41	119.03	111.02
1	A	1174	ALA	CB-CA-C	-6.40	97.69	110.42
5	F	407	GLU	CB-CA-C	-6.38	96.59	109.55
5	F	624	LEU	N-CA-C	6.38	118.96	109.59
5	F	128	TYR	N-CA-C	6.34	118.94	108.48
5	F	612	THR	CB-CA-C	-6.27	101.39	109.92
5	F	520	ASN	CB-CA-C	-6.24	99.27	110.37
5	F	450	ASN	N-CA-C	6.24	124.08	110.80
5	F	664	LEU	N-CA-C	6.17	118.83	108.02
5	F	900	SER	CB-CA-C	-6.16	99.39	110.36
5	F	605	GLY	O-C-N	6.13	129.94	123.45
5	F	607	ARG	CB-CA-C	6.08	120.25	110.16
5	F	787	GLY	CA-C-N	5.94	127.26	119.84
5	F	787	GLY	C-N-CA	5.94	127.26	119.84
1	A	440	LEU	CB-CA-C	5.92	121.58	110.63
5	F	1023	SER	N-CA-C	5.89	117.81	110.91
5	F	220	TYR	O-C-N	-5.88	115.66	121.19
5	F	610	THR	CB-CA-C	-5.82	97.68	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	976	LYS	O-C-N	5.78	130.10	122.36
5	F	670	CYS	N-CA-C	5.77	117.43	111.03
1	A	1102	ILE	N-CA-C	5.76	114.59	108.95
1	A	897	ARG	CB-CA-C	5.53	120.25	110.85
4	E	210	ASN	CA-C-N	-5.51	112.95	119.84
4	E	210	ASN	C-N-CA	-5.51	112.95	119.84
5	F	549	ASN	CA-C-N	5.48	131.84	121.97
5	F	549	ASN	C-N-CA	5.48	131.84	121.97
5	F	622	LEU	CB-CA-C	-5.48	100.75	109.80
5	F	1052	GLN	CA-C-N	-5.48	112.99	119.84
5	F	1052	GLN	C-N-CA	-5.48	112.99	119.84
5	F	1065	ASN	N-CA-C	5.46	117.29	110.91
5	F	873	GLN	CB-CA-C	5.45	119.20	110.09
5	F	608	THR	CA-C-N	-5.45	114.04	122.59
5	F	608	THR	C-N-CA	-5.45	114.04	122.59
5	F	1058	GLY	CA-C-N	-5.38	113.11	119.84
5	F	1058	GLY	C-N-CA	-5.38	113.11	119.84
4	E	207	MET	CA-C-N	-5.37	113.13	119.84
4	E	207	MET	C-N-CA	-5.37	113.13	119.84
1	A	266	PRO	CB-CA-C	-5.33	104.03	110.00
5	F	451	VAL	N-CA-CB	5.32	120.00	111.23
5	F	600	ARG	N-CA-C	-5.31	106.86	113.55
5	F	609	TYR	CA-CB-CG	5.31	123.46	113.90
5	F	509	CYS	CA-C-N	-5.31	113.20	119.84
5	F	509	CYS	C-N-CA	-5.31	113.20	119.84
5	F	219	TYR	CB-CA-C	-5.27	102.93	110.62
5	F	295	SER	CB-CA-C	-5.27	100.61	109.83
1	A	171	ARG	N-CA-C	5.23	120.59	113.16
1	A	897	ARG	N-CA-C	-5.21	105.67	111.36
1	A	1440	PRO	CA-C-N	5.21	131.50	121.54
1	A	1440	PRO	C-N-CA	5.21	131.50	121.54
1	A	215	LEU	N-CA-C	5.18	117.01	111.36
5	F	299	ASN	CB-CA-C	-5.14	107.97	114.40
1	A	1044	PHE	N-CA-C	-5.12	105.61	111.14
5	F	1062	CYS	O-C-N	-5.12	115.78	122.59
5	F	1016	LEU	N-CA-C	5.12	117.03	108.99
5	F	243	ARG	CA-C-N	-5.10	113.47	119.84
5	F	243	ARG	C-N-CA	-5.10	113.47	119.84
1	A	256	ILE	N-CA-C	-5.08	107.39	111.91
5	F	1026	THR	CA-C-N	5.03	128.02	120.83
5	F	1026	THR	C-N-CA	5.03	128.02	120.83

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1344	TYR	Peptide
1	A	1440	PRO	Peptide
1	A	1441	HIS	Peptide
1	A	228	TYR	Peptide
1	A	229	ILE	Peptide
1	A	237	VAL	Peptide
1	A	266	PRO	Peptide
1	A	268	PRO	Peptide
1	A	456	GLN	Peptide
1	A	628	GLY	Peptide
1	A	629	GLY	Peptide
3	C	281	GLY	Peptide,Mainchain
5	F	1023	SER	Peptide
5	F	1024	LYS	Peptide
5	F	1074	CYS	Peptide,Mainchain
5	F	175	TYR	Peptide
5	F	220	TYR	Peptide
5	F	406	CYS	Mainchain
5	F	476	GLU	Peptide
5	F	522	TYR	Peptide
5	F	600	ARG	Peptide
5	F	70	TYR	Peptide
5	F	785	LYS	Peptide
5	F	786	SER	Peptide
5	F	805	ILE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10183	0	10143	405	0
2	B	710	0	633	1	0
3	C	1367	0	1343	10	0
4	E	1304	0	1330	68	0
5	F	7567	0	7399	323	0
6	D	28	0	25	0	0
6	G	28	0	25	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	28	0	25	1	0
6	K	28	0	25	0	0
7	H	39	0	34	0	0
7	I	39	0	34	0	0
8	L	42	0	37	0	0
9	A	14	0	13	0	0
9	F	98	0	91	0	0
10	A	426	0	675	21	0
11	A	2	0	0	0	0
11	F	1	0	0	0	0
All	All	21904	0	21832	788	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 18.

All (788) 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:A:1389:ARG:HD2	1:A:1391:TRP:CE3	1.43	1.51
5:F:669:TYR:HD1	5:F:670:CYS:N	1.28	1.29
4:E:208:PRO:CG	4:E:214:SER:HA	1.64	1.26
1:A:1203:ASP:OD2	1:A:1229:ARG:HD2	1.15	1.24
1:A:1389:ARG:HB2	1:A:1391:TRP:CZ3	1.71	1.24
5:F:411:TYR:CD1	5:F:1074:CYS:HA	1.71	1.22
4:E:15:CYS:SG	4:E:191:LEU:CD2	2.28	1.21
1:A:956:SER:HB3	1:A:1022:ARG:NH1	1.53	1.21
1:A:475:PHE:CE2	1:A:537:LYS:HE3	1.77	1.20
1:A:224:LYS:O	1:A:266:PRO:HG3	1.44	1.16
1:A:1389:ARG:HD2	1:A:1391:TRP:CD2	1.82	1.15
5:F:529:LEU:O	5:F:530:GLN:HG2	1.48	1.14
4:E:15:CYS:SG	4:E:191:LEU:HD21	1.87	1.13
1:A:1060:PHE:HZ	1:A:1376:PHE:CE1	1.68	1.10
1:A:1015:GLY:HA3	1:A:1326:GLN:HE22	1.03	1.09
1:A:1389:ARG:CD	1:A:1391:TRP:CE3	2.34	1.09
1:A:956:SER:HB3	1:A:1022:ARG:HH11	0.92	1.08
4:E:208:PRO:HG3	4:E:214:SER:HA	1.28	1.08
1:A:1262:LYS:HE3	4:E:209:GLN:O	1.52	1.08
5:F:564:LEU:HD11	5:F:569:GLU:HG3	1.31	1.07
1:A:1046:ILE:HD12	10:A:1914:PC1:H392	1.36	1.06
5:F:174:ILE:HG22	5:F:175:TYR:H	1.21	1.06
5:F:315[B]:ARG:HH21	5:F:1049:MET:HE3	1.16	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:669:TYR:CD1	5:F:670:CYS:N	2.09	1.05
1:A:128:ILE:HG13	1:A:171:ARG:HH11	1.16	1.05
1:A:1391:TRP:HE1	1:A:1397:HIS:CD2	1.73	1.04
5:F:564:LEU:CD1	5:F:569:GLU:HG3	1.87	1.04
4:E:19:GLY:HA3	4:E:191:LEU:CD1	1.88	1.04
5:F:894:VAL:HG21	5:F:993:PHE:CE2	1.93	1.03
5:F:297:ASN:ND2	5:F:330:LYS:O	1.91	1.03
4:E:208:PRO:HG2	4:E:214:SER:HA	1.39	1.02
4:E:19:GLY:CA	4:E:191:LEU:CD1	2.38	1.02
5:F:661:TYR:CE2	5:F:663:PHE:CZ	2.48	1.02
1:A:362:ASP:OD1	3:C:437:ASN:ND2	1.93	1.01
5:F:643:THR:HG22	5:F:647:TYR:CE2	1.95	1.01
5:F:647:TYR:CE1	5:F:713:GLY:HA3	1.96	1.00
5:F:644:GLN:HA	5:F:647:TYR:HD2	1.25	1.00
5:F:534:ILE:HG22	5:F:904:GLN:HG2	1.40	0.99
1:A:1015:GLY:CA	1:A:1326:GLN:HE22	1.75	0.99
1:A:942:PHE:HD2	1:A:1048:TYR:CD1	1.81	0.99
1:A:1337:LEU:CD1	1:A:1350:TYR:HE1	1.76	0.98
5:F:248:GLN:OE1	5:F:447:GLN:HB3	1.63	0.98
1:A:1203:ASP:OD2	1:A:1229:ARG:CD	2.11	0.98
1:A:529:CYS:SG	1:A:945:ILE:HG13	2.03	0.97
1:A:1015:GLY:HA3	1:A:1326:GLN:NE2	1.80	0.97
4:E:19:GLY:CA	4:E:191:LEU:HD12	1.94	0.97
5:F:732:VAL:O	5:F:820:ASP:HB2	1.63	0.96
1:A:942:PHE:HD2	1:A:1048:TYR:HD1	1.00	0.96
5:F:315[B]:ARG:HH21	5:F:1049:MET:CE	1.78	0.96
5:F:174:ILE:HG22	5:F:175:TYR:N	1.75	0.96
5:F:315[B]:ARG:NH2	5:F:1049:MET:HE3	1.81	0.95
1:A:955:PHE:CE1	1:A:992:HIS:ND1	2.34	0.95
4:E:19:GLY:HA3	4:E:191:LEU:HD13	1.48	0.95
1:A:1262:LYS:CE	4:E:209:GLN:O	2.15	0.95
5:F:528:ASN:O	5:F:528:ASN:ND2	1.98	0.95
1:A:955:PHE:CE1	1:A:992:HIS:CE1	2.54	0.95
1:A:614:GLU:OE2	1:A:615:ASP:HB2	1.68	0.94
5:F:30:PRO:CG	5:F:1020:MET:HE1	1.97	0.94
6:G:1:NAG:C6	6:G:2:NAG:H82	1.98	0.94
4:E:19:GLY:N	4:E:191:LEU:CD1	2.32	0.93
1:A:1390:ASP:O	1:A:1392:SER:N	2.02	0.93
5:F:382:LYS:NZ	5:F:407:GLU:O	2.02	0.93
1:A:1042:ALA:O	1:A:1046:ILE:HG13	1.69	0.92
1:A:1389:ARG:HB2	1:A:1391:TRP:HZ3	1.25	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:174:ILE:CG2	5:F:175:TYR:H	1.81	0.92
5:F:1036:GLN:HE21	5:F:1037:ALA:H	1.17	0.92
5:F:661:TYR:CD2	5:F:663:PHE:CZ	2.58	0.92
1:A:1299:GLN:NE2	1:A:1327:GLU:OE1	2.03	0.92
1:A:836:ASP:OD2	1:A:900:ARG:NH1	2.02	0.92
5:F:290:PHE:HD2	5:F:310:VAL:O	1.52	0.91
5:F:647:TYR:CD1	5:F:713:GLY:HA3	2.05	0.91
1:A:942:PHE:CD2	1:A:1048:TYR:HD1	1.88	0.91
1:A:1043:ILE:HG12	1:A:1047:ILE:HD11	1.52	0.90
1:A:1337:LEU:HG	1:A:1350:TYR:CE1	2.05	0.90
1:A:956:SER:CB	1:A:1022:ARG:HH11	1.84	0.90
1:A:1389:ARG:HB2	1:A:1391:TRP:CE3	2.06	0.89
1:A:1060:PHE:CZ	1:A:1376:PHE:CE1	2.60	0.89
1:A:587:PHE:CE2	1:A:625:MET:HE3	2.08	0.89
1:A:587:PHE:HE2	1:A:625:MET:CE	1.85	0.89
1:A:1262:LYS:HE3	4:E:209:GLN:C	1.98	0.87
1:A:820:ASP:HB2	1:A:821:PRO:HA	1.56	0.86
1:A:1096:ARG:NH2	4:E:213:GLU:OE2	2.08	0.86
5:F:1062:CYS:O	5:F:1063:PHE:CD1	2.28	0.86
5:F:510:PRO:HG2	5:F:767:TYR:CE2	2.11	0.86
5:F:536:VAL:HG12	5:F:537:GLY:H	1.37	0.86
5:F:478:LYS:O	5:F:480:ASN:N	2.09	0.85
5:F:30:PRO:HG2	5:F:1020:MET:HE1	1.58	0.85
5:F:477:ASN:O	5:F:478:LYS:HB2	1.75	0.85
1:A:510:GLU:OE2	1:A:531:ARG:HD3	1.76	0.85
5:F:297:ASN:HD21	5:F:331:GLY:HA3	1.40	0.85
1:A:1391:TRP:NE1	1:A:1397:HIS:CD2	2.45	0.85
4:E:15:CYS:SG	4:E:191:LEU:HD23	2.14	0.84
5:F:661:TYR:HD2	5:F:663:PHE:CE2	1.96	0.84
1:A:841:SER:O	1:A:845:VAL:HG23	1.76	0.84
5:F:1036:GLN:NE2	5:F:1037:ALA:H	1.75	0.84
5:F:643:THR:HG22	5:F:647:TYR:HE2	1.42	0.83
5:F:894:VAL:HG11	5:F:993:PHE:CE2	2.13	0.83
1:A:965:GLU:OE1	1:A:990:TRP:NE1	2.11	0.83
1:A:1134:CYS:SG	1:A:1153:LEU:CD1	2.67	0.83
1:A:1391:TRP:NE1	1:A:1397:HIS:HD2	1.76	0.83
5:F:534:ILE:HG22	5:F:904:GLN:CG	2.09	0.82
5:F:894:VAL:HG21	5:F:993:PHE:HE2	1.41	0.82
1:A:538:ILE:O	1:A:541:TYR:HD1	1.62	0.82
5:F:290:PHE:CD2	5:F:310:VAL:O	2.32	0.82
5:F:661:TYR:HE2	5:F:663:PHE:CZ	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:894:VAL:HG21	5:F:993:PHE:CZ	2.14	0.81
4:E:208:PRO:HG2	4:E:214:SER:CA	2.10	0.81
5:F:515:PHE:HE2	5:F:563:PHE:CE1	1.97	0.81
5:F:247:ILE:HG23	5:F:429:LEU:HD11	1.61	0.81
1:A:262:ARG:HG2	1:A:262:ARG:HH11	1.46	0.81
1:A:1046:ILE:CD1	10:A:1914:PC1:H392	2.11	0.80
1:A:128:ILE:HG13	1:A:171:ARG:NH1	1.94	0.80
5:F:30:PRO:HG3	5:F:1020:MET:HE1	1.62	0.80
5:F:174:ILE:CG2	5:F:175:TYR:N	2.43	0.80
1:A:1134:CYS:SG	1:A:1153:LEU:HD12	2.22	0.80
5:F:671:SER:O	5:F:672:ASP:OD1	1.99	0.80
1:A:840:THR:O	1:A:844:THR:HG23	1.82	0.79
5:F:733:LYS:NZ	5:F:792:GLU:O	2.14	0.79
1:A:1337:LEU:CD1	1:A:1350:TYR:CE1	2.66	0.79
1:A:955:PHE:HE1	1:A:992:HIS:CE1	2.00	0.79
1:A:1046:ILE:O	1:A:1049:ILE:HG22	1.84	0.78
1:A:591:GLU:OE2	1:A:593:ARG:NH1	2.15	0.78
5:F:353:ARG:HB2	5:F:353:ARG:HH11	1.48	0.78
1:A:819:GLU:CD	1:A:897:ARG:HH21	1.91	0.78
1:A:955:PHE:CD1	1:A:992:HIS:ND1	2.51	0.78
5:F:598:ASP:C	5:F:599:GLU:HG3	2.08	0.77
1:A:1384:PHE:O	1:A:1388:THR:HG23	1.85	0.77
1:A:215:LEU:O	1:A:219:LYS:HG3	1.83	0.77
5:F:478:LYS:O	5:F:479:THR:C	2.27	0.77
5:F:644:GLN:HA	5:F:647:TYR:CD2	2.16	0.77
5:F:1061:VAL:HG23	5:F:1062:CYS:H	1.48	0.77
5:F:564:LEU:CD1	5:F:569:GLU:CG	2.63	0.77
1:A:821:PRO:HG3	1:A:1286:MET:HG2	1.67	0.77
5:F:411:TYR:CE1	5:F:1074:CYS:HA	2.19	0.77
5:F:894:VAL:HG11	5:F:993:PHE:HE2	1.49	0.77
1:A:1020:LEU:HD12	1:A:1020:LEU:O	1.85	0.76
1:A:903:ARG:HB2	1:A:904:PRO:HD3	1.66	0.76
1:A:1337:LEU:HD12	1:A:1350:TYR:HE1	1.50	0.76
1:A:820:ASP:H	1:A:821:PRO:HA	1.50	0.76
1:A:955:PHE:CD1	1:A:992:HIS:CE1	2.73	0.76
5:F:315[B]:ARG:NH2	5:F:1049:MET:CE	2.46	0.76
1:A:1390:ASP:HB3	1:A:1393:ILE:CD1	2.16	0.75
5:F:661:TYR:CD2	5:F:663:PHE:CE2	2.74	0.75
5:F:76:ASN:O	5:F:78:ARG:N	2.20	0.75
5:F:411:TYR:CD1	5:F:1074:CYS:CA	2.63	0.75
5:F:894:VAL:CG2	5:F:993:PHE:CE2	2.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1060:PHE:HZ	1:A:1376:PHE:CD1	2.04	0.75
1:A:468:ASN:ND2	1:A:531:ARG:NH2	2.35	0.75
1:A:475:PHE:CZ	1:A:537:LYS:HE3	2.21	0.75
1:A:902:LEU:HD11	1:A:905:LEU:HD12	1.69	0.75
1:A:206:MET:HE2	1:A:317:LEU:HD12	1.68	0.74
1:A:587:PHE:HE2	1:A:625:MET:HE3	1.48	0.74
1:A:1325:TRP:HA	1:A:1328:ILE:HD12	1.68	0.74
4:E:19:GLY:CA	4:E:191:LEU:HD13	2.11	0.74
5:F:503:THR:HB	5:F:514:TYR:HD2	1.53	0.74
5:F:510:PRO:HG2	5:F:767:TYR:HE2	1.52	0.74
1:A:1389:ARG:CB	1:A:1391:TRP:CZ3	2.63	0.74
4:E:19:GLY:HA3	4:E:191:LEU:HD12	1.60	0.74
5:F:450:ASN:O	5:F:451:VAL:HG22	1.88	0.74
5:F:452:TYR:OH	5:F:463:THR:CG2	2.36	0.73
1:A:820:ASP:HB2	1:A:821:PRO:CA	2.18	0.73
5:F:661:TYR:CE2	5:F:663:PHE:HZ	2.02	0.73
1:A:171:ARG:O	1:A:174:ARG:HB2	1.88	0.73
1:A:224:LYS:O	1:A:266:PRO:CG	2.32	0.73
5:F:732:VAL:HG23	5:F:733:LYS:N	2.02	0.73
1:A:1235:PHE:HE2	4:E:153:VAL:CG2	2.02	0.73
1:A:1389:ARG:HE	1:A:1391:TRP:HB2	1.54	0.72
1:A:902:LEU:CD1	1:A:905:LEU:HD12	2.19	0.72
5:F:586:GLY:HA3	5:F:611:TRP:CZ2	2.24	0.72
1:A:262:ARG:HG2	1:A:262:ARG:NH1	1.99	0.72
1:A:820:ASP:CB	1:A:821:PRO:CA	2.68	0.72
4:E:19:GLY:H	4:E:191:LEU:CD1	2.01	0.72
5:F:530:GLN:OE1	5:F:532:LYS:NZ	2.22	0.72
1:A:1195:ILE:HD11	4:E:113:PHE:CD2	2.25	0.72
1:A:1299:GLN:HG2	1:A:1327:GLU:HB3	1.71	0.72
5:F:1074:CYS:SG	5:F:1075:ETA:N	2.63	0.72
5:F:30:PRO:HG3	5:F:1020:MET:CE	2.19	0.72
1:A:544:SER:OG	1:A:547:ASN:HB3	1.90	0.71
1:A:843:PHE:CE2	1:A:871:LEU:HA	2.25	0.71
1:A:1134:CYS:SG	1:A:1153:LEU:HD13	2.30	0.71
5:F:669:TYR:CE1	5:F:670:CYS:HB2	2.25	0.71
5:F:353:ARG:HB2	5:F:353:ARG:NH1	2.05	0.71
1:A:587:PHE:CE2	1:A:625:MET:CE	2.68	0.71
1:A:439:ILE:HG12	1:A:541:TYR:OH	1.91	0.71
5:F:366:GLY:HA2	5:F:401:ILE:HD11	1.72	0.71
1:A:1014:GLU:OE2	1:A:1326:GLN:NE2	2.23	0.71
1:A:1329:LEU:HD11	1:A:1358:TYR:CD1	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:ILE:HD11	1:A:1276:MET:HG2	1.74	0.70
5:F:409:LYS:HE2	5:F:1071:TYR:CE1	2.26	0.70
1:A:1391:TRP:CD1	1:A:1397:HIS:HD2	2.09	0.70
5:F:892:ILE:O	5:F:892:ILE:HD12	1.91	0.70
1:A:632:TYR:HB3	1:A:633:PRO:HD3	1.71	0.70
1:A:911:ALA:O	1:A:915:LYS:HE3	1.92	0.70
5:F:529:LEU:O	5:F:530:GLN:CG	2.35	0.70
1:A:1249[A]:ARG:O	1:A:1249[A]:ARG:HD3	1.92	0.69
1:A:538:ILE:O	1:A:541:TYR:CD1	2.46	0.69
5:F:595:LYS:HE3	5:F:983:GLN:HE22	1.56	0.69
5:F:671:SER:C	5:F:672:ASP:OD1	2.35	0.69
1:A:245:CYS:SG	1:A:246:ALA:N	2.66	0.69
1:A:268:PRO:HB2	1:A:273:THR:HB	1.73	0.69
1:A:587:PHE:HE2	1:A:625:MET:HE2	1.56	0.69
5:F:511:ASN:HB3	5:F:607:ARG:HH12	1.56	0.69
1:A:1235:PHE:HE2	4:E:153:VAL:HG21	1.58	0.69
1:A:994:ASP:HB3	1:A:1330:LEU:HD21	1.75	0.68
4:E:208:PRO:O	4:E:210:ASN:N	2.27	0.68
6:G:1:NAG:H62	6:G:2:NAG:H82	1.76	0.68
5:F:318:LYS:HG2	5:F:536:VAL:HG13	1.75	0.68
1:A:1235:PHE:CE2	4:E:153:VAL:HG21	2.28	0.68
1:A:1337:LEU:CG	1:A:1350:TYR:CE1	2.76	0.68
5:F:564:LEU:HD12	5:F:569:GLU:CG	2.24	0.68
1:A:820:ASP:CB	1:A:821:PRO:HA	2.19	0.68
1:A:1071:GLN:NE2	1:A:1381:MET:SD	2.67	0.68
4:E:206:ARG:O	4:E:207:MET:C	2.36	0.67
5:F:351:VAL:HG12	5:F:352:SER:N	2.09	0.67
1:A:843:PHE:HE2	1:A:871:LEU:CA	2.07	0.67
1:A:1417:ILE:O	1:A:1460:THR:HA	1.95	0.67
1:A:1305:ASN:HD22	1:A:1311:GLN:HG3	1.59	0.66
1:A:1047:ILE:O	1:A:1051:LEU:HG	1.94	0.66
1:A:1391:TRP:CZ2	1:A:1396:PRO:HD2	2.30	0.66
5:F:77:ALA:O	5:F:81:VAL:HG23	1.95	0.66
6:G:1:NAG:H61	6:G:2:NAG:H82	1.75	0.66
5:F:503:THR:HB	5:F:514:TYR:CD2	2.29	0.66
1:A:843:PHE:O	1:A:846:GLU:HG3	1.95	0.66
5:F:649:GLU:OE1	5:F:655:ASN:ND2	2.29	0.66
5:F:302:ASP:O	5:F:304:SER:N	2.29	0.66
1:A:996:HIS:ND1	1:A:998:ASP:HB2	2.11	0.65
5:F:586:GLY:O	5:F:611:TRP:CD2	2.49	0.65
5:F:506:PHE:HA	5:F:762:TYR:HE2	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:991:LYS:HB3	5:F:1010:LYS:HB2	1.78	0.65
5:F:667:ARG:NH1	5:F:668:ASP:O	2.30	0.65
1:A:915:LYS:HD3	1:A:915:LYS:N	2.11	0.65
1:A:231:THR:O	1:A:262:ARG:NH2	2.29	0.65
1:A:1264:PHE:CE1	1:A:1267:LEU:HD23	2.32	0.65
1:A:1060:PHE:CZ	1:A:1376:PHE:CD1	2.82	0.65
1:A:1192:GLY:HA3	1:A:1238:PHE:CD2	2.31	0.65
1:A:45:ILE:HG12	1:A:107:ALA:HA	1.78	0.65
1:A:439:ILE:CG1	1:A:541:TYR:OH	2.45	0.65
1:A:843:PHE:CE2	1:A:871:LEU:CA	2.80	0.65
5:F:297:ASN:ND2	5:F:331:GLY:HA3	2.10	0.65
1:A:1430:GLN:HG3	1:A:1432:PRO:HD2	1.79	0.64
5:F:536:VAL:HG12	5:F:537:GLY:N	2.10	0.64
1:A:1060:PHE:HZ	1:A:1376:PHE:CZ	2.14	0.64
1:A:1248:SER:HB3	1:A:1249[B]:ARG:HD3	1.78	0.64
5:F:647:TYR:CD1	5:F:713:GLY:CA	2.78	0.64
1:A:1334:TYR:CE1	1:A:1351:THR:HG23	2.33	0.64
5:F:449:THR:O	5:F:462:ILE:HG13	1.97	0.64
5:F:661:TYR:HE2	5:F:663:PHE:HZ	1.38	0.64
5:F:736:PHE:CZ	5:F:796:MET:SD	2.90	0.64
1:A:1139:HIS:CD2	1:A:1142:GLN:HB3	2.33	0.64
5:F:76:ASN:ND2	5:F:79:GLN:HB2	2.13	0.64
5:F:283:GLU:OE2	5:F:321:LYS:NZ	2.31	0.64
5:F:529:LEU:C	5:F:530:GLN:HG2	2.20	0.64
5:F:597:GLN:NE2	5:F:763:GLU:O	2.31	0.63
5:F:153:ASP:OD1	5:F:160:GLN:HG2	1.98	0.63
1:A:303:ASP:OD2	1:A:1302:ARG:NH1	2.31	0.63
1:A:372:GLN:NE2	1:A:486:LEU:O	2.31	0.63
5:F:667:ARG:HH21	5:F:686:PHE:HE1	1.45	0.63
5:F:894:VAL:CB	5:F:993:PHE:CE2	2.82	0.63
1:A:1195:ILE:HD11	4:E:113:PHE:HD2	1.62	0.63
1:A:1389:ARG:HD2	1:A:1391:TRP:CZ3	2.25	0.63
5:F:407:GLU:O	5:F:407:GLU:HG2	1.98	0.63
5:F:452:TYR:OH	5:F:463:THR:HG21	1.99	0.62
1:A:468:ASN:HD21	1:A:531:ARG:HD3	1.65	0.62
1:A:1019:LEU:HD21	1:A:1045:PHE:CZ	2.35	0.62
1:A:822:ILE:HD12	1:A:822:ILE:O	2.00	0.61
1:A:608:PHE:CZ	1:A:1050:ILE:HD11	2.35	0.61
1:A:820:ASP:N	1:A:821:PRO:HA	2.11	0.61
1:A:843:PHE:O	1:A:846:GLU:CG	2.48	0.61
1:A:1258:TRP:HE1	4:E:208:PRO:HD2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:351:VAL:O	5:F:352:SER:HB3	1.98	0.61
5:F:482:LYS:O	5:F:482:LYS:HG2	1.99	0.61
5:F:647:TYR:HE1	5:F:713:GLY:HA3	1.60	0.61
1:A:965:GLU:CD	1:A:990:TRP:HE1	2.08	0.61
1:A:1260:PHE:HA	1:A:1263:SER:OG	1.99	0.61
1:A:823:ARG:HG2	1:A:823:ARG:HH21	1.65	0.61
5:F:858:ASP:HB2	5:F:1015:ASN:OD1	1.99	0.61
5:F:669:TYR:HE1	5:F:670:CYS:HB2	1.64	0.61
5:F:163:TYR:OH	5:F:199:ARG:NH2	2.34	0.61
5:F:894:VAL:CG1	5:F:993:PHE:CE2	2.84	0.61
4:E:30:ASP:OD2	4:E:55:ARG:NH2	2.34	0.61
5:F:531:PRO:O	5:F:532:LYS:HG3	2.01	0.60
5:F:731:GLY:O	5:F:732:VAL:HG22	2.01	0.60
5:F:310:VAL:HG12	5:F:1050:VAL:HG21	1.83	0.60
5:F:101:ARG:HH12	5:F:201:GLU:HG2	1.64	0.60
1:A:265:TRP:HZ2	1:A:271:GLY:HA2	1.66	0.60
1:A:823:ARG:HH21	1:A:823:ARG:CG	2.14	0.60
1:A:942:PHE:HA	1:A:945:ILE:HG22	1.83	0.60
1:A:1389:ARG:CB	1:A:1391:TRP:CE3	2.81	0.60
5:F:579:LYS:O	5:F:583:GLY:HA3	2.01	0.60
1:A:587:PHE:CD2	1:A:625:MET:HE3	2.36	0.60
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.37	0.60
1:A:1020:LEU:HD12	1:A:1020:LEU:C	2.27	0.60
5:F:243:ARG:HH11	5:F:243:ARG:CG	2.15	0.60
5:F:411:TYR:HD1	5:F:1074:CYS:HA	1.56	0.59
1:A:637:VAL:HG22	10:A:1903:PC1:H291	1.84	0.59
1:A:541:TYR:O	1:A:542:TRP:HB2	2.02	0.59
5:F:309:LEU:HD12	5:F:353:ARG:HD2	1.84	0.59
5:F:981:GLN:NE2	5:F:1038:GLU:OE2	2.35	0.59
5:F:586:GLY:O	5:F:611:TRP:CE2	2.56	0.59
1:A:1195:ILE:CD1	4:E:113:PHE:CD2	2.86	0.59
5:F:256:MET:HB3	5:F:291:VAL:HG12	1.83	0.59
5:F:303:VAL:O	5:F:303:VAL:HG22	2.02	0.59
5:F:309:LEU:HD12	5:F:353:ARG:CD	2.33	0.59
5:F:302:ASP:OD1	5:F:341:PHE:HE2	1.86	0.58
5:F:894:VAL:CG1	5:F:993:PHE:HE2	2.15	0.58
5:F:643:THR:O	5:F:647:TYR:CD2	2.57	0.58
1:A:822:ILE:HG21	1:A:1291:LYS:H	1.68	0.58
1:A:982:GLN:HG2	5:F:547:ARG:HE	1.67	0.58
5:F:225:TRP:NE1	5:F:236:ASP:OD2	2.36	0.58
1:A:469:ARG:HG2	1:A:511:LEU:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:TRP:O	1:A:1020:LEU:N	2.28	0.58
4:E:208:PRO:CG	4:E:214:SER:CA	2.58	0.58
5:F:206:LEU:HD13	5:F:458:LEU:HD21	1.85	0.58
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.15	0.58
5:F:894:VAL:CG2	5:F:993:PHE:HE2	2.10	0.58
1:A:108:TYR:HB2	1:A:112:PHE:HB2	1.86	0.57
1:A:482:LYS:HE2	1:A:486:LEU:HD22	1.86	0.57
1:A:820:ASP:HB2	1:A:821:PRO:C	2.30	0.57
1:A:183:GLN:O	1:A:187:ASN:ND2	2.38	0.57
1:A:591:GLU:OE2	1:A:593:ARG:NH2	2.36	0.57
5:F:365:ASP:O	5:F:394:HIS:NE2	2.37	0.57
5:F:679:ASN:HD21	5:F:759:PRO:HG3	1.68	0.57
1:A:225:THR:HG23	1:A:266:PRO:HB3	1.86	0.57
1:A:1094:LYS:HD3	4:E:212:TRP:CZ2	2.40	0.57
1:A:900:ARG:HD2	1:A:903:ARG:HH11	1.70	0.57
1:A:1262:LYS:HE2	4:E:209:GLN:OE1	2.04	0.57
1:A:1416:ARG:HA	1:A:1461:VAL:O	2.04	0.57
1:A:369:TRP:HD1	1:A:369:TRP:O	1.87	0.57
1:A:468:ASN:HD22	1:A:531:ARG:NH2	2.02	0.57
1:A:1249[A]:ARG:HH21	1:A:1249[A]:ARG:CG	2.17	0.57
5:F:505:ARG:O	5:F:505:ARG:HG2	2.03	0.57
5:F:586:GLY:CA	5:F:611:TRP:CZ2	2.88	0.57
5:F:825:ILE:HA	5:F:864:MET:HE1	1.85	0.57
1:A:529:CYS:SG	1:A:945:ILE:CG1	2.89	0.56
1:A:1244:ILE:CG2	1:A:1247:LEU:HD21	2.35	0.56
1:A:475:PHE:CE2	1:A:537:LYS:CE	2.70	0.56
4:E:206:ARG:HB3	4:E:206:ARG:CZ	2.33	0.56
5:F:638:ILE:HG21	5:F:644:GLN:HB3	1.87	0.56
1:A:542:TRP:HE3	1:A:542:TRP:N	2.04	0.56
4:E:19:GLY:N	4:E:191:LEU:HD13	2.14	0.56
1:A:1144:GLU:O	1:A:1148:HIS:ND1	2.30	0.56
1:A:1390:ASP:HB3	1:A:1393:ILE:HD12	1.86	0.56
5:F:597:GLN:HB2	5:F:768:LYS:HZ1	1.69	0.56
1:A:1339:ASP:O	1:A:1341:GLU:N	2.34	0.56
5:F:981:GLN:HG2	5:F:1038:GLU:HG2	1.87	0.56
5:F:515:PHE:HD1	5:F:623:ALA:O	1.89	0.56
1:A:252:ARG:HD2	1:A:1302:ARG:HH11	1.70	0.56
5:F:270:THR:HG22	5:F:392:GLY:HA3	1.87	0.56
1:A:843:PHE:CD2	1:A:871:LEU:HA	2.41	0.56
1:A:959:ASP:OD2	1:A:988:ARG:NH1	2.38	0.56
1:A:1099:ARG:O	1:A:1100:CYS:SG	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1389:ARG:CD	1:A:1391:TRP:CD2	2.73	0.56
1:A:454:HIS:HB2	1:A:998:ASP:OD1	2.05	0.56
5:F:64:GLU:O	5:F:67:GLN:NE2	2.38	0.55
1:A:1264:PHE:CE1	1:A:1267:LEU:CD2	2.90	0.55
5:F:452:TYR:N	5:F:452:TYR:CD1	2.73	0.55
1:A:445:ASN:HD21	1:A:534:ARG:HD3	1.71	0.55
10:A:1911:PC1:H322	10:A:1911:PC1:H262	1.89	0.55
5:F:389:PHE:N	5:F:389:PHE:CD1	2.73	0.55
5:F:497:GLU:O	5:F:501:ARG:HD3	2.05	0.55
5:F:1036:GLN:HE21	5:F:1037:ALA:N	1.97	0.55
1:A:1389:ARG:CG	1:A:1391:TRP:CE3	2.88	0.55
5:F:732:VAL:O	5:F:820:ASP:CB	2.48	0.55
1:A:1139:HIS:HD2	1:A:1142:GLN:HB3	1.69	0.55
1:A:1124:MET:HE2	1:A:1164:GLU:HB2	1.87	0.55
5:F:530:GLN:HG2	5:F:904:GLN:HE22	1.70	0.55
1:A:74:MET:HB3	1:A:78:ASP:HB3	1.88	0.55
1:A:206:MET:CE	1:A:317:LEU:HD12	2.34	0.55
1:A:1043:ILE:O	1:A:1047:ILE:HG13	2.07	0.55
5:F:518:ASP:O	5:F:520:ASN:N	2.40	0.55
1:A:1391:TRP:CE2	1:A:1396:PRO:HD2	2.42	0.55
1:A:1019:LEU:CD2	1:A:1045:PHE:CZ	2.90	0.54
1:A:1046:ILE:O	1:A:1050:ILE:HG12	2.07	0.54
4:E:15:CYS:O	4:E:191:LEU:HD11	2.07	0.54
5:F:510:PRO:HG3	5:F:762:TYR:CD1	2.42	0.54
5:F:647:TYR:HD1	5:F:713:GLY:CA	2.20	0.54
4:E:37:PRO:HA	4:E:174:ILE:HA	1.90	0.54
5:F:428:TYR:CD1	5:F:428:TYR:C	2.85	0.54
5:F:880:GLU:HA	5:F:1033:LEU:HD22	1.89	0.54
1:A:1046:ILE:HD13	10:A:1914:PC1:H381	1.90	0.54
1:A:513:LEU:HD23	1:A:527:LEU:HD11	1.90	0.54
1:A:216:GLU:OE2	1:A:1239:ARG:NH2	2.37	0.54
1:A:1262:LYS:CD	4:E:209:GLN:O	2.56	0.54
4:E:19:GLY:N	4:E:191:LEU:HD11	2.18	0.54
4:E:123:ILE:HG22	4:E:127:MET:HE2	1.89	0.54
4:E:206:ARG:HB3	4:E:206:ARG:NH1	2.23	0.54
1:A:820:ASP:OD2	1:A:829:ASN:ND2	2.40	0.54
1:A:1173:LYS:O	1:A:1175:ARG:N	2.40	0.54
5:F:247:ILE:HG22	5:F:247:ILE:O	2.08	0.54
1:A:957:CYS:SG	1:A:958:ASN:N	2.81	0.54
1:A:1043:ILE:CG2	10:A:1904:PC1:H291	2.37	0.54
1:A:1016:TRP:CG	1:A:1017:PRO:HD3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TRP:NE1	3:C:293:MET:HA	2.23	0.53
5:F:510:PRO:HG2	5:F:767:TYR:CD2	2.42	0.53
5:F:586:GLY:C	5:F:611:TRP:CZ2	2.87	0.53
5:F:634:ILE:HB	5:F:707:ARG:HH12	1.73	0.53
1:A:1244:ILE:O	1:A:1247:LEU:HD23	2.09	0.53
1:A:573:PHE:O	1:A:640:TYR:OH	2.25	0.53
1:A:942:PHE:CD2	1:A:1048:TYR:CD1	2.73	0.53
1:A:969:ARG:HB3	5:F:176:GLU:HG3	1.90	0.53
1:A:541:TYR:CD1	1:A:541:TYR:N	2.76	0.53
5:F:252:SER:OG	5:F:357:ASN:OD1	2.26	0.53
1:A:1264:PHE:CZ	1:A:1267:LEU:HD23	2.44	0.53
1:A:1334:TYR:CE1	1:A:1351:THR:CG2	2.92	0.53
5:F:452:TYR:N	5:F:452:TYR:HD1	2.05	0.53
5:F:669:TYR:CD1	5:F:670:CYS:CB	2.92	0.53
1:A:820:ASP:CG	1:A:829:ASN:HD21	2.17	0.53
5:F:1061:VAL:HG23	5:F:1062:CYS:N	2.20	0.53
1:A:333:LEU:HD11	1:A:1064:VAL:HG11	1.91	0.53
1:A:1101:TYR:H	1:A:1101:TYR:HD1	1.56	0.53
1:A:1337:LEU:HD12	1:A:1350:TYR:CE1	2.39	0.53
5:F:531:PRO:C	5:F:532:LYS:HG3	2.34	0.53
1:A:1101:TYR:CD1	1:A:1101:TYR:N	2.74	0.53
5:F:356:CYS:SG	5:F:357:ASN:N	2.76	0.53
5:F:55:GLY:HA3	5:F:718:LEU:HD11	1.91	0.52
1:A:542:TRP:N	1:A:542:TRP:CE3	2.76	0.52
5:F:478:LYS:O	5:F:480:ASN:CG	2.52	0.52
1:A:816:LEU:HD21	1:A:901:VAL:HG12	1.91	0.52
5:F:411:TYR:CE1	5:F:1074:CYS:CA	2.88	0.52
5:F:478:LYS:C	5:F:480:ASN:N	2.66	0.52
1:A:1014:GLU:OE2	1:A:1015:GLY:N	2.43	0.52
1:A:1015:GLY:CA	1:A:1326:GLN:NE2	2.55	0.52
5:F:669:TYR:HD1	5:F:670:CYS:CA	2.15	0.52
5:F:77:ALA:HA	5:F:624:LEU:CD2	2.38	0.52
5:F:515:PHE:CD1	5:F:623:ALA:O	2.63	0.52
5:F:515:PHE:CE2	5:F:563:PHE:CE1	2.88	0.52
1:A:953:LYS:HE2	1:A:1038:ARG:HH12	1.75	0.52
5:F:359:ILE:HD11	5:F:432:LEU:HD21	1.91	0.52
1:A:217:LEU:HD11	1:A:1237:LEU:HD11	1.91	0.52
1:A:276:ASP:O	1:A:277:ASN:CB	2.57	0.52
1:A:366:TYR:O	1:A:369:TRP:HB3	2.10	0.52
1:A:632:TYR:HB3	1:A:633:PRO:CD	2.39	0.52
5:F:243:ARG:NH1	5:F:243:ARG:HG3	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:303:VAL:O	5:F:323:ALA:HB1	2.10	0.52
5:F:321:LYS:O	5:F:325:ASN:ND2	2.43	0.52
5:F:733:LYS:NZ	5:F:793:SER:HA	2.25	0.52
5:F:805:ILE:O	5:F:807:GLY:N	2.38	0.52
1:A:1306:PHE:CD2	1:A:1315:LEU:HD13	2.45	0.52
4:E:7:PRO:HA	4:E:10:ARG:HB2	1.92	0.52
1:A:820:ASP:CB	1:A:821:PRO:C	2.83	0.51
5:F:1011:LEU:HD22	5:F:1016:LEU:HD12	1.92	0.51
1:A:1016:TRP:N	1:A:1017:PRO:CD	2.73	0.51
5:F:1007:HIS:NE2	5:F:1009:GLU:OE2	2.43	0.51
1:A:843:PHE:HE2	1:A:871:LEU:HA	1.68	0.51
5:F:309:LEU:HD12	5:F:353:ARG:CG	2.40	0.51
1:A:819:GLU:CG	1:A:897:ARG:HH21	2.24	0.51
1:A:843:PHE:HE2	1:A:871:LEU:N	2.09	0.51
1:A:1416:ARG:HB3	1:A:1460:THR:HB	1.91	0.51
5:F:102:LEU:HB3	5:F:490:MET:HE3	1.91	0.51
5:F:1008:VAL:HG22	5:F:1019:ILE:HG12	1.92	0.51
1:A:225:THR:HA	1:A:266:PRO:HB3	1.92	0.51
4:E:131:LYS:HB3	4:E:133:ARG:HE	1.76	0.51
5:F:398:ARG:NH1	5:F:414:GLU:OE2	2.43	0.51
5:F:510:PRO:HG3	5:F:762:TYR:CE1	2.46	0.51
1:A:468:ASN:HD21	1:A:531:ARG:HH21	1.59	0.51
5:F:669:TYR:CD1	5:F:670:CYS:HB2	2.46	0.51
1:A:1249[A]:ARG:NH2	1:A:1249[A]:ARG:HG2	2.24	0.51
4:E:19:GLY:H	4:E:191:LEU:HD13	1.70	0.51
5:F:198:ASN:HB2	5:F:208:GLN:HE22	1.76	0.51
5:F:894:VAL:HG11	5:F:993:PHE:CD2	2.44	0.51
1:A:287:GLN:NE2	1:A:621:TYR:OH	2.35	0.51
3:C:265:VAL:HG12	3:C:265:VAL:O	2.10	0.51
5:F:131:ALA:HB2	5:F:167:ALA:HB1	1.92	0.51
1:A:468:ASN:ND2	1:A:531:ARG:HH21	2.08	0.50
5:F:243:ARG:CG	5:F:243:ARG:NH1	2.73	0.50
1:A:974:VAL:HG21	1:A:986:ARG:HD2	1.93	0.50
1:A:1235:PHE:CE2	4:E:153:VAL:CG2	2.87	0.50
1:A:1244:ILE:HG23	1:A:1247:LEU:HD21	1.93	0.50
5:F:1052:GLN:O	5:F:1052:GLN:HG2	2.12	0.50
6:G:1:NAG:H61	6:G:2:NAG:C8	2.41	0.50
1:A:526:VAL:O	1:A:530:ILE:HG13	2.10	0.50
1:A:1337:LEU:HD11	1:A:1350:TYR:HE1	1.70	0.50
5:F:77:ALA:HA	5:F:624:LEU:HD21	1.93	0.50
5:F:993:PHE:HB2	5:F:1008:VAL:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:MET:HB2	10:A:1911:PC1:H352	1.92	0.50
5:F:245:TRP:O	5:F:465:THR:HG21	2.12	0.50
1:A:1418:LYS:HG3	1:A:1420:LEU:H	1.77	0.50
5:F:75:ASN:O	5:F:76:ASN:HB3	2.11	0.50
5:F:173:ASP:CB	5:F:422:ARG:HH22	2.25	0.50
5:F:1073:ASP:O	5:F:1074:CYS:C	2.54	0.50
1:A:57:ILE:HA	1:A:60:THR:HG22	1.93	0.50
1:A:529:CYS:HA	1:A:532:LEU:HD12	1.94	0.50
1:A:591:GLU:OE2	1:A:593:ARG:CZ	2.59	0.50
4:E:107:ALA:HA	4:E:110:ILE:HD12	1.93	0.50
5:F:638:ILE:HD11	5:F:710:LEU:HB2	1.94	0.49
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.95	0.49
1:A:915:LYS:HD3	1:A:915:LYS:H	1.75	0.49
1:A:170:LEU:HD12	1:A:173:LEU:HD13	1.95	0.49
10:A:1902:PC1:H221	10:A:1902:PC1:H321	1.94	0.49
5:F:438:LEU:HD12	5:F:1068:LEU:HD12	1.95	0.49
1:A:844:THR:O	1:A:847:ILE:HG13	2.12	0.49
1:A:993:ASN:O	1:A:995:PHE:N	2.39	0.49
1:A:1046:ILE:CD1	10:A:1914:PC1:C39	2.89	0.49
5:F:315[B]:ARG:HE	5:F:1049:MET:HE2	1.77	0.49
5:F:394:HIS:HD2	5:F:396:TYR:HB2	1.78	0.49
5:F:985:PHE:HZ	6:J:1:NAG:H61	1.77	0.49
5:F:389:PHE:N	5:F:389:PHE:HD1	2.10	0.49
5:F:482:LYS:HE3	5:F:485:LEU:HD12	1.93	0.49
5:F:584:GLU:O	5:F:613:PRO:HD3	2.12	0.49
5:F:153:ASP:OD1	5:F:160:GLN:CG	2.59	0.49
5:F:564:LEU:HD12	5:F:569:GLU:CB	2.43	0.49
5:F:744:THR:HG1	5:F:755:TRP:HZ3	1.60	0.49
1:A:49:GLU:O	1:A:50:TRP:O	2.31	0.49
1:A:206:MET:HE2	1:A:317:LEU:CD1	2.41	0.49
1:A:1060:PHE:CZ	1:A:1376:PHE:CZ	2.96	0.49
1:A:363:LEU:HD22	3:C:399:ARG:HD3	1.95	0.49
1:A:1334:TYR:CZ	1:A:1351:THR:HG23	2.47	0.49
5:F:417:SER:OG	5:F:418:ILE:N	2.46	0.49
5:F:513:TYR:OH	5:F:567:GLU:OE2	2.28	0.49
5:F:95:ARG:HD3	5:F:494:VAL:HG22	1.95	0.49
1:A:808:PHE:HE2	1:A:903:ARG:HH22	1.61	0.48
5:F:333:THR:HG21	5:F:335:TYR:CE2	2.47	0.48
5:F:564:LEU:CD1	5:F:569:GLU:CB	2.90	0.48
5:F:733:LYS:HD2	5:F:793:SER:O	2.13	0.48
1:A:842:VAL:O	1:A:845:VAL:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:333:THR:HG21	5:F:335:TYR:HE2	1.78	0.48
5:F:733:LYS:CD	5:F:793:SER:O	2.61	0.48
1:A:974:VAL:HG23	1:A:986:ARG:HG3	1.95	0.48
1:A:1293:ALA:HB2	1:A:1339:ASP:H	1.77	0.48
1:A:1318:ARG:HH21	1:A:1328:ILE:HD11	1.79	0.48
4:E:208:PRO:HG2	4:E:214:SER:CB	2.43	0.48
5:F:184:GLU:OE2	5:F:212:SER:OG	2.27	0.48
5:F:744:THR:HB	5:F:755:TRP:CH2	2.48	0.48
1:A:269:ASN:ND2	1:A:273:THR:OG1	2.42	0.48
5:F:1062:CYS:O	5:F:1063:PHE:HD1	1.88	0.48
1:A:510:GLU:OE2	1:A:531:ARG:CD	2.55	0.48
1:A:542:TRP:HE3	1:A:542:TRP:H	1.61	0.48
1:A:1081:LEU:HD22	1:A:1085:GLN:HE21	1.79	0.48
4:E:161:SER:HA	4:E:164:ARG:HD3	1.95	0.48
5:F:105:GLU:HG3	5:F:194:VAL:HG21	1.95	0.48
5:F:190:ALA:C	5:F:192:ASP:H	2.21	0.48
1:A:172:PRO:HB2	1:A:572:ILE:HD11	1.95	0.48
1:A:974:VAL:CG2	1:A:986:ARG:HG3	2.44	0.48
5:F:173:ASP:OD2	5:F:422:ARG:NH2	2.47	0.48
5:F:726:GLN:HB3	5:F:729:ILE:HD11	1.96	0.48
1:A:500:ASP:OD1	1:A:537:LYS:NZ	2.47	0.47
1:A:1258:TRP:NE1	4:E:208:PRO:HD2	2.29	0.47
1:A:1046:ILE:C	1:A:1049:ILE:HG22	2.37	0.47
4:E:207:MET:O	4:E:209:GLN:N	2.47	0.47
5:F:615:ASN:OD1	6:G:1:NAG:O5	2.32	0.47
1:A:1262:LYS:CG	4:E:209:GLN:O	2.62	0.47
1:A:1370:PHE:CD1	1:A:1370:PHE:C	2.91	0.47
4:E:19:GLY:HA2	4:E:191:LEU:HD12	1.87	0.47
5:F:732:VAL:HG23	5:F:733:LYS:H	1.74	0.47
1:A:539:THR:C	1:A:541:TYR:N	2.68	0.47
5:F:644:GLN:CA	5:F:647:TYR:HD2	2.12	0.47
1:A:534:ARG:O	1:A:537:LYS:HB2	2.14	0.47
1:A:594:ARG:NH2	1:A:1025:ASP:OD1	2.31	0.47
1:A:965:GLU:HA	1:A:990:TRP:CZ2	2.49	0.47
1:A:1390:ASP:HB3	1:A:1393:ILE:HD13	1.94	0.47
5:F:348:ASN:O	5:F:350:ASN:N	2.47	0.47
5:F:733:LYS:HZ3	5:F:793:SER:HA	1.79	0.47
5:F:509:CYS:C	5:F:511:ASN:N	2.73	0.47
1:A:433:VAL:O	1:A:437:LEU:N	2.44	0.47
1:A:813:SER:HA	1:A:816:LEU:HB3	1.96	0.47
1:A:1199:LEU:HD12	1:A:1232:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:ASP:OD2	1:A:1302:ARG:NH2	2.47	0.47
4:E:15:CYS:O	4:E:191:LEU:HD21	2.15	0.47
5:F:38:TRP:HE1	5:F:831:THR:HB	1.79	0.47
5:F:348:ASN:C	5:F:350:ASN:N	2.71	0.47
1:A:843:PHE:CE2	1:A:871:LEU:CB	2.98	0.47
5:F:531:PRO:C	5:F:532:LYS:CG	2.85	0.47
1:A:1067:THR:HG21	1:A:1377:VAL:HG13	1.97	0.47
1:A:1429:ILE:HG21	1:A:1433:LEU:HD12	1.96	0.46
5:F:302:ASP:OD1	5:F:341:PHE:CE2	2.67	0.46
5:F:598:ASP:O	5:F:599:GLU:HG3	2.14	0.46
5:F:669:TYR:HD1	5:F:670:CYS:CB	2.26	0.46
5:F:1068:LEU:N	5:F:1068:LEU:HD23	2.30	0.46
4:E:211:PRO:O	4:E:212:TRP:CD1	2.68	0.46
5:F:536:VAL:CG1	5:F:537:GLY:H	2.18	0.46
5:F:563:PHE:HB3	5:F:577:ARG:HD3	1.97	0.46
1:A:165:ARG:HG3	1:A:165:ARG:HH11	1.80	0.46
1:A:533:LEU:HG	1:A:533:LEU:O	2.14	0.46
1:A:1154:ASN:O	1:A:1158:THR:HG23	2.15	0.46
5:F:297:ASN:HD21	5:F:331:GLY:CA	2.21	0.46
5:F:656:PHE:O	5:F:660:GLY:HA2	2.14	0.46
1:A:213:ILE:HG13	1:A:1240:VAL:HG11	1.97	0.46
5:F:159:ARG:NH2	5:F:224:PRO:O	2.49	0.46
5:F:219:TYR:O	5:F:219:TYR:CD2	2.68	0.46
1:A:332:VAL:HB	1:A:657:LEU:HD11	1.97	0.46
1:A:632:TYR:CD1	1:A:632:TYR:C	2.92	0.46
5:F:106:ALA:HB2	5:F:191:LEU:HD21	1.97	0.46
5:F:563:PHE:HD2	5:F:577:ARG:HD3	1.80	0.46
1:A:121:GLY:HA3	1:A:174:ARG:NH2	2.31	0.46
1:A:912[B]:LYS:HA	1:A:915:LYS:HE3	1.97	0.46
1:A:1390:ASP:C	1:A:1392:SER:N	2.74	0.46
1:A:536:PHE:O	1:A:539:THR:OG1	2.30	0.46
5:F:518:ASP:O	5:F:521:GLY:N	2.39	0.46
5:F:795:ILE:O	5:F:819:ILE:N	2.49	0.46
1:A:911:ALA:O	1:A:915:LYS:CE	2.63	0.46
1:A:1016:TRP:CZ3	1:A:1020:LEU:HD23	2.51	0.46
1:A:823:ARG:CG	1:A:823:ARG:NH2	2.73	0.46
5:F:30:PRO:CG	5:F:1020:MET:CE	2.79	0.46
5:F:979:THR:HB	5:F:1038:GLU:HB3	1.98	0.46
10:A:1915:PC1:H321	10:A:1915:PC1:H31	1.71	0.45
5:F:458:LEU:HD23	5:F:461:VAL:HG11	1.97	0.45
5:F:445:GLN:O	5:F:466:LEU:CD1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:207:MET:C	4:E:209:GLN:N	2.75	0.45
1:A:1305:ASN:HD22	1:A:1311:GLN:CG	2.28	0.45
5:F:242:ARG:HA	5:F:247:ILE:HD11	1.99	0.45
1:A:614:GLU:HG3	1:A:1017:PRO:HG2	1.99	0.45
1:A:877:ALA:O	1:A:881:ILE:N	2.46	0.45
1:A:903:ARG:CB	1:A:904:PRO:HD3	2.42	0.45
1:A:1016:TRP:CZ3	1:A:1020:LEU:CD2	3.00	0.45
5:F:586:GLY:O	5:F:611:TRP:CE3	2.69	0.45
1:A:369:TRP:CE3	3:C:293:MET:HE3	2.52	0.45
5:F:598:ASP:C	5:F:599:GLU:CG	2.85	0.45
5:F:207:TRP:HE1	5:F:458:LEU:HD22	1.82	0.45
1:A:72:LEU:HD22	1:A:74:MET:HE2	1.99	0.45
1:A:1261:ILE:HG22	4:E:207:MET:SD	2.57	0.45
4:E:211:PRO:C	4:E:212:TRP:CD1	2.95	0.45
1:A:276:ASP:O	1:A:277:ASN:HB3	2.16	0.45
1:A:1281:TYR:O	1:A:1360:TYR:OH	2.33	0.45
5:F:47:VAL:HG13	5:F:776:TYR:HE2	1.81	0.45
5:F:587:GLU:HB3	5:F:610:THR:HG22	1.99	0.45
5:F:733:LYS:HB3	5:F:818:LYS:O	2.17	0.45
5:F:1068:LEU:HB2	5:F:1069:GLU:H	1.66	0.45
1:A:295:THR:HG22	1:A:1323:GLU:OE2	2.17	0.44
1:A:1334:TYR:O	1:A:1334:TYR:CG	2.70	0.44
1:A:376:MET:SD	1:A:422:ARG:NH1	2.90	0.44
4:E:206:ARG:C	4:E:207:MET:O	2.58	0.44
1:A:1254:ARG:HG3	1:A:1255:THR:N	2.32	0.44
5:F:509:CYS:C	5:F:511:ASN:H	2.25	0.44
5:F:900:SER:OG	5:F:901:TYR:N	2.50	0.44
1:A:210:TYR:O	1:A:313:TYR:OH	2.35	0.44
1:A:820:ASP:N	1:A:821:PRO:CA	2.79	0.44
4:E:207:MET:C	4:E:209:GLN:H	2.24	0.44
1:A:305:ILE:HG23	10:A:1902:PC1:H121	1.99	0.44
1:A:896:LEU:HD23	1:A:899:LEU:HD12	2.00	0.44
4:E:19:GLY:H	4:E:191:LEU:HD11	1.77	0.44
5:F:96:SER:O	5:F:99:LEU:HB2	2.18	0.44
1:A:587:PHE:HB3	1:A:593:ARG:HH21	1.82	0.44
1:A:1094:LYS:HD3	4:E:212:TRP:CH2	2.53	0.44
1:A:1244:ILE:O	1:A:1247:LEU:CD2	2.65	0.44
5:F:894:VAL:HA	5:F:895:TYR:HA	1.68	0.44
1:A:1262:LYS:CE	4:E:209:GLN:OE1	2.65	0.44
5:F:147:ILE:HG22	5:F:149:PRO:HD3	1.99	0.44
1:A:468:ASN:ND2	1:A:531:ARG:CZ	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:PHE:CZ	1:A:537:LYS:CE	2.99	0.44
1:A:1120:PHE:HZ	1:A:1167:LEU:HD12	1.83	0.44
1:A:1121:GLU:CG	1:A:1249[A]:ARG:HH22	2.30	0.44
4:E:209:GLN:HG3	4:E:210:ASN:N	2.33	0.44
5:F:564:LEU:HD12	5:F:569:GLU:HB2	1.99	0.44
5:F:738:VAL:HG13	5:F:744:THR:HG22	2.00	0.44
5:F:892:ILE:O	5:F:893:SER:HB3	2.18	0.44
1:A:902:LEU:HD12	1:A:905:LEU:HD12	1.95	0.43
1:A:1046:ILE:HA	1:A:1049:ILE:HG22	2.00	0.43
1:A:1334:TYR:O	1:A:1334:TYR:CD1	2.70	0.43
3:C:398:GLN:HG2	3:C:402:LYS:HD2	2.00	0.43
5:F:428:TYR:CD1	5:F:428:TYR:O	2.70	0.43
5:F:508:LEU:N	5:F:508:LEU:HD23	2.33	0.43
5:F:515:PHE:CD1	5:F:515:PHE:C	2.93	0.43
1:A:423:TRP:HA	1:A:426:HIS:HD2	1.83	0.43
5:F:168:VAL:HG22	5:F:218:ARG:HG2	2.00	0.43
5:F:594:VAL:HG21	5:F:607:ARG:HH21	1.84	0.43
5:F:1068:LEU:O	5:F:1070:ASP:N	2.52	0.43
1:A:468:ASN:HD21	1:A:531:ARG:CD	2.30	0.43
5:F:509:CYS:O	5:F:511:ASN:N	2.52	0.43
5:F:860:GLY:O	5:F:878:PHE:N	2.44	0.43
1:A:225:THR:HG21	1:A:227:TYR:CZ	2.53	0.43
1:A:1016:TRP:HZ3	1:A:1020:LEU:CD2	2.31	0.43
1:A:307:ASN:OD1	1:A:307:ASN:N	2.46	0.43
1:A:540:LYS:HE3	1:A:540:LYS:HB2	1.74	0.43
1:A:846:GLU:HG3	1:A:847:ILE:N	2.33	0.43
5:F:656:PHE:CD1	5:F:660:GLY:O	2.71	0.43
1:A:794[B]:ARG:HE	1:A:794[B]:ARG:HB3	1.54	0.43
1:A:1044:PHE:HB2	10:A:1904:PC1:H2A1	2.00	0.43
5:F:298:SER:OG	5:F:299:ASN:N	2.51	0.43
5:F:598:ASP:N	5:F:598:ASP:OD1	2.50	0.43
1:A:1263:SER:O	1:A:1265:GLN:N	2.41	0.43
1:A:1403:LYS:HA	1:A:1406:TRP:HD1	1.83	0.43
2:B:169:ARG:NH1	2:B:173:GLU:OE1	2.51	0.43
4:E:17:LEU:HD23	4:E:20:ILE:HD12	2.00	0.43
1:A:964:THR:OG1	1:A:965:GLU:N	2.50	0.43
1:A:1384:PHE:CE1	1:A:1388:THR:HG21	2.53	0.43
5:F:411:TYR:HA	5:F:1074:CYS:HB2	1.99	0.43
1:A:1321:THR:HG22	10:A:1909:PC1:H3D2	2.00	0.43
1:A:1331:ALA:O	1:A:1336:LYS:HG3	2.19	0.43
1:A:369:TRP:CD1	1:A:369:TRP:C	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:712:ALA:HA	5:F:715:THR:HG22	2.01	0.43
1:A:165:ARG:O	1:A:168:ARG:HG2	2.19	0.42
1:A:172:PRO:O	1:A:175:LEU:HB3	2.19	0.42
1:A:252:ARG:HD2	1:A:1302:ARG:NH1	2.33	0.42
1:A:449:ILE:HD12	1:A:449:ILE:HA	1.90	0.42
1:A:1244:ILE:HG22	1:A:1247:LEU:HD21	2.00	0.42
5:F:661:TYR:HD2	5:F:663:PHE:CZ	2.13	0.42
5:F:790:ALA:N	5:F:793:SER:OG	2.52	0.42
1:A:1091:TYR:CZ	1:A:1399:LEU:HB3	2.54	0.42
1:A:1104:LYS:HG3	1:A:1105:ASN:H	1.84	0.42
1:A:1389:ARG:HE	1:A:1391:TRP:CB	2.29	0.42
10:A:1912:PC1:H142	10:A:1912:PC1:H112	1.86	0.42
5:F:989:ASP:HB3	5:F:990:SER:H	1.69	0.42
1:A:370:ILE:HG21	3:C:404:ARG:NH1	2.34	0.42
5:F:309:LEU:HD12	5:F:353:ARG:HG2	2.00	0.42
1:A:1127:LEU:HD13	1:A:1160:ILE:HG21	2.00	0.42
5:F:381:ASP:HB3	5:F:383:LYS:HE3	2.00	0.42
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.33	0.42
1:A:559:ILE:HG22	1:A:563:LEU:HB2	2.01	0.42
1:A:614:GLU:HG3	1:A:1017:PRO:CG	2.49	0.42
1:A:1195:ILE:CD1	4:E:113:PHE:CE2	3.03	0.42
5:F:52:THR:O	5:F:722:TYR:OH	2.30	0.42
5:F:784:ASN:O	5:F:787:GLY:N	2.50	0.42
1:A:1293:ALA:O	1:A:1295:VAL:N	2.52	0.42
4:E:55:ARG:HD2	4:E:80:CYS:HB3	2.01	0.42
1:A:1249[A]:ARG:CG	1:A:1249[A]:ARG:NH2	2.75	0.42
5:F:248:GLN:HE21	5:F:248:GLN:HB3	1.66	0.42
5:F:515:PHE:HE2	5:F:563:PHE:HE1	1.59	0.42
1:A:902:LEU:O	1:A:905:LEU:HB2	2.20	0.42
1:A:1132:THR:HG21	10:A:1912:PC1:H3A1	2.01	0.42
5:F:805:ILE:HB	5:F:808:LYS:HE2	2.02	0.42
5:F:886:MET:SD	5:F:895:TYR:CE1	3.13	0.42
5:F:496:LEU:HD23	5:F:499:ILE:HD12	2.02	0.42
1:A:1020:LEU:HD13	1:A:1045:PHE:HD2	1.85	0.42
1:A:632:TYR:CB	1:A:633:PRO:CD	2.98	0.41
1:A:945:ILE:HD11	10:A:1904:PC1:H361	2.02	0.41
1:A:1262:LYS:HG2	4:E:209:GLN:HA	2.01	0.41
1:A:1304:ASN:HD22	1:A:1304:ASN:HA	1.60	0.41
5:F:586:GLY:CA	5:F:611:TRP:CE2	3.02	0.41
5:F:594:VAL:HG21	5:F:607:ARG:HE	1.85	0.41
5:F:856:LEU:HD12	5:F:856:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:1061:VAL:CG2	5:F:1062:CYS:H	2.19	0.41
1:A:1265:GLN:HE21	1:A:1265:GLN:HB3	1.65	0.41
1:A:1389:ARG:HH21	1:A:1389:ARG:HG2	1.84	0.41
5:F:1073:ASP:O	5:F:1074:CYS:O	2.38	0.41
1:A:1049:ILE:HG23	1:A:1050:ILE:N	2.34	0.41
5:F:878:PHE:HB3	5:F:886:MET:HE3	2.01	0.41
1:A:265:TRP:CZ2	1:A:271:GLY:HA2	2.52	0.41
1:A:1096:ARG:HB3	1:A:1097:PRO:HD2	2.02	0.41
1:A:1102:ILE:HG13	1:A:1411:PRO:HB2	2.02	0.41
3:C:282:PRO:HA	3:C:389:ILE:O	2.21	0.41
5:F:76:ASN:HD22	5:F:79:GLN:HB2	1.84	0.41
5:F:413:TYR:OH	5:F:428:TYR:HA	2.20	0.41
5:F:649:GLU:C	5:F:649:GLU:CD	2.88	0.41
5:F:767:TYR:OH	5:F:812:PRO:O	2.35	0.41
5:F:769:ARG:HH22	5:F:858:ASP:HB3	1.86	0.41
1:A:49:GLU:C	1:A:50:TRP:O	2.63	0.41
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.92	0.41
1:A:526:VAL:HG22	10:A:1904:PC1:H331	2.02	0.41
5:F:509:CYS:HB2	5:F:630:SER:HB3	2.03	0.41
1:A:999:ASN:HB2	1:A:1002:SER:H	1.86	0.41
1:A:1052:ILE:HD13	1:A:1052:ILE:HA	1.90	0.41
10:A:1903:PC1:H2E2	10:A:1903:PC1:H3C2	2.03	0.41
5:F:55:GLY:O	5:F:59:LEU:N	2.46	0.41
5:F:190:ALA:C	5:F:192:ASP:N	2.79	0.41
5:F:382:LYS:NZ	5:F:407:GLU:HG2	2.35	0.41
5:F:681:GLU:O	5:F:685:ASN:ND2	2.54	0.41
5:F:894:VAL:CB	5:F:993:PHE:HE2	2.29	0.41
1:A:113:HIS:O	1:A:119:ARG:NE	2.36	0.41
1:A:1389:ARG:NE	1:A:1391:TRP:HB2	2.29	0.41
10:A:1909:PC1:H3C2	10:A:1909:PC1:H391	1.74	0.41
5:F:243:ARG:HH11	5:F:243:ARG:HG3	1.84	0.41
5:F:303:VAL:O	5:F:303:VAL:HG13	2.21	0.41
5:F:315[B]:ARG:HH21	5:F:1049:MET:HE2	1.76	0.41
1:A:189:ILE:HG13	1:A:654:ASN:HD22	1.85	0.41
1:A:248:THR:HG22	1:A:249:GLY:H	1.86	0.41
1:A:369:TRP:O	1:A:369:TRP:CD1	2.71	0.41
1:A:591:GLU:CD	1:A:593:ARG:HH12	2.25	0.41
1:A:604:LEU:HA	1:A:604:LEU:HD12	1.89	0.41
1:A:794[B]:ARG:NH2	1:A:795:ILE:HD11	2.36	0.41
1:A:821:PRO:HG3	1:A:1286:MET:CG	2.42	0.41
1:A:965:GLU:HA	1:A:990:TRP:HZ2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1043:ILE:CG1	1:A:1047:ILE:HD11	2.37	0.41
10:A:1912:PC1:H231	10:A:1912:PC1:H261	1.53	0.41
5:F:736:PHE:CE1	5:F:796:MET:SD	3.14	0.41
4:E:113:PHE:HD1	4:E:113:PHE:HA	1.69	0.41
5:F:436:MET:HE2	5:F:436:MET:HB3	1.89	0.40
1:A:292:GLU:CD	1:A:292:GLU:C	2.89	0.40
1:A:578:MET:HE1	1:A:600:PHE:HD1	1.87	0.40
1:A:794[A]:ARG:NH1	1:A:798:ALA:CB	2.84	0.40
1:A:1201:GLU:O	1:A:1204:THR:OG1	2.37	0.40
1:A:1391:TRP:CD1	1:A:1397:HIS:CD2	2.98	0.40
5:F:628:THR:HA	5:F:631:PHE:HE2	1.86	0.40
1:A:656:PHE:CE1	1:A:1060:PHE:HD2	2.39	0.40
1:A:1057:MET:HE2	10:A:1906:PC1:H2G1	2.03	0.40
1:A:1122:TYR:HD1	1:A:1122:TYR:HA	1.77	0.40
1:A:1391:TRP:CZ2	1:A:1396:PRO:CD	3.02	0.40
3:C:388:TYR:HB2	3:C:430:PHE:CD1	2.56	0.40
5:F:530:GLN:CG	5:F:904:GLN:HE22	2.34	0.40
5:F:895:TYR:CD1	5:F:895:TYR:N	2.90	0.40
1:A:299:TYR:O	1:A:303:ASP:HB2	2.22	0.40
1:A:369:TRP:CD1	3:C:293:MET:HA	2.56	0.40
1:A:611:LEU:HD12	1:A:611:LEU:HA	1.86	0.40
4:E:15:CYS:O	4:E:191:LEU:CD1	2.70	0.40
5:F:451:VAL:HG23	5:F:559:VAL:O	2.20	0.40
5:F:584:GLU:O	5:F:613:PRO:CD	2.69	0.40
1:A:1249[B]:ARG:HA	1:A:1249[B]:ARG:HD2	1.97	0.40
1:A:1441:HIS:HB3	1:A:1443:VAL:N	2.36	0.40
5:F:1002:CYS:SG	5:F:1026:THR:OG1	2.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1268/1873 (68%)	1103 (87%)	143 (11%)	22 (2%)	7	35
2	B	98/106 (92%)	90 (92%)	8 (8%)	0	100	100
3	C	174/199 (87%)	171 (98%)	3 (2%)	0	100	100
4	E	156/222 (70%)	142 (91%)	12 (8%)	2 (1%)	9	39
5	F	929/1106 (84%)	764 (82%)	137 (15%)	28 (3%)	3	25
All	All	2625/3506 (75%)	2270 (86%)	303 (12%)	52 (2%)	8	32

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	977	ASP
1	A	1174	ALA
1	A	1391	TRP
1	A	1441	HIS
5	F	77	ALA
5	F	303	VAL
5	F	351	VAL
5	F	352	SER
5	F	451	VAL
5	F	478	LYS
5	F	479	THR
5	F	536	VAL
5	F	598	ASP
5	F	785	LYS
5	F	806	GLN
5	F	1061	VAL
1	A	80	ASN
1	A	1440	PRO
4	E	209	GLN
5	F	732	VAL
5	F	733	LYS
5	F	1068	LEU
1	A	819	GLU
1	A	1344	TYR
1	A	1354	THR
5	F	297	ASN
5	F	349	TYR
5	F	353	ARG
5	F	531	PRO
5	F	786	SER

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Mol	Chain	Res	Type
1	A	994	ASP
1	A	1138	GLN
1	A	1333	SER
1	A	1355	ASN
5	F	175	TYR
5	F	313	ASN
5	F	734	ALA
5	F	1069	GLU
1	A	820	ASP
1	A	903	ARG
1	A	1323	GLU
4	E	212	TRP
1	A	542	TRP
1	A	1294	LEU
5	F	532	LYS
5	F	894	VAL
5	F	1062	CYS
5	F	519	PRO
1	A	457	PRO
1	A	252	ARG
1	A	630	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	1073/1628 (66%)	1022 (95%)	51 (5%)	23	50
2	B	59/91 (65%)	56 (95%)	3 (5%)	21	49
3	C	143/179 (80%)	142 (99%)	1 (1%)	76	78
4	E	141/192 (73%)	134 (95%)	7 (5%)	22	49
5	F	837/974 (86%)	794 (95%)	43 (5%)	21	49
All	All	2253/3064 (74%)	2148 (95%)	105 (5%)	26	50

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	174	ARG
1	A	206	MET
1	A	221	LYS
1	A	224	LYS
1	A	262	ARG
1	A	276	ASP
1	A	277	ASN
1	A	327	ASN
1	A	422	ARG
1	A	525	SER
1	A	529	CYS
1	A	531	ARG
1	A	540	LYS
1	A	541	TYR
1	A	542	TRP
1	A	597	PHE
1	A	643	ILE
1	A	649	ASN
1	A	794[A]	ARG
1	A	794[B]	ARG
1	A	800	TRP
1	A	822	ILE
1	A	823	ARG
1	A	846	GLU
1	A	915	LYS
1	A	926	ARG
1	A	930	ASN
1	A	954	PHE
1	A	982	GLN
1	A	986	ARG
1	A	1020	LEU
1	A	1101	TYR
1	A	1120	PHE
1	A	1121	GLU
1	A	1122	TYR
1	A	1199	LEU
1	A	1229	ARG
1	A	1239	ARG
1	A	1247	LEU
1	A	1249[A]	ARG
1	A	1249[B]	ARG
1	A	1262	LYS

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Mol	Chain	Res	Type
1	A	1264	PHE
1	A	1265	GLN
1	A	1276	MET
1	A	1304	ASN
1	A	1329	LEU
1	A	1376	PHE
1	A	1380	ILE
1	A	1388	THR
2	B	115	PRO
2	B	167	SER
2	B	170	LEU
3	C	299	ASP
4	E	10	ARG
4	E	15	CYS
4	E	113	PHE
4	E	191	LEU
4	E	206	ARG
4	E	207	MET
4	E	212	TRP
5	F	95	ARG
5	F	97	LYS
5	F	243	ARG
5	F	299	ASN
5	F	311	GLN
5	F	315[A]	ARG
5	F	315[B]	ARG
5	F	333	THR
5	F	348	ASN
5	F	353	ARG
5	F	389	PHE
5	F	428	TYR
5	F	447	GLN
5	F	452	TYR
5	F	478	LYS
5	F	501	ARG
5	F	508	LEU
5	F	509	CYS
5	F	515	PHE
5	F	528	ASN
5	F	529	LEU
5	F	532	LYS
5	F	544	ARG

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Mol	Chain	Res	Type
5	F	564	LEU
5	F	591	ARG
5	F	599	GLU
5	F	615	ASN
5	F	733	LYS
5	F	755	TRP
5	F	796	MET
5	F	895	TYR
5	F	989	ASP
5	F	991	LYS
5	F	1020	MET
5	F	1032	ARG
5	F	1036	GLN
5	F	1049	MET
5	F	1052	GLN
5	F	1062	CYS
5	F	1068	LEU
5	F	1070	ASP
5	F	1071	TYR
5	F	1072	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	426	HIS
1	A	445	ASN
1	A	456	GLN
1	A	468	ASN
1	A	579	GLN
1	A	859	HIS
1	A	916	HIS
1	A	948	GLN
1	A	1036	ASN
1	A	1071	GLN
1	A	1085	GLN
1	A	1139	HIS
1	A	1154	ASN
1	A	1265	GLN
1	A	1304	ASN
1	A	1305	ASN
1	A	1311	GLN

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Mol	Chain	Res	Type
1	A	1326	GLN
1	A	1397	HIS
1	A	1456	ASN
3	C	398	GLN
4	E	209	GLN
5	F	76	ASN
5	F	311	GLN
5	F	313	ASN
5	F	316	ASN
5	F	325	ASN
5	F	348	ASN
5	F	484	GLN
5	F	511	ASN
5	F	556	GLN
5	F	679	ASN
5	F	806	GLN
5	F	888	HIS
5	F	1036	GLN
5	F	1052	GLN
5	F	1066	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ETA	F	1075	5	3,3,3	0.45	0	2,2,2	0.51	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
5	ETA	F	1075	5	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1075	ETA	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1075	ETA	1	0

5.5 Carbohydrates

17 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	$\# Z > 2$
6	NAG	D	1	5,6	14,14,15	0.67	1 (7%)	17,19,21	0.97	1 (5%)
6	NAG	D	2	6	14,14,15	0.47	0	17,19,21	0.44	0
6	NAG	G	1	5,6	14,14,15	0.29	0	17,19,21	0.56	0
6	NAG	G	2	6	14,14,15	0.30	0	17,19,21	0.56	0
7	NAG	H	1	5,7	14,14,15	0.64	0	17,19,21	0.59	0
7	NAG	H	2	7	14,14,15	0.26	0	17,19,21	0.82	1 (5%)
7	BMA	H	3	7	11,11,12	0.85	0	15,15,17	0.78	0
7	NAG	I	1	5,7	14,14,15	0.30	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	I	2	7	14,14,15	0.33	0	17,19,21	0.58	0
7	BMA	I	3	7	11,11,12	0.59	0	15,15,17	0.91	1 (6%)
6	NAG	J	1	5,6	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	J	2	6	14,14,15	0.27	0	17,19,21	0.52	0
6	NAG	K	1	5,6	14,14,15	0.56	0	17,19,21	0.96	1 (5%)
6	NAG	K	2	6	14,14,15	0.62	0	17,19,21	1.07	1 (5%)
8	NAG	L	1	5,8	14,14,15	0.35	0	17,19,21	0.65	0
8	NAG	L	2	8	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
8	NAG	L	3	8	14,14,15	0.46	0	17,19,21	0.69	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	1	5,6	-	4/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
7	NAG	H	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	BMA	H	3	7	-	0/2/19/22	0/1/1/1
7	NAG	I	1	5,7	-	2/6/23/26	0/1/1/1
7	NAG	I	2	7	-	2/6/23/26	0/1/1/1
7	BMA	I	3	7	-	2/2/19/22	0/1/1/1
6	NAG	J	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	NAG	K	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1
8	NAG	L	1	5,8	-	1/6/23/26	0/1/1/1
8	NAG	L	2	8	-	2/6/23/26	0/1/1/1
8	NAG	L	3	8	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1	NAG	C1-C2	2.34	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	K	1	NAG	C1-O5-C5	3.43	116.79	112.19
6	K	2	NAG	C2-N2-C7	3.22	127.21	122.90
6	D	1	NAG	C2-N2-C7	2.95	126.85	122.90
8	L	2	NAG	C1-O5-C5	2.93	116.11	112.19
7	H	2	NAG	C1-O5-C5	2.70	115.80	112.19
8	L	3	NAG	C1-O5-C5	2.37	115.36	112.19
7	I	3	BMA	C1-O5-C5	2.26	115.21	112.19

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	3	NAG	O5-C5-C6-O6
8	L	2	NAG	O5-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
7	H	2	NAG	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
8	L	2	NAG	C4-C5-C6-O6
7	H	1	NAG	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
8	L	3	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
7	I	2	NAG	C4-C5-C6-O6
6	G	1	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
7	H	1	NAG	C4-C5-C6-O6
6	G	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C3-C2-N2-C7
6	K	2	NAG	O5-C5-C6-O6

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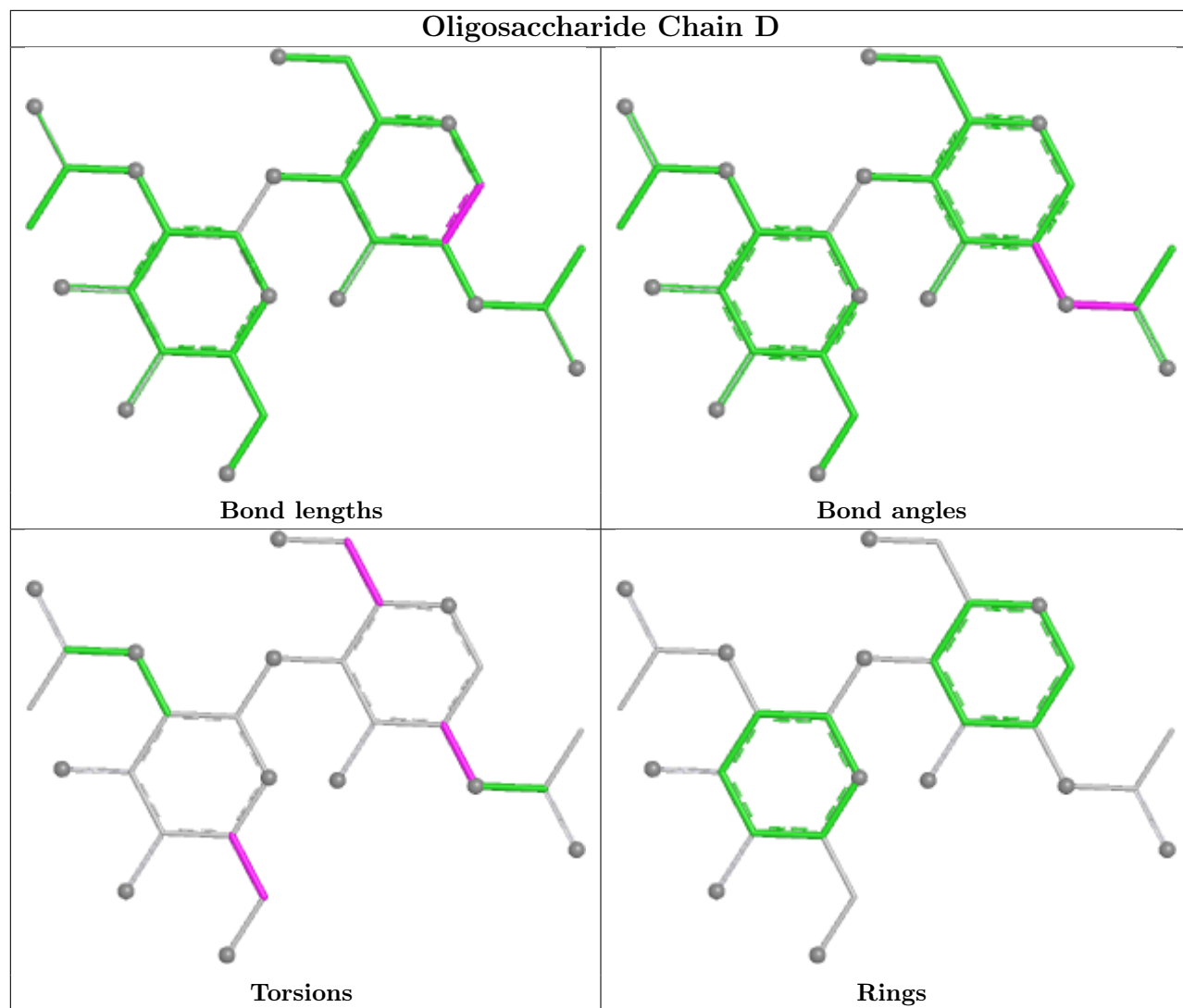
Mol	Chain	Res	Type	Atoms
8	L	1	NAG	C4-C5-C6-O6
6	D	1	NAG	C1-C2-N2-C7
6	J	1	NAG	C1-C2-N2-C7
6	K	2	NAG	C1-C2-N2-C7
6	D	1	NAG	C3-C2-N2-C7
6	G	1	NAG	C4-C5-C6-O6
6	G	2	NAG	C8-C7-N2-C2
6	G	2	NAG	O7-C7-N2-C2

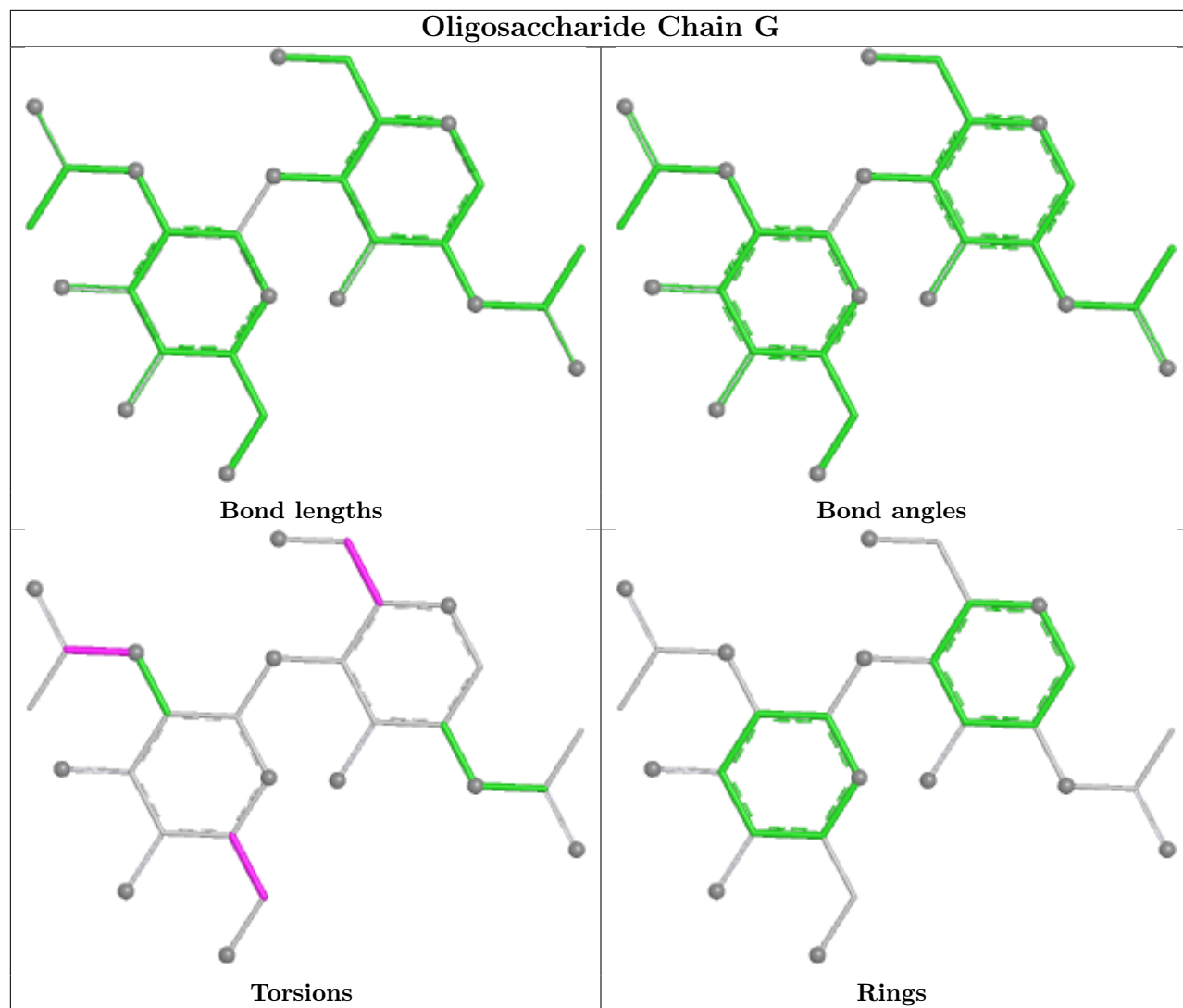
There are no ring outliers.

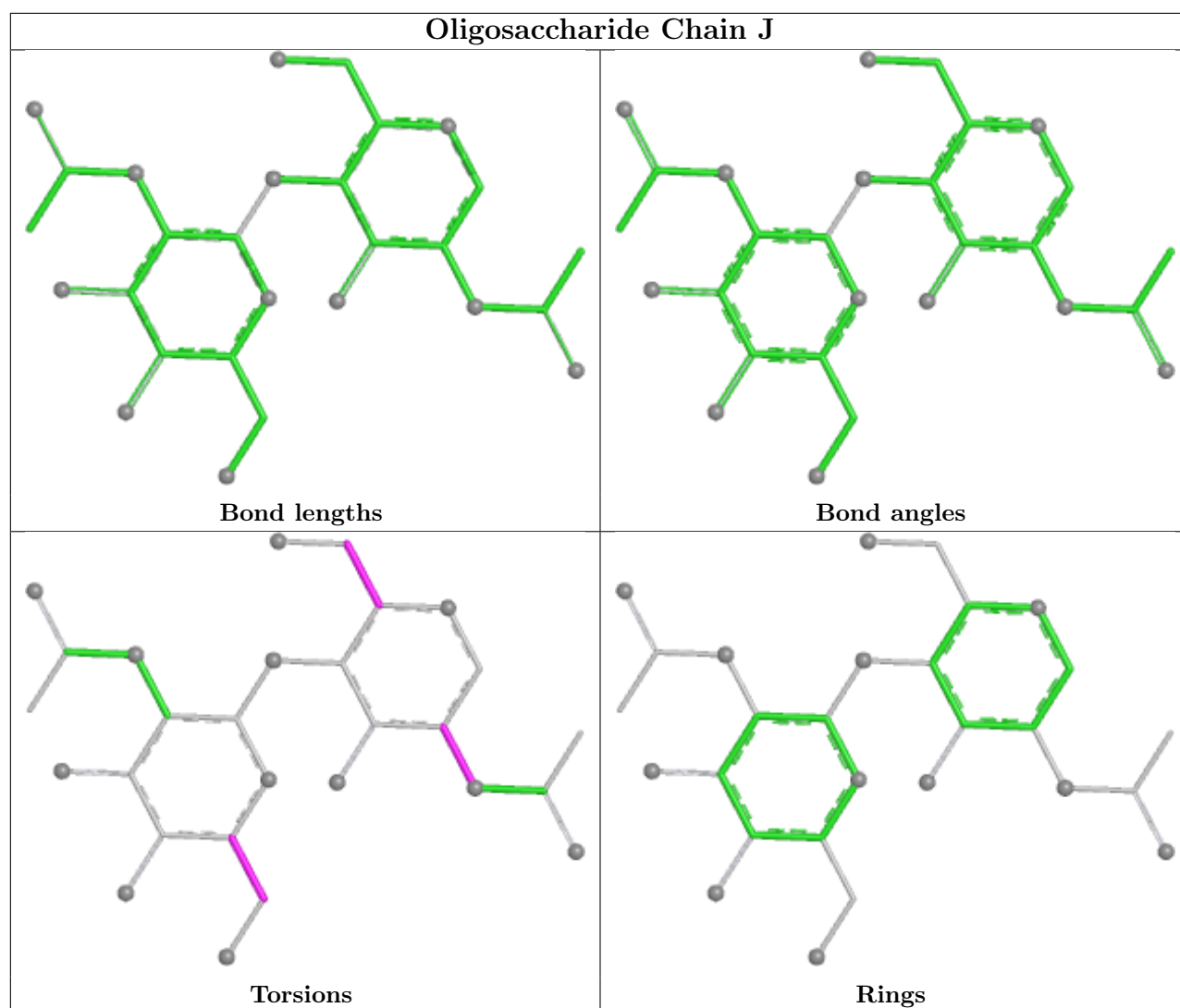
3 monomers are involved in 6 short contacts:

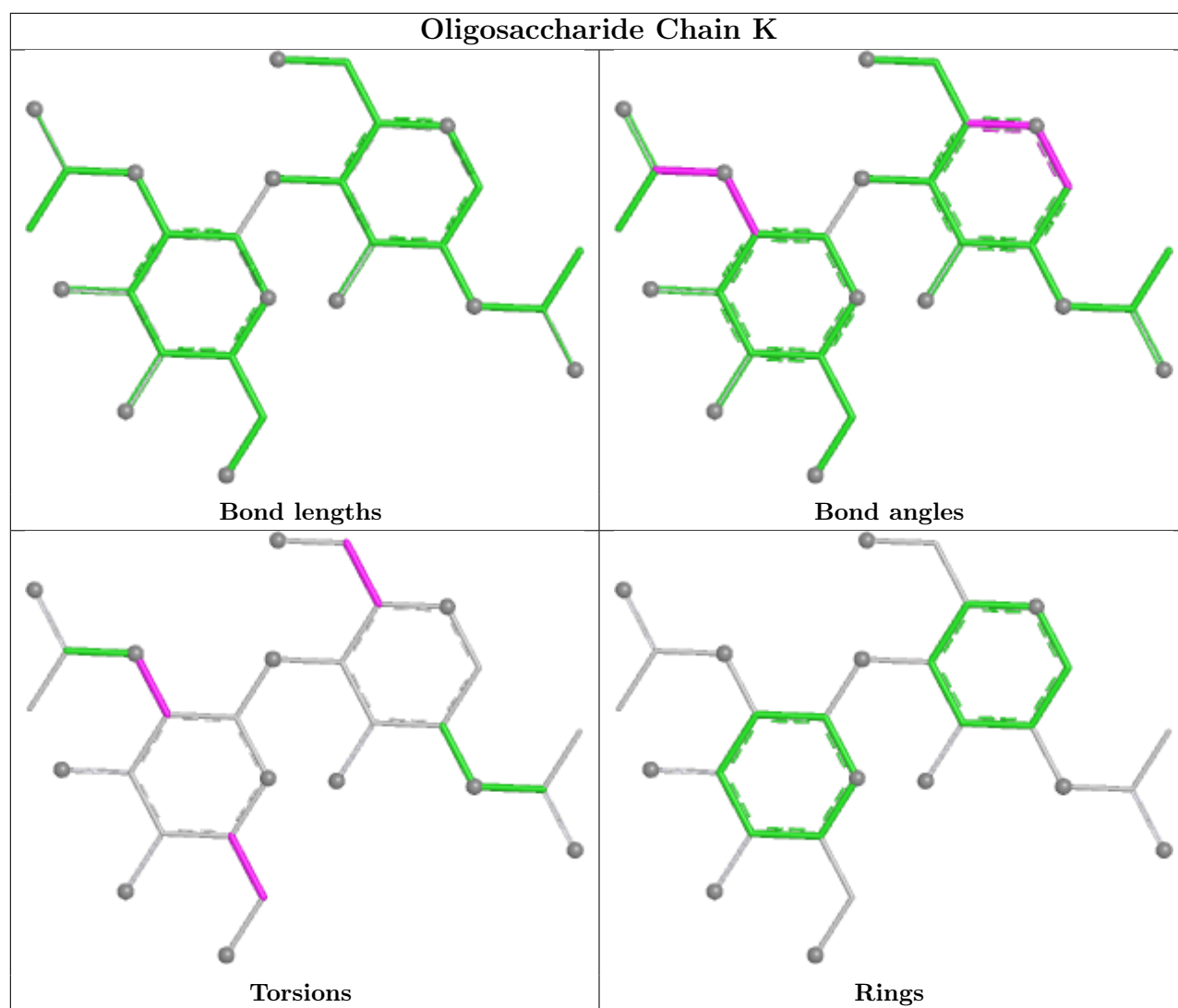
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	2	NAG	4	0
6	J	1	NAG	1	0
6	G	1	NAG	5	0

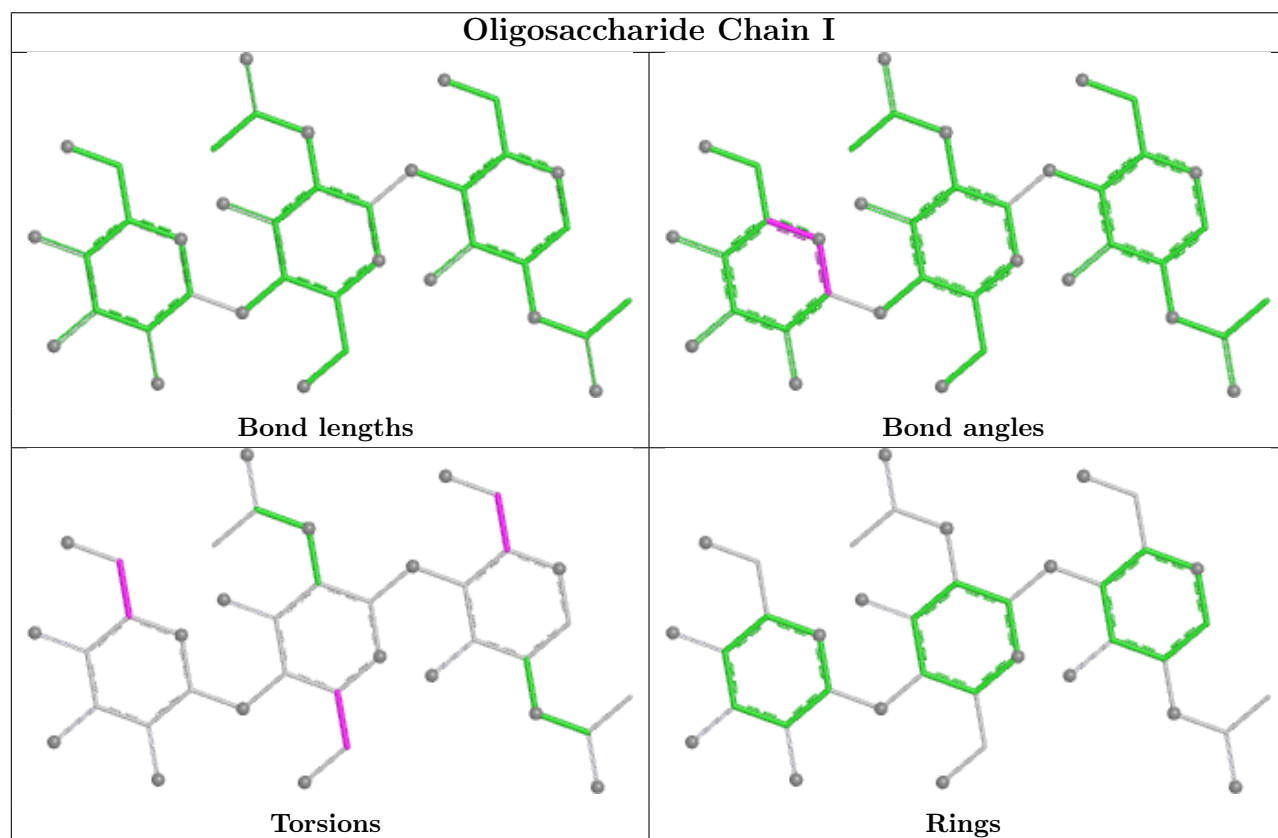
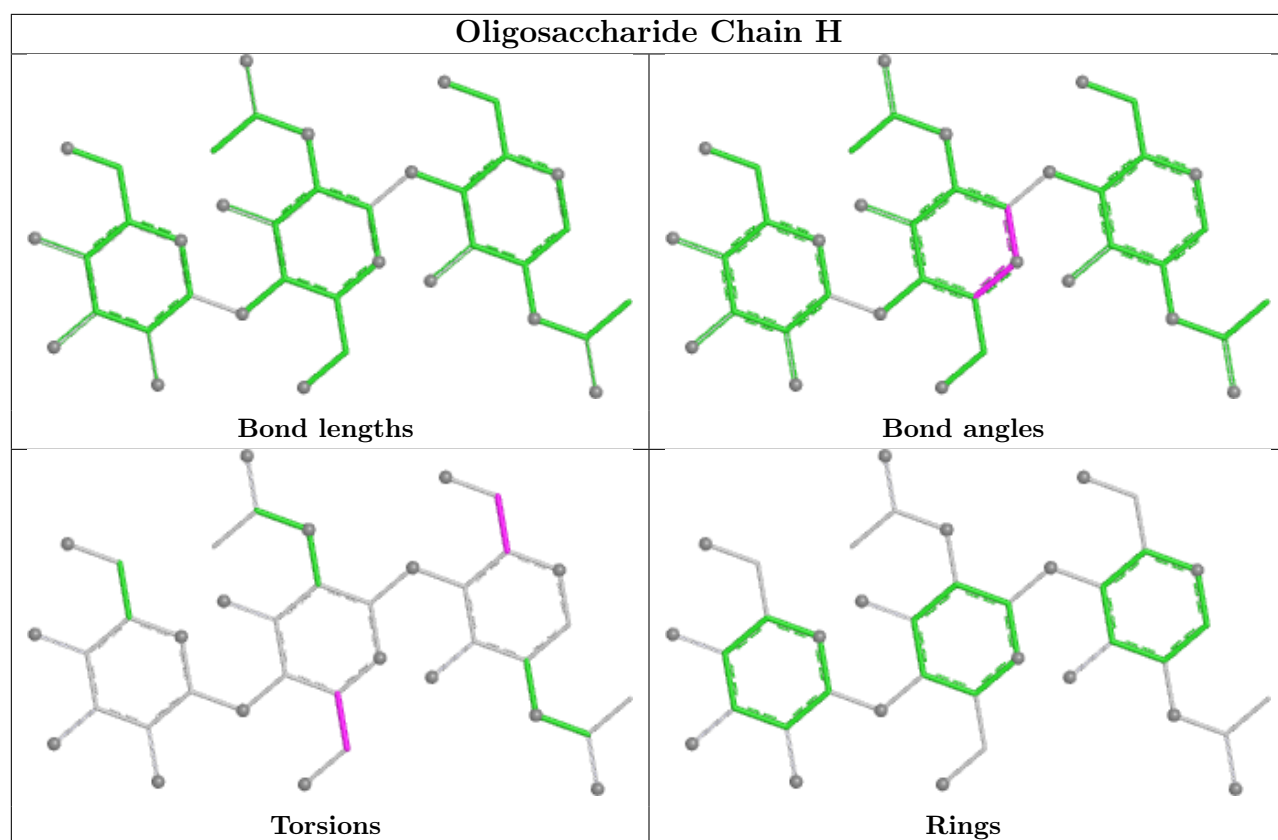
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

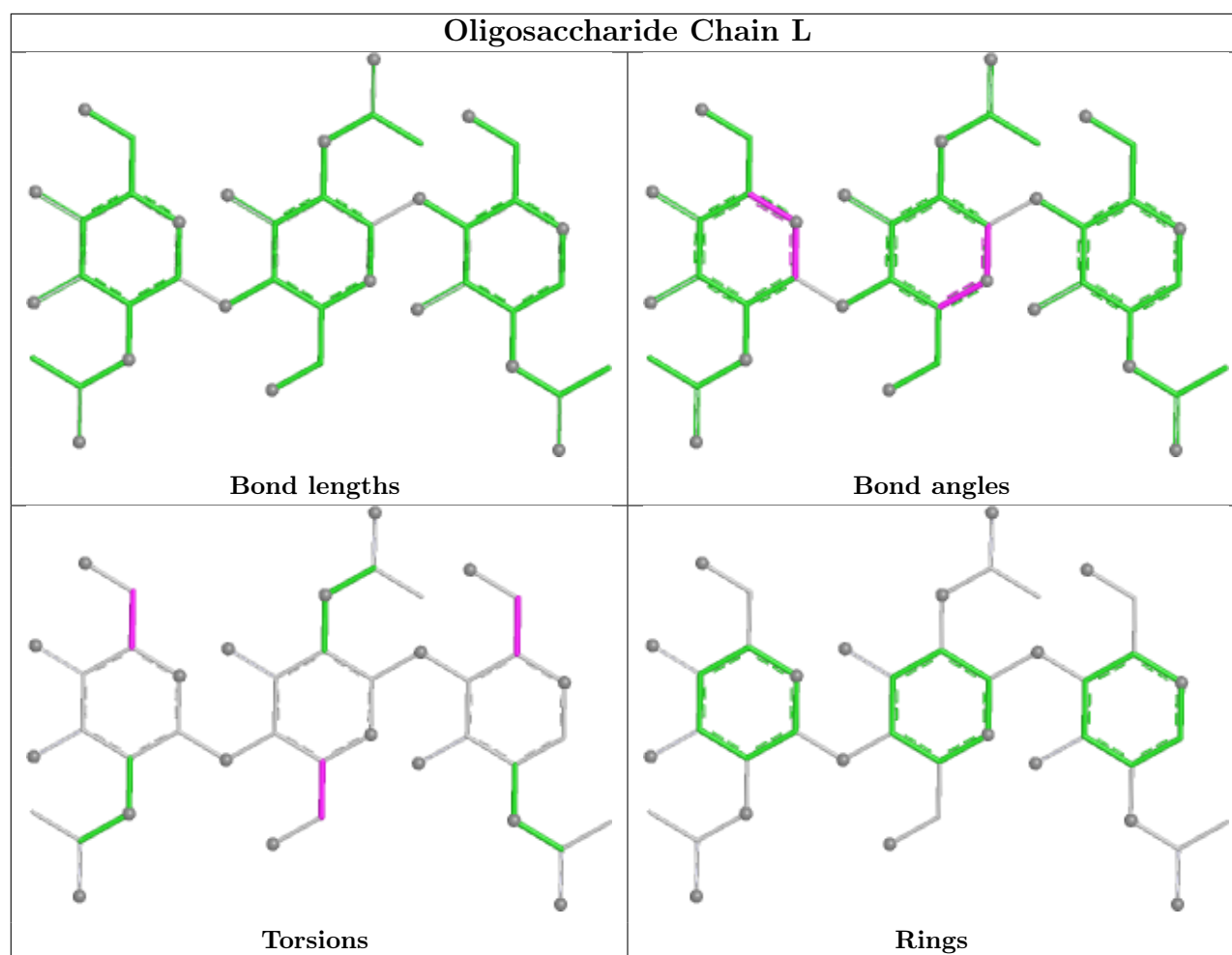












5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
10	PC1	A	1915	-	47,47,53	1.20	3 (6%)	53,55,61	1.22	4 (7%)
9	NAG	F	1206	5	14,14,15	0.52	0	17,19,21	0.40	0
10	PC1	A	1907	-	11,11,53	0.76	0	10,10,61	0.37	0
9	NAG	F	1203	5	14,14,15	0.28	0	17,19,21	0.48	0
9	NAG	F	1220	5	14,14,15	0.84	1 (7%)	17,19,21	1.07	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NAG	F	1214	5	14,14,15	0.67	1 (7%)	17,19,21	0.57	0
10	PC1	A	1912	-	44,44,53	1.21	3 (6%)	50,52,61	1.10	3 (6%)
9	NAG	A	1901	1	14,14,15	0.40	0	17,19,21	0.57	0
10	PC1	A	1904	-	41,41,53	1.25	4 (9%)	47,49,61	1.19	4 (8%)
10	PC1	A	1913	-	17,17,53	0.78	0	16,16,61	0.39	0
10	PC1	A	1914	-	13,13,53	0.61	0	12,12,61	0.49	0
9	NAG	F	1219	5	14,14,15	0.39	0	17,19,21	0.46	0
10	PC1	A	1906	-	17,17,53	0.74	0	16,16,61	0.48	0
10	PC1	A	1902	-	43,43,53	1.21	5 (11%)	49,51,61	1.19	3 (6%)
10	PC1	A	1909	-	14,14,53	0.67	0	13,13,61	0.43	0
10	PC1	A	1908	-	11,11,53	0.66	0	10,10,61	0.32	0
10	PC1	A	1903	-	53,53,53	1.11	3 (5%)	59,61,61	1.03	3 (5%)
9	NAG	F	1213	5	14,14,15	0.45	0	17,19,21	0.71	1 (5%)
9	NAG	F	1221	5	14,14,15	0.57	0	17,19,21	0.61	0
10	PC1	A	1910	-	17,17,53	0.83	0	16,16,61	0.38	0
10	PC1	A	1905	-	37,37,53	1.26	4 (10%)	43,45,61	1.15	4 (9%)
10	PC1	A	1911	-	47,47,53	1.11	3 (6%)	53,55,61	1.10	4 (7%)

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
10	PC1	A	1915	-	-	28/51/51/57	-
9	NAG	F	1206	5	-	0/6/23/26	0/1/1/1
10	PC1	A	1907	-	-	4/9/9/57	-
9	NAG	F	1203	5	-	0/6/23/26	0/1/1/1
9	NAG	F	1220	5	-	0/6/23/26	0/1/1/1
9	NAG	F	1214	5	-	0/6/23/26	0/1/1/1
10	PC1	A	1912	-	-	23/48/48/57	-
9	NAG	A	1901	1	-	2/6/23/26	0/1/1/1
10	PC1	A	1904	-	-	19/45/45/57	-
10	PC1	A	1913	-	-	4/15/15/57	-
10	PC1	A	1914	-	-	6/11/11/57	-
9	NAG	F	1219	5	-	2/6/23/26	0/1/1/1
10	PC1	A	1906	-	-	9/15/15/57	-
10	PC1	A	1902	-	-	22/47/47/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PC1	A	1909	-	-	7/12/12/57	-
10	PC1	A	1908	-	-	5/9/9/57	-
10	PC1	A	1903	-	-	27/57/57/57	-
9	NAG	F	1213	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1221	5	-	1/6/23/26	0/1/1/1
10	PC1	A	1910	-	-	9/15/15/57	-
10	PC1	A	1905	-	-	27/41/41/57	-
10	PC1	A	1911	-	-	30/51/51/57	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1904	PC1	O31-C31	3.30	1.43	1.33
10	A	1902	PC1	O21-C21	3.24	1.43	1.34
10	A	1912	PC1	O31-C31	3.23	1.42	1.33
10	A	1903	PC1	O31-C31	3.22	1.42	1.33
10	A	1915	PC1	O31-C31	3.19	1.42	1.33
10	A	1905	PC1	O21-C21	3.11	1.43	1.34
10	A	1915	PC1	O21-C21	3.10	1.43	1.34
10	A	1905	PC1	O31-C31	3.02	1.42	1.33
10	A	1902	PC1	O31-C31	2.97	1.42	1.33
10	A	1903	PC1	O21-C21	2.96	1.42	1.34
10	A	1911	PC1	O21-C2	-2.94	1.39	1.46
10	A	1904	PC1	O21-C21	2.89	1.42	1.34
10	A	1912	PC1	O21-C2	-2.85	1.39	1.46
10	A	1915	PC1	O21-C2	-2.82	1.40	1.46
10	A	1912	PC1	O21-C21	2.75	1.42	1.34
10	A	1911	PC1	O31-C31	2.67	1.41	1.33
10	A	1903	PC1	O21-C2	-2.61	1.40	1.46
10	A	1904	PC1	O21-C2	-2.59	1.40	1.46
10	A	1911	PC1	O21-C21	2.58	1.41	1.34
9	F	1220	NAG	C1-C2	2.53	1.55	1.52
10	A	1902	PC1	O21-C2	-2.31	1.41	1.46
10	A	1902	PC1	C22-C21	2.13	1.56	1.50
9	F	1214	NAG	C1-C2	2.11	1.55	1.52
10	A	1905	PC1	O21-C2	-2.07	1.41	1.46
10	A	1902	PC1	P-O11	2.05	1.67	1.59
10	A	1904	PC1	C22-C21	2.01	1.56	1.50
10	A	1905	PC1	P-O13	2.00	1.67	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1915	PC1	O21-C21-C22	5.39	123.15	111.48
10	A	1902	PC1	O21-C21-C22	5.04	122.38	111.48
10	A	1912	PC1	O21-C21-C22	4.36	120.91	111.48
10	A	1904	PC1	O21-C21-C22	4.07	120.28	111.48
10	A	1904	PC1	C15-N-C13	3.94	119.32	108.98
9	F	1220	NAG	C1-O5-C5	3.77	117.24	112.19
10	A	1905	PC1	C15-N-C13	3.74	118.80	108.98
10	A	1911	PC1	C15-N-C13	3.62	118.49	108.98
10	A	1902	PC1	C15-N-C13	3.62	118.49	108.98
10	A	1903	PC1	C15-N-C13	3.56	118.32	108.98
10	A	1903	PC1	O21-C21-C22	3.55	119.16	111.48
10	A	1905	PC1	O21-C21-C22	3.52	119.10	111.48
10	A	1912	PC1	C15-N-C13	3.44	118.02	108.98
10	A	1911	PC1	O21-C21-C22	3.43	118.89	111.48
10	A	1904	PC1	O31-C31-C32	3.42	122.25	111.83
10	A	1915	PC1	C15-N-C13	3.28	117.60	108.98
10	A	1915	PC1	O31-C31-C32	3.07	121.19	111.83
10	A	1903	PC1	O31-C31-C32	2.93	120.76	111.83
10	A	1902	PC1	O31-C31-C32	2.72	120.13	111.83
10	A	1912	PC1	O31-C31-C32	2.57	119.66	111.83
10	A	1911	PC1	O31-C31-C32	2.49	119.44	111.83
10	A	1915	PC1	O21-C21-O22	-2.43	118.03	123.70
10	A	1905	PC1	O31-C31-C32	2.28	118.79	111.83
9	F	1213	NAG	C1-O5-C5	2.28	115.24	112.19
10	A	1904	PC1	O31-C31-O32	-2.13	118.30	123.63
10	A	1911	PC1	C2-O21-C21	-2.09	112.79	117.80
10	A	1905	PC1	O21-C2-C1	2.02	115.58	108.34

There are no chirality outliers.

All (227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1902	PC1	C1-O11-P-O12
10	A	1902	PC1	O13-C11-C12-N
10	A	1903	PC1	C11-O13-P-O14
10	A	1903	PC1	C11-O13-P-O11
10	A	1903	PC1	C22-C21-O21-C2
10	A	1904	PC1	C11-O13-P-O12
10	A	1904	PC1	C11-O13-P-O14
10	A	1904	PC1	C11-O13-P-O11
10	A	1904	PC1	C1-O11-P-O12
10	A	1904	PC1	C1-O11-P-O13
10	A	1904	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
10	A	1904	PC1	O11-C1-C2-O21
10	A	1904	PC1	O22-C21-O21-C2
10	A	1904	PC1	O32-C31-O31-C3
10	A	1904	PC1	C32-C31-O31-C3
10	A	1905	PC1	C11-O13-P-O14
10	A	1905	PC1	C1-O11-P-O12
10	A	1905	PC1	C1-O11-P-O14
10	A	1905	PC1	C1-O11-P-O13
10	A	1905	PC1	C22-C21-O21-C2
10	A	1911	PC1	C11-O13-P-O12
10	A	1911	PC1	C11-O13-P-O14
10	A	1911	PC1	C11-O13-P-O11
10	A	1911	PC1	C1-O11-P-O12
10	A	1911	PC1	C1-O11-P-O14
10	A	1911	PC1	C1-O11-P-O13
10	A	1911	PC1	O13-C11-C12-N
10	A	1911	PC1	O22-C21-O21-C2
10	A	1912	PC1	C1-O11-P-O12
10	A	1912	PC1	C1-O11-P-O14
10	A	1912	PC1	C1-O11-P-O13
10	A	1912	PC1	O13-C11-C12-N
10	A	1912	PC1	C22-C21-O21-C2
10	A	1915	PC1	C11-O13-P-O12
10	A	1915	PC1	C11-O13-P-O11
10	A	1915	PC1	C1-O11-P-O12
10	A	1915	PC1	C1-O11-P-O14
10	A	1915	PC1	C1-O11-P-O13
10	A	1915	PC1	O22-C21-O21-C2
10	A	1915	PC1	C22-C21-O21-C2
10	A	1915	PC1	O32-C31-O31-C3
10	A	1915	PC1	C32-C31-O31-C3
9	A	1901	NAG	O5-C5-C6-O6
10	A	1903	PC1	O22-C21-O21-C2
10	A	1905	PC1	O22-C21-O21-C2
10	A	1912	PC1	O22-C21-O21-C2
9	F	1213	NAG	C4-C5-C6-O6
10	A	1904	PC1	C22-C21-O21-C2
10	A	1911	PC1	C22-C21-O21-C2
9	F	1213	NAG	O5-C5-C6-O6
10	A	1908	PC1	C39-C3A-C3B-C3C
10	A	1911	PC1	C32-C31-O31-C3
9	A	1901	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	F	1219	NAG	O5-C5-C6-O6
10	A	1911	PC1	O32-C31-O31-C3
9	F	1219	NAG	C4-C5-C6-O6
10	A	1910	PC1	C2E-C2F-C2G-C2H
10	A	1912	PC1	C31-C32-C33-C34
10	A	1902	PC1	O21-C2-C3-O31
10	A	1915	PC1	C36-C37-C38-C39
10	A	1912	PC1	C23-C24-C25-C26
10	A	1904	PC1	C21-C22-C23-C24
10	A	1902	PC1	C22-C23-C24-C25
10	A	1909	PC1	C35-C36-C37-C38
10	A	1905	PC1	C1-C2-O21-C21
10	A	1902	PC1	C34-C35-C36-C37
10	A	1911	PC1	C28-C29-C2A-C2B
10	A	1911	PC1	C2D-C2E-C2F-C2G
10	A	1906	PC1	C29-C2A-C2B-C2C
10	A	1909	PC1	C3B-C3C-C3D-C3E
10	A	1915	PC1	C26-C27-C28-C29
10	A	1915	PC1	C38-C39-C3A-C3B
10	A	1905	PC1	C25-C26-C27-C28
10	A	1915	PC1	C2A-C2B-C2C-C2D
10	A	1914	PC1	C3B-C3C-C3D-C3E
10	A	1915	PC1	C2E-C2F-C2G-C2H
10	A	1911	PC1	C2B-C2C-C2D-C2E
10	A	1906	PC1	C24-C25-C26-C27
10	A	1902	PC1	C22-C21-O21-C2
10	A	1902	PC1	C33-C34-C35-C36
10	A	1903	PC1	C2E-C2F-C2G-C2H
10	A	1906	PC1	C25-C26-C27-C28
10	A	1915	PC1	C22-C23-C24-C25
10	A	1912	PC1	C34-C35-C36-C37
10	A	1915	PC1	C34-C35-C36-C37
10	A	1902	PC1	C24-C25-C26-C27
10	A	1904	PC1	C27-C28-C29-C2A
10	A	1903	PC1	C32-C31-O31-C3
10	A	1903	PC1	C22-C23-C24-C25
10	A	1906	PC1	C27-C28-C29-C2A
10	A	1910	PC1	C25-C26-C27-C28
10	A	1915	PC1	C24-C25-C26-C27
10	A	1905	PC1	C21-C22-C23-C24
10	A	1903	PC1	C37-C38-C39-C3A
10	A	1905	PC1	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
10	A	1905	PC1	C34-C35-C36-C37
10	A	1902	PC1	C3A-C3B-C3C-C3D
10	A	1912	PC1	C24-C25-C26-C27
10	A	1912	PC1	C36-C37-C38-C39
10	A	1913	PC1	C27-C28-C29-C2A
10	A	1903	PC1	C29-C2A-C2B-C2C
10	A	1902	PC1	O22-C21-O21-C2
10	A	1914	PC1	C3E-C3F-C3G-C3H
10	A	1904	PC1	C24-C25-C26-C27
10	A	1915	PC1	C23-C24-C25-C26
10	A	1903	PC1	C25-C26-C27-C28
10	A	1906	PC1	C2D-C2E-C2F-C2G
10	A	1903	PC1	O32-C31-O31-C3
10	A	1911	PC1	C37-C38-C39-C3A
10	A	1912	PC1	C27-C28-C29-C2A
10	A	1905	PC1	C32-C31-O31-C3
10	A	1915	PC1	C21-C22-C23-C24
10	A	1902	PC1	C35-C36-C37-C38
9	F	1221	NAG	O5-C5-C6-O6
10	A	1903	PC1	C3E-C3F-C3G-C3H
10	A	1904	PC1	C22-C23-C24-C25
10	A	1903	PC1	C3D-C3E-C3F-C3G
10	A	1911	PC1	O21-C2-C3-O31
10	A	1903	PC1	C26-C27-C28-C29
10	A	1915	PC1	C33-C34-C35-C36
10	A	1912	PC1	C33-C34-C35-C36
10	A	1911	PC1	C25-C26-C27-C28
10	A	1909	PC1	C39-C3A-C3B-C3C
10	A	1915	PC1	C37-C38-C39-C3A
10	A	1913	PC1	C26-C27-C28-C29
10	A	1903	PC1	C35-C36-C37-C38
10	A	1911	PC1	C24-C25-C26-C27
10	A	1907	PC1	C32-C33-C34-C35
10	A	1902	PC1	C1-C2-C3-O31
10	A	1915	PC1	C29-C2A-C2B-C2C
10	A	1905	PC1	O32-C31-O31-C3
10	A	1903	PC1	C24-C25-C26-C27
10	A	1912	PC1	C38-C39-C3A-C3B
10	A	1907	PC1	C39-C3A-C3B-C3C
10	A	1902	PC1	O11-C1-C2-O21
10	A	1910	PC1	C22-C23-C24-C25
10	A	1910	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
10	A	1915	PC1	C39-C3A-C3B-C3C
10	A	1903	PC1	C38-C39-C3A-C3B
10	A	1903	PC1	C2F-C2G-C2H-C2I
10	A	1904	PC1	C32-C33-C34-C35
10	A	1905	PC1	C37-C38-C39-C3A
10	A	1915	PC1	C32-C33-C34-C35
10	A	1903	PC1	C34-C35-C36-C37
10	A	1902	PC1	O11-C1-C2-C3
10	A	1904	PC1	O11-C1-C2-C3
10	A	1903	PC1	C32-C33-C34-C35
10	A	1912	PC1	C21-C22-C23-C24
10	A	1905	PC1	C23-C24-C25-C26
10	A	1911	PC1	C36-C37-C38-C39
10	A	1912	PC1	C22-C23-C24-C25
10	A	1911	PC1	C1-C2-C3-O31
10	A	1908	PC1	C3A-C3B-C3C-C3D
10	A	1905	PC1	C2-C1-O11-P
10	A	1911	PC1	C2-C1-O11-P
10	A	1905	PC1	C33-C34-C35-C36
10	A	1906	PC1	C2C-C2D-C2E-C2F
10	A	1908	PC1	C3E-C3F-C3G-C3H
10	A	1910	PC1	C27-C28-C29-C2A
10	A	1910	PC1	C2B-C2C-C2D-C2E
10	A	1911	PC1	C22-C23-C24-C25
10	A	1912	PC1	C25-C26-C27-C28
10	A	1914	PC1	C38-C39-C3A-C3B
10	A	1914	PC1	C3C-C3D-C3E-C3F
10	A	1911	PC1	O11-C1-C2-C3
10	A	1911	PC1	C32-C33-C34-C35
10	A	1904	PC1	C35-C36-C37-C38
10	A	1903	PC1	C31-C32-C33-C34
10	A	1911	PC1	C23-C24-C25-C26
10	A	1907	PC1	C35-C36-C37-C38
10	A	1909	PC1	C37-C38-C39-C3A
10	A	1915	PC1	C12-C11-O13-P
10	A	1912	PC1	O21-C2-C3-O31
10	A	1915	PC1	O21-C2-C3-O31
10	A	1911	PC1	C29-C2A-C2B-C2C
10	A	1903	PC1	O13-C11-C12-N
10	A	1905	PC1	O13-C11-C12-N
10	A	1915	PC1	O13-C11-C12-N
10	A	1915	PC1	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
10	A	1902	PC1	C3D-C3E-C3F-C3G
10	A	1914	PC1	C37-C38-C39-C3A
10	A	1911	PC1	O11-C1-C2-O21
10	A	1906	PC1	C2E-C2F-C2G-C2H
10	A	1912	PC1	C32-C33-C34-C35
10	A	1912	PC1	C1-C2-C3-O31
10	A	1902	PC1	C1-O11-P-O14
10	A	1902	PC1	C1-O11-P-O13
10	A	1903	PC1	C11-O13-P-O12
10	A	1905	PC1	C11-O13-P-O12
10	A	1905	PC1	C11-O13-P-O11
10	A	1911	PC1	C33-C34-C35-C36
10	A	1912	PC1	C2A-C2B-C2C-C2D
10	A	1905	PC1	C11-C12-N-C15
10	A	1908	PC1	C3F-C3G-C3H-C3I
10	A	1902	PC1	C23-C24-C25-C26
10	A	1913	PC1	C24-C25-C26-C27
10	A	1905	PC1	C26-C27-C28-C29
10	A	1905	PC1	C38-C39-C3A-C3B
10	A	1909	PC1	C3F-C3G-C3H-C3I
10	A	1905	PC1	C32-C33-C34-C35
10	A	1910	PC1	C29-C2A-C2B-C2C
10	A	1906	PC1	C23-C24-C25-C26
10	A	1914	PC1	C36-C37-C38-C39
10	A	1908	PC1	C3D-C3E-C3F-C3G
10	A	1911	PC1	C34-C35-C36-C37
10	A	1903	PC1	C3C-C3D-C3E-C3F
10	A	1910	PC1	C24-C25-C26-C27
10	A	1910	PC1	C2C-C2D-C2E-C2F
10	A	1902	PC1	O32-C31-O31-C3
10	A	1902	PC1	C32-C31-O31-C3
10	A	1907	PC1	C34-C35-C36-C37
10	A	1906	PC1	C21-C22-C23-C24
10	A	1905	PC1	C11-C12-N-C14
10	A	1913	PC1	C2D-C2E-C2F-C2G
10	A	1909	PC1	C34-C35-C36-C37
10	A	1905	PC1	O21-C21-C22-C23
10	A	1903	PC1	O31-C31-C32-C33
10	A	1902	PC1	C3C-C3D-C3E-C3F
10	A	1903	PC1	C27-C28-C29-C2A
10	A	1912	PC1	O31-C31-C32-C33
10	A	1902	PC1	C3B-C3C-C3D-C3E

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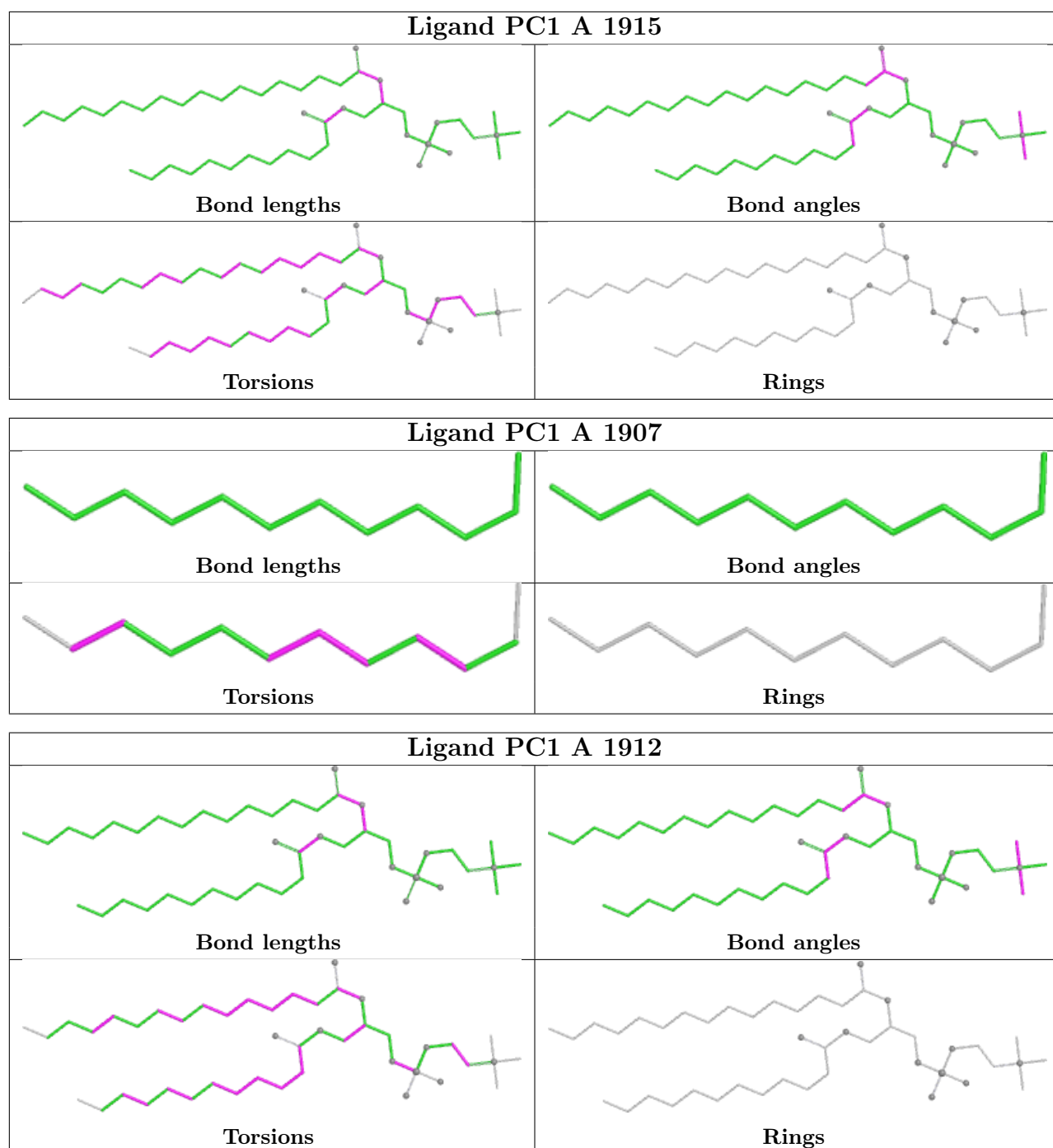
Mol	Chain	Res	Type	Atoms
10	A	1905	PC1	O22-C21-C22-C23
10	A	1909	PC1	C3A-C3B-C3C-C3D
10	A	1912	PC1	O32-C31-C32-C33
10	A	1904	PC1	C34-C35-C36-C37
10	A	1903	PC1	O32-C31-C32-C33
10	A	1911	PC1	O21-C21-C22-C23

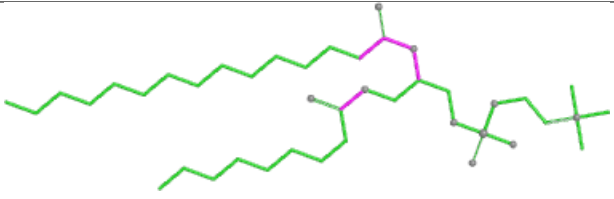
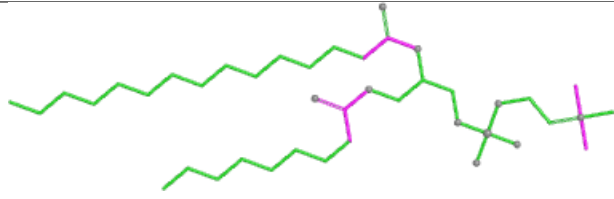
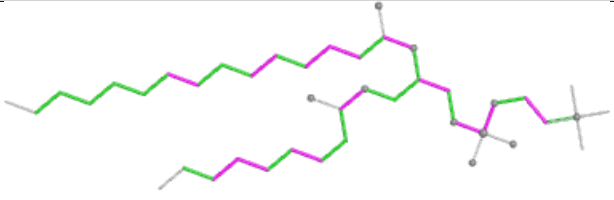
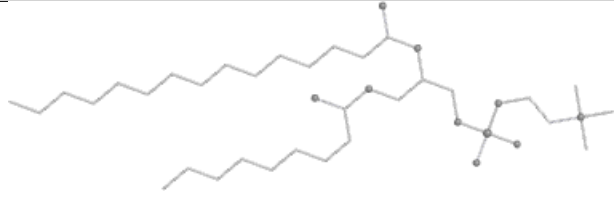
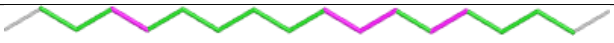
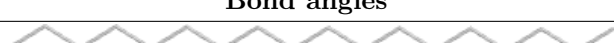
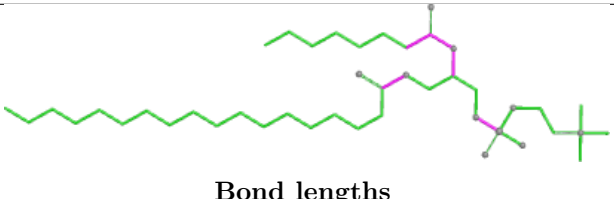
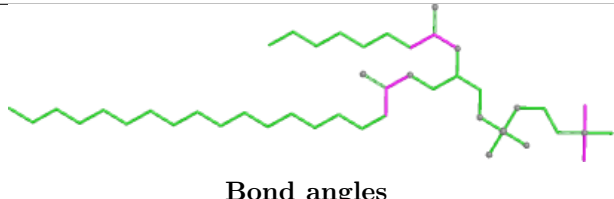
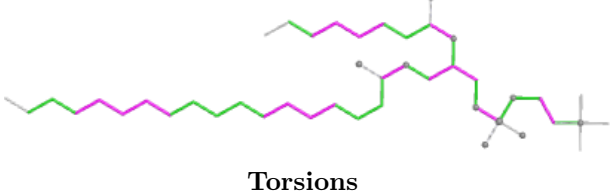
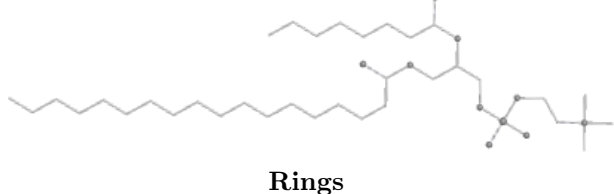
There are no ring outliers.

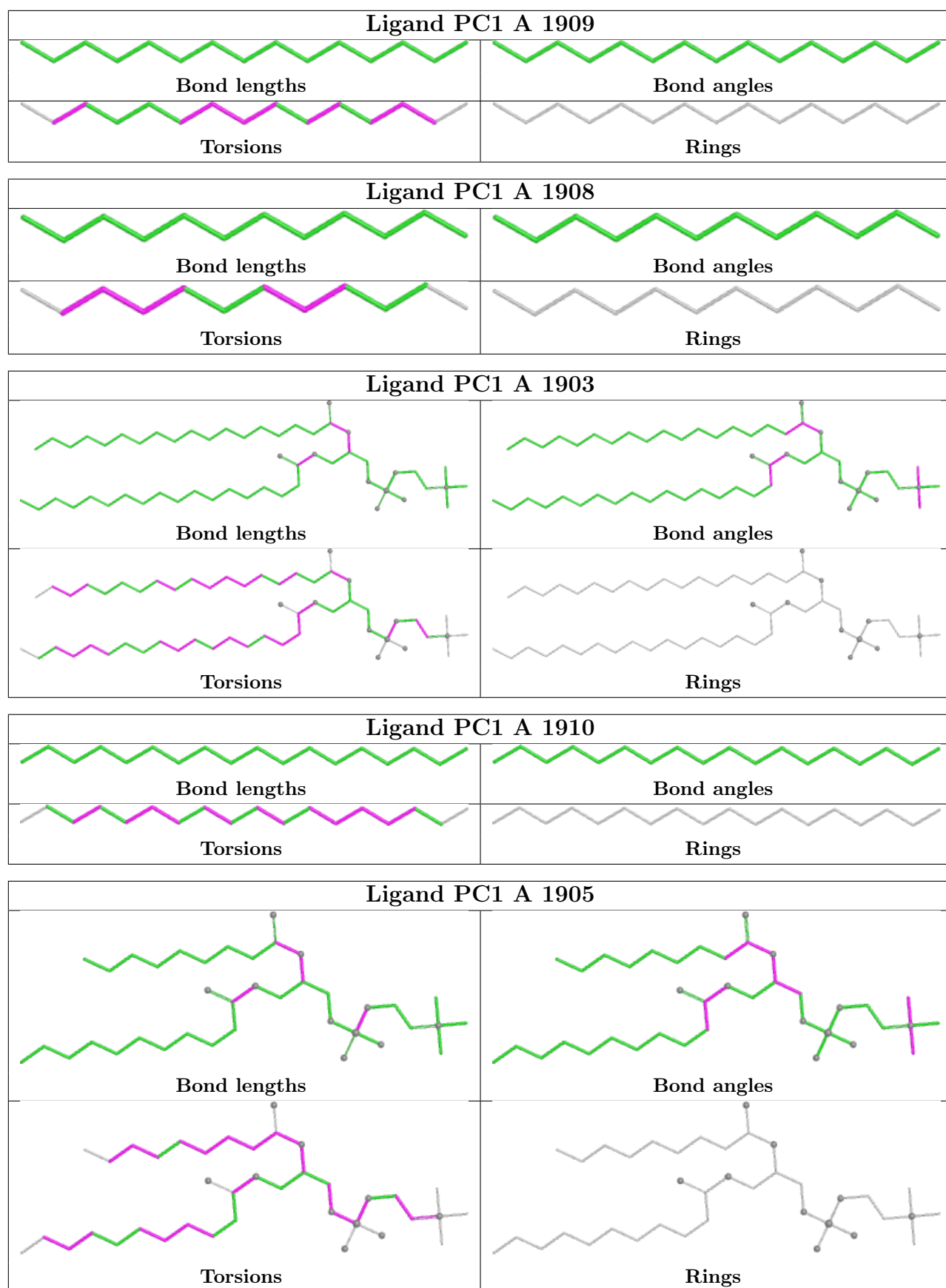
9 monomers are involved in 21 short contacts:

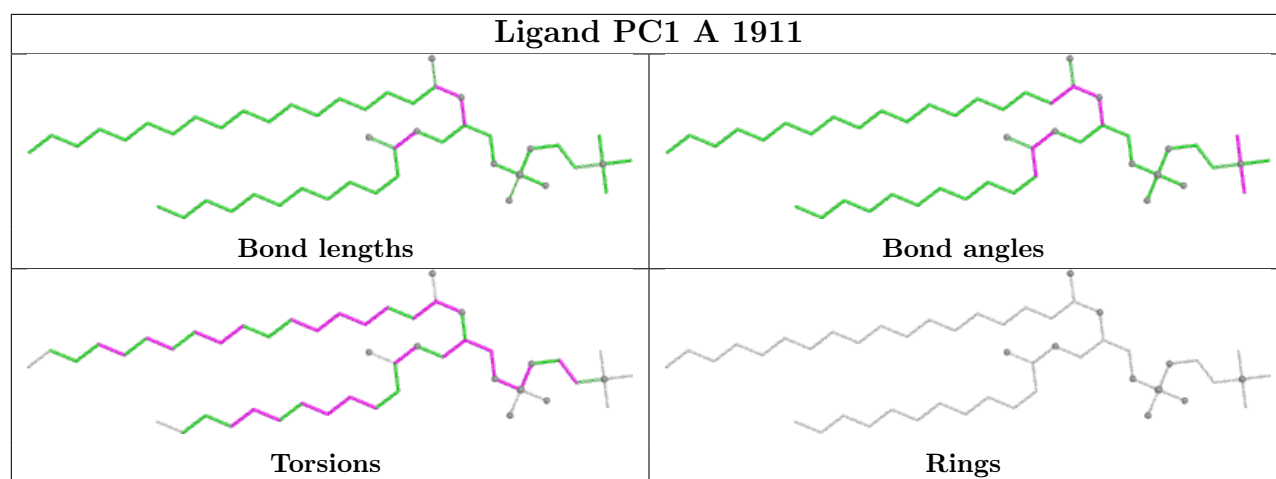
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1915	PC1	1	0
10	A	1912	PC1	3	0
10	A	1904	PC1	4	0
10	A	1914	PC1	4	0
10	A	1906	PC1	1	0
10	A	1902	PC1	2	0
10	A	1909	PC1	2	0
10	A	1903	PC1	2	0
10	A	1911	PC1	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand PC1 A 1904	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 1913	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 1914	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 1906	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 A 1902	
 Bond lengths	 Bond angles
 Torsions	 Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

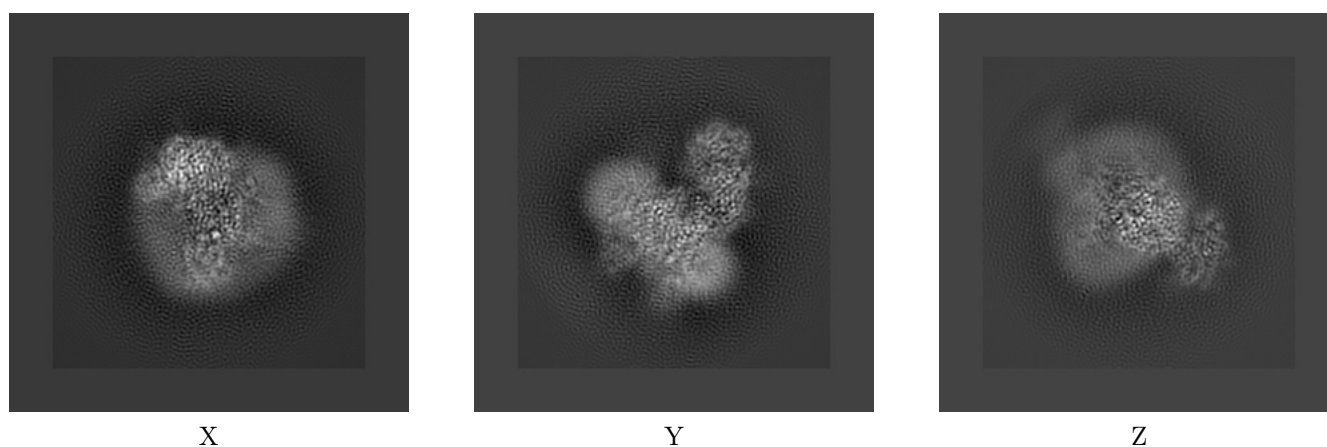
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9513. 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](#)

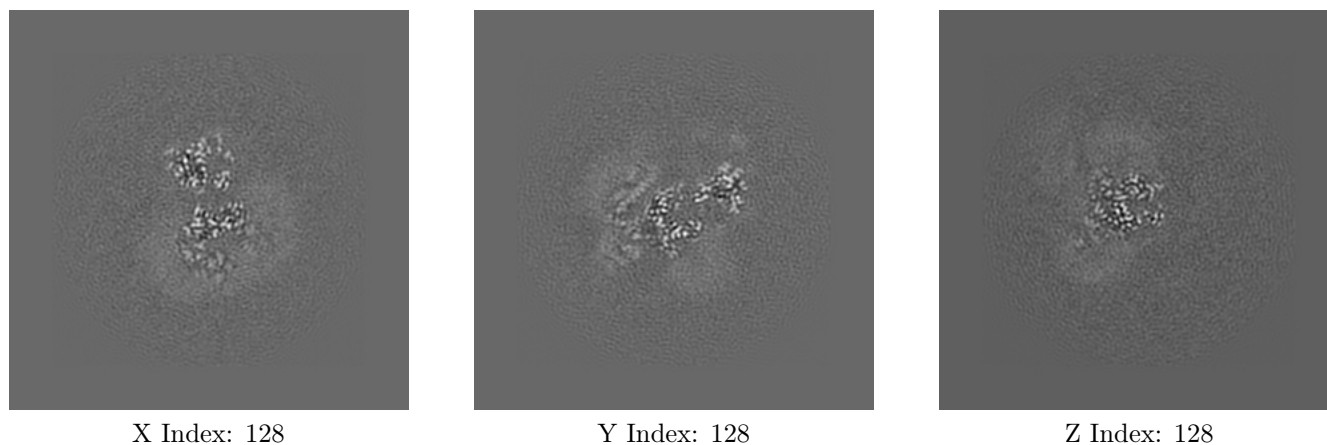
6.1.1 Primary map



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

6.2 Central slices [i](#)

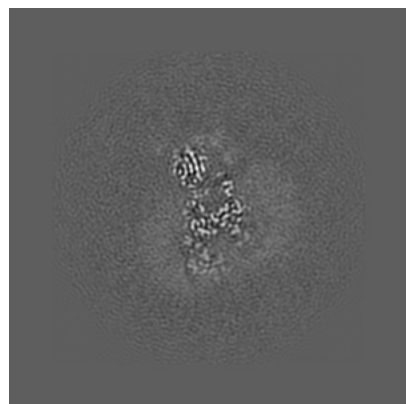
6.2.1 Primary map



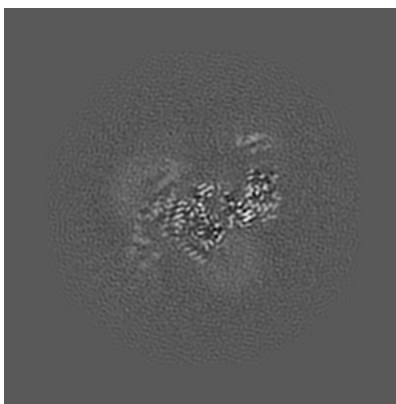
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

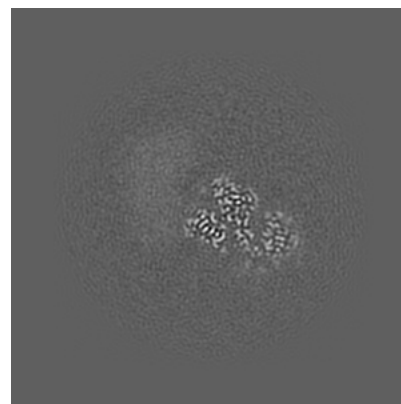
6.3.1 Primary map



X Index: 123



Y Index: 123

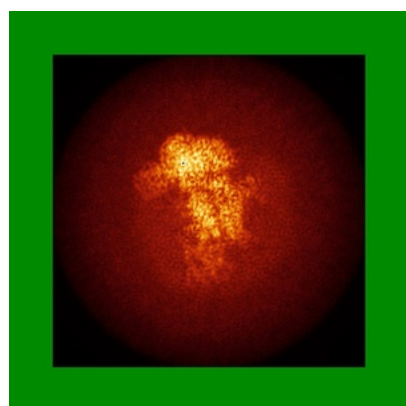


Z Index: 159

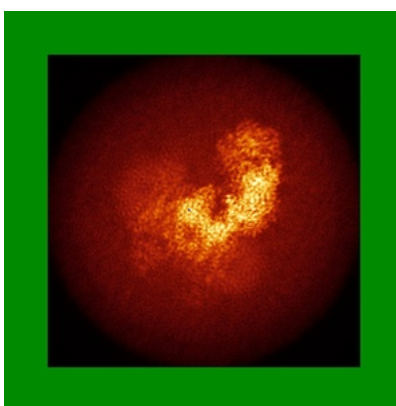
The images above show the largest variance slices of the map in three orthogonal directions.

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

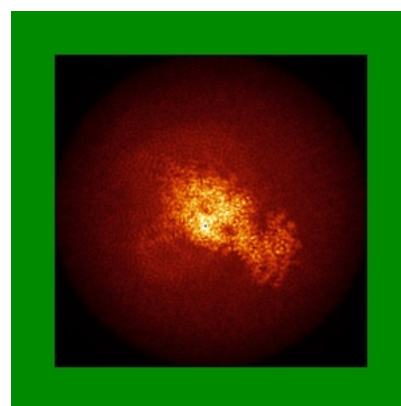
6.4.1 Primary map



X



Y

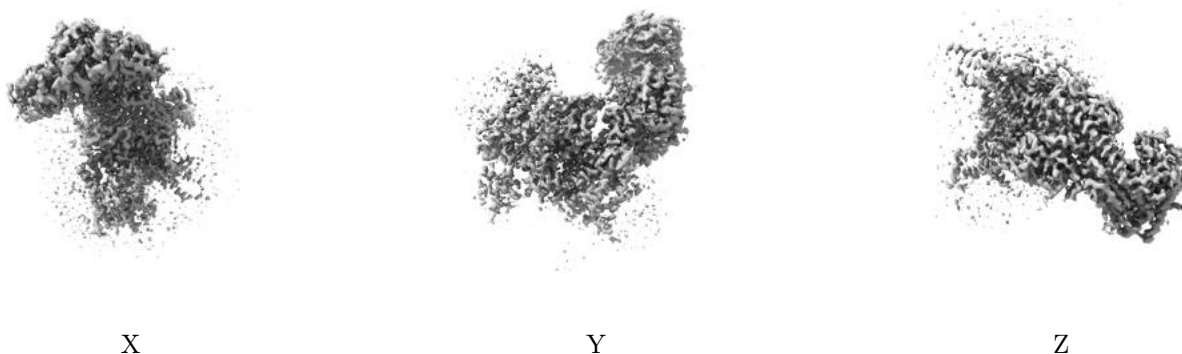


Z

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

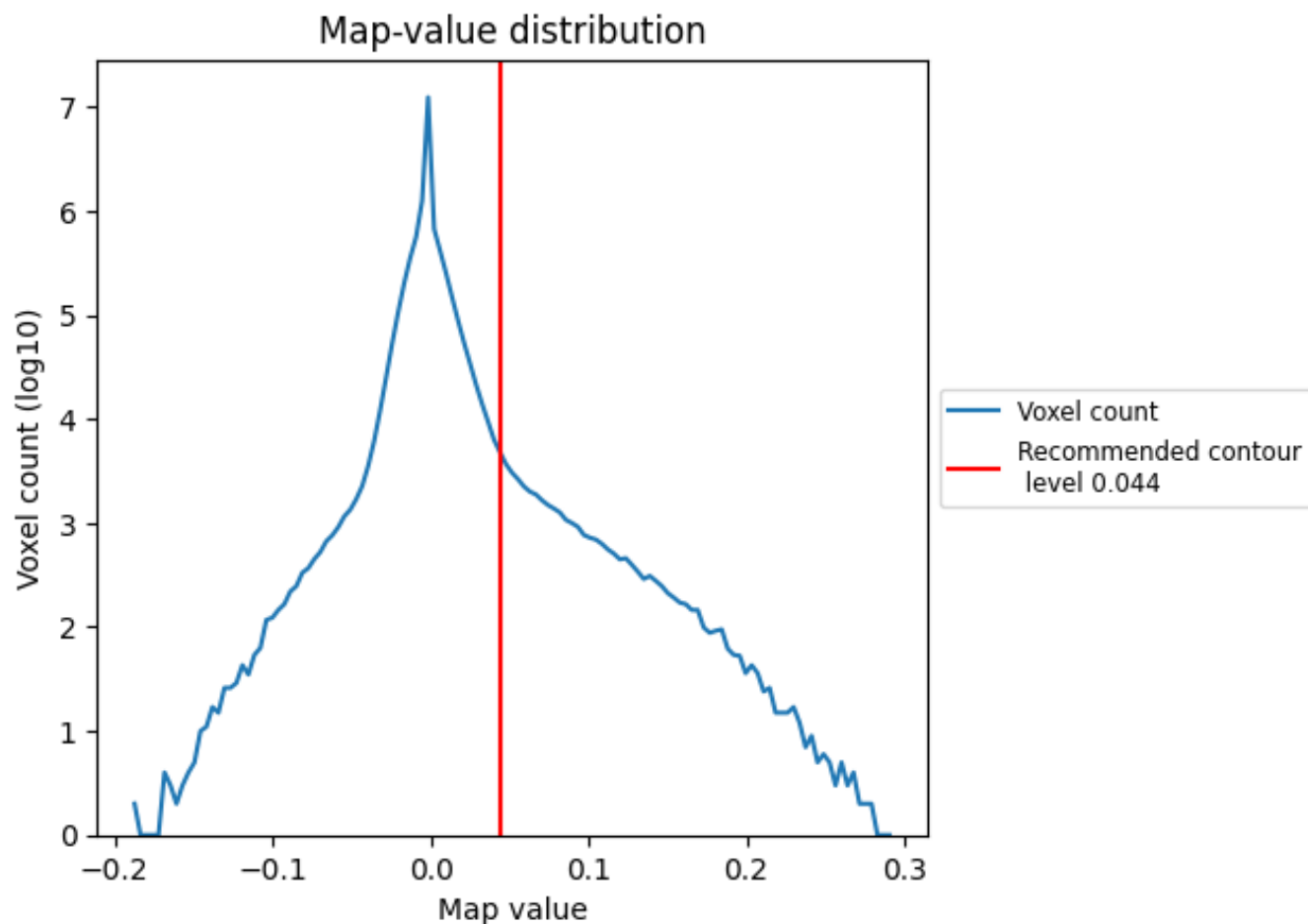
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

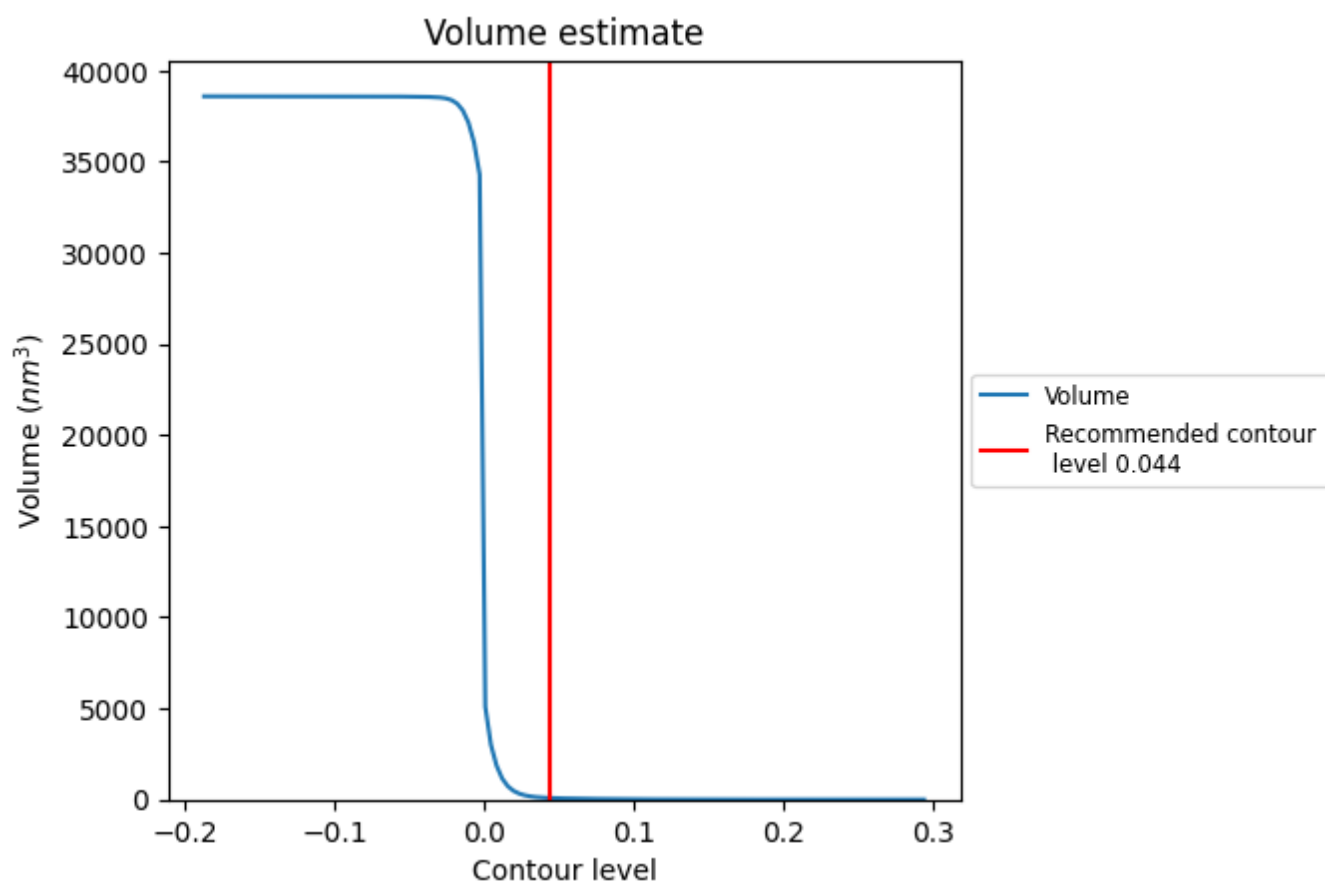
This section contains the results of statistical analysis of the map.

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.

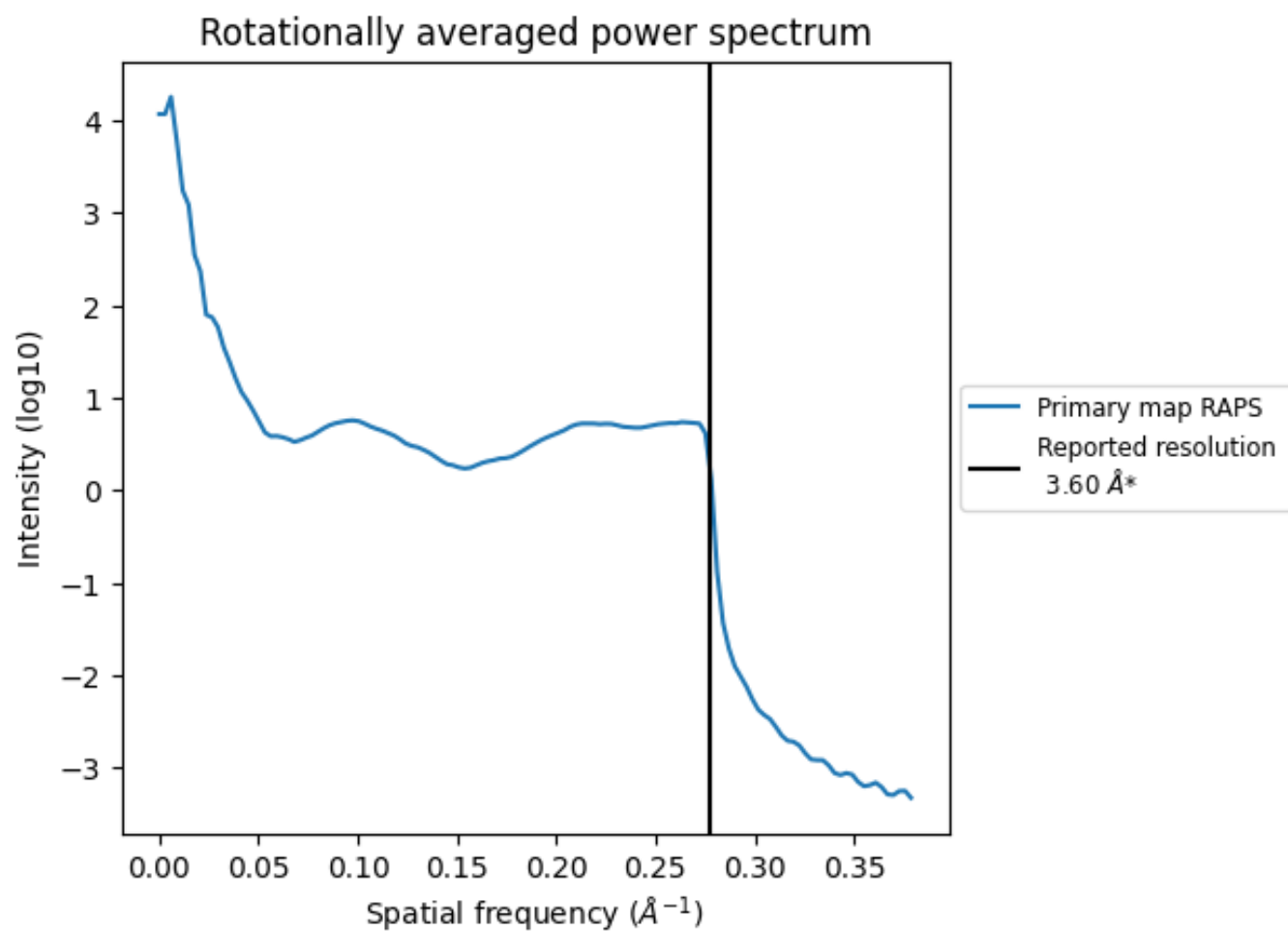
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 87 nm³; this corresponds to an approximate mass of 79 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 0.278 Å⁻¹

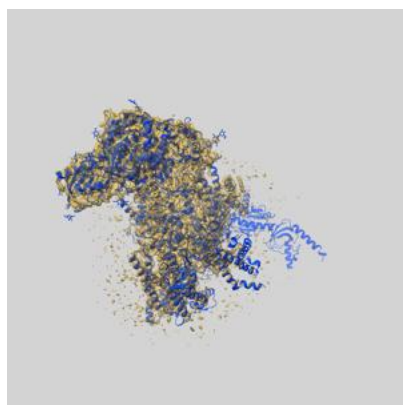
8 Fourier-Shell correlation ⓘ

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

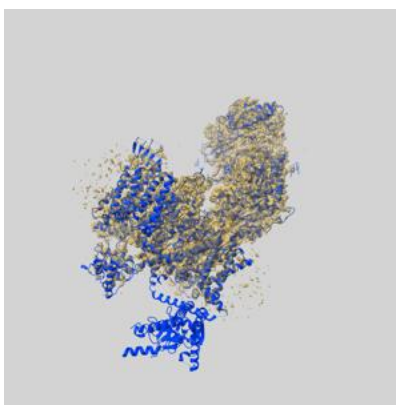
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9513 and PDB model 5GJV. Per-residue inclusion information can be found in section 3 on page 9.

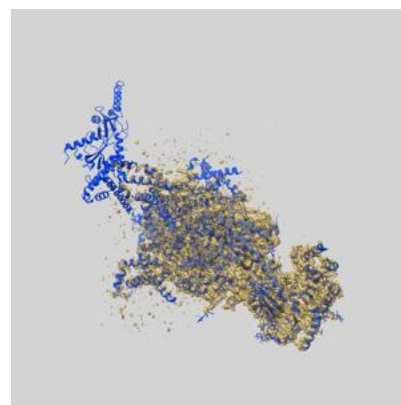
9.1 Map-model overlay [i](#)



X



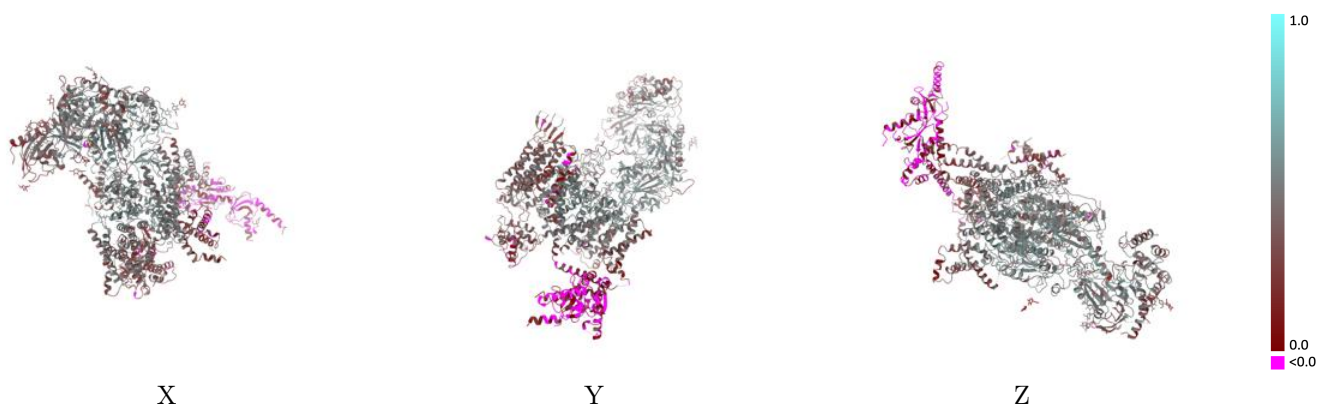
Y



Z

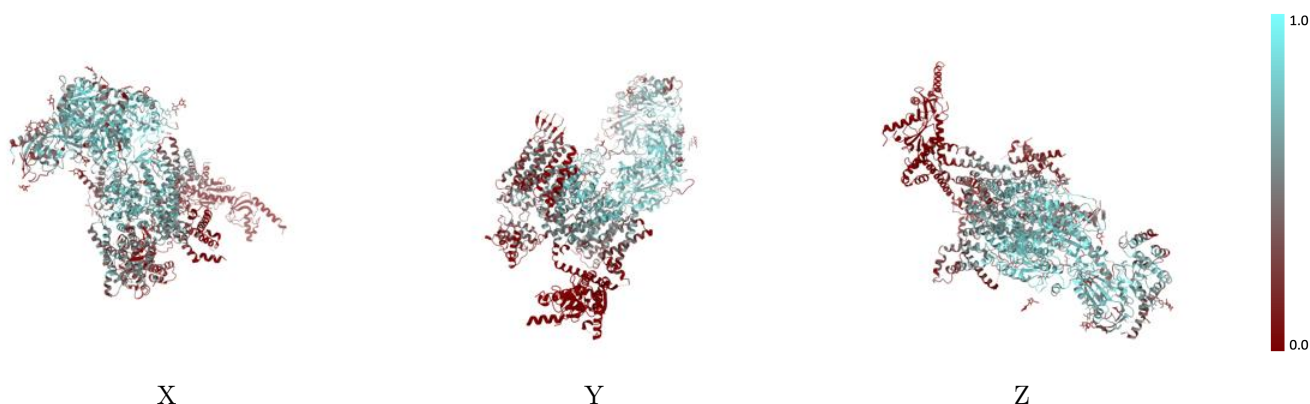
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



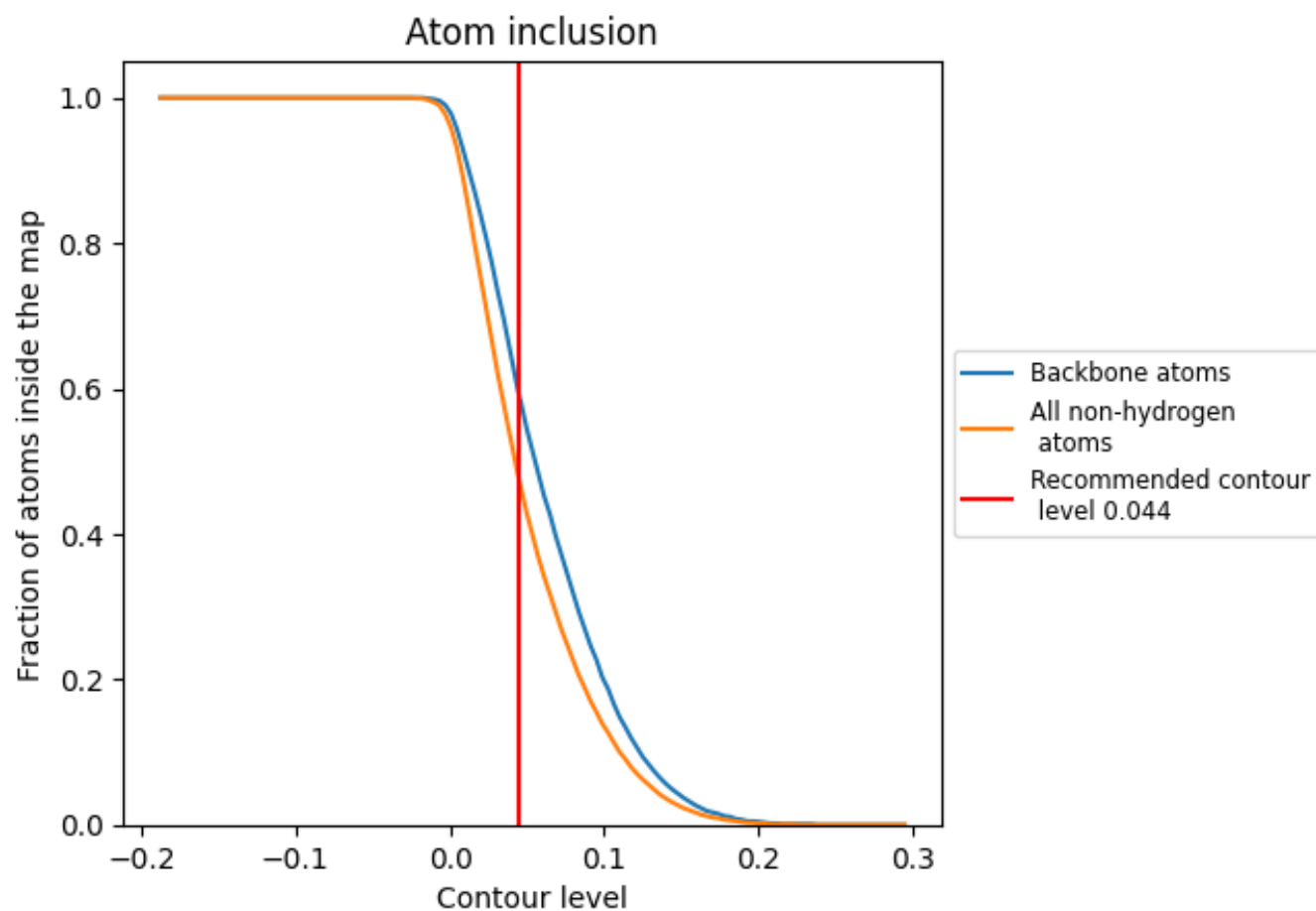
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 48% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4820	0.3850
A	0.4760	0.4090
B	0.0000	0.0240
C	0.0000	0.0110
D	0.0710	0.0690
E	0.3030	0.3460
F	0.6540	0.4590
G	0.1790	0.3650
H	0.3330	0.3700
I	0.6920	0.5200
J	0.5360	0.4920
K	0.2500	0.3890
L	0.2860	0.2870

1.0

0.0

<0.0