



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 01:37 AM JST

PDB ID : 6JPA
EMDB ID : EMD-9868
Title : Rabbit Cav1.1-Verapamil Complex
Authors : Zhao, Y.; Huang, G.; Wu, J.; Yan, N.
Deposited on : 2019-03-26
Resolution : 2.60 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.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

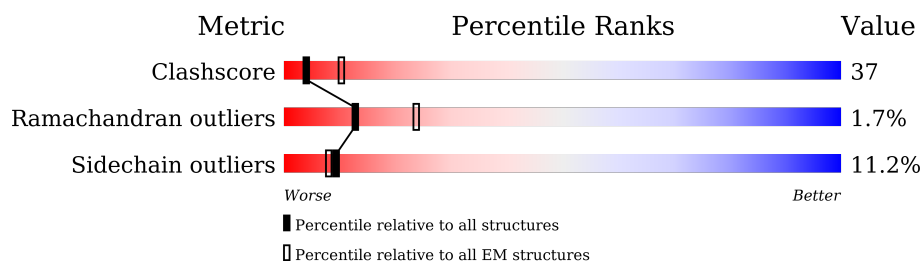
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1506	
2	E	222	
3	B	450	
4	C	524	
5	F	1046	
6	D	2	
6	G	2	
6	J	2	

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Mol	Chain	Length	Quality of chain
6	K	2	<div> <div>100%</div> <div>100%</div> </div>
7	H	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
7	I	3	<div> <div>67%</div> <div>33%</div> </div>
8	L	3	<div> <div>67%</div> <div>33%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	ETA	F	1101	-	-	X	-
6	NAG	D	1	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 22232 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	1274	Total	C	N	O	S	0	0
			10219	6728	1668	1753	70		

- Molecule 2 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	169	Total	C	N	O	S	0	0
			1326	872	216	220	18		

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

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

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	973	Total	C	N	O	S	1	0
			7804	4942	1320	1510	32		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	SER	See sequence details	UNP P13806

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-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.



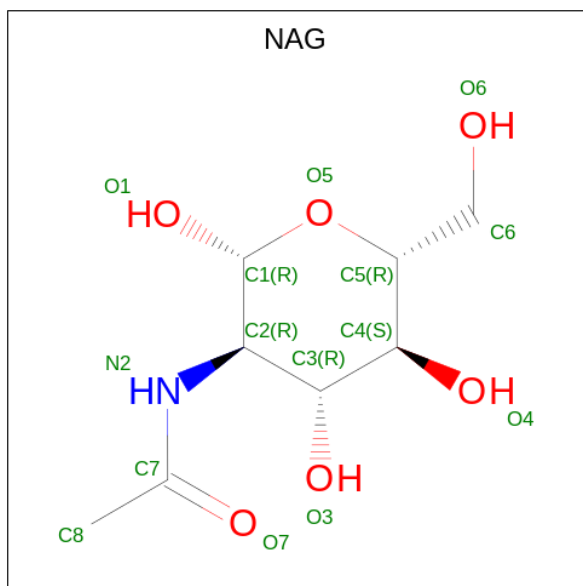
Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	3	Total	C	N	O	0	0
			39	22	2	15		
7	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

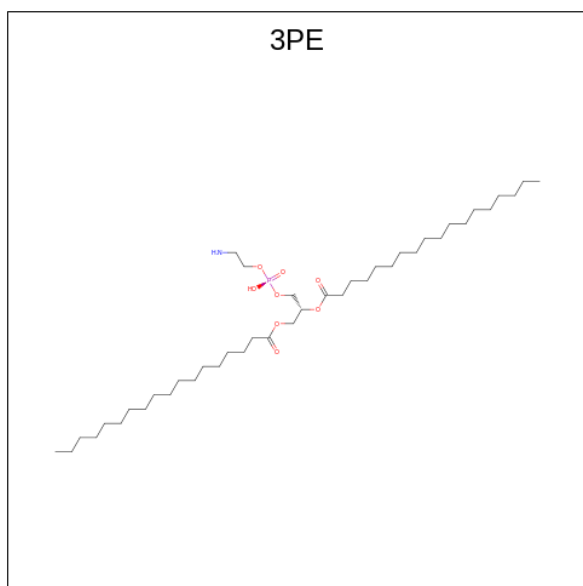


Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	
9	F	1	Total	C	N	O	0
			98	56	7	35	

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

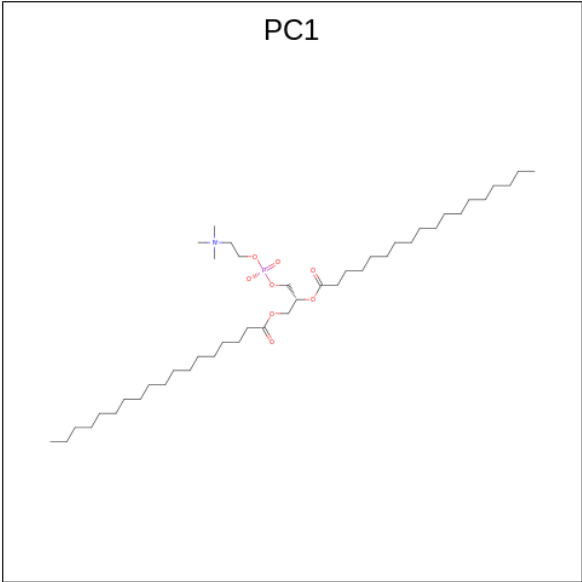
Mol	Chain	Residues	Atoms		AltConf
10	A	3	Total	Ca	0
			3	3	

- Molecule 11 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: C₄₁H₈₂NO₈P).



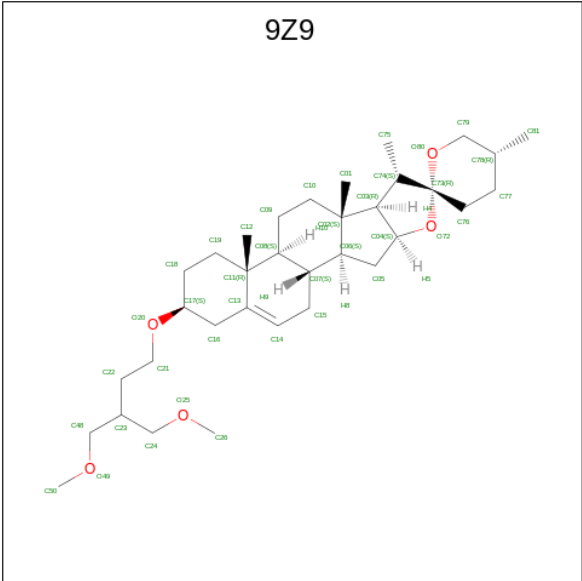
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			266	189	7	62	8	
11	A	1	Total	C	N	O	P	0
			266	189	7	62	8	
11	A	1	Total	C	N	O	P	0
			266	189	7	62	8	
11	A	1	Total	C	N	O	P	0
			266	189	7	62	8	
11	A	1	Total	C	N	O	P	0
			266	189	7	62	8	
11	A	1	Total	C	N	O	P	0
			266	189	7	62	8	
11	A	1	Total	C	N	O	P	0
			266	189	7	62	8	

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	N	O	P	0
			93	73	2	16	2	
12	A	1	Total	C	N	O	P	0
			93	73	2	16	2	

- Molecule 13 is (3beta,14beta,17beta,25R)-3-[4-methoxy-3-(methoxymethyl)butoxy]spirost-5-en (three-letter code: 9Z9) (formula: C₃₄H₅₆O₅).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			30	27	3	

-
- The chemical structure of 4YH is shown with atom labels. The pyridine ring is labeled with N1, C2, C3, C4, C5, and C6. The butyl chain is labeled with C7, C8, C9, and C10. The phenyl ring is labeled with C11, C12, C13, C14, C15, and C16. The methyl group is labeled with C17. The ethyl group is labeled with C18 and C19. The oxygen atoms are labeled with O20, O21, O22, and O23. The structure is drawn with stereochemistry: the bond between C7 and C8 is a wedge, the bond between C8 and C9 is a dash, and the bond between C9 and C10 is a wedge. The bond between C11 and C12 is a wedge, and the bond between C12 and C13 is a dash. The bond between C14 and C15 is a wedge, and the bond between C15 and C16 is a dash. The bond between C17 and C18 is a wedge, and the bond between C18 and C19 is a dash.

Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total 66	C 54	N 4	O 8	1
14	A	1	Total 66	C 54	N 4	O 8	1

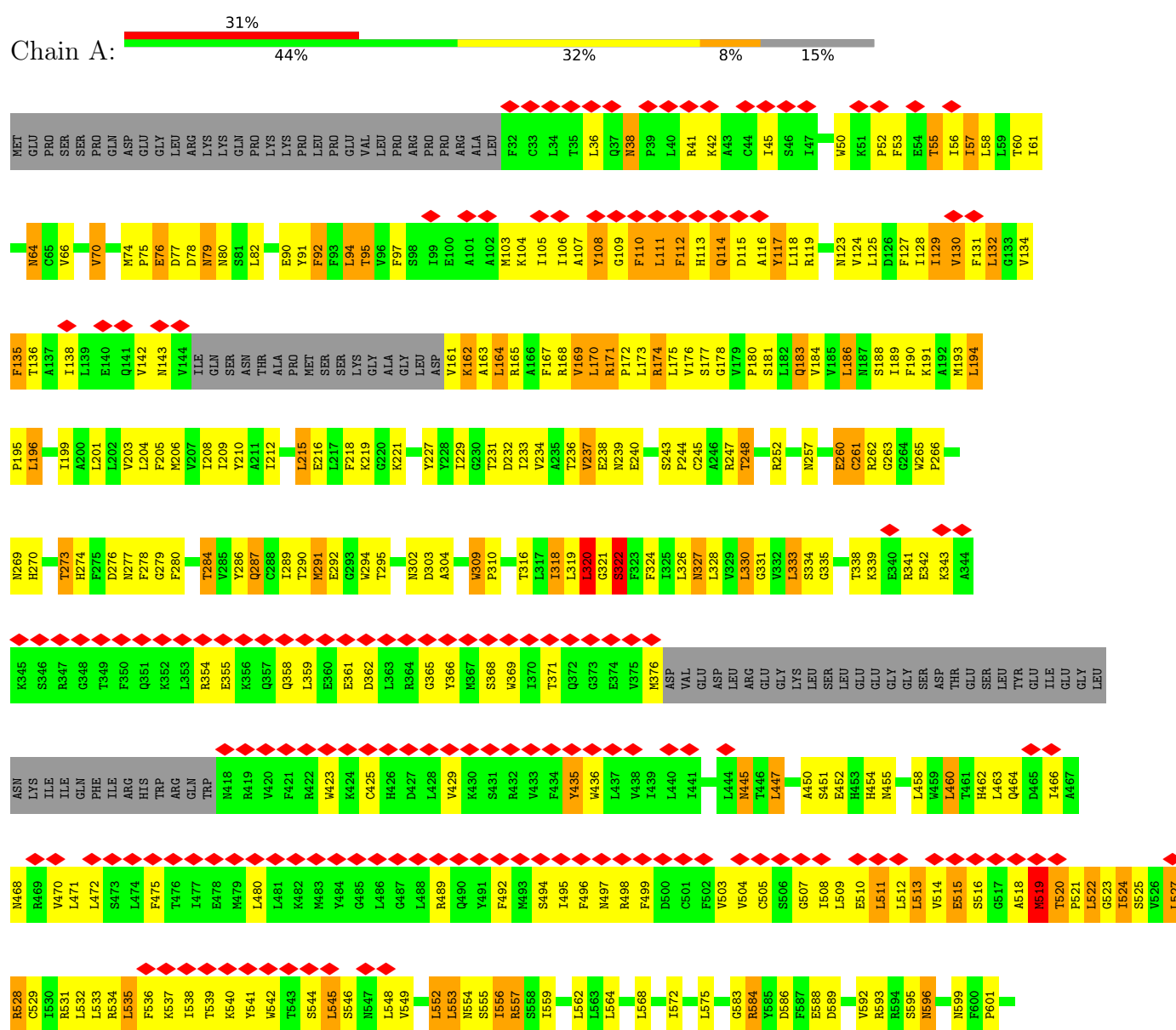
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- Chemical structure of Ethanolamine (ETA) is shown. The structure consists of a central carbon atom bonded to a hydrogen atom (H), an amino group (H₂N), a hydroxyl group (OH), and a methyl group (CH₃). The amino group is labeled 'CA' and the hydroxyl group is labeled 'CB'.

Mol	Chain	Residues	Atoms				AltConf
15	F	1	Total	C	N	O	0
			4	2	1	1	

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.

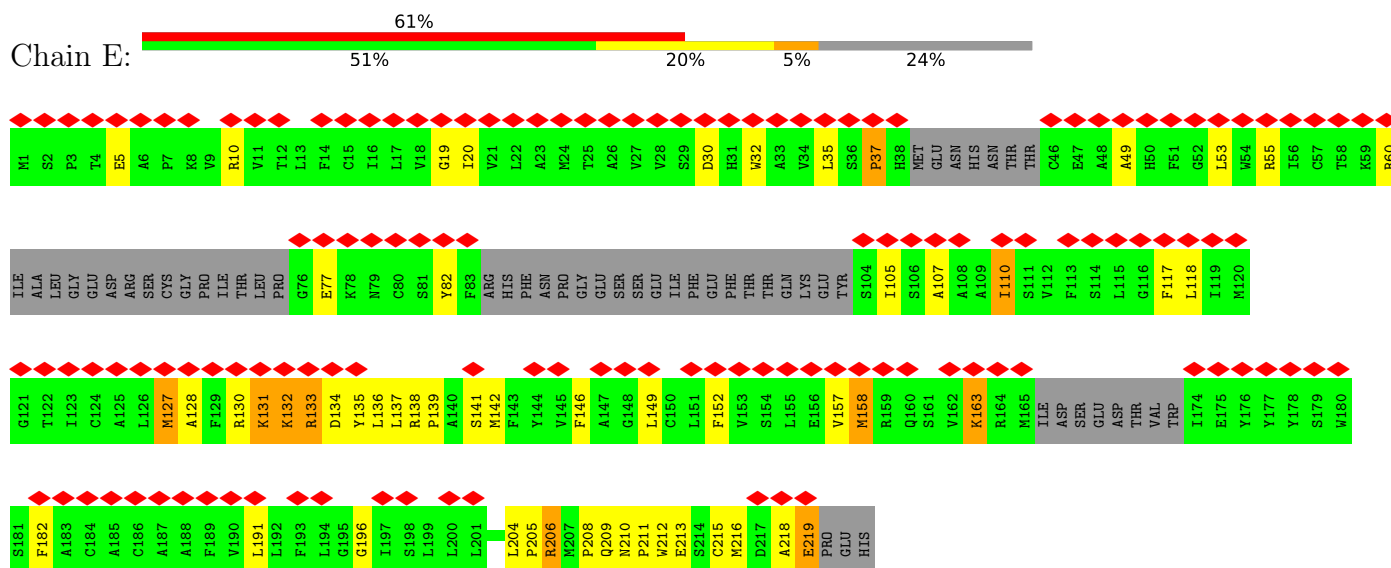
- Molecule 1: Voltage-dependent L-type calcium channel subunit alpha-1S



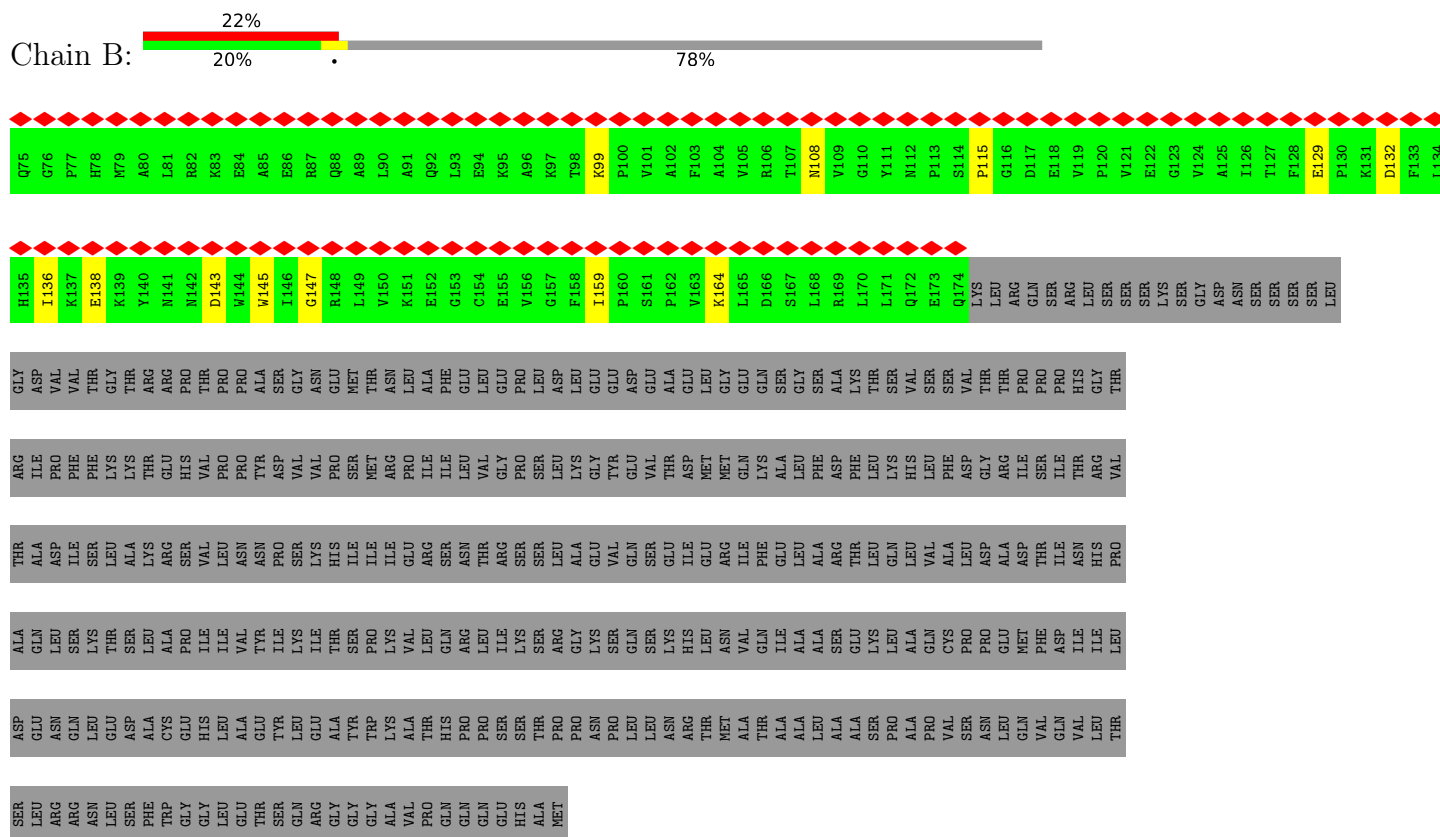




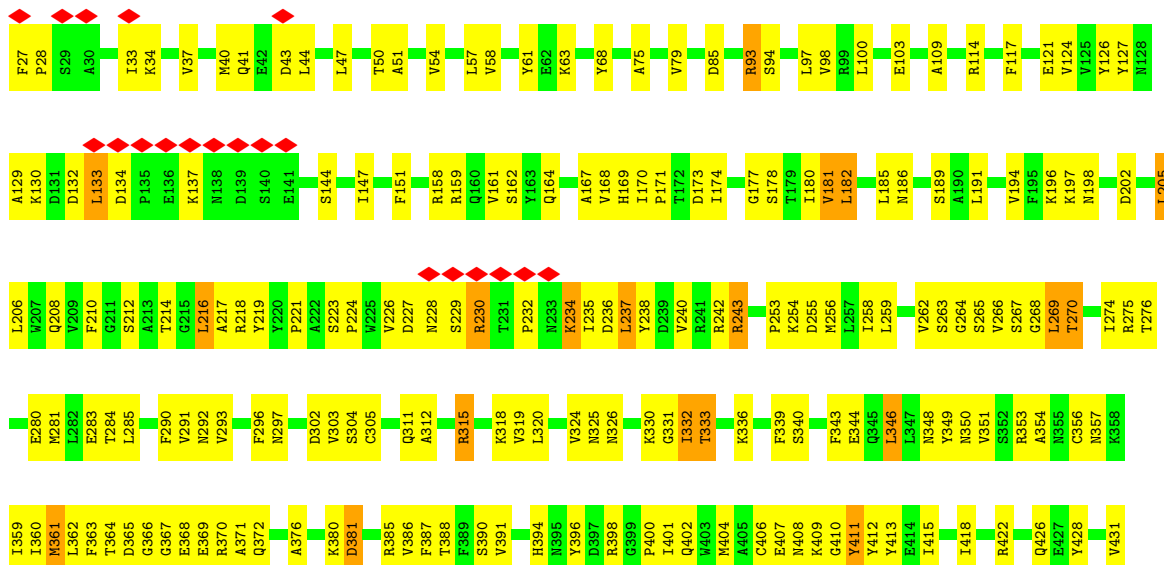
• Molecule 2: Voltage-dependent calcium channel gamma-1 subunit



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



• Molecule 4: Voltage-dependent L-type calcium channel subunit beta-1







- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-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



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	433477	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.142	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	349.12, 349.12, 349.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ETA, CA, PC1, 4YH, NAG, 3PE, 9Z9, BMA

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	0.43	0/10463	0.62	0/14191
2	E	0.55	0/1358	0.69	0/1832
3	B	0.29	0/723	0.45	0/979
4	C	0.31	0/1394	0.49	0/1892
5	F	0.80	1/7974 (0.0%)	0.78	0/10816
All	All	0.59	1/21912 (0.0%)	0.67	0/29710

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	665	ALA	C-N	-6.89	1.21	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10219	0	10305	935	0
2	E	1326	0	1345	124	0
3	B	710	0	633	6	0
4	C	1367	0	1343	96	0
5	F	7804	0	7608	541	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	28	0	25	8	0
6	G	28	0	25	1	0
6	J	28	0	25	0	0
6	K	28	0	25	8	0
7	H	39	0	34	4	0
7	I	39	0	34	1	0
8	L	42	0	37	11	0
9	A	14	0	13	3	0
9	F	98	0	91	15	0
10	A	3	0	0	0	0
11	A	266	0	341	49	0
12	A	93	0	140	13	0
13	A	30	0	0	6	0
14	A	66	0	76	12	0
15	F	4	0	7	4	0
All	All	22232	0	22107	1642	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 37.

All (1642) 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:462:HIS:CE1	1:A:466:ILE:HD11	1.40	1.56
5:F:784:ASN:ND2	9:F:1120:NAG:C1	1.69	1.52
5:F:678:ASN:HD21	6:K:1:NAG:C1	1.19	1.52
5:F:326:ASN:ND2	9:F:1104:NAG:C1	1.72	1.51
1:A:136:THR:HG22	1:A:164:LEU:CD2	1.42	1.49
5:F:988:ASN:HD21	9:F:1122:NAG:C1	1.18	1.49
1:A:1097:PRO:HG2	2:E:218:ALA:CB	1.42	1.46
5:F:1001:ASN:HD21	9:F:1121:NAG:C1	1.27	1.45
1:A:496:PHE:CE2	1:A:537:LYS:HA	1.54	1.43
1:A:136:THR:CG2	1:A:164:LEU:HD23	1.45	1.42
5:F:1001:ASN:ND2	9:F:1121:NAG:C1	1.81	1.40
1:A:366:TYR:CE2	4:C:396:VAL:HG12	1.61	1.36
5:F:678:ASN:ND2	6:K:1:NAG:C1	1.87	1.34
5:F:988:ASN:ND2	9:F:1122:NAG:C1	1.87	1.34
1:A:1097:PRO:HG3	1:A:1413:ALA:CB	1.57	1.31
1:A:366:TYR:CD1	4:C:400:LEU:HD11	1.68	1.28
1:A:539:THR:CG2	1:A:545:LEU:HD12	1.67	1.24
1:A:435:TYR:HE1	1:A:436:TRP:CE3	1.57	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:326:ASN:ND2	9:F:1104:NAG:O5	1.62	1.22
5:F:1070:ASP:OD1	5:F:1072:THR:HG22	1.36	1.22
1:A:109:GLY:C	1:A:113:HIS:HB2	1.63	1.20
1:A:366:TYR:CB	4:C:400:LEU:HD21	1.68	1.19
1:A:1188:LEU:HD12	2:E:142:MET:SD	1.81	1.19
1:A:366:TYR:CE2	4:C:396:VAL:CG1	2.24	1.19
5:F:255:ASP:OD1	5:F:354:ALA:HB3	1.42	1.19
8:L:3:NAG:H82	8:L:3:NAG:C1	1.71	1.18
5:F:132:ASP:OD2	5:F:137:LYS:HG2	1.45	1.17
1:A:1097:PRO:CG	1:A:1413:ALA:CB	2.22	1.16
4:C:290:THR:HA	4:C:293:MET:CE	1.75	1.16
1:A:542:TRP:CH2	1:A:933:LEU:HD12	1.81	1.15
1:A:1068:PHE:CE1	1:A:1381:MET:HE3	1.79	1.15
1:A:366:TYR:HE2	4:C:396:VAL:CG1	1.59	1.15
1:A:269:ASN:HB2	1:A:273:THR:HG23	1.26	1.15
1:A:496:PHE:CE2	1:A:537:LYS:CA	2.31	1.14
1:A:462:HIS:NE2	1:A:466:ILE:HD11	1.60	1.14
5:F:100:LEU:CD1	5:F:198:ASN:HD21	1.59	1.14
1:A:117:TYR:CE1	1:A:118:LEU:CD2	2.31	1.13
1:A:496:PHE:HZ	1:A:537:LYS:HB3	1.13	1.13
1:A:462:HIS:CE1	1:A:466:ILE:CD1	2.30	1.13
1:A:875:VAL:HG11	1:A:906:ARG:NH1	1.64	1.13
1:A:435:TYR:HA	1:A:541:TYR:HE2	1.06	1.13
2:E:134:ASP:HA	2:E:137:LEU:CD2	1.79	1.13
1:A:664:LEU:HD13	13:A:1914:9Z9:C18	1.78	1.12
1:A:109:GLY:CA	1:A:113:HIS:HB2	1.78	1.12
1:A:117:TYR:CE1	1:A:118:LEU:HD21	1.84	1.12
5:F:359:ILE:HG22	5:F:385:ARG:HB2	1.16	1.12
1:A:45:ILE:HG13	1:A:106:ILE:HD12	1.30	1.12
4:C:279:LEU:HD22	4:C:387:VAL:CB	1.80	1.12
5:F:161:VAL:HG21	5:F:221:PRO:HG2	1.19	1.11
5:F:465:THR:CG2	5:F:489:VAL:CG1	2.28	1.11
5:F:47:LEU:HG	8:L:1:NAG:H81	1.27	1.11
1:A:1366:MET:HE2	11:A:1912:3PE:H2A2	1.27	1.11
5:F:100:LEU:HD11	5:F:198:ASN:HD21	1.13	1.11
1:A:1097:PRO:CG	1:A:1413:ALA:HB2	1.78	1.11
1:A:1188:LEU:CD1	2:E:142:MET:SD	2.39	1.10
1:A:542:TRP:CZ2	1:A:933:LEU:HD12	1.86	1.10
1:A:928:ILE:HG22	1:A:932:VAL:HG23	1.28	1.10
4:C:290:THR:HA	4:C:293:MET:HE2	1.18	1.10
1:A:366:TYR:HB3	4:C:400:LEU:HD21	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:PHE:CZ	1:A:537:LYS:HA	1.86	1.09
1:A:435:TYR:CE1	1:A:436:TRP:CE3	2.41	1.09
1:A:1097:PRO:CG	2:E:218:ALA:CB	2.30	1.09
5:F:889:LEU:HD12	5:F:892:ILE:CD1	1.83	1.09
1:A:927:THR:HB	1:A:1066:VAL:HG21	1.35	1.08
2:E:32:TRP:NE1	2:E:158:MET:HG3	1.68	1.08
1:A:257:ASN:HD21	9:A:1901:NAG:C1	1.66	1.08
1:A:1062:GLY:O	1:A:1065:ILE:HG13	1.54	1.08
6:K:2:NAG:H82	6:K:2:NAG:H3	1.36	1.07
1:A:1097:PRO:HG3	1:A:1413:ALA:HB1	1.27	1.07
1:A:1097:PRO:HG2	2:E:218:ALA:HB2	1.34	1.06
1:A:1239:ARG:O	1:A:1242:ARG:HG3	1.52	1.06
1:A:189:ILE:HD13	1:A:654:ASN:ND2	1.71	1.06
2:E:32:TRP:HE1	2:E:158:MET:HG3	0.99	1.06
1:A:45:ILE:HG21	1:A:106:ILE:HD11	1.06	1.05
4:C:279:LEU:CD2	4:C:387:VAL:HB	1.86	1.05
1:A:366:TYR:HB3	4:C:400:LEU:CD2	1.86	1.05
1:A:109:GLY:HA3	1:A:113:HIS:CB	1.86	1.04
1:A:366:TYR:CG	4:C:400:LEU:HD11	1.92	1.04
1:A:45:ILE:HG13	1:A:106:ILE:CD1	1.88	1.04
4:C:279:LEU:HD22	4:C:387:VAL:HB	1.09	1.04
5:F:1074:CYS:O	15:F:1101:ETA:N	1.88	1.04
2:E:20:ILE:HG13	2:E:118:LEU:HD11	1.38	1.04
8:L:3:NAG:C1	8:L:3:NAG:C8	2.31	1.04
5:F:889:LEU:O	5:F:894:VAL:HG12	1.56	1.04
1:A:257:ASN:ND2	9:A:1901:NAG:C1	2.22	1.03
1:A:1046:ILE:CD1	11:A:1908:3PE:H232	1.88	1.03
5:F:178:SER:HB3	5:F:181:VAL:HG12	1.39	1.03
4:C:285:LYS:HA	4:C:290:THR:HG21	1.40	1.03
5:F:889:LEU:HG	5:F:894:VAL:HG11	1.39	1.03
1:A:1069:GLN:O	1:A:1074:THR:HB	1.57	1.03
5:F:100:LEU:HD11	5:F:198:ASN:ND2	1.71	1.03
1:A:504:VAL:O	1:A:508:ILE:HG22	1.58	1.02
1:A:510:GLU:HG3	1:A:527:LEU:HG	1.39	1.02
1:A:544:SER:HB3	1:A:930:ASN:OD1	1.58	1.02
5:F:480:ASN:O	5:F:480:ASN:ND2	1.92	1.02
1:A:496:PHE:HE2	1:A:537:LYS:HA	1.23	1.02
1:A:366:TYR:CG	4:C:400:LEU:HD21	1.94	1.01
1:A:539:THR:HG23	1:A:545:LEU:HD12	1.02	1.01
1:A:291:MET:HG2	1:A:1321:THR:HG23	1.40	1.01
1:A:875:VAL:CG1	1:A:906:ARG:HH12	1.74	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HG21	1:A:106:ILE:CD1	1.90	1.01
1:A:1097:PRO:CG	2:E:218:ALA:HB1	1.87	1.01
1:A:1091:TYR:HD1	1:A:1091:TYR:O	1.43	1.00
1:A:496:PHE:CZ	1:A:537:LYS:CA	2.44	1.00
1:A:1155:VAL:HG22	1:A:1197:VAL:CG1	1.91	1.00
5:F:161:VAL:CG2	5:F:221:PRO:HG2	1.92	1.00
1:A:1366:MET:CE	11:A:1912:3PE:H2A2	1.91	1.00
5:F:889:LEU:CD1	5:F:892:ILE:HD11	1.91	1.00
1:A:1097:PRO:HG2	2:E:218:ALA:HB1	1.05	0.99
1:A:1076:TYR:HE2	1:A:1078:ASN:ND2	1.61	0.99
1:A:1195:ILE:HD11	2:E:117:PHE:CZ	1.97	0.99
5:F:993:PHE:HB2	5:F:1008:VAL:CG1	1.92	0.99
1:A:105:ILE:HG22	1:A:114:GLN:HG3	1.39	0.99
1:A:1168:LYS:O	1:A:1172:PHE:HD2	1.45	0.99
2:E:134:ASP:CA	2:E:137:LEU:HD23	1.92	0.99
5:F:332:ILE:HG22	5:F:333:THR:H	1.23	0.99
1:A:366:TYR:CE1	4:C:400:LEU:HD11	1.96	0.98
5:F:889:LEU:HD12	5:F:892:ILE:HD11	1.00	0.98
5:F:362:LEU:HD11	5:F:401:ILE:HD11	1.42	0.98
1:A:875:VAL:HG11	1:A:906:ARG:HH12	1.24	0.98
4:C:280:VAL:HG21	4:C:371:ILE:HG22	1.42	0.98
1:A:664:LEU:CD1	13:A:1914:9Z9:C18	2.41	0.97
1:A:664:LEU:HD23	1:A:664:LEU:O	1.64	0.97
2:E:134:ASP:HA	2:E:137:LEU:HD23	1.44	0.97
5:F:168:VAL:CG1	5:F:216:LEU:HD21	1.94	0.97
1:A:435:TYR:HA	1:A:541:TYR:CE2	1.99	0.97
1:A:1162:THR:HG21	1:A:1194:ILE:HD11	1.47	0.97
1:A:435:TYR:HE1	1:A:436:TRP:CZ3	1.82	0.97
1:A:75:PRO:HG2	5:F:265:SER:HA	1.45	0.97
1:A:496:PHE:HZ	1:A:537:LYS:CB	1.78	0.97
5:F:510:PRO:HG2	5:F:767:TYR:CE2	1.99	0.97
1:A:210:TYR:OH	1:A:316:THR:HG22	1.65	0.96
5:F:114:ARG:NH2	7:H:1:NAG:H62	1.79	0.96
1:A:366:TYR:CD2	4:C:396:VAL:HG12	1.99	0.96
1:A:309:TRP:CZ3	12:A:1909:PC1:H332	2.01	0.96
2:E:208:PRO:HB3	2:E:213:GLU:CB	1.95	0.96
1:A:792:CYS:O	1:A:796:VAL:HG12	1.64	0.96
5:F:336:LYS:HE3	5:F:369:GLU:OE2	1.66	0.95
1:A:868:PHE:CB	1:A:909:ASN:ND2	2.28	0.95
1:A:1076:TYR:O	1:A:1077:LYS:HE2	1.66	0.95
2:E:135:TYR:HA	2:E:138:ARG:NH1	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:476:GLU:OE1	5:F:478:LYS:HB2	1.65	0.95
1:A:540:LYS:HD2	1:A:541:TYR:HE1	1.32	0.95
1:A:1046:ILE:HD12	11:A:1908:3PE:H232	1.47	0.95
1:A:1096:ARG:HG3	1:A:1097:PRO:HD2	1.48	0.94
5:F:159:ARG:HH22	5:F:226:VAL:HG12	1.32	0.94
5:F:465:THR:HG21	5:F:489:VAL:HG11	1.45	0.94
1:A:540:LYS:HD2	1:A:541:TYR:CE1	2.02	0.94
5:F:659:SER:O	5:F:719:VAL:HG11	1.67	0.94
1:A:539:THR:HG23	1:A:545:LEU:CD1	1.96	0.94
1:A:1096:ARG:HB2	1:A:1096:ARG:CZ	1.98	0.94
5:F:291:VAL:HG12	5:F:312:ALA:HB2	1.49	0.94
5:F:356:CYS:SG	5:F:1062:CYS:HB2	2.07	0.94
1:A:868:PHE:HB3	1:A:909:ASN:HD22	1.32	0.94
2:E:20:ILE:HD11	2:E:118:LEU:HD21	1.47	0.93
1:A:545:LEU:O	1:A:549:VAL:HG23	1.67	0.93
1:A:170:LEU:CD1	11:A:1906:3PE:H3B2	1.98	0.93
5:F:825:ILE:HG21	5:F:846:ARG:NH2	1.82	0.93
1:A:280:PHE:O	1:A:284:THR:HG22	1.67	0.93
1:A:1195:ILE:HD11	2:E:117:PHE:HZ	1.26	0.93
1:A:109:GLY:CA	1:A:113:HIS:CB	2.43	0.92
1:A:1342:SER:O	1:A:1344:TYR:CE1	2.22	0.92
1:A:519:MET:HA	1:A:519:MET:CE	1.97	0.92
1:A:1096:ARG:HG3	1:A:1097:PRO:CD	1.99	0.92
5:F:993:PHE:O	5:F:1008:VAL:HG12	1.70	0.92
4:C:418:ALA:O	4:C:422:LEU:HD23	1.68	0.92
5:F:388:THR:HB	5:F:401:ILE:HG13	1.50	0.92
1:A:435:TYR:CE1	1:A:436:TRP:HE3	1.88	0.92
5:F:161:VAL:HG21	5:F:221:PRO:CG	1.99	0.92
1:A:868:PHE:CE2	1:A:915:LYS:NZ	2.37	0.92
1:A:976:LYS:HD2	1:A:984:GLU:OE2	1.70	0.92
2:E:138:ARG:HD3	2:E:204:LEU:HD23	1.52	0.91
1:A:496:PHE:CZ	1:A:537:LYS:HB3	2.06	0.91
5:F:824:TRP:CG	5:F:864:MET:CE	2.52	0.91
1:A:221:LYS:NZ	12:A:1909:PC1:H121	1.84	0.91
1:A:309:TRP:CZ2	2:E:152:PHE:HZ	1.87	0.91
1:A:1007:LEU:HA	1:A:1010:VAL:HG12	1.51	0.91
1:A:1007:LEU:HA	1:A:1010:VAL:CG1	2.01	0.91
1:A:1366:MET:CE	11:A:1912:3PE:C2A	2.47	0.91
1:A:519:MET:O	1:A:520:THR:HG22	1.70	0.90
5:F:266:VAL:O	5:F:270:THR:HG23	1.71	0.90
5:F:669:TYR:CD1	5:F:704:LEU:CD2	2.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:THR:CG2	1:A:545:LEU:CD1	2.50	0.90
1:A:1097:PRO:CG	1:A:1413:ALA:HB1	1.95	0.90
1:A:475:PHE:HE2	1:A:534:ARG:HD3	1.34	0.90
1:A:559:ILE:HD13	1:A:659:ILE:HD11	1.54	0.90
1:A:508:ILE:HD12	1:A:511:LEU:HD23	1.54	0.90
5:F:159:ARG:NH2	5:F:226:VAL:HG12	1.86	0.89
1:A:1338:CYS:SG	1:A:1352:CYS:HB2	2.12	0.89
5:F:117:PHE:CG	5:F:182:LEU:HD12	2.08	0.89
1:A:976:LYS:NZ	1:A:984:GLU:HG3	1.88	0.89
5:F:892:ILE:HG13	5:F:894:VAL:HG12	1.55	0.89
1:A:109:GLY:HA3	1:A:113:HIS:HB2	1.51	0.89
2:E:134:ASP:O	2:E:137:LEU:HD23	1.70	0.89
5:F:1070:ASP:CG	5:F:1072:THR:HG22	1.91	0.89
1:A:45:ILE:CG2	1:A:106:ILE:HD11	2.00	0.89
1:A:1065:ILE:HD12	1:A:1066:VAL:N	1.87	0.89
1:A:1389:ARG:HH21	1:A:1389:ARG:HG3	1.37	0.89
2:E:134:ASP:C	2:E:137:LEU:HD23	1.92	0.89
5:F:710:LEU:HD21	5:F:714:PHE:CZ	2.08	0.89
2:E:134:ASP:HA	2:E:137:LEU:HD21	1.54	0.88
1:A:959:ASP:HB3	1:A:972:TYR:CD2	2.08	0.88
5:F:824:TRP:CG	5:F:864:MET:HE1	2.08	0.88
1:A:170:LEU:HD13	11:A:1906:3PE:H3B2	1.56	0.88
1:A:925:ILE:HD11	1:A:1370:PHE:CZ	2.08	0.88
5:F:350:ASN:HD21	6:D:1:NAG:C1	1.87	0.88
5:F:993:PHE:HB2	5:F:1008:VAL:HG13	1.54	0.88
1:A:496:PHE:CE2	1:A:537:LYS:O	2.26	0.88
1:A:181:SER:O	1:A:184:VAL:HG22	1.72	0.88
1:A:117:TYR:CE1	1:A:118:LEU:HD23	2.08	0.88
1:A:291:MET:HG2	1:A:1321:THR:CG2	2.04	0.88
1:A:366:TYR:HE2	4:C:396:VAL:CB	1.87	0.88
1:A:462:HIS:O	1:A:466:ILE:HG13	1.74	0.88
5:F:276:THR:O	5:F:280:GLU:HG2	1.74	0.88
5:F:367:GLY:O	5:F:400:PRO:HG2	1.73	0.87
5:F:510:PRO:HG2	5:F:767:TYR:CD2	2.08	0.87
1:A:520:THR:OG1	1:A:521:PRO:HD2	1.74	0.87
1:A:1180:ASP:HB3	1:A:1183:ASN:ND2	1.89	0.87
1:A:269:ASN:HD22	1:A:273:THR:HG21	1.40	0.86
4:C:285:LYS:HA	4:C:290:THR:CG2	2.06	0.86
1:A:976:LYS:HZ3	1:A:984:GLU:HG3	1.39	0.86
1:A:52:PRO:O	1:A:56:ILE:HG23	1.75	0.86
1:A:113:HIS:O	1:A:116:ALA:HB3	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:O	1:A:57:ILE:HG22	1.73	0.86
1:A:94:LEU:HD11	1:A:134:VAL:CG1	2.06	0.86
11:A:1912:3PE:H221	11:A:1912:3PE:O31	1.74	0.86
1:A:1064:VAL:O	1:A:1067:THR:HG22	1.75	0.86
1:A:1266:ALA:C	1:A:1267:LEU:HD13	1.95	0.86
2:E:132:LYS:HD3	2:E:132:LYS:N	1.88	0.86
2:E:208:PRO:HB3	2:E:213:GLU:HB3	1.58	0.86
5:F:480:ASN:HA	5:F:483:ASN:HB2	1.58	0.86
1:A:535:LEU:O	1:A:538:ILE:HG22	1.76	0.85
5:F:591:ARG:HH22	9:F:1115:NAG:HN2	1.23	0.85
5:F:889:LEU:O	5:F:894:VAL:CG1	2.24	0.85
1:A:528:ARG:O	1:A:531:ARG:HG3	1.76	0.85
1:A:545:LEU:HD22	1:A:549:VAL:HG23	1.56	0.85
1:A:631:SER:O	1:A:635:VAL:HG22	1.76	0.85
4:C:283:SER:HB3	4:C:290:THR:HB	1.55	0.85
1:A:927:THR:HB	1:A:1066:VAL:CG2	2.05	0.85
5:F:263:SER:O	5:F:266:VAL:HG22	1.75	0.85
1:A:542:TRP:CE3	1:A:545:LEU:HB2	2.11	0.85
1:A:793:HIS:HA	1:A:796:VAL:CG1	2.07	0.85
5:F:361:MET:HE2	5:F:387:PHE:CD1	2.12	0.85
1:A:496:PHE:HE2	1:A:537:LYS:CA	1.77	0.84
1:A:545:LEU:O	1:A:545:LEU:HD22	1.77	0.84
1:A:928:ILE:CG2	1:A:932:VAL:HG23	2.07	0.84
1:A:1155:VAL:HG22	1:A:1197:VAL:HG13	1.57	0.84
5:F:465:THR:CG2	5:F:489:VAL:HG11	2.04	0.84
1:A:548:LEU:HD13	1:A:930:ASN:HB3	1.59	0.84
6:D:1:NAG:H83	6:D:2:NAG:C7	2.07	0.84
1:A:1068:PHE:CE1	1:A:1381:MET:CE	2.60	0.84
1:A:1097:PRO:CB	1:A:1413:ALA:CB	2.55	0.84
1:A:45:ILE:CG1	1:A:106:ILE:HD12	2.08	0.84
1:A:1336:LYS:HB2	1:A:1352:CYS:O	1.78	0.84
4:C:418:ALA:O	4:C:422:LEU:CD2	2.25	0.84
1:A:435:TYR:CD2	1:A:541:TYR:HD2	1.95	0.84
1:A:1105:ASN:O	1:A:1109:TYR:HB3	1.77	0.84
1:A:138:ILE:O	1:A:142:VAL:HG23	1.78	0.83
5:F:168:VAL:CG1	5:F:216:LEU:CD2	2.56	0.83
5:F:168:VAL:HG13	5:F:216:LEU:HD21	1.60	0.83
1:A:927:THR:CB	1:A:1066:VAL:HG21	2.07	0.83
1:A:330:LEU:HD21	13:A:1914:9Z9:C76	2.08	0.83
1:A:494:SER:HB3	1:A:497:ASN:HB2	1.59	0.83
1:A:496:PHE:CZ	1:A:537:LYS:CB	2.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PHE:CB	1:A:909:ASN:HD22	1.90	0.83
5:F:206:LEU:CD2	5:F:458:LEU:HD21	2.08	0.83
5:F:361:MET:CE	5:F:387:PHE:CD1	2.61	0.83
5:F:824:TRP:C	5:F:864:MET:HE1	1.99	0.83
5:F:134:ASP:HB2	5:F:137:LYS:HD3	1.60	0.83
1:A:376:MET:O	4:C:295:LYS:HE3	1.78	0.83
4:C:290:THR:CA	4:C:293:MET:HE2	2.06	0.83
1:A:662:ASP:O	1:A:666:GLU:HG2	1.79	0.83
1:A:114:GLN:O	1:A:117:TYR:HD1	1.61	0.82
1:A:901:VAL:O	1:A:904:PRO:HD2	1.79	0.82
5:F:170:ILE:HD13	5:F:216:LEU:HD23	1.58	0.82
5:F:350:ASN:ND2	6:D:1:NAG:C1	2.41	0.82
5:F:1010:LYS:CG	5:F:1017:ILE:HG13	2.09	0.82
1:A:868:PHE:CD2	1:A:915:LYS:NZ	2.47	0.82
2:E:138:ARG:HD3	2:E:204:LEU:CD2	2.10	0.82
1:A:976:LYS:NZ	1:A:984:GLU:CG	2.43	0.82
5:F:243:ARG:HH21	5:F:243:ARG:HG3	1.45	0.82
1:A:519:MET:O	1:A:520:THR:CG2	2.28	0.82
1:A:903:ARG:O	1:A:906:ARG:HG2	1.79	0.82
1:A:868:PHE:HB2	1:A:909:ASN:ND2	1.94	0.82
1:A:599:ASN:HD22	1:A:601:PRO:HD2	1.44	0.81
1:A:1136:GLY:O	11:A:1911:3PE:H251	1.79	0.81
2:E:20:ILE:CD1	2:E:118:LEU:HD21	2.10	0.81
1:A:117:TYR:HE1	1:A:118:LEU:HD21	1.41	0.81
1:A:664:LEU:HD23	1:A:664:LEU:C	1.99	0.81
1:A:106:ILE:HG13	1:A:107:ALA:H	1.44	0.81
1:A:494:SER:HB3	1:A:497:ASN:CG	2.00	0.81
1:A:798:ALA:HB1	1:A:800:TRP:CZ3	2.14	0.81
5:F:515:PHE:HE2	5:F:580:MET:HE3	1.46	0.81
1:A:1162:THR:HG22	1:A:1190:VAL:CG1	2.11	0.81
5:F:47:LEU:HG	8:L:1:NAG:C8	2.09	0.81
5:F:1070:ASP:OD1	5:F:1072:THR:CG2	2.24	0.81
1:A:61:ILE:HD11	1:A:171:ARG:O	1.81	0.81
1:A:116:ALA:O	1:A:119:ARG:HB2	1.79	0.81
1:A:921:VAL:HG13	1:A:1370:PHE:HE2	1.45	0.81
1:A:1096:ARG:HB2	1:A:1096:ARG:NH1	1.96	0.81
5:F:781:PRO:O	5:F:875:GLY:HA3	1.81	0.81
1:A:1155:VAL:CG2	1:A:1197:VAL:HG13	2.11	0.80
5:F:43:ASP:OD1	8:L:1:NAG:H2	1.81	0.80
5:F:465:THR:CG2	5:F:489:VAL:HG12	2.11	0.80
1:A:366:TYR:HE2	4:C:396:VAL:HG12	1.07	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:VAL:CG1	1:A:1055:PHE:HE2	1.94	0.80
5:F:824:TRP:CD1	5:F:864:MET:HE1	2.17	0.80
1:A:1096:ARG:HG3	1:A:1097:PRO:N	1.95	0.80
1:A:1188:LEU:HD13	2:E:142:MET:SD	2.20	0.80
5:F:858:ASP:HA	5:F:986:PHE:CZ	2.17	0.80
1:A:338:THR:O	1:A:342:GLU:HG2	1.80	0.80
5:F:887:ARG:O	5:F:890:VAL:HG22	1.82	0.80
1:A:180:PRO:HA	1:A:183:GLN:NE2	1.96	0.80
1:A:494:SER:HB3	1:A:497:ASN:CB	2.11	0.80
1:A:927:THR:CB	1:A:1066:VAL:CG2	2.60	0.80
5:F:359:ILE:CG2	5:F:385:ARG:HB2	2.08	0.80
1:A:91:TYR:O	1:A:95:THR:HG23	1.81	0.79
1:A:1342:SER:O	1:A:1344:TYR:HE1	1.64	0.79
5:F:481:LEU:HD23	5:F:482:LYS:H	1.46	0.79
1:A:1068:PHE:CG	1:A:1073:GLU:HG2	2.18	0.79
1:A:435:TYR:CD2	1:A:541:TYR:CD2	2.71	0.79
1:A:1366:MET:HE1	11:A:1912:3PE:H2A1	1.65	0.78
1:A:1366:MET:HE3	11:A:1912:3PE:H2C1	1.65	0.78
2:E:32:TRP:HE1	2:E:158:MET:CG	1.91	0.78
5:F:168:VAL:HG22	5:F:218:ARG:HG2	1.64	0.78
1:A:56:ILE:HG13	1:A:57:ILE:N	1.97	0.78
5:F:1010:LYS:HG3	5:F:1017:ILE:HG13	1.64	0.78
1:A:309:TRP:CZ2	2:E:152:PHE:CZ	2.71	0.78
1:A:542:TRP:CD2	1:A:545:LEU:HB2	2.18	0.78
1:A:221:LYS:HZ3	12:A:1909:PC1:H121	1.46	0.78
1:A:519:MET:O	1:A:520:THR:CB	2.32	0.78
5:F:356:CYS:SG	5:F:1062:CYS:CB	2.71	0.78
5:F:465:THR:HG23	5:F:489:VAL:HG12	1.66	0.78
5:F:663:PHE:HB2	5:F:744:THR:HG23	1.63	0.78
1:A:105:ILE:CG2	1:A:114:GLN:HG3	2.14	0.77
5:F:669:TYR:CE1	5:F:704:LEU:HD21	2.19	0.77
1:A:868:PHE:CD2	1:A:909:ASN:ND2	2.53	0.77
5:F:590:PHE:CD2	5:F:592:THR:HG23	2.18	0.77
1:A:104:LYS:O	1:A:108:TYR:HD2	1.68	0.77
11:A:1907:3PE:H111	11:A:1908:3PE:H121	1.65	0.77
5:F:669:TYR:CE1	5:F:704:LEU:CD2	2.68	0.77
2:E:138:ARG:CD	2:E:204:LEU:HD23	2.14	0.77
5:F:591:ARG:NH2	9:F:1115:NAG:HN2	1.81	0.77
1:A:868:PHE:HB2	1:A:909:ASN:HD21	1.49	0.77
1:A:928:ILE:HG21	1:A:1059:ILE:HG23	1.65	0.77
1:A:1249:ARG:HE	1:A:1249:ARG:HA	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:LEU:HD12	1:A:1329:LEU:O	1.84	0.76
2:E:30:ASP:OD2	2:E:55:ARG:HG3	1.85	0.76
1:A:425:CYS:O	1:A:429:VAL:HG23	1.85	0.76
8:L:1:NAG:O3	8:L:1:NAG:H83	1.86	0.76
1:A:134:VAL:O	1:A:138:ILE:HG12	1.85	0.76
5:F:259:LEU:O	5:F:362:LEU:HA	1.86	0.76
5:F:1008:VAL:HG23	5:F:1019:ILE:HG22	1.67	0.76
1:A:559:ILE:CD1	1:A:659:ILE:HD11	2.16	0.76
1:A:1091:TYR:O	1:A:1091:TYR:CD1	2.34	0.76
1:A:947:VAL:O	1:A:951:LYS:HB2	1.85	0.76
5:F:465:THR:HG22	5:F:489:VAL:CG1	2.16	0.76
1:A:1242:ARG:O	1:A:1245:LYS:HG3	1.86	0.76
4:C:280:VAL:HB	4:C:371:ILE:O	1.85	0.76
1:A:112:PHE:O	1:A:115:ASP:HB3	1.86	0.75
1:A:1389:ARG:HG3	1:A:1389:ARG:NH2	1.98	0.75
1:A:868:PHE:HD2	1:A:909:ASN:ND2	1.83	0.75
1:A:1162:THR:CG2	1:A:1194:ILE:HD11	2.16	0.75
14:A:1915[A]:4YH:H30	14:A:1915[A]:4YH:H20	1.68	0.75
5:F:178:SER:HB3	5:F:181:VAL:CG1	2.14	0.75
5:F:359:ILE:HG22	5:F:385:ARG:CB	2.07	0.75
2:E:127:MET:CG	2:E:136:LEU:HD21	2.16	0.75
5:F:388:THR:CB	5:F:401:ILE:HG13	2.16	0.75
5:F:1074:CYS:C	15:F:1101:ETA:HB1	2.08	0.75
1:A:556:ILE:HG12	1:A:556:ILE:O	1.85	0.74
1:A:1097:PRO:CB	1:A:1413:ALA:HB1	2.17	0.74
1:A:905:LEU:CD2	1:A:1280:ILE:HD11	2.16	0.74
1:A:601:PRO:HB3	11:A:1908:3PE:H32	1.69	0.74
5:F:824:TRP:CG	5:F:864:MET:HE3	2.22	0.74
1:A:1132:THR:HG23	1:A:1243:LEU:HD11	1.67	0.74
5:F:256:MET:HB2	5:F:359:ILE:CD1	2.18	0.74
5:F:855:ILE:O	5:F:856:LEU:HD12	1.87	0.74
1:A:934:VAL:HG11	1:A:1055:PHE:HE2	1.51	0.74
1:A:964:THR:HG22	1:A:966:GLU:H	1.51	0.74
1:A:496:PHE:CE2	1:A:537:LYS:C	2.60	0.74
5:F:332:ILE:HG22	5:F:333:THR:N	2.01	0.74
1:A:103:MET:HA	1:A:106:ILE:HG12	1.70	0.73
1:A:959:ASP:HB3	1:A:972:TYR:CE2	2.22	0.73
1:A:435:TYR:HD2	1:A:541:TYR:CD2	2.06	0.73
11:A:1912:3PE:H221	11:A:1912:3PE:C3	2.18	0.73
1:A:1096:ARG:CG	1:A:1097:PRO:HD2	2.18	0.73
2:E:136:LEU:C	2:E:139:PRO:HD2	2.09	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:590:PHE:HD2	5:F:592:THR:HG23	1.52	0.73
5:F:515:PHE:HE2	5:F:580:MET:CE	2.00	0.73
1:A:294:TRP:HE1	1:A:1321:THR:HG21	1.54	0.73
1:A:435:TYR:CE1	1:A:436:TRP:CZ3	2.73	0.73
1:A:902:LEU:HD23	1:A:902:LEU:O	1.87	0.73
5:F:206:LEU:HD23	5:F:458:LEU:CD2	2.19	0.73
5:F:889:LEU:CG	5:F:894:VAL:HG11	2.17	0.73
1:A:520:THR:OG1	1:A:521:PRO:CD	2.37	0.73
5:F:117:PHE:CD1	5:F:182:LEU:HD12	2.23	0.73
5:F:825:ILE:CG2	5:F:846:ARG:NH2	2.51	0.73
1:A:1069:GLN:HA	1:A:1073:GLU:HB2	1.71	0.73
5:F:275:ARG:HD2	5:F:325:ASN:HA	1.69	0.73
5:F:590:PHE:HE2	5:F:592:THR:HG21	1.53	0.73
1:A:269:ASN:HB2	1:A:273:THR:CG2	2.15	0.72
1:A:463:LEU:HD22	1:A:463:LEU:O	1.89	0.72
1:A:496:PHE:HE2	1:A:537:LYS:C	1.90	0.72
2:E:127:MET:HG2	2:E:136:LEU:HD21	1.70	0.72
5:F:243:ARG:HG3	5:F:243:ARG:NH2	2.00	0.72
1:A:934:VAL:CG1	1:A:1055:PHE:CE2	2.72	0.72
1:A:895:ILE:HG23	1:A:896:LEU:HD23	1.70	0.72
1:A:366:TYR:CD1	4:C:400:LEU:CD1	2.63	0.72
1:A:94:LEU:HD11	1:A:134:VAL:HG12	1.71	0.72
5:F:255:ASP:OD1	5:F:354:ALA:CB	2.31	0.72
1:A:365:GLY:HA2	4:C:437:ASN:O	1.90	0.72
1:A:898:VAL:O	1:A:901:VAL:HG12	1.89	0.72
5:F:205:LEU:HD21	5:F:492:VAL:CG2	2.19	0.72
5:F:513:TYR:O	5:F:624:LEU:HD12	1.90	0.72
1:A:172:PRO:O	1:A:175:LEU:HB2	1.89	0.72
1:A:247:ARG:O	1:A:248:THR:OG1	2.05	0.71
5:F:100:LEU:CD1	5:F:198:ASN:ND2	2.38	0.71
1:A:318:ILE:O	1:A:322:SER:HB2	1.89	0.71
1:A:366:TYR:CE2	4:C:396:VAL:CB	2.68	0.71
5:F:229:SER:O	5:F:235:ILE:HG22	1.91	0.71
5:F:669:TYR:CD1	5:F:704:LEU:HD22	2.24	0.71
5:F:133:LEU:H	5:F:133:LEU:CD2	2.03	0.71
5:F:235:ILE:O	5:F:235:ILE:HD12	1.91	0.71
5:F:847:ASN:ND2	5:F:847:ASN:O	2.24	0.71
1:A:545:LEU:HD22	1:A:549:VAL:CG2	2.19	0.71
1:A:875:VAL:CG1	1:A:906:ARG:NH1	2.40	0.71
1:A:1111:VAL:HG12	1:A:1171:ALA:HB2	1.71	0.71
1:A:114:GLN:O	1:A:117:TYR:CD1	2.44	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:604:LEU:HB3	11:A:1908:3PE:H221	1.73	0.71
5:F:478:LYS:HD3	5:F:478:LYS:C	2.11	0.71
11:A:1907:3PE:H111	11:A:1908:3PE:C12	2.20	0.71
5:F:159:ARG:NH2	5:F:226:VAL:CG1	2.54	0.71
1:A:132:LEU:O	1:A:136:THR:HG23	1.90	0.71
1:A:559:ILE:HD13	1:A:659:ILE:CD1	2.19	0.71
1:A:1373:ILE:HG12	13:A:1914:9Z9:C79	2.21	0.71
1:A:1091:TYR:CE1	2:E:212:TRP:HB3	2.26	0.70
1:A:366:TYR:CG	4:C:400:LEU:CD1	2.74	0.70
1:A:976:LYS:N	1:A:976:LYS:HE3	2.06	0.70
1:A:1172:PHE:O	1:A:1174:ALA:N	2.24	0.70
5:F:705:ILE:HD12	5:F:706:ASN:N	2.06	0.70
1:A:138:ILE:N	1:A:138:ILE:HD13	2.03	0.70
1:A:366:TYR:OH	4:C:391:ILE:CG2	2.40	0.70
1:A:435:TYR:CA	1:A:541:TYR:HE2	1.95	0.70
1:A:868:PHE:HE2	1:A:915:LYS:NZ	1.89	0.70
1:A:927:THR:HG21	1:A:1066:VAL:HG22	1.73	0.70
5:F:510:PRO:HG2	5:F:767:TYR:HE2	1.57	0.70
5:F:93:ARG:NH1	5:F:202:ASP:OD2	2.25	0.70
1:A:1162:THR:HG22	1:A:1190:VAL:HG13	1.72	0.70
5:F:595:LYS:HD3	5:F:599:GLU:OE1	1.91	0.70
1:A:1007:LEU:CA	1:A:1010:VAL:HG12	2.22	0.70
1:A:1076:TYR:O	1:A:1077:LYS:CE	2.38	0.70
5:F:210:PHE:HB2	5:F:490:MET:HE2	1.73	0.70
5:F:988:ASN:CG	9:F:1122:NAG:C1	2.60	0.70
5:F:411:TYR:CD1	5:F:1074:CYS:HA	2.27	0.69
1:A:1161:PHE:O	1:A:1164:GLU:HG3	1.91	0.69
2:E:127:MET:CG	2:E:136:LEU:CD2	2.69	0.69
1:A:106:ILE:HG13	1:A:107:ALA:N	2.08	0.69
1:A:1155:VAL:HG22	1:A:1197:VAL:HG11	1.70	0.69
2:E:208:PRO:HB3	2:E:213:GLU:HB2	1.73	0.69
1:A:519:MET:O	1:A:520:THR:HB	1.92	0.69
1:A:905:LEU:HD23	1:A:1280:ILE:HD11	1.75	0.69
1:A:976:LYS:HZ3	1:A:984:GLU:CG	2.06	0.69
1:A:1097:PRO:CG	2:E:218:ALA:HB2	2.13	0.69
5:F:850:VAL:HG22	5:F:851:MET:HG2	1.72	0.69
1:A:1068:PHE:CZ	1:A:1381:MET:CE	2.75	0.69
1:A:1338:CYS:HG	1:A:1352:CYS:CB	2.06	0.69
1:A:1366:MET:HE1	11:A:1912:3PE:C2A	2.21	0.69
1:A:199:ILE:O	1:A:203:VAL:HG23	1.93	0.69
4:C:280:VAL:HG12	4:C:285:LYS:NZ	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:339:PHE:CZ	5:F:362:LEU:HD23	2.28	0.69
5:F:1074:CYS:C	15:F:1101:ETA:HN1	1.95	0.69
2:E:130:ARG:O	2:E:131:LYS:HB2	1.92	0.69
2:E:132:LYS:HD3	2:E:132:LYS:H	1.57	0.69
4:C:285:LYS:CA	4:C:290:THR:HG21	2.21	0.69
5:F:388:THR:HB	5:F:401:ILE:CG1	2.23	0.69
1:A:1097:PRO:HG2	1:A:1413:ALA:HB2	1.73	0.69
1:A:1155:VAL:CG2	1:A:1197:VAL:CG1	2.67	0.69
1:A:1320:ALA:O	14:A:1916[B]:4YH:H33	1.93	0.69
5:F:478:LYS:HD3	5:F:478:LYS:O	1.93	0.69
5:F:996:VAL:HG23	5:F:1004:ARG:O	1.92	0.69
1:A:53:PHE:HA	1:A:56:ILE:HG12	1.73	0.68
1:A:295:THR:HG21	1:A:1318:ARG:HG3	1.75	0.68
5:F:370:ARG:CD	5:F:372:GLN:HE21	2.06	0.68
1:A:210:TYR:OH	1:A:316:THR:CG2	2.41	0.68
1:A:539:THR:HG21	1:A:545:LEU:HD12	1.72	0.68
5:F:206:LEU:CD2	5:F:458:LEU:CD2	2.71	0.68
1:A:934:VAL:HG12	1:A:1055:PHE:CE2	2.28	0.68
5:F:124:VAL:HG21	5:F:182:LEU:HD13	1.75	0.68
5:F:590:PHE:CE2	5:F:592:THR:HG21	2.28	0.68
1:A:366:TYR:CE2	4:C:396:VAL:HB	2.29	0.68
1:A:542:TRP:CE3	1:A:545:LEU:CB	2.76	0.68
1:A:1097:PRO:CB	1:A:1413:ALA:HB2	2.19	0.68
5:F:461:VAL:HG12	5:F:495:SER:HA	1.74	0.68
5:F:478:LYS:HD2	5:F:479:THR:HG23	1.73	0.68
1:A:269:ASN:CB	1:A:273:THR:HG23	2.16	0.68
1:A:1076:TYR:CE2	1:A:1078:ASN:ND2	2.53	0.68
5:F:889:LEU:O	5:F:892:ILE:HG13	1.92	0.68
5:F:889:LEU:HA	5:F:892:ILE:HD11	1.75	0.68
2:E:134:ASP:CA	2:E:137:LEU:CD2	2.57	0.68
5:F:311:GLN:HE22	5:F:520:ASN:HD21	1.41	0.68
5:F:359:ILE:HD13	5:F:361:MET:HE3	1.74	0.68
5:F:993:PHE:HB2	5:F:1008:VAL:HG11	1.75	0.68
1:A:309:TRP:HB3	12:A:1909:PC1:H221	1.75	0.68
1:A:976:LYS:HD2	1:A:984:GLU:CD	2.14	0.68
5:F:168:VAL:HG11	5:F:216:LEU:HD21	1.76	0.68
5:F:398:ARG:O	5:F:402:GLN:HG3	1.94	0.68
1:A:926:ARG:HG3	1:A:926:ARG:O	1.94	0.68
5:F:411:TYR:CE1	5:F:1074:CYS:HA	2.29	0.68
1:A:508:ILE:HG13	1:A:508:ILE:O	1.93	0.67
1:A:1097:PRO:C	2:E:218:ALA:HB2	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:O	1:A:61:ILE:HG13	1.94	0.67
1:A:291:MET:HE2	11:A:1913:3PE:H12	1.76	0.67
5:F:162:SER:O	5:F:221:PRO:HB2	1.93	0.67
1:A:539:THR:HG21	1:A:545:LEU:CD1	2.23	0.67
5:F:132:ASP:OD2	5:F:137:LYS:CG	2.36	0.67
1:A:976:LYS:HZ2	1:A:984:GLU:CG	2.05	0.67
1:A:75:PRO:O	1:A:77:ASP:N	2.28	0.67
1:A:1025:ASP:HB3	1:A:1033:PRO:HB3	1.77	0.67
1:A:1091:TYR:HD1	1:A:1091:TYR:C	1.98	0.67
1:A:542:TRP:CH2	1:A:933:LEU:CD1	2.71	0.67
5:F:44:LEU:HD11	5:F:824:TRP:CZ2	2.29	0.67
1:A:331:GLY:HA2	1:A:1380:ILE:HD12	1.75	0.67
1:A:116:ALA:HA	1:A:119:ARG:CG	2.25	0.67
1:A:513:LEU:HD22	1:A:519:MET:SD	2.34	0.67
1:A:1259:THR:CG2	1:A:1383:ASN:OD1	2.43	0.67
1:A:1329:LEU:HD12	1:A:1329:LEU:C	2.15	0.67
1:A:454:HIS:HD2	1:A:1029:GLU:OE2	1.78	0.66
5:F:858:ASP:HA	5:F:986:PHE:CE1	2.30	0.66
1:A:919:GLN:O	1:A:923:VAL:HG23	1.96	0.66
5:F:705:ILE:HD12	5:F:705:ILE:C	2.15	0.66
4:C:284:LEU:HG	4:C:418:ALA:HB3	1.75	0.66
5:F:515:PHE:CE2	5:F:580:MET:HE3	2.30	0.66
5:F:858:ASP:HB3	5:F:986:PHE:CE2	2.30	0.66
1:A:365:GLY:CA	4:C:437:ASN:O	2.43	0.66
1:A:564:LEU:HD21	11:A:1907:3PE:H3E1	1.77	0.66
1:A:664:LEU:C	1:A:664:LEU:CD2	2.63	0.66
12:A:1910:PC1:H272	12:A:1910:PC1:H2C1	1.78	0.66
5:F:783:PHE:CE1	5:F:873:GLN:HB2	2.31	0.66
1:A:1091:TYR:HA	2:E:212:TRP:CE3	2.31	0.66
1:A:1236:ARG:HG2	1:A:1239:ARG:CZ	2.25	0.66
5:F:478:LYS:CD	5:F:479:THR:HG23	2.26	0.66
1:A:601:PRO:HG3	11:A:1907:3PE:O22	1.96	0.66
1:A:227:TYR:CD2	1:A:262:ARG:HB3	2.30	0.66
1:A:1140:TYR:O	1:A:1141:HIS:HB2	1.94	0.66
1:A:1199:LEU:HD23	1:A:1232:SER:OG	1.95	0.66
1:A:1334:TYR:O	1:A:1353:GLY:HA3	1.95	0.66
2:E:208:PRO:O	2:E:209:GLN:HB2	1.95	0.66
5:F:348:ASN:O	5:F:350:ASN:N	2.29	0.66
1:A:104:LYS:O	1:A:108:TYR:CD2	2.49	0.65
1:A:94:LEU:HD11	1:A:134:VAL:HG13	1.78	0.65
1:A:435:TYR:CD1	1:A:436:TRP:HE3	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LYS:HE2	4:C:445:HIS:CG	2.31	0.65
1:A:1112:TRP:O	1:A:1116:THR:HG23	1.96	0.65
5:F:114:ARG:HH21	7:H:1:NAG:H62	1.61	0.65
1:A:269:ASN:O	1:A:270:HIS:HB2	1.95	0.65
1:A:1282:ALA:O	1:A:1286:MET:HG3	1.95	0.65
5:F:339:PHE:O	5:F:343:PHE:HD2	1.79	0.65
5:F:891:ASN:OD1	9:F:1107:NAG:O5	2.08	0.65
1:A:189:ILE:CD1	1:A:654:ASN:ND2	2.55	0.65
1:A:636:LEU:O	1:A:639:ILE:HG23	1.97	0.65
1:A:1168:LYS:O	1:A:1172:PHE:CD2	2.38	0.65
11:A:1905:3PE:C35	11:A:1913:3PE:C39	2.74	0.65
5:F:256:MET:HB2	5:F:359:ILE:HD11	1.79	0.65
1:A:905:LEU:O	1:A:908:ILE:HG23	1.96	0.65
1:A:1096:ARG:HG3	2:E:218:ALA:HB3	1.77	0.65
5:F:361:MET:HE2	5:F:387:PHE:HD1	1.62	0.65
5:F:783:PHE:HE1	5:F:873:GLN:CB	2.09	0.65
1:A:57:ILE:HD11	1:A:174:ARG:HH12	1.61	0.65
1:A:109:GLY:HA3	1:A:113:HIS:HB3	1.74	0.65
1:A:109:GLY:O	1:A:110:PHE:O	2.15	0.65
1:A:169:VAL:CG2	1:A:575:LEU:HB2	2.27	0.65
1:A:295:THR:HG21	1:A:1318:ARG:CG	2.26	0.65
5:F:339:PHE:HZ	5:F:362:LEU:HD23	1.62	0.65
1:A:1121:GLU:HA	1:A:1121:GLU:OE1	1.94	0.65
5:F:366:GLY:HA3	5:F:396:TYR:CB	2.26	0.65
5:F:783:PHE:HE1	5:F:873:GLN:HA	1.62	0.65
1:A:124:VAL:O	1:A:128:ILE:HG13	1.97	0.65
1:A:1333:SER:O	1:A:1336:LYS:HG2	1.96	0.65
6:K:1:NAG:H82	6:K:2:NAG:H2	1.79	0.65
1:A:552:LEU:O	1:A:556:ILE:HG22	1.97	0.64
1:A:793:HIS:HA	1:A:796:VAL:HG12	1.79	0.64
14:A:1916[B]:4YH:H24	14:A:1916[B]:4YH:C12	2.27	0.64
2:E:127:MET:HG3	2:E:136:LEU:CD2	2.27	0.64
5:F:506:PHE:CZ	5:F:667:ARG:HG3	2.32	0.64
1:A:1068:PHE:CZ	1:A:1381:MET:HE3	2.32	0.64
2:E:135:TYR:HA	2:E:138:ARG:HH12	1.59	0.64
5:F:114:ARG:CZ	7:H:1:NAG:H62	2.27	0.64
1:A:269:ASN:HD22	1:A:273:THR:CG2	2.08	0.64
1:A:548:LEU:CD2	1:A:934:VAL:HG21	2.28	0.64
5:F:159:ARG:HH22	5:F:226:VAL:CG1	2.06	0.64
1:A:366:TYR:CG	4:C:400:LEU:CD2	2.76	0.64
5:F:28:PRO:HD3	5:F:851:MET:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:LYS:HZ2	1:A:984:GLU:HG2	1.63	0.64
5:F:892:ILE:O	5:F:893:SER:HB3	1.97	0.64
1:A:1430:GLN:HG3	1:A:1432:PRO:HD2	1.80	0.64
2:E:137:LEU:N	2:E:137:LEU:HD22	2.13	0.64
5:F:28:PRO:HD3	5:F:851:MET:HE3	1.80	0.64
1:A:78:ASP:O	1:A:79:ASN:HB2	1.98	0.64
4:C:280:VAL:HG12	4:C:285:LYS:HZ1	1.62	0.64
8:L:3:NAG:H83	8:L:3:NAG:O5	1.97	0.64
1:A:366:TYR:CD2	4:C:400:LEU:HD21	2.33	0.63
1:A:798:ALA:HB1	1:A:800:TRP:CH2	2.33	0.63
2:E:118:LEU:HD23	2:E:118:LEU:C	2.19	0.63
1:A:1076:TYR:HE2	1:A:1078:ASN:CG	2.02	0.63
5:F:130:LYS:HA	5:F:228:ASN:HD22	1.63	0.63
1:A:97:PHE:O	1:A:130:VAL:HG11	1.99	0.63
1:A:661:VAL:HG13	1:A:662:ASP:OD1	1.97	0.63
1:A:366:TYR:CD2	4:C:400:LEU:HD11	2.32	0.63
1:A:1099:ARG:HH21	2:E:219:GLU:HA	1.64	0.63
5:F:340:SER:O	5:F:344:GLU:HG2	1.97	0.63
5:F:103:GLU:HG3	5:F:194:VAL:HG21	1.81	0.63
5:F:895:TYR:CZ	5:F:986:PHE:HE1	2.17	0.63
1:A:1472:ARG:HH12	1:A:1483:PHE:HA	1.63	0.63
5:F:269:LEU:HD22	5:F:269:LEU:O	1.99	0.63
1:A:52:PRO:HA	1:A:55:THR:OG1	1.99	0.63
1:A:496:PHE:CD2	1:A:540:LYS:HB2	2.34	0.63
1:A:976:LYS:CD	1:A:984:GLU:OE2	2.47	0.63
2:E:107:ALA:N	2:E:157:VAL:HG11	2.13	0.63
1:A:524:ILE:O	1:A:524:ILE:HG12	1.97	0.62
1:A:1096:ARG:CG	2:E:218:ALA:HB3	2.29	0.62
1:A:1199:LEU:HD11	2:E:110:ILE:HD11	1.81	0.62
5:F:783:PHE:CE1	5:F:873:GLN:CB	2.82	0.62
1:A:1091:TYR:CD1	1:A:1091:TYR:C	2.70	0.62
5:F:178:SER:OG	5:F:180:ILE:HG22	2.00	0.62
1:A:189:ILE:HD13	1:A:654:ASN:HD22	1.64	0.62
1:A:330:LEU:CD2	13:A:1914:9Z9:C76	2.77	0.62
1:A:1156:ALA:O	1:A:1160:ILE:HG13	1.99	0.62
1:A:237:VAL:HG12	1:A:238:GLU:H	1.64	0.62
1:A:339:LYS:HB2	1:A:339:LYS:NZ	2.15	0.62
1:A:475:PHE:CE2	1:A:534:ARG:HD3	2.26	0.62
1:A:366:TYR:CE1	4:C:400:LEU:CD1	2.78	0.62
1:A:366:TYR:OH	4:C:391:ILE:HG21	1.99	0.62
5:F:159:ARG:NH1	5:F:224:PRO:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:3:NAG:C8	8:L:3:NAG:O5	2.47	0.62
1:A:110:PHE:O	1:A:113:HIS:N	2.33	0.62
1:A:545:LEU:CD2	1:A:549:VAL:CG2	2.77	0.62
1:A:557:ARG:HG3	1:A:557:ARG:HH11	1.63	0.62
5:F:97:LEU:HD11	5:F:464:GLY:O	1.99	0.62
5:F:528:ASN:HD22	5:F:528:ASN:C	2.02	0.62
5:F:825:ILE:HD13	5:F:846:ARG:HH22	1.64	0.62
1:A:548:LEU:HD22	1:A:934:VAL:HG21	1.81	0.62
1:A:1046:ILE:HD13	11:A:1908:3PE:H232	1.78	0.62
1:A:1096:ARG:HD2	2:E:218:ALA:O	1.98	0.62
5:F:1008:VAL:CG2	5:F:1019:ILE:HG22	2.29	0.62
1:A:110:PHE:O	1:A:111:LEU:C	2.37	0.62
1:A:912:LYS:HD3	1:A:912:LYS:H	1.64	0.62
1:A:1166:ILE:O	1:A:1170:LEU:HG	1.99	0.62
5:F:161:VAL:CG2	5:F:221:PRO:CG	2.70	0.62
1:A:462:HIS:CE1	1:A:466:ILE:CG1	2.82	0.61
5:F:880:GLU:HG2	5:F:1035:ILE:HG22	1.82	0.61
5:F:889:LEU:HG	5:F:894:VAL:CG1	2.23	0.61
1:A:180:PRO:HA	1:A:183:GLN:HE21	1.62	0.61
1:A:173:LEU:O	1:A:176:VAL:HG12	1.99	0.61
5:F:1010:LYS:HG2	5:F:1017:ILE:HG13	1.83	0.61
1:A:97:PHE:C	1:A:130:VAL:HG11	2.21	0.61
1:A:366:TYR:CD2	4:C:400:LEU:CG	2.84	0.61
5:F:206:LEU:HD21	5:F:458:LEU:HD21	1.81	0.61
5:F:370:ARG:HD3	5:F:372:GLN:HE21	1.65	0.61
5:F:376:ALA:O	5:F:380:LYS:HB2	2.01	0.61
5:F:993:PHE:O	5:F:1008:VAL:CG1	2.47	0.61
2:E:215:CYS:O	2:E:216:MET:HB3	2.00	0.61
1:A:668:GLU:OE1	1:A:669:SER:N	2.33	0.61
1:A:1068:PHE:CD1	1:A:1381:MET:HE3	2.35	0.61
1:A:1338:CYS:SG	1:A:1352:CYS:CB	2.85	0.61
5:F:465:THR:HG22	5:F:489:VAL:HG13	1.81	0.61
5:F:256:MET:HB2	5:F:359:ILE:HD12	1.83	0.61
5:F:856:LEU:O	5:F:1017:ILE:HG22	2.01	0.61
1:A:105:ILE:HG21	1:A:114:GLN:HE21	1.66	0.61
1:A:227:TYR:CE2	1:A:262:ARG:HB3	2.35	0.61
2:E:137:LEU:HD22	2:E:137:LEU:H	1.65	0.61
5:F:133:LEU:H	5:F:133:LEU:HD23	1.66	0.61
5:F:781:PRO:CG	5:F:795:ILE:HG13	2.31	0.61
1:A:604:LEU:HB3	11:A:1908:3PE:C22	2.31	0.61
1:A:1389:ARG:NH1	1:A:1396:PRO:HD2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:TYR:CD1	2:E:212:TRP:HB3	2.35	0.60
1:A:1338:CYS:HG	1:A:1352:CYS:HB2	1.64	0.60
12:A:1909:PC1:H133	12:A:1909:PC1:O13	2.01	0.60
1:A:466:ILE:O	1:A:470:VAL:HG23	2.02	0.60
1:A:1067:THR:HG21	1:A:1377:VAL:HG11	1.83	0.60
1:A:793:HIS:O	1:A:797:ASN:CB	2.49	0.60
1:A:1249:ARG:HA	1:A:1249:ARG:NE	2.10	0.60
2:E:210:ASN:ND2	2:E:213:GLU:OE1	2.33	0.60
1:A:1083:LYS:NZ	1:A:1087:GLN:OE1	2.35	0.60
5:F:868:ASP:HA	5:F:871:THR:HG22	1.82	0.60
1:A:116:ALA:HA	1:A:119:ARG:HG2	1.84	0.60
1:A:1343:ASP:C	1:A:1344:TYR:CD1	2.74	0.60
5:F:1068:LEU:HD12	5:F:1068:LEU:O	2.01	0.60
1:A:161:VAL:O	1:A:163:ALA:N	2.35	0.60
2:E:20:ILE:HG13	2:E:118:LEU:CD1	2.24	0.60
1:A:639:ILE:HD11	11:A:1906:3PE:H292	1.83	0.60
1:A:1154:ASN:ND2	1:A:1239:ARG:NH1	2.50	0.60
1:A:1259:THR:HG22	1:A:1383:ASN:OD1	2.02	0.60
5:F:391:VAL:HG12	5:F:415:ILE:HB	1.84	0.60
1:A:76:GLU:HA	1:A:76:GLU:OE1	2.01	0.60
1:A:542:TRP:CZ3	1:A:545:LEU:HB2	2.36	0.60
1:A:1161:PHE:HA	1:A:1164:GLU:HG2	1.82	0.60
6:D:1:NAG:H83	6:D:2:NAG:C8	2.31	0.60
1:A:557:ARG:HG3	1:A:557:ARG:NH1	2.17	0.60
1:A:1105:ASN:O	1:A:1109:TYR:CB	2.48	0.60
5:F:476:GLU:OE1	5:F:478:LYS:CB	2.47	0.60
1:A:174:ARG:CG	1:A:174:ARG:HH21	2.13	0.59
1:A:545:LEU:HD22	1:A:545:LEU:C	2.23	0.59
5:F:109:ALA:HB2	5:F:471:ILE:O	2.02	0.59
4:C:280:VAL:HG11	4:C:371:ILE:HB	1.85	0.59
5:F:449:THR:HG22	5:F:450:ASN:N	2.17	0.59
5:F:710:LEU:CD2	5:F:714:PHE:CZ	2.82	0.59
5:F:1045:ASP:OD1	5:F:1046:PRO:HD2	2.02	0.59
1:A:274:HIS:HD2	1:A:276:ASP:H	1.49	0.59
5:F:33:ILE:HG21	5:F:1007:HIS:ND1	2.17	0.59
5:F:43:ASP:CG	8:L:1:NAG:H2	2.23	0.59
5:F:704:LEU:C	5:F:704:LEU:HD23	2.23	0.59
1:A:45:ILE:CG1	1:A:106:ILE:CD1	2.71	0.59
1:A:798:ALA:HB1	1:A:800:TRP:CE3	2.37	0.59
1:A:1076:TYR:CE2	1:A:1078:ASN:CG	2.75	0.59
4:C:278:ILE:C	4:C:279:LEU:HD23	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:889:LEU:HA	5:F:892:ILE:CD1	2.32	0.59
1:A:520:THR:O	1:A:524:ILE:HG22	2.02	0.59
5:F:796:MET:HB3	5:F:818:LYS:HD2	1.83	0.59
1:A:470:VAL:HG12	1:A:470:VAL:O	2.01	0.59
1:A:1071:GLN:CG	1:A:1072:GLY:H	2.15	0.59
5:F:217:ALA:HB2	5:F:240:VAL:HG21	1.84	0.59
1:A:447:LEU:HD22	1:A:447:LEU:O	2.02	0.59
1:A:1076:TYR:CE2	1:A:1078:ASN:HB3	2.37	0.59
1:A:630:PRO:HA	1:A:635:VAL:HG13	1.85	0.59
1:A:793:HIS:O	1:A:797:ASN:HB2	2.02	0.59
1:A:798:ALA:CB	1:A:800:TRP:CH2	2.86	0.59
1:A:1097:PRO:CD	2:E:218:ALA:CB	2.80	0.59
5:F:262:VAL:HG22	5:F:296:PHE:O	2.03	0.59
5:F:521:GLY:O	5:F:562:ASP:OD1	2.21	0.59
1:A:366:TYR:CZ	4:C:400:LEU:HD11	2.38	0.59
1:A:1294:LEU:HD11	1:A:1307:GLN:OE1	2.02	0.59
5:F:590:PHE:CE2	5:F:592:THR:CG2	2.86	0.59
1:A:445:ASN:OD1	1:A:534:ARG:NH1	2.33	0.59
1:A:559:ILE:HD13	1:A:659:ILE:CG1	2.33	0.59
1:A:905:LEU:HD21	1:A:1280:ILE:HD11	1.83	0.59
1:A:109:GLY:HA3	1:A:113:HIS:CG	2.37	0.58
2:E:138:ARG:HE	2:E:204:LEU:HA	1.67	0.58
5:F:85:ASP:HB3	5:F:502:LEU:HD22	1.84	0.58
5:F:590:PHE:CD2	5:F:592:THR:CG2	2.85	0.58
1:A:115:ASP:O	1:A:119:ARG:N	2.35	0.58
1:A:294:TRP:NE1	1:A:1321:THR:HG21	2.17	0.58
1:A:1068:PHE:CB	1:A:1073:GLU:HG2	2.33	0.58
1:A:1426:LEU:HD13	1:A:1429:ILE:HD12	1.85	0.58
1:A:309:TRP:HZ2	2:E:152:PHE:HZ	1.48	0.58
1:A:1068:PHE:CZ	1:A:1381:MET:HE1	2.38	0.58
1:A:1309:PHE:HB3	1:A:1310:PRO:HD3	1.86	0.58
5:F:792:GLU:OE1	5:F:792:GLU:N	2.22	0.58
5:F:851:MET:SD	5:F:1020:MET:SD	3.01	0.58
1:A:664:LEU:HD12	13:A:1914:9Z9:C18	2.31	0.58
1:A:901:VAL:O	1:A:901:VAL:HG22	2.03	0.58
1:A:1406:TRP:NE1	1:A:1410:ASP:OD2	2.36	0.58
2:E:136:LEU:O	2:E:139:PRO:HG2	2.04	0.58
5:F:170:ILE:CD1	5:F:216:LEU:HD23	2.30	0.58
1:A:454:HIS:CD2	1:A:1029:GLU:OE2	2.56	0.58
1:A:964:THR:HG22	1:A:965:GLU:N	2.17	0.58
2:E:205:PRO:O	2:E:206:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:284:LEU:O	4:C:290:THR:HG21	2.03	0.58
5:F:291:VAL:CG1	5:F:312:ALA:HB2	2.28	0.58
5:F:408:ASN:C	5:F:409:LYS:HG3	2.24	0.58
5:F:651:LEU:O	5:F:687:ASN:ND2	2.37	0.58
5:F:702:THR:O	5:F:706:ASN:HB2	2.03	0.58
5:F:780:ALA:HB2	5:F:863:LEU:HD21	1.84	0.58
5:F:887:ARG:NH2	5:F:1032:ARG:O	2.36	0.58
1:A:1195:ILE:HD11	2:E:117:PHE:CE2	2.36	0.58
12:A:1909:PC1:O13	12:A:1909:PC1:H152	2.01	0.58
5:F:168:VAL:HG13	5:F:216:LEU:CD2	2.24	0.58
5:F:523:VAL:HG21	5:F:526:HIS:HB2	1.85	0.58
1:A:463:LEU:C	1:A:463:LEU:HD13	2.24	0.58
1:A:519:MET:HA	1:A:519:MET:HE2	1.83	0.58
1:A:540:LYS:CD	1:A:541:TYR:HE1	2.13	0.58
5:F:361:MET:HE1	5:F:387:PHE:CD1	2.38	0.58
6:K:2:NAG:H82	6:K:2:NAG:C3	2.21	0.58
1:A:342:GLU:OE1	1:A:342:GLU:HA	2.02	0.58
1:A:1091:TYR:CZ	2:E:212:TRP:HA	2.38	0.58
2:E:128:ALA:HB1	2:E:137:LEU:HD22	1.85	0.58
5:F:256:MET:HE3	5:F:258:ILE:HG13	1.84	0.58
1:A:452:GLU:HG2	1:A:464:GLN:OE1	2.04	0.57
1:A:1366:MET:HE3	11:A:1912:3PE:C2C	2.34	0.57
5:F:693:LYS:NZ	5:F:696:ASN:OD1	2.37	0.57
1:A:169:VAL:HG21	1:A:575:LEU:HB2	1.85	0.57
1:A:333:LEU:HB3	1:A:657:LEU:CD2	2.34	0.57
1:A:1366:MET:CE	11:A:1912:3PE:H2C1	2.34	0.57
1:A:1431:PRO:HB3	1:A:1436:GLY:HA2	1.84	0.57
5:F:456:LEU:O	5:F:457:GLU:HB2	2.03	0.57
5:F:1011:LEU:HD12	5:F:1011:LEU:N	2.19	0.57
1:A:1266:ALA:O	1:A:1267:LEU:HD13	2.03	0.57
5:F:256:MET:CB	5:F:359:ILE:HD11	2.33	0.57
1:A:542:TRP:CD2	1:A:545:LEU:CB	2.86	0.57
1:A:1135:LEU:O	1:A:1138:GLN:HG2	2.04	0.57
5:F:357:ASN:ND2	5:F:1064:ASP:HB3	2.18	0.57
5:F:824:TRP:C	5:F:864:MET:CE	2.71	0.57
1:A:45:ILE:CG2	1:A:106:ILE:CD1	2.73	0.57
1:A:366:TYR:CD2	4:C:400:LEU:HG	2.39	0.57
5:F:132:ASP:CG	5:F:137:LYS:HG2	2.22	0.57
5:F:824:TRP:O	5:F:864:MET:HE1	2.03	0.57
1:A:494:SER:O	1:A:498:ARG:HG3	2.05	0.57
1:A:515:GLU:HA	1:A:515:GLU:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:118:LEU:HD23	2:E:118:LEU:O	2.04	0.57
2:E:133:ARG:HB2	2:E:135:TYR:CE2	2.38	0.57
5:F:824:TRP:CB	5:F:864:MET:CE	2.83	0.57
1:A:129:ILE:HG22	1:A:130:VAL:N	2.18	0.57
5:F:366:GLY:HA3	5:F:396:TYR:HB3	1.85	0.57
1:A:168:ARG:C	1:A:170:LEU:H	2.07	0.57
1:A:291:MET:CG	1:A:1321:THR:HG23	2.27	0.57
1:A:316:THR:O	1:A:320:LEU:HB2	2.05	0.57
1:A:1234:PHE:CE1	2:E:149:LEU:HD13	2.40	0.57
1:A:1271:ALA:HB1	12:A:1910:PC1:H3G2	1.85	0.57
5:F:332:ILE:CG2	5:F:333:THR:H	2.06	0.57
1:A:1046:ILE:CD1	11:A:1908:3PE:C23	2.76	0.57
1:A:1096:ARG:HD3	1:A:1097:PRO:HD2	1.87	0.57
5:F:844:CYS:HB3	5:F:866:ASN:ND2	2.20	0.57
1:A:97:PHE:HB3	1:A:130:VAL:HG13	1.86	0.56
1:A:1247:LEU:HD21	1:A:1253:VAL:HG12	1.87	0.56
5:F:339:PHE:O	5:F:343:PHE:CD2	2.58	0.56
1:A:107:ALA:O	1:A:108:TYR:HB2	2.03	0.56
1:A:875:VAL:HG11	1:A:906:ARG:CZ	2.31	0.56
1:A:651:ILE:HD11	11:A:1913:3PE:C2H	2.35	0.56
1:A:664:LEU:HG	1:A:1065:ILE:HG22	1.87	0.56
1:A:822:ILE:HD12	1:A:1341:GLU:HG3	1.86	0.56
1:A:1309:PHE:CE2	12:A:1910:PC1:H2B2	2.40	0.56
5:F:205:LEU:HD21	5:F:492:VAL:HG21	1.87	0.56
5:F:523:VAL:HG13	5:F:523:VAL:O	2.05	0.56
5:F:889:LEU:O	5:F:892:ILE:CG1	2.54	0.56
1:A:112:PHE:CE1	1:A:115:ASP:OD2	2.58	0.56
1:A:494:SER:CB	1:A:497:ASN:CG	2.73	0.56
1:A:1497:ILE:O	1:A:1498:TRP:CB	2.52	0.56
5:F:365:ASP:OD1	5:F:366:GLY:N	2.38	0.56
1:A:964:THR:HB	1:A:967:GLU:HG2	1.87	0.56
5:F:100:LEU:HD13	5:F:198:ASN:HD21	1.62	0.56
5:F:121:GLU:HA	5:F:121:GLU:OE1	2.05	0.56
1:A:1095:ALA:HA	2:E:212:TRP:HB2	1.86	0.56
2:E:218:ALA:O	2:E:219:GLU:HG2	2.04	0.56
5:F:784:ASN:CG	9:F:1120:NAG:C1	2.65	0.56
5:F:895:TYR:CE1	5:F:986:PHE:HE1	2.23	0.56
4:C:418:ALA:O	4:C:422:LEU:HD22	2.06	0.56
5:F:37:VAL:HG13	5:F:1011:LEU:HG	1.88	0.56
1:A:277:ASN:ND2	11:A:1905:3PE:O14	2.39	0.56
1:A:892:VAL:HG12	1:A:895:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:137:LEU:CD2	2:E:137:LEU:H	2.19	0.56
5:F:326:ASN:ND2	9:F:1104:NAG:C2	2.65	0.56
5:F:1061:VAL:HG23	5:F:1061:VAL:O	2.05	0.56
1:A:962:LYS:HG2	1:A:967:GLU:C	2.27	0.56
1:A:1245:LYS:O	1:A:1248:SER:HB3	2.05	0.56
4:C:279:LEU:HD22	4:C:387:VAL:CG1	2.34	0.56
5:F:366:GLY:HA3	5:F:396:TYR:HB2	1.88	0.56
1:A:910:ARG:HD3	1:A:910:ARG:N	2.16	0.56
1:A:1065:ILE:HD12	1:A:1065:ILE:C	2.26	0.56
1:A:1173:LYS:O	1:A:1174:ALA:HB3	2.05	0.55
1:A:1180:ASP:HB3	1:A:1183:ASN:HD22	1.68	0.55
1:A:1358:TYR:HB3	11:A:1912:3PE:H222	1.87	0.55
6:D:1:NAG:C8	6:D:2:NAG:C7	2.83	0.55
5:F:476:GLU:CD	5:F:478:LYS:HB2	2.26	0.55
1:A:339:LYS:O	1:A:343:LYS:HG2	2.06	0.55
1:A:632:TYR:HB3	1:A:633:PRO:CD	2.36	0.55
1:A:925:ILE:CD1	1:A:1370:PHE:CZ	2.84	0.55
5:F:444:LYS:NZ	5:F:467:PRO:O	2.39	0.55
5:F:1010:LYS:HG3	5:F:1017:ILE:CG1	2.35	0.55
1:A:908:ILE:O	1:A:915:LYS:HG3	2.05	0.55
1:A:1096:ARG:CD	1:A:1097:PRO:HD2	2.37	0.55
5:F:773:ASN:HD22	5:F:777:VAL:HG21	1.71	0.55
5:F:474:GLN:O	5:F:475:PHE:C	2.44	0.55
1:A:112:PHE:CD1	1:A:115:ASP:OD2	2.60	0.55
1:A:339:LYS:HB2	1:A:339:LYS:HZ2	1.71	0.55
1:A:1247:LEU:HD11	1:A:1257:LEU:HD12	1.89	0.55
1:A:338:THR:HB	1:A:1388:THR:CG2	2.36	0.55
1:A:462:HIS:NE2	1:A:466:ILE:CD1	2.52	0.55
1:A:1098:LEU:N	2:E:218:ALA:HB2	2.22	0.55
5:F:227:ASP:HB2	5:F:236:ASP:HB3	1.89	0.55
5:F:449:THR:HG22	5:F:450:ASN:H	1.71	0.55
1:A:221:LYS:HZ1	12:A:1909:PC1:H121	1.66	0.55
1:A:542:TRP:CZ2	1:A:933:LEU:CD1	2.77	0.55
2:E:128:ALA:HB1	2:E:137:LEU:CD2	2.37	0.55
2:E:53:LEU:HD23	2:E:158:MET:HE2	1.88	0.55
4:C:283:SER:HB3	4:C:290:THR:CB	2.32	0.55
5:F:37:VAL:CG2	5:F:1018:PHE:CD2	2.90	0.55
1:A:362:ASP:OD2	4:C:396:VAL:HG21	2.07	0.55
1:A:1267:LEU:HD13	1:A:1267:LEU:N	2.20	0.55
1:A:161:VAL:C	1:A:163:ALA:H	2.11	0.54
1:A:928:ILE:CG2	1:A:932:VAL:CG2	2.83	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1501:THR:O	1:A:1505:LEU:N	2.38	0.54
1:A:109:GLY:CA	1:A:113:HIS:HB3	2.32	0.54
1:A:529:CYS:HB2	1:A:948:GLN:HG3	1.88	0.54
1:A:792:CYS:O	1:A:796:VAL:CG1	2.49	0.54
1:A:1068:PHE:HB3	1:A:1073:GLU:CG	2.37	0.54
5:F:129:ALA:O	5:F:130:LYS:HG2	2.07	0.54
5:F:243:ARG:HH21	5:F:243:ARG:CG	2.15	0.54
5:F:370:ARG:HG3	5:F:372:GLN:HG3	1.89	0.54
1:A:76:GLU:HB2	5:F:264:GLY:O	2.08	0.54
1:A:237:VAL:HG23	1:A:240:GLU:OE1	2.07	0.54
1:A:505:CYS:O	1:A:509:LEU:HB2	2.08	0.54
5:F:216:LEU:C	5:F:216:LEU:HD13	2.28	0.54
5:F:570:ASN:HD21	5:F:592:THR:CG2	2.20	0.54
1:A:1188:LEU:HD13	2:E:142:MET:CE	2.37	0.54
1:A:1234:PHE:CZ	2:E:149:LEU:HD13	2.42	0.54
1:A:1358:TYR:O	1:A:1362:ILE:HG13	2.06	0.54
1:A:233:ILE:HG21	5:F:547:ARG:NH2	2.22	0.54
1:A:927:THR:CB	1:A:1066:VAL:HG22	2.37	0.54
1:A:1128:ILE:O	1:A:1132:THR:OG1	2.26	0.54
5:F:441:ASP:N	5:F:441:ASP:OD1	2.40	0.54
1:A:900:ARG:O	1:A:903:ARG:HD2	2.07	0.54
1:A:1334:TYR:HA	1:A:1353:GLY:C	2.27	0.54
14:A:1916[B]:4YH:C12	14:A:1916[B]:4YH:C27	2.85	0.54
1:A:1366:MET:HE2	11:A:1912:3PE:C2A	2.10	0.54
11:A:1904:3PE:H241	11:A:1904:3PE:O22	2.07	0.54
3:B:143:ASP:HB3	3:B:164:LYS:HD3	1.89	0.54
5:F:528:ASN:O	5:F:528:ASN:ND2	2.27	0.54
5:F:825:ILE:HG21	5:F:846:ARG:HH22	1.66	0.54
5:F:858:ASP:CA	5:F:986:PHE:CZ	2.88	0.54
1:A:280:PHE:HZ	1:A:630:PRO:HB2	1.71	0.54
5:F:171:PRO:HG2	5:F:174:ILE:HD12	1.88	0.54
5:F:780:ALA:CB	5:F:863:LEU:HD21	2.38	0.54
5:F:896:ALA:CB	5:F:987:ASP:HB3	2.38	0.54
1:A:651:ILE:HD11	11:A:1913:3PE:H2H2	1.90	0.53
1:A:908:ILE:O	1:A:915:LYS:CG	2.55	0.53
3:B:145:TRP:HB2	3:B:159:ILE:HB	1.90	0.53
5:F:385:ARG:HH12	5:F:431:VAL:HG12	1.73	0.53
5:F:570:ASN:ND2	5:F:592:THR:CG2	2.70	0.53
5:F:597:GLN:OE1	5:F:768:LYS:NZ	2.38	0.53
2:E:32:TRP:HB2	2:E:182:PHE:HB2	1.90	0.53
5:F:411:TYR:HD2	5:F:413:TYR:HH	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD11	1:A:174:ARG:NH1	2.22	0.53
1:A:1136:GLY:O	11:A:1911:3PE:C25	2.55	0.53
5:F:824:TRP:HB3	5:F:864:MET:HE3	1.91	0.53
1:A:97:PHE:HB3	1:A:130:VAL:CG1	2.39	0.53
1:A:280:PHE:CZ	1:A:630:PRO:HB2	2.43	0.53
1:A:1390:ASP:O	1:A:1392:SER:N	2.41	0.53
2:E:30:ASP:OD2	2:E:55:ARG:CG	2.55	0.53
5:F:284:THR:HG21	5:F:428:TYR:OH	2.09	0.53
1:A:170:LEU:HD11	11:A:1906:3PE:H3B2	1.88	0.53
1:A:205:PHE:O	1:A:209:ILE:HG13	2.08	0.53
1:A:277:ASN:HD22	1:A:279:GLY:H	1.57	0.53
1:A:928:ILE:CG2	1:A:1059:ILE:HG23	2.37	0.53
5:F:230:ARG:N	5:F:230:ARG:HD3	2.23	0.53
5:F:515:PHE:CE2	5:F:580:MET:CE	2.88	0.53
5:F:795:ILE:HD11	5:F:874:ILE:HD11	1.90	0.53
5:F:992:SER:O	5:F:993:PHE:CD1	2.62	0.53
1:A:234:VAL:HG12	1:A:236:THR:HG23	1.91	0.53
1:A:1249:ARG:O	1:A:1251:GLU:HG3	2.09	0.53
5:F:783:PHE:CE1	5:F:873:GLN:HA	2.44	0.53
1:A:927:THR:O	1:A:927:THR:HG22	2.09	0.53
1:A:930:ASN:O	1:A:934:VAL:HG23	2.09	0.53
1:A:1039:VAL:HG12	1:A:1039:VAL:O	2.07	0.53
1:A:934:VAL:HG11	1:A:1055:PHE:CE2	2.35	0.53
1:A:1071:GLN:HG2	1:A:1072:GLY:N	2.23	0.53
1:A:927:THR:CG2	1:A:1066:VAL:HG22	2.38	0.52
1:A:979:ASP:O	1:A:981:THR:N	2.42	0.52
1:A:1249:ARG:HE	1:A:1249:ARG:CA	2.19	0.52
1:A:1345:ALA:O	1:A:1347:GLY:N	2.43	0.52
6:K:2:NAG:H3	6:K:2:NAG:C8	2.19	0.52
1:A:76:GLU:HB2	5:F:264:GLY:CA	2.39	0.52
1:A:1320:ALA:O	14:A:1916[B]:4YH:H35	2.09	0.52
5:F:361:MET:CE	5:F:387:PHE:HD1	2.19	0.52
1:A:522:LEU:HG	1:A:522:LEU:O	2.09	0.52
1:A:611:LEU:HB3	14:A:1915[A]:4YH:H38	1.92	0.52
5:F:178:SER:O	5:F:181:VAL:HG13	2.09	0.52
5:F:359:ILE:HD13	5:F:361:MET:CE	2.37	0.52
1:A:257:ASN:ND2	9:A:1901:NAG:O5	2.35	0.52
1:A:1199:LEU:CD2	1:A:1232:SER:OG	2.57	0.52
5:F:993:PHE:CB	5:F:1008:VAL:CG1	2.77	0.52
1:A:227:TYR:CD2	1:A:262:ARG:CB	2.93	0.52
1:A:366:TYR:CD2	4:C:396:VAL:CG1	2.79	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:HIS:CD2	1:A:466:ILE:HD11	2.41	0.52
1:A:925:ILE:HD11	1:A:1370:PHE:CE1	2.43	0.52
1:A:1062:GLY:O	1:A:1065:ILE:CG1	2.43	0.52
1:A:1247:LEU:HD11	1:A:1257:LEU:CD1	2.39	0.52
5:F:339:PHE:CZ	5:F:362:LEU:CD2	2.92	0.52
5:F:824:TRP:CD1	5:F:864:MET:CE	2.87	0.52
5:F:847:ASN:C	5:F:847:ASN:HD22	2.09	0.52
5:F:1011:LEU:N	5:F:1011:LEU:CD1	2.73	0.52
1:A:1136:GLY:O	11:A:1911:3PE:H262	2.09	0.52
1:A:1155:VAL:O	1:A:1159:ILE:HG13	2.10	0.52
1:A:1345:ALA:HB3	1:A:1348:GLU:HG3	1.92	0.52
11:A:1904:3PE:O22	11:A:1904:3PE:H31	2.04	0.52
5:F:61:TYR:O	5:F:68:TYR:OH	2.24	0.52
2:E:135:TYR:HA	2:E:138:ARG:HH11	1.72	0.52
5:F:845:LYS:CD	5:F:847:ASN:ND2	2.73	0.52
1:A:117:TYR:CD1	1:A:118:LEU:HD23	2.44	0.52
1:A:928:ILE:HG22	1:A:932:VAL:CG2	2.18	0.52
1:A:1071:GLN:CG	1:A:1072:GLY:N	2.73	0.52
14:A:1916[B]:4YH:H31	14:A:1916[B]:4YH:N8	2.24	0.52
5:F:826:GLU:O	5:F:830:LYS:HG2	2.09	0.52
5:F:1066:ASN:HD22	5:F:1067:VAL:H	1.57	0.52
1:A:339:LYS:NZ	1:A:339:LYS:CB	2.73	0.52
4:C:289:VAL:HG12	4:C:293:MET:HE1	1.92	0.52
5:F:367:GLY:O	5:F:400:PRO:CG	2.51	0.52
1:A:174:ARG:CG	1:A:174:ARG:NH2	2.73	0.52
1:A:650:TYR:HD2	11:A:1913:3PE:H2F1	1.75	0.52
1:A:793:HIS:CA	1:A:796:VAL:HG12	2.40	0.52
5:F:1010:LYS:CG	5:F:1017:ILE:CG1	2.85	0.52
1:A:194:LEU:N	1:A:195:PRO:HD2	2.25	0.51
1:A:262:ARG:HG2	1:A:263:GLY:H	1.74	0.51
1:A:335:GLY:HA2	1:A:1388:THR:HG23	1.91	0.51
2:E:208:PRO:O	2:E:213:GLU:CD	2.48	0.51
5:F:34:LYS:CD	5:F:1009:GLU:OE2	2.59	0.51
5:F:532:LYS:NZ	5:F:532:LYS:CB	2.73	0.51
5:F:777:VAL:O	5:F:797:VAL:HA	2.10	0.51
1:A:1334:TYR:HA	1:A:1353:GLY:CA	2.39	0.51
1:A:535:LEU:CD1	1:A:536:PHE:N	2.73	0.51
1:A:1155:VAL:HG22	1:A:1197:VAL:CG2	2.40	0.51
1:A:1172:PHE:C	1:A:1174:ALA:H	2.14	0.51
5:F:1008:VAL:HG23	5:F:1019:ILE:CG2	2.37	0.51
1:A:75:PRO:HB3	1:A:583:GLY:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:ARG:C	1:A:586:ASP:H	2.13	0.51
1:A:868:PHE:CG	1:A:909:ASN:ND2	2.79	0.51
5:F:127:TYR:HB2	5:F:147:ILE:HB	1.92	0.51
5:F:177:GLY:HA2	5:F:182:LEU:HD23	1.91	0.51
5:F:867:HIS:O	5:F:868:ASP:CB	2.57	0.51
5:F:889:LEU:HA	5:F:892:ILE:CG1	2.41	0.51
1:A:1261:ILE:HG22	1:A:1261:ILE:O	2.09	0.51
1:A:1333:SER:O	1:A:1353:GLY:HA3	2.10	0.51
2:E:20:ILE:CG1	2:E:118:LEU:HD11	2.26	0.51
5:F:346:LEU:O	5:F:353:ARG:NH2	2.43	0.51
5:F:1070:ASP:OD1	5:F:1072:THR:N	2.40	0.51
1:A:117:TYR:CZ	1:A:118:LEU:CD2	2.90	0.51
1:A:1334:TYR:HA	1:A:1353:GLY:HA3	1.92	0.51
1:A:1029:GLU:O	1:A:1030:ASP:HB2	2.11	0.51
1:A:1096:ARG:NH1	1:A:1096:ARG:CB	2.73	0.51
1:A:66:VAL:O	1:A:70:VAL:HG22	2.11	0.51
1:A:1119:TYR:CD1	1:A:1119:TYR:N	2.75	0.51
1:A:1236:ARG:HG2	1:A:1239:ARG:NH2	2.25	0.51
1:A:535:LEU:HD12	1:A:536:PHE:H	1.76	0.51
1:A:169:VAL:CG2	1:A:575:LEU:CB	2.89	0.51
1:A:1299:GLN:HB2	1:A:1331:ALA:HB2	1.92	0.51
2:E:127:MET:HG2	2:E:136:LEU:CD2	2.38	0.51
5:F:386:VAL:O	5:F:410:GLY:HA3	2.10	0.51
5:F:487:LEU:HD22	7:I:1:NAG:H82	1.93	0.51
5:F:1021:VAL:HG22	5:F:1022:GLU:N	2.26	0.50
1:A:138:ILE:HD13	1:A:138:ILE:H	1.73	0.50
1:A:174:ARG:NH2	1:A:174:ARG:HG2	2.27	0.50
1:A:176:VAL:HG21	1:A:186:LEU:HD12	1.93	0.50
1:A:964:THR:CG2	1:A:965:GLU:N	2.73	0.50
1:A:1389:ARG:HH21	1:A:1389:ARG:CG	2.14	0.50
5:F:690:ILE:HG23	5:F:695:PRO:HG3	1.93	0.50
1:A:868:PHE:HB3	1:A:909:ASN:ND2	2.01	0.50
2:E:208:PRO:HB3	2:E:213:GLU:C	2.31	0.50
5:F:167:ALA:HB3	5:F:219:TYR:CZ	2.46	0.50
5:F:783:PHE:HE1	5:F:873:GLN:CA	2.22	0.50
1:A:109:GLY:O	1:A:113:HIS:HB2	2.09	0.50
1:A:117:TYR:O	1:A:123:ASN:OD1	2.29	0.50
1:A:204:LEU:O	1:A:208:ILE:HG13	2.11	0.50
1:A:540:LYS:HD2	1:A:541:TYR:CD1	2.46	0.50
1:A:1069:GLN:CA	1:A:1073:GLU:HB2	2.39	0.50
1:A:1112:TRP:HA	1:A:1171:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:PHE:C	1:A:1174:ALA:N	2.65	0.50
5:F:291:VAL:O	5:F:291:VAL:HG13	2.11	0.50
5:F:339:PHE:HZ	5:F:362:LEU:CD2	2.24	0.50
5:F:712:ALA:HB2	5:F:743:ILE:HD13	1.93	0.50
1:A:82:LEU:HD12	1:A:82:LEU:O	2.11	0.50
1:A:1068:PHE:CG	1:A:1073:GLU:CG	2.94	0.50
1:A:1309:PHE:HE2	12:A:1910:PC1:H2B2	1.76	0.50
2:E:32:TRP:NE1	2:E:158:MET:CG	2.59	0.50
5:F:237:LEU:HD12	5:F:237:LEU:H	1.76	0.50
5:F:454:ASP:OD1	5:F:455:ALA:N	2.44	0.50
5:F:479:THR:O	5:F:480:ASN:HB3	2.12	0.50
5:F:629:TYR:CB	5:F:809:LEU:HD23	2.42	0.50
1:A:489:ARG:O	1:A:492:PHE:HB2	2.11	0.50
1:A:661:VAL:HG13	1:A:662:ASP:N	2.26	0.50
1:A:892:VAL:O	1:A:895:ILE:HG22	2.11	0.50
1:A:1132:THR:CG2	1:A:1243:LEU:HD21	2.41	0.50
1:A:1162:THR:O	1:A:1166:ILE:HG13	2.11	0.50
4:C:373:HIS:HB3	4:C:376:GLN:HB2	1.93	0.50
5:F:510:PRO:CG	5:F:767:TYR:CE2	2.84	0.50
1:A:136:THR:CG2	1:A:164:LEU:CD2	2.35	0.50
1:A:875:VAL:HG12	1:A:906:ARG:HH12	1.71	0.50
1:A:976:LYS:HE3	1:A:976:LYS:CA	2.41	0.50
5:F:262:VAL:CG2	5:F:296:PHE:O	2.59	0.50
5:F:506:PHE:CZ	5:F:667:ARG:CG	2.94	0.50
5:F:781:PRO:HD3	5:F:795:ILE:HG13	1.93	0.50
2:E:208:PRO:CB	2:E:213:GLU:HB3	2.36	0.50
1:A:135:PHE:C	1:A:135:PHE:CD1	2.85	0.50
1:A:260:GLU:HG2	1:A:261:CYS:N	2.26	0.50
2:E:210:ASN:HB2	2:E:213:GLU:OE1	2.11	0.50
5:F:726:GLN:HB3	5:F:729:ILE:HD11	1.94	0.50
4:C:289:VAL:O	4:C:293:MET:HG3	2.12	0.49
5:F:33:ILE:HG23	5:F:1018:PHE:HE2	1.77	0.49
5:F:465:THR:HG23	5:F:489:VAL:CG1	2.23	0.49
5:F:476:GLU:OE1	5:F:478:LYS:N	2.45	0.49
5:F:1074:CYS:O	15:F:1101:ETA:HB1	2.11	0.49
1:A:309:TRP:CB	12:A:1909:PC1:H221	2.41	0.49
1:A:892:VAL:HG12	1:A:895:ILE:H	1.77	0.49
1:A:1016:TRP:N	1:A:1017:PRO:CD	2.75	0.49
1:A:1125:PHE:CD1	1:A:1125:PHE:C	2.86	0.49
5:F:336:LYS:CE	5:F:369:GLU:OE2	2.52	0.49
1:A:962:LYS:HG3	1:A:967:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:262:VAL:HG23	5:F:297:ASN:HB3	1.94	0.49
5:F:385:ARG:NH1	5:F:431:VAL:HG12	2.27	0.49
5:F:1008:VAL:CB	5:F:1019:ILE:HG22	2.41	0.49
1:A:117:TYR:CD1	1:A:118:LEU:CD2	2.91	0.49
1:A:366:TYR:CD2	4:C:400:LEU:CD1	2.96	0.49
1:A:450:ALA:HA	1:A:1000:VAL:HG21	1.94	0.49
1:A:533:LEU:O	1:A:536:PHE:HD2	1.96	0.49
1:A:632:TYR:CD1	1:A:632:TYR:C	2.85	0.49
14:A:1916[B]:4YH:C12	14:A:1916[B]:4YH:N8	2.75	0.49
2:E:5:GLU:OE1	2:E:10:ARG:NH2	2.45	0.49
5:F:242:ARG:NH1	5:F:426:GLN:HB3	2.28	0.49
1:A:92:PHE:CD1	1:A:92:PHE:C	2.86	0.49
1:A:324:PHE:O	1:A:328:LEU:HD13	2.12	0.49
1:A:366:TYR:OH	4:C:391:ILE:HG23	2.12	0.49
1:A:503:VAL:O	1:A:507:GLY:N	2.46	0.49
5:F:210:PHE:HB2	5:F:490:MET:CE	2.42	0.49
4:C:299:ASP:OD1	4:C:299:ASP:O	2.30	0.49
5:F:205:LEU:HD21	5:F:492:VAL:HG23	1.95	0.49
5:F:629:TYR:CD1	5:F:629:TYR:C	2.84	0.49
5:F:710:LEU:HD23	5:F:710:LEU:O	2.12	0.49
5:F:824:TRP:CB	5:F:864:MET:HE1	2.41	0.49
1:A:1334:TYR:O	1:A:1353:GLY:CA	2.60	0.49
1:A:1342:SER:O	1:A:1344:TYR:CD1	2.64	0.49
1:A:278:PHE:CD2	11:A:1911:3PE:H271	2.47	0.49
1:A:1068:PHE:HB3	1:A:1073:GLU:HG2	1.94	0.49
1:A:1343:ASP:C	1:A:1344:TYR:HD1	2.16	0.49
1:A:1381:MET:C	1:A:1383:ASN:H	2.16	0.49
5:F:57:LEU:HD23	5:F:801:VAL:HG21	1.94	0.49
5:F:216:LEU:HD13	5:F:216:LEU:O	2.12	0.49
5:F:481:LEU:HD23	5:F:482:LYS:N	2.22	0.49
5:F:663:PHE:CB	5:F:744:THR:HG23	2.39	0.49
5:F:775:ASN:HB2	5:F:1013:ASN:O	2.12	0.49
1:A:519:MET:HA	1:A:519:MET:HE3	1.89	0.49
1:A:60:THR:HG22	1:A:97:PHE:CZ	2.48	0.48
1:A:189:ILE:HD11	1:A:562:LEU:HD21	1.95	0.48
1:A:1321:THR:O	1:A:1321:THR:HG22	2.12	0.48
5:F:206:LEU:HD23	5:F:458:LEU:HD23	1.93	0.48
5:F:348:ASN:C	5:F:350:ASN:H	2.16	0.48
5:F:481:LEU:CD2	5:F:482:LYS:H	2.22	0.48
1:A:265:TRP:CD1	1:A:266:PRO:HD2	2.47	0.48
1:A:1097:PRO:HB2	1:A:1413:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:19:GLY:HA3	2:E:191:LEU:HD22	1.95	0.48
2:E:107:ALA:HB2	2:E:157:VAL:HG12	1.95	0.48
2:E:136:LEU:O	2:E:139:PRO:HD2	2.12	0.48
1:A:105:ILE:CG2	1:A:114:GLN:HE21	2.26	0.48
1:A:1247:LEU:HD21	1:A:1253:VAL:CG1	2.43	0.48
4:C:290:THR:HA	4:C:293:MET:HE1	1.87	0.48
5:F:34:LYS:HD2	5:F:1009:GLU:OE2	2.13	0.48
5:F:281:MET:O	5:F:284:THR:HB	2.12	0.48
5:F:460:LEU:HD13	5:F:529:LEU:CD1	2.43	0.48
5:F:477:ASN:N	5:F:477:ASN:ND2	2.60	0.48
6:D:1:NAG:H83	6:D:2:NAG:O7	2.12	0.48
1:A:958:ASN:ND2	1:A:989:GLN:HG2	2.29	0.48
1:A:1028:GLU:OE1	1:A:1028:GLU:HA	2.12	0.48
5:F:516:ALA:HB3	5:F:525:LEU:N	2.28	0.48
1:A:135:PHE:C	1:A:135:PHE:HD1	2.17	0.48
1:A:165:ARG:O	1:A:168:ARG:HG3	2.14	0.48
1:A:302:ASN:OD1	1:A:310:PRO:HG2	2.13	0.48
1:A:685:LYS:HE2	4:C:445:HIS:CB	2.43	0.48
5:F:151:PHE:CZ	5:F:224:PRO:HD3	2.48	0.48
5:F:161:VAL:HG23	5:F:223:SER:OG	2.14	0.48
1:A:376:MET:HB2	4:C:299:ASP:OD2	2.14	0.48
1:A:1014:GLU:CD	1:A:1322:GLY:O	2.51	0.48
5:F:562:ASP:OD1	5:F:563:PHE:N	2.46	0.48
5:F:845:LYS:HD2	5:F:847:ASN:ND2	2.28	0.48
5:F:993:PHE:CB	5:F:1008:VAL:HG13	2.37	0.48
1:A:924:ALA:HB1	1:A:1063:PHE:CD1	2.48	0.48
1:A:1396:PRO:HA	1:A:1399:LEU:HB2	1.94	0.48
4:C:290:THR:CA	4:C:293:MET:CE	2.69	0.48
5:F:627:PRO:HG2	5:F:630:SER:HB3	1.94	0.48
5:F:824:TRP:CB	5:F:864:MET:HE3	2.42	0.48
1:A:212:ILE:O	1:A:216:GLU:HG3	2.14	0.48
1:A:962:LYS:HG2	1:A:967:GLU:O	2.14	0.48
1:A:997:PHE:HD2	1:A:1003:ALA:HB1	1.78	0.48
11:A:1904:3PE:H342	11:A:1904:3PE:O32	2.14	0.48
5:F:357:ASN:ND2	5:F:1064:ASP:CB	2.76	0.48
5:F:390:SER:HB2	5:F:412:TYR:OH	2.14	0.48
1:A:45:ILE:CB	1:A:106:ILE:HD12	2.44	0.48
1:A:588:GLU:HG2	5:F:268:GLY:O	2.14	0.48
1:A:1074:THR:CG2	1:A:1075:GLU:N	2.77	0.48
5:F:365:ASP:O	5:F:394:HIS:CE1	2.66	0.48
5:F:889:LEU:HA	5:F:892:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:GLY:CA	1:A:1380:ILE:HD12	2.41	0.47
2:E:107:ALA:HB2	2:E:157:VAL:CG1	2.44	0.47
1:A:94:LEU:CD1	1:A:134:VAL:HG12	2.40	0.47
1:A:169:VAL:HG23	1:A:575:LEU:CB	2.44	0.47
1:A:60:THR:HG22	1:A:97:PHE:CE1	2.49	0.47
1:A:366:TYR:CD2	4:C:400:LEU:CD2	2.96	0.47
1:A:1263:SER:O	1:A:1267:LEU:HD22	2.15	0.47
5:F:720:GLN:O	5:F:724:SER:OG	2.32	0.47
1:A:103:MET:CA	1:A:106:ILE:HG12	2.41	0.47
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.76	0.47
1:A:1289:PHE:CE1	1:A:1354:THR:CG2	2.98	0.47
1:A:1292:ILE:HG23	1:A:1336:LYS:HB3	1.96	0.47
14:A:1915[A]:4YH:H12	14:A:1915[A]:4YH:C11	2.43	0.47
5:F:256:MET:HE2	5:F:258:ILE:HD11	1.96	0.47
5:F:285:LEU:CD1	5:F:291:VAL:HG21	2.45	0.47
1:A:132:LEU:O	1:A:135:PHE:HB3	2.14	0.47
1:A:435:TYR:CD1	1:A:435:TYR:C	2.85	0.47
5:F:51:ALA:HB3	5:F:817:ILE:HD11	1.96	0.47
1:A:56:ILE:HG13	1:A:57:ILE:H	1.76	0.47
1:A:542:TRP:CE2	1:A:545:LEU:HB2	2.49	0.47
5:F:370:ARG:HD2	5:F:372:GLN:HE21	1.78	0.47
5:F:669:TYR:HE1	5:F:708:VAL:HG21	1.78	0.47
5:F:711:ASP:OD2	5:F:739:THR:CG2	2.63	0.47
1:A:97:PHE:CB	1:A:130:VAL:CG1	2.92	0.47
1:A:113:HIS:O	1:A:116:ALA:CB	2.56	0.47
1:A:161:VAL:C	1:A:163:ALA:N	2.68	0.47
1:A:539:THR:O	1:A:542:TRP:N	2.47	0.47
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.49	0.47
1:A:1062:GLY:C	1:A:1065:ILE:HG13	2.32	0.47
1:A:1076:TYR:CE2	1:A:1078:ASN:CB	2.98	0.47
4:C:292:MET:SD	4:C:404:ARG:NH2	2.88	0.47
5:F:133:LEU:HD23	5:F:133:LEU:N	2.28	0.47
5:F:284:THR:CG2	5:F:428:TYR:OH	2.62	0.47
5:F:570:ASN:ND2	5:F:592:THR:HG22	2.30	0.47
5:F:710:LEU:CD2	5:F:714:PHE:CE1	2.98	0.47
5:F:781:PRO:CD	5:F:795:ILE:HG13	2.45	0.47
4:C:276:PRO:HG2	4:C:384:PRO:HB3	1.97	0.47
5:F:33:ILE:HG23	5:F:1018:PHE:CE2	2.50	0.47
5:F:510:PRO:CG	5:F:767:TYR:HE2	2.22	0.47
5:F:1010:LYS:HG3	5:F:1017:ILE:CD1	2.45	0.47
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:669:TYR:CE1	5:F:708:VAL:HG21	2.50	0.47
5:F:896:ALA:HB2	5:F:987:ASP:HB3	1.95	0.47
1:A:901:VAL:O	1:A:904:PRO:CD	2.55	0.47
1:A:1094:LYS:O	1:A:1095:ALA:O	2.33	0.47
5:F:54:VAL:HG22	5:F:815:VAL:HG21	1.97	0.47
5:F:792:GLU:H	5:F:792:GLU:CD	2.12	0.47
1:A:912:LYS:H	1:A:912:LYS:CD	2.28	0.46
1:A:923:VAL:HG12	1:A:923:VAL:O	2.15	0.46
1:A:1258:TRP:HE1	2:E:208:PRO:HD2	1.80	0.46
5:F:711:ASP:OD2	5:F:739:THR:HG23	2.15	0.46
1:A:685:LYS:HE2	4:C:445:HIS:CD2	2.51	0.46
1:A:900:ARG:O	1:A:900:ARG:HG3	2.15	0.46
1:A:1094:LYS:HD2	2:E:212:TRP:CZ2	2.50	0.46
1:A:1097:PRO:HB2	1:A:1413:ALA:CB	2.41	0.46
1:A:1099:ARG:NH2	2:E:219:GLU:HA	2.29	0.46
2:E:136:LEU:HD12	2:E:139:PRO:HG2	1.97	0.46
5:F:285:LEU:HD11	5:F:291:VAL:HG21	1.97	0.46
5:F:466:LEU:HD12	5:F:467:PRO:HD2	1.97	0.46
1:A:369:TRP:HB3	4:C:293:MET:HA	1.96	0.46
1:A:927:THR:CG2	1:A:1066:VAL:CG2	2.94	0.46
5:F:283:GLU:OE1	5:F:283:GLU:HA	2.15	0.46
5:F:304:SER:HB2	5:F:305:CYS:H	1.54	0.46
6:G:1:NAG:H62	6:G:2:NAG:HN2	1.80	0.46
5:F:126:TYR:HE1	5:F:144:SER:HB2	1.80	0.46
5:F:516:ALA:CB	5:F:524:LEU:HB3	2.46	0.46
5:F:1012:MET:O	5:F:1013:ASN:CB	2.63	0.46
1:A:997:PHE:HD2	1:A:1003:ALA:CB	2.29	0.46
1:A:193:MET:O	1:A:193:MET:HG2	2.15	0.46
1:A:309:TRP:CH2	2:E:152:PHE:CZ	3.03	0.46
1:A:472:LEU:CD2	1:A:511:LEU:HD22	2.45	0.46
1:A:525:SER:O	1:A:528:ARG:N	2.48	0.46
1:A:822:ILE:HA	1:A:1291:LYS:HD3	1.96	0.46
5:F:33:ILE:HG21	5:F:1007:HIS:CE1	2.50	0.46
5:F:178:SER:CB	5:F:181:VAL:HG12	2.28	0.46
5:F:191:LEU:HD22	5:F:490:MET:HE1	1.96	0.46
5:F:532:LYS:HZ2	5:F:532:LYS:HB2	1.80	0.46
5:F:710:LEU:HD21	5:F:714:PHE:CE1	2.46	0.46
5:F:1070:ASP:OD2	5:F:1072:THR:HG22	2.15	0.46
1:A:76:GLU:HG2	5:F:267:SER:OG	2.15	0.46
1:A:280:PHE:O	1:A:284:THR:CG2	2.53	0.46
1:A:309:TRP:HZ2	2:E:152:PHE:CZ	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:VAL:CG1	1:A:895:ILE:HG22	2.45	0.46
1:A:962:LYS:CG	1:A:967:GLU:HB3	2.45	0.46
1:A:1063:PHE:HE2	1:A:1373:ILE:HG22	1.80	0.46
4:C:288:GLU:HB3	4:C:404:ARG:HH21	1.81	0.46
5:F:50:THR:O	5:F:722:TYR:OH	2.29	0.46
5:F:133:LEU:CD2	5:F:133:LEU:N	2.73	0.46
5:F:895:TYR:CE1	5:F:986:PHE:CE1	3.03	0.46
1:A:338:THR:HB	1:A:1388:THR:HG21	1.98	0.46
5:F:539:PRO:HD3	5:F:977:CYS:HB3	1.98	0.46
5:F:628:THR:O	5:F:629:TYR:CD2	2.69	0.46
5:F:629:TYR:HB2	5:F:809:LEU:HD23	1.98	0.46
5:F:856:LEU:HD21	5:F:878:PHE:CG	2.51	0.46
1:A:639:ILE:C	1:A:639:ILE:HD12	2.37	0.46
1:A:931:ILE:HG23	1:A:932:VAL:N	2.30	0.46
1:A:1263:SER:C	1:A:1265:GLN:H	2.19	0.46
2:E:117:PHE:CD2	2:E:146:PHE:HB3	2.51	0.46
3:B:99:LYS:NZ	3:B:138:GLU:OE1	2.40	0.46
5:F:161:VAL:HG22	5:F:162:SER:N	2.30	0.46
5:F:320:LEU:O	5:F:324:VAL:HG23	2.16	0.46
5:F:845:LYS:CD	5:F:847:ASN:HD21	2.29	0.46
1:A:592:VAL:HG23	1:A:592:VAL:O	2.14	0.46
1:A:593:ARG:O	1:A:596:ASN:ND2	2.49	0.46
1:A:903:ARG:N	1:A:904:PRO:CD	2.78	0.46
1:A:977:ASP:OD1	1:A:977:ASP:N	2.47	0.46
5:F:234:LYS:HB2	5:F:551:GLN:HG2	1.96	0.46
5:F:1001:ASN:HD22	9:F:1121:NAG:C1	2.09	0.46
1:A:510:GLU:HA	1:A:513:LEU:HB2	1.97	0.45
1:A:1262:LYS:HD3	2:E:209:GLN:HA	1.99	0.45
1:A:1334:TYR:CA	1:A:1353:GLY:HA3	2.46	0.45
2:E:35:LEU:HG	2:E:37:PRO:HD3	1.98	0.45
3:B:129:GLU:N	3:B:132:ASP:OD2	2.47	0.45
5:F:41:GLN:HB3	5:F:1011:LEU:HB3	1.98	0.45
5:F:336:LYS:HG3	5:F:369:GLU:OE2	2.16	0.45
5:F:364:THR:O	5:F:390:SER:HA	2.15	0.45
1:A:333:LEU:HB3	1:A:657:LEU:HD23	1.98	0.45
1:A:954:PHE:CD2	1:A:1022:ARG:HG2	2.51	0.45
2:E:20:ILE:CG1	2:E:118:LEU:HD21	2.47	0.45
2:E:128:ALA:HB3	2:E:137:LEU:HD13	1.97	0.45
5:F:285:LEU:HD13	5:F:291:VAL:HB	1.99	0.45
5:F:607:ARG:HA	5:F:607:ARG:HD3	1.80	0.45
5:F:824:TRP:CD2	5:F:864:MET:HE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LEU:CD1	1:A:941:MET:HG3	2.46	0.45
1:A:541:TYR:CD1	1:A:541:TYR:N	2.84	0.45
1:A:796:VAL:HG13	1:A:797:ASN:N	2.31	0.45
1:A:938:LEU:HD12	1:A:938:LEU:HA	1.77	0.45
1:A:1181:PRO:HG2	2:E:215:CYS:SG	2.56	0.45
1:A:1334:TYR:O	1:A:1336:LYS:N	2.47	0.45
1:A:1403:LYS:HA	1:A:1406:TRP:HB3	1.98	0.45
1:A:1416:ARG:H	1:A:1416:ARG:HD3	1.81	0.45
4:C:436:GLU:HG2	4:C:441:ASP:HB3	1.98	0.45
1:A:247:ARG:HE	1:A:261:CYS:HB3	1.81	0.45
1:A:318:ILE:O	1:A:322:SER:CB	2.62	0.45
1:A:460:LEU:HD22	1:A:464:GLN:HE21	1.82	0.45
1:A:901:VAL:HG21	1:A:1283:VAL:HB	1.98	0.45
1:A:1249:ARG:NE	1:A:1249:ARG:CA	2.73	0.45
5:F:79:VAL:HG12	5:F:612:THR:HG22	1.99	0.45
5:F:362:LEU:HD12	5:F:362:LEU:O	2.17	0.45
1:A:117:TYR:CZ	1:A:118:LEU:HD23	2.49	0.45
1:A:175:LEU:HD13	11:A:1907:3PE:H3C1	1.97	0.45
1:A:216:GLU:HG2	1:A:1138:GLN:HE22	1.81	0.45
1:A:365:GLY:HA3	4:C:437:ASN:O	2.15	0.45
1:A:541:TYR:N	1:A:541:TYR:HD1	2.15	0.45
1:A:1052:ILE:HD13	1:A:1052:ILE:HA	1.71	0.45
1:A:1162:THR:CG2	1:A:1190:VAL:HG13	2.42	0.45
4:C:279:LEU:HD22	4:C:387:VAL:CG2	2.44	0.45
8:L:1:NAG:H61	8:L:2:NAG:O5	2.17	0.45
1:A:190:PHE:O	1:A:194:LEU:HD23	2.17	0.45
1:A:475:PHE:HE2	1:A:534:ARG:CD	2.17	0.45
1:A:496:PHE:HE2	1:A:537:LYS:O	1.82	0.45
1:A:1016:TRP:CG	1:A:1017:PRO:HD3	2.52	0.45
1:A:1349:GLU:H	1:A:1349:GLU:HG2	1.53	0.45
2:E:35:LEU:HB3	2:E:49:ALA:H	1.81	0.45
5:F:75:ALA:O	5:F:79:VAL:HG23	2.17	0.45
5:F:773:ASN:HD22	5:F:777:VAL:CG2	2.30	0.45
5:F:1006:PHE:O	5:F:1006:PHE:CD1	2.70	0.45
1:A:472:LEU:HD23	1:A:511:LEU:CD2	2.46	0.45
1:A:1104:LYS:O	1:A:1105:ASN:HB2	2.16	0.45
1:A:1245:LYS:O	1:A:1248:SER:N	2.36	0.45
1:A:1288:MET:HG2	1:A:1356:PHE:CD2	2.52	0.45
1:A:1289:PHE:HE1	1:A:1354:THR:CG2	2.30	0.45
1:A:1389:ARG:O	1:A:1389:ARG:HG2	2.16	0.45
2:E:137:LEU:CD2	2:E:137:LEU:N	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:41:GLN:OE1	5:F:1012:MET:O	2.34	0.45
5:F:243:ARG:HA	5:F:243:ARG:HD2	1.74	0.45
5:F:628:THR:O	5:F:629:TYR:CG	2.69	0.45
5:F:821:VAL:O	5:F:825:ILE:HG13	2.17	0.45
1:A:376:MET:O	4:C:295:LYS:CE	2.57	0.45
1:A:651:ILE:HD11	11:A:1913:3PE:H2H1	1.98	0.45
5:F:368:GLU:O	5:F:368:GLU:HG2	2.16	0.45
5:F:511:ASN:HB2	5:F:627:PRO:HG3	1.99	0.45
5:F:771:LEU:O	5:F:811:LYS:NZ	2.49	0.45
1:A:64:ASN:HD22	1:A:64:ASN:C	2.10	0.45
1:A:905:LEU:HD22	1:A:905:LEU:HA	1.69	0.45
1:A:1469:ALA:HA	1:A:1472:ARG:HB3	1.98	0.45
4:C:426:PRO:HA	4:C:427:PRO:HD3	1.89	0.45
5:F:292:ASN:OD1	5:F:293:VAL:N	2.47	0.45
5:F:523:VAL:CG2	5:F:526:HIS:HB2	2.46	0.45
5:F:845:LYS:HG2	5:F:846:ARG:N	2.31	0.45
1:A:117:TYR:HH	1:A:127:PHE:HD2	1.63	0.45
1:A:290:THR:O	1:A:291:MET:HB2	2.17	0.45
1:A:295:THR:HG21	1:A:1318:ARG:HG2	1.99	0.45
1:A:553:LEU:HA	1:A:556:ILE:CG2	2.47	0.45
1:A:1195:ILE:CD1	2:E:117:PHE:CE2	3.00	0.45
1:A:1498:TRP:O	1:A:1499:LYS:CB	2.65	0.45
2:E:135:TYR:O	2:E:139:PRO:HD2	2.17	0.45
5:F:319:VAL:HG21	5:F:1046:PRO:HG3	1.98	0.45
5:F:350:ASN:CG	6:D:1:NAG:C1	2.85	0.45
5:F:515:PHE:CZ	5:F:623:ALA:HB3	2.52	0.45
5:F:516:ALA:HB3	5:F:525:LEU:H	1.82	0.45
5:F:576:ILE:HD11	5:F:588:LYS:HG2	1.99	0.45
1:A:868:PHE:HE2	1:A:915:LYS:HZ2	1.54	0.44
1:A:1337:LEU:HD22	1:A:1338:CYS:N	2.32	0.44
2:E:136:LEU:HD12	2:E:139:PRO:CG	2.47	0.44
4:C:275:ARG:NH2	4:C:384:PRO:O	2.50	0.44
5:F:705:ILE:CD1	5:F:706:ASN:N	2.78	0.44
5:F:1010:LYS:CG	5:F:1017:ILE:CD1	2.95	0.44
1:A:532:LEU:O	1:A:535:LEU:HG	2.16	0.44
1:A:1164:GLU:HG3	1:A:1165:MET:N	2.32	0.44
5:F:27:PHE:CE1	5:F:1020:MET:HG2	2.52	0.44
1:A:112:PHE:HD1	1:A:115:ASP:CB	2.30	0.44
1:A:330:LEU:HD12	1:A:330:LEU:HA	1.82	0.44
1:A:366:TYR:OH	4:C:396:VAL:HB	2.17	0.44
1:A:533:LEU:O	1:A:536:PHE:CD2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LEU:O	1:A:572:ILE:HG13	2.17	0.44
1:A:921:VAL:HG13	1:A:1370:PHE:CE2	2.35	0.44
1:A:1113:TYR:CD1	1:A:1113:TYR:O	2.70	0.44
1:A:1263:SER:OG	1:A:1383:ASN:ND2	2.51	0.44
5:F:94:SER:O	5:F:98:VAL:HG23	2.17	0.44
5:F:465:THR:HG22	5:F:466:LEU:N	2.32	0.44
1:A:368:SER:HA	1:A:371:THR:HG22	2.00	0.44
1:A:903:ARG:H	1:A:903:ARG:HG3	1.62	0.44
1:A:924:ALA:HB1	1:A:1063:PHE:HD1	1.82	0.44
1:A:1000:VAL:HG12	1:A:1000:VAL:O	2.17	0.44
1:A:1155:VAL:CG2	1:A:1197:VAL:HG11	2.43	0.44
5:F:702:THR:HG23	5:F:703:ASP:N	2.32	0.44
5:F:803:ILE:HD12	5:F:805:ILE:HD11	1.99	0.44
1:A:532:LEU:O	1:A:532:LEU:HD22	2.18	0.44
1:A:661:VAL:CG1	1:A:662:ASP:N	2.80	0.44
1:A:929:GLY:O	1:A:933:LEU:HB2	2.17	0.44
1:A:1007:LEU:CA	1:A:1010:VAL:CG1	2.85	0.44
2:E:118:LEU:C	2:E:118:LEU:CD2	2.85	0.44
5:F:867:HIS:O	5:F:868:ASP:HB3	2.16	0.44
1:A:80:ASN:ND2	1:A:82:LEU:HB3	2.33	0.44
1:A:117:TYR:OH	1:A:127:PHE:HD2	2.01	0.44
1:A:125:LEU:HA	1:A:128:ILE:HD12	2.00	0.44
1:A:1113:TYR:CD1	1:A:1113:TYR:C	2.90	0.44
5:F:704:LEU:HD23	5:F:704:LEU:O	2.18	0.44
1:A:58:LEU:HA	1:A:61:ILE:HG22	1.99	0.44
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.82	0.44
1:A:229:ILE:HG12	1:A:260:GLU:HB3	1.99	0.44
1:A:341:ARG:HH11	1:A:665:ALA:HB1	1.83	0.44
5:F:669:TYR:CD1	5:F:704:LEU:HD21	2.37	0.44
1:A:53:PHE:O	1:A:57:ILE:CG2	2.57	0.44
1:A:656:PHE:CE2	14:A:1915[A]:4YH:N4	2.86	0.44
1:A:957:CYS:SG	1:A:958:ASN:N	2.91	0.44
5:F:263:SER:HB3	5:F:332:ILE:O	2.18	0.44
1:A:66:VAL:O	1:A:66:VAL:HG12	2.18	0.44
1:A:170:LEU:O	1:A:173:LEU:HB2	2.18	0.44
1:A:196:LEU:HD11	1:A:333:LEU:HD13	2.00	0.44
1:A:535:LEU:HD13	1:A:536:PHE:N	2.33	0.44
1:A:816:LEU:CD1	1:A:901:VAL:HA	2.47	0.44
1:A:868:PHE:HD2	1:A:915:LYS:NZ	2.10	0.44
1:A:1007:LEU:O	1:A:1010:VAL:HG13	2.18	0.44
11:A:1912:3PE:C3	11:A:1912:3PE:C22	2.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:214:THR:HG22	5:F:214:THR:O	2.17	0.44
5:F:390:SER:CB	5:F:412:TYR:OH	2.66	0.44
5:F:781:PRO:O	5:F:875:GLY:CA	2.60	0.44
6:D:1:NAG:H82	6:D:1:NAG:H3	2.00	0.44
1:A:509:LEU:O	1:A:509:LEU:HD13	2.18	0.43
1:A:980:PRO:HG3	5:F:276:THR:HG21	2.00	0.43
5:F:164:GLN:O	5:F:196:LYS:NZ	2.44	0.43
5:F:481:LEU:HD23	5:F:481:LEU:N	2.33	0.43
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.82	0.43
1:A:341:ARG:HD3	1:A:665:ALA:CB	2.49	0.43
1:A:341:ARG:NH1	1:A:665:ALA:HB1	2.33	0.43
1:A:997:PHE:CD2	1:A:1003:ALA:CB	3.01	0.43
1:A:1065:ILE:HD12	1:A:1066:VAL:CA	2.49	0.43
5:F:516:ALA:HB3	5:F:524:LEU:HB3	2.01	0.43
5:F:826:GLU:OE1	5:F:826:GLU:HA	2.17	0.43
1:A:131:PHE:CD1	1:A:131:PHE:C	2.91	0.43
1:A:219:LYS:NZ	1:A:1138:GLN:OE1	2.51	0.43
1:A:813:SER:HB3	1:A:1279:PHE:CZ	2.53	0.43
1:A:1014:GLU:OE2	1:A:1322:GLY:O	2.36	0.43
1:A:1171:ALA:O	1:A:1172:PHE:CG	2.72	0.43
2:E:32:TRP:HH2	2:E:53:LEU:HG	1.83	0.43
2:E:138:ARG:NE	2:E:204:LEU:HD23	2.33	0.43
5:F:133:LEU:H	5:F:133:LEU:HD22	1.80	0.43
5:F:198:ASN:HB2	5:F:208:GLN:OE1	2.18	0.43
5:F:513:TYR:CZ	5:F:625:VAL:HG21	2.54	0.43
5:F:669:TYR:HD1	5:F:704:LEU:CD2	2.25	0.43
5:F:739:THR:HG22	5:F:743:ILE:O	2.17	0.43
5:F:824:TRP:HB3	5:F:864:MET:CE	2.48	0.43
1:A:94:LEU:CD1	1:A:94:LEU:C	2.85	0.43
1:A:354:ARG:HH22	1:A:673:ALA:CB	2.31	0.43
1:A:979:ASP:C	1:A:981:THR:H	2.21	0.43
4:C:279:LEU:HD23	4:C:279:LEU:N	2.32	0.43
4:C:361:LEU:HB3	4:C:458:HIS:HE2	1.84	0.43
5:F:1010:LYS:HG2	5:F:1017:ILE:CG1	2.47	0.43
1:A:123:ASN:N	1:A:123:ASN:HD22	2.15	0.43
1:A:136:THR:HA	1:A:164:LEU:HD22	2.00	0.43
1:A:309:TRP:H	1:A:310:PRO:HD2	1.83	0.43
1:A:536:PHE:O	1:A:539:THR:HB	2.19	0.43
1:A:1164:GLU:HG3	1:A:1165:MET:H	1.83	0.43
5:F:253:PRO:O	5:F:356:CYS:HB3	2.19	0.43
5:F:346:LEU:HD21	5:F:360:ILE:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:400:PRO:O	5:F:404:MET:HG3	2.18	0.43
5:F:661:TYR:HD2	5:F:752:GLY:HA3	1.83	0.43
1:A:167:PHE:O	1:A:170:LEU:HB2	2.18	0.43
1:A:366:TYR:CG	4:C:400:LEU:CG	3.00	0.43
1:A:807:LEU:HA	1:A:810:LEU:HB2	2.00	0.43
1:A:1295:VAL:O	1:A:1298:THR:OG1	2.30	0.43
5:F:242:ARG:NH2	5:F:280:GLU:O	2.52	0.43
5:F:281:MET:CE	5:F:363:PHE:HZ	2.31	0.43
5:F:532:LYS:H	5:F:532:LYS:HG3	1.56	0.43
1:A:980:PRO:HD3	5:F:418:ILE:HD13	2.01	0.43
5:F:205:LEU:HD23	5:F:206:LEU:N	2.34	0.43
1:A:56:ILE:CG1	1:A:57:ILE:N	2.73	0.43
1:A:327:ASN:C	1:A:327:ASN:HD22	2.21	0.43
2:E:163:LYS:HA	2:E:163:LYS:HD2	1.30	0.43
5:F:169:HIS:CE1	5:F:238:TYR:HD1	2.37	0.43
1:A:366:TYR:CZ	4:C:400:LEU:CD1	3.01	0.43
1:A:958:ASN:HB3	1:A:972:TYR:CZ	2.54	0.43
1:A:1074:THR:HG22	1:A:1075:GLU:HG3	2.01	0.43
1:A:1189:ILE:HD11	1:A:1241:MET:HB3	2.00	0.43
1:A:1390:ASP:C	1:A:1392:SER:H	2.22	0.43
5:F:41:GLN:HB3	5:F:1011:LEU:CG	2.49	0.43
5:F:100:LEU:HD12	5:F:194:VAL:HG12	2.00	0.43
5:F:208:GLN:O	5:F:219:TYR:HA	2.19	0.43
1:A:1007:LEU:C	1:A:1010:VAL:HG12	2.39	0.43
1:A:1068:PHE:CE2	1:A:1073:GLU:OE2	2.72	0.43
4:C:279:LEU:C	4:C:280:VAL:CG1	2.87	0.43
5:F:33:ILE:CG2	5:F:1007:HIS:CE1	3.02	0.43
1:A:38:ASN:HD22	1:A:38:ASN:HA	1.50	0.42
5:F:44:LEU:HD11	5:F:824:TRP:HZ2	1.82	0.42
5:F:381:ASP:OD1	5:F:381:ASP:N	2.37	0.42
1:A:1136:GLY:C	11:A:1911:3PE:H262	2.39	0.42
5:F:981:GLN:HG2	5:F:1038:GLU:HG2	2.01	0.42
1:A:291:MET:CE	11:A:1913:3PE:H12	2.46	0.42
1:A:354:ARG:HH22	1:A:673:ALA:HB1	1.84	0.42
5:F:41:GLN:CB	5:F:1011:LEU:HB3	2.49	0.42
5:F:590:PHE:CD1	5:F:590:PHE:N	2.87	0.42
5:F:1005:ILE:HG23	5:F:1005:ILE:O	2.19	0.42
1:A:499:PHE:HZ	1:A:533:LEU:HB3	1.84	0.42
1:A:535:LEU:HD12	1:A:536:PHE:N	2.33	0.42
1:A:545:LEU:O	1:A:549:VAL:CG2	2.52	0.42
1:A:979:ASP:C	1:A:981:THR:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1263:SER:C	1:A:1265:GLN:N	2.73	0.42
1:A:1347:GLY:C	1:A:1348:GLU:HG2	2.40	0.42
14:A:1916[B]:4YH:H20	14:A:1916[B]:4YH:H25	1.49	0.42
5:F:845:LYS:HD3	5:F:847:ASN:HD21	1.84	0.42
5:F:1008:VAL:HB	5:F:1019:ILE:HG22	2.02	0.42
1:A:614:GLU:HG2	1:A:1017:PRO:HD3	2.01	0.42
1:A:976:LYS:CD	1:A:984:GLU:CD	2.85	0.42
1:A:1106:PRO:O	1:A:1110:GLN:HB2	2.19	0.42
1:A:109:GLY:HA3	1:A:113:HIS:ND1	2.35	0.42
1:A:136:THR:CB	1:A:164:LEU:CD2	2.98	0.42
1:A:632:TYR:CB	1:A:633:PRO:CD	2.98	0.42
1:A:1107:TYR:O	1:A:1111:VAL:HG23	2.19	0.42
1:A:1199:LEU:C	1:A:1201:GLU:N	2.72	0.42
5:F:319:VAL:CG2	5:F:1046:PRO:HG3	2.49	0.42
5:F:988:ASN:OD1	9:F:1122:NAG:O5	2.37	0.42
1:A:94:LEU:C	1:A:94:LEU:HD12	2.40	0.42
1:A:1091:TYR:CE1	2:E:212:TRP:CB	2.99	0.42
1:A:1366:MET:CE	11:A:1912:3PE:C2C	2.98	0.42
4:C:279:LEU:O	4:C:280:VAL:HG12	2.20	0.42
5:F:844:CYS:HB3	5:F:866:ASN:HD21	1.85	0.42
5:F:1011:LEU:CD1	5:F:1011:LEU:H	2.32	0.42
1:A:163:ALA:C	1:A:165:ARG:N	2.73	0.42
1:A:358:GLN:HA	1:A:361:GLU:HG2	2.01	0.42
1:A:658:ALA:O	1:A:661:VAL:HG12	2.18	0.42
1:A:1068:PHE:HB3	1:A:1073:GLU:HG3	2.01	0.42
2:E:32:TRP:CH2	2:E:53:LEU:HG	2.53	0.42
5:F:182:LEU:HD22	5:F:182:LEU:HA	1.80	0.42
5:F:212:SER:CB	5:F:216:LEU:O	2.67	0.42
5:F:845:LYS:O	5:F:866:ASN:ND2	2.53	0.42
1:A:366:TYR:CE2	4:C:400:LEU:HD11	2.54	0.42
14:A:1915[A]:4YH:H18	14:A:1915[A]:4YH:H15	1.82	0.42
5:F:178:SER:O	5:F:181:VAL:CG1	2.68	0.42
5:F:733:LYS:HE3	5:F:733:LYS:HB2	1.82	0.42
1:A:523:GLY:C	1:A:525:SER:N	2.73	0.42
1:A:931:ILE:HD12	1:A:931:ILE:HA	1.89	0.42
1:A:1076:TYR:HE2	1:A:1078:ASN:HD22	1.56	0.42
2:E:60:ARG:NE	2:E:77:GLU:OE1	2.49	0.42
5:F:28:PRO:HD3	5:F:851:MET:HE1	2.00	0.42
5:F:478:LYS:HD3	5:F:479:THR:HG23	2.00	0.42
5:F:570:ASN:ND2	5:F:592:THR:HG21	2.34	0.42
1:A:66:VAL:HG13	11:A:1907:3PE:O32	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LEU:HD13	1:A:480:LEU:O	2.20	0.41
1:A:1010:VAL:HG23	1:A:1016:TRP:HB2	2.02	0.41
3:B:108:ASN:ND2	4:C:266:PRO:O	2.53	0.41
5:F:704:LEU:O	5:F:708:VAL:HG23	2.20	0.41
1:A:1381:MET:C	1:A:1383:ASN:N	2.73	0.41
5:F:481:LEU:CD2	5:F:481:LEU:H	2.34	0.41
5:F:705:ILE:HD12	5:F:706:ASN:CA	2.50	0.41
5:F:1066:ASN:HD22	5:F:1067:VAL:N	2.17	0.41
1:A:331:GLY:CA	1:A:1380:ILE:CD1	2.98	0.41
1:A:355:GLU:O	1:A:359:LEU:N	2.38	0.41
1:A:468:ASN:O	1:A:472:LEU:N	2.46	0.41
1:A:525:SER:C	1:A:527:LEU:N	2.73	0.41
1:A:666:GLU:HA	1:A:666:GLU:OE1	2.21	0.41
1:A:823:ARG:HG2	1:A:1341:GLU:HB3	2.03	0.41
1:A:1155:VAL:HG21	1:A:1197:VAL:HG13	1.98	0.41
2:E:141:SER:OG	2:E:196:GLY:O	2.37	0.41
4:C:393:SER:HB3	4:C:396:VAL:HG23	2.02	0.41
5:F:346:LEU:HD12	5:F:346:LEU:HA	1.86	0.41
5:F:471:ILE:O	5:F:471:ILE:HG13	2.19	0.41
6:K:1:NAG:H82	6:K:2:NAG:C2	2.47	0.41
1:A:191:LYS:HB3	1:A:191:LYS:HE3	1.82	0.41
1:A:286:TYR:O	1:A:290:THR:HG23	2.20	0.41
1:A:341:ARG:HD3	1:A:665:ALA:HB2	2.02	0.41
1:A:366:TYR:CZ	4:C:396:VAL:HB	2.55	0.41
5:F:63:LYS:NZ	5:F:717:GLU:OE2	2.36	0.41
5:F:509:CYS:HB2	5:F:510:PRO:CD	2.49	0.41
1:A:532:LEU:HD11	1:A:941:MET:HG3	2.02	0.41
1:A:664:LEU:HG	1:A:1065:ILE:CG2	2.48	0.41
1:A:821:PRO:O	1:A:1291:LYS:HE3	2.21	0.41
1:A:1243:LEU:O	1:A:1246:LEU:HB2	2.21	0.41
2:E:130:ARG:O	2:E:133:ARG:HD2	2.20	0.41
3:B:136:ILE:HA	3:B:147:GLY:HA3	2.01	0.41
5:F:206:LEU:CD2	5:F:495:SER:HB2	2.49	0.41
5:F:315:ARG:HD3	5:F:315:ARG:HA	1.97	0.41
5:F:346:LEU:CD2	5:F:360:ILE:CG2	2.98	0.41
5:F:510:PRO:HG3	5:F:762:TYR:CD1	2.55	0.41
5:F:851:MET:HA	5:F:1023:SER:N	2.36	0.41
1:A:302:ASN:O	1:A:304:ALA:N	2.54	0.41
1:A:460:LEU:HD23	1:A:460:LEU:HA	1.86	0.41
1:A:525:SER:O	1:A:527:LEU:N	2.53	0.41
1:A:927:THR:HG21	1:A:1066:VAL:CG2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:THR:HG22	1:A:1075:GLU:N	2.36	0.41
4:C:450:LEU:HA	4:C:453:TYR:HB3	2.02	0.41
5:F:114:ARG:HH21	7:H:1:NAG:C6	2.29	0.41
5:F:477:ASN:N	5:F:477:ASN:HD22	2.18	0.41
1:A:976:LYS:H	1:A:976:LYS:HG2	1.58	0.41
1:A:1109:TYR:O	1:A:1112:TRP:HB3	2.21	0.41
1:A:1343:ASP:OD1	1:A:1343:ASP:N	2.53	0.41
1:A:1430:GLN:HA	1:A:1431:PRO:HD3	1.93	0.41
2:E:205:PRO:O	2:E:206:ARG:CB	2.69	0.41
4:C:427:PRO:HA	4:C:430:PHE:HD2	1.86	0.41
5:F:232:PRO:HB2	5:F:234:LYS:HD3	2.01	0.41
5:F:369:GLU:HG2	5:F:371:ALA:H	1.85	0.41
1:A:650:TYR:CD2	11:A:1913:3PE:H2F1	2.54	0.41
1:A:1007:LEU:HA	1:A:1010:VAL:HG11	1.95	0.41
1:A:1286:MET:O	1:A:1290:GLY:N	2.53	0.41
12:A:1910:PC1:H111	12:A:1910:PC1:H133	1.84	0.41
4:C:393:SER:HB3	4:C:396:VAL:CG2	2.51	0.41
5:F:185:LEU:O	5:F:189:SER:OG	2.36	0.41
5:F:629:TYR:C	5:F:629:TYR:HD1	2.23	0.41
1:A:287:GLN:NE2	1:A:292:GLU:O	2.46	0.41
1:A:423:TRP:CZ2	4:C:303:HIS:NE2	2.89	0.41
1:A:868:PHE:CB	1:A:909:ASN:HD21	2.11	0.41
1:A:1091:TYR:CE2	2:E:211:PRO:HB2	2.56	0.41
1:A:1250:ALA:O	1:A:1254:ARG:HB2	2.21	0.41
1:A:1299:GLN:HB2	1:A:1331:ALA:CB	2.51	0.41
1:A:1326:GLN:H	1:A:1326:GLN:HG3	1.49	0.41
5:F:58:VAL:HG13	5:F:803:ILE:HG22	2.01	0.41
5:F:117:PHE:CD2	5:F:182:LEU:HD12	2.52	0.41
5:F:151:PHE:CE2	5:F:224:PRO:HD3	2.56	0.41
5:F:330:LYS:HG2	5:F:331:GLY:N	2.35	0.41
5:F:351:VAL:HG23	5:F:353:ARG:HG3	2.03	0.41
5:F:361:MET:HE2	5:F:387:PHE:HB2	2.02	0.41
6:K:1:NAG:H83	6:K:1:NAG:H2	1.91	0.41
1:A:57:ILE:O	1:A:61:ILE:HG22	2.21	0.41
1:A:559:ILE:HD13	1:A:659:ILE:HG12	2.03	0.41
1:A:1113:TYR:O	1:A:1113:TYR:HD1	2.04	0.41
1:A:1389:ARG:HD2	1:A:1391:TRP:CE3	2.55	0.41
4:C:281:GLY:HA3	4:C:422:LEU:HG	2.01	0.41
4:C:398:GLN:HA	4:C:401:ILE:HD12	2.02	0.41
1:A:244:PRO:HB2	1:A:304:ALA:HB2	2.02	0.40
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:1907:3PE:H3B1	11:A:1907:3PE:H3E2	1.83	0.40
5:F:217:ALA:HB2	5:F:240:VAL:CG2	2.50	0.40
5:F:290:PHE:HD1	5:F:354:ALA:HB2	1.86	0.40
1:A:169:VAL:HG21	1:A:575:LEU:CB	2.51	0.40
1:A:496:PHE:CZ	1:A:537:LYS:O	2.72	0.40
1:A:1104:LYS:O	1:A:1105:ASN:CB	2.70	0.40
5:F:398:ARG:O	5:F:401:ILE:HG22	2.21	0.40
5:F:466:LEU:HD12	5:F:466:LEU:HA	1.87	0.40
5:F:729:ILE:CG2	8:L:2:NAG:H82	2.51	0.40
5:F:817:ILE:HG21	5:F:817:ILE:HD13	1.86	0.40
1:A:52:PRO:HA	1:A:55:THR:HG1	1.85	0.40
1:A:361:GLU:O	4:C:437:ASN:HB2	2.20	0.40
1:A:584:ARG:C	1:A:586:ASP:N	2.75	0.40
1:A:941:MET:O	1:A:945:ILE:HG13	2.21	0.40
1:A:168:ARG:C	1:A:170:LEU:N	2.73	0.40
1:A:925:ILE:CD1	1:A:1370:PHE:CE1	3.03	0.40
1:A:973:TYR:CE2	5:F:173:ASP:HB3	2.57	0.40
1:A:1115:VAL:CG1	1:A:1168:LYS:HD3	2.51	0.40
1:A:1301:ASN:HB2	1:A:1302:ARG:H	1.74	0.40
5:F:274:ILE:CG1	5:F:391:VAL:HG21	2.51	0.40
1:A:231:THR:O	1:A:262:ARG:NH2	2.46	0.40
1:A:584:ARG:O	1:A:586:ASP:N	2.52	0.40
1:A:1097:PRO:CD	2:E:218:ALA:HB3	2.50	0.40
2:E:208:PRO:CB	2:E:213:GLU:HB2	2.46	0.40
4:C:279:LEU:HA	4:C:387:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1260/1506 (84%)	1106 (88%)	117 (9%)	37 (3%)	4 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	159/222 (72%)	146 (92%)	11 (7%)	2 (1%)	12	24
3	B	98/450 (22%)	89 (91%)	9 (9%)	0	100	100
4	C	174/524 (33%)	164 (94%)	10 (6%)	0	100	100
5	F	968/1046 (92%)	876 (90%)	86 (9%)	6 (1%)	25	47
All	All	2659/3748 (71%)	2381 (90%)	233 (9%)	45 (2%)	13	18

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	76	GLU
1	A	110	PHE
1	A	129	ILE
1	A	237	VAL
1	A	320	LEU
1	A	322	SER
1	A	520	THR
1	A	632	TYR
1	A	1095	ALA
1	A	1173	LYS
1	A	1334	TYR
2	E	206	ARG
5	F	349	TYR
1	A	162	LYS
1	A	215	LEU
1	A	303	ASP
1	A	321	GLY
1	A	519	MET
1	A	1141	HIS
1	A	1335	GLY
1	A	1391	TRP
5	F	629	TYR
5	F	661	TYR
1	A	50	TRP
1	A	79	ASN
1	A	169	VAL
1	A	1037	ASN
1	A	1105	ASN
5	F	790	ALA
1	A	108	TYR
1	A	111	LEU

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Mol	Chain	Res	Type
1	A	248	THR
1	A	518	ALA
1	A	1097	PRO
1	A	1346	PRO
1	A	309	TRP
1	A	522	LEU
1	A	644	LEU
1	A	980	PRO
1	A	1382	ASP
1	A	178	GLY
5	F	627	PRO
2	E	37	PRO
5	F	332	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1097/1327 (83%)	923 (84%)	174 (16%)	2	4
2	E	143/192 (74%)	133 (93%)	10 (7%)	15	30
3	B	58/391 (15%)	57 (98%)	1 (2%)	60	81
4	C	143/460 (31%)	141 (99%)	2 (1%)	67	85
5	F	868/924 (94%)	796 (92%)	72 (8%)	11	22
All	All	2309/3294 (70%)	2050 (89%)	259 (11%)	9	10

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	41	ARG
1	A	42	LYS
1	A	55	THR
1	A	57	ILE
1	A	64	ASN

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Mol	Chain	Res	Type
1	A	70	VAL
1	A	74	MET
1	A	90	GLU
1	A	92	PHE
1	A	94	LEU
1	A	95	THR
1	A	112	PHE
1	A	114	GLN
1	A	117	TYR
1	A	130	VAL
1	A	132	LEU
1	A	135	PHE
1	A	143	ASN
1	A	162	LYS
1	A	164	LEU
1	A	170	LEU
1	A	171	ARG
1	A	174	ARG
1	A	177	SER
1	A	183	GLN
1	A	186	LEU
1	A	188	SER
1	A	194	LEU
1	A	196	LEU
1	A	201	LEU
1	A	206	MET
1	A	215	LEU
1	A	218	PHE
1	A	232	ASP
1	A	239	ASN
1	A	243	SER
1	A	245	CYS
1	A	252	ARG
1	A	260	GLU
1	A	261	CYS
1	A	273	THR
1	A	284	THR
1	A	287	GLN
1	A	289	ILE
1	A	291	MET
1	A	318	ILE
1	A	320	LEU

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Mol	Chain	Res	Type
1	A	322	SER
1	A	326	LEU
1	A	327	ASN
1	A	330	LEU
1	A	333	LEU
1	A	334	SER
1	A	435	TYR
1	A	445	ASN
1	A	447	LEU
1	A	451	SER
1	A	455	ASN
1	A	458	LEU
1	A	460	LEU
1	A	495	ILE
1	A	511	LEU
1	A	512	LEU
1	A	513	LEU
1	A	514	VAL
1	A	515	GLU
1	A	516	SER
1	A	519	MET
1	A	524	ILE
1	A	527	LEU
1	A	528	ARG
1	A	535	LEU
1	A	545	LEU
1	A	546	SER
1	A	552	LEU
1	A	553	LEU
1	A	554	ASN
1	A	555	SER
1	A	556	ILE
1	A	557	ARG
1	A	584	ARG
1	A	589	ASP
1	A	595	SER
1	A	596	ASN
1	A	604	LEU
1	A	636	LEU
1	A	637	VAL
1	A	639	ILE
1	A	652	LEU

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Mol	Chain	Res	Type
1	A	653	LEU
1	A	657	LEU
1	A	894	LYS
1	A	896	LEU
1	A	899	LEU
1	A	900	ARG
1	A	905	LEU
1	A	906	ARG
1	A	908	ILE
1	A	910	ARG
1	A	912	LYS
1	A	919	GLN
1	A	922	PHE
1	A	926	ARG
1	A	930	ASN
1	A	933	LEU
1	A	938	LEU
1	A	939	GLN
1	A	951	LYS
1	A	961	SER
1	A	962	LYS
1	A	976	LYS
1	A	977	ASP
1	A	983	MET
1	A	984	GLU
1	A	991	ILE
1	A	999	ASN
1	A	1004	MET
1	A	1018	GLN
1	A	1037	ASN
1	A	1038	ARG
1	A	1056	MET
1	A	1063	PHE
1	A	1068	PHE
1	A	1074	THR
1	A	1091	TYR
1	A	1096	ARG
1	A	1117	SER
1	A	1118	SER
1	A	1119	TYR
1	A	1120	PHE
1	A	1124	MET

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Mol	Chain	Res	Type
1	A	1131	ASN
1	A	1132	THR
1	A	1142	GLN
1	A	1163	LEU
1	A	1164	GLU
1	A	1175	ARG
1	A	1188	LEU
1	A	1201	GLU
1	A	1241	MET
1	A	1246	LEU
1	A	1247	LEU
1	A	1249	ARG
1	A	1256	LEU
1	A	1262	LYS
1	A	1267	LEU
1	A	1272	LEU
1	A	1277	LEU
1	A	1287	GLN
1	A	1288	MET
1	A	1289	PHE
1	A	1295	VAL
1	A	1307	GLN
1	A	1314	LEU
1	A	1318	ARG
1	A	1326	GLN
1	A	1329	LEU
1	A	1337	LEU
1	A	1343	ASP
1	A	1349	GLU
1	A	1352	CYS
1	A	1366	MET
1	A	1371	LEU
1	A	1381	MET
1	A	1383	ASN
1	A	1384	PHE
1	A	1385	ASP
1	A	1387	LEU
1	A	1388	THR
1	A	1416	ARG
1	A	1427	ARG
1	A	1451	MET
1	A	1464	ASN

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Mol	Chain	Res	Type
2	E	82	TYR
2	E	105	ILE
2	E	110	ILE
2	E	127	MET
2	E	131	LYS
2	E	132	LYS
2	E	133	ARG
2	E	158	MET
2	E	163	LYS
2	E	219	GLU
3	B	115	PRO
4	C	279	LEU
4	C	280	VAL
5	F	40	MET
5	F	93	ARG
5	F	133	LEU
5	F	158	ARG
5	F	181	VAL
5	F	182	LEU
5	F	186	ASN
5	F	197	LYS
5	F	205	LEU
5	F	216	LEU
5	F	230	ARG
5	F	234	LYS
5	F	237	LEU
5	F	243	ARG
5	F	254	LYS
5	F	269	LEU
5	F	270	THR
5	F	302	ASP
5	F	303	VAL
5	F	315	ARG
5	F	318	LYS
5	F	333	THR
5	F	346	LEU
5	F	361	MET
5	F	381	ASP
5	F	406	CYS
5	F	407	GLU
5	F	411	TYR
5	F	422	ARG

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Mol	Chain	Res	Type
5	F	441	ASP
5	F	442	LYS
5	F	471	ILE
5	F	472	THR
5	F	474	GLN
5	F	476	GLU
5	F	477	ASN
5	F	480	ASN
5	F	505	ARG
5	F	508	LEU
5	F	520	ASN
5	F	525	LEU
5	F	528	ASN
5	F	530	GLN
5	F	532	LYS
5	F	542	ASN
5	F	577	ARG
5	F	593	LEU
5	F	629	TYR
5	F	657	GLU
5	F	658	GLU
5	F	662	THR
5	F	707	ARG
5	F	710	LEU
5	F	743	ILE
5	F	744	THR
5	F	785	LYS
5	F	793	SER
5	F	847	ASN
5	F	849	ASP
5	F	850	VAL
5	F	851	MET
5	F	853	CYS
5	F	987	ASP
5	F	988	ASN
5	F	989	ASP
5	F	990	SER
5	F	991	LYS
5	F	1013	ASN
5	F	1062	CYS
5	F	1065	ASN
5	F	1066	ASN

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Mol	Chain	Res	Type
5	F	1068	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	114	GLN
1	A	123	ASN
1	A	143	ASN
1	A	183	GLN
1	A	257	ASN
1	A	269	ASN
1	A	274	HIS
1	A	277	ASN
1	A	327	ASN
1	A	454	HIS
1	A	456	GLN
1	A	464	GLN
1	A	599	ASN
1	A	654	ASN
1	A	909	ASN
1	A	939	GLN
1	A	999	ASN
1	A	1037	ASN
1	A	1085	GLN
1	A	1105	ASN
1	A	1131	ASN
1	A	1154	ASN
1	A	1183	ASN
1	A	1374	ASN
2	E	50	HIS
5	F	56	GLN
5	F	108	GLN
5	F	228	ASN
5	F	299	ASN
5	F	350	ASN
5	F	357	ASN
5	F	372	GLN
5	F	395	ASN
5	F	450	ASN
5	F	477	ASN
5	F	511	ASN

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Mol	Chain	Res	Type
5	F	520	ASN
5	F	530	GLN
5	F	570	ASN
5	F	678	ASN
5	F	697	ASN
5	F	773	ASN
5	F	847	ASN
5	F	866	ASN
5	F	988	ASN
5	F	1001	ASN
5	F	1013	ASN
5	F	1065	ASN
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 ⓘ

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

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	6	14,14,15	0.28	0	17,19,21	1.02	1 (5%)
6	NAG	D	2	6	14,14,15	0.32	0	17,19,21	0.56	0
6	NAG	G	1	6,5	14,14,15	0.28	0	17,19,21	0.63	0
6	NAG	G	2	6	14,14,15	0.28	0	17,19,21	0.58	0
7	NAG	H	1	5,7	14,14,15	0.73	1 (7%)	17,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	H	2	7	14,14,15	0.37	0	17,19,21	0.77	0
7	BMA	H	3	7	11,11,12	0.74	0	15,15,17	0.97	1 (6%)
7	NAG	I	1	5,7	14,14,15	0.84	1 (7%)	17,19,21	0.82	0
7	NAG	I	2	7	14,14,15	1.63	1 (7%)	17,19,21	0.91	1 (5%)
7	BMA	I	3	7	11,11,12	0.92	0	15,15,17	1.04	1 (6%)
6	NAG	J	1	6,5	14,14,15	0.56	0	17,19,21	0.62	0
6	NAG	J	2	6	14,14,15	0.33	0	17,19,21	0.39	0
6	NAG	K	1	6	14,14,15	0.28	0	17,19,21	0.65	0
6	NAG	K	2	6	14,14,15	0.29	0	17,19,21	0.57	0
8	NAG	L	1	5,8	14,14,15	0.29	0	17,19,21	0.65	0
8	NAG	L	2	8	14,14,15	0.31	0	17,19,21	0.69	0
8	NAG	L	3	8	14,14,15	0.29	0	17,19,21	1.34	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	6	-	5/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	G	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	G	2	6	-	3/6/23/26	0/1/1/1
7	NAG	H	1	5,7	-	0/6/23/26	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	6,5	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	NAG	K	1	6	-	4/6/23/26	0/1/1/1
6	NAG	K	2	6	-	6/6/23/26	0/1/1/1
8	NAG	L	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	L	2	8	-	5/6/23/26	0/1/1/1
8	NAG	L	3	8	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	2	NAG	O5-C1	-5.91	1.34	1.43
7	I	1	NAG	O5-C1	-2.67	1.39	1.43
7	H	1	NAG	O5-C1	-2.36	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	3	NAG	C1-O5-C5	4.38	118.13	112.19
6	D	1	NAG	C3-C4-C5	2.52	114.73	110.24
7	H	3	BMA	C1-O5-C5	2.41	115.46	112.19
7	I	2	NAG	C4-C3-C2	2.24	114.30	111.02
7	I	3	BMA	O5-C1-C2	-2.02	107.66	110.77

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C8-C7-N2-C2
6	D	1	NAG	O7-C7-N2-C2
6	K	1	NAG	C8-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
8	L	1	NAG	C8-C7-N2-C2
8	L	1	NAG	O7-C7-N2-C2
8	L	3	NAG	C1-C2-N2-C7
8	L	3	NAG	C8-C7-N2-C2
8	L	3	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
8	L	2	NAG	C8-C7-N2-C2
8	L	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C1-C2-N2-C7
6	J	1	NAG	O5-C5-C6-O6
8	L	2	NAG	C4-C5-C6-O6
6	K	2	NAG	O7-C7-N2-C2
6	K	1	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
8	L	2	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
8	L	2	NAG	C1-C2-N2-C7
7	H	2	NAG	O5-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6

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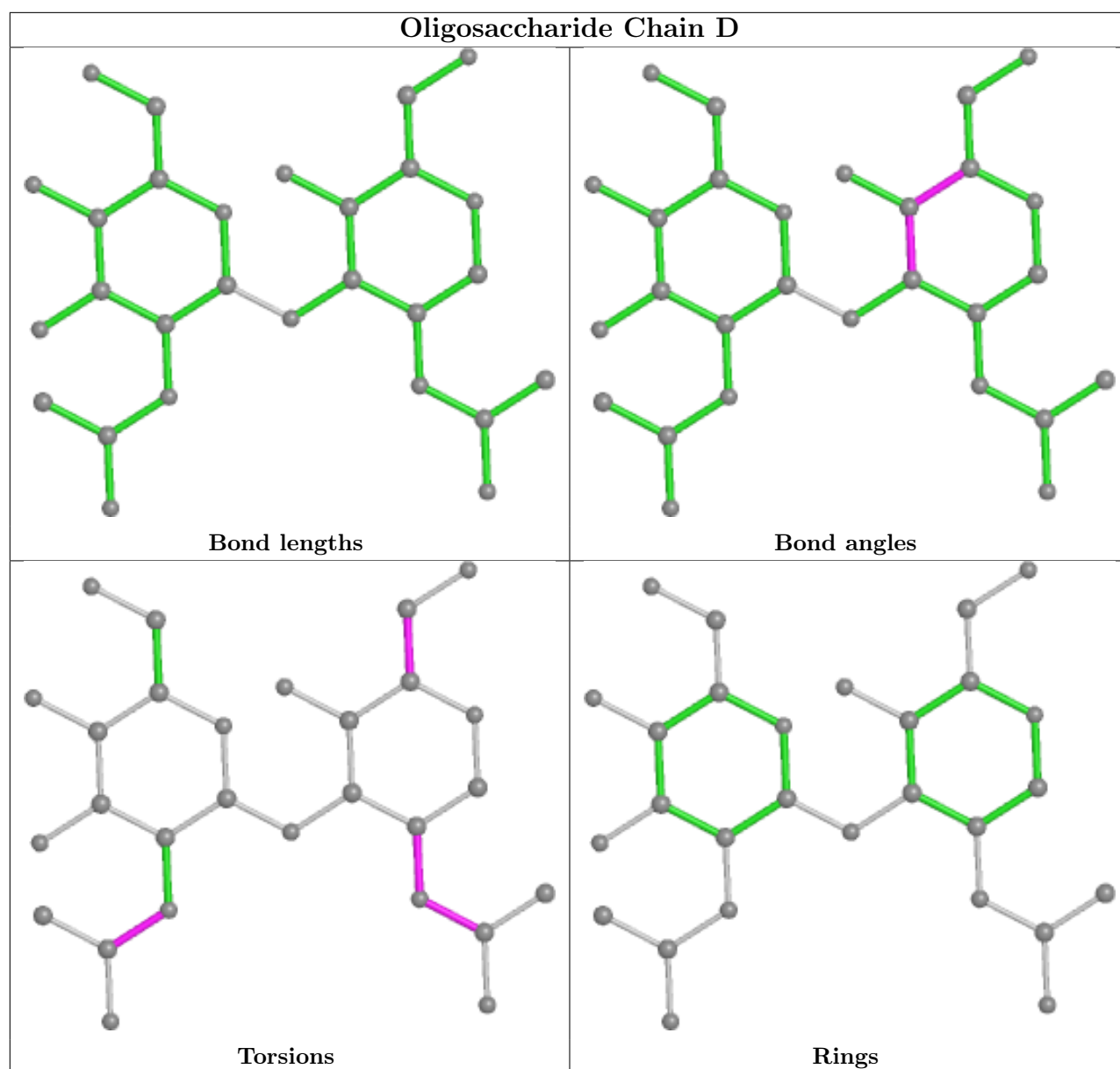
Mol	Chain	Res	Type	Atoms
6	K	2	NAG	C4-C5-C6-O6
7	I	2	NAG	O5-C5-C6-O6
7	I	3	BMA	C4-C5-C6-O6
6	D	2	NAG	C8-C7-N2-C2
6	D	1	NAG	C1-C2-N2-C7
6	K	2	NAG	O5-C5-C6-O6
7	I	3	BMA	O5-C5-C6-O6
7	I	1	NAG	O5-C5-C6-O6
6	D	2	NAG	O7-C7-N2-C2
8	L	3	NAG	O5-C5-C6-O6
6	G	2	NAG	C1-C2-N2-C7
7	I	2	NAG	C4-C5-C6-O6
6	G	2	NAG	O5-C5-C6-O6
7	I	1	NAG	C4-C5-C6-O6
6	K	2	NAG	C3-C2-N2-C7
6	G	2	NAG	C3-C2-N2-C7

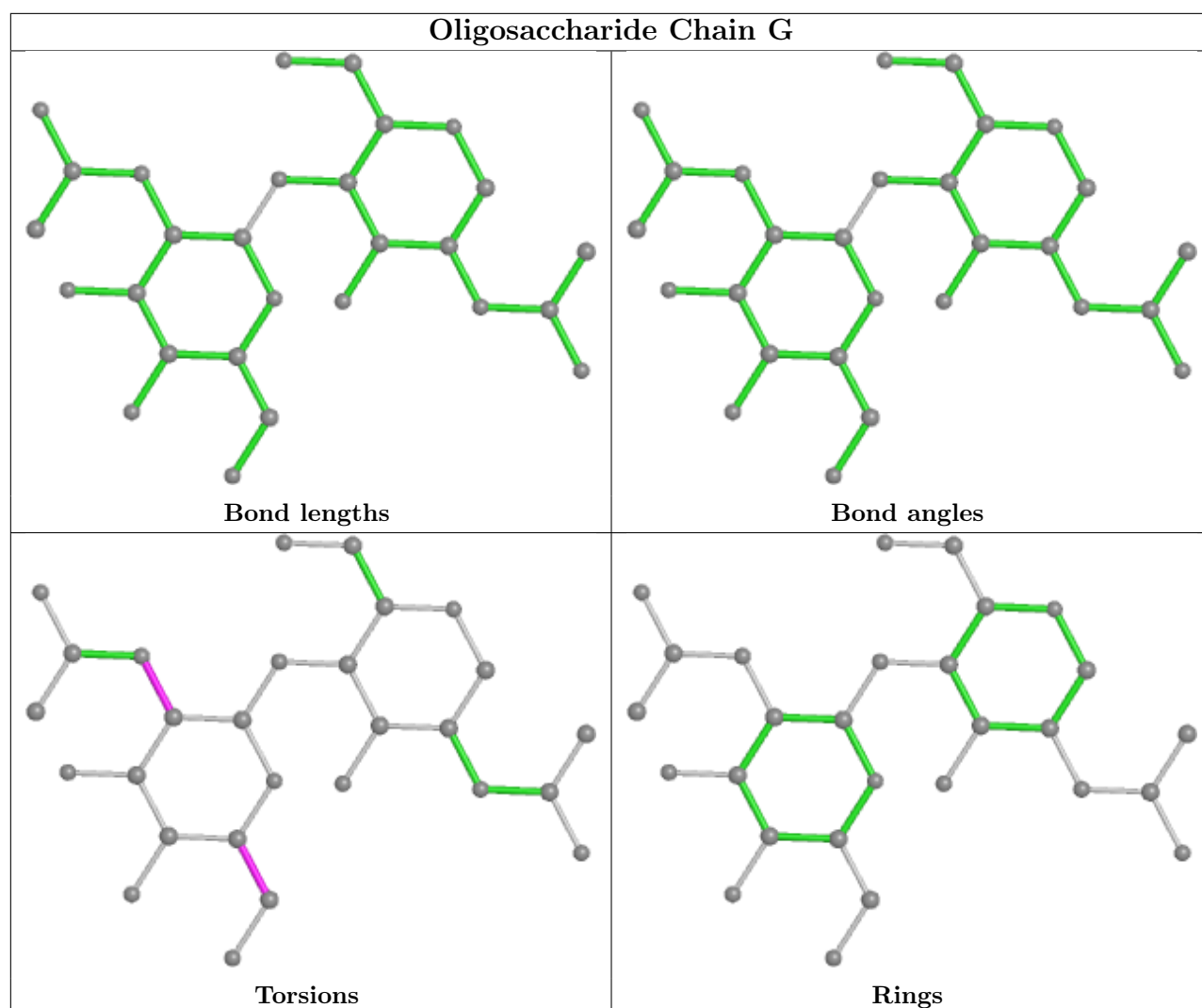
There are no ring outliers.

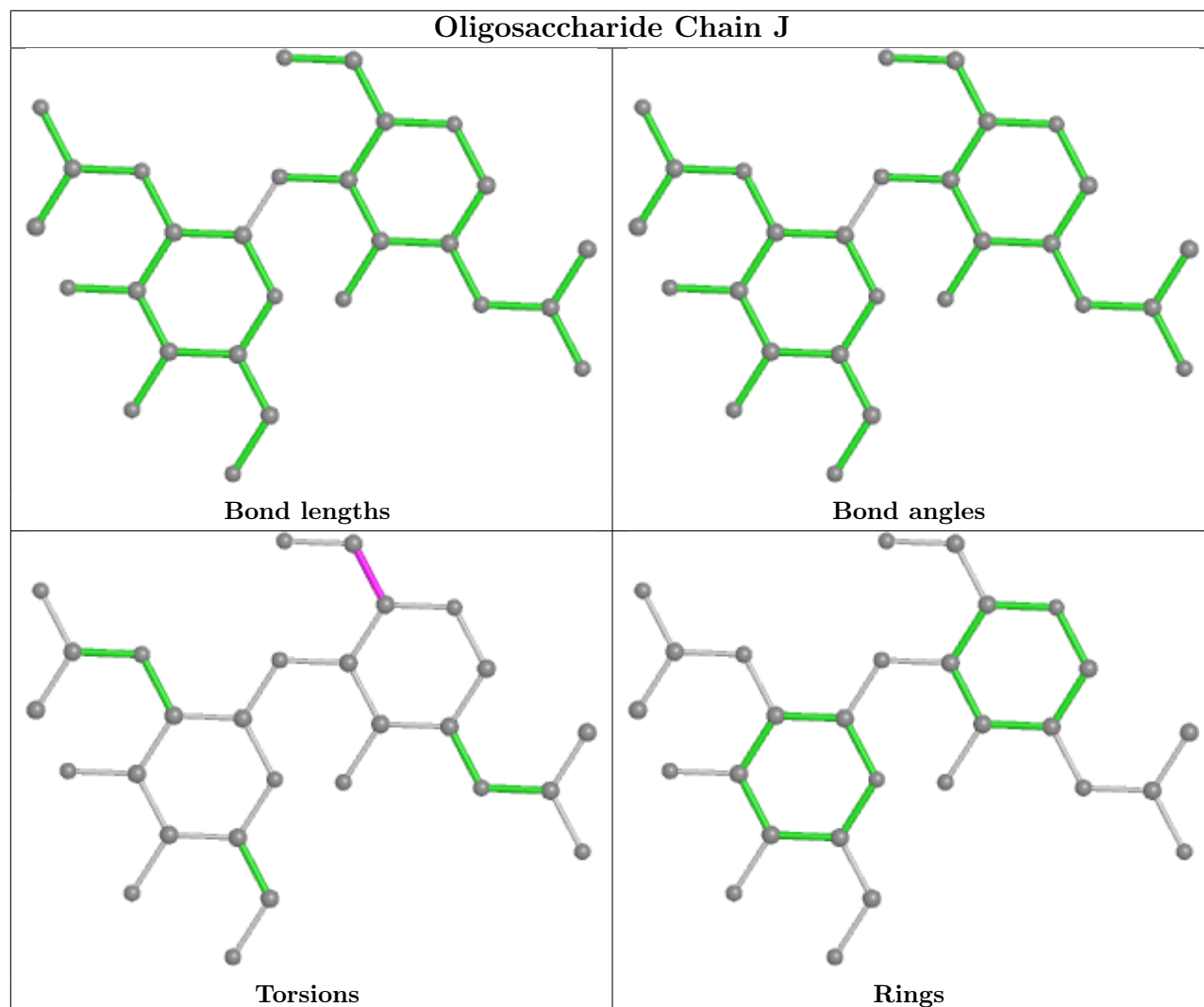
11 monomers are involved in 33 short contacts:

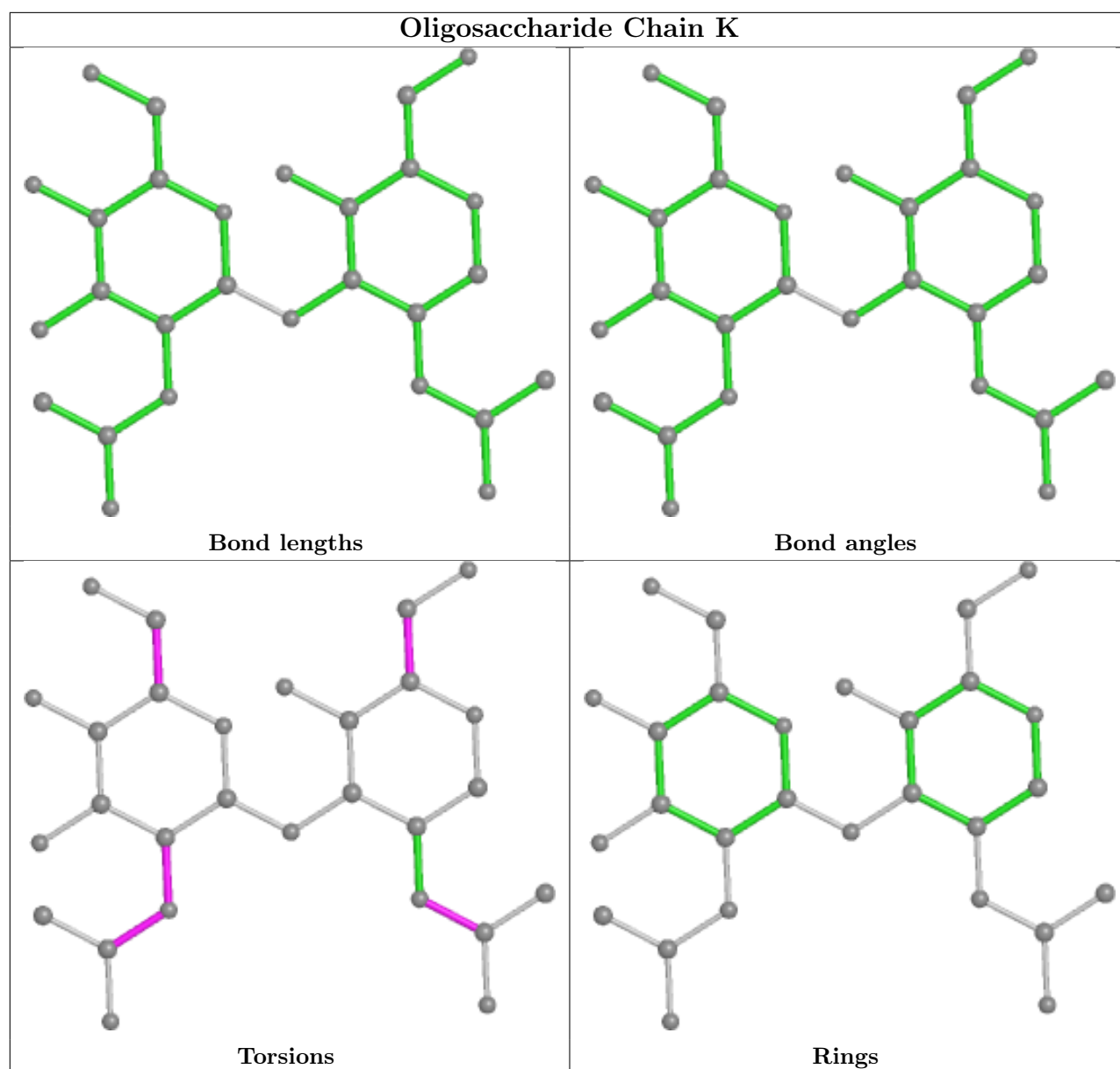
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	1	NAG	1	0
6	D	2	NAG	4	0
6	D	1	NAG	8	0
6	K	2	NAG	5	0
8	L	2	NAG	2	0
8	L	3	NAG	4	0
7	H	1	NAG	4	0
7	I	1	NAG	1	0
6	K	1	NAG	5	0
6	G	2	NAG	1	0
8	L	1	NAG	6	0

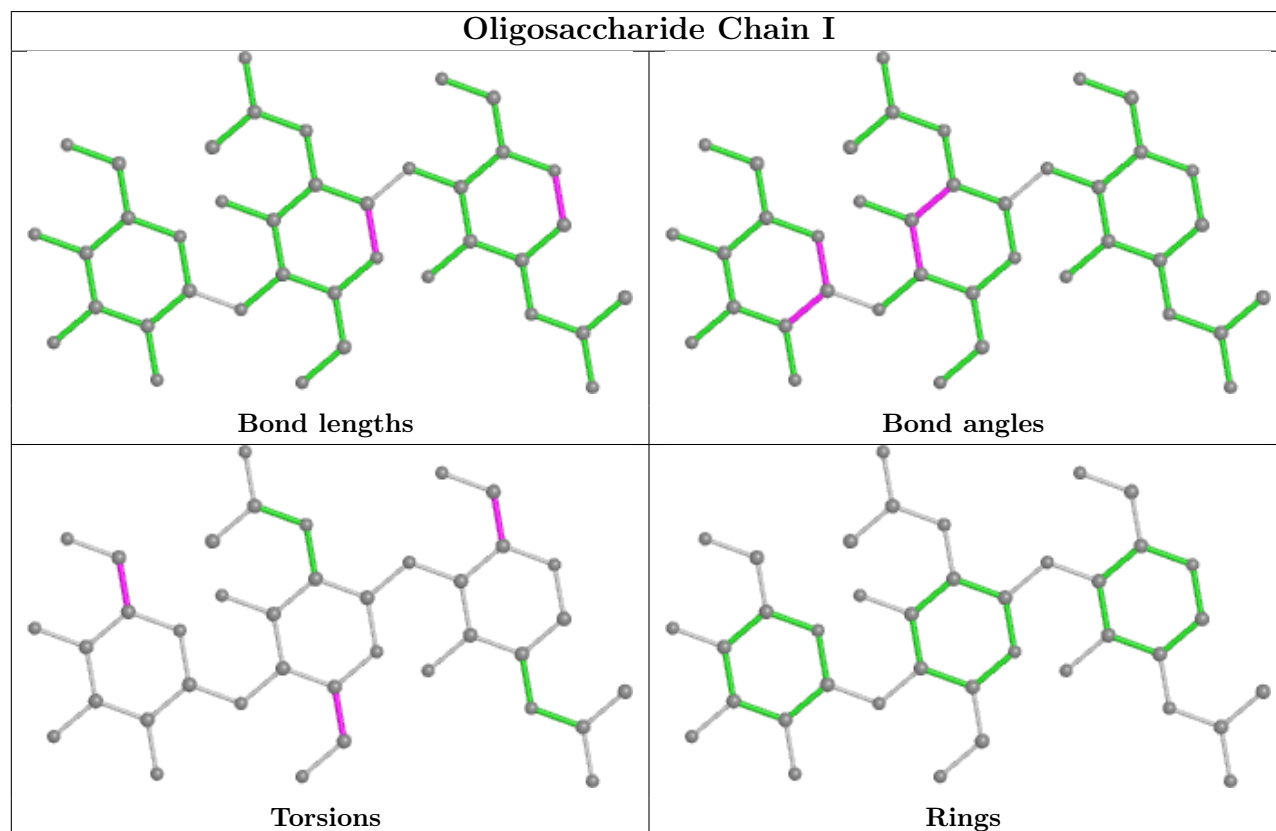
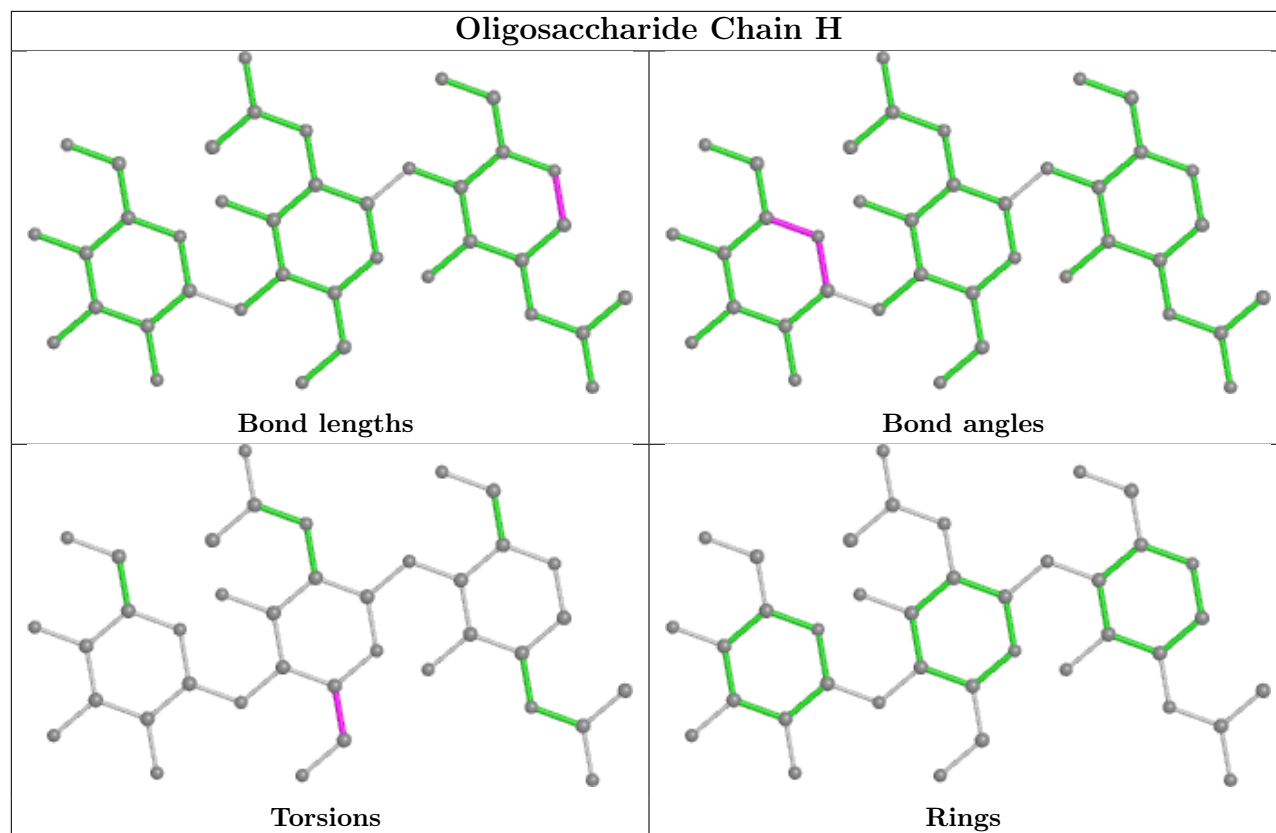
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

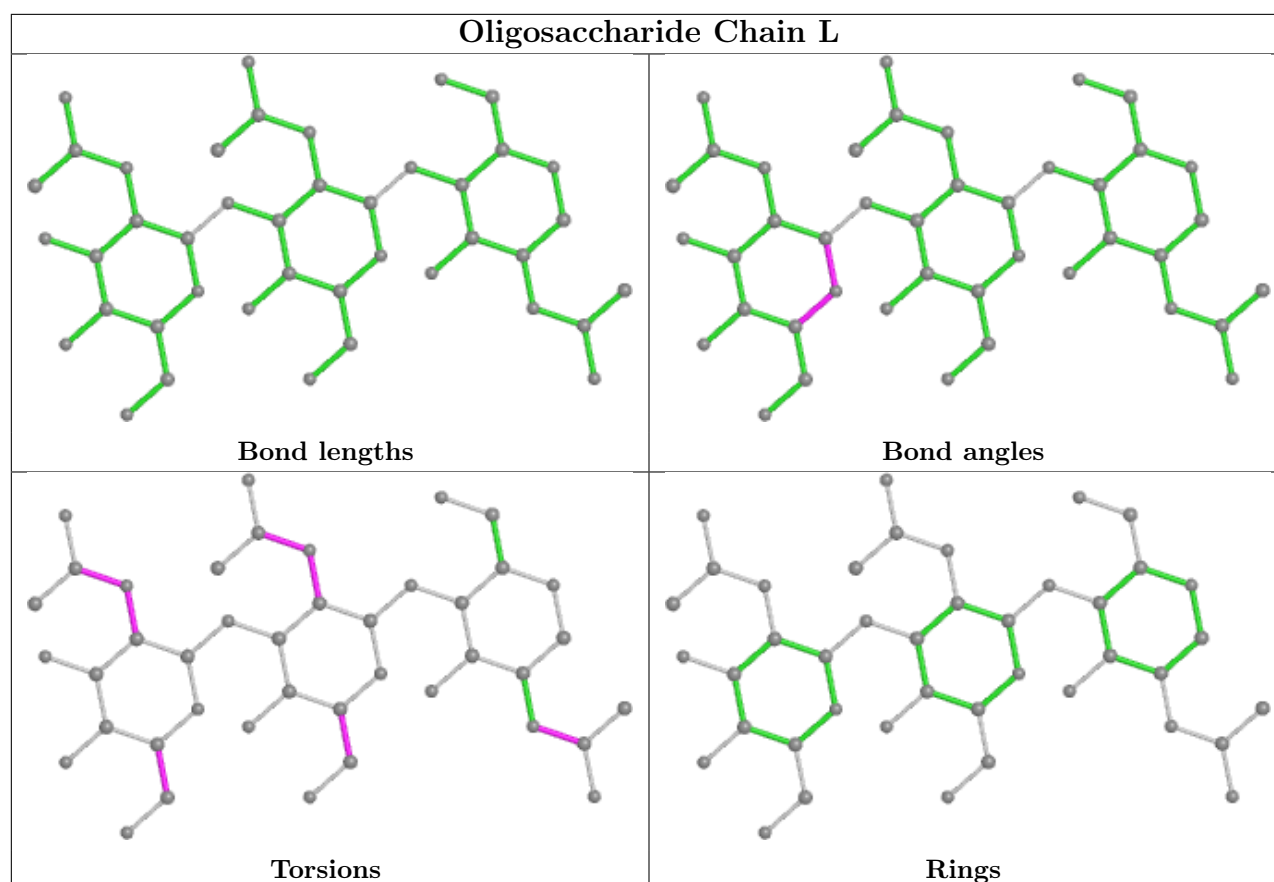












5.6 Ligand geometry [i](#)

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	$\# Z > 2$
12	PC1	A	1909	-	38,38,53	1.06	2 (5%)	44,46,61	1.06	2 (4%)
9	NAG	F	1114	5	14,14,15	0.23	0	17,19,21	0.65	1 (5%)
14	4YH	A	1916[B]	-	32,34,34	0.97	3 (9%)	36,46,46	1.66	11 (30%)
15	ETA	F	1101	-	3,3,3	0.41	0	2,2,2	0.52	0
9	NAG	F	1104	-	14,14,15	0.30	0	17,19,21	0.71	0
11	3PE	A	1912	-	41,41,50	1.00	2 (4%)	44,46,55	1.18	3 (6%)
13	9Z9	A	1914	-	35,35,44	0.64	1 (2%)	58,58,68	1.09	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	3PE	A	1913	-	38,38,50	1.11	2 (5%)	42,43,55	1.08	3 (7%)
11	3PE	A	1906	-	41,41,50	1.04	2 (4%)	44,46,55	1.12	4 (9%)
11	3PE	A	1911	-	34,34,50	1.11	2 (5%)	37,39,55	1.21	4 (10%)
9	NAG	F	1107	5	14,14,15	0.29	0	17,19,21	0.64	0
9	NAG	F	1115	5	14,14,15	0.81	1 (7%)	17,19,21	1.00	1 (5%)
12	PC1	A	1910	-	53,53,53	0.89	2 (3%)	59,61,61	1.03	5 (8%)
9	NAG	A	1901	-	14,14,15	0.70	1 (7%)	17,19,21	0.81	0
9	NAG	F	1120	-	14,14,15	0.30	0	17,19,21	0.62	0
9	NAG	F	1121	-	14,14,15	0.45	0	17,19,21	0.52	0
11	3PE	A	1904	-	32,32,50	1.14	2 (6%)	35,37,55	1.25	2 (5%)
9	NAG	F	1122	-	14,14,15	0.29	0	17,19,21	0.62	0
11	3PE	A	1908	-	19,19,50	1.03	1 (5%)	21,23,55	1.19	2 (9%)
14	4YH	A	1915[A]	-	32,34,34	3.66	14 (43%)	36,46,46	1.88	11 (30%)
11	3PE	A	1907	-	35,35,50	1.10	2 (5%)	38,40,55	1.18	4 (10%)
11	3PE	A	1905	-	18,18,50	1.07	1 (5%)	20,22,55	1.07	2 (10%)

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
12	PC1	A	1909	-	-	11/42/42/57	-
9	NAG	F	1114	5	-	0/6/23/26	0/1/1/1
14	4YH	A	1916[B]	-	-	14/32/35/35	0/2/2/2
15	ETA	F	1101	-	-	1/1/1/1	-
9	NAG	F	1104	-	-	3/6/23/26	0/1/1/1
11	3PE	A	1912	-	-	20/45/45/54	-
13	9Z9	A	1914	-	-	-	0/6/6/6
11	3PE	A	1913	-	-	15/40/40/54	-
11	3PE	A	1906	-	-	23/45/45/54	-
11	3PE	A	1911	-	-	19/38/38/54	-
9	NAG	F	1107	5	-	2/6/23/26	0/1/1/1
9	NAG	F	1115	5	-	0/6/23/26	0/1/1/1
12	PC1	A	1910	-	-	31/57/57/57	-
9	NAG	A	1901	-	-	2/6/23/26	0/1/1/1
9	NAG	F	1120	-	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	F	1121	-	-	0/6/23/26	0/1/1/1
11	3PE	A	1904	-	-	20/36/36/54	-
9	NAG	F	1122	-	-	2/6/23/26	0/1/1/1
11	3PE	A	1908	-	-	7/22/22/54	-
14	4YH	A	1915[A]	-	-	14/32/35/35	0/2/2/2
11	3PE	A	1907	-	-	10/39/39/54	-
11	3PE	A	1905	-	-	7/20/20/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1915[A]	4YH	C5-C2	8.32	1.53	1.39
14	A	1915[A]	4YH	C11-C13	7.81	1.53	1.38
14	A	1915[A]	4YH	C14-C18	7.74	1.52	1.38
14	A	1915[A]	4YH	C12-C17	7.60	1.52	1.39
14	A	1915[A]	4YH	C9-C6	5.66	1.52	1.40
14	A	1915[A]	4YH	C7-C10	5.59	1.52	1.40
11	A	1913	3PE	O31-C31	4.50	1.46	1.33
11	A	1906	3PE	O31-C31	4.43	1.46	1.33
14	A	1915[A]	4YH	C11-C2	-4.42	1.32	1.39
11	A	1907	3PE	O21-C21	4.27	1.46	1.34
11	A	1904	3PE	O21-C21	4.18	1.46	1.34
11	A	1907	3PE	O31-C31	4.18	1.45	1.33
11	A	1904	3PE	O31-C31	4.17	1.45	1.33
11	A	1911	3PE	O31-C31	4.17	1.45	1.33
11	A	1913	3PE	O21-C21	4.17	1.46	1.34
11	A	1912	3PE	O21-C21	4.16	1.46	1.34
11	A	1905	3PE	O31-C31	4.12	1.45	1.33
11	A	1906	3PE	O21-C21	4.11	1.45	1.34
11	A	1911	3PE	O21-C21	4.08	1.45	1.34
12	A	1909	PC1	O31-C31	4.05	1.45	1.33
12	A	1910	PC1	O21-C21	4.03	1.45	1.34
14	A	1915[A]	4YH	C12-C7	-3.98	1.31	1.38
12	A	1909	PC1	O21-C21	3.96	1.45	1.34
12	A	1910	PC1	O31-C31	3.87	1.44	1.33
11	A	1912	3PE	O31-C31	3.86	1.44	1.33
11	A	1908	3PE	O21-C21	3.82	1.45	1.34
14	A	1915[A]	4YH	C14-C10	-3.81	1.31	1.39
14	A	1915[A]	4YH	C13-C9	-3.78	1.31	1.39
14	A	1915[A]	4YH	C5-C6	-3.69	1.32	1.38
14	A	1915[A]	4YH	C18-C17	-3.35	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	1915[A]	4YH	C1-C3	2.96	1.53	1.47
14	A	1916[B]	4YH	C1-C3	2.71	1.53	1.47
14	A	1915[A]	4YH	O19-C6	2.66	1.41	1.37
9	F	1115	NAG	C1-C2	2.41	1.55	1.52
9	A	1901	NAG	O5-C1	-2.19	1.40	1.43
14	A	1916[B]	4YH	O24-C10	2.09	1.40	1.37
14	A	1916[B]	4YH	O20-C7	2.04	1.40	1.37
13	A	1914	9Z9	O80-C79	-2.04	1.40	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1912	3PE	O21-C21-C22	4.95	122.18	111.50
14	A	1915[A]	4YH	C21-C16-N8	-4.83	104.86	112.56
11	A	1904	3PE	O21-C21-C22	4.63	121.49	111.50
13	A	1914	9Z9	O80-C73-C76	4.63	115.07	110.77
11	A	1906	3PE	O21-C21-C22	4.21	120.58	111.50
11	A	1907	3PE	O21-C21-C22	4.18	120.52	111.50
11	A	1911	3PE	O21-C21-C22	4.18	120.50	111.50
12	A	1910	PC1	O21-C21-C22	4.03	120.19	111.50
12	A	1909	PC1	O21-C21-C22	3.96	120.03	111.50
14	A	1916[B]	4YH	O23-C9-C6	3.80	120.70	115.41
9	F	1115	NAG	C1-O5-C5	3.61	117.08	112.19
14	A	1915[A]	4YH	O23-C9-C6	3.58	120.40	115.41
11	A	1913	3PE	O21-C21-C22	3.50	119.04	111.50
11	A	1908	3PE	O21-C21-C22	3.44	118.92	111.50
14	A	1915[A]	4YH	O20-C7-C10	3.38	120.12	115.41
14	A	1915[A]	4YH	C33-O24-C10	-3.31	112.54	117.53
14	A	1916[B]	4YH	O20-C7-C10	3.24	119.93	115.41
14	A	1915[A]	4YH	C22-C26-C25	-3.21	106.46	112.78
14	A	1916[B]	4YH	O24-C10-C7	3.17	119.83	115.41
12	A	1910	PC1	O31-C31-C32	3.15	121.78	111.91
14	A	1915[A]	4YH	O24-C10-C7	3.12	119.75	115.41
11	A	1907	3PE	O31-C31-C32	3.11	121.66	111.91
13	A	1914	9Z9	C77-C78-C79	3.09	112.86	108.56
11	A	1904	3PE	O31-C31-C32	2.94	121.13	111.91
14	A	1915[A]	4YH	O23-C9-C13	-2.92	119.36	124.37
14	A	1916[B]	4YH	O19-C6-C5	-2.90	119.13	124.12
14	A	1915[A]	4YH	O19-C6-C9	2.88	119.42	115.41
11	A	1905	3PE	O31-C31-C32	2.81	120.71	111.91
11	A	1913	3PE	O31-C31-C32	2.74	120.51	111.91
14	A	1915[A]	4YH	O24-C10-C14	-2.73	119.68	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	1911	3PE	O31-C31-C32	2.73	120.49	111.91
12	A	1910	PC1	O31-C31-O32	-2.67	116.84	123.59
11	A	1906	3PE	O31-C31-C32	2.60	120.08	111.91
12	A	1909	PC1	O31-C31-C32	2.59	120.05	111.91
14	A	1916[B]	4YH	O23-C9-C13	-2.58	119.95	124.37
14	A	1916[B]	4YH	O20-C7-C12	-2.52	119.79	124.12
14	A	1916[B]	4YH	C32-O23-C9	-2.44	113.85	117.53
13	A	1914	9Z9	C79-O80-C73	2.38	118.23	113.72
14	A	1916[B]	4YH	C31-O20-C7	-2.36	113.96	117.53
11	A	1908	3PE	C2-O21-C21	-2.35	112.00	117.79
11	A	1905	3PE	O31-C31-O32	-2.32	117.73	123.59
11	A	1912	3PE	O31-C31-C32	2.31	119.15	111.91
9	F	1114	NAG	C1-O5-C5	2.31	115.32	112.19
14	A	1916[B]	4YH	O19-C6-C9	2.27	118.57	115.41
12	A	1910	PC1	O21-C2-C1	2.25	116.56	108.40
14	A	1916[B]	4YH	C30-O19-C6	-2.21	114.19	117.53
11	A	1907	3PE	O31-C31-O32	-2.21	118.02	123.59
12	A	1910	PC1	O21-C21-O22	-2.18	118.44	123.70
11	A	1907	3PE	O21-C21-O22	-2.17	118.45	123.70
11	A	1913	3PE	O12-P-O14	2.13	119.02	110.68
14	A	1915[A]	4YH	O20-C7-C12	-2.11	120.50	124.12
11	A	1906	3PE	O21-C21-O22	-2.10	118.62	123.70
11	A	1912	3PE	O21-C21-O22	-2.10	118.64	123.70
11	A	1911	3PE	O21-C21-O22	-2.08	118.67	123.70
11	A	1906	3PE	C2-O21-C21	-2.07	112.69	117.79
11	A	1911	3PE	C2-O21-C21	-2.05	112.73	117.79
13	A	1914	9Z9	O80-C73-O72	-2.02	104.16	109.78
14	A	1915[A]	4YH	C32-O23-C9	-2.01	114.49	117.53
14	A	1916[B]	4YH	O24-C10-C14	-2.00	120.94	124.37

There are no chirality outliers.

All (203) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	F	1104	NAG	C8-C7-N2-C2
9	F	1104	NAG	O7-C7-N2-C2
11	A	1904	3PE	C1-O11-P-O12
11	A	1904	3PE	C1-O11-P-O13
11	A	1904	3PE	C1-O11-P-O14
11	A	1904	3PE	O13-C11-C12-N
11	A	1904	3PE	C3-C2-O21-C21
11	A	1904	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
11	A	1905	3PE	C1-O11-P-O12
11	A	1905	3PE	C1-O11-P-O13
11	A	1905	3PE	C11-O13-P-O14
11	A	1906	3PE	C1-O11-P-O12
11	A	1906	3PE	C1-O11-P-O13
11	A	1906	3PE	C1-O11-P-O14
11	A	1907	3PE	C1-O11-P-O12
11	A	1907	3PE	C1-O11-P-O13
11	A	1907	3PE	C1-O11-P-O14
11	A	1908	3PE	C1-O11-P-O12
11	A	1908	3PE	C1-O11-P-O13
11	A	1908	3PE	C1-O11-P-O14
11	A	1911	3PE	C1-O11-P-O12
11	A	1911	3PE	C1-O11-P-O14
11	A	1911	3PE	O13-C11-C12-N
11	A	1911	3PE	C22-C21-O21-C2
11	A	1912	3PE	O13-C11-C12-N
11	A	1912	3PE	O22-C21-O21-C2
11	A	1912	3PE	C22-C21-O21-C2
11	A	1913	3PE	O21-C2-C3-O31
12	A	1909	PC1	O13-C11-C12-N
12	A	1910	PC1	C1-O11-P-O14
12	A	1910	PC1	O13-C11-C12-N
14	A	1915[A]	4YH	C2-C1-C22-C26
14	A	1916[B]	4YH	C2-C1-C15-C29
14	A	1916[B]	4YH	C2-C1-C15-C28
14	A	1916[B]	4YH	C3-C1-C15-C29
14	A	1916[B]	4YH	C3-C1-C15-C28
14	A	1916[B]	4YH	C22-C1-C15-C29
14	A	1916[B]	4YH	C22-C1-C15-C28
11	A	1906	3PE	O32-C31-O31-C3
11	A	1911	3PE	O22-C21-O21-C2
11	A	1906	3PE	C32-C31-O31-C3
9	F	1120	NAG	O5-C5-C6-O6
11	A	1904	3PE	O22-C21-O21-C2
9	F	1120	NAG	C4-C5-C6-O6
12	A	1910	PC1	C22-C21-O21-C2
14	A	1916[B]	4YH	C10-C7-O20-C31
14	A	1915[A]	4YH	C10-C7-O20-C31
11	A	1904	3PE	C32-C31-O31-C3
12	A	1910	PC1	C21-C22-C23-C24
14	A	1916[B]	4YH	N8-C25-C26-C22

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Mol	Chain	Res	Type	Atoms
9	A	1901	NAG	O5-C5-C6-O6
14	A	1916[B]	4YH	C9-C6-O19-C30
11	A	1906	3PE	C21-C22-C23-C24
11	A	1912	3PE	C31-C32-C33-C34
14	A	1916[B]	4YH	C12-C7-O20-C31
12	A	1910	PC1	O22-C21-O21-C2
14	A	1915[A]	4YH	C12-C7-O20-C31
14	A	1915[A]	4YH	C13-C9-O23-C32
12	A	1909	PC1	C22-C21-O21-C2
9	A	1901	NAG	C4-C5-C6-O6
14	A	1915[A]	4YH	C14-C10-O24-C33
11	A	1904	3PE	O32-C31-O31-C3
11	A	1908	3PE	C22-C21-O21-C2
11	A	1908	3PE	C11-O13-P-O11
11	A	1911	3PE	C1-O11-P-O13
12	A	1910	PC1	C11-O13-P-O11
14	A	1916[B]	4YH	C5-C6-O19-C30
11	A	1908	3PE	O22-C21-O21-C2
12	A	1909	PC1	O22-C21-O21-C2
11	A	1907	3PE	C32-C33-C34-C35
11	A	1913	3PE	C26-C27-C28-C29
12	A	1910	PC1	C24-C25-C26-C27
11	A	1906	3PE	C39-C3A-C3B-C3C
11	A	1911	3PE	C24-C25-C26-C27
12	A	1910	PC1	C1-C2-O21-C21
11	A	1912	3PE	C2C-C2D-C2E-C2F
12	A	1910	PC1	C22-C23-C24-C25
12	A	1910	PC1	C29-C2A-C2B-C2C
11	A	1904	3PE	C23-C24-C25-C26
12	A	1910	PC1	C2A-C2B-C2C-C2D
14	A	1915[A]	4YH	C6-C9-O23-C32
11	A	1911	3PE	C23-C24-C25-C26
11	A	1912	3PE	C22-C23-C24-C25
11	A	1913	3PE	C2B-C2C-C2D-C2E
11	A	1911	3PE	C32-C33-C34-C35
11	A	1913	3PE	C35-C36-C37-C38
12	A	1910	PC1	C2B-C2C-C2D-C2E
11	A	1913	3PE	C32-C33-C34-C35
11	A	1906	3PE	C36-C37-C38-C39
12	A	1910	PC1	C3C-C3D-C3E-C3F
12	A	1910	PC1	C39-C3A-C3B-C3C
11	A	1912	3PE	C2F-C2G-C2H-C2I

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Mol	Chain	Res	Type	Atoms
11	A	1912	3PE	C24-C25-C26-C27
11	A	1912	3PE	C25-C26-C27-C28
12	A	1909	PC1	C27-C28-C29-C2A
11	A	1907	3PE	C22-C21-O21-C2
11	A	1904	3PE	C33-C34-C35-C36
11	A	1904	3PE	C25-C26-C27-C28
12	A	1910	PC1	C38-C39-C3A-C3B
11	A	1906	3PE	C31-C32-C33-C34
11	A	1904	3PE	C35-C36-C37-C38
12	A	1910	PC1	C25-C26-C27-C28
11	A	1906	3PE	C37-C38-C39-C3A
11	A	1912	3PE	C21-C22-C23-C24
11	A	1906	3PE	C22-C21-O21-C2
11	A	1906	3PE	O22-C21-O21-C2
11	A	1907	3PE	O22-C21-O21-C2
11	A	1911	3PE	C34-C35-C36-C37
14	A	1915[A]	4YH	C7-C10-O24-C33
11	A	1906	3PE	C38-C39-C3A-C3B
11	A	1913	3PE	C2A-C2B-C2C-C2D
11	A	1906	3PE	C3A-C3B-C3C-C3D
11	A	1911	3PE	C1-C2-C3-O31
11	A	1913	3PE	C1-C2-C3-O31
11	A	1904	3PE	C27-C28-C29-C2A
12	A	1910	PC1	C2E-C2F-C2G-C2H
12	A	1910	PC1	C3B-C3C-C3D-C3E
11	A	1905	3PE	C31-C32-C33-C34
11	A	1913	3PE	C32-C31-O31-C3
11	A	1913	3PE	C27-C28-C29-C2A
11	A	1912	3PE	C2A-C2B-C2C-C2D
11	A	1906	3PE	O21-C2-C3-O31
11	A	1911	3PE	O21-C2-C3-O31
14	A	1915[A]	4YH	C21-C16-N8-C27
12	A	1910	PC1	C23-C24-C25-C26
11	A	1913	3PE	C2F-C2G-C2H-C2I
14	A	1915[A]	4YH	C21-C16-N8-C25
11	A	1911	3PE	O11-C1-C2-C3
12	A	1910	PC1	O11-C1-C2-C3
11	A	1906	3PE	O13-C11-C12-N
11	A	1907	3PE	C38-C39-C3A-C3B
11	A	1904	3PE	C1-C2-C3-O31
11	A	1913	3PE	O32-C31-O31-C3
12	A	1910	PC1	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
11	A	1912	3PE	C36-C37-C38-C39
11	A	1904	3PE	O21-C2-C3-O31
11	A	1906	3PE	C22-C23-C24-C25
12	A	1909	PC1	O11-C1-C2-C3
12	A	1909	PC1	C23-C24-C25-C26
11	A	1911	3PE	C33-C34-C35-C36
12	A	1910	PC1	C3D-C3E-C3F-C3G
11	A	1912	3PE	C1-C2-C3-O31
11	A	1911	3PE	O11-C1-C2-O21
12	A	1909	PC1	O11-C1-C2-O21
12	A	1910	PC1	C36-C37-C38-C39
12	A	1909	PC1	C33-C34-C35-C36
12	A	1910	PC1	O21-C2-C3-O31
14	A	1915[A]	4YH	C9-C6-O19-C30
11	A	1912	3PE	C35-C36-C37-C38
11	A	1904	3PE	C11-O13-P-O11
11	A	1905	3PE	C11-O13-P-O11
11	A	1912	3PE	C1-O11-P-O13
12	A	1910	PC1	C1-O11-P-O13
12	A	1910	PC1	C28-C29-C2A-C2B
11	A	1905	3PE	C1-O11-P-O14
11	A	1908	3PE	C11-O13-P-O14
12	A	1910	PC1	C11-O13-P-O14
9	F	1104	NAG	C1-C2-N2-C7
12	A	1910	PC1	O11-C1-C2-O21
12	A	1910	PC1	C2C-C2D-C2E-C2F
12	A	1910	PC1	C37-C38-C39-C3A
12	A	1909	PC1	O21-C21-C22-C23
14	A	1915[A]	4YH	C3-C1-C2-C5
14	A	1915[A]	4YH	C15-C1-C22-C26
14	A	1915[A]	4YH	C3-C1-C22-C26
11	A	1912	3PE	O21-C2-C3-O31
11	A	1911	3PE	C25-C26-C27-C28
11	A	1911	3PE	C26-C27-C28-C29
11	A	1912	3PE	C3-C2-O21-C21
11	A	1906	3PE	C28-C29-C2A-C2B
11	A	1911	3PE	C11-O13-P-O11
11	A	1906	3PE	C1-C2-C3-O31
12	A	1910	PC1	C1-C2-C3-O31
9	F	1122	NAG	C4-C5-C6-O6
14	A	1916[B]	4YH	C21-C16-N8-C27
11	A	1907	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
12	A	1909	PC1	C26-C27-C28-C29
14	A	1916[B]	4YH	C1-C22-C26-C25
9	F	1107	NAG	C4-C5-C6-O6
11	A	1912	3PE	O11-C1-C2-O21
14	A	1915[A]	4YH	C5-C6-O19-C30
11	A	1904	3PE	C24-C25-C26-C27
11	A	1906	3PE	C3-C2-O21-C21
9	F	1122	NAG	O5-C5-C6-O6
9	F	1107	NAG	O5-C5-C6-O6
11	A	1906	3PE	C23-C24-C25-C26
11	A	1905	3PE	O13-C11-C12-N
12	A	1909	PC1	O21-C2-C3-O31
11	A	1912	3PE	C23-C24-C25-C26
11	A	1906	3PE	C33-C34-C35-C36
11	A	1904	3PE	O11-C1-C2-O21
11	A	1911	3PE	C2A-C2B-C2C-C2D
11	A	1907	3PE	C33-C34-C35-C36
11	A	1913	3PE	C33-C34-C35-C36
11	A	1913	3PE	O31-C31-C32-C33
14	A	1916[B]	4YH	C21-C16-N8-C25
11	A	1907	3PE	C11-O13-P-O11
11	A	1904	3PE	C2-C1-O11-P
11	A	1913	3PE	O32-C31-C32-C33
11	A	1906	3PE	C12-C11-O13-P
11	A	1912	3PE	C12-C11-O13-P
15	F	1101	ETA	N-CA-CB-O
11	A	1913	3PE	C21-C22-C23-C24

There are no ring outliers.

21 monomers are involved in 102 short contacts:

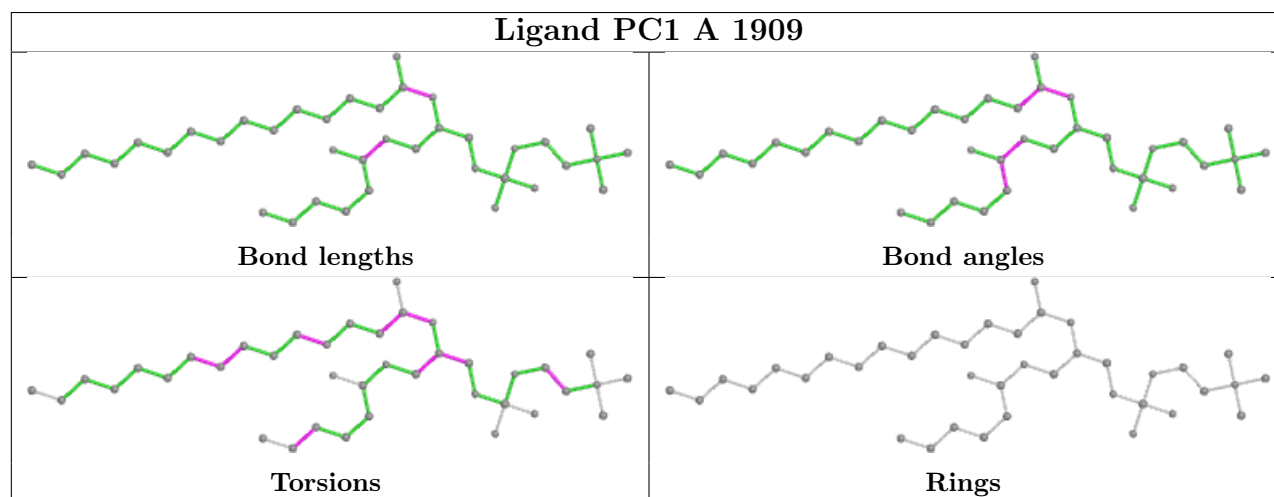
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1909	PC1	8	0
14	A	1916[B]	4YH	7	0
15	F	1101	ETA	4	0
9	F	1104	NAG	3	0
11	A	1912	3PE	14	0
13	A	1914	9Z9	6	0
11	A	1913	3PE	8	0
11	A	1906	3PE	4	0
11	A	1911	3PE	5	0
9	F	1107	NAG	1	0

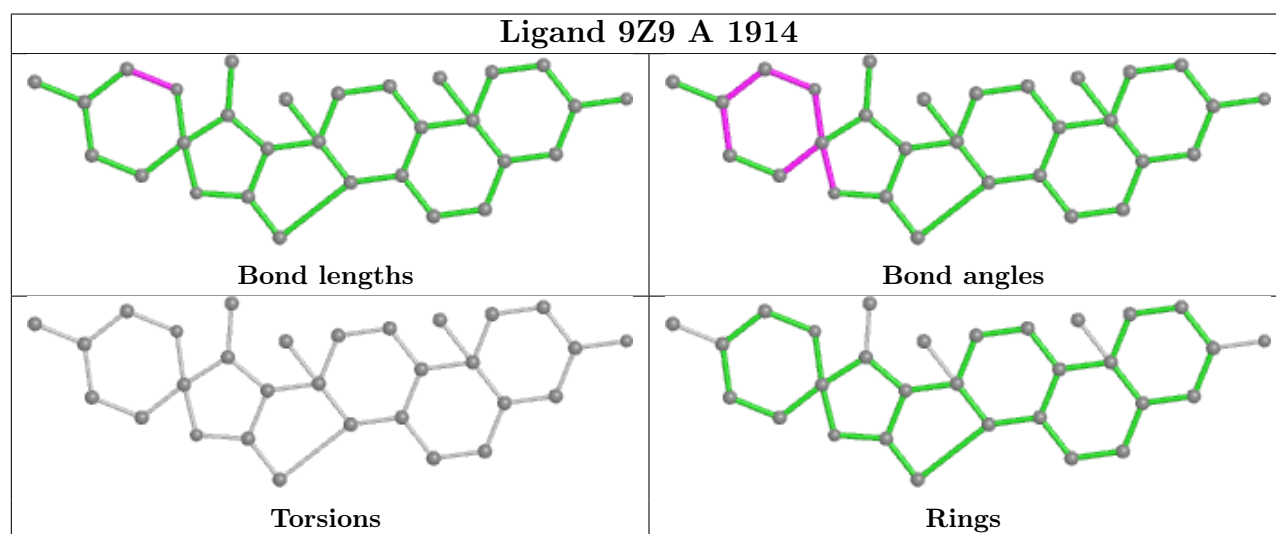
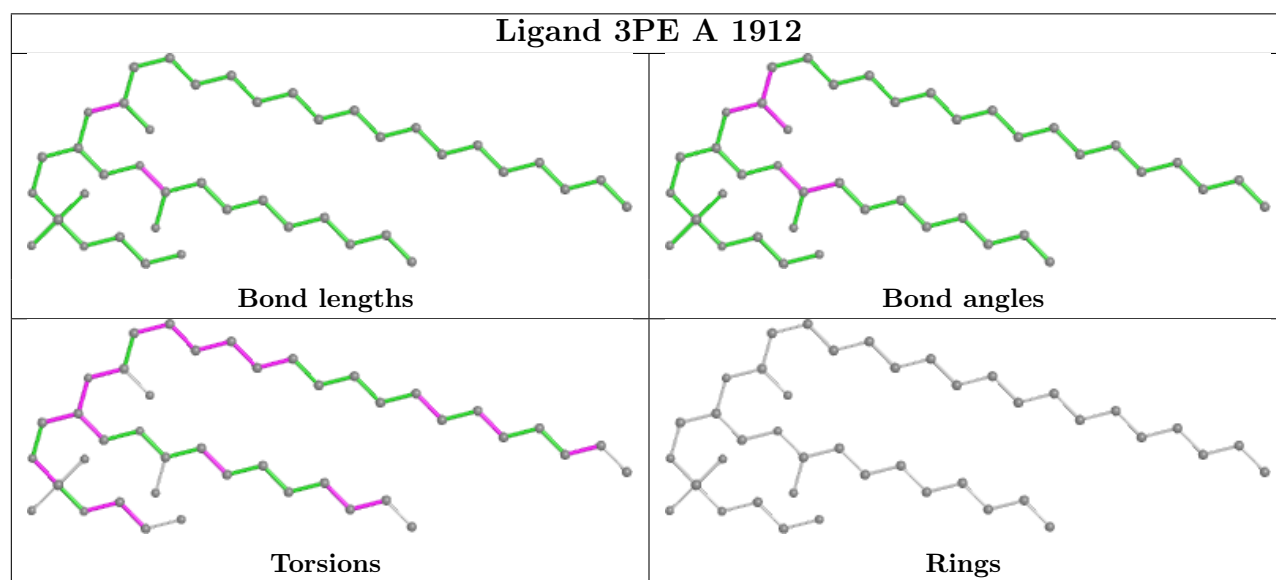
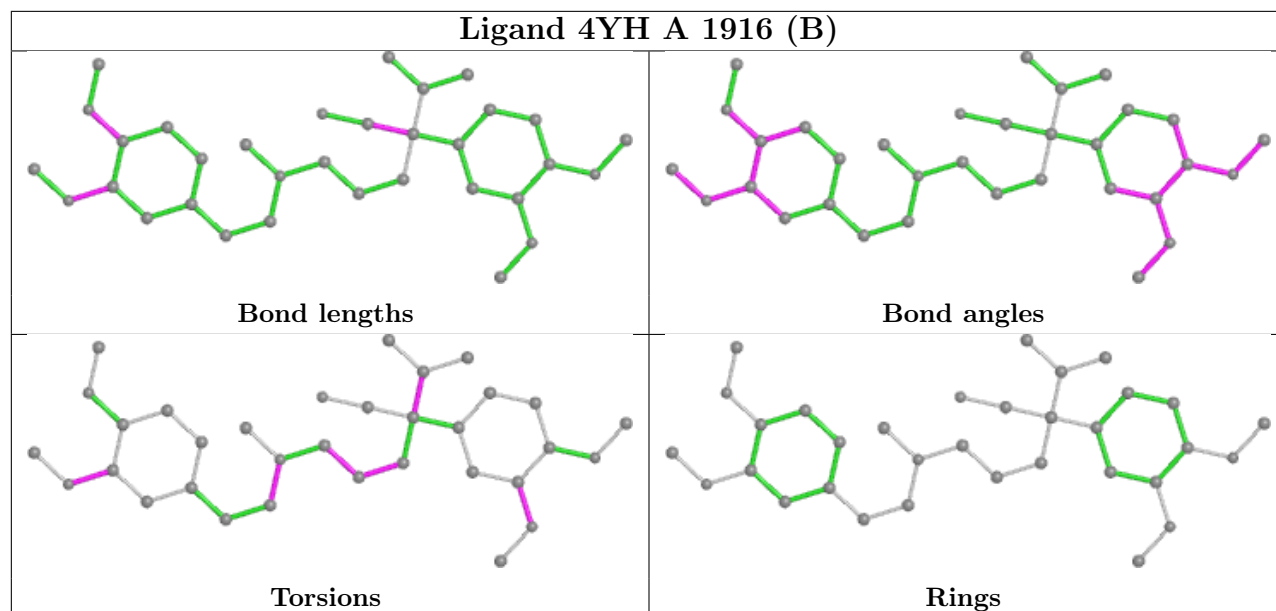
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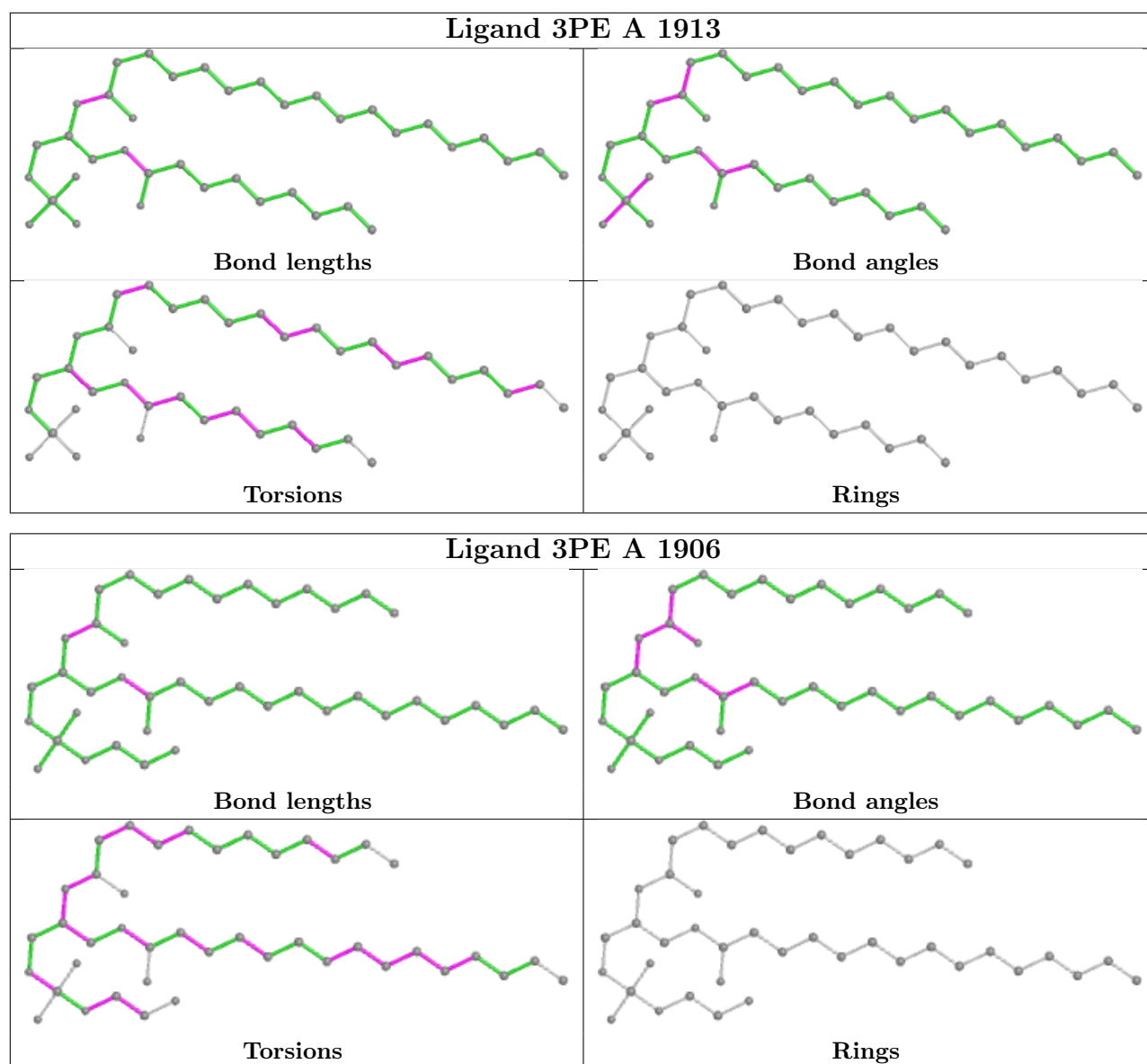
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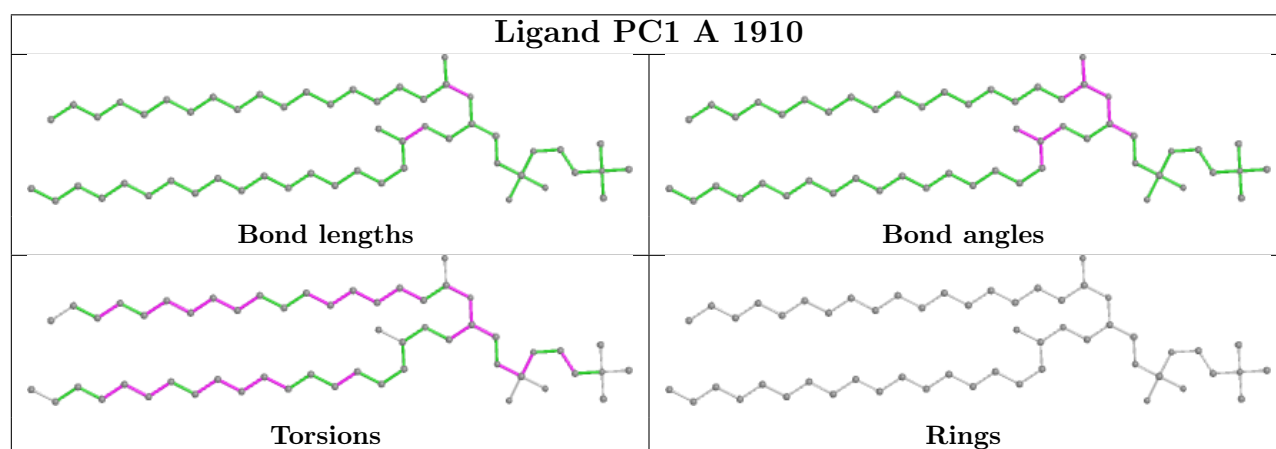
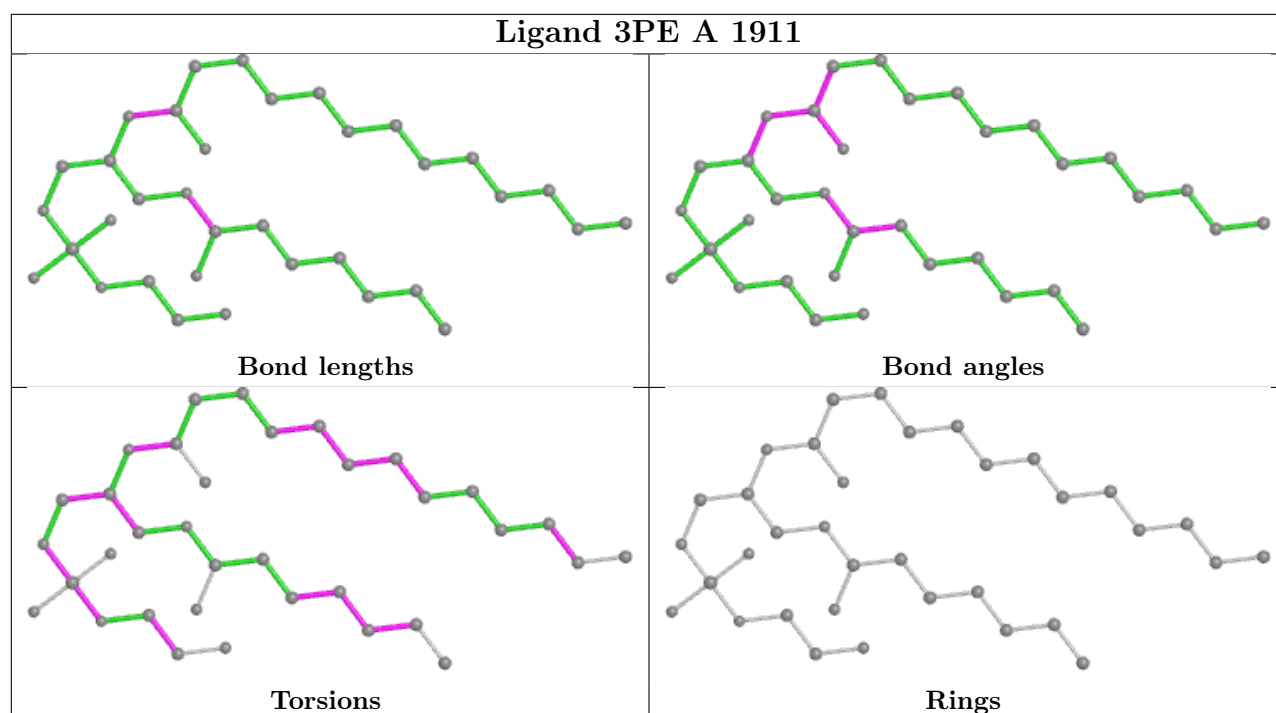
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1115	NAG	2	0
12	A	1910	PC1	5	0
9	A	1901	NAG	3	0
9	F	1120	NAG	2	0
9	F	1121	NAG	3	0
11	A	1904	3PE	3	0
9	F	1122	NAG	4	0
11	A	1908	3PE	9	0
14	A	1915[A]	4YH	5	0
11	A	1907	3PE	7	0
11	A	1905	3PE	2	0

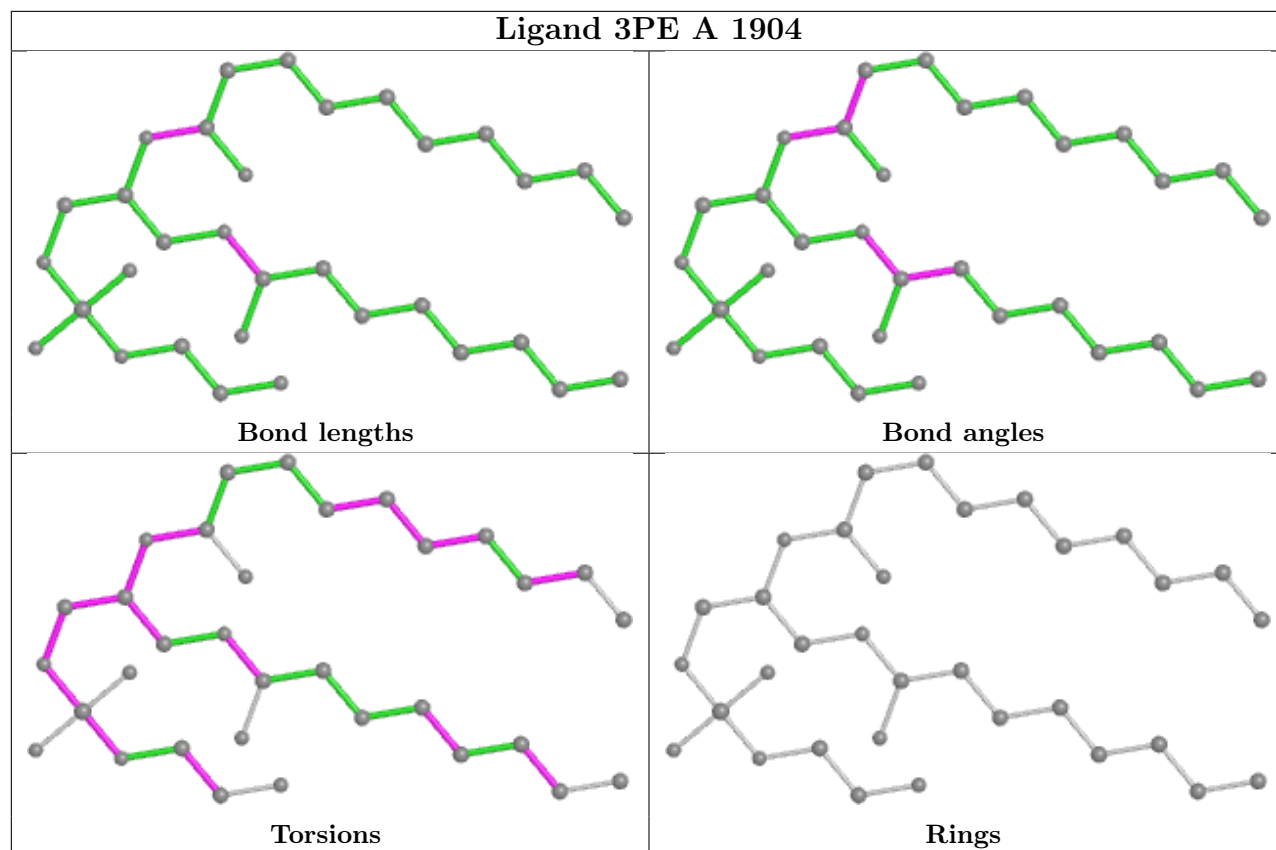
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

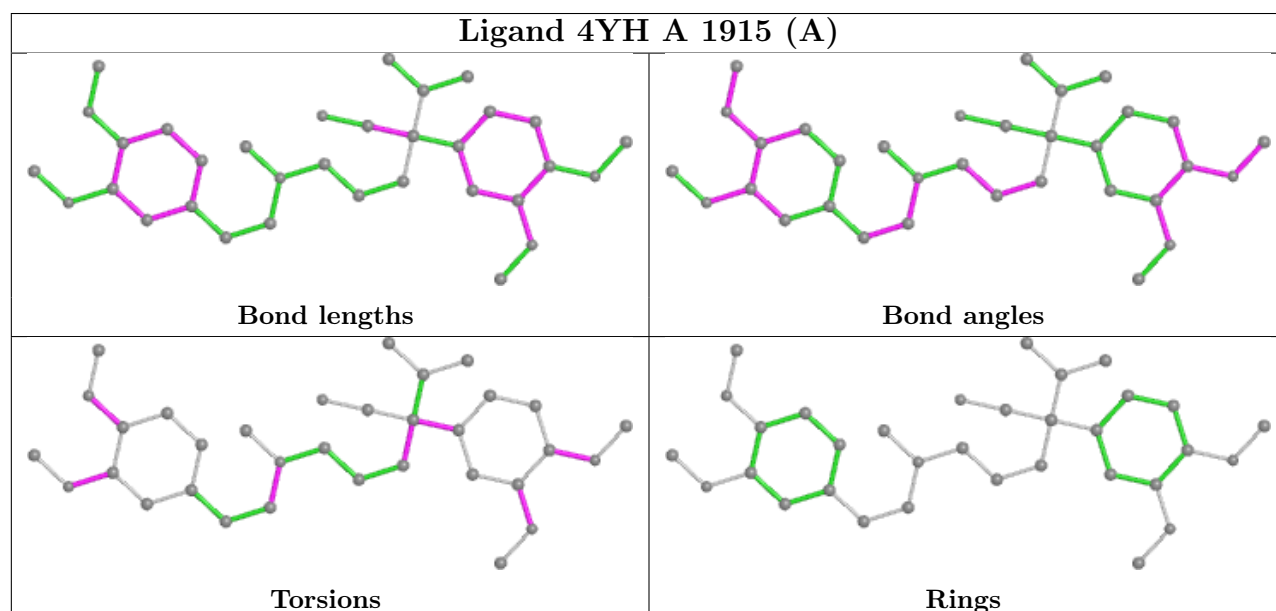
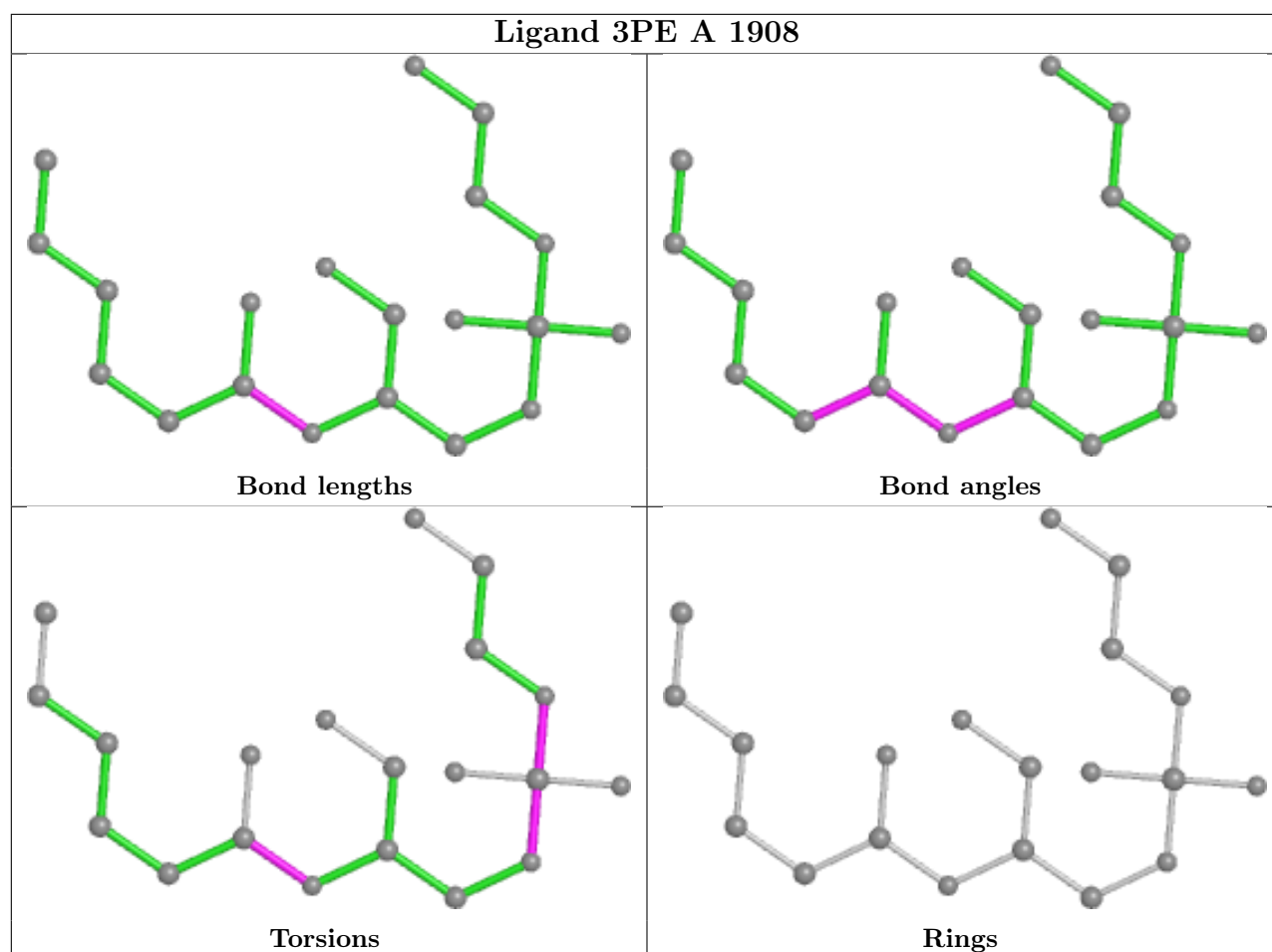


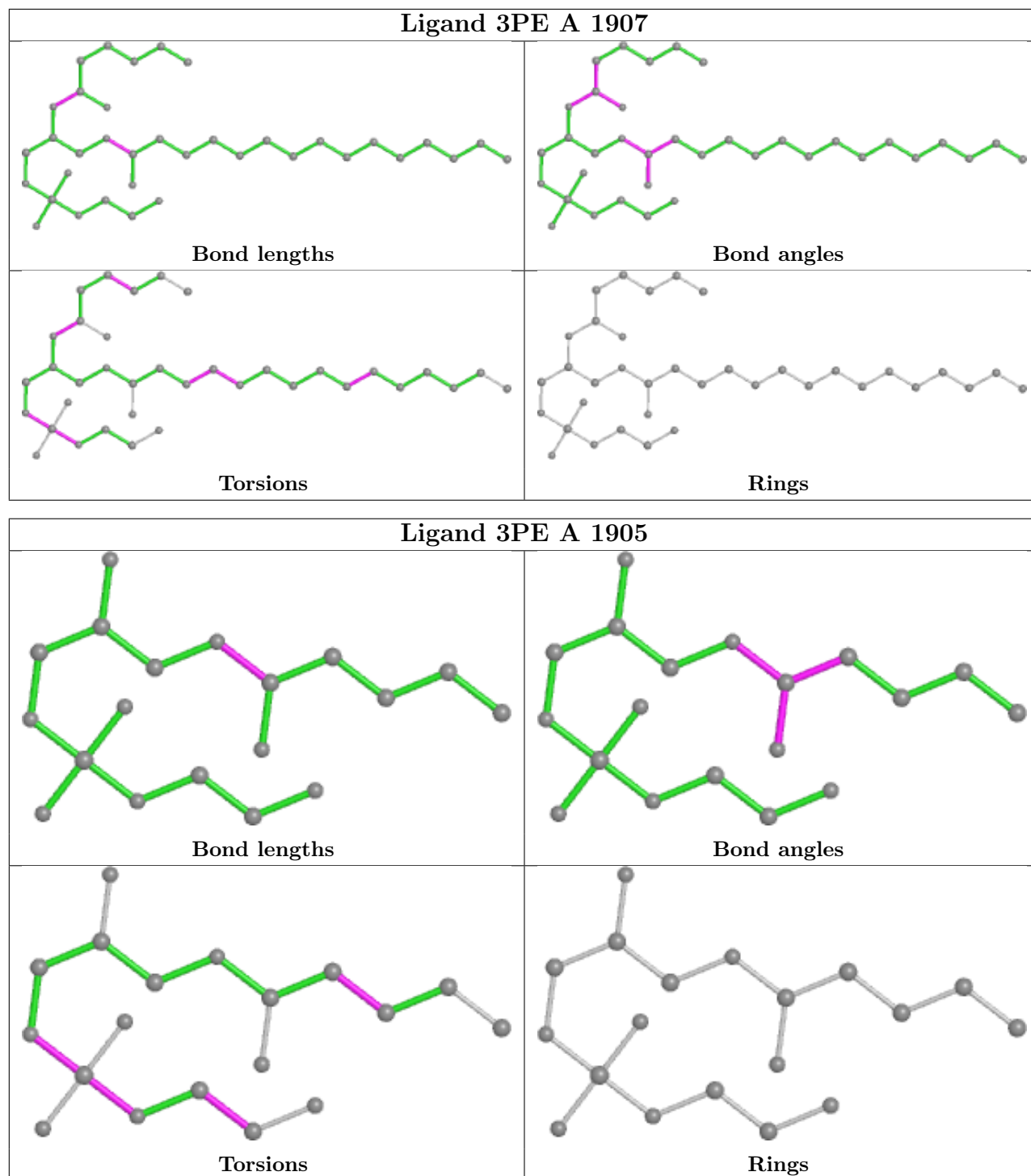












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

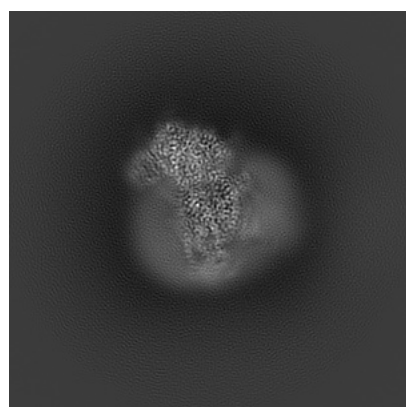
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9868. These allow visual inspection of the internal detail of the map and identification of artifacts.

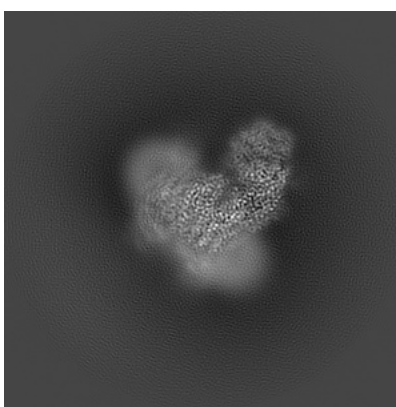
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

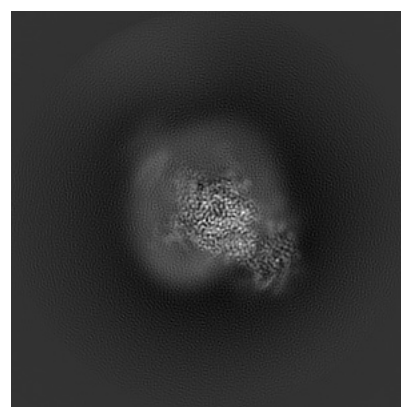
6.1.1 Primary map



X



Y

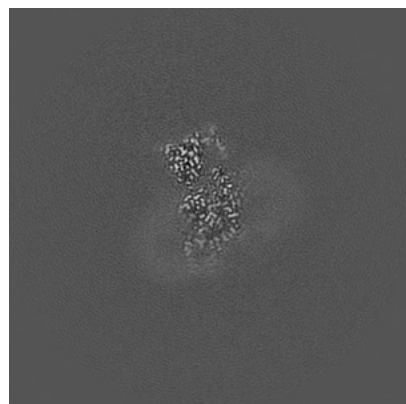


Z

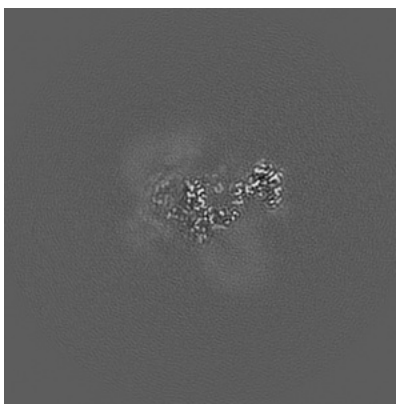
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

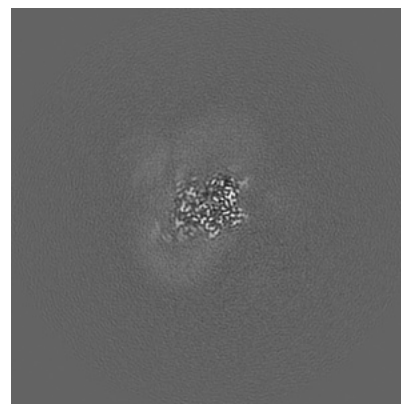
6.2.1 Primary map



X Index: 160



Y Index: 160

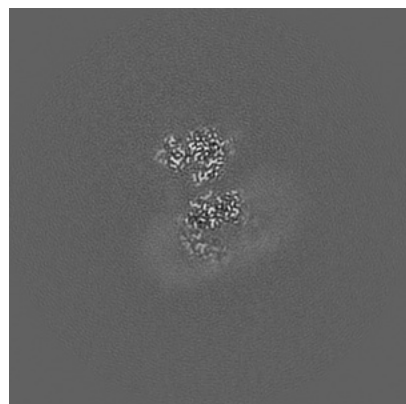


Z Index: 160

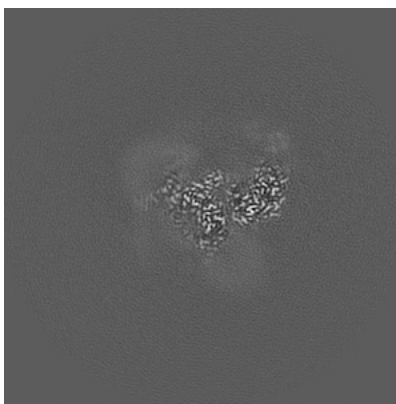
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

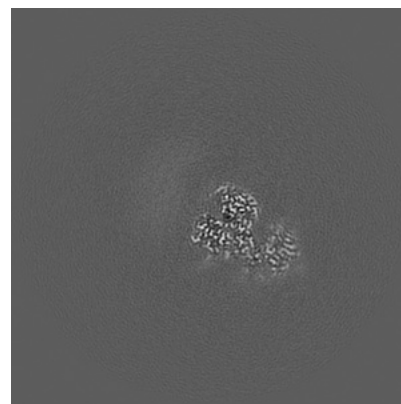
6.3.1 Primary map



X Index: 173



Y Index: 150



Z Index: 205

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

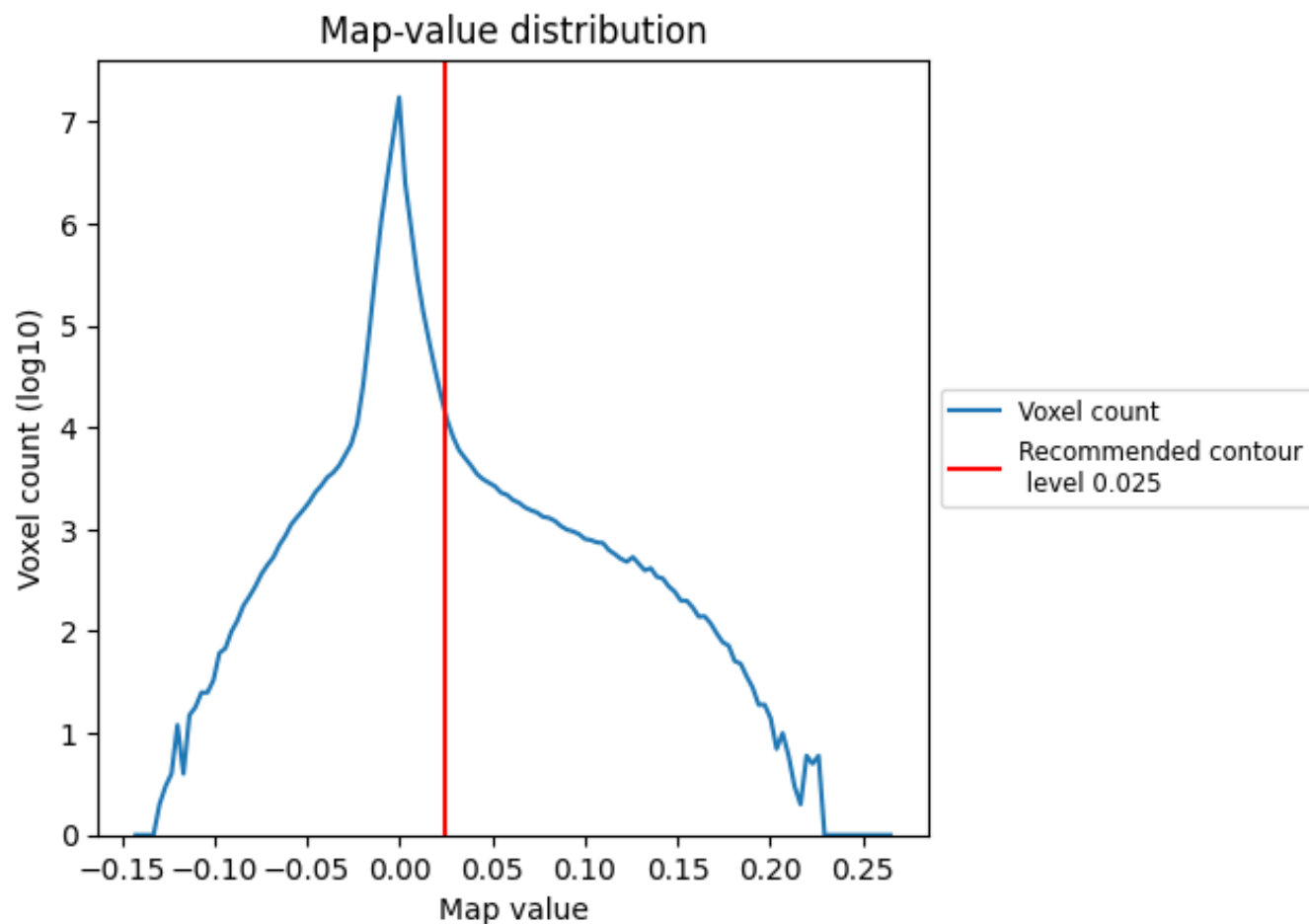
6.5 Mask visualisation

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

7 Map analysis [i](#)

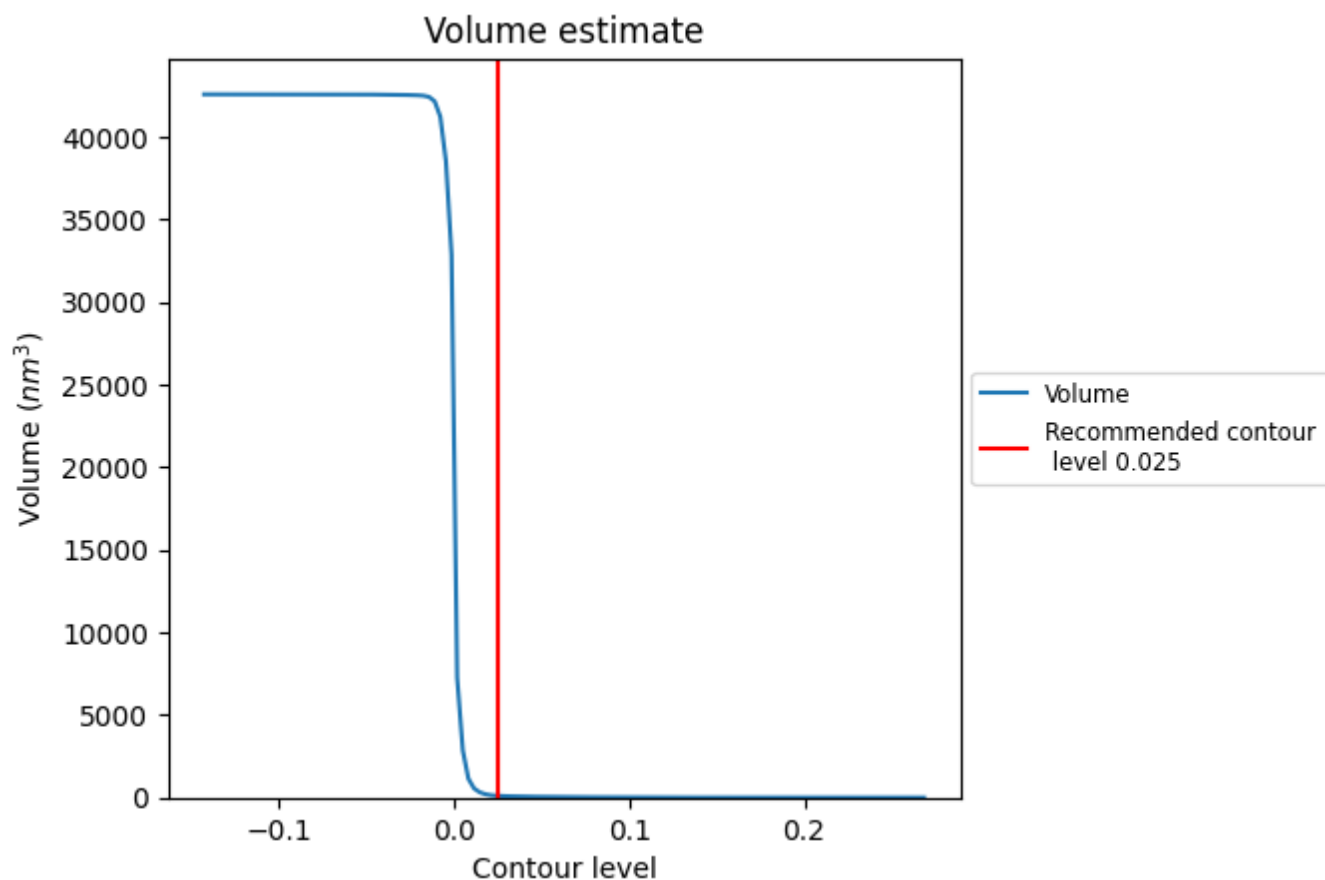
This section contains the results of statistical analysis of the map.

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.

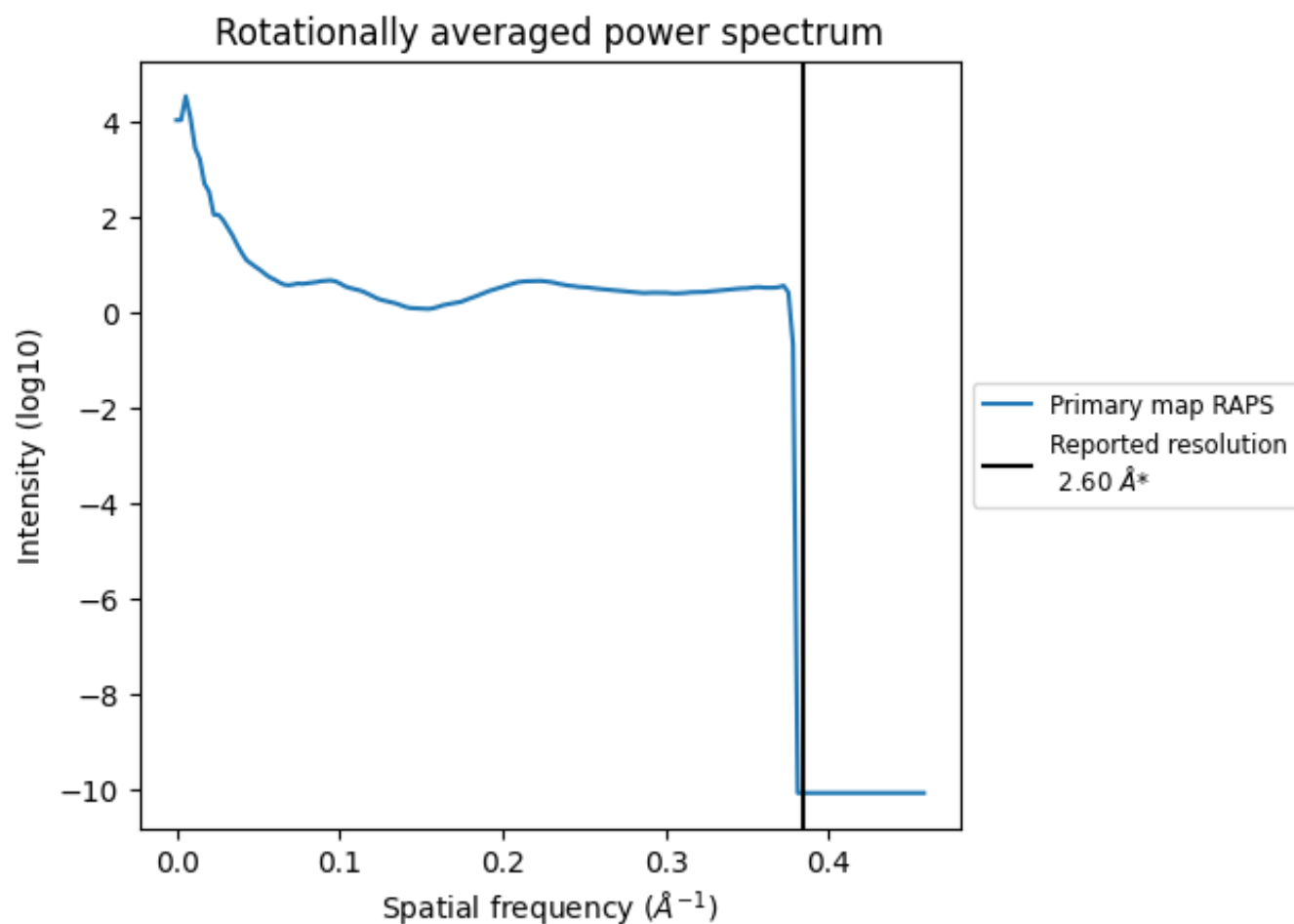
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 106 nm^3 ; this corresponds to an approximate mass of 96 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 0.385 Å⁻¹

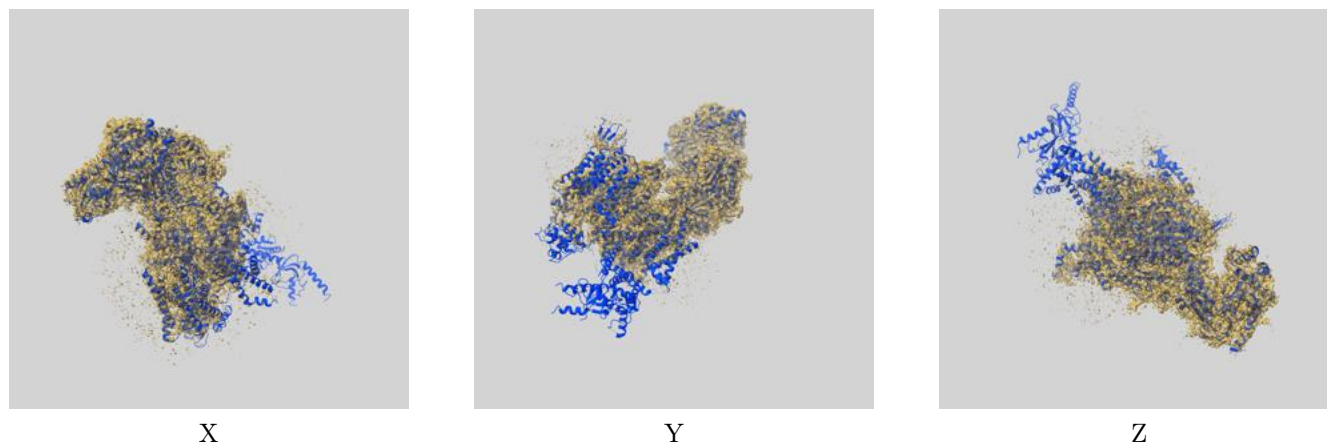
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

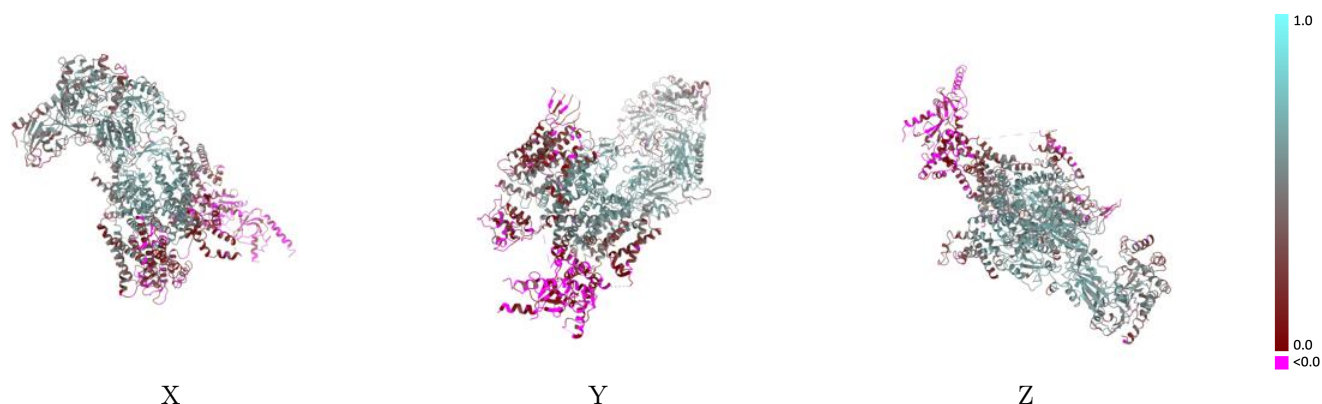
This section contains information regarding the fit between EMDB map EMD-9868 and PDB model 6JPA. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



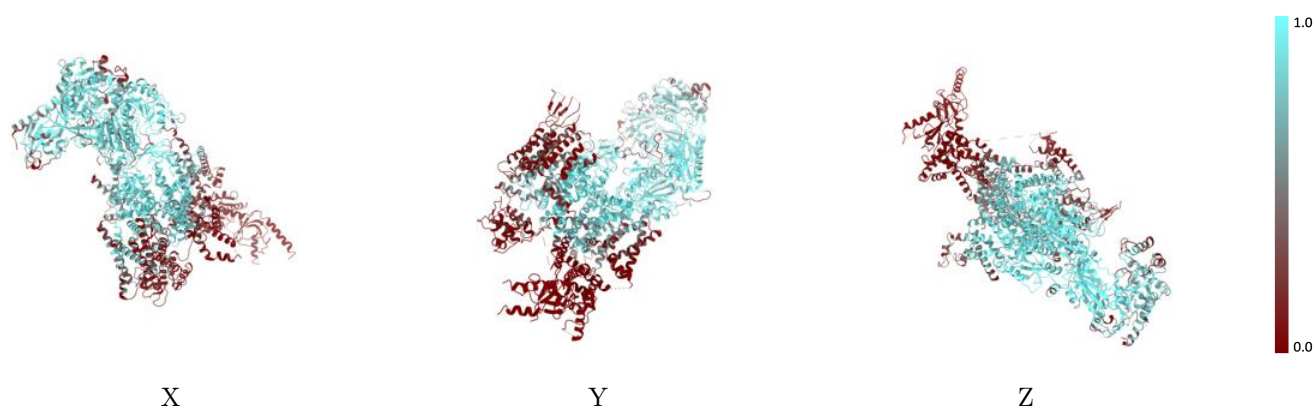
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



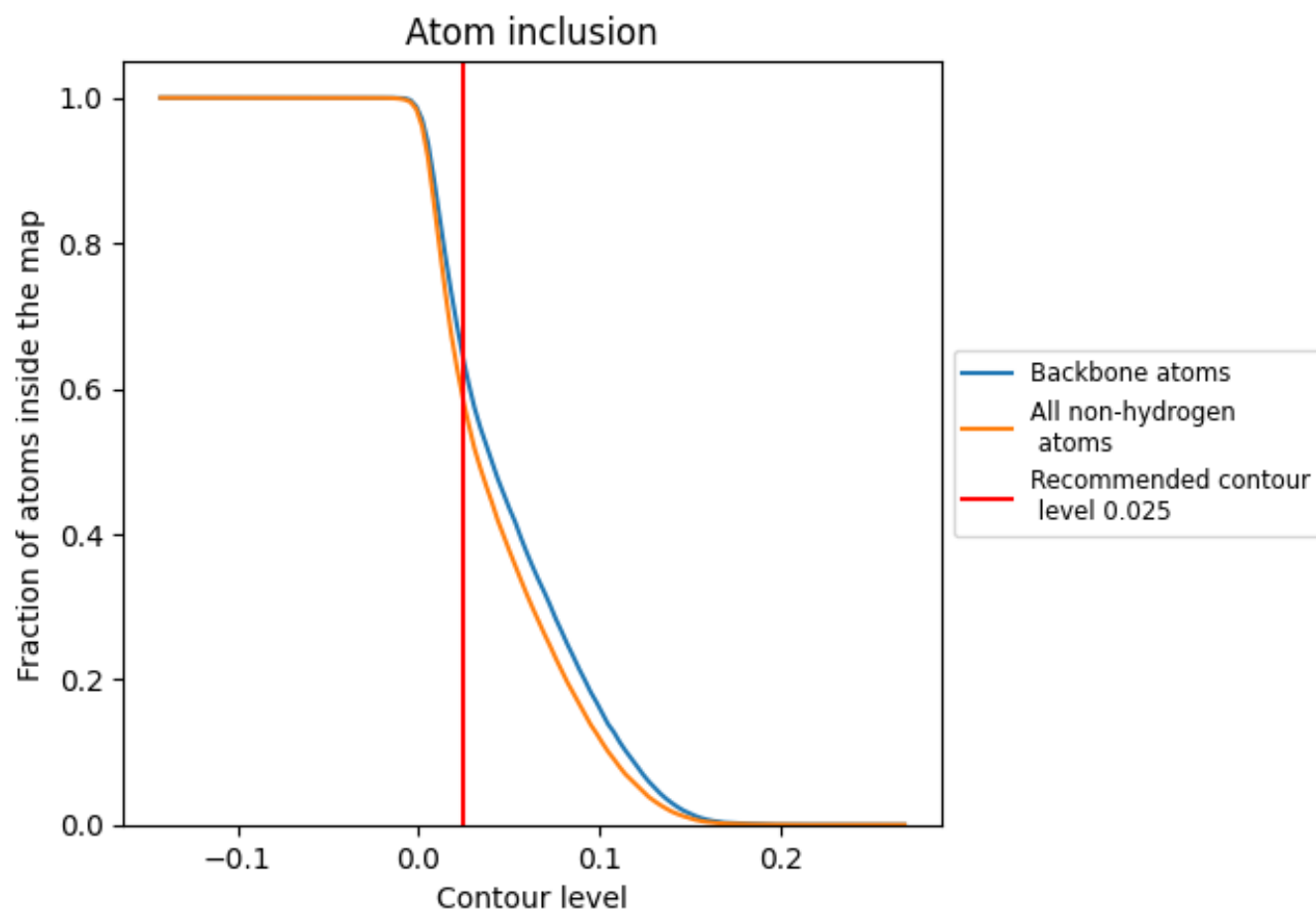
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5798	<div></div> 0.4000
A	<div></div> 0.5912	<div></div> 0.4260
B	<div></div> 0.0000	<div></div> -0.0070
C	<div></div> 0.0000	<div></div> 0.0090
D	<div></div> 0.3929	<div></div> 0.3430
E	<div></div> 0.2142	<div></div> 0.1960
F	<div></div> 0.7828	<div></div> 0.5060
G	<div></div> 0.4286	<div></div> 0.3500
H	<div></div> 0.4872	<div></div> 0.2720
I	<div></div> 0.8718	<div></div> 0.5240
J	<div></div> 0.6071	<div></div> 0.4340
K	<div></div> 0.1071	<div></div> 0.2320
L	<div></div> 0.1905	<div></div> 0.1980

1.0

0.0

<0.0