



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 12:44 PM EST

PDB ID : 7LKP
EMDB ID : EMD-23409
Title : Structure of ATP-free human ABCA4
Authors : Liu, F.; Lee, J.; Chen, J.
Deposited on : 2021-02-02
Resolution : 3.27 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

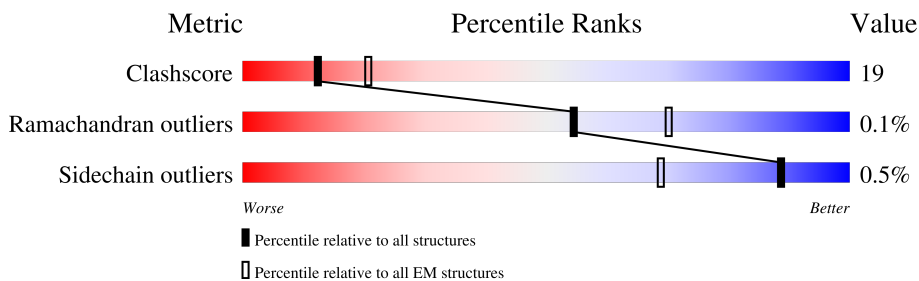
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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	2273	
2	B	3	
3	C	5	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	2307	-	-	X	-
7	AJP	A	2310	X	-	-	-

2 Entry composition [i](#)

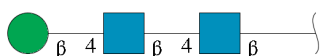
There are 7 unique types of molecules in this entry. The entry contains 15789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Retinal-specific phospholipid-transporting ATPase ABCA4.

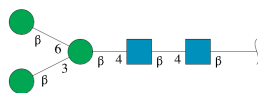
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1941	15274	9874	2554	2762	84	0	0

- Molecule 2 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
			Total	C	N	O		
2	B	3	39	22	2	15	0	0

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



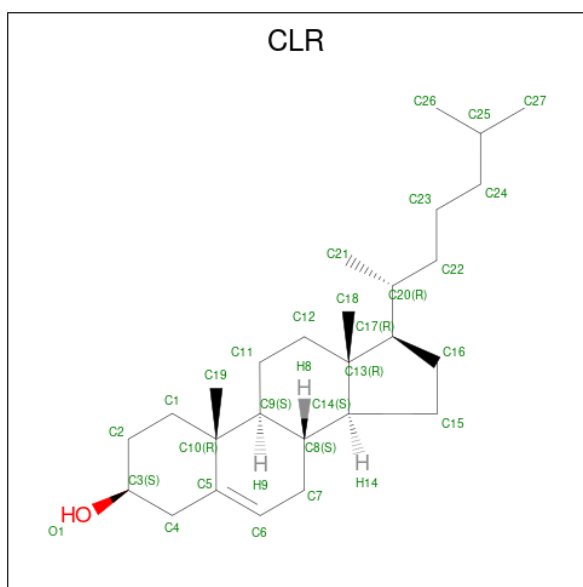
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	5	61	34	2	25	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



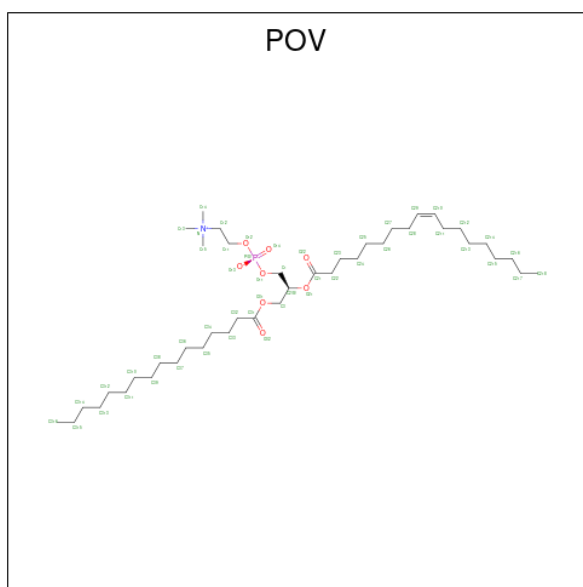
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	
4	A	1	Total	C	N	O	0
			84	48	6	30	

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O).



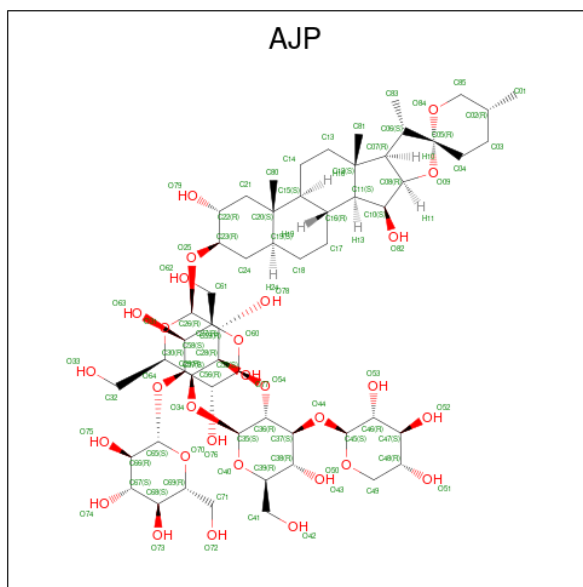
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			174	167	7	
5	A	1	Total	C	O	0
			174	167	7	
5	A	1	Total	C	O	0
			174	167	7	
5	A	1	Total	C	O	0
			174	167	7	
5	A	1	Total	C	O	0
			174	167	7	
5	A	1	Total	C	O	0
			174	167	7	

- Molecule 6 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: C₄₂H₈₂NO₈P).



Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total C 83 83	0
6	A	1	Total C 83 83	0
6	A	1	Total C 83 83	0
6	A	1	Total C 83 83	0
6	A	1	Total C 83 83	0
6	A	1	Total C 83 83	0
6	A	1	Total C 83 83	0

- Molecule 7 is Digitonin (three-letter code: AJP) (formula: C₅₆H₉₂O₂₉).

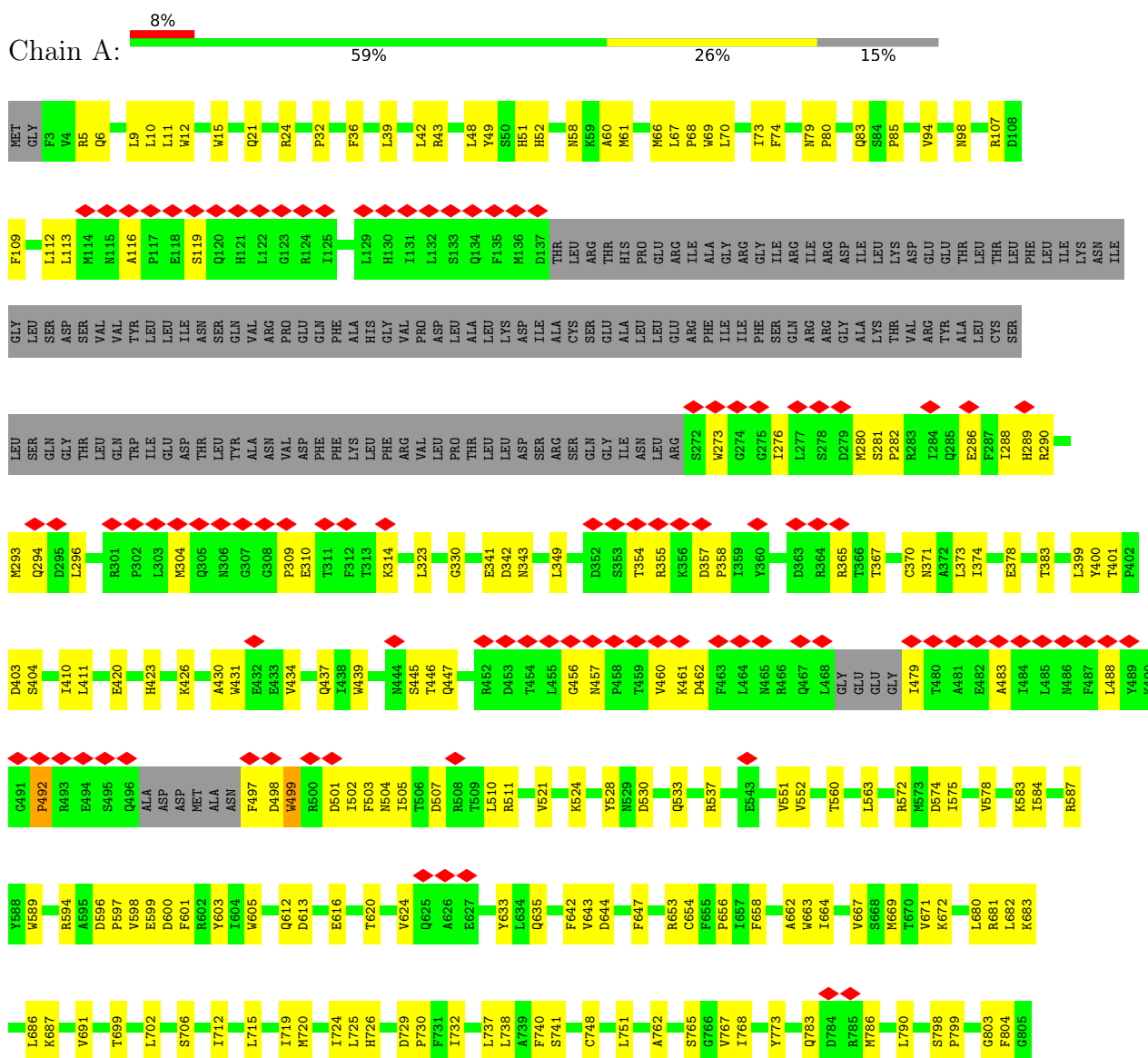


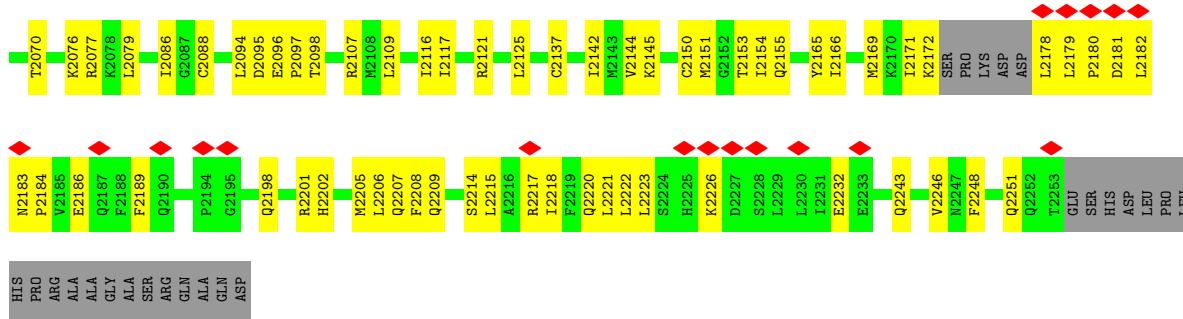
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	C O	0
			74	50 24	

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: Retinal-specific phospholipid-transporting ATPase ABCA4

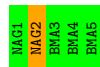
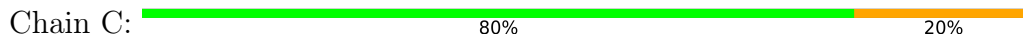




- Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	320102	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.737	Depositor
Minimum map value	-2.317	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.461	Depositor
Map size (\AA)	362.56, 362.56, 362.56	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.03, 1.03, 1.03	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: AJP, POV, BMA, CLR, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/15651	0.54	1/21271 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	PRO	N-CA-CB	6.09	110.61	103.30

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	15274	0	15124	581	0
2	B	39	0	34	0	0
3	C	61	0	52	1	0
4	A	84	0	76	2	0
5	A	174	0	270	88	0
6	A	83	0	133	7	0
7	A	74	0	0	9	0
All	All	15789	0	15689	599	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 19.

All (599) 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:2178:LEU:CD1	1:A:2179:LEU:H	1.23	1.51
1:A:2178:LEU:HD12	1:A:2179:LEU:N	1.19	1.44
1:A:1793:VAL:HG22	5:A:2307:CLR:C21	1.50	1.41
1:A:1793:VAL:CG2	5:A:2307:CLR:C21	1.98	1.40
1:A:1475:GLN:NE2	1:A:1476:LYS:HD3	1.36	1.35
1:A:1475:GLN:NE2	1:A:1476:LYS:CD	1.95	1.28
1:A:1793:VAL:CG2	5:A:2307:CLR:H211	1.62	1.26
1:A:1363:PHE:CD2	5:A:2311:CLR:H191	1.69	1.26
1:A:1796:SER:OG	5:A:2307:CLR:H272	1.34	1.24
1:A:1363:PHE:CD2	5:A:2311:CLR:C19	2.24	1.19
1:A:1796:SER:OG	5:A:2307:CLR:C27	1.91	1.16
1:A:1793:VAL:HG23	5:A:2307:CLR:H212	1.24	1.15
1:A:1373:PHE:HB2	5:A:2312:CLR:C7	1.76	1.13
1:A:1793:VAL:CG2	5:A:2307:CLR:H212	1.66	1.13
1:A:1373:PHE:HB2	5:A:2312:CLR:H72	1.29	1.12
1:A:15:TRP:CD1	5:A:2309:CLR:C11	2.32	1.11
1:A:1796:SER:CB	5:A:2307:CLR:H272	1.80	1.11
1:A:2172:LYS:CG	1:A:2232:GLU:OE2	1.99	1.11
1:A:1373:PHE:HB2	5:A:2312:CLR:C6	1.81	1.10
1:A:1789:SER:CB	5:A:2307:CLR:H112	1.80	1.10
1:A:2179:LEU:HG	1:A:2180:PRO:HD3	1.12	1.09
1:A:2172:LYS:HG2	1:A:2232:GLU:OE2	1.53	1.08
1:A:1475:GLN:NE2	1:A:1476:LYS:CE	2.17	1.06
1:A:1472:GLN:NE2	1:A:1476:LYS:HG3	1.68	1.06
1:A:1789:SER:HA	5:A:2307:CLR:C11	1.85	1.06
1:A:15:TRP:CD1	5:A:2309:CLR:H112	1.90	1.05
1:A:1475:GLN:HE21	1:A:1476:LYS:HE2	1.23	1.03
1:A:357:ASP:OD1	1:A:358:PRO:HD2	1.65	0.95
1:A:1373:PHE:CB	5:A:2312:CLR:H6	1.95	0.95
1:A:1789:SER:CA	5:A:2307:CLR:H112	1.97	0.94
1:A:2179:LEU:CG	1:A:2180:PRO:HD3	1.96	0.94
1:A:1475:GLN:HE21	1:A:1476:LYS:CE	1.74	0.94
1:A:1373:PHE:CB	5:A:2312:CLR:C6	2.45	0.93
1:A:1789:SER:HA	5:A:2307:CLR:H112	1.49	0.93
1:A:1789:SER:HB2	5:A:2307:CLR:H112	1.53	0.91
1:A:1443:ARG:HE	1:A:1453:TYR:HB3	1.35	0.90
1:A:2172:LYS:HG3	1:A:2232:GLU:OE2	1.70	0.90
1:A:1363:PHE:CE2	5:A:2311:CLR:H191	2.07	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:GLN:HE22	1:A:1476:LYS:CD	1.69	0.89
1:A:15:TRP:CD1	5:A:2309:CLR:H111	2.09	0.88
1:A:1363:PHE:HE2	5:A:2311:CLR:H182	1.39	0.88
1:A:1792:TYR:CD1	5:A:2307:CLR:C18	2.56	0.88
1:A:1789:SER:HA	5:A:2307:CLR:H111	1.56	0.86
1:A:1831:LYS:HE3	1:A:1831:LYS:HA	1.56	0.85
1:A:2178:LEU:HD12	1:A:2179:LEU:CA	2.08	0.84
1:A:1792:TYR:CD1	5:A:2307:CLR:H181	2.13	0.83
1:A:1157:LEU:HB3	1:A:1231:PHE:HB2	1.60	0.83
1:A:1363:PHE:CD2	5:A:2311:CLR:H193	2.14	0.83
1:A:1796:SER:HB3	5:A:2307:CLR:H272	1.62	0.81
1:A:1098:ARG:HG3	1:A:2246:VAL:HG21	1.62	0.81
1:A:1475:GLN:HE22	1:A:1476:LYS:HD3	1.00	0.81
1:A:1796:SER:OG	5:A:2307:CLR:H271	1.80	0.81
1:A:15:TRP:HD1	5:A:2309:CLR:H111	1.43	0.81
1:A:2178:LEU:HD11	1:A:2179:LEU:HD23	1.62	0.80
1:A:1792:TYR:CG	5:A:2307:CLR:C18	2.65	0.80
1:A:521:VAL:O	1:A:524:LYS:NZ	2.14	0.79
1:A:1793:VAL:HG22	5:A:2307:CLR:H211	0.79	0.78
1:A:1373:PHE:HB3	5:A:2312:CLR:H6	1.65	0.77
1:A:2098:THR:HG22	1:A:2109:LEU:HD13	1.67	0.77
1:A:1229:LEU:C	1:A:1229:LEU:HD23	2.05	0.77
1:A:1240:HIS:HB2	1:A:1241:ARG:HH21	1.49	0.77
1:A:656:PRO:HG3	1:A:806:THR:HG21	1.68	0.76
1:A:1789:SER:HB3	5:A:2307:CLR:H11	1.66	0.76
1:A:119:SER:HA	1:A:280:MET:SD	2.26	0.76
1:A:1699:LEU:CD1	5:A:2307:CLR:C19	2.65	0.75
1:A:12:TRP:HD1	5:A:2309:CLR:H191	1.48	0.75
1:A:2178:LEU:HD11	1:A:2179:LEU:CD2	2.17	0.74
1:A:1699:LEU:HD11	5:A:2307:CLR:H191	1.69	0.73
1:A:1472:GLN:O	1:A:1476:LYS:HG2	1.88	0.73
1:A:1844:GLY:HA2	1:A:1875:ILE:HD11	1.69	0.73
1:A:1229:LEU:HD21	1:A:1231:PHE:CD2	2.23	0.72
1:A:1373:PHE:CB	5:A:2312:CLR:H72	2.17	0.71
1:A:1239:LYS:HZ1	1:A:1241:ARG:HB2	1.55	0.71
1:A:2179:LEU:HG	1:A:2180:PRO:CD	2.06	0.70
1:A:1699:LEU:HD13	5:A:2307:CLR:H192	1.73	0.70
1:A:1371:LYS:CE	5:A:2307:CLR:H41	2.21	0.70
1:A:1372:ASP:O	1:A:1376:GLN:HB2	1.90	0.70
1:A:773:TYR:HA	1:A:799:PRO:HB2	1.73	0.70
1:A:1545:SER:HB2	1:A:1555:GLN:HE22	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:HB3	1:A:635:GLN:HG2	1.73	0.70
1:A:1724:TRP:HE1	1:A:1897:GLN:HG3	1.57	0.70
1:A:12:TRP:CD1	5:A:2309:CLR:H191	2.27	0.70
1:A:790:LEU:C	1:A:790:LEU:HD23	2.12	0.70
1:A:613:ASP:OD1	1:A:1635:HIS:NE2	2.24	0.69
1:A:706:SER:HB3	5:A:2309:CLR:H263	1.74	0.69
1:A:1731:ASP:OD2	1:A:1779:TYR:OH	2.08	0.69
1:A:1699:LEU:HD13	5:A:2307:CLR:C19	2.23	0.69
1:A:1155:LEU:HD12	1:A:1155:LEU:O	1.92	0.69
1:A:2178:LEU:HD12	1:A:2179:LEU:CB	2.23	0.69
1:A:1488:CYS:HB2	1:A:1503:PRO:HD2	1.74	0.68
1:A:1699:LEU:HD11	5:A:2307:CLR:C19	2.23	0.68
1:A:488:LEU:CB	1:A:499:TRP:H	2.05	0.68
1:A:1443:ARG:NH2	1:A:1518:SER:O	2.26	0.68
1:A:367:THR:O	1:A:371:ASN:ND2	2.26	0.68
1:A:1699:LEU:CD1	5:A:2307:CLR:H191	2.24	0.68
1:A:1925:ARG:HH12	1:A:1957:ARG:HG2	1.57	0.68
1:A:370:CYS:O	1:A:374:ILE:HG13	1.94	0.68
1:A:2007:ILE:HG12	1:A:2011:HIS:CE1	2.28	0.68
1:A:2182:LEU:HD12	1:A:2182:LEU:O	1.94	0.68
1:A:488:LEU:HA	1:A:498:ASP:HB2	1.76	0.68
1:A:15:TRP:HD1	5:A:2309:CLR:C11	1.93	0.68
1:A:15:TRP:NE1	5:A:2309:CLR:H112	2.07	0.67
1:A:965:ASN:OD1	1:A:970:THR:OG1	2.11	0.67
1:A:1892:LEU:C	1:A:1892:LEU:HD23	2.15	0.67
1:A:1895:LEU:C	1:A:1895:LEU:HD23	2.14	0.67
1:A:1240:HIS:HB3	1:A:2223:LEU:HG	1.77	0.67
1:A:1363:PHE:HD2	5:A:2311:CLR:H193	1.56	0.67
1:A:2215:LEU:HA	1:A:2218:ILE:HD13	1.77	0.67
1:A:1363:PHE:CG	5:A:2311:CLR:C19	2.78	0.67
1:A:1793:VAL:HG21	5:A:2307:CLR:C21	2.22	0.67
1:A:399:LEU:HD23	1:A:528:TYR:HE2	1.60	0.66
1:A:410:ILE:HD11	1:A:563:LEU:HD21	1.77	0.66
1:A:1524:ASP:OD1	1:A:1526:THR:OG1	2.13	0.66
1:A:1970:LEU:O	1:A:1970:LEU:HD23	1.96	0.66
1:A:431:TRP:HA	1:A:434:VAL:HG12	1.77	0.65
1:A:2178:LEU:CD1	1:A:2179:LEU:HG	2.26	0.65
1:A:1373:PHE:HB2	5:A:2312:CLR:H6	1.59	0.65
1:A:2178:LEU:CD1	1:A:2179:LEU:CG	2.75	0.65
1:A:977:THR:HG22	1:A:1005:LEU:HD21	1.79	0.65
1:A:2178:LEU:HD11	1:A:2179:LEU:CG	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2178:LEU:CG	1:A:2179:LEU:H	2.05	0.64
1:A:1414:TYR:N	1:A:1555:GLN:O	2.25	0.64
1:A:1751:LYS:O	1:A:1755:THR:OG1	2.16	0.64
1:A:2206:LEU:HD23	1:A:2206:LEU:H	1.63	0.64
1:A:1576:LEU:HD23	1:A:1606:LEU:HD11	1.80	0.64
1:A:1594:ILE:HA	1:A:1597:GLU:HG2	1.80	0.64
1:A:993:ASP:OD1	1:A:994:ILE:N	2.31	0.64
1:A:1704:GLU:OE1	1:A:1723:TYR:OH	2.14	0.64
1:A:936:LYS:HZ1	1:A:980:LEU:HD21	1.63	0.63
1:A:370:CYS:HA	1:A:373:LEU:HB3	1.81	0.63
1:A:1156:TYR:HE2	1:A:1267:THR:HA	1.61	0.63
1:A:1636:ASN:HB3	1:A:1640:ARG:HH21	1.62	0.63
5:A:2311:CLR:O1	5:A:2312:CLR:H272	1.99	0.63
1:A:574:ASP:OD1	1:A:575:ILE:N	2.32	0.63
1:A:357:ASP:OD1	1:A:358:PRO:CD	2.43	0.62
1:A:720:MET:HG3	1:A:730:PRO:HB3	1.82	0.62
1:A:948:ARG:HB3	1:A:1137:ARG:HH22	1.64	0.62
1:A:1240:HIS:HB2	1:A:1241:ARG:NH2	2.13	0.62
1:A:960:ALA:HB3	1:A:1130:ILE:HG22	1.79	0.62
1:A:1244:ALA:HB1	1:A:1248:ARG:HH12	1.63	0.62
1:A:751:LEU:HD21	1:A:768:ILE:HG21	1.82	0.62
1:A:1098:ARG:CG	1:A:2246:VAL:HG21	2.29	0.62
1:A:1943:LEU:HD21	1:A:1984:MET:SD	2.40	0.62
1:A:1784:LEU:CB	5:A:2313:CLR:H6	2.29	0.62
1:A:119:SER:CB	1:A:280:MET:CE	2.78	0.61
1:A:383:THR:HG22	6:A:2316:POV:H32	1.82	0.61
1:A:1405:LEU:HB2	1:A:1656:VAL:HG13	1.81	0.61
1:A:1511:PRO:HG2	1:A:1523:GLN:HG2	1.82	0.61
1:A:1792:TYR:CG	5:A:2307:CLR:H182	2.35	0.61
1:A:2217:ARG:HA	1:A:2220:GLN:HE21	1.66	0.61
1:A:1150:CYS:HG	1:A:1151:PHE:HD1	1.48	0.61
1:A:681:ARG:HD3	1:A:865:TYR:CG	2.35	0.61
1:A:2023:ILE:HD11	1:A:2076:LYS:HG2	1.82	0.61
1:A:1493:ARG:HD3	1:A:1494:GLU:H	1.66	0.61
1:A:2181:ASP:O	1:A:2184:PRO:HD2	2.01	0.61
1:A:36:PHE:CD2	1:A:715:LEU:HD11	2.37	0.60
1:A:1472:GLN:HG2	1:A:1476:LYS:HE2	1.83	0.60
1:A:2035:LEU:HD23	1:A:2039:LEU:HD13	1.82	0.60
1:A:1600:LYS:NZ	1:A:1601:GLU:OE1	2.31	0.60
1:A:32:PRO:HB3	1:A:662:ALA:HB1	1.83	0.60
1:A:1753:ALA:HA	1:A:1852:GLN:HG2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2314:CLR:H183	5:A:2314:CLR:H212	1.83	0.60
1:A:423:HIS:HE1	1:A:1601:GLU:HB2	1.67	0.59
1:A:804:PHE:HB3	1:A:834:PHE:HE2	1.66	0.59
1:A:1475:GLN:HE21	1:A:1476:LYS:CD	1.91	0.59
1:A:933:ASN:HA	1:A:948:ARG:HH12	1.65	0.59
1:A:1121:ASP:OD1	1:A:1122:GLU:N	2.35	0.59
1:A:1214:HIS:CD2	1:A:1215:HIS:HD2	2.20	0.59
1:A:52:HIS:CD2	1:A:83:GLN:HB2	2.36	0.59
1:A:1098:ARG:HG3	1:A:2246:VAL:CG2	2.32	0.59
1:A:12:TRP:HD1	5:A:2309:CLR:C19	2.15	0.59
1:A:1792:TYR:HB3	5:A:2307:CLR:H183	1.85	0.59
1:A:1391:SER:HB2	1:A:1682:VAL:HG21	1.85	0.59
1:A:2094:LEU:HD23	1:A:2097:PRO:HG3	1.83	0.59
1:A:1472:GLN:HE21	1:A:1476:LYS:HE3	1.67	0.58
1:A:1225:ILE:HG22	1:A:1228:GLU:HB2	1.85	0.58
1:A:1363:PHE:CE2	5:A:2311:CLR:H182	2.29	0.58
1:A:790:LEU:HD23	1:A:790:LEU:O	2.04	0.58
1:A:1464:PRO:HG2	1:A:1510:PRO:HB2	1.86	0.58
5:A:2311:CLR:O1	5:A:2312:CLR:C27	2.52	0.58
1:A:1472:GLN:NE2	1:A:1476:LYS:CG	2.56	0.58
1:A:404:SER:OG	1:A:560:THR:O	2.21	0.58
1:A:1425:GLU:OE1	1:A:1425:GLU:N	2.28	0.58
1:A:1705:ARG:NH2	1:A:1786:ASP:OD1	2.24	0.58
1:A:21:GLN:OE1	1:A:24:ARG:NH2	2.36	0.57
1:A:2178:LEU:HD11	1:A:2179:LEU:HG	1.85	0.57
1:A:36:PHE:HE1	1:A:658:PHE:HB3	1.69	0.57
1:A:1008:CYS:SG	1:A:1068:ARG:NH1	2.77	0.57
1:A:1792:TYR:CD1	5:A:2307:CLR:H183	2.40	0.57
1:A:1152:GLY:HA2	1:A:1272:ILE:HD11	1.85	0.57
1:A:1573:GLY:HA2	1:A:1606:LEU:HD12	1.86	0.57
1:A:1950:THR:HG23	1:A:1952:SER:H	1.69	0.57
1:A:1155:LEU:HD11	1:A:1233:LEU:HD12	1.87	0.57
1:A:401:THR:HG22	1:A:552:VAL:HA	1.87	0.57
1:A:1214:HIS:HD2	1:A:1215:HIS:HD2	1.52	0.57
6:A:2308:POV:H25	6:A:2321:POV:H22	1.86	0.57
1:A:119:SER:HA	1:A:280:MET:CE	2.34	0.57
1:A:1687:ILE:HD11	1:A:1803:GLY:HA3	1.87	0.57
1:A:1475:GLN:NE2	1:A:1476:LYS:HE2	1.93	0.56
1:A:426:LYS:HG2	1:A:1598:ALA:HB2	1.87	0.56
1:A:1204:ASP:OD1	1:A:1205:VAL:N	2.37	0.56
1:A:2198:GLN:H	1:A:2198:GLN:CD	2.07	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2218:ILE:HD12	1:A:2218:ILE:H	1.70	0.56
1:A:920:ARG:HH11	1:A:920:ARG:HG2	1.71	0.56
1:A:1752:LYS:O	1:A:1756:SER:OG	2.22	0.56
1:A:1648:SER:OG	1:A:1651:GLU:OE2	2.24	0.56
1:A:2182:LEU:HD13	1:A:2206:LEU:HD22	1.87	0.56
1:A:1159:LEU:HB3	1:A:1259:LEU:HD11	1.88	0.56
1:A:584:ILE:HG22	1:A:1625:HIS:HD2	1.71	0.56
1:A:948:ARG:HB3	1:A:1137:ARG:NH2	2.21	0.56
1:A:310:GLU:H	1:A:314:LYS:NZ	2.04	0.56
7:A:2310:AJP:O78	7:A:2310:AJP:C24	2.54	0.56
1:A:572:ARG:HH11	1:A:572:ARG:HG2	1.71	0.56
7:A:2310:AJP:O76	7:A:2310:AJP:C36	2.54	0.56
1:A:2109:LEU:C	1:A:2109:LEU:HD23	2.26	0.55
1:A:1159:LEU:HD12	1:A:1229:LEU:HD22	1.87	0.55
1:A:349:LEU:HD23	1:A:1816:PHE:HE1	1.71	0.55
1:A:1792:TYR:HB3	5:A:2307:CLR:C18	2.37	0.55
1:A:51:HIS:HB3	1:A:642:PHE:CE1	2.41	0.55
1:A:1243:TYR:O	1:A:1247:PHE:HD1	1.90	0.55
1:A:1955:VAL:HB	1:A:1958:LEU:HD11	1.88	0.55
1:A:1547:LYS:O	1:A:1548:SER:OG	2.22	0.55
1:A:860:VAL:HG12	1:A:861:PHE:CD1	2.42	0.54
1:A:119:SER:CB	1:A:280:MET:HE1	2.37	0.54
1:A:860:VAL:HG12	1:A:861:PHE:HD1	1.73	0.54
1:A:2088:CYS:SG	1:A:2121:ARG:NH2	2.80	0.54
1:A:2179:LEU:N	1:A:2180:PRO:CD	2.70	0.54
1:A:2049:LYS:NZ	1:A:2053:TRP:HB2	2.22	0.54
1:A:2205:MET:HG3	1:A:2205:MET:O	2.07	0.54
1:A:1632:ASN:O	1:A:1636:ASN:ND2	2.36	0.54
1:A:664:ILE:HG21	5:A:2314:CLR:C26	2.37	0.54
1:A:1053:HIS:HE1	1:A:1054:LYS:NZ	2.05	0.54
1:A:1632:ASN:OD1	1:A:1636:ASN:ND2	2.41	0.54
7:A:2310:AJP:C61	7:A:2310:AJP:C56	2.81	0.54
1:A:664:ILE:HG21	5:A:2314:CLR:H261	1.89	0.53
1:A:2052:ASN:HA	1:A:2055:ILE:HG22	1.90	0.53
1:A:1667:GLN:O	1:A:1671:ILE:HG12	2.08	0.53
1:A:1683:ALA:O	1:A:1687:ILE:HG23	2.09	0.53
1:A:273:TRP:HZ3	1:A:276:ILE:HG13	1.74	0.53
1:A:664:ILE:CG2	5:A:2314:CLR:C26	2.87	0.53
1:A:1008:CYS:HB2	1:A:1075:ALA:HB2	1.90	0.53
1:A:2171:ILE:HD13	1:A:2182:LEU:HB2	1.90	0.53
1:A:15:TRP:CD1	5:A:2309:CLR:C12	2.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:HD11	1:A:741:SER:HB2	1.91	0.53
1:A:2178:LEU:HD12	1:A:2179:LEU:H	0.42	0.53
5:A:2314:CLR:C16	5:A:2314:CLR:H232	2.38	0.53
1:A:1249:GLU:O	1:A:1253:THR:OG1	2.24	0.53
1:A:2178:LEU:CD1	1:A:2179:LEU:CB	2.86	0.53
1:A:6:GLN:HG2	1:A:691:VAL:HG12	1.91	0.52
1:A:445:SER:HB3	1:A:447:GLN:HG3	1.92	0.52
1:A:664:ILE:CG2	5:A:2314:CLR:H263	2.38	0.52
1:A:24:ARG:HG3	1:A:669:MET:HG3	1.92	0.52
1:A:1438:PRO:HB2	1:A:1640:ARG:HH11	1.74	0.52
4:A:2306:NAG:H83	4:A:2306:NAG:H3	1.89	0.52
1:A:1371:LYS:HE2	5:A:2307:CLR:H41	1.92	0.52
1:A:1530:ILE:O	1:A:1534:LEU:HG	2.09	0.52
1:A:2178:LEU:CD1	1:A:2179:LEU:N	2.09	0.52
1:A:12:TRP:CD1	5:A:2309:CLR:C19	2.93	0.52
1:A:1784:LEU:HB2	5:A:2313:CLR:H6	1.91	0.52
1:A:52:HIS:HD2	1:A:83:GLN:HB2	1.74	0.52
1:A:2005:THR:OG1	1:A:2006:ASN:OD1	2.27	0.52
1:A:430:ALA:HB2	1:A:1594:ILE:HG12	1.92	0.52
1:A:1031:LYS:HD2	1:A:1078:GLY:HA3	1.91	0.52
1:A:2243:GLN:OE1	1:A:2243:GLN:HA	2.10	0.52
1:A:958:ILE:HG23	1:A:1113:ILE:HB	1.92	0.51
1:A:1241:ARG:HH22	1:A:2220:GLN:HA	1.74	0.51
1:A:1373:PHE:CG	5:A:2312:CLR:C6	2.94	0.51
1:A:1156:TYR:HA	1:A:1232:LEU:HA	1.93	0.51
1:A:74:PHE:HB2	6:A:2318:POV:H26A	1.92	0.51
1:A:1747:ILE:HA	1:A:1755:THR:HG21	1.93	0.51
1:A:2220:GLN:OE1	1:A:2221:LEU:HD23	2.10	0.51
1:A:2178:LEU:HD12	1:A:2179:LEU:CG	2.41	0.51
1:A:971:THR:O	1:A:975:ILE:HG13	2.10	0.51
1:A:1776:PRO:HB2	1:A:1889:TYR:HB2	1.93	0.51
1:A:1093:ASP:N	1:A:1093:ASP:OD1	2.43	0.51
1:A:273:TRP:CZ3	1:A:276:ILE:HG13	2.45	0.51
1:A:1043:GLU:OE1	1:A:1055:ARG:NH2	2.39	0.51
1:A:39:LEU:HD11	1:A:654:CYS:SG	2.51	0.50
1:A:2178:LEU:HD12	1:A:2179:LEU:HG	1.93	0.50
7:A:2310:AJP:C83	7:A:2310:AJP:C81	2.89	0.50
1:A:310:GLU:H	1:A:314:LYS:HZ1	1.59	0.50
1:A:1238:PHE:HE2	1:A:1240:HIS:HB3	1.76	0.50
1:A:1378:VAL:O	1:A:1382:THR:HG23	2.12	0.50
1:A:2144:VAL:HG13	1:A:2145:LYS:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1506:ALA:HB1	1:A:1536:LYS:HB3	1.92	0.50
1:A:1735:TYR:CE1	1:A:1771:GLY:HA3	2.47	0.50
1:A:12:TRP:HZ3	1:A:1026:PHE:HB2	1.76	0.50
1:A:537:ARG:HG2	1:A:537:ARG:HH21	1.76	0.50
1:A:1013:ILE:O	1:A:1014:LEU:HD23	2.12	0.50
1:A:1146:PHE:HD1	1:A:1147:LEU:HD23	1.76	0.50
1:A:1784:LEU:CG	5:A:2313:CLR:H6	2.42	0.50
1:A:798:SER:N	1:A:799:PRO:CD	2.75	0.50
1:A:1229:LEU:C	1:A:1229:LEU:CD2	2.79	0.50
1:A:1705:ARG:HH11	1:A:1783:PHE:HA	1.77	0.50
1:A:1940:LEU:HD12	1:A:1960:VAL:HG22	1.93	0.50
1:A:354:THR:OG1	1:A:355:ARG:N	2.44	0.50
1:A:1034:SER:OG	1:A:1035:GLN:N	2.45	0.50
1:A:1701:LEU:HD21	1:A:1727:ASN:ND2	2.26	0.50
1:A:1892:LEU:HD23	1:A:1892:LEU:O	2.11	0.50
1:A:819:LEU:HD21	1:A:836:PHE:CE2	2.47	0.49
1:A:1239:LYS:NZ	1:A:1242:ALA:H	2.09	0.49
1:A:1967:CYS:SG	1:A:2125:LEU:HD23	2.51	0.49
1:A:1053:HIS:HE1	1:A:1054:LYS:HZ3	1.59	0.49
1:A:94:VAL:HG12	1:A:1616:LYS:HE3	1.93	0.49
1:A:288:ILE:O	1:A:294:GLN:NE2	2.45	0.49
1:A:399:LEU:HD23	1:A:528:TYR:CE2	2.45	0.49
1:A:1929:ILE:HD11	1:A:1942:GLU:OE2	2.12	0.49
1:A:1228:GLU:OE1	1:A:2153:THR:HB	2.12	0.49
1:A:1840:CYS:HB3	1:A:1882:MET:HE2	1.94	0.49
7:A:2310:AJP:O25	7:A:2310:AJP:C32	2.60	0.49
1:A:931:VAL:HG23	1:A:987:VAL:HG22	1.95	0.49
1:A:1240:HIS:HD2	1:A:1241:ARG:HE	1.61	0.49
1:A:479:ILE:O	1:A:483:ALA:N	2.43	0.49
1:A:594:ARG:HD3	1:A:1621:ASN:ND2	2.28	0.49
1:A:374:ILE:HG22	1:A:378:GLU:HG3	1.94	0.49
1:A:1754:TYR:HB3	1:A:1763:LEU:HD22	1.95	0.49
1:A:2198:GLN:OE1	1:A:2198:GLN:N	2.30	0.49
1:A:726:HIS:N	1:A:813:GLU:OE2	2.45	0.49
1:A:783:GLN:OE1	1:A:783:GLN:N	2.37	0.49
1:A:1239:LYS:HZ2	1:A:1242:ALA:H	1.60	0.49
1:A:1919:ASP:N	1:A:1919:ASP:OD1	2.43	0.49
1:A:1982:PHE:O	1:A:1986:THR:HG23	2.12	0.49
1:A:921:GLU:HB3	1:A:954:TYR:OH	2.12	0.48
1:A:936:LYS:HD2	1:A:937:ILE:H	1.78	0.48
1:A:947:ASP:OD1	1:A:947:ASP:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:ILE:HD12	1:A:1140:CYS:SG	2.53	0.48
1:A:1566:LEU:HD12	1:A:1567:PRO:HD2	1.95	0.48
1:A:1829:LEU:HD23	1:A:1829:LEU:C	2.34	0.48
1:A:1015:PHE:HE2	1:A:1026:PHE:HE2	1.60	0.48
1:A:85:PRO:HD2	3:C:2:NAG:H2	1.94	0.48
1:A:2198:GLN:HG3	1:A:2208:PHE:CE1	2.48	0.48
1:A:957:GLN:HB3	1:A:1128:ASP:HB2	1.94	0.48
1:A:2107:ARG:HD2	1:A:2107:ARG:HA	1.60	0.48
1:A:1415:THR:O	1:A:1522:LEU:HA	2.13	0.48
1:A:2222:LEU:O	1:A:2226:LYS:HG2	2.14	0.48
7:A:2310:AJP:C45	7:A:2310:AJP:O54	2.62	0.48
1:A:672:LYS:HG3	1:A:762:ALA:HB2	1.95	0.48
1:A:1475:GLN:NE2	1:A:1476:LYS:CG	2.73	0.48
1:A:1893:THR:O	1:A:1896:VAL:HG12	2.12	0.48
1:A:1414:TYR:HD2	1:A:1523:GLN:NE2	2.11	0.48
1:A:15:TRP:CG	5:A:2309:CLR:H121	2.49	0.48
1:A:589:TRP:HE3	1:A:1549:LYS:HE3	1.79	0.48
1:A:681:ARG:HD3	1:A:865:TYR:CD1	2.48	0.47
1:A:1229:LEU:HD23	1:A:1230:ILE:N	2.29	0.47
1:A:1105:LEU:O	1:A:1108:ARG:HG2	2.13	0.47
1:A:1236:LYS:HD3	1:A:1236:LYS:N	2.30	0.47
1:A:507:ASP:O	1:A:511:ARG:HG2	2.14	0.47
1:A:2166:ILE:HG12	1:A:2209:GLN:HG2	1.95	0.47
1:A:1828:VAL:O	1:A:1832:LEU:HG	2.14	0.47
1:A:612:GLN:O	1:A:616:GLU:HG3	2.14	0.47
1:A:1967:CYS:HB2	1:A:2117:ILE:HD11	1.95	0.47
1:A:66:MET:HG2	1:A:420:GLU:HG2	1.97	0.47
1:A:80:PRO:HB3	1:A:330:GLY:O	2.15	0.47
1:A:510:LEU:HD23	1:A:510:LEU:HA	1.76	0.47
1:A:683:LYS:O	1:A:687:LYS:HG3	2.15	0.47
1:A:1414:TYR:CD1	1:A:1555:GLN:HB3	2.49	0.47
1:A:1521:ILE:HD12	1:A:1521:ILE:H	1.80	0.47
1:A:36:PHE:CE2	1:A:719:ILE:HD11	2.50	0.47
1:A:286:GLU:HA	1:A:289:HIS:HB2	1.95	0.47
1:A:1162:LYS:NZ	1:A:1258:GLY:O	2.47	0.47
1:A:1263:GLY:HA3	1:A:2155:GLN:NE2	2.30	0.47
1:A:2171:ILE:HD13	1:A:2182:LEU:HA	1.97	0.47
1:A:2178:LEU:CD1	1:A:2179:LEU:HD23	2.38	0.47
1:A:1371:LYS:HE3	5:A:2307:CLR:H41	1.96	0.47
1:A:119:SER:HA	1:A:280:MET:HE2	1.97	0.47
1:A:457:ASN:HA	1:A:461:LYS:H	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1779:TYR:HB3	1:A:1893:THR:HG21	1.97	0.47
1:A:1247:PHE:CE2	1:A:1264:ILE:HG13	2.49	0.47
1:A:67:LEU:HB3	1:A:68:PRO:HD3	1.96	0.46
1:A:98:ASN:HB2	1:A:107:ARG:NH2	2.31	0.46
1:A:1391:SER:OG	1:A:1751:LYS:NZ	2.42	0.46
1:A:1583:LEU:O	1:A:1587:MET:HG2	2.14	0.46
1:A:2019:GLN:O	1:A:2077:ARG:NH2	2.48	0.46
1:A:457:ASN:O	1:A:462:ASP:N	2.47	0.46
1:A:1792:TYR:CB	5:A:2307:CLR:C18	2.94	0.46
1:A:1895:LEU:HD23	1:A:1895:LEU:O	2.15	0.46
1:A:293:MET:HA	1:A:296:LEU:O	2.14	0.46
1:A:530:ASP:OD1	1:A:533:GLN:NE2	2.44	0.46
1:A:686:LEU:O	1:A:691:VAL:HG22	2.16	0.46
1:A:1691:SER:OG	1:A:1799:ASN:ND2	2.49	0.46
1:A:1713:GLN:O	1:A:1718:VAL:HG12	2.16	0.46
1:A:2066:CYS:HG	1:A:2070:THR:HG1	1.57	0.46
1:A:1820:ARG:HD2	1:A:1821:THR:N	2.31	0.46
1:A:400:TYR:HA	1:A:551:VAL:O	2.16	0.46
1:A:445:SER:OG	1:A:446:THR:N	2.49	0.46
1:A:1878:ASN:O	1:A:1882:MET:HB2	2.15	0.46
1:A:2049:LYS:HZ1	1:A:2053:TRP:HB2	1.81	0.46
1:A:355:ARG:HA	1:A:355:ARG:HD3	1.75	0.46
1:A:977:THR:HG21	1:A:1007:MET:SD	2.55	0.46
1:A:790:LEU:C	1:A:790:LEU:CD2	2.82	0.46
1:A:1520:GLU:O	1:A:1520:GLU:HG3	2.16	0.46
6:A:2317:POV:H214	6:A:2317:POV:H21A	1.56	0.46
1:A:24:ARG:NH1	1:A:669:MET:HB3	2.30	0.46
1:A:671:VAL:HG11	1:A:765:SER:CB	2.46	0.46
1:A:1366:THR:HG21	1:A:1730:TRP:HZ2	1.80	0.46
1:A:1421:GLU:O	1:A:1421:GLU:HG2	2.14	0.46
1:A:1943:LEU:HD23	1:A:1944:THR:N	2.31	0.46
1:A:49:TYR:HB3	1:A:644:ASP:HB3	1.98	0.45
1:A:1491:SER:HB2	1:A:1497:THR:H	1.82	0.45
1:A:1934:LYS:HD3	1:A:1934:LYS:N	2.31	0.45
1:A:12:TRP:HA	5:A:2309:CLR:H182	1.99	0.45
1:A:1112:THR:O	1:A:1112:THR:HG22	2.16	0.45
1:A:2045:GLU:OE1	1:A:2045:GLU:N	2.47	0.45
1:A:15:TRP:CD1	5:A:2309:CLR:H121	2.52	0.45
1:A:341:GLU:OE2	1:A:583:LYS:NZ	2.44	0.45
1:A:1159:LEU:O	1:A:1229:LEU:N	2.50	0.45
1:A:1101:TRP:O	1:A:1105:LEU:HD23	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1818:ASN:ND2	1:A:1820:ARG:O	2.49	0.45
1:A:2095:ASP:OD1	1:A:2096:GLU:HG3	2.16	0.45
1:A:930:CYS:SG	1:A:988:LEU:HB3	2.57	0.45
1:A:1418:SER:HB2	1:A:1530:ILE:HD11	1.99	0.45
1:A:439:TRP:HD1	1:A:503:PHE:CE2	2.34	0.45
1:A:2186:GLU:HG3	1:A:2201:ARG:HH22	1.82	0.45
1:A:401:THR:HG21	1:A:552:VAL:HG13	1.99	0.45
1:A:1488:CYS:HB2	1:A:1502:CYS:HB2	1.49	0.45
1:A:1818:ASN:OD1	1:A:1819:ASN:N	2.49	0.45
7:A:2310:AJP:C24	7:A:2310:AJP:C27	2.94	0.45
1:A:70:LEU:HA	1:A:73:ILE:HG22	1.99	0.45
1:A:528:TYR:OH	1:A:537:ARG:HG2	2.17	0.45
1:A:1070:LEU:O	1:A:1074:ILE:HG23	2.17	0.45
1:A:1789:SER:CA	5:A:2307:CLR:C11	2.62	0.45
1:A:1449:TRP:CG	1:A:1450:LEU:N	2.84	0.45
1:A:365:ARG:O	1:A:365:ARG:HG2	2.17	0.45
1:A:933:ASN:CA	1:A:948:ARG:HH12	2.30	0.44
1:A:1220:LYS:HD2	1:A:1220:LYS:N	2.32	0.44
1:A:1433:VAL:O	1:A:1438:PRO:HD2	2.17	0.44
1:A:1433:VAL:HG11	1:A:1640:ARG:HB3	1.99	0.44
1:A:1694:PRO:HB2	1:A:1778:MET:CE	2.47	0.44
1:A:1074:ILE:HA	1:A:1077:VAL:HG13	2.00	0.44
1:A:1576:LEU:HD12	1:A:1580:LEU:HD23	2.00	0.44
1:A:1895:LEU:C	1:A:1895:LEU:CD2	2.86	0.44
1:A:2142:ILE:HB	1:A:2150:CYS:SG	2.58	0.44
1:A:36:PHE:HD2	1:A:715:LEU:HD11	1.78	0.44
1:A:1354:HIS:O	1:A:1358:LEU:HD23	2.18	0.44
1:A:1017:HIS:HA	1:A:1058:GLU:OE1	2.17	0.44
1:A:2137:CYS:SG	1:A:2154:ILE:HD11	2.58	0.44
1:A:1229:LEU:C	1:A:1230:ILE:HD12	2.38	0.44
1:A:1455:CYS:HB2	1:A:1517:ARG:O	2.18	0.44
1:A:1474:PHE:CZ	1:A:1508:GLY:HA2	2.52	0.44
1:A:49:TYR:CE1	1:A:51:HIS:HB2	2.53	0.44
1:A:488:LEU:CA	1:A:498:ASP:HB2	2.46	0.44
1:A:667:VAL:HG13	1:A:748:CYS:SG	2.57	0.44
1:A:1784:LEU:HG	5:A:2313:CLR:H6	1.99	0.44
1:A:504:ASN:HD22	4:A:2302:NAG:H83	1.83	0.44
1:A:1960:VAL:HG12	1:A:2151:MET:HE1	1.99	0.44
1:A:738:LEU:HD23	1:A:738:LEU:HA	1.86	0.44
1:A:1155:LEU:HD12	1:A:1155:LEU:C	2.38	0.44
1:A:1246:LEU:HD23	1:A:1250:LEU:HD23	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1577:VAL:HB	1:A:1602:ILE:HG21	2.00	0.44
1:A:1776:PRO:HB2	1:A:1889:TYR:CB	2.48	0.44
1:A:2169:MET:HE3	1:A:2206:LEU:HD21	1.99	0.44
7:A:2310:AJP:C13	5:A:2314:CLR:H71	2.48	0.44
1:A:488:LEU:CB	1:A:498:ASP:HB2	2.48	0.43
1:A:572:ARG:HG2	1:A:572:ARG:NH1	2.32	0.43
1:A:706:SER:HB3	5:A:2309:CLR:C26	2.45	0.43
1:A:767:VAL:HG21	5:A:2307:CLR:H221	1.99	0.43
1:A:74:PHE:CE2	1:A:323:LEU:HD12	2.53	0.43
1:A:729:ASP:O	1:A:732:ILE:HG22	2.18	0.43
1:A:815:GLN:HG3	1:A:817:LEU:HD12	2.00	0.43
1:A:1573:GLY:O	1:A:1577:VAL:HG12	2.18	0.43
1:A:1687:ILE:HG22	1:A:1841:LEU:HD22	2.00	0.43
1:A:2198:GLN:HG3	1:A:2208:PHE:CZ	2.53	0.43
1:A:43:ARG:HB2	1:A:647:PHE:CE2	2.53	0.43
1:A:79:ASN:HB2	1:A:597:PRO:HG3	2.00	0.43
1:A:1238:PHE:CE2	1:A:1240:HIS:HB3	2.52	0.43
1:A:1438:PRO:HG3	1:A:1640:ARG:HD2	1.98	0.43
1:A:119:SER:CB	1:A:280:MET:HE2	2.46	0.43
1:A:598:VAL:HG12	1:A:599:GLU:HG3	2.00	0.43
1:A:948:ARG:HA	1:A:948:ARG:HD2	1.86	0.43
1:A:1354:HIS:CD2	1:A:1718:VAL:HA	2.54	0.43
1:A:61:MET:HB3	1:A:613:ASP:OD2	2.17	0.43
1:A:437:GLN:HE22	1:A:1590:SER:H	1.66	0.43
1:A:1402:ALA:HA	1:A:1659:GLN:HB2	2.00	0.43
1:A:1789:SER:HB3	5:A:2307:CLR:C1	2.43	0.43
1:A:1892:LEU:C	1:A:1892:LEU:CD2	2.86	0.43
1:A:2165:TYR:CZ	1:A:2215:LEU:HD13	2.54	0.43
1:A:724:ILE:HG22	1:A:725:LEU:HD12	1.99	0.43
1:A:1157:LEU:HA	1:A:1264:ILE:HD13	2.01	0.43
1:A:1602:ILE:N	1:A:1603:PRO:HD2	2.34	0.43
1:A:2206:LEU:O	1:A:2206:LEU:HG	2.18	0.43
1:A:2207:GLN:O	1:A:2207:GLN:HG2	2.19	0.43
1:A:341:GLU:O	1:A:342:ASP:HB3	2.18	0.43
1:A:572:ARG:HH12	1:A:1659:GLN:CD	2.21	0.43
1:A:824:ILE:HD11	1:A:836:PHE:HD2	1.84	0.43
1:A:1036:GLU:H	1:A:1036:GLU:CD	2.22	0.43
1:A:1153:THR:HG22	1:A:1154:GLY:H	1.83	0.43
1:A:1159:LEU:HB2	1:A:1229:LEU:HB3	2.00	0.43
1:A:1885:GLU:HG2	1:A:1889:TYR:CZ	2.54	0.43
1:A:1970:LEU:HD23	1:A:1970:LEU:C	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:ARG:HG3	1:A:1494:GLU:OE2	2.19	0.43
1:A:1960:VAL:CG1	1:A:2151:MET:HE1	2.49	0.43
1:A:2198:GLN:CD	1:A:2198:GLN:N	2.69	0.43
1:A:1159:LEU:HD23	1:A:1262:PHE:HB2	2.01	0.43
1:A:1475:GLN:HE22	1:A:1476:LYS:CE	2.04	0.43
1:A:1606:LEU:HD23	1:A:1606:LEU:HA	1.85	0.43
1:A:1852:GLN:HA	1:A:1852:GLN:OE1	2.19	0.43
1:A:48:LEU:HD11	1:A:1496:LEU:HD22	2.00	0.43
1:A:410:ILE:HG22	1:A:411:LEU:HD12	2.01	0.43
1:A:1371:LYS:HZ3	5:A:2307:CLR:C3	2.32	0.43
1:A:281:SER:N	1:A:282:PRO:HD2	2.33	0.42
1:A:403:ASP:HB2	1:A:528:TYR:O	2.19	0.42
1:A:1225:ILE:CG2	1:A:1228:GLU:HB2	2.49	0.42
1:A:1701:LEU:HA	1:A:1701:LEU:HD23	1.74	0.42
6:A:2316:POV:H36A	6:A:2316:POV:H33	1.90	0.42
1:A:423:HIS:CE1	1:A:1601:GLU:HB2	2.51	0.42
1:A:1093:ASP:OD2	1:A:1974:ASN:ND2	2.30	0.42
1:A:1417:PHE:HE1	1:A:1419:MET:HB2	1.83	0.42
1:A:1493:ARG:HA	1:A:1493:ARG:NE	2.34	0.42
1:A:1862:GLY:C	1:A:1863:GLU:OE1	2.57	0.42
1:A:289:HIS:HA	1:A:294:GLN:HE22	1.83	0.42
1:A:60:ALA:HB3	1:A:69:TRP:HA	2.01	0.42
1:A:1869:PRO:O	1:A:1875:ILE:HB	2.20	0.42
1:A:2004:LEU:HD12	1:A:2004:LEU:H	1.85	0.42
1:A:2066:CYS:SG	1:A:2067:LEU:N	2.92	0.42
1:A:2232:GLU:OE1	1:A:2232:GLU:N	2.52	0.42
1:A:341:GLU:OE1	1:A:587:ARG:N	2.29	0.42
1:A:921:GLU:OE1	1:A:954:TYR:OH	2.34	0.42
1:A:1397:PHE:CD2	1:A:1671:ILE:HG21	2.54	0.42
1:A:1945:LYS:HA	1:A:1992:THR:HB	2.02	0.42
1:A:2005:THR:OG1	1:A:2006:ASN:N	2.52	0.42
1:A:10:LEU:HB2	1:A:699:THR:HG21	2.01	0.42
1:A:112:LEU:O	1:A:116:ALA:HB2	2.20	0.42
1:A:1796:SER:CB	5:A:2307:CLR:C27	2.69	0.42
1:A:2086:ILE:HD12	1:A:2086:ILE:HA	1.91	0.42
1:A:584:ILE:HG22	1:A:1625:HIS:CD2	2.54	0.42
1:A:1251:GLU:OE2	1:A:2214:SER:HA	2.20	0.42
1:A:1978:LYS:HA	1:A:1981:THR:HG22	2.00	0.42
1:A:5:ARG:O	1:A:9:LEU:HG	2.20	0.42
1:A:73:ILE:HD11	6:A:2317:POV:H29	2.01	0.42
7:A:2310:AJP:C41	7:A:2310:AJP:O34	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:LEU:HD23	1:A:737:LEU:HA	1.85	0.42
1:A:1472:GLN:HG2	1:A:1476:LYS:CE	2.48	0.42
1:A:2067:LEU:O	1:A:2070:THR:OG1	2.37	0.42
1:A:2183:ASN:N	1:A:2184:PRO:CD	2.82	0.42
1:A:2205:MET:O	1:A:2205:MET:CG	2.68	0.42
1:A:1010:GLN:O	1:A:1068:ARG:NH2	2.53	0.41
1:A:11:LEU:HD11	1:A:702:LEU:HD23	2.02	0.41
1:A:1532:ASP:OD1	1:A:1536:LYS:HD2	2.19	0.41
1:A:653:ARG:O	1:A:656:PRO:HD2	2.20	0.41
1:A:1383:PHE:HB3	1:A:1689:SER:HB2	2.02	0.41
1:A:1831:LYS:HA	1:A:1831:LYS:CE	2.35	0.41
1:A:601:PHE:O	1:A:605:TRP:NE1	2.53	0.41
1:A:1137:ARG:HA	1:A:1137:ARG:HD3	1.89	0.41
1:A:1792:TYR:CE1	5:A:2307:CLR:H181	2.54	0.41
1:A:1820:ARG:O	1:A:1821:THR:OG1	2.36	0.41
1:A:2023:ILE:HG21	1:A:2079:LEU:HD23	2.03	0.41
1:A:289:HIS:HA	1:A:294:GLN:NE2	2.35	0.41
1:A:1519:THR:O	1:A:1519:THR:HG22	2.21	0.41
1:A:109:PHE:O	1:A:113:LEU:HB2	2.20	0.41
1:A:119:SER:CA	1:A:280:MET:CE	2.99	0.41
1:A:643:VAL:HG22	1:A:1498:MET:HA	2.02	0.41
1:A:1013:ILE:HG13	1:A:1074:ILE:HD11	2.03	0.41
1:A:1963:ARG:HB2	1:A:1966:GLU:HG3	2.02	0.41
1:A:304:MET:HB2	1:A:309:PRO:HG3	2.03	0.41
1:A:589:TRP:CD1	1:A:1552:VAL:HG11	2.55	0.41
1:A:620:THR:O	1:A:624:VAL:HG22	2.20	0.41
1:A:786:MET:HE3	1:A:790:LEU:HD22	2.03	0.41
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.93	0.41
1:A:112:LEU:HD11	1:A:290:ARG:HH21	1.86	0.41
1:A:936:LYS:HD2	1:A:937:ILE:N	2.36	0.41
1:A:1033:LYS:HZ2	1:A:1078:GLY:HA2	1.86	0.41
1:A:1157:LEU:HB3	1:A:1231:PHE:CB	2.43	0.41
1:A:1449:TRP:CE2	1:A:1450:LEU:HD23	2.56	0.41
1:A:1668:LEU:HD23	1:A:1668:LEU:HA	1.89	0.41
1:A:2002:SER:OG	1:A:2003:ILE:N	2.54	0.41
1:A:2116:ILE:HD12	1:A:2121:ARG:NH1	2.36	0.41
1:A:456:GLY:O	1:A:460:VAL:N	2.54	0.41
1:A:1153:THR:HG22	1:A:1154:GLY:N	2.36	0.41
1:A:1155:LEU:O	1:A:1155:LEU:CD1	2.67	0.41
1:A:1238:PHE:HE2	1:A:2223:LEU:HG	1.84	0.41
1:A:2248:PHE:O	1:A:2251:GLN:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:C	1:A:343:ASN:H	2.24	0.40
1:A:497:PHE:N	1:A:501:ASP:OD2	2.55	0.40
1:A:502:ILE:HA	1:A:505:ILE:HG22	2.03	0.40
1:A:663:TRP:HZ3	1:A:740:PHE:HD2	1.69	0.40
1:A:680:LEU:HB2	1:A:682:LEU:CD1	2.51	0.40
1:A:922:HIS:CE1	1:A:924:GLY:H	2.39	0.40
1:A:1350:LEU:O	1:A:1354:HIS:ND1	2.55	0.40
1:A:672:LYS:HE2	1:A:672:LYS:HB3	1.86	0.40
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.89	0.40
1:A:1405:LEU:HD23	1:A:1405:LEU:HA	1.86	0.40
1:A:1554:GLU:OE1	1:A:1557:TYR:OH	2.34	0.40
1:A:1819:ASN:HA	1:A:1823:LEU:HB2	2.02	0.40
1:A:2182:LEU:HD11	1:A:2206:LEU:HB3	2.04	0.40
1:A:2189:PHE:CE1	1:A:2222:LEU:HD21	2.57	0.40
1:A:578:VAL:HG13	1:A:603:TYR:HE1	1.86	0.40
1:A:596:ASP:N	1:A:600:ASP:OD2	2.28	0.40
1:A:633:TYR:HE2	1:A:1614:ASN:HD22	1.69	0.40
1:A:1582:ASP:O	1:A:1586:ILE:HG12	2.21	0.40
1:A:2183:ASN:HB3	1:A:2184:PRO:HD3	2.02	0.40
1:A:803:GLY:HA2	1:A:806:THR:HG22	2.04	0.40
1:A:1266:ASP:OD1	1:A:1267:THR:N	2.54	0.40
1:A:1470:ILE:H	1:A:1470:ILE:HD12	1.86	0.40
1:A:1844:GLY:HA2	1:A:1875:ILE:CD1	2.46	0.40
6:A:2308:POV:H25	6:A:2321:POV:C22	2.50	0.40
1:A:1053:HIS:CE1	1:A:1054:LYS:HG3	2.57	0.40
1:A:1443:ARG:HA	1:A:1449:TRP:CD1	2.56	0.40
1:A:1766:LEU:HD23	1:A:1766:LEU:HA	1.95	0.40
1:A:1928:ILE:HD13	1:A:1928:ILE:HA	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1923/2273 (85%)	1813 (94%)	109 (6%)	1 (0%)	51 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	492	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1656/1990 (83%)	1648 (100%)	8 (0%)	88 93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	499	TRP
1	A	992	ARG
1	A	1240	HIS
1	A	1529	ASN
1	A	1826	ASN
1	A	1896	VAL
1	A	1933	ASN
1	A	2202	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	HIS
1	A	1053	HIS
1	A	1214	HIS
1	A	1240	HIS
1	A	1472	GLN
1	A	1475	GLN
1	A	1621	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1826	ASN
1	A	2011	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	2,1	14,14,15	0.31	0	17,19,21	0.46	0
2	NAG	B	2	2	14,14,15	1.04	1 (7%)	17,19,21	2.02	1 (5%)
2	BMA	B	3	2	11,11,12	0.56	0	15,15,17	0.76	0
3	NAG	C	1	3,1	14,14,15	0.36	0	17,19,21	0.45	0
3	NAG	C	2	3	14,14,15	0.80	1 (7%)	17,19,21	1.34	1 (5%)
3	BMA	C	3	3	11,11,12	0.56	0	15,15,17	0.89	0
3	BMA	C	4	3	11,11,12	0.53	0	15,15,17	0.72	0
3	BMA	C	5	3	11,11,12	0.57	0	15,15,17	0.88	0

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2	2	-	1/6/23/26	0/1/1/1
2	BMA	B	3	2	-	0/2/19/22	0/1/1/1
3	NAG	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1
3	BMA	C	3	3	-	2/2/19/22	0/1/1/1
3	BMA	C	4	3	-	0/2/19/22	0/1/1/1
3	BMA	C	5	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	3.62	1.49	1.43
3	C	2	NAG	O5-C1	2.87	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	NAG	C1-O5-C5	7.70	122.63	112.19
3	C	2	NAG	C1-O5-C5	5.06	119.05	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

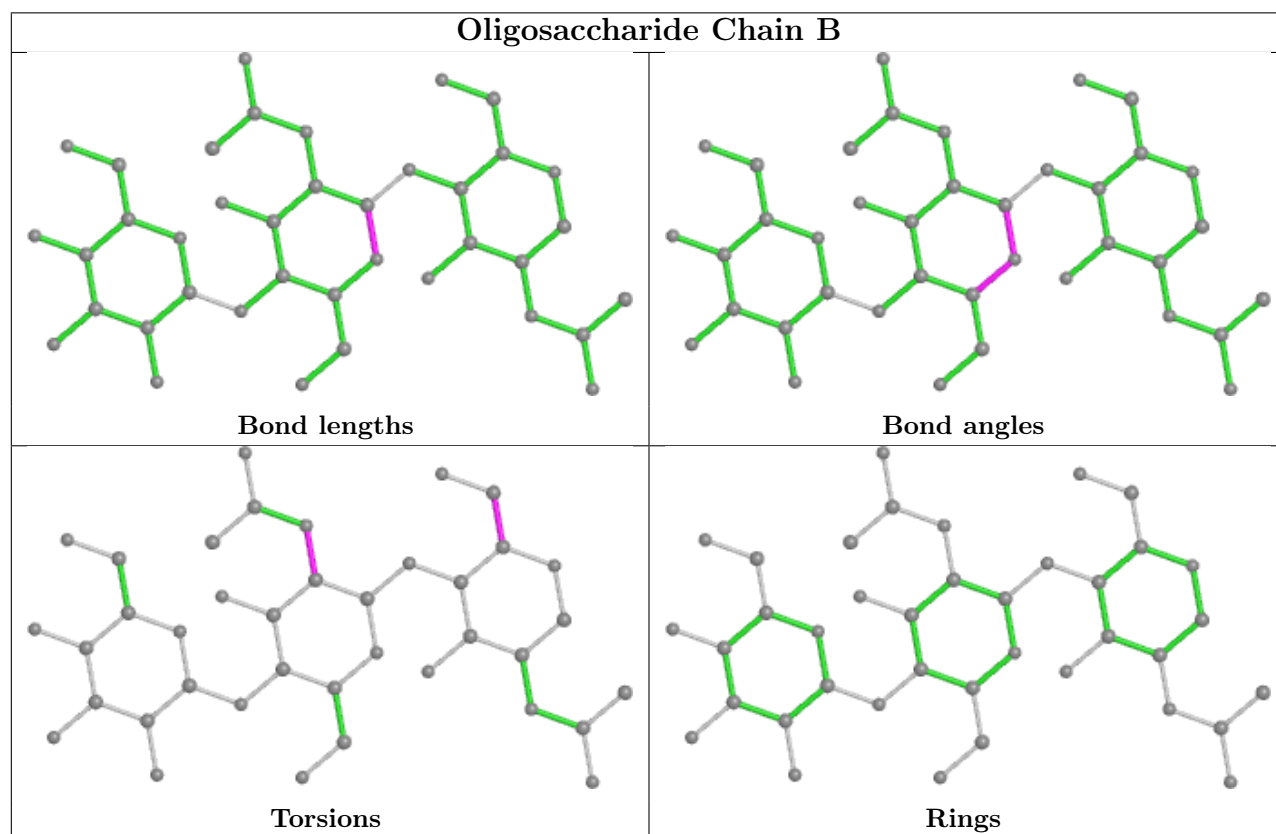
Mol	Chain	Res	Type	Atoms
3	C	3	BMA	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C1-C2-N2-C7
3	C	2	NAG	O5-C5-C6-O6
3	C	3	BMA	C4-C5-C6-O6
2	B	1	NAG	C4-C5-C6-O6
2	B	2	NAG	C3-C2-N2-C7
3	C	1	NAG	C3-C2-N2-C7
3	C	2	NAG	C3-C2-N2-C7

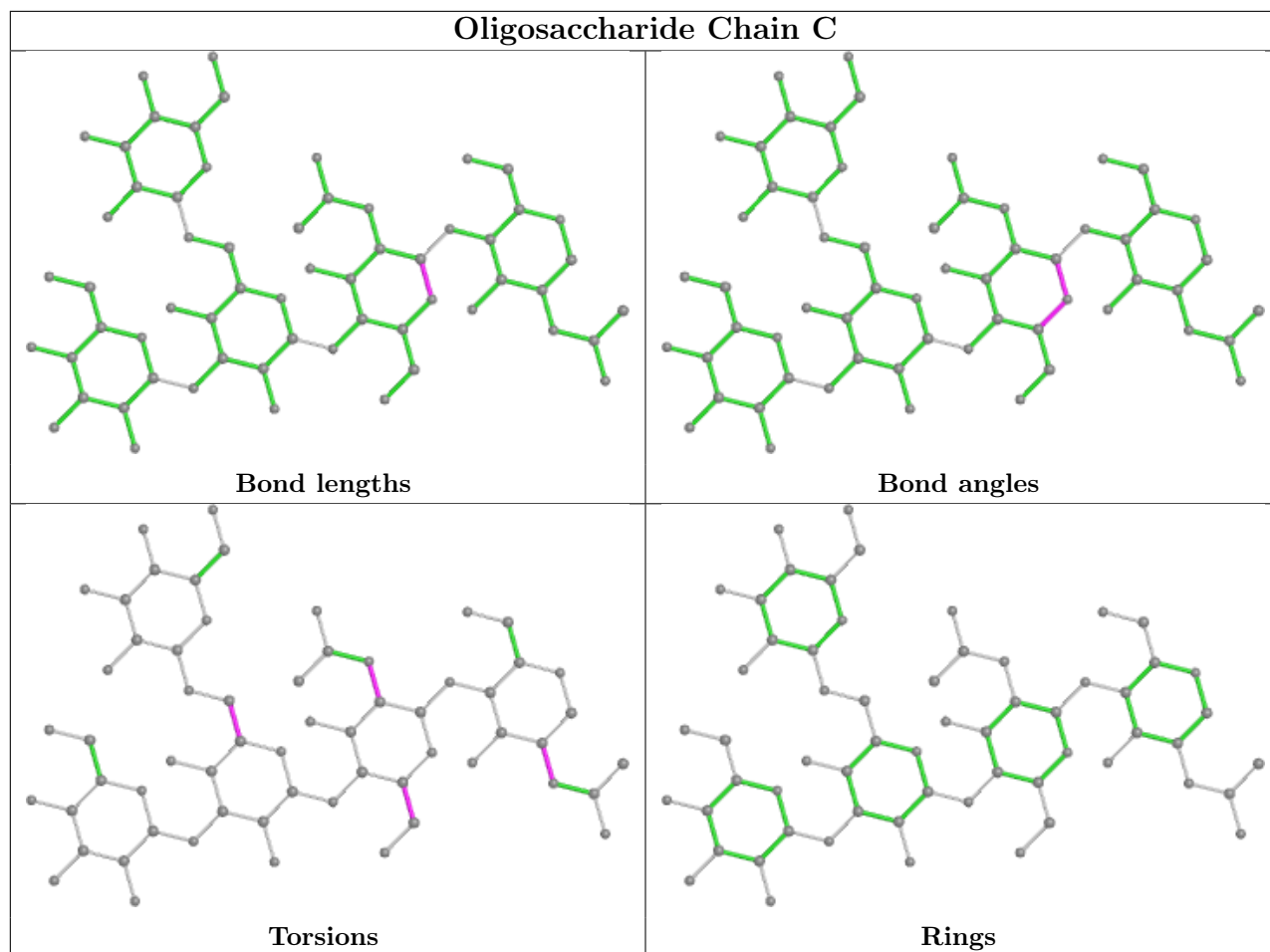
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	NAG	1	0

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





5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	CLR	A	2314	-	31,31,31	0.31	0	48,48,48	0.49	0
6	POV	A	2317	-	14,14,51	0.97	1 (7%)	13,13,59	1.12	2 (15%)
4	NAG	A	2301	1	14,14,15	0.20	0	17,19,21	0.38	0
5	CLR	A	2312	-	31,31,31	0.29	0	48,48,48	0.42	0
5	CLR	A	2309	-	31,31,31	0.29	0	48,48,48	0.52	0
5	CLR	A	2311	-	23,23,31	0.48	0	37,37,48	1.27	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2302	1	14,14,15	0.56	0	17,19,21	0.54	0
6	POV	A	2321	-	10,10,51	0.25	0	9,9,59	0.30	0
6	POV	A	2320	-	10,10,51	0.29	0	9,9,59	0.83	0
4	NAG	A	2303	1	14,14,15	0.36	0	17,19,21	0.36	0
4	NAG	A	2306	1	14,14,15	0.53	0	17,19,21	1.58	4 (23%)
4	NAG	A	2305	1	14,14,15	0.23	0	17,19,21	0.34	0
5	CLR	A	2315	-	24,24,31	0.35	0	37,39,48	0.61	1 (2%)
6	POV	A	2318	-	17,17,51	0.32	0	16,16,59	0.79	0
4	NAG	A	2304	1	14,14,15	0.26	0	17,19,21	0.51	0
6	POV	A	2308	-	8,8,51	0.43	0	7,7,59	0.86	0
7	AJP	A	2310	-	83,83,95	0.34	0	125,131,149	0.96	6 (4%)
5	CLR	A	2313	-	24,24,31	0.36	0	37,39,48	0.57	1 (2%)
5	CLR	A	2307	-	31,31,31	0.30	0	48,48,48	0.49	0
6	POV	A	2319	-	9,9,51	0.40	0	8,8,59	0.90	0
6	POV	A	2316	-	8,8,51	0.30	0	7,7,59	0.72	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	A	2314	-	-	6/10/68/68	0/4/4/4
6	POV	A	2317	-	-	7/12/12/55	-
4	NAG	A	2301	1	-	4/6/23/26	0/1/1/1
5	CLR	A	2312	-	-	0/10/68/68	0/4/4/4
5	CLR	A	2309	-	-	1/10/68/68	0/4/4/4
5	CLR	A	2311	-	-	-	0/4/4/4
4	NAG	A	2302	1	-	4/6/23/26	0/1/1/1
6	POV	A	2321	-	-	3/8/8/55	-
6	POV	A	2320	-	-	7/8/8/55	-
4	NAG	A	2303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2306	1	-	5/6/23/26	0/1/1/1
4	NAG	A	2305	1	-	1/6/23/26	0/1/1/1
5	CLR	A	2315	-	-	-	0/4/4/4
6	POV	A	2318	-	-	8/15/15/55	-
4	NAG	A	2304	1	-	4/6/23/26	0/1/1/1
6	POV	A	2308	-	-	1/6/6/55	-
7	AJP	A	2310	-	29/29/33/38	15/22/194/220	0/10/10/11

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLR	A	2313	-	-	-	0/4/4/4
5	CLR	A	2307	-	-	3/10/68/68	0/4/4/4
6	POV	A	2319	-	-	1/7/7/55	-
6	POV	A	2316	-	-	2/6/6/55	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2317	POV	C29-C210	3.53	1.52	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	2310	AJP	C12-C07-C08	-4.61	99.90	104.88
4	A	2306	NAG	C2-N2-C7	4.45	129.24	122.90
7	A	2310	AJP	O09-C08-C10	3.92	118.24	110.17
5	A	2311	CLR	C11-C9-C10	3.26	117.38	113.08
5	A	2311	CLR	C14-C8-C9	-3.18	104.84	109.09
7	A	2310	AJP	C26-O25-C23	3.01	119.99	115.33
5	A	2311	CLR	C16-C15-C14	-2.88	100.11	104.71
5	A	2311	CLR	C15-C14-C8	2.57	123.31	119.08
4	A	2306	NAG	C1-O5-C5	2.55	115.64	112.19
5	A	2315	CLR	C20-C17-C13	2.55	120.80	115.89
5	A	2311	CLR	C7-C8-C14	2.49	114.51	110.91
4	A	2306	NAG	C1-C2-N2	2.42	114.62	110.49
7	A	2310	AJP	C06-C07-C08	-2.41	99.96	104.34
4	A	2306	NAG	C3-C4-C5	2.35	114.44	110.24
7	A	2310	AJP	O09-C08-C07	-2.34	98.45	104.06
5	A	2313	CLR	C20-C17-C13	2.34	120.40	115.89
6	A	2317	POV	C211-C210-C29	-2.13	108.42	124.73
6	A	2317	POV	C28-C29-C210	-2.11	108.50	124.73
7	A	2310	AJP	C13-C12-C07	2.05	118.74	115.46

All (29) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	2310	AJP	C39
7	A	2310	AJP	C26
7	A	2310	AJP	C10
7	A	2310	AJP	C28
7	A	2310	AJP	C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
7	A	2310	AJP	C15
7	A	2310	AJP	C22
7	A	2310	AJP	C36
7	A	2310	AJP	C35
7	A	2310	AJP	C05
7	A	2310	AJP	C56
7	A	2310	AJP	C19
7	A	2310	AJP	C59
7	A	2310	AJP	C07
7	A	2310	AJP	C30
7	A	2310	AJP	C57
7	A	2310	AJP	C02
7	A	2310	AJP	C23
7	A	2310	AJP	C47
7	A	2310	AJP	C11
7	A	2310	AJP	C37
7	A	2310	AJP	C55
7	A	2310	AJP	C46
7	A	2310	AJP	C20
7	A	2310	AJP	C12
7	A	2310	AJP	C48
7	A	2310	AJP	C38
7	A	2310	AJP	C45
7	A	2310	AJP	C16

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2310	AJP	C35-C36-O54-C55
7	A	2310	AJP	O60-C55-O54-C36
7	A	2310	AJP	C56-C55-O54-C36
4	A	2302	NAG	C4-C5-C6-O6
4	A	2302	NAG	O5-C5-C6-O6
7	A	2310	AJP	O31-C26-O25-C23
4	A	2306	NAG	C4-C5-C6-O6
7	A	2310	AJP	C27-C26-O25-C23
4	A	2304	NAG	O5-C5-C6-O6
4	A	2301	NAG	O5-C5-C6-O6
4	A	2306	NAG	O5-C5-C6-O6
7	A	2310	AJP	C30-C29-O34-C35
7	A	2310	AJP	C36-C37-O44-C45
4	A	2301	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	2301	NAG	O7-C7-N2-C2
4	A	2302	NAG	C8-C7-N2-C2
4	A	2302	NAG	O7-C7-N2-C2
4	A	2303	NAG	C8-C7-N2-C2
4	A	2303	NAG	O7-C7-N2-C2
4	A	2304	NAG	C8-C7-N2-C2
4	A	2304	NAG	O7-C7-N2-C2
4	A	2306	NAG	C8-C7-N2-C2
4	A	2306	NAG	O7-C7-N2-C2
5	A	2307	CLR	C17-C20-C22-C23
4	A	2301	NAG	C4-C5-C6-O6
5	A	2307	CLR	C21-C20-C22-C23
6	A	2317	POV	C211-C212-C213-C214
5	A	2309	CLR	C21-C20-C22-C23
7	A	2310	AJP	C38-C37-O44-C45
6	A	2317	POV	C25-C26-C27-C28
6	A	2318	POV	C211-C212-C213-C214
7	A	2310	AJP	C28-C29-O34-C35
6	A	2318	POV	C23-C24-C25-C26
6	A	2318	POV	C22-C23-C24-C25
7	A	2310	AJP	C37-C36-O54-C55
4	A	2304	NAG	C4-C5-C6-O6
6	A	2317	POV	C26-C27-C28-C29
6	A	2318	POV	C26-C27-C28-C29
6	A	2317	POV	C213-C214-C215-C216
5	A	2314	CLR	C13-C17-C20-C21
7	A	2310	AJP	O50-C45-O44-C37
6	A	2319	POV	C24-C25-C26-C27
7	A	2310	AJP	O40-C39-C41-O42
4	A	2305	NAG	O5-C5-C6-O6
7	A	2310	AJP	O60-C59-C61-O62
6	A	2317	POV	C210-C211-C212-C213
6	A	2316	POV	C35-C36-C37-C38
5	A	2314	CLR	C21-C20-C22-C23
6	A	2320	POV	C311-C312-C313-C314
6	A	2320	POV	C34-C35-C36-C37
6	A	2321	POV	C25-C26-C27-C28
6	A	2316	POV	C31-C32-C33-C34
6	A	2320	POV	C39-C310-C311-C312
6	A	2320	POV	C36-C37-C38-C39
6	A	2320	POV	C35-C36-C37-C38
6	A	2318	POV	C215-C216-C217-C218

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	2320	POV	C311-C310-C39-C38
5	A	2314	CLR	C16-C17-C20-C22
6	A	2321	POV	C24-C25-C26-C27
5	A	2314	CLR	C17-C20-C22-C23
6	A	2320	POV	C37-C38-C39-C310
6	A	2318	POV	C214-C215-C216-C217
6	A	2318	POV	C21-C22-C23-C24
4	A	2306	NAG	C3-C2-N2-C7
5	A	2314	CLR	C20-C22-C23-C24
6	A	2317	POV	C29-C210-C211-C212
6	A	2318	POV	C25-C26-C27-C28
6	A	2308	POV	C27-C28-C29-C210
5	A	2314	CLR	C13-C17-C20-C22
7	A	2310	AJP	C46-C45-O44-C37
6	A	2321	POV	C21-C22-C23-C24
7	A	2310	AJP	C22-C23-O25-C26
6	A	2317	POV	C24-C25-C26-C27
5	A	2307	CLR	C16-C17-C20-C22

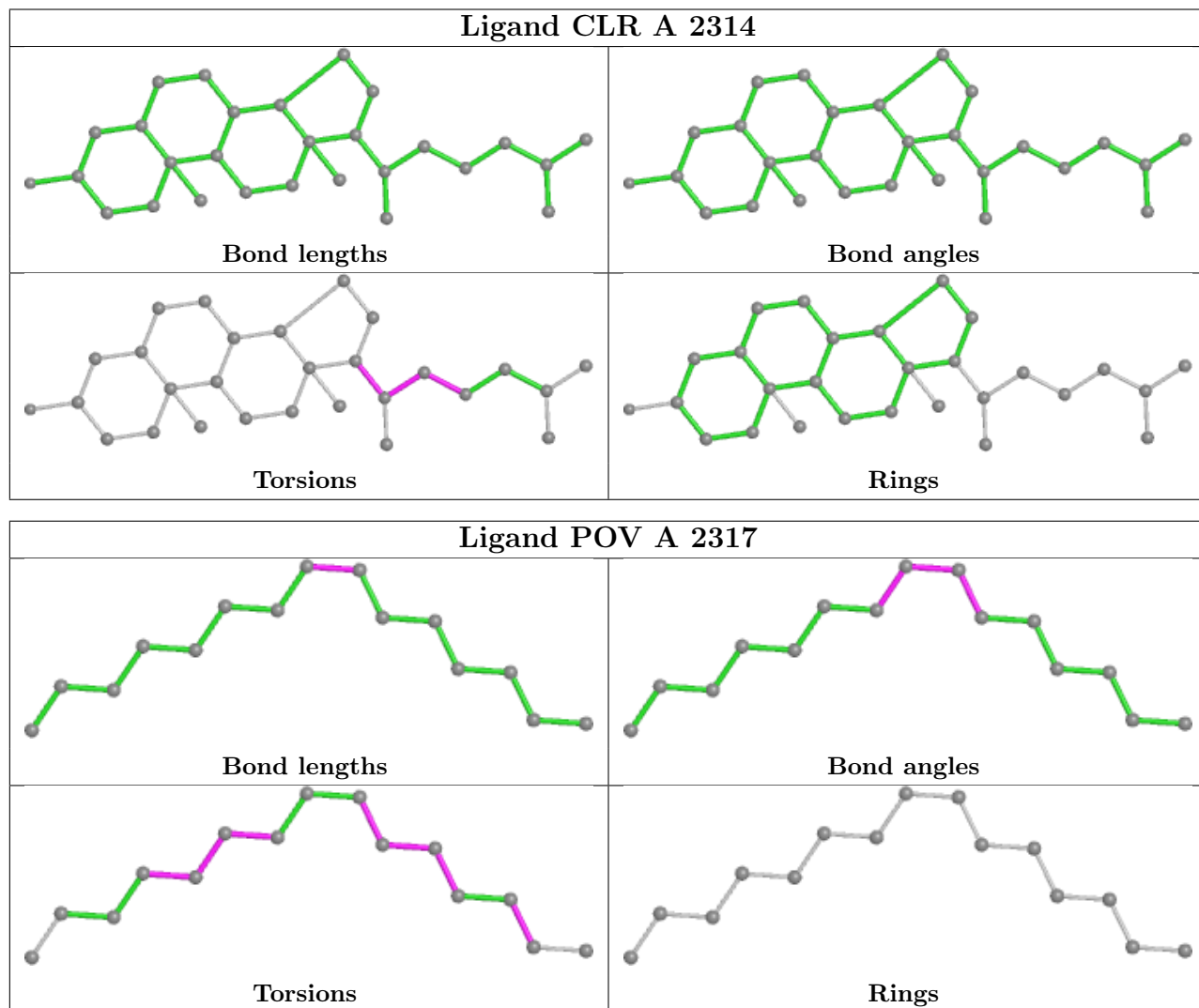
There are no ring outliers.

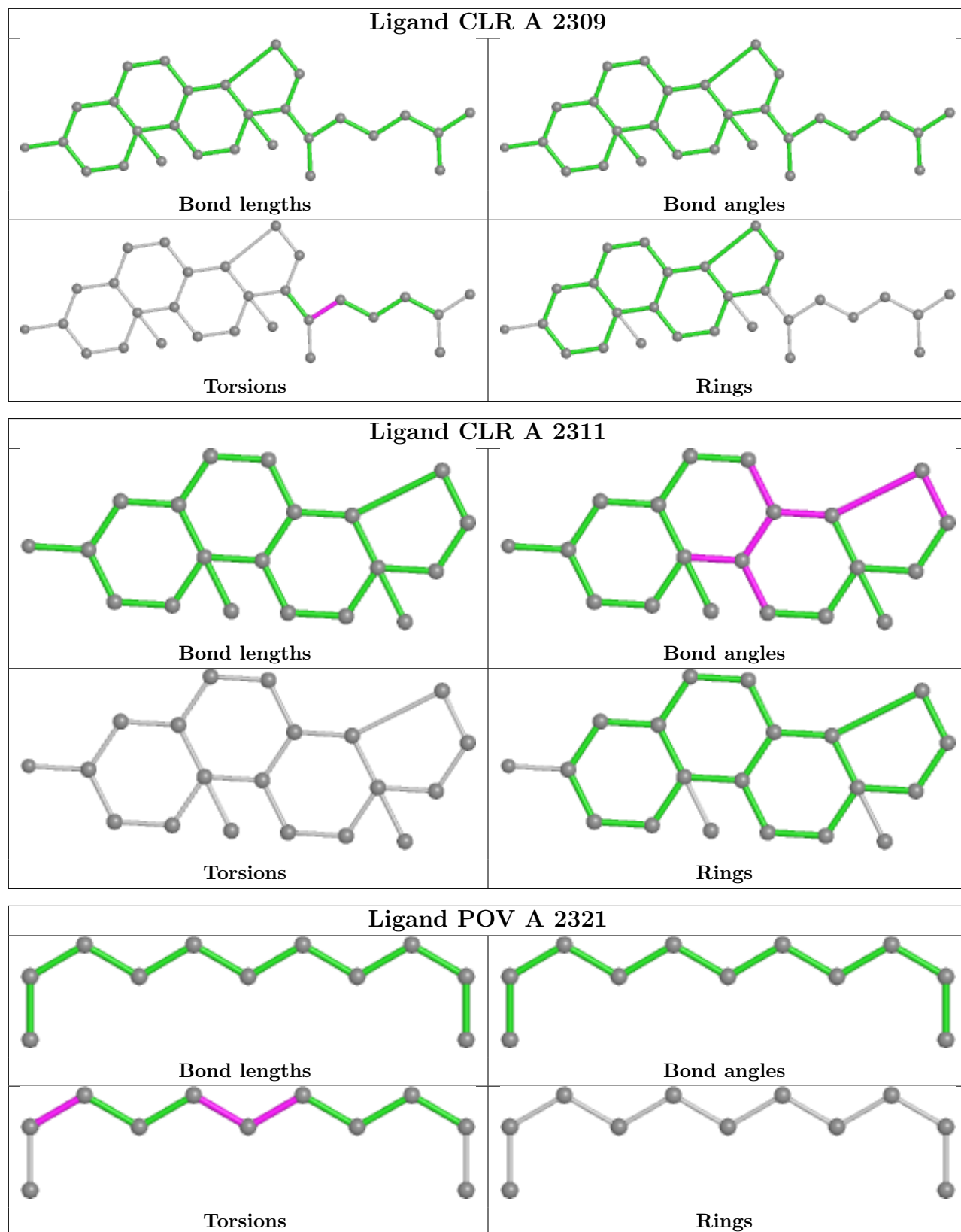
14 monomers are involved in 105 short contacts:

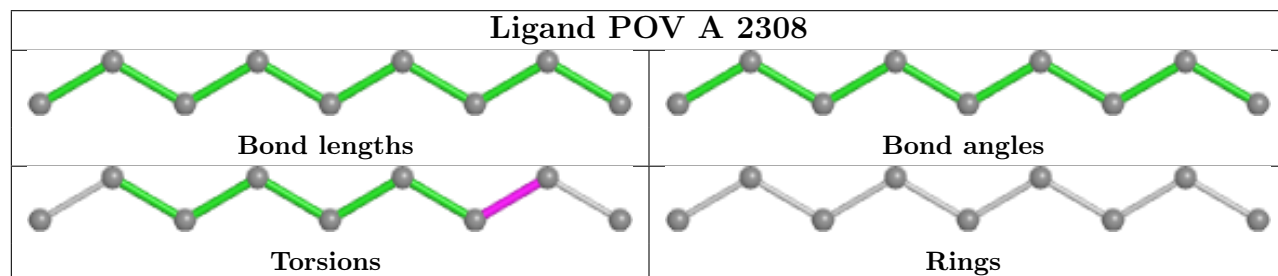
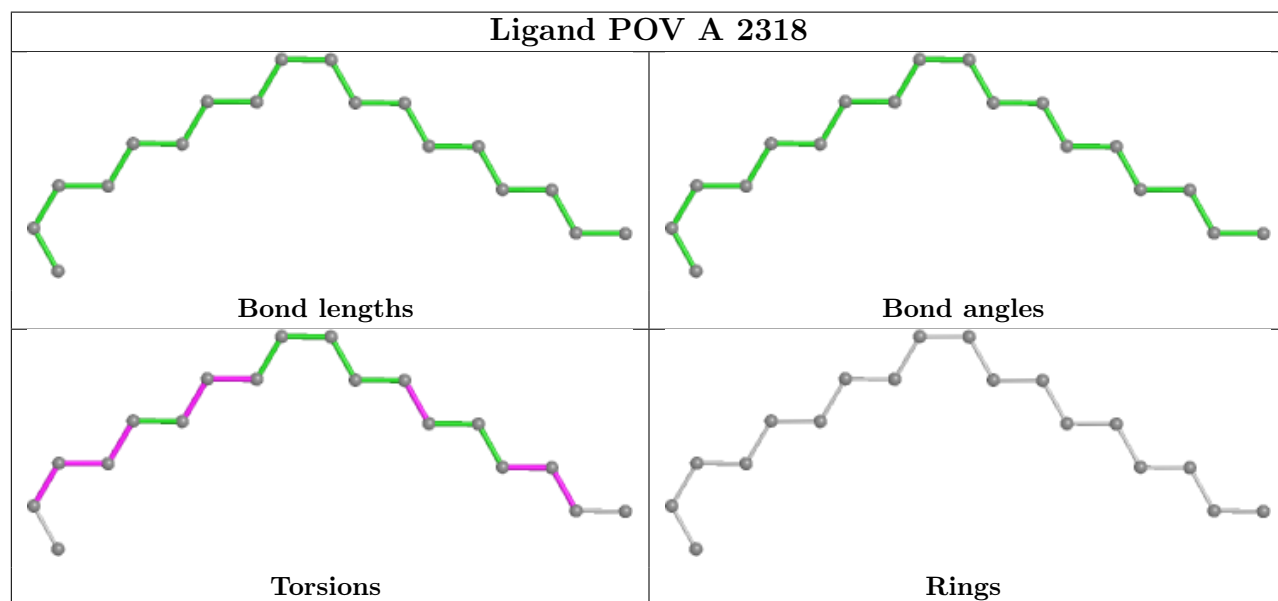
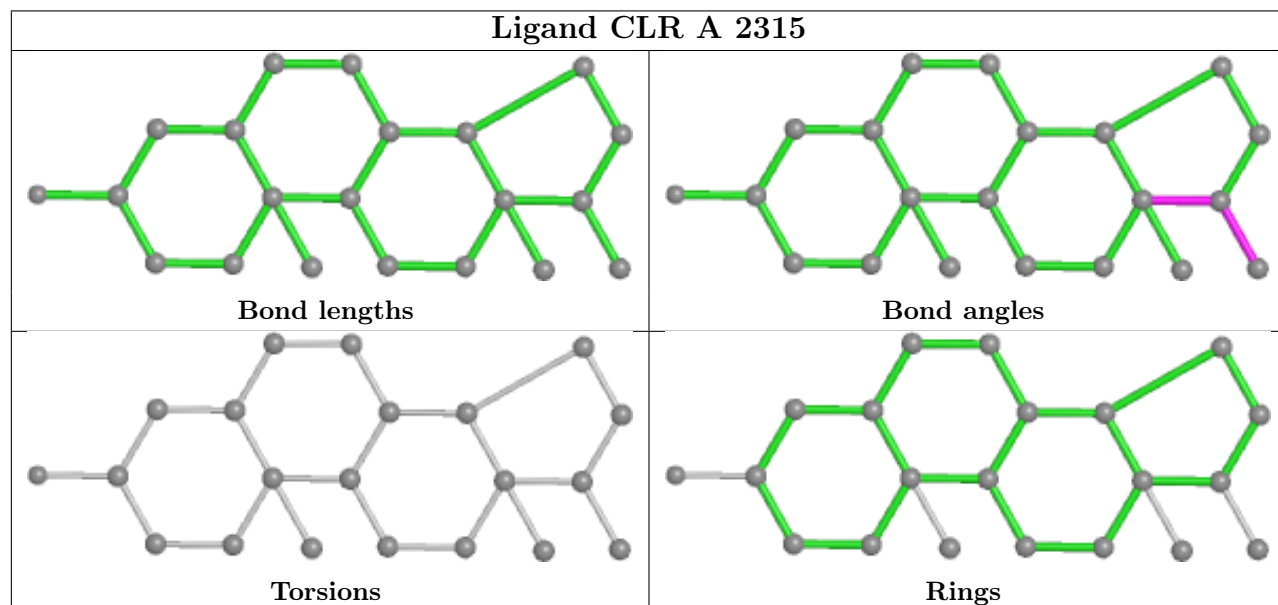
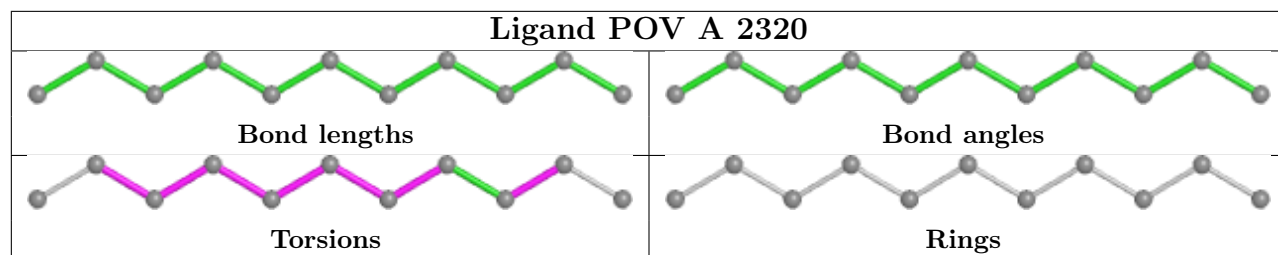
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2314	CLR	7	0
6	A	2317	POV	2	0
5	A	2312	CLR	11	0
5	A	2309	CLR	16	0
5	A	2311	CLR	10	0
4	A	2302	NAG	1	0
6	A	2321	POV	2	0
4	A	2306	NAG	1	0
6	A	2318	POV	1	0
6	A	2308	POV	2	0
7	A	2310	AJP	9	0
5	A	2313	CLR	4	0
5	A	2307	CLR	42	0
6	A	2316	POV	2	0

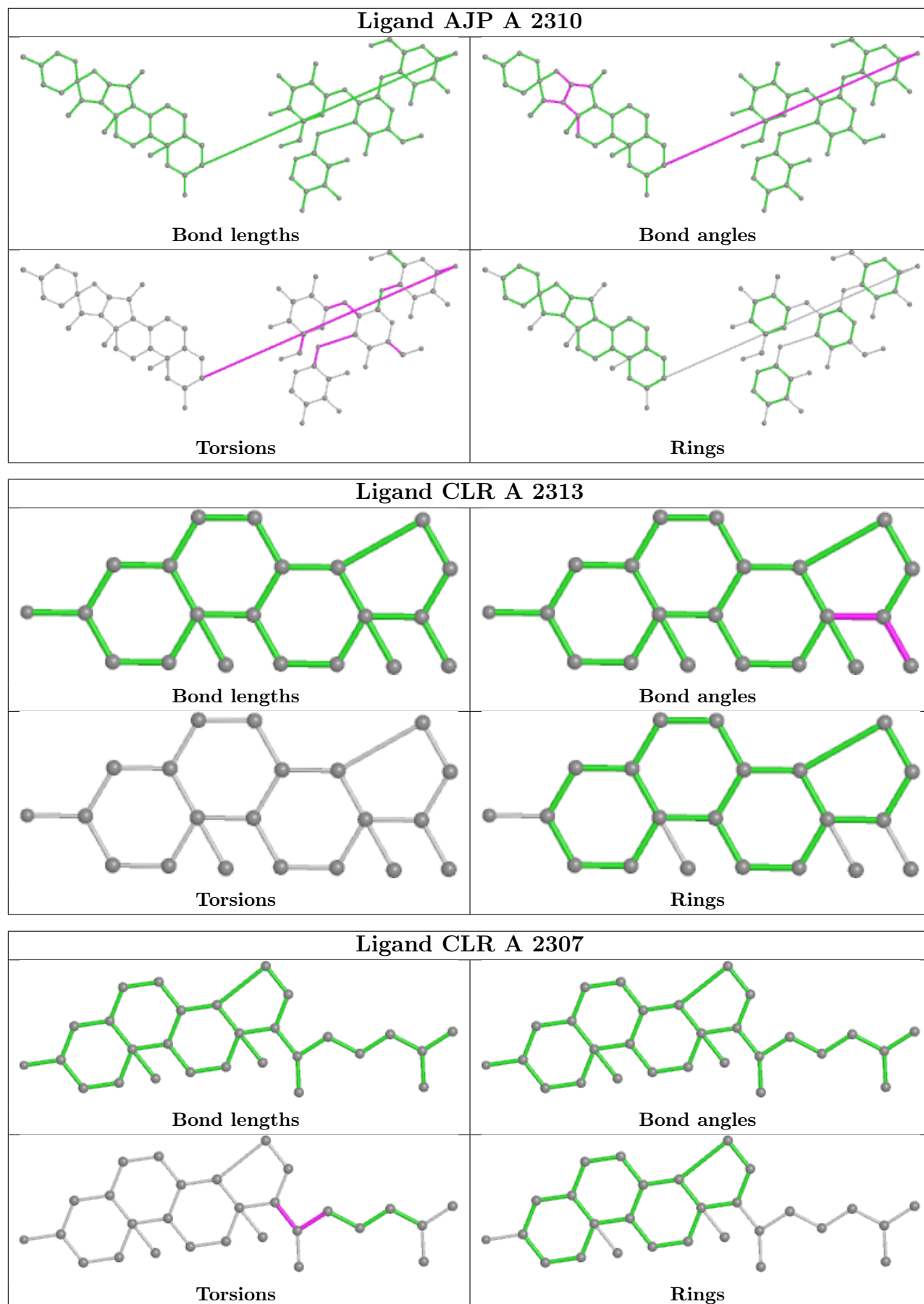
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

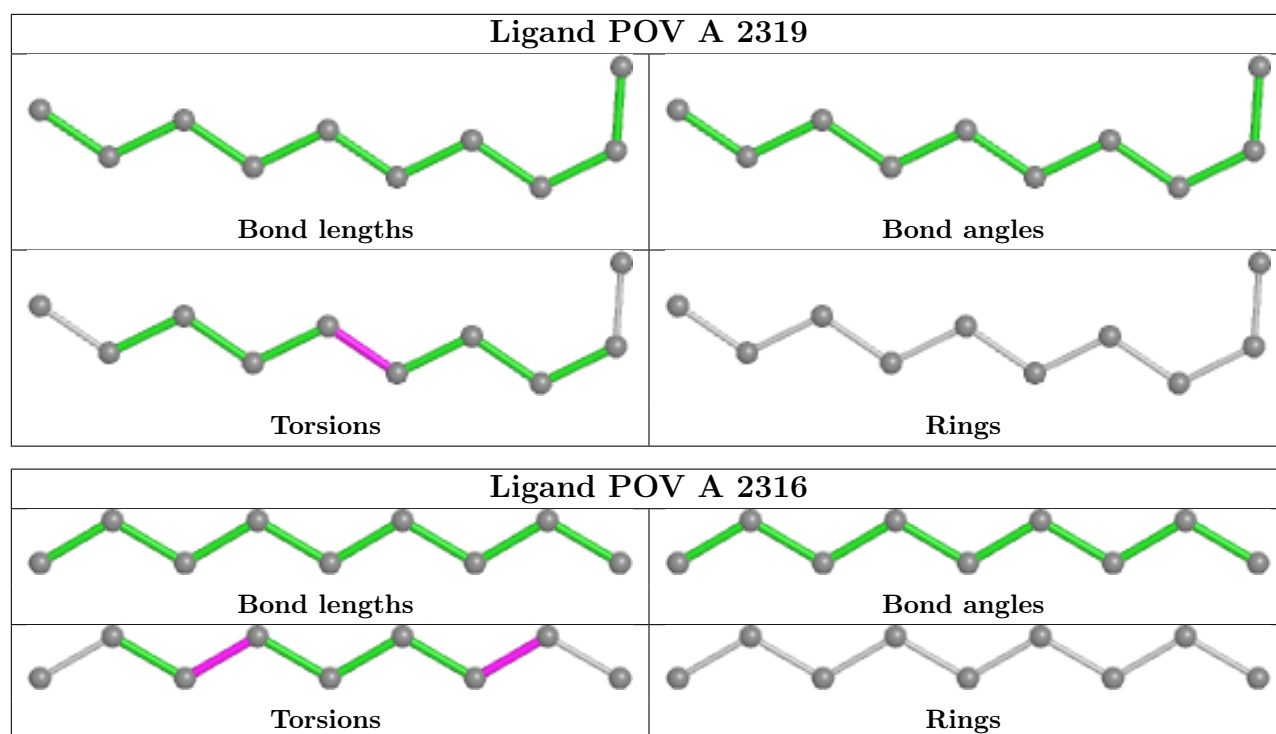
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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 [\(i\)](#)

There are no chain breaks in this entry.

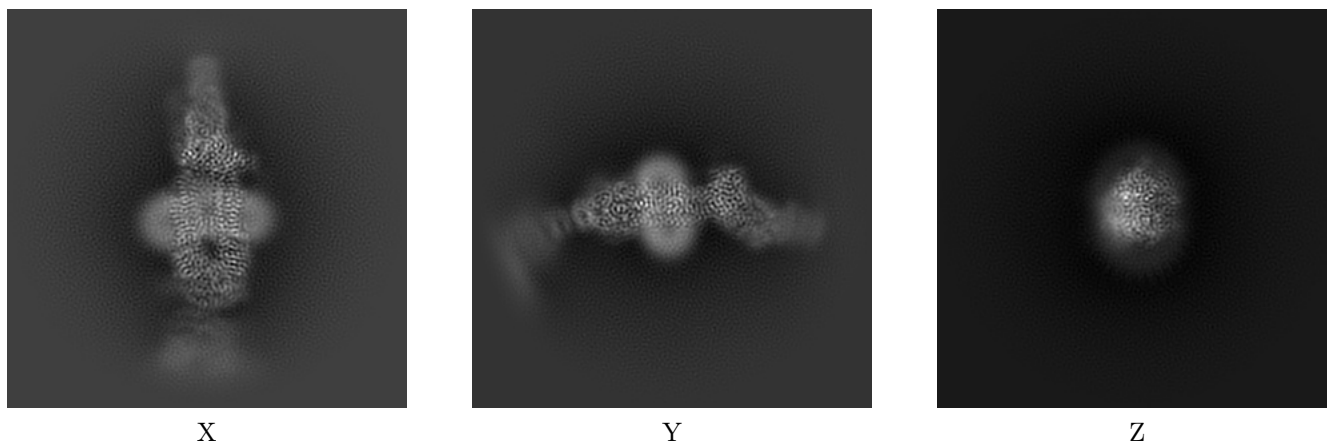
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23409. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

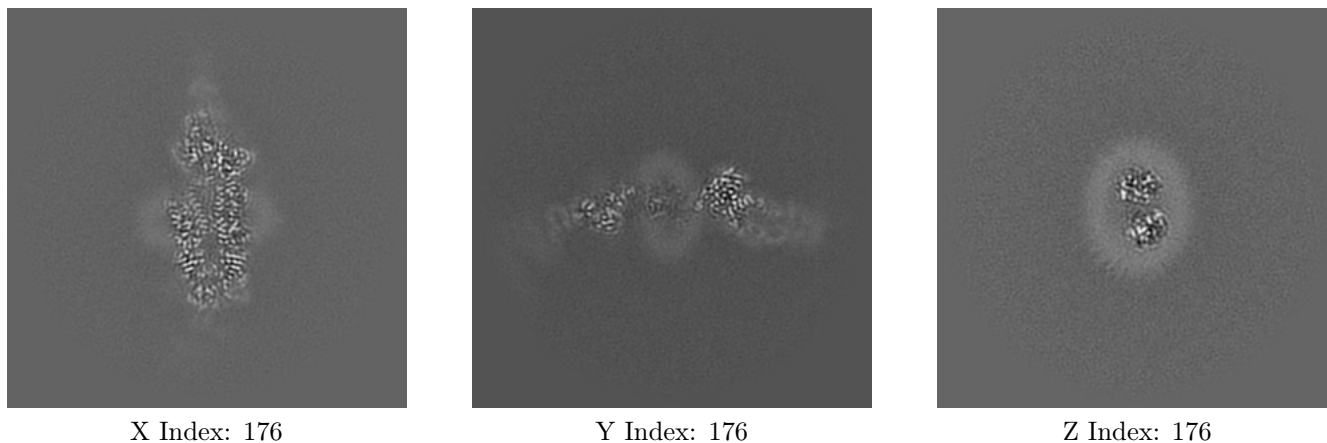
6.1.1 Primary map



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

6.2 Central slices [i](#)

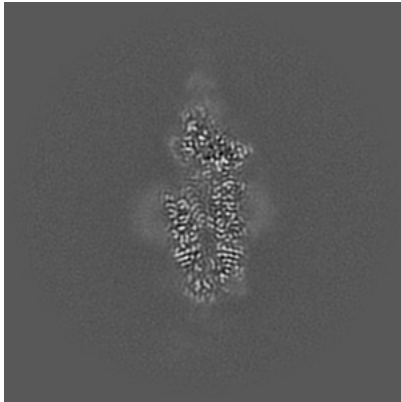
6.2.1 Primary map



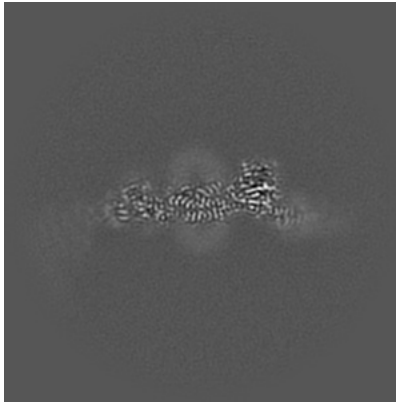
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

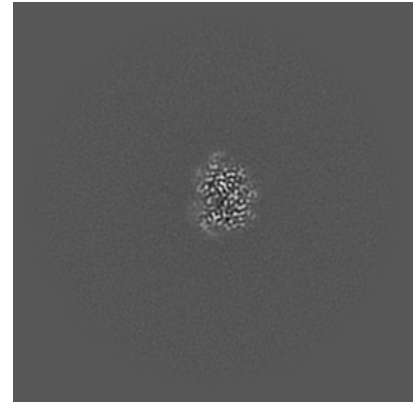
6.3.1 Primary map



X Index: 177



Y Index: 187



Z Index: 222

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

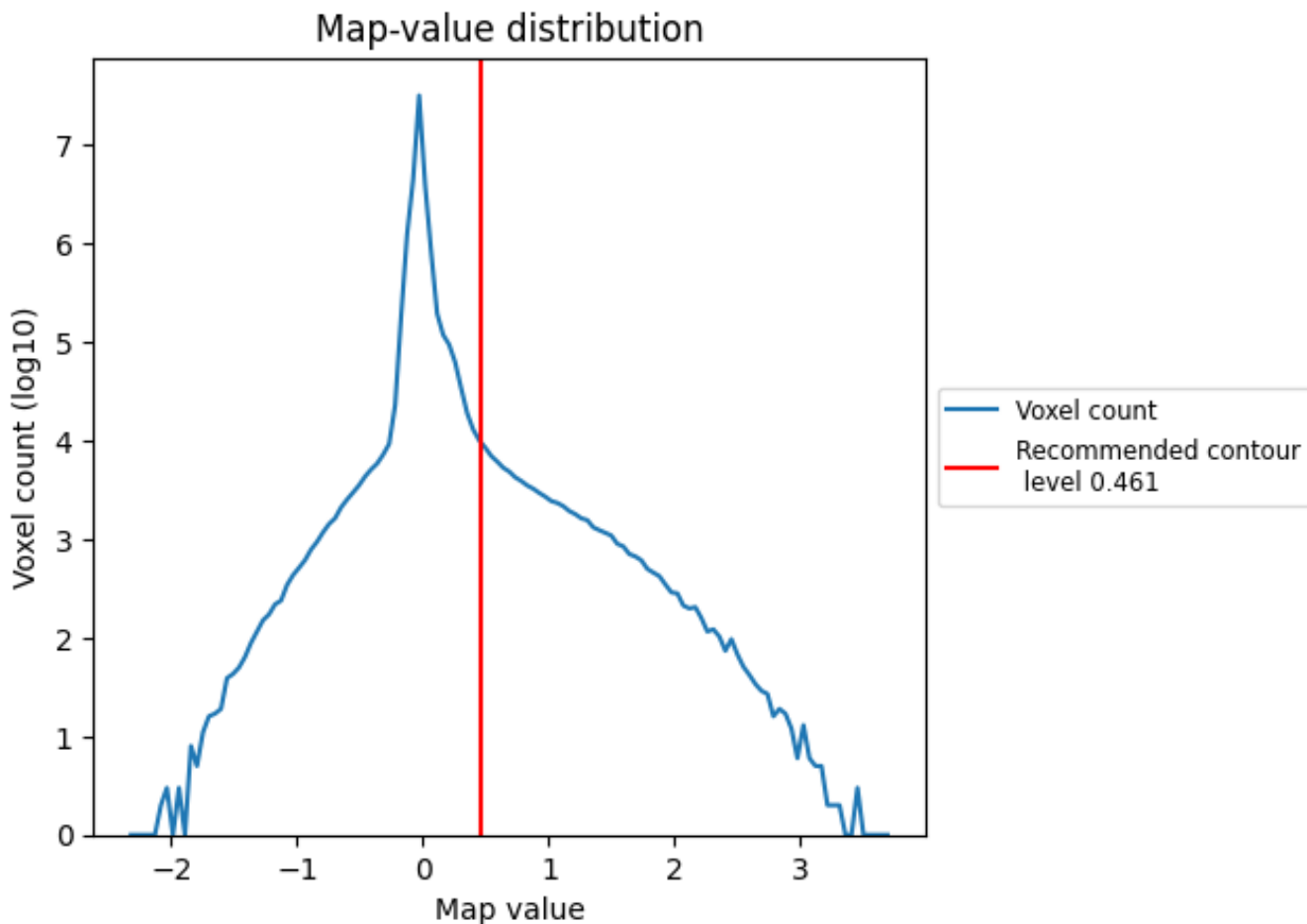
6.5 Mask visualisation

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

7 Map analysis [i](#)

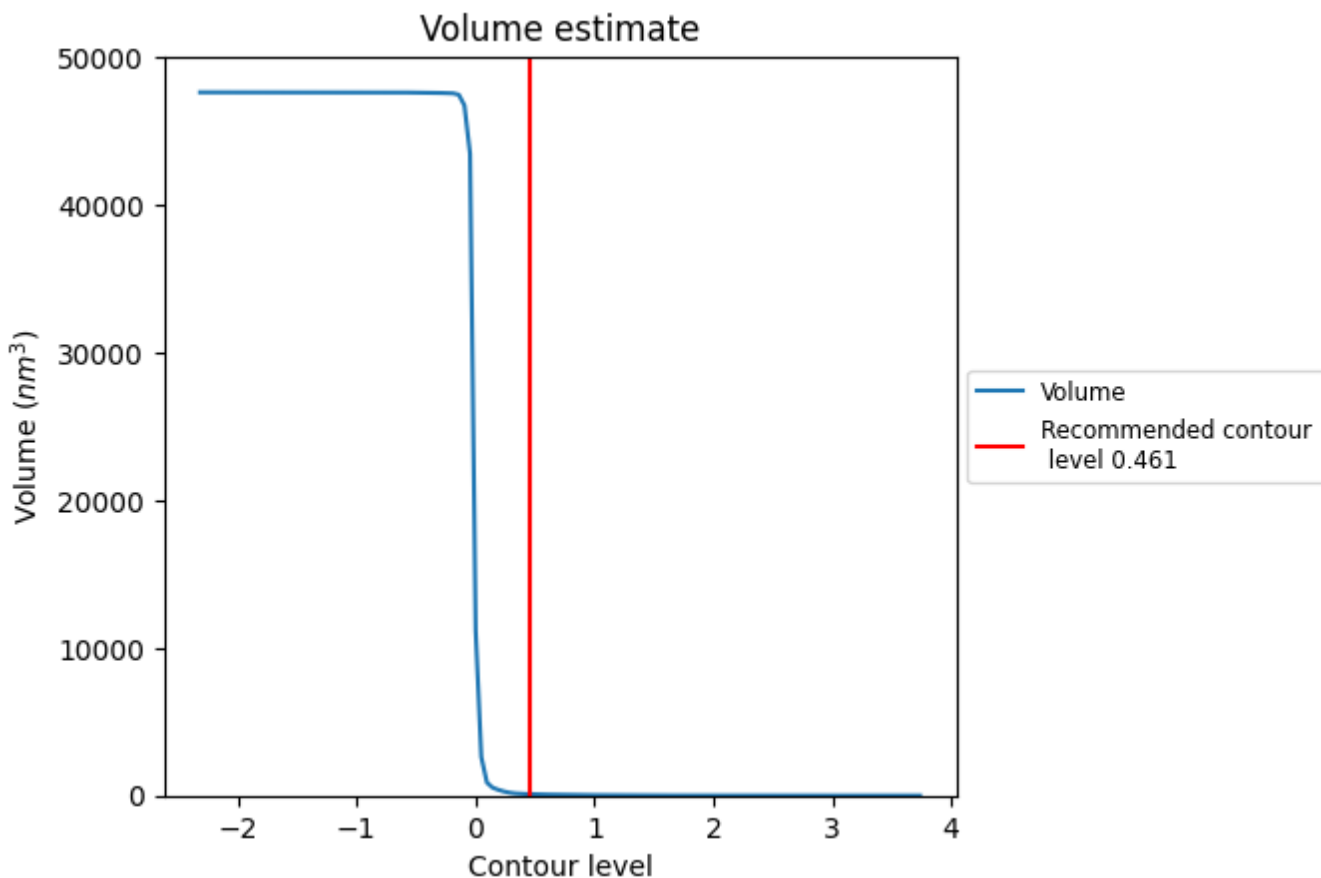
This section contains the results of statistical analysis of the map.

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.

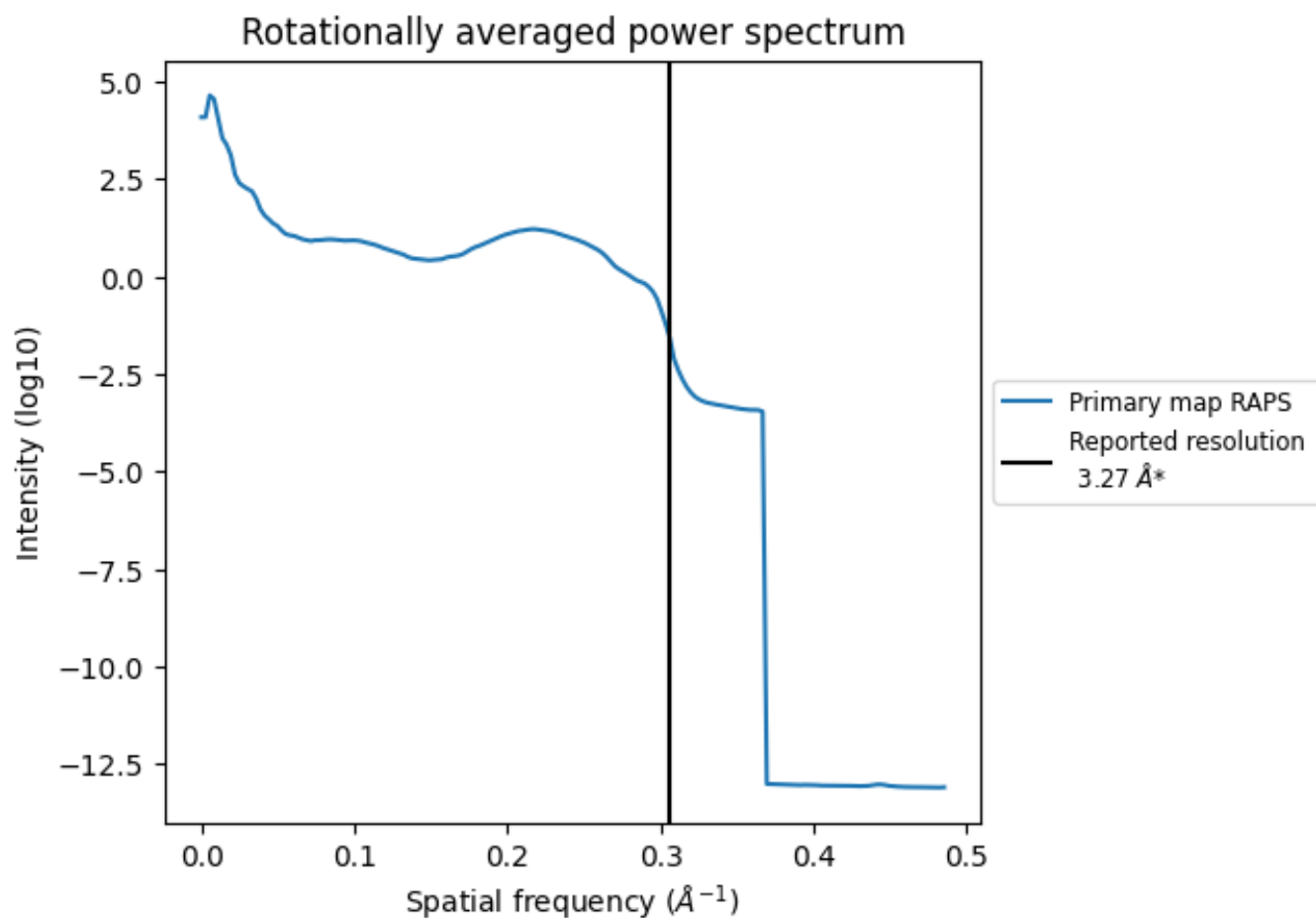
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 95 nm³; this corresponds to an approximate mass of 85 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.306\AA^{-1}

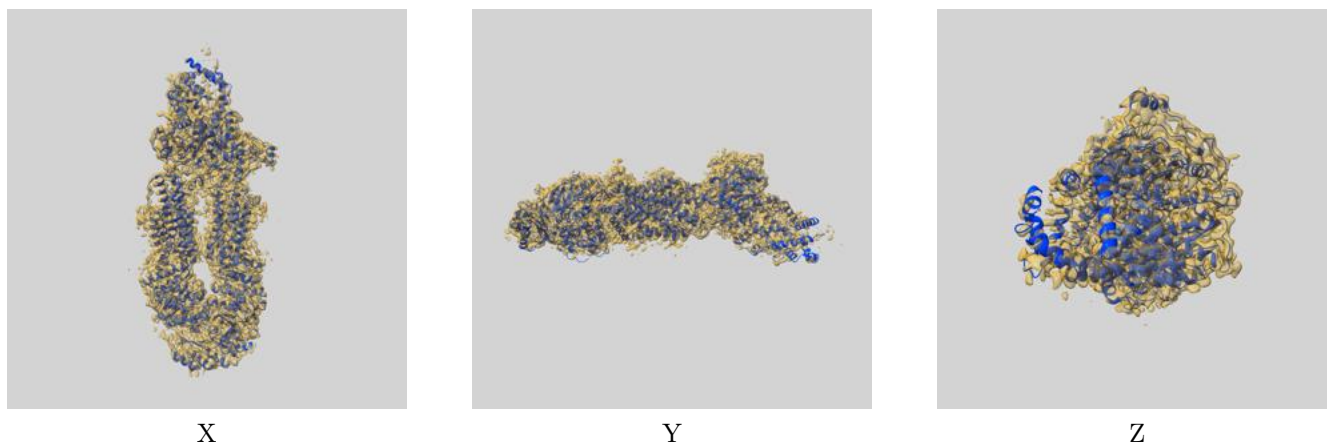
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

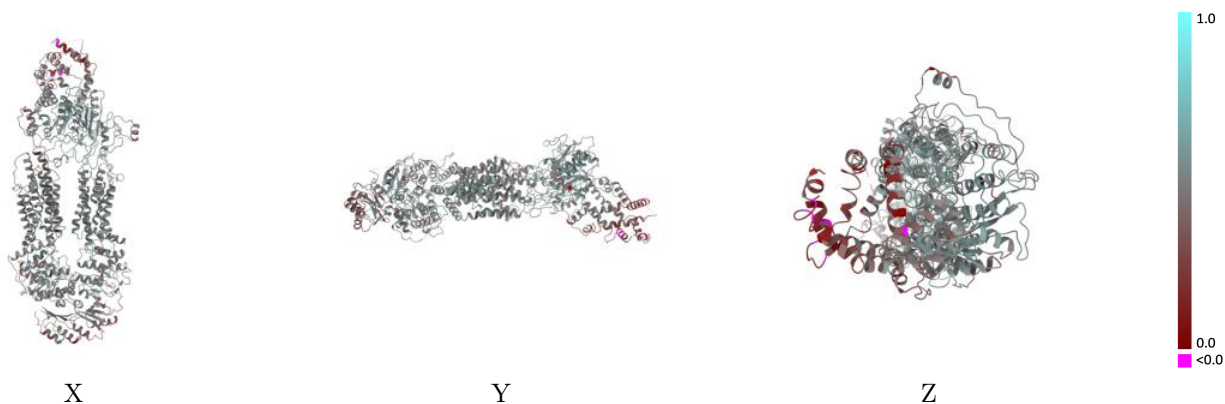
This section contains information regarding the fit between EMDB map EMD-23409 and PDB model 7LKP. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



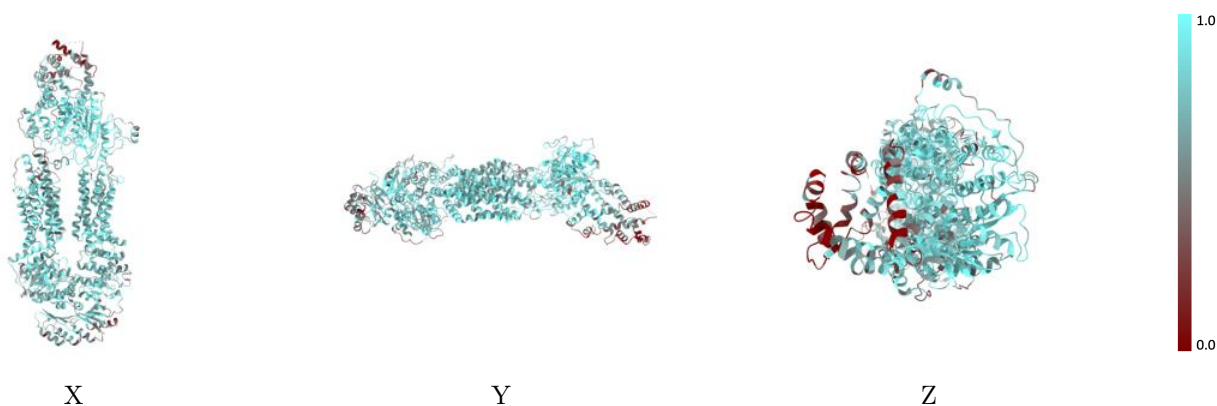
The images above show the 3D surface view of the map at the recommended contour level 0.461 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



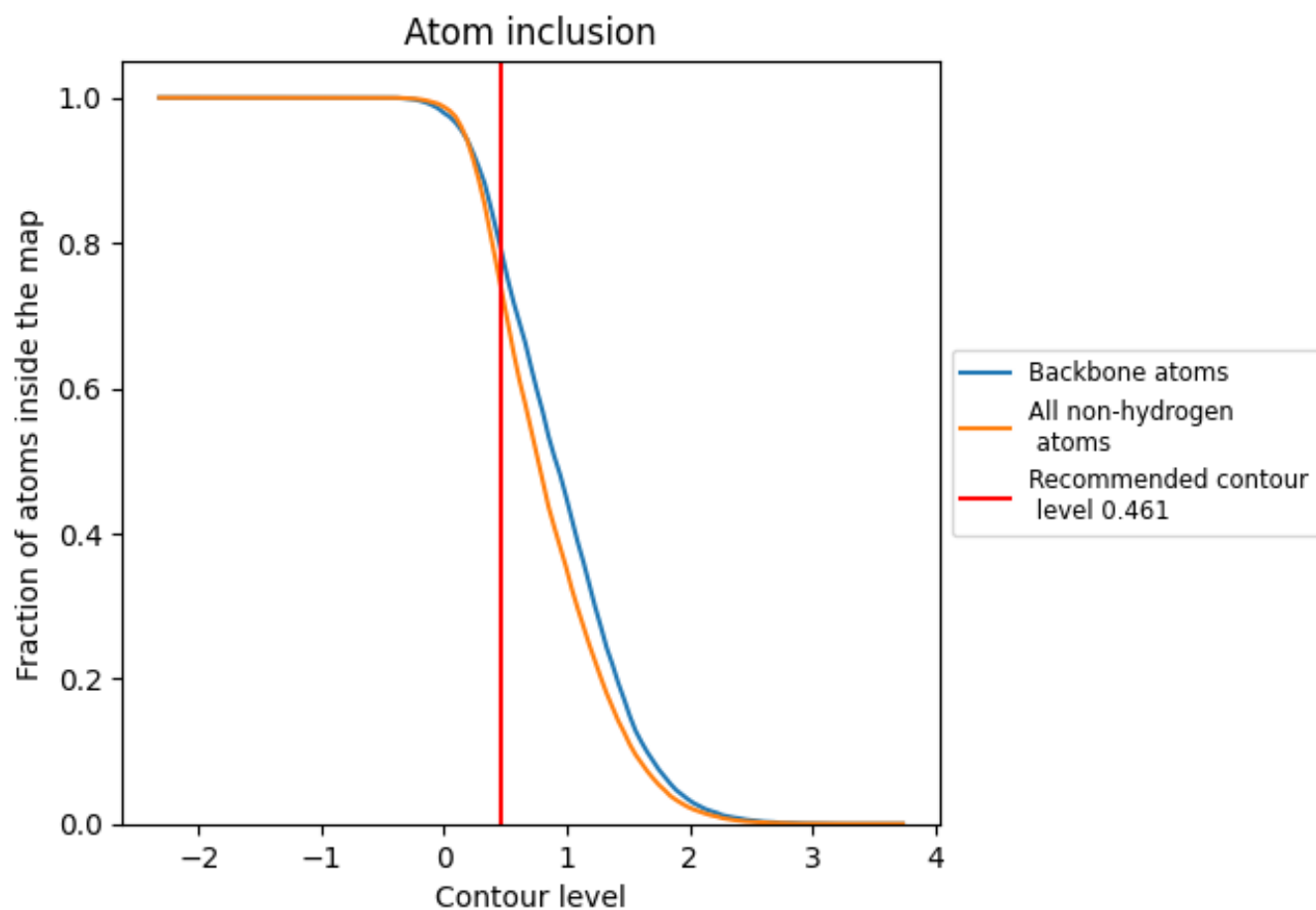
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.461).








9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 74% 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 (0.461) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7411	 0.4770
A	 0.7409	 0.4770
B	 0.7692	 0.4810
C	 0.7705	 0.4710

