



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 05:11 PM JST

PDB ID : 4WW3
Title : Crystal structure of the lumi intermediate of squid rhodopsin
Authors : Murakami, M.; Kouyama, T.
Deposited on : 2014-11-10
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

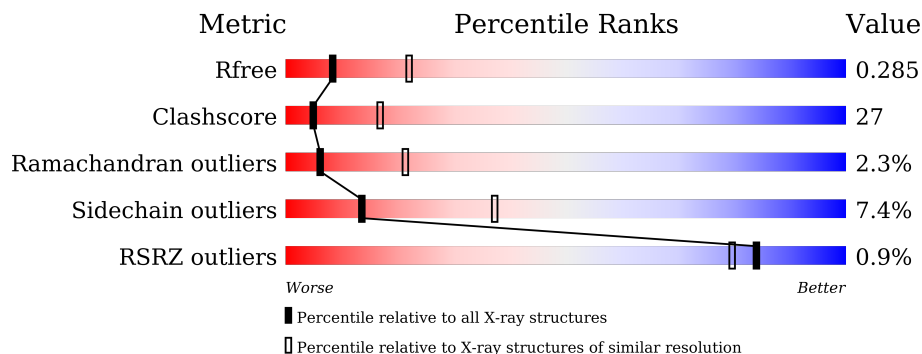
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	350	
1	B	350	

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
4	TWT	A	404	-	-	-	X

2 Entry composition [i](#)

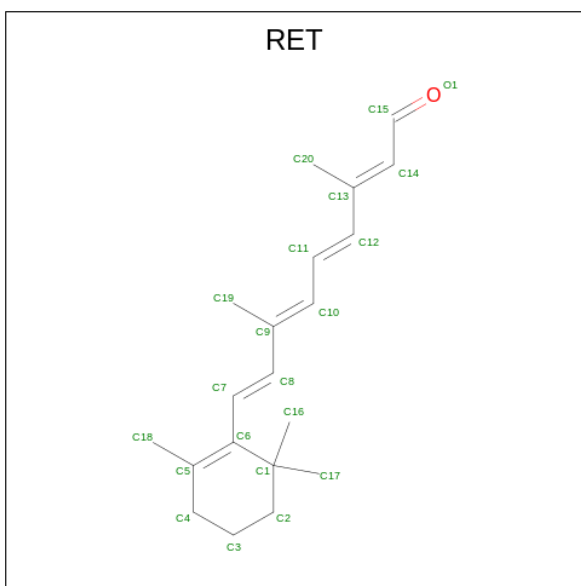
There are 8 unique types of molecules in this entry. The entry contains 5838 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Rhodopsin.

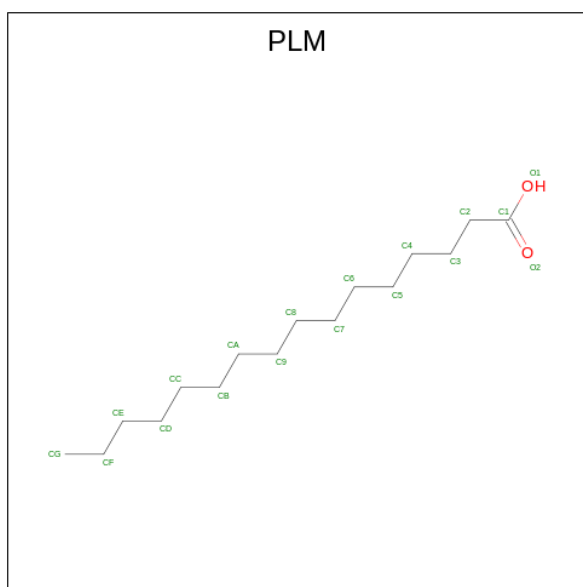
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	350	Total 2781	C 1838	N 443	O 474	S 26	0	0	0
1	B	347	Total 2762	C 1828	N 440	O 468	S 26	0	0	0

- Molecule 2 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



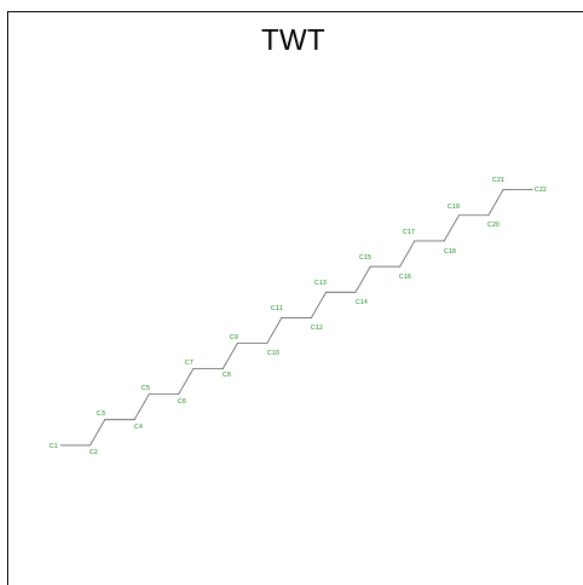
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 20	C 20	0	0
2	B	1	Total 20	C 20	0	0

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



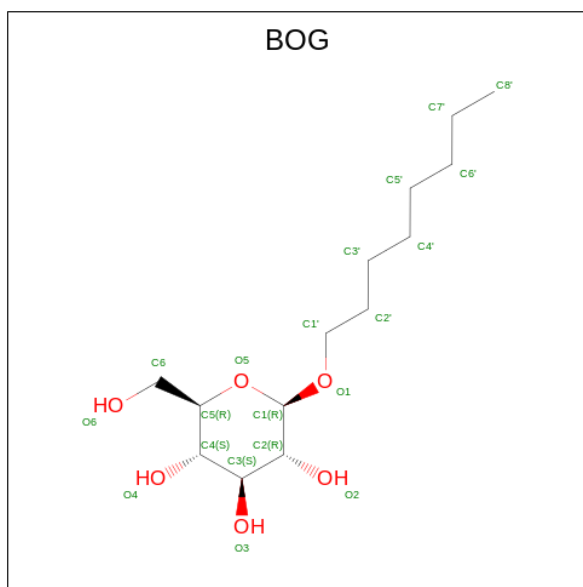
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 17 16 1	0	0
3	A	1	Total C O 17 16 1	0	0
3	B	1	Total C O 17 16 1	0	0
3	B	1	Total C O 17 16 1	0	0

- Molecule 4 is DOCOSANE (three-letter code: TWT) (formula: $C_{22}H_{46}$).



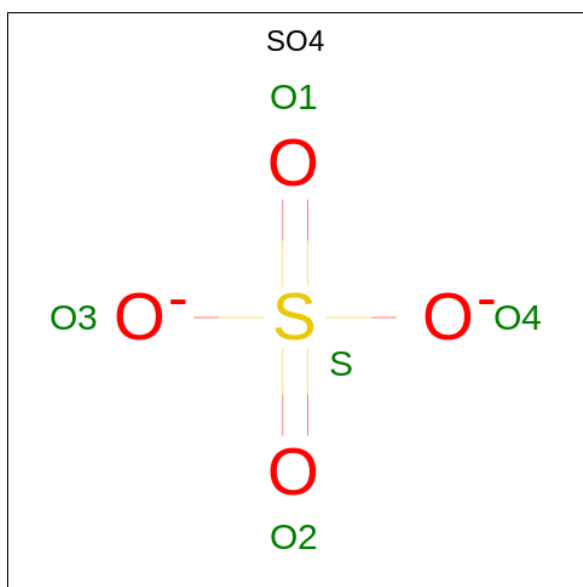
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 22 22	0	0
4	B	1	Total C 22 22	0	0

- Molecule 5 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



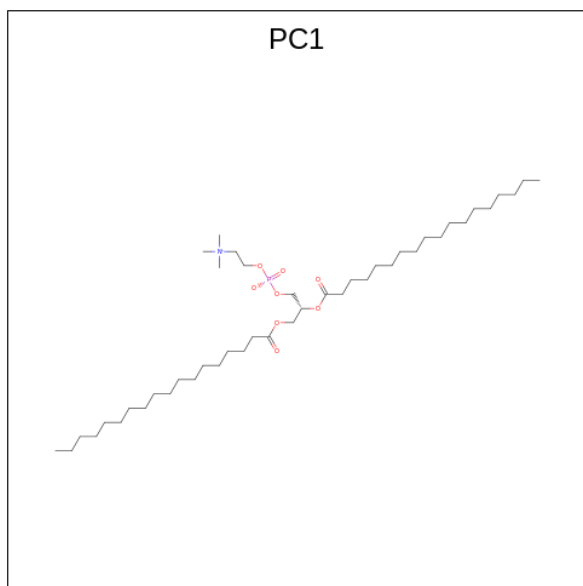
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 20 14 6	0	0
5	B	1	Total C O 20 14 6	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	P	0	0
			39	30	8	1		

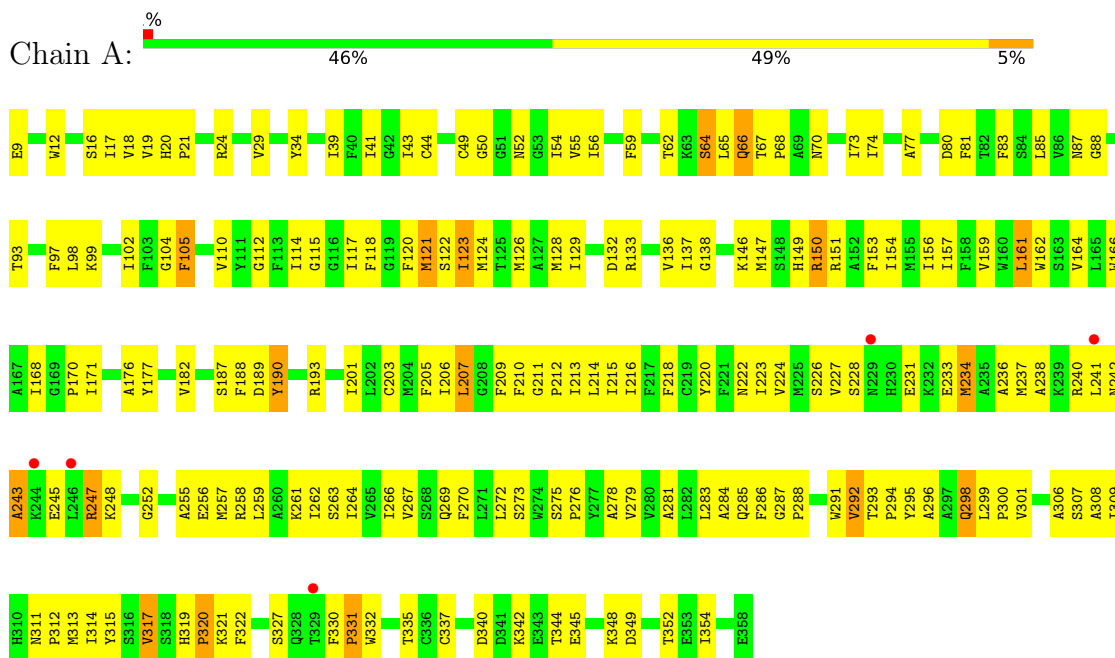
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	29	Total O 29 29	0	0
8	B	30	Total O 30 30	0	0

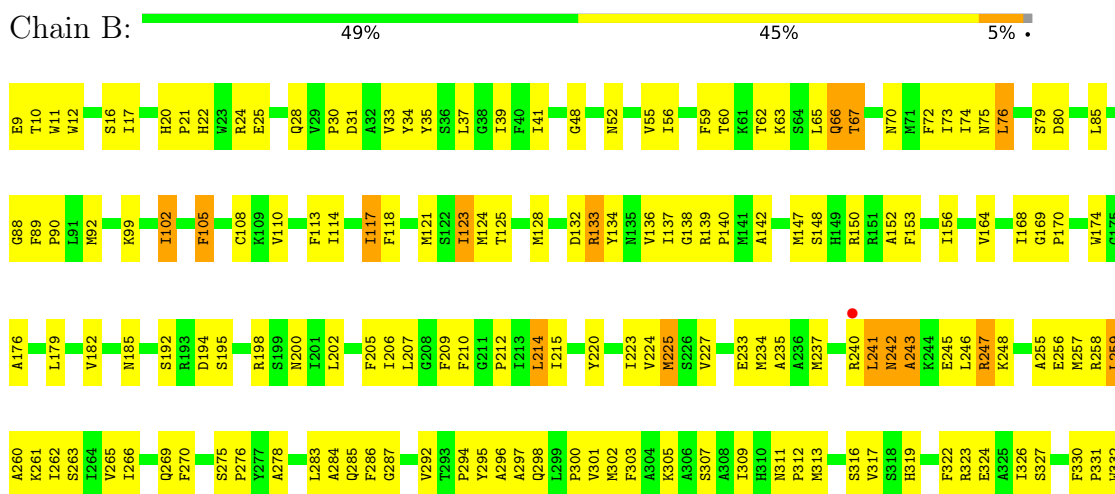
3 Residue-property plots i

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Rhodopsin



- Molecule 1: Rhodopsin



V333	L334	T335	C336	C337	Q338	F339	K342	E343	T344	E345	D346	A350	E351	T352	E353	I354	F355	ALA	GLY	GLU
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	122.39Å 122.39Å 158.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.08 – 2.80 44.08 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.5 (44.08-2.80) 83.6 (44.08-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.81Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.290 , 0.296 0.278 , 0.285	Depositor DCC
R_{free} test set	1351 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.127 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5838	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PLM, SO4, TWT, PC1, RET, BOG

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	0.46	0/2866	0.63	0/3889
1	B	0.47	0/2847	0.64	0/3865
All	All	0.47	0/5713	0.64	0/7754

There are no bond length outliers.

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	2781	0	2766	181	0
1	B	2762	0	2752	141	0
2	A	20	0	27	3	0
2	B	20	0	27	0	0
3	A	34	0	62	1	0
3	B	34	0	62	1	0
4	A	22	0	46	0	0
4	B	22	0	46	0	0
5	A	20	0	28	5	0
5	B	20	0	28	2	0
6	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	39	0	49	1	0
8	A	29	0	0	8	0
8	B	30	0	0	3	0
All	All	5838	0	5893	320	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 27.

All (320) 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:21:PRO:HA	1:A:24:ARG:HD3	1.32	1.11
1:A:59:PHE:HB3	1:A:74:ILE:HD11	1.36	1.06
1:A:284:ALA:HB2	1:A:292:VAL:HG21	1.42	0.98
1:B:150:ARG:H	1:B:150:ARG:HD2	1.28	0.96
1:B:113:PHE:O	1:B:117:ILE:HG22	1.69	0.91
1:A:298:GLN:O	1:A:301:VAL:HG12	1.72	0.87
1:A:20:HIS:ND1	1:A:21:PRO:HD2	1.92	0.85
1:A:218:PHE:O	1:A:222:ASN:HB2	1.79	0.82
1:A:21:PRO:CA	1:A:24:ARG:HD3	2.08	0.82
1:A:220:TYR:OH	1:A:263:SER:HB3	1.82	0.79
1:B:170:PRO:HB3	1:B:176:ALA:CA	2.13	0.79
1:A:115:GLY:HA3	2:A:401:RET:H203	1.66	0.78
1:B:117:ILE:HD12	1:B:164:VAL:HG22	1.64	0.78
1:B:150:ARG:HD2	1:B:150:ARG:N	2.02	0.75
1:A:209:PHE:CE2	1:A:213:ILE:HD11	2.22	0.75
1:B:234:MET:HA	1:B:237:MET:HE3	1.69	0.75
1:B:137:ILE:HD11	1:B:256:GLU:HB3	1.69	0.75
1:B:354:ILE:HD13	1:B:354:ILE:H	1.51	0.74
1:A:212:PRO:HA	1:A:215:ILE:HD12	1.68	0.74
1:A:146:LYS:HE2	5:A:405:BOG:H61	1.68	0.74
1:B:258:ARG:O	1:B:262:ILE:HG13	1.88	0.74
1:A:201:ILE:HD12	1:A:285:GLN:HE21	1.54	0.73
1:A:299:LEU:HD12	1:A:299:LEU:H	1.53	0.72
1:B:150:ARG:H	1:B:150:ARG:CD	2.00	0.72
1:B:311:ASN:HB2	1:B:312:PRO:HD3	1.69	0.72
1:B:79:SER:HB2	1:B:121:MET:CE	2.20	0.71
1:A:293:THR:H	1:A:296:ALA:HB3	1.54	0.71
1:A:201:ILE:HD12	1:A:285:GLN:NE2	2.06	0.71
1:B:63:LYS:HD2	1:B:66:GLN:NE2	2.07	0.70
1:B:257:MET:HG3	1:B:261:LYS:HE3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:HA	1:A:133:ARG:NE	2.07	0.69
1:A:209:PHE:O	1:A:213:ILE:HG13	1.94	0.68
1:A:73:ILE:HD11	5:A:405:BOG:H7'2	1.75	0.68
1:A:284:ALA:CB	1:A:292:VAL:HG21	2.23	0.67
1:B:63:LYS:HD2	1:B:66:GLN:HE22	1.58	0.67
1:B:202:LEU:HD12	7:B:406:PC1:H361	1.75	0.67
1:B:298:GLN:O	1:B:301:VAL:HG12	1.93	0.67
1:A:201:ILE:CD1	1:A:285:GLN:HE21	2.08	0.67
1:B:284:ALA:HB2	1:B:292:VAL:HG21	1.77	0.67
1:A:278:ALA:O	1:A:281:ALA:HB3	1.95	0.66
1:A:190:TYR:HA	1:A:201:ILE:HD11	1.77	0.66
1:A:306:ALA:O	1:A:309:ILE:HG12	1.97	0.65
1:A:188:PHE:CE1	1:A:190:TYR:HB3	2.32	0.65
1:A:12:TRP:CD2	1:A:24:ARG:HG2	2.32	0.64
1:A:188:PHE:HE1	1:A:190:TYR:HB3	1.63	0.64
1:B:110:VAL:O	1:B:114:ILE:HG13	1.98	0.64
1:A:137:ILE:HD11	1:A:256:GLU:HB2	1.80	0.64
1:A:50:GLY:O	1:A:54:ILE:HG13	1.97	0.64
1:B:170:PRO:HB3	1:B:176:ALA:N	2.12	0.63
1:A:311:ASN:HB2	1:A:312:PRO:HD3	1.80	0.63
1:B:52:ASN:HD21	1:B:80:ASP:HB3	1.64	0.63
1:B:170:PRO:HB3	1:B:176:ALA:HA	1.80	0.63
1:A:340:ASP:OD2	1:A:342:LYS:HB2	1.98	0.63
1:A:20:HIS:CE1	1:A:21:PRO:HD2	2.33	0.63
1:B:136:VAL:O	1:B:137:ILE:HD13	1.99	0.63
1:A:21:PRO:HA	1:A:24:ARG:CD	2.21	0.63
1:B:248:LYS:HE3	1:B:350:ALA:O	1.99	0.62
1:A:133:ARG:NH2	1:A:136:VAL:HG11	2.15	0.62
1:A:263:SER:O	1:A:267:VAL:HG23	2.00	0.62
1:B:20:HIS:ND1	1:B:21:PRO:HD2	2.15	0.61
1:B:324:GLU:HG3	1:B:339:PHE:CE2	2.35	0.61
1:B:118:PHE:HA	1:B:121:MET:HB3	1.82	0.61
1:B:41:ILE:HG13	1:B:88:GLY:HA2	1.82	0.61
1:A:59:PHE:HB3	1:A:74:ILE:CD1	2.22	0.61
1:A:293:THR:N	1:A:296:ALA:HB3	2.16	0.61
1:B:313:MET:O	1:B:317:VAL:HG23	2.00	0.60
1:A:150:ARG:HD3	1:A:150:ARG:N	2.16	0.60
1:A:34:TYR:CD1	1:A:99:LYS:HG2	2.37	0.60
1:B:52:ASN:HA	1:B:55:VAL:HG12	1.82	0.60
1:A:137:ILE:HG22	1:A:223:ILE:HG23	1.82	0.60
1:B:79:SER:HB2	1:B:121:MET:HE1	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:HB2	8:B:501:HOH:O	2.01	0.59
1:A:209:PHE:CZ	1:A:213:ILE:HD11	2.37	0.58
1:A:354:ILE:HD12	1:A:354:ILE:O	2.02	0.58
1:B:153:PHE:O	1:B:156:ILE:HG13	2.02	0.58
1:B:132:ASP:OD2	1:B:147:MET:HB2	2.02	0.58
1:A:177:TYR:HA	1:A:187:SER:O	2.03	0.58
1:B:296:ALA:O	1:B:300:PRO:HG2	2.04	0.58
1:A:283:LEU:O	1:A:287:GLY:N	2.34	0.57
1:B:33:VAL:O	1:B:37:LEU:HG	2.05	0.56
1:A:170:PRO:HB3	1:A:176:ALA:CA	2.36	0.56
1:A:122:SER:O	1:A:126:MET:HG3	2.05	0.56
1:A:224:VAL:HA	1:A:227:VAL:HG23	1.88	0.56
1:B:11:TRP:HB2	1:B:28:GLN:OE1	2.06	0.56
1:A:114:ILE:O	1:A:117:ILE:HG22	2.06	0.56
1:A:12:TRP:CE3	1:A:24:ARG:HG2	2.40	0.56
1:A:257:MET:O	1:A:261:LYS:HG3	2.05	0.56
1:B:102:ILE:HD13	1:B:102:ILE:H	1.70	0.56
1:A:313:MET:O	1:A:317:VAL:HG22	2.06	0.56
1:B:79:SER:HB2	1:B:121:MET:HE2	1.87	0.56
1:B:240:ARG:HD3	1:B:241:LEU:HD13	1.87	0.56
1:A:236:ALA:O	1:A:240:ARG:HB2	2.06	0.55
1:B:322:PHE:CE2	1:B:326:ILE:HD11	2.42	0.55
1:A:29:VAL:HG22	8:A:519:HOH:O	2.06	0.55
1:A:269:GLN:NE2	1:A:307:SER:OG	2.40	0.55
1:B:48:GLY:HA3	1:B:309:ILE:HG22	1.88	0.55
1:B:297:ALA:O	1:B:300:PRO:HD2	2.07	0.55
1:B:48:GLY:CA	1:B:309:ILE:HG22	2.37	0.55
1:A:12:TRP:HA	8:A:521:HOH:O	2.07	0.55
1:B:113:PHE:CZ	1:B:168:ILE:HD12	2.42	0.55
1:A:263:SER:O	1:A:266:ILE:HG12	2.07	0.54
1:A:77:ALA:HA	8:A:518:HOH:O	2.07	0.54
1:A:49:CYS:HB3	1:A:81:PHE:HE1	1.72	0.54
1:A:190:TYR:HA	1:A:201:ILE:CD1	2.37	0.54
1:A:49:CYS:HB3	1:A:81:PHE:CE1	2.43	0.54
1:B:324:GLU:OE2	1:B:344:THR:HG21	2.07	0.54
1:A:52:ASN:HA	1:A:55:VAL:HG12	1.88	0.53
1:B:220:TYR:O	1:B:224:VAL:HG23	2.08	0.53
1:B:248:LYS:NZ	1:B:353:GLU:HA	2.24	0.53
1:A:342:LYS:HA	1:A:345:GLU:HG3	1.91	0.53
1:B:319:HIS:HB3	1:B:322:PHE:HB3	1.89	0.53
1:A:327:SER:O	1:A:331:PRO:HB3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:O	1:A:59:PHE:HB2	2.08	0.53
1:A:19:VAL:O	1:A:24:ARG:HD2	2.09	0.53
1:A:12:TRP:HZ2	1:B:25:GLU:HB2	1.74	0.52
1:B:237:MET:O	1:B:242:ASN:HB2	2.09	0.52
1:B:322:PHE:CZ	1:B:326:ILE:HD11	2.45	0.52
1:A:319:HIS:HB3	1:A:322:PHE:HB3	1.92	0.52
1:B:257:MET:O	1:B:261:LYS:HG3	2.09	0.52
1:A:110:VAL:O	1:A:114:ILE:HG12	2.10	0.52
1:A:259:LEU:HD12	5:A:405:BOG:H6'1	1.91	0.52
1:A:291:TRP:O	1:A:293:THR:HG23	2.10	0.52
1:B:205:PHE:HE1	1:B:278:ALA:HB1	1.75	0.52
1:B:34:TYR:CG	1:B:99:LYS:HG2	2.45	0.52
1:A:67:THR:HG21	5:A:405:BOG:H5	1.92	0.52
1:A:295:TYR:HB3	1:A:299:LEU:HD13	1.92	0.52
1:A:293:THR:HB	1:A:294:PRO:HD2	1.91	0.51
1:A:170:PRO:HB3	1:A:176:ALA:HA	1.92	0.51
1:A:293:THR:H	1:A:296:ALA:CB	2.21	0.51
1:A:344:THR:O	1:A:348:LYS:HG3	2.11	0.51
1:A:153:PHE:CE2	1:A:157:ILE:HD11	2.46	0.51
1:A:228:SER:HA	1:A:231:GLU:HB2	1.91	0.51
1:A:279:VAL:O	1:A:283:LEU:HD13	2.11	0.51
1:B:133:ARG:HA	1:B:133:ARG:NH1	2.26	0.51
1:A:243:ALA:HB3	1:A:245:GLU:OE2	2.11	0.51
1:A:98:LEU:HD12	1:A:102:ILE:HD13	1.93	0.50
1:A:206:ILE:HA	1:A:210:PHE:CD2	2.46	0.50
1:B:207:LEU:N	1:B:207:LEU:HD22	2.25	0.50
1:B:125:THR:O	1:B:128:MET:HB2	2.11	0.50
1:A:133:ARG:HA	1:A:133:ARG:HE	1.74	0.50
1:B:22:HIS:O	1:B:25:GLU:HG2	2.12	0.50
1:B:263:SER:O	1:B:266:ILE:HG12	2.12	0.50
1:B:336:CYS:SG	3:B:404:PLM:H21	2.51	0.50
1:A:342:LYS:O	1:A:345:GLU:HG3	2.11	0.50
1:B:275:SER:HB2	1:B:276:PRO:HD3	1.93	0.50
1:B:330:PHE:N	1:B:331:PRO:CD	2.75	0.50
1:A:293:THR:HB	1:A:294:PRO:CD	2.42	0.50
1:B:133:ARG:HG2	1:B:260:ALA:HA	1.93	0.50
1:A:112:GLY:HA2	2:A:401:RET:H202	1.93	0.50
1:B:182:VAL:HG22	1:B:298:GLN:OE1	2.12	0.49
1:A:330:PHE:N	1:A:331:PRO:CD	2.75	0.49
1:B:48:GLY:O	1:B:52:ASN:HB2	2.12	0.49
1:A:345:GLU:HA	1:A:348:LYS:HD2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:O	1:A:87:ASN:HB2	2.12	0.49
1:B:247:ARG:O	1:B:247:ARG:HD3	2.12	0.49
1:B:316:SER:O	1:B:323:ARG:NH1	2.40	0.49
1:A:233:GLU:O	1:A:237:MET:HG2	2.13	0.49
1:B:137:ILE:HD11	1:B:256:GLU:CB	2.39	0.49
1:B:297:ALA:C	1:B:300:PRO:HD2	2.32	0.49
1:A:247:ARG:HH21	1:A:247:ARG:HB2	1.78	0.49
1:B:76:LEU:HD13	1:B:311:ASN:HD22	1.77	0.49
1:B:259:LEU:HB3	5:B:407:BOG:H6'1	1.95	0.48
1:B:327:SER:O	1:B:331:PRO:HB3	2.13	0.48
1:B:132:ASP:HB2	1:B:147:MET:HE2	1.96	0.48
1:A:273:SER:HB3	1:A:307:SER:HB2	1.95	0.48
1:B:269:GLN:NE2	1:B:307:SER:OG	2.44	0.48
1:A:20:HIS:ND1	1:A:21:PRO:CD	2.70	0.48
1:A:176:ALA:O	1:A:189:ASP:N	2.46	0.48
1:B:132:ASP:OD1	1:B:133:ARG:NH1	2.46	0.48
1:B:206:ILE:HA	1:B:210:PHE:CD2	2.48	0.48
1:B:123:ILE:HG12	1:B:270:PHE:CZ	2.48	0.48
1:B:192:SER:HB3	1:B:194:ASP:OD1	2.14	0.48
1:A:157:ILE:HG22	1:A:161:LEU:HD23	1.96	0.48
1:A:311:ASN:OD1	8:A:501:HOH:O	2.20	0.48
1:A:16:SER:HB2	1:A:17:ILE:HD12	1.95	0.48
1:A:288:PRO:O	1:A:291:TRP:HB2	2.13	0.48
1:A:153:PHE:CZ	1:A:157:ILE:HD11	2.49	0.47
1:B:214:LEU:HD23	1:B:215:ILE:N	2.28	0.47
1:B:67:THR:O	1:B:70:ASN:HB2	2.13	0.47
1:B:92:MET:HG3	1:B:185:ASN:HB3	1.96	0.47
1:A:216:ILE:HD13	1:A:267:VAL:HG11	1.95	0.47
1:A:224:VAL:O	1:A:227:VAL:HG23	2.14	0.47
1:A:49:CYS:HA	1:A:81:PHE:CD1	2.49	0.47
1:A:52:ASN:O	1:A:56:ILE:HG13	2.15	0.47
1:A:67:THR:HB	8:A:527:HOH:O	2.14	0.47
1:B:52:ASN:O	1:B:55:VAL:HG12	2.15	0.47
1:B:89:PHE:CD2	1:B:90:PRO:HA	2.49	0.47
1:B:255:ALA:O	1:B:259:LEU:HD22	2.15	0.47
1:A:62:THR:HG22	1:A:64:SER:H	1.80	0.47
1:A:146:LYS:HE2	5:A:405:BOG:C6	2.42	0.47
1:A:205:PHE:CE1	1:A:278:ALA:HB1	2.50	0.47
1:A:288:PRO:HB2	1:A:291:TRP:CG	2.50	0.46
1:B:332:TRP:O	1:B:335:THR:HG23	2.14	0.46
1:A:193:ARG:HH11	1:A:286:PHE:CA	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:TYR:O	1:B:39:ILE:HG12	2.15	0.46
1:A:240:ARG:HH11	1:A:241:LEU:HD13	1.80	0.46
1:B:330:PHE:O	1:B:333:VAL:HG23	2.15	0.46
1:A:12:TRP:CZ2	1:B:25:GLU:HB2	2.50	0.46
1:A:39:ILE:O	1:A:43:ILE:HG13	2.15	0.46
1:A:93:THR:HG22	1:A:97:PHE:CE2	2.51	0.46
1:A:52:ASN:O	1:A:55:VAL:HG12	2.16	0.46
1:A:220:TYR:CD1	1:A:264:ILE:HD11	2.51	0.46
1:B:59:PHE:CD2	1:B:65:LEU:HD13	2.51	0.46
1:A:123:ILE:HG12	1:A:270:PHE:CZ	2.51	0.46
1:A:133:ARG:NE	1:A:133:ARG:CA	2.76	0.46
1:B:52:ASN:CA	1:B:55:VAL:HG12	2.46	0.46
1:A:18:VAL:HG12	1:A:18:VAL:O	2.15	0.45
1:A:133:ARG:HE	1:A:133:ARG:CA	2.29	0.45
1:A:150:ARG:N	1:A:150:ARG:CD	2.79	0.45
1:A:124:MET:HG3	1:A:159:VAL:HG22	1.99	0.45
1:B:124:MET:O	1:B:128:MET:HG2	2.16	0.45
1:B:233:GLU:O	1:B:237:MET:HG3	2.16	0.45
1:B:301:VAL:O	1:B:305:LYS:HG3	2.15	0.45
1:A:270:PHE:O	1:A:273:SER:HB2	2.15	0.45
1:B:21:PRO:HA	1:B:24:ARG:HG3	1.98	0.45
1:B:52:ASN:HA	1:B:55:VAL:CG1	2.46	0.45
1:A:150:ARG:CD	1:A:150:ARG:H	2.30	0.45
1:A:17:ILE:HG13	1:A:105:PHE:CD2	2.52	0.45
1:A:147:MET:SD	1:A:151:ARG:HB3	2.56	0.45
1:A:206:ILE:HA	1:A:210:PHE:HD2	1.79	0.45
1:A:237:MET:HA	1:A:240:ARG:CB	2.47	0.44
1:B:298:GLN:O	1:B:302:MET:HG2	2.18	0.44
1:B:224:VAL:O	1:B:227:VAL:HG22	2.17	0.44
1:A:150:ARG:O	1:A:154:ILE:HG13	2.18	0.44
1:B:148:SER:HB2	1:B:150:ARG:HH21	1.82	0.44
1:B:220:TYR:CD1	1:B:223:ILE:HD12	2.53	0.44
1:B:52:ASN:O	1:B:56:ILE:HG13	2.17	0.44
1:B:337:CYS:O	1:B:338:GLN:C	2.56	0.44
1:B:35:TYR:N	1:B:35:TYR:CD2	2.86	0.44
1:B:30:PRO:O	1:B:31:ASP:C	2.56	0.44
1:A:150:ARG:HD3	1:A:150:ARG:H	1.82	0.44
1:A:348:LYS:O	1:A:352:THR:HG23	2.18	0.44
1:B:206:ILE:HG22	1:B:207:LEU:HD22	2.00	0.44
1:A:330:PHE:O	1:A:332:TRP:N	2.51	0.43
1:A:332:TRP:O	1:A:335:THR:HG23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:CG	1:B:260:ALA:HA	2.48	0.43
1:A:118:PHE:HA	1:A:121:MET:HB3	2.00	0.43
1:A:153:PHE:O	1:A:157:ILE:HG13	2.18	0.43
1:B:52:ASN:ND2	1:B:80:ASP:HB3	2.31	0.43
1:B:275:SER:O	1:B:276:PRO:C	2.57	0.43
1:B:33:VAL:HG21	1:B:295:TYR:OH	2.18	0.43
1:B:75:ASN:OD1	1:B:121:MET:HE3	2.18	0.43
1:B:198:ARG:O	1:B:202:LEU:HG	2.18	0.43
1:A:299:LEU:HB2	1:A:300:PRO:HD3	2.01	0.43
1:B:220:TYR:OH	1:B:263:SER:HB3	2.18	0.43
1:A:252:GLY:O	1:A:255:ALA:HB3	2.18	0.43
1:A:266:ILE:HG22	1:A:314:ILE:HD12	2.01	0.43
1:A:275:SER:HB2	1:A:276:PRO:HD3	2.00	0.43
1:B:235:ALA:C	1:B:237:MET:H	2.22	0.43
1:A:29:VAL:HG21	1:A:182:VAL:HG11	1.99	0.43
1:A:205:PHE:HE1	1:A:278:ALA:HB1	1.83	0.43
1:A:276:PRO:HB2	8:A:502:HOH:O	2.18	0.43
1:B:243:ALA:N	1:B:245:GLU:HG2	2.34	0.42
1:A:41:ILE:HG13	1:A:88:GLY:HA2	1.99	0.42
1:A:124:MET:O	1:A:128:MET:HE3	2.18	0.42
1:A:136:VAL:HG22	1:A:136:VAL:O	2.19	0.42
1:A:240:ARG:HA	1:A:240:ARG:NE	2.33	0.42
1:B:52:ASN:O	1:B:55:VAL:CG1	2.67	0.42
1:A:166:TRP:CH2	1:A:207:LEU:HD23	2.54	0.42
1:B:55:VAL:HG13	1:B:56:ILE:N	2.34	0.42
1:B:73:ILE:HD11	5:B:407:BOG:H7'2	2.01	0.42
1:B:169:GLY:HA3	8:B:515:HOH:O	2.19	0.42
1:A:193:ARG:HH11	1:A:286:PHE:C	2.22	0.42
1:B:72:PHE:CZ	1:B:152:ALA:HA	2.53	0.42
1:A:132:ASP:OD1	1:A:133:ARG:NH2	2.53	0.42
1:B:59:PHE:CE2	1:B:65:LEU:HD13	2.55	0.42
1:B:105:PHE:O	1:B:108:CYS:HB3	2.19	0.42
1:B:285:GLN:NE2	1:B:285:GLN:HA	2.35	0.42
1:A:299:LEU:H	1:A:299:LEU:CD1	2.28	0.42
1:B:17:ILE:CG2	1:B:179:LEU:HD12	2.49	0.42
1:B:20:HIS:CE1	1:B:21:PRO:HD2	2.55	0.42
1:B:248:LYS:HZ3	1:B:353:GLU:HA	1.85	0.42
1:B:324:GLU:CD	1:B:344:THR:HG21	2.40	0.42
1:A:120:PHE:CZ	2:A:401:RET:H7	2.55	0.42
1:A:234:MET:O	1:A:238:ALA:HB2	2.20	0.42
1:A:258:ARG:NH2	1:A:258:ARG:HG3	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:O	1:A:262:ILE:HG13	2.20	0.42
1:B:234:MET:O	1:B:237:MET:HB2	2.20	0.42
1:A:218:PHE:CD1	1:A:218:PHE:C	2.93	0.41
1:A:117:ILE:HD11	1:A:164:VAL:HG22	2.01	0.41
1:A:161:LEU:HD13	1:A:161:LEU:HA	1.63	0.41
1:A:170:PRO:HB3	1:A:176:ALA:N	2.35	0.41
1:A:233:GLU:O	1:A:233:GLU:HG2	2.19	0.41
1:B:12:TRP:CH2	1:B:24:ARG:HD3	2.55	0.41
1:A:80:ASP:HB3	1:A:308:ALA:O	2.19	0.41
1:A:168:ILE:O	1:A:171:ILE:HB	2.20	0.41
1:A:337:CYS:SG	3:A:403:PLM:O2	2.77	0.41
1:B:60:THR:CG2	1:B:74:ILE:HD13	2.50	0.41
1:B:140:PRO:C	1:B:142:ALA:N	2.74	0.41
1:A:114:ILE:HA	1:A:117:ILE:HG22	2.02	0.41
1:A:216:ILE:HG23	1:A:220:TYR:CE2	2.54	0.41
1:B:261:LYS:O	1:B:265:VAL:HG23	2.20	0.41
1:A:220:TYR:O	1:A:224:VAL:HG23	2.20	0.41
1:A:65:LEU:HD21	1:A:321:LYS:HB3	2.02	0.41
1:A:68:PRO:HG3	1:A:149:HIS:CE1	2.56	0.41
1:A:114:ILE:HA	1:A:117:ILE:CG2	2.50	0.41
1:A:129:ILE:O	1:A:133:ARG:HG2	2.21	0.41
1:A:224:VAL:C	1:A:226:SER:H	2.24	0.41
1:A:258:ARG:HG3	1:A:258:ARG:HH21	1.86	0.41
1:A:299:LEU:HD12	1:A:299:LEU:N	2.30	0.41
1:A:312:PRO:HA	1:A:315:TYR:HD1	1.85	0.41
1:B:124:MET:HB2	8:B:528:HOH:O	2.20	0.41
1:B:242:ASN:HA	1:B:245:GLU:HG3	2.03	0.41
1:A:44:CYS:HB3	8:A:528:HOH:O	2.21	0.40
1:A:138:GLY:CA	1:A:223:ILE:HG12	2.50	0.40
1:B:133:ARG:HA	1:B:133:ARG:HH11	1.85	0.40
1:A:136:VAL:HG13	1:A:137:ILE:HG12	2.04	0.40
1:A:275:SER:O	1:A:276:PRO:C	2.59	0.40
1:A:320:PRO:HG2	8:A:525:HOH:O	2.21	0.40
1:B:234:MET:HE1	1:B:246:LEU:HD12	2.04	0.40
1:B:283:LEU:O	1:B:287:GLY:N	2.53	0.40
1:A:17:ILE:HD12	1:A:17:ILE:N	2.36	0.40
1:B:174:TRP:CD1	1:B:200:ASN:HB2	2.57	0.40
1:B:202:LEU:HD21	1:B:286:PHE:HZ	1.87	0.40
1:B:209:PHE:O	1:B:212:PRO:HG2	2.21	0.40
1:B:342:LYS:HA	1:B:345:GLU:OE1	2.21	0.40
1:A:166:TRP:CZ3	1:A:207:LEU:HD23	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:SER:HB3	1:A:104:GLY:HA2	2.04	0.40
1:A:345:GLU:HA	1:A:348:LYS:CD	2.51	0.40
1:B:137:ILE:C	1:B:139:ARG:H	2.25	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 X-ray entries followed by that with respect to entries of similar resolution.

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	348/350 (99%)	299 (86%)	39 (11%)	10 (3%)	4	15
1	B	345/350 (99%)	306 (89%)	33 (10%)	6 (2%)	9	29
All	All	693/700 (99%)	605 (87%)	72 (10%)	16 (2%)	6	21

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ALA
1	A	298	GLN
1	B	241	LEU
1	B	243	ALA
1	B	352	THR
1	A	66	GLN
1	A	162	TRP
1	A	211	GLY
1	A	248	LYS
1	A	331	PRO
1	B	62	THR
1	B	225	MET
1	A	70	ASN
1	A	292	VAL
1	B	138	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	320	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 X-ray entries followed by that with respect to entries of similar resolution.

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	296/296 (100%)	276 (93%)	20 (7%)	16	42
1	B	295/296 (100%)	271 (92%)	24 (8%)	11	33
All	All	591/592 (100%)	547 (93%)	44 (7%)	13	37

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	64	SER
1	A	66	GLN
1	A	85	LEU
1	A	105	PHE
1	A	121	MET
1	A	123	ILE
1	A	150	ARG
1	A	156	ILE
1	A	161	LEU
1	A	190	TYR
1	A	203	CYS
1	A	207	LEU
1	A	214	LEU
1	A	234	MET
1	A	242	ASN
1	A	247	ARG
1	A	272	LEU
1	A	317	VAL
1	A	349	ASP
1	B	9	GLU
1	B	10	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	16	SER
1	B	66	GLN
1	B	67	THR
1	B	76	LEU
1	B	85	LEU
1	B	102	ILE
1	B	105	PHE
1	B	117	ILE
1	B	123	ILE
1	B	133	ARG
1	B	134	TYR
1	B	195	SER
1	B	214	LEU
1	B	225	MET
1	B	242	ASN
1	B	247	ARG
1	B	259	LEU
1	B	294	PRO
1	B	303	PHE
1	B	338	GLN
1	B	346	ASP
1	B	354	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	87	ASN
1	A	229	ASN
1	A	230	HIS
1	A	242	ASN
1	A	254	ASN
1	A	269	GLN
1	A	338	GLN
1	B	52	ASN
1	B	70	ASN
1	B	87	ASN
1	B	149	HIS
1	B	222	ASN
1	B	230	HIS
1	B	269	GLN
1	B	328	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	338	GLN

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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	BOG	B	407	-	20,20,20	1.80	7 (35%)	25,25,25	2.77	11 (44%)
5	BOG	A	405	-	20,20,20	1.81	8 (40%)	25,25,25	2.80	11 (44%)
2	RET	B	402	1	20,20,21	1.68	5 (25%)	27,27,28	2.31	8 (29%)
4	TWT	A	404	-	21,21,21	0.32	0	20,20,20	1.67	4 (20%)
2	RET	A	401	1	20,20,21	2.04	5 (25%)	27,27,28	2.38	8 (29%)
3	PLM	A	403	-	16,16,17	0.28	0	15,15,17	0.69	0
3	PLM	B	403	-	16,16,17	0.35	0	15,15,17	0.64	0
4	TWT	B	405	-	21,21,21	0.27	0	20,20,20	1.73	6 (30%)
7	PC1	B	406	-	38,38,53	1.62	3 (7%)	41,43,61	1.01	1 (2%)
6	SO4	B	401	-	4,4,4	0.29	0	6,6,6	0.06	0
3	PLM	A	402	-	16,16,17	0.42	0	15,15,17	0.59	0
3	PLM	B	404	-	16,16,17	0.29	0	15,15,17	0.68	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	BOG	B	407	-	-	6/11/31/31	0/1/1/1
5	BOG	A	405	-	-	4/11/31/31	0/1/1/1
2	RET	B	402	1	-	2/13/30/31	0/1/1/1
4	TWT	A	404	-	-	9/19/19/19	-
2	RET	A	401	1	-	2/13/30/31	0/1/1/1
3	PLM	A	403	-	-	7/13/14/15	-
3	PLM	B	403	-	-	4/13/14/15	-
4	TWT	B	405	-	-	8/19/19/19	-
7	PC1	B	406	-	-	15/42/42/57	-
3	PLM	A	402	-	-	5/13/14/15	-
3	PLM	B	404	-	-	8/13/14/15	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	406	PC1	O21-C21	7.56	1.55	1.34
2	A	401	RET	C1-C6	5.41	1.61	1.53
2	A	401	RET	C14-C13	4.56	1.37	1.33
2	B	402	RET	C1-C6	4.11	1.59	1.53
7	B	406	PC1	O31-C31	4.01	1.45	1.33
5	A	405	BOG	O5-C1	3.73	1.51	1.41
5	B	407	BOG	O5-C1	3.70	1.51	1.41
2	A	401	RET	C2-C3	-3.69	1.43	1.52
2	B	402	RET	C2-C3	-3.43	1.44	1.52
2	B	402	RET	C14-C13	2.86	1.36	1.33
5	A	405	BOG	C4-C3	2.71	1.59	1.52
5	B	407	BOG	C4-C3	2.70	1.59	1.52
5	B	407	BOG	C4-C5	-2.56	1.47	1.53
5	A	405	BOG	O6-C6	2.55	1.53	1.42
5	B	407	BOG	O6-C6	2.53	1.53	1.42
2	A	401	RET	C7-C6	2.46	1.53	1.45
5	A	405	BOG	O2-C2	2.39	1.48	1.43
5	B	407	BOG	O2-C2	2.25	1.48	1.43
5	A	405	BOG	C3-C2	-2.21	1.46	1.52
5	A	405	BOG	C4-C5	-2.17	1.48	1.53
5	B	407	BOG	C3-C2	-2.15	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	RET	C7-C6	2.15	1.52	1.45
2	A	401	RET	C5-C6	2.14	1.38	1.34
5	A	405	BOG	C6-C5	2.13	1.59	1.51
5	B	407	BOG	C6-C5	2.11	1.58	1.51
5	A	405	BOG	O1-C1	-2.07	1.36	1.40
7	B	406	PC1	P-O14	2.05	1.58	1.50
2	B	402	RET	C5-C6	2.05	1.38	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	407	BOG	C1'-O1-C1	-8.30	100.08	113.84
5	A	405	BOG	C1'-O1-C1	-8.22	100.20	113.84
2	A	401	RET	C11-C10-C9	6.92	137.19	127.31
2	B	402	RET	C11-C10-C9	5.79	135.57	127.31
2	B	402	RET	C8-C9-C10	-5.75	110.12	118.94
2	B	402	RET	C7-C8-C9	5.63	134.74	126.23
2	A	401	RET	C7-C8-C9	5.50	134.54	126.23
2	A	401	RET	C8-C9-C10	-5.45	110.57	118.94
5	A	405	BOG	O1-C1-C2	-4.87	100.70	108.30
5	B	407	BOG	O1-C1-C2	-4.38	101.47	108.30
5	B	407	BOG	C1-C2-C3	-4.36	100.92	110.00
5	A	405	BOG	O5-C5-C4	-4.33	101.83	109.69
5	A	405	BOG	C1-C2-C3	-4.16	101.34	110.00
5	B	407	BOG	O5-C5-C4	-4.15	102.15	109.69
5	A	405	BOG	O3-C3-C2	-3.81	101.55	110.35
5	B	407	BOG	O3-C3-C2	-3.75	101.68	110.35
4	B	405	TWT	C14-C13-C12	-3.38	97.28	114.42
2	A	401	RET	C19-C9-C10	3.35	127.62	122.92
4	A	404	TWT	C14-C13-C12	-3.32	97.57	114.42
2	B	402	RET	C19-C9-C8	3.23	123.16	118.08
4	A	404	TWT	C16-C15-C14	-3.13	98.55	114.42
7	B	406	PC1	O21-C21-C22	3.04	118.06	111.50
4	B	405	TWT	C16-C15-C14	-3.01	99.14	114.42
4	B	405	TWT	C12-C11-C10	-3.00	99.21	114.42
4	B	405	TWT	C18-C17-C16	-2.97	99.34	114.42
4	A	404	TWT	C12-C11-C10	-2.94	99.49	114.42
5	B	407	BOG	O4-C4-C5	-2.82	102.30	109.30
2	B	402	RET	C19-C9-C10	2.71	126.72	122.92
4	A	404	TWT	C18-C17-C16	-2.66	100.90	114.42
5	A	405	BOG	O4-C4-C5	-2.66	102.69	109.30
5	B	407	BOG	C4'-C3'-C2'	-2.65	100.97	114.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	407	BOG	C3'-C2'-C1'	-2.59	102.01	113.49
5	A	405	BOG	C4'-C3'-C2'	-2.58	101.32	114.42
5	A	405	BOG	C6'-C5'-C4'	-2.56	101.45	114.42
5	A	405	BOG	C3'-C2'-C1'	-2.55	102.19	113.49
4	B	405	TWT	C20-C19-C18	-2.54	101.51	114.42
5	A	405	BOG	O1-C1'-C2'	-2.52	100.73	109.56
5	B	407	BOG	C6'-C5'-C4'	-2.48	101.82	114.42
2	B	402	RET	C10-C11-C12	-2.39	115.75	123.22
2	A	401	RET	C19-C9-C8	2.37	121.81	118.08
2	A	401	RET	C10-C11-C12	-2.31	116.01	123.22
2	B	402	RET	C8-C7-C6	-2.23	120.93	127.20
5	B	407	BOG	C5'-C4'-C3'	-2.15	103.53	114.42
5	B	407	BOG	O1-C1'-C2'	-2.14	102.06	109.56
4	B	405	TWT	C10-C9-C8	-2.10	103.77	114.42
5	A	405	BOG	C5'-C4'-C3'	-2.10	103.78	114.42
2	A	401	RET	C11-C12-C13	2.09	132.30	126.42
2	B	402	RET	C18-C5-C6	2.02	126.80	124.53
2	A	401	RET	C18-C5-C6	2.01	126.78	124.53

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	402	RET	C1-C6-C7-C8
3	A	402	PLM	C1-C2-C3-C4
3	A	403	PLM	C1-C2-C3-C4
3	B	403	PLM	C1-C2-C3-C4
7	B	406	PC1	C1-O11-P-O12
7	B	406	PC1	C1-O11-P-O14
7	B	406	PC1	C32-C31-O31-C3
7	B	406	PC1	C21-C22-C23-C24
7	B	406	PC1	O32-C31-O31-C3
5	A	405	BOG	O1-C1'-C2'-C3'
7	B	406	PC1	C1-O11-P-O13
5	B	407	BOG	O1-C1'-C2'-C3'
3	A	402	PLM	C7-C8-C9-CA
3	A	403	PLM	CB-CC-CD-CE
4	B	405	TWT	C6-C7-C8-C9
3	B	404	PLM	CB-CC-CD-CE
4	A	404	TWT	C3-C4-C5-C6
3	B	403	PLM	C7-C8-C9-CA
3	A	402	PLM	C9-CA-CB-CC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	404	PLM	C2-C3-C4-C5
3	A	403	PLM	C7-C8-C9-CA
3	B	404	PLM	C8-C9-CA-CB
4	A	404	TWT	C6-C7-C8-C9
7	B	406	PC1	C22-C23-C24-C25
3	B	403	PLM	C6-C7-C8-C9
7	B	406	PC1	C26-C27-C28-C29
3	A	403	PLM	CC-CD-CE-CF
4	B	405	TWT	C4-C5-C6-C7
4	B	405	TWT	C7-C8-C9-C10
4	B	405	TWT	C3-C4-C5-C6
4	A	404	TWT	C15-C16-C17-C18
3	A	403	PLM	C8-C9-CA-CB
3	B	403	PLM	C2-C3-C4-C5
3	B	404	PLM	C6-C7-C8-C9
3	B	404	PLM	CC-CD-CE-CF
4	A	404	TWT	C4-C5-C6-C7
5	A	405	BOG	C3'-C4'-C5'-C6'
2	A	401	RET	C1-C6-C7-C8
2	A	401	RET	C5-C6-C7-C8
5	B	407	BOG	C3'-C4'-C5'-C6'
4	A	404	TWT	C7-C8-C9-C10
3	A	402	PLM	C8-C9-CA-CB
7	B	406	PC1	C2B-C2C-C2D-C2E
7	B	406	PC1	C23-C24-C25-C26
3	B	404	PLM	C4-C5-C6-C7
4	A	404	TWT	C14-C15-C16-C17
7	B	406	PC1	C2C-C2D-C2E-C2F
3	A	403	PLM	C6-C7-C8-C9
4	B	405	TWT	C15-C16-C17-C18
4	B	405	TWT	C14-C15-C16-C17
3	B	404	PLM	C7-C8-C9-CA
7	B	406	PC1	C32-C33-C34-C35
4	A	404	TWT	C11-C10-C9-C8
4	B	405	TWT	C5-C6-C7-C8
2	B	402	RET	C5-C6-C7-C8
5	A	405	BOG	C5'-C6'-C7'-C8'
4	B	405	TWT	C12-C13-C14-C15
3	A	403	PLM	C4-C5-C6-C7
7	B	406	PC1	C11-O13-P-O11
3	B	404	PLM	C9-CA-CB-CC
5	B	407	BOG	C1'-C2'-C3'-C4'

Continued on next page...

Continued from previous page...

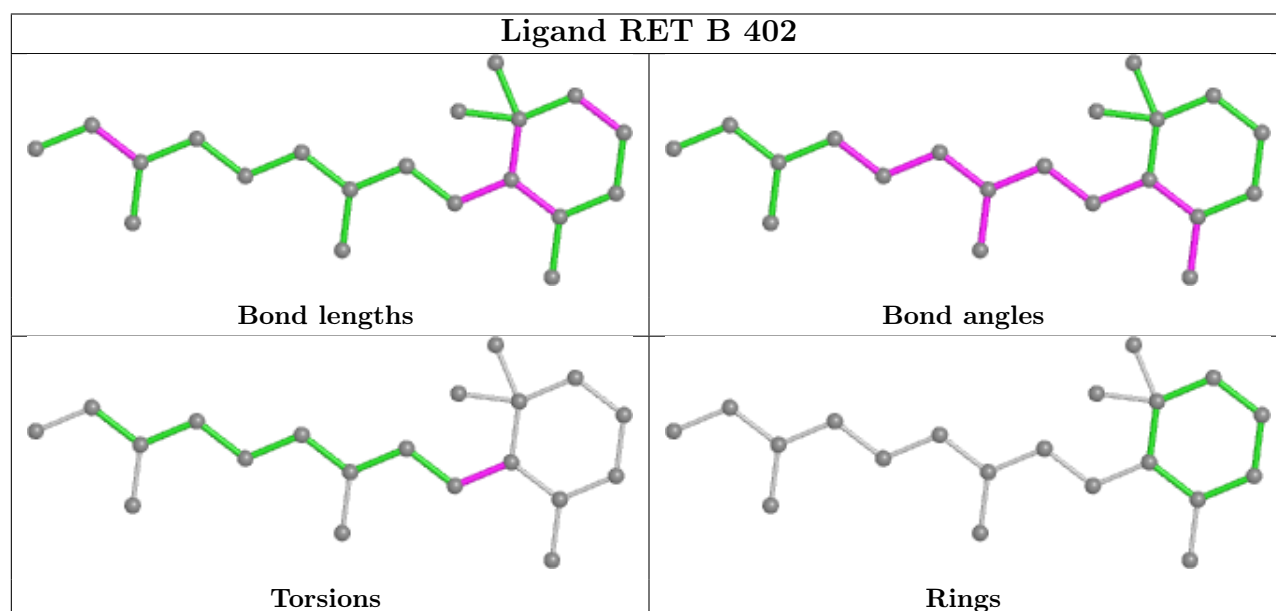
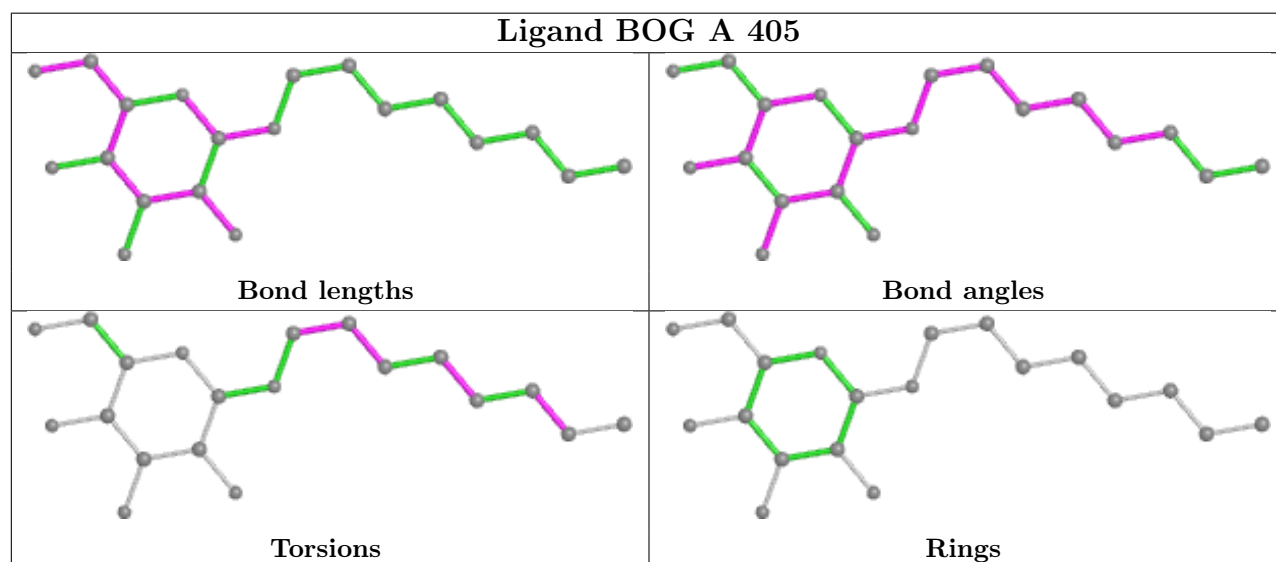
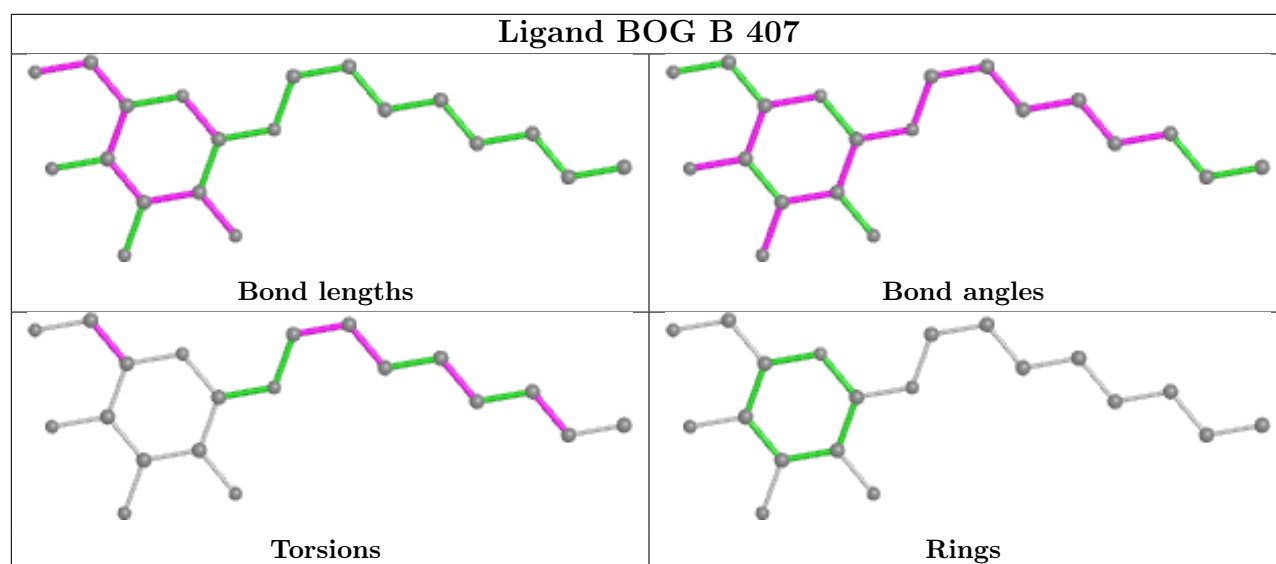
Mol	Chain	Res	Type	Atoms
5	B	407	BOG	C4-C5-C6-O6
5	B	407	BOG	O5-C5-C6-O6
4	A	404	TWT	C5-C6-C7-C8
5	B	407	BOG	C5'-C6'-C7'-C8'
7	B	406	PC1	O21-C21-C22-C23
4	A	404	TWT	C13-C14-C15-C16
5	A	405	BOG	C1'-C2'-C3'-C4'
7	B	406	PC1	O22-C21-C22-C23
3	A	402	PLM	CB-CC-CD-CE

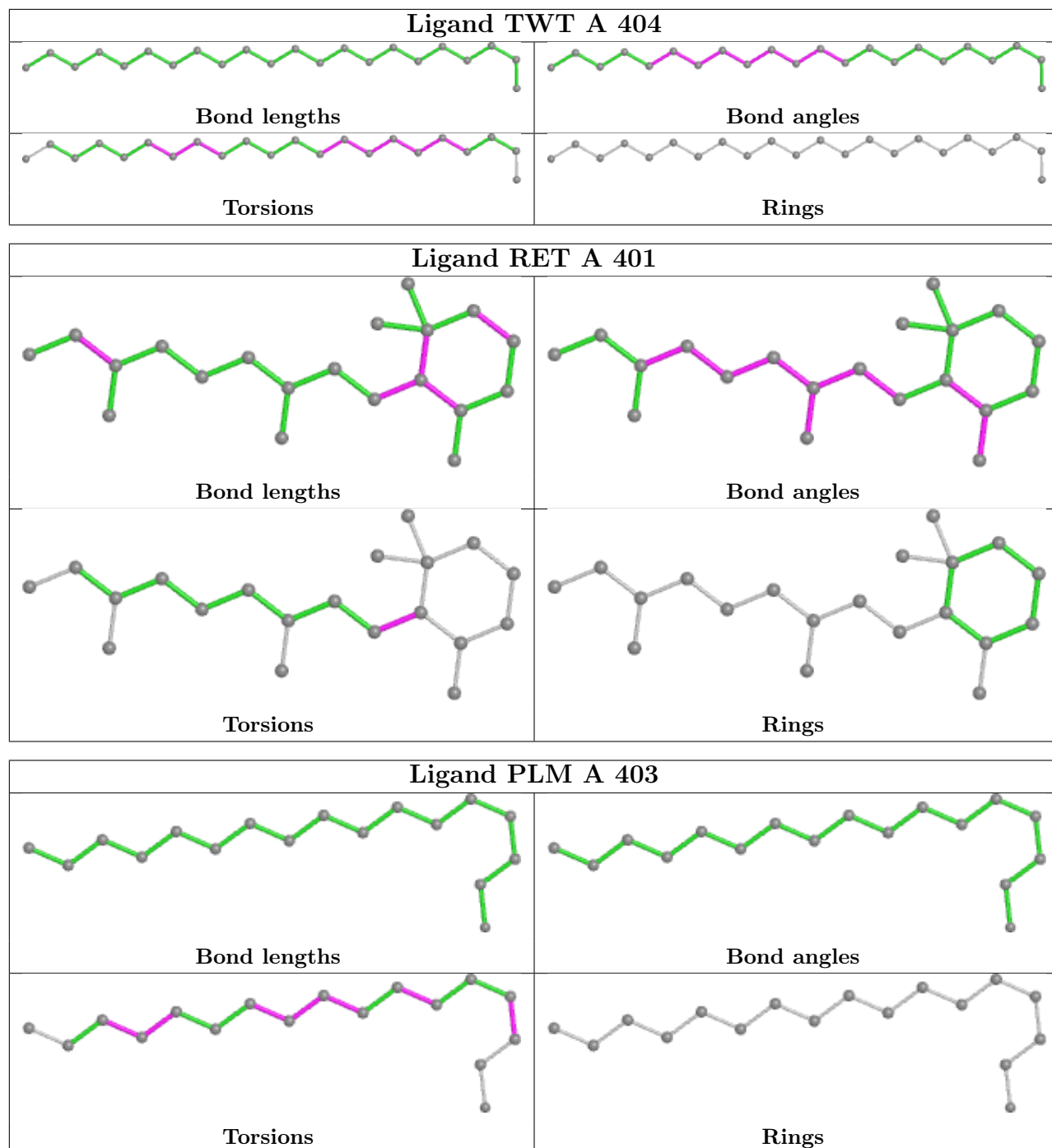
There are no ring outliers.

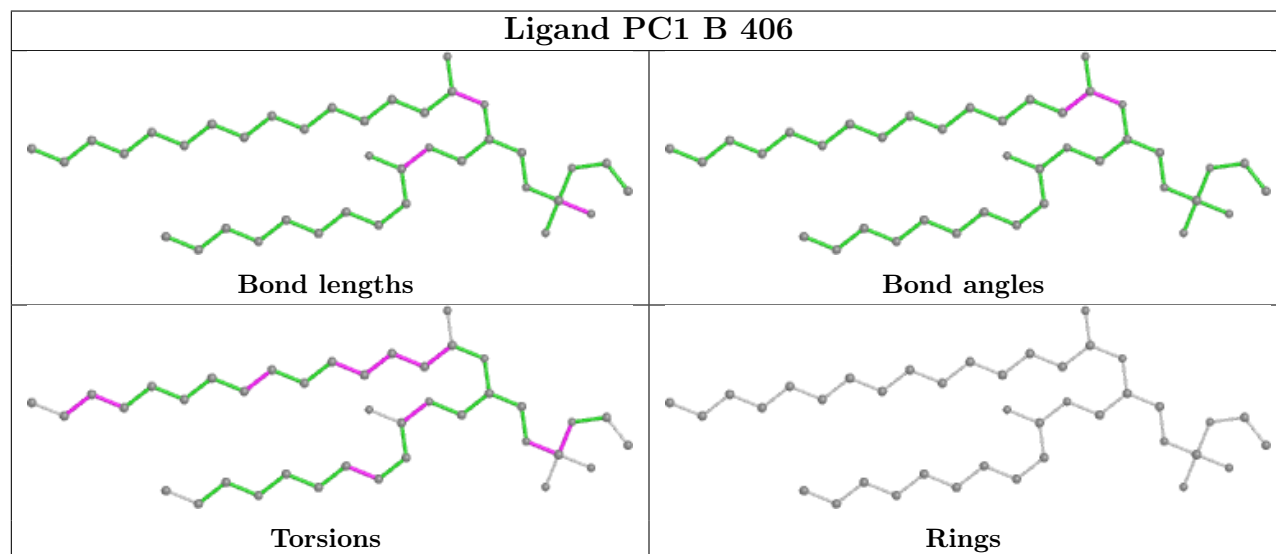
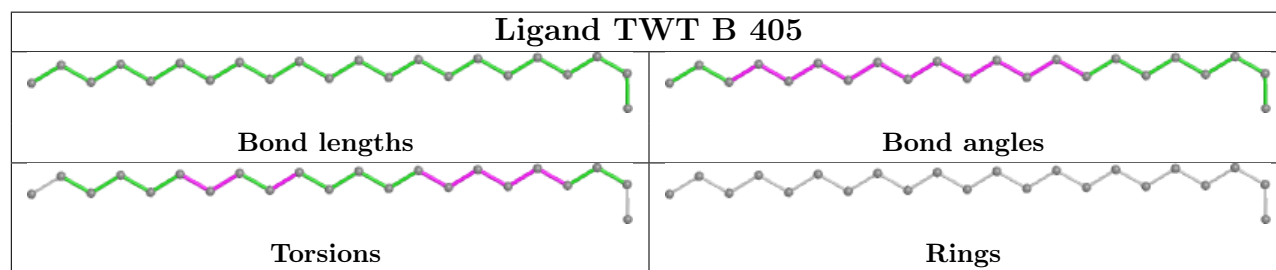
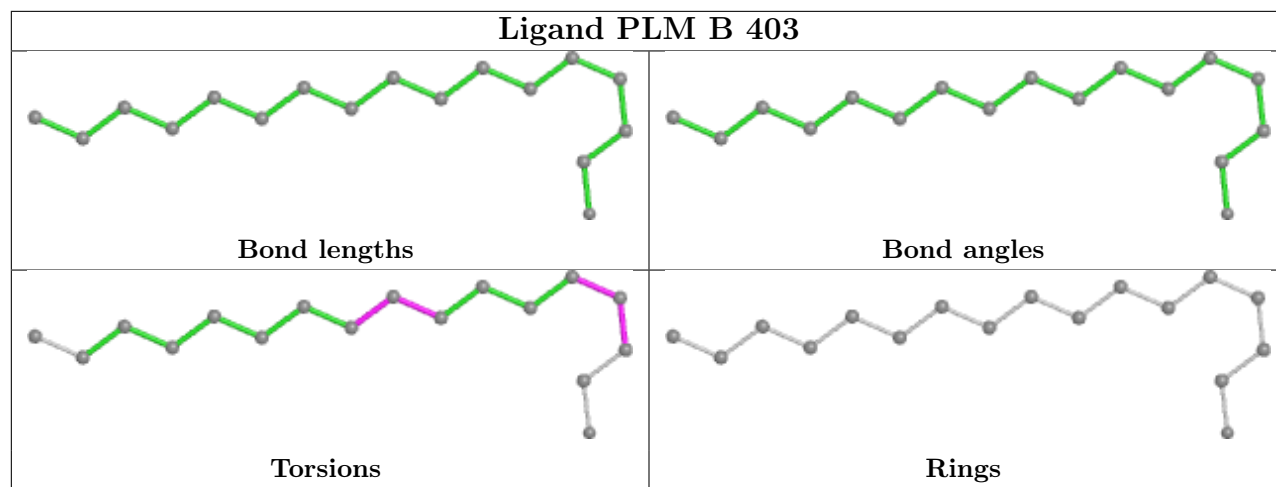
6 monomers are involved in 13 short contacts:

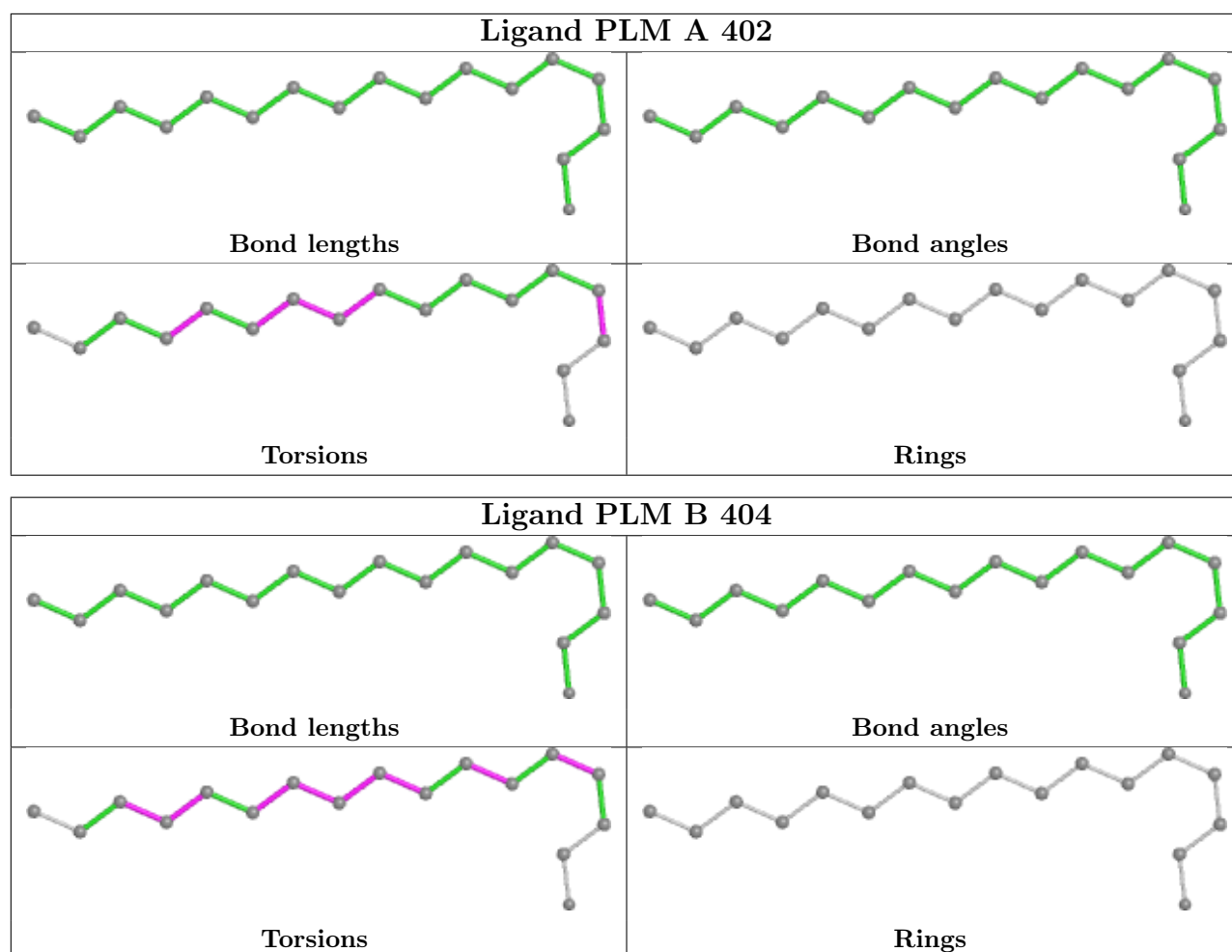
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	407	BOG	2	0
5	A	405	BOG	5	0
2	A	401	RET	3	0
3	A	403	PLM	1	0
7	B	406	PC1	1	0
3	B	404	PLM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/350 (100%)	-0.00	5 (1%) 75 70	33, 62, 145, 158	0
1	B	347/350 (99%)	-0.05	1 (0%) 94 93	32, 60, 124, 143	0
All	All	697/700 (99%)	-0.03	6 (0%) 84 80	32, 61, 135, 158	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	244	LYS	3.7
1	A	241	LEU	3.6
1	A	229	ASN	3.2
1	A	329	THR	2.5
1	A	246	LEU	2.1
1	B	240	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

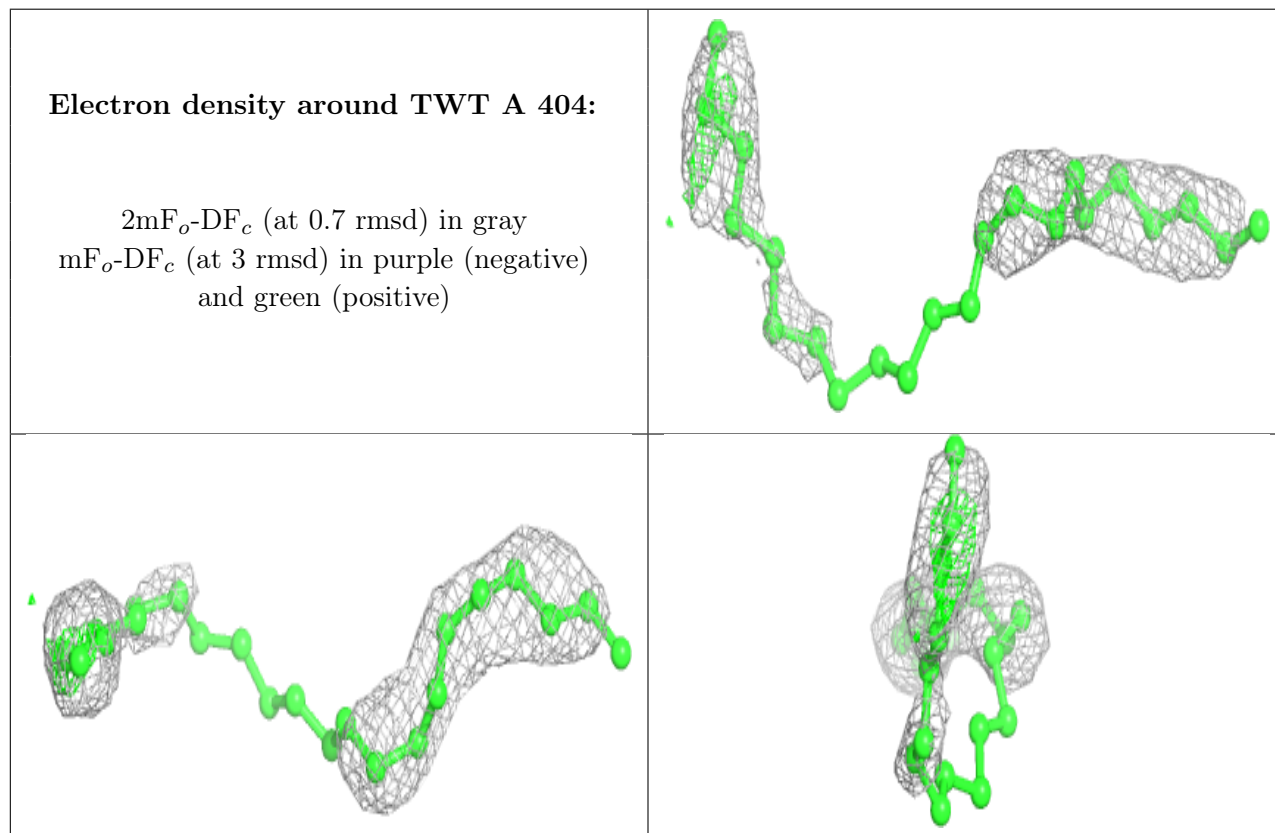
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

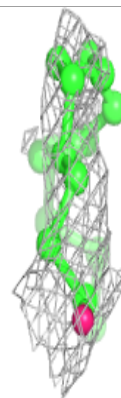
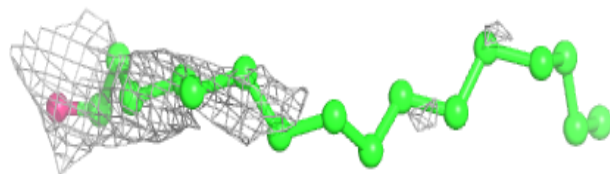
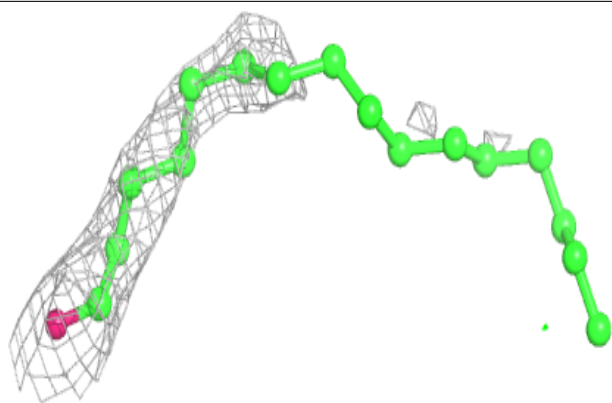
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	TWT	A	404	22/22	0.79	0.58	79,92,105,106	0
3	PLM	A	403	17/18	0.81	0.56	98,108,111,111	0
7	PC1	B	406	39/54	0.82	0.28	71,88,131,131	0
3	PLM	B	404	17/18	0.83	0.81	115,115,117,118	0
3	PLM	A	402	17/18	0.84	0.27	50,57,62,63	0
4	TWT	B	405	22/22	0.86	0.55	82,86,90,90	0
3	PLM	B	403	17/18	0.86	0.31	63,69,73,74	0
5	BOG	A	405	20/20	0.90	0.21	57,105,111,112	0
5	BOG	B	407	20/20	0.93	0.36	102,116,118,119	0
6	SO4	B	401	5/5	0.95	0.10	141,141,142,142	0
2	RET	A	401	20/21	0.97	0.26	45,50,53,53	0
2	RET	B	402	20/21	0.97	0.22	37,42,46,49	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

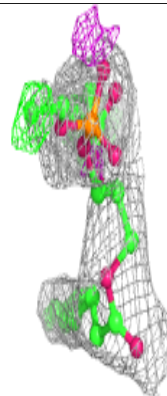
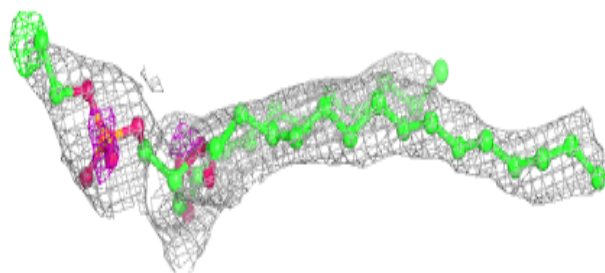
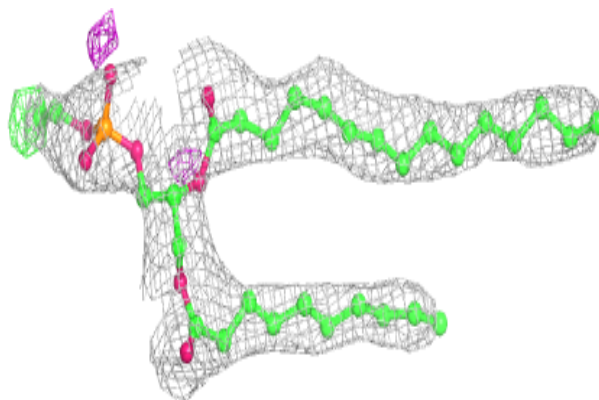


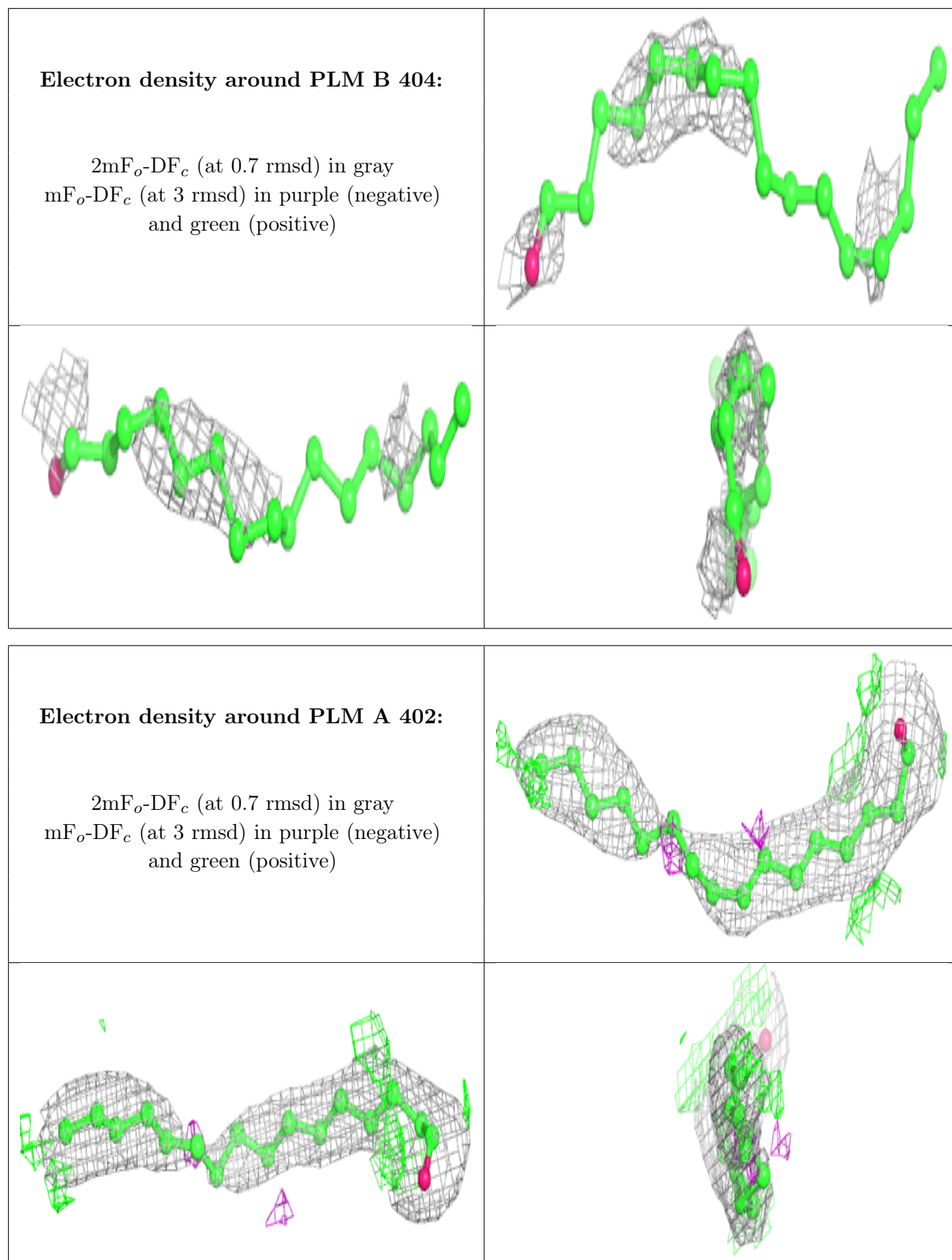
Electron density around PLM A 403:

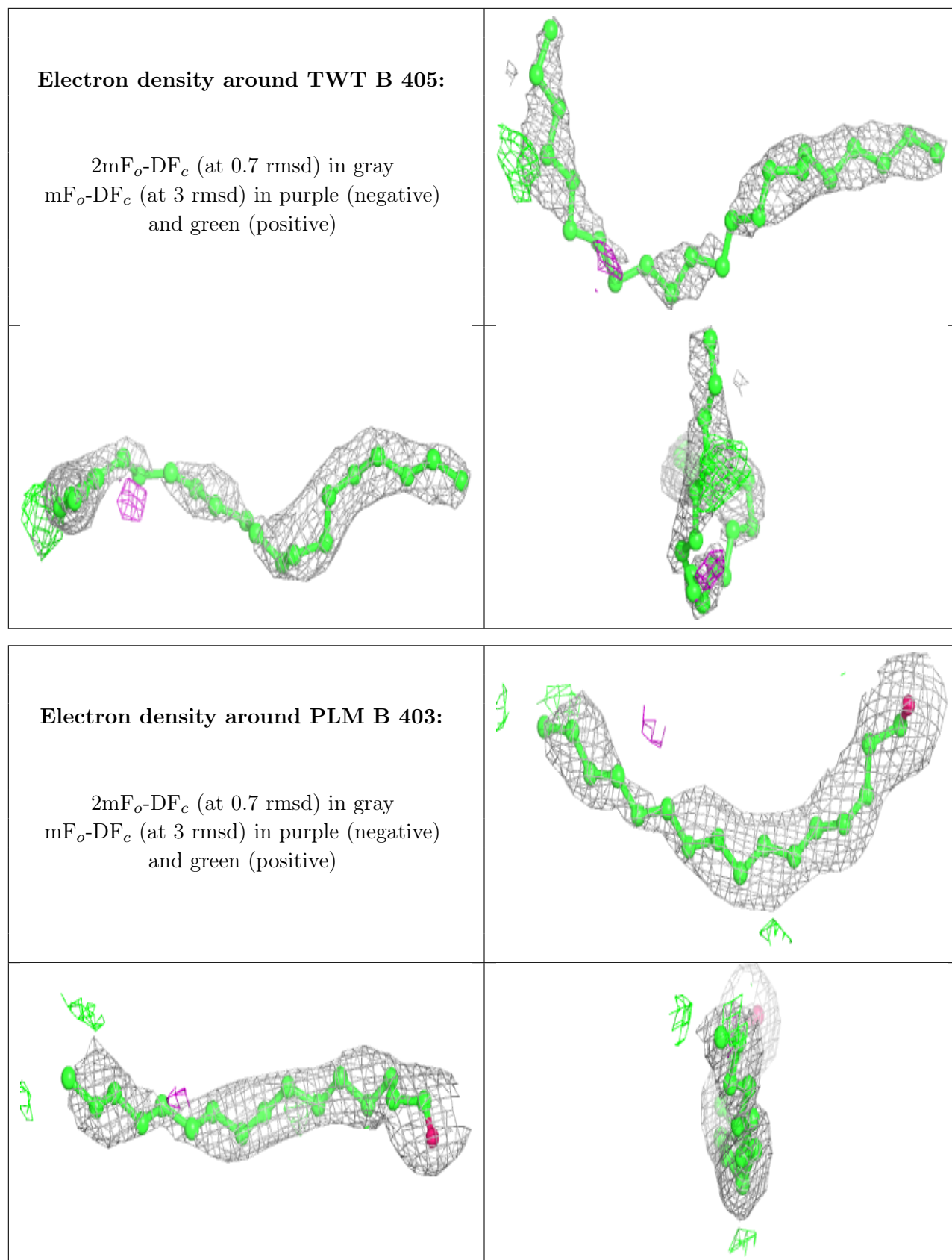
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PC1 B 406:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

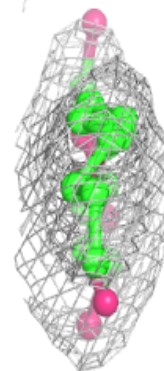
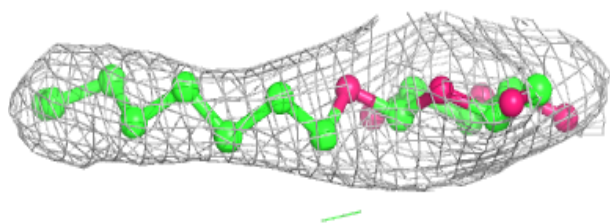
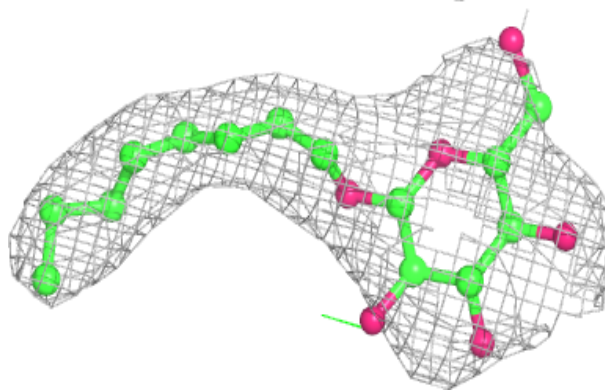




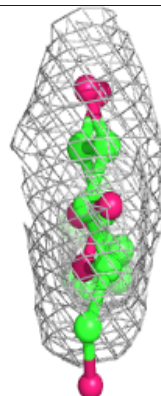
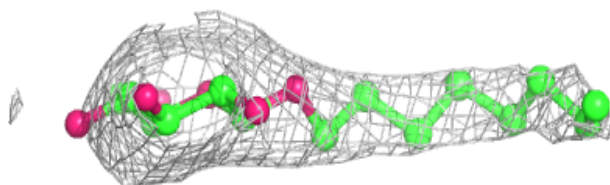
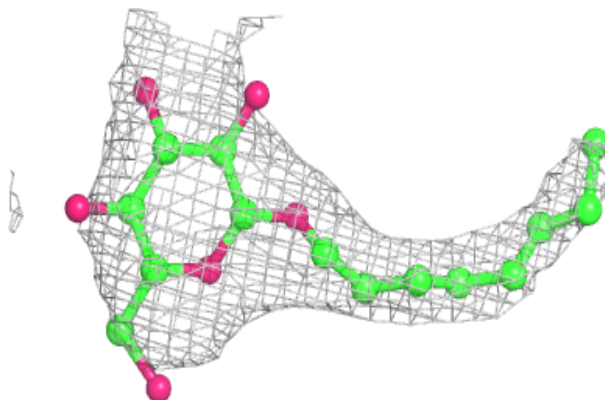


Electron density around BOG A 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

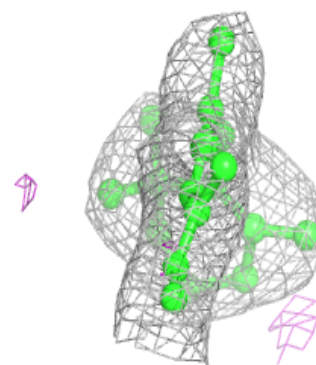
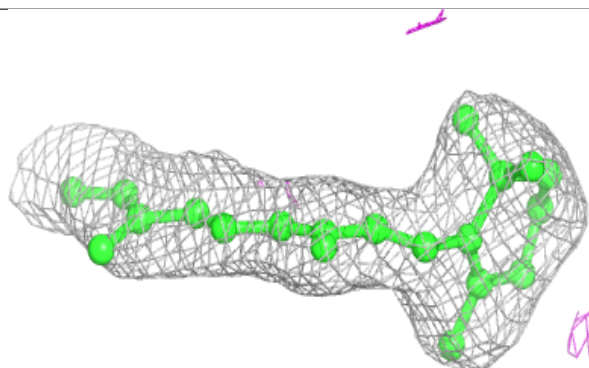
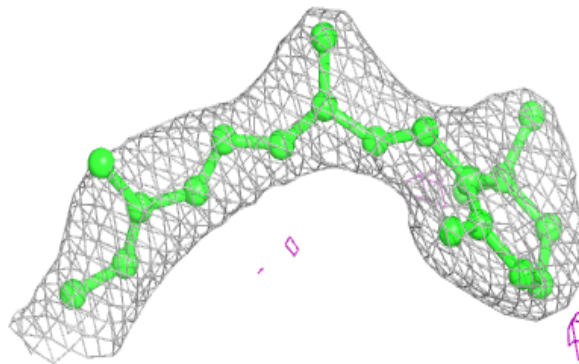
**Electron density around BOG B 407:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

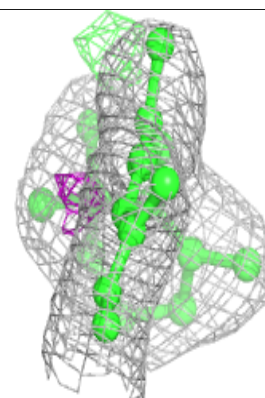
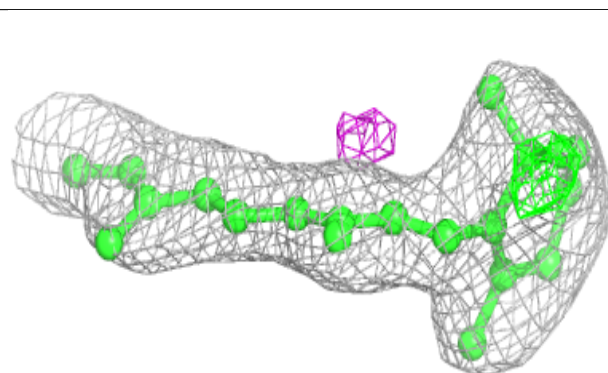
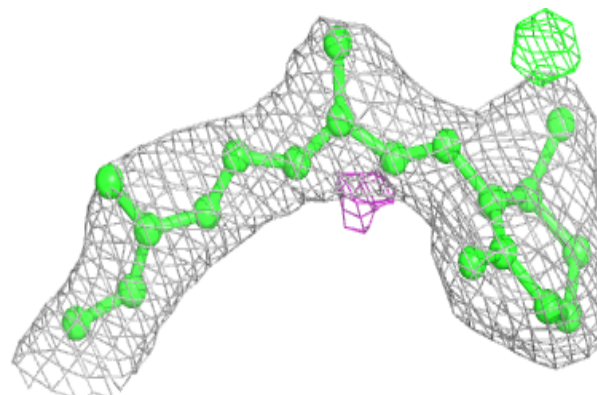


Electron density around RET A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around RET B 402:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.