



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 04:17 PM EDT

PDB ID : 4IRE  
Title : Crystal structure of GLIC with mutations at the loop C region  
Authors : Chen, Q.; Pan, J.; Liang, Y.H.; Xu, Y.; Tang, P.  
Deposited on : 2013-01-14  
Resolution : 3.19 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](mailto: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 : 2.35.1  
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) : 2.35.1

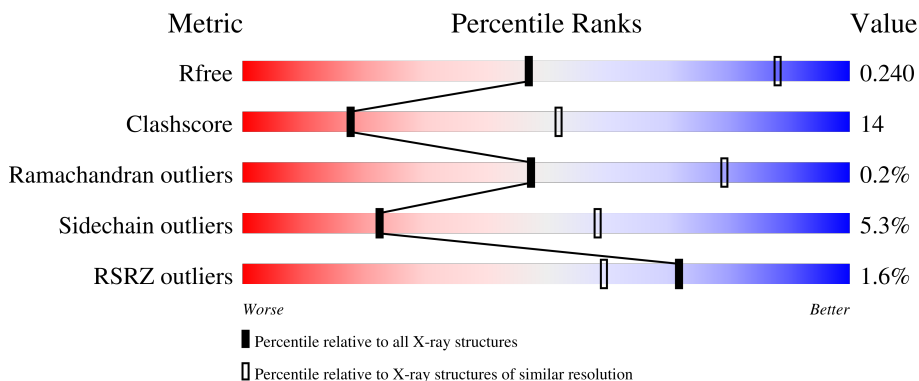
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	 2% 69% 28% ..
1	B	317	 % 70% 27% ..
1	C	317	 3% 69% 28% ..
1	D	317	 % 68% 30% ..
1	E	317	 % 71% 26% ..

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
2	LMD	E	404	-	-	-	X
3	PC1	A	402	-	-	-	X
3	PC1	B	401	-	-	-	X
3	PC1	C	403	-	-	-	X
3	PC1	C	404	-	-	-	X
3	PC1	D	502	-	-	-	X
3	PC1	E	405	-	-	-	X
3	PC1	E	406	-	-	-	X
4	OXL	A	406	-	X	-	-
4	OXL	B	404	-	X	-	-
4	OXL	C	405	-	X	-	-
4	OXL	C	406	-	X	-	-
4	OXL	D	504	-	X	-	-
4	OXL	D	505	-	X	-	-
4	OXL	D	506	-	X	-	-
4	OXL	D	507	-	X	-	-
4	OXL	E	407	-	X	-	-
4	OXL	E	408	-	X	-	-
4	OXL	E	409	-	-	X	-
4	OXL	E	410	-	X	-	-
5	ACT	B	406	-	-	-	X
5	ACT	E	411	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13440 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.

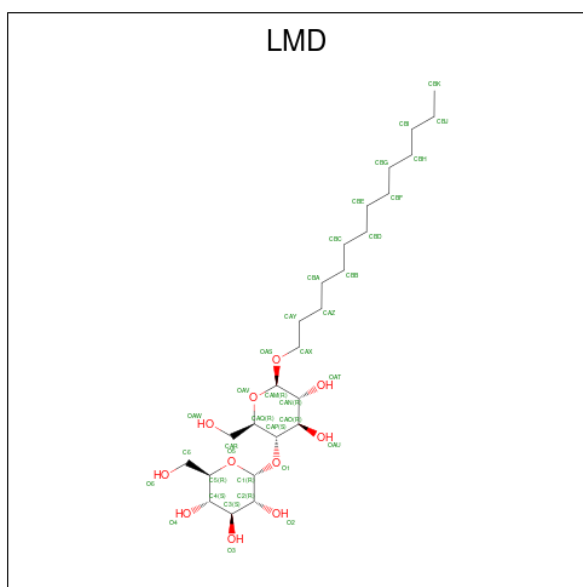
- Molecule 1 is a protein called Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	312	Total 2538	C 1672	N 409	O 452	S 5	0	1	0
1	B	313	Total 2542	C 1674	N 410	O 453	S 5	0	1	0
1	C	311	Total 2530	C 1667	N 408	O 451	S 4	0	1	0
1	D	313	Total 2542	C 1674	N 410	O 453	S 5	0	1	0
1	E	312	Total 2534	C 1669	N 409	O 452	S 4	0	1	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASN	ASP	engineered mutation	UNP Q7NDN8
A	177	GLN	GLU	engineered mutation	UNP Q7NDN8
A	178	ASN	ASP	engineered mutation	UNP Q7NDN8
B	91	ASN	ASP	engineered mutation	UNP Q7NDN8
B	177	GLN	GLU	engineered mutation	UNP Q7NDN8
B	178	ASN	ASP	engineered mutation	UNP Q7NDN8
C	91	ASN	ASP	engineered mutation	UNP Q7NDN8
C	177	GLN	GLU	engineered mutation	UNP Q7NDN8
C	178	ASN	ASP	engineered mutation	UNP Q7NDN8
D	91	ASN	ASP	engineered mutation	UNP Q7NDN8
D	177	GLN	GLU	engineered mutation	UNP Q7NDN8
D	178	ASN	ASP	engineered mutation	UNP Q7NDN8
E	91	ASN	ASP	engineered mutation	UNP Q7NDN8
E	177	GLN	GLU	engineered mutation	UNP Q7NDN8
E	178	ASN	ASP	engineered mutation	UNP Q7NDN8

- Molecule 2 is tetradecyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: LMD) (formula: C<sub>26</sub>H<sub>50</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			37	26	11		
2	C	1	Total	C	O	0	0
			37	26	11		
2	C	1	Total	C	O	0	0
			25	20	5		
2	E	1	Total	C	O	0	0
			21	19	2		
2	E	1	Total	C	O	0	0
			26	20	6		
2	E	1	Total	C	O	0	0
			37	26	11		

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 37	27	1	8	1	0	0
3	A	1	Total 39	29	1	8	1	0	0
3	B	1	Total 39	29	1	8	1	0	0
3	B	1	Total 38	28	1	8	1	0	0
3	C	1	Total 38	28	1	8	1	0	0
3	C	1	Total 32	22	1	8	1	0	0
3	D	1	Total 37	27	1	8	1	0	0
3	D	1	Total 37	27	1	8	1	0	0
3	E	1	Total 38	28	1	8	1	0	0
3	E	1	Total 38	28	1	8	1	0	0

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).



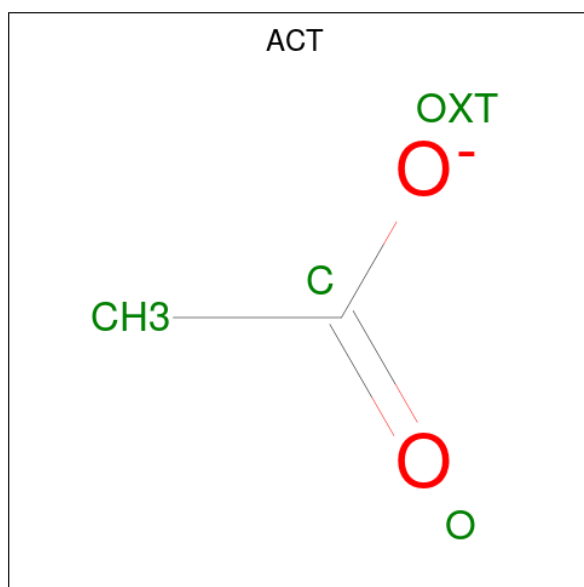
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 2 4	0	0
4	A	1	Total C O 6 2 4	0	0
4	A	1	Total C O 6 2 4	0	0
4	B	1	Total C O 6 2 4	0	0
4	B	1	Total C O 6 2 4	0	0
4	C	1	Total C O 6 2 4	0	0
4	C	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0
4	D	1	Total C O 6 2 4	0	0
4	E	1	Total C O 6 2 4	0	0
4	E	1	Total C O 6 2 4	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 6 2 4	0	0
4	E	1	Total C O 6 2 4	0	0
4	E	1	Total C O 6 2 4	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

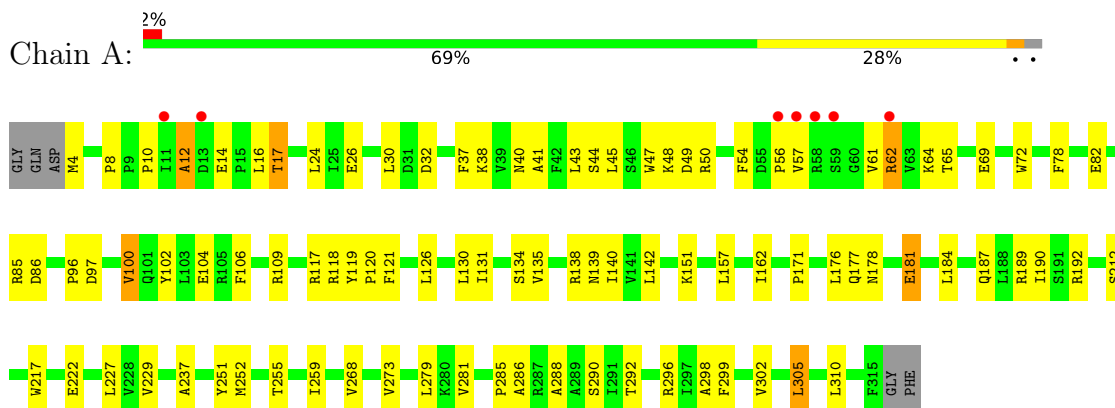
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	5		
6	B	12	Total	O	0	0
			12	12		
6	C	12	Total	O	0	0
			12	12		
6	D	12	Total	O	0	0
			12	12		
6	E	15	Total	O	0	0
			15	15		

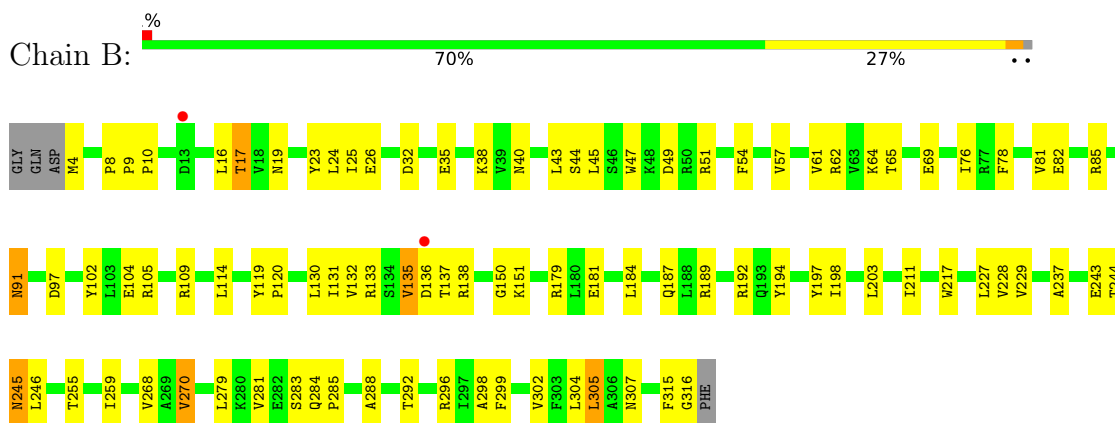
### 3 Residue-property plots [i](#)

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.

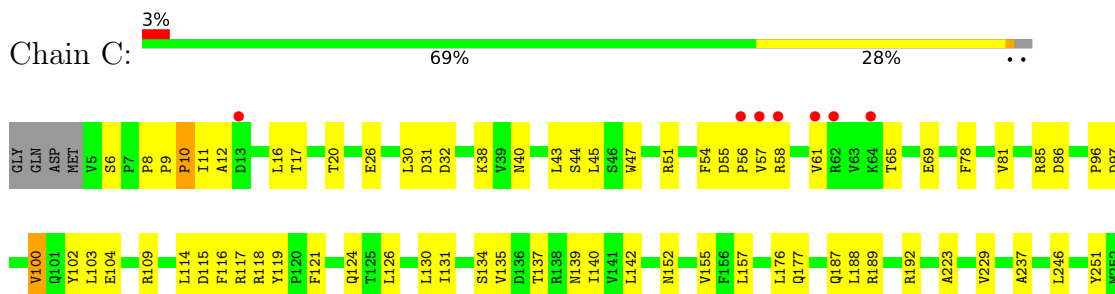
- Molecule 1: Proton-gated ion channel



- Molecule 1: Proton-gated ion channel

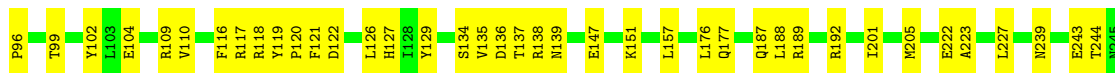


- Molecule 1: Proton-gated ion channel

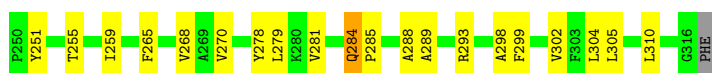
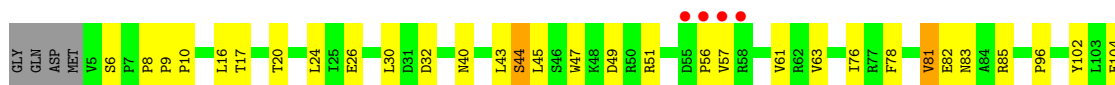




- Molecule 1: Proton-gated ion channel



- Molecule 1: Proton-gated ion channel



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.03Å 133.62Å 161.43Å 90.00° 102.57° 90.00°	Depositor
Resolution (Å)	29.86 – 3.19 29.86 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.86-3.19) 97.7 (29.86-3.19)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 3.18Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.204 , 0.243 0.204 , 0.240	Depositor DCC
$R_{free}$ test set	1000 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.0	Xtrriage
Anisotropy	0.259	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 62.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13440	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LMD, ACT, PC1, OXL

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	0.44	0/2609	0.64	0/3566
1	B	0.45	0/2613	0.61	0/3571
1	C	0.44	0/2601	0.64	0/3556
1	D	0.45	0/2613	0.62	0/3571
1	E	0.44	0/2605	0.63	0/3561
All	All	0.45	0/13041	0.63	0/17825

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	2538	0	2566	57	0
1	B	2542	0	2569	55	0
1	C	2530	0	2557	56	0
1	D	2542	0	2569	70	0
1	E	2534	0	2560	59	0
2	A	37	0	50	4	0
2	C	62	0	88	12	0
2	E	84	0	119	13	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	76	0	100	18	0
3	B	77	0	102	16	0
3	C	70	0	88	15	0
3	D	74	0	96	11	0
3	E	76	0	100	8	0
4	A	18	0	0	0	0
4	B	12	0	0	0	0
4	C	12	0	0	1	0
4	D	30	0	0	1	0
4	E	30	0	0	4	0
5	A	8	0	6	1	0
5	B	8	0	6	0	0
5	C	8	0	6	2	0
5	D	8	0	6	0	0
5	E	8	0	6	5	0
6	A	5	0	0	0	0
6	B	12	0	0	0	0
6	C	12	0	0	0	0
6	D	12	0	0	1	0
6	E	15	0	0	2	0
All	All	13440	0	13594	367	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 14.

All (367) 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)
3:A:403:PC1:H322	3:A:403:PC1:H241	1.34	1.06
1:E:131:ILE:HD13	5:E:411:ACT:CH3	1.88	1.01
1:E:131:ILE:CD1	5:E:411:ACT:H2	1.91	1.00
3:A:403:PC1:H261	3:A:403:PC1:H341	1.43	0.99
3:D:503:PC1:H281	3:D:503:PC1:H321	1.47	0.94
1:E:131:ILE:HD13	5:E:411:ACT:H2	0.94	0.92
3:C:404:PC1:H31	3:C:404:PC1:H251	1.52	0.90
3:B:401:PC1:H221	3:B:401:PC1:H31	1.61	0.82
3:C:403:PC1:H2A2	3:C:403:PC1:H361	1.63	0.79
3:D:503:PC1:H281	3:D:503:PC1:C32	2.13	0.79
2:C:402:LMD:H26	1:D:244:THR:HG21	1.65	0.78
1:D:26:GLU:HB2	1:D:40[B]:ASN:HB2	1.67	0.77
2:A:401:LMD:H7	2:E:401:LMD:H28	1.68	0.75

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:LMD:H12	2:E:401:LMD:H21	1.66	0.75
3:A:403:PC1:H241	3:A:403:PC1:H32	1.69	0.75
1:D:5:VAL:O	1:D:72:TRP:HB2	1.86	0.74
3:A:403:PC1:H341	3:A:403:PC1:C26	2.17	0.72
1:C:32:ASP:OD2	1:C:192:ARG:NH2	2.22	0.72
3:E:406:PC1:H252	3:E:406:PC1:H352	1.73	0.71
1:D:5:VAL:O	1:D:72:TRP:CD1	2.44	0.71
3:D:502:PC1:H322	3:D:502:PC1:H262	1.73	0.70
1:D:32:ASP:OD2	1:D:192:ARG:NH2	2.26	0.69
1:A:187:GLN:OE1	1:A:189:ARG:NH2	2.26	0.68
1:C:85:ARG:N	4:C:405:OXL:O4	2.22	0.68
1:C:26:GLU:HB2	1:C:40[B]:ASN:HB2	1.76	0.68
3:B:401:PC1:H221	3:B:401:PC1:H322	1.75	0.67
1:D:7:PRO:HG3	1:D:72:TRP:NE1	2.10	0.67
1:D:16:LEU:HD11	1:D:47:TRP:HB2	1.77	0.67
1:D:5:VAL:O	1:D:72:TRP:HD1	1.77	0.66
1:C:30:LEU:HD12	1:C:157:LEU:HD21	1.76	0.66
3:C:403:PC1:H262	3:C:403:PC1:C32	2.26	0.66
3:B:401:PC1:H322	3:B:401:PC1:H251	1.77	0.66
1:C:187:GLN:OE1	1:C:189:ARG:NH2	2.29	0.66
1:A:26:GLU:HB2	1:A:40[B]:ASN:HB2	1.76	0.65
1:A:237:ALA:HB2	2:C:401:LMD:H3	1.78	0.65
1:D:5:VAL:HG23	1:D:6:SER:N	2.12	0.65
1:C:131:ILE:HD13	5:C:407:ACT:H2	1.79	0.65
1:D:9:PRO:HD3	1:D:51:ARG:HH11	1.62	0.65
3:C:403:PC1:H342	3:C:403:PC1:H281	1.78	0.65
1:E:237:ALA:HA	2:E:404:LMD:H15	1.77	0.64
1:B:43:LEU:HB3	1:B:104:GLU:HG2	1.80	0.64
1:A:252:MET:H	3:A:403:PC1:H221	1.61	0.64
1:A:10:PRO:HD3	1:A:138:ARG:HD2	1.78	0.63
1:E:32:ASP:OD2	1:E:192:ARG:NH2	2.31	0.63
1:E:187:GLN:OE1	1:E:189:ARG:NH2	2.32	0.63
1:D:223:ALA:HB2	1:E:222:GLU:HG3	1.80	0.62
3:B:402:PC1:H322	3:B:402:PC1:H251	1.81	0.62
1:C:126:LEU:HB2	1:C:188:LEU:HB3	1.82	0.62
1:E:78:PHE:N	4:E:408:OXL:O3	2.29	0.62
1:A:32:ASP:OD2	1:A:192:ARG:NH2	2.32	0.62
1:B:187:GLN:OE1	1:B:189:ARG:NH2	2.33	0.61
3:E:406:PC1:H332	3:E:406:PC1:H232	1.81	0.61
3:A:403:PC1:H362	3:A:403:PC1:C28	2.31	0.61
1:D:85:ARG:N	4:D:504:OXL:O3	2.27	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:LEU:HB2	1:E:288:ALA:HB2	1.83	0.61
1:D:7:PRO:HG3	1:D:72:TRP:HE1	1.65	0.61
1:D:26:GLU:HB2	1:D:40[A]:ASN:HB3	1.82	0.61
1:C:16:LEU:HD11	1:C:47:TRP:HB2	1.82	0.61
1:D:268:VAL:HG12	1:D:299:PHE:HZ	1.66	0.61
1:B:268:VAL:HG12	1:B:299:PHE:HZ	1.66	0.61
1:D:176:LEU:HD12	1:D:177:GLN:HG3	1.83	0.60
1:D:9:PRO:HD3	1:D:51:ARG:NH1	2.16	0.60
1:E:6:SER:O	1:E:51:ARG:NH2	2.34	0.60
3:A:403:PC1:O32	3:A:403:PC1:H12	2.02	0.60
1:E:131:ILE:HG21	5:E:411:ACT:CH3	2.32	0.59
3:C:403:PC1:H361	3:C:403:PC1:C2A	2.31	0.58
1:E:45:LEU:HB2	1:E:102:TYR:HB3	1.84	0.58
1:C:47:TRP:O	1:C:100:VAL:HG23	2.04	0.58
1:C:279:LEU:HB2	1:C:288:ALA:HB2	1.86	0.58
1:E:268:VAL:HG12	1:E:299:PHE:HZ	1.68	0.58
1:D:45:LEU:HB2	1:D:102:TYR:HB3	1.85	0.58
1:E:16:LEU:HD11	1:E:47:TRP:HB2	1.86	0.58
1:D:134:SER:HB3	1:D:139:ASN:HA	1.85	0.58
1:A:78:PHE:HE2	1:A:85:ARG:HD3	1.68	0.58
2:A:401:LMD:H12	2:E:401:LMD:H27	1.84	0.58
1:D:279:LEU:HB2	1:D:288:ALA:HB2	1.85	0.58
3:C:403:PC1:H262	3:C:403:PC1:H321	1.85	0.57
1:E:10:PRO:HD3	1:E:138:ARG:HD2	1.85	0.57
1:E:298:ALA:O	1:E:302:VAL:HG23	2.04	0.57
3:D:503:PC1:H321	3:D:503:PC1:C28	2.29	0.57
3:E:406:PC1:O12	3:E:406:PC1:H31	2.05	0.57
1:E:43:LEU:HB3	1:E:104:GLU:HG2	1.86	0.57
1:A:54:PHE:CE1	1:A:96:PRO:HA	2.40	0.56
1:C:6:SER:O	1:C:51:ARG:NH2	2.36	0.56
1:A:16:LEU:HD11	1:A:47:TRP:HB2	1.88	0.56
1:C:55:ASP:HB3	1:C:58:ARG:HB3	1.88	0.56
1:B:24:LEU:HB2	1:B:151:LYS:HB2	1.88	0.56
1:A:78:PHE:CE2	1:A:85:ARG:HD3	2.41	0.56
1:D:254:TYR:OH	3:D:502:PC1:H341	2.05	0.56
1:A:56:PRO:HD3	1:A:96:PRO:HB3	1.86	0.56
1:A:45:LEU:HB2	1:A:102:TYR:HB3	1.87	0.56
1:B:45:LEU:HB2	1:B:102:TYR:HB3	1.88	0.56
3:C:404:PC1:H31	3:C:404:PC1:H222	1.87	0.56
3:C:403:PC1:H262	3:C:403:PC1:H322	1.88	0.55
1:A:268:VAL:HG12	1:A:299:PHE:HZ	1.72	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ASN:HB2	1:D:46:SER:HB3	1.87	0.55
1:B:268:VAL:HG12	1:B:299:PHE:CZ	2.42	0.55
1:B:198:ILE:HD11	3:B:401:PC1:H272	1.89	0.55
1:E:78:PHE:HE2	1:E:85:ARG:HD3	1.72	0.54
1:D:10:PRO:HD3	1:D:138:ARG:HD2	1.89	0.54
1:E:122:ASP:OD2	1:E:192:ARG:NH1	2.41	0.54
1:A:43:LEU:HB3	1:A:104:GLU:HG2	1.88	0.54
3:C:403:PC1:H281	3:C:403:PC1:C34	2.37	0.54
1:A:12:ALA:HB3	1:A:14:GLU:OE1	2.06	0.54
1:D:5:VAL:HG23	1:D:6:SER:H	1.72	0.54
1:E:255:THR:O	1:E:259:ILE:HG13	2.08	0.54
1:E:56:PRO:HD3	1:E:96:PRO:HB3	1.89	0.54
1:B:32:ASP:OD2	1:B:192:ARG:NH2	2.37	0.54
3:A:403:PC1:H32	3:A:403:PC1:C22	2.35	0.53
1:C:54:PHE:CE1	1:C:96:PRO:HA	2.42	0.53
1:C:152:ASN:HB3	1:C:155:VAL:HG23	1.89	0.53
1:E:152:ASN:ND2	6:E:509:HOH:O	2.42	0.53
1:E:131:ILE:HG21	5:E:411:ACT:H2	1.90	0.53
3:B:401:PC1:H31	3:B:401:PC1:C22	2.22	0.53
1:A:131:ILE:HD13	5:A:407:ACT:H2	1.90	0.53
1:B:237:ALA:HA	2:C:401:LMD:H14	1.91	0.53
1:C:56:PRO:HD3	1:C:96:PRO:HB3	1.91	0.53
1:C:237:ALA:HB2	2:E:402:LMD:H3	1.90	0.53
3:A:403:PC1:H12	3:A:403:PC1:C31	2.39	0.53
1:E:117:ARG:NH2	6:E:507:HOH:O	2.41	0.53
1:C:237:ALA:HA	2:C:402:LMD:H13	1.89	0.52
1:E:85:ARG:NH2	4:E:409:OXL:O3	2.42	0.52
3:A:403:PC1:H241	3:A:403:PC1:C32	2.24	0.52
1:D:16:LEU:HD12	1:D:17:THR:N	2.24	0.52
1:D:239:ASN:ND2	1:D:243:GLU:OE1	2.43	0.52
1:A:16:LEU:HD12	1:A:17:THR:N	2.25	0.52
1:C:268:VAL:HG12	1:C:299:PHE:HZ	1.74	0.52
3:A:403:PC1:H32	3:A:403:PC1:C24	2.38	0.52
1:C:8:PRO:HG2	1:C:16:LEU:HD22	1.92	0.52
1:D:285:PRO:HA	1:D:288:ALA:HB3	1.92	0.52
1:A:47:TRP:O	1:A:100:VAL:HG23	2.09	0.51
1:E:126:LEU:HB2	1:E:188:LEU:HB3	1.93	0.51
1:C:289:ALA:O	1:C:293:ARG:HB2	2.11	0.51
1:C:116:PHE:O	1:C:253:THR:HG22	2.11	0.51
1:E:81:VAL:HB	1:E:83:ASN:O	2.10	0.51
1:A:26:GLU:HB2	1:A:40[A]:ASN:HB3	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:LYS:NZ	1:C:109:ARG:HD2	2.26	0.50
2:A:401:LMD:H26	1:B:244:THR:HG21	1.92	0.50
1:D:118:ARG:O	1:D:121:PHE:N	2.38	0.50
1:E:85:ARG:HH22	4:E:409:OXL:C2	2.25	0.50
1:E:228:VAL:HG11	1:E:270:VAL:HG23	1.93	0.50
1:E:245:ASN:ND2	2:E:404:LMD:OAT	2.44	0.50
1:A:176:LEU:HD12	1:A:177:GLN:HG3	1.93	0.50
1:B:78:PHE:CE2	1:B:85:ARG:HD3	2.46	0.50
1:E:82:GLU:HG3	1:E:109:ARG:HD3	1.93	0.50
1:D:298:ALA:O	1:D:302:VAL:HG23	2.12	0.49
1:B:120:PRO:HB2	1:B:192:ARG:HD3	1.95	0.49
1:D:8:PRO:HB3	1:D:49:ASP:OD1	2.12	0.49
1:A:62:ARG:H	1:A:62:ARG:NE	2.11	0.49
1:E:16:LEU:HD12	1:E:17:THR:N	2.28	0.49
1:E:78:PHE:CE2	1:E:85:ARG:HD3	2.47	0.49
1:A:268:VAL:HG12	1:A:299:PHE:CZ	2.46	0.49
1:A:24:LEU:HB2	1:A:151:LYS:HB2	1.95	0.49
1:A:131:ILE:HD11	1:A:181:GLU:HG2	1.94	0.49
1:B:61:VAL:HG21	1:B:64:LYS:HG2	1.94	0.49
3:C:403:PC1:C32	3:C:403:PC1:H242	2.42	0.49
1:D:78:PHE:HE2	1:D:85:ARG:HD3	1.78	0.49
1:A:212:SER:HA	1:A:227:LEU:HD22	1.95	0.48
1:D:43:LEU:HB3	1:D:104:GLU:HG2	1.95	0.48
1:B:315:PHE:CD1	1:B:315:PHE:N	2.81	0.48
1:E:26:GLU:HB2	1:E:40[B]:ASN:HB2	1.95	0.48
1:E:240:ILE:HD13	2:E:402:LMD:H18	1.94	0.48
1:A:118:ARG:O	1:A:121:PHE:N	2.40	0.48
1:C:55:ASP:HB2	1:C:58:ARG:HH21	1.79	0.48
1:A:54:PHE:CZ	1:A:64:LYS:HG3	2.49	0.48
1:C:30:LEU:HB2	1:C:157:LEU:HD11	1.95	0.48
1:D:54:PHE:CE1	1:D:96:PRO:HA	2.49	0.48
1:D:78:PHE:CE2	1:D:85:ARG:HD3	2.49	0.48
1:E:198:ILE:HD11	3:E:405:PC1:H281	1.96	0.48
1:B:279:LEU:HB2	1:B:288:ALA:HB2	1.95	0.48
1:E:8:PRO:HA	1:E:9:PRO:HD3	1.64	0.48
1:A:38:LYS:NZ	1:A:109:ARG:HD2	2.28	0.48
1:B:91:ASN:OD1	5:C:408:ACT:H1	2.14	0.48
1:D:30:LEU:HD12	1:D:157:LEU:HD21	1.96	0.48
1:E:152:ASN:HB3	1:E:155:VAL:HG23	1.96	0.48
1:C:115:ASP:O	1:C:124:GLN:NE2	2.48	0.47
3:B:402:PC1:H111	3:B:402:PC1:H143	1.54	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:VAL:HG12	1:D:299:PHE:CZ	2.48	0.47
1:E:8:PRO:HB3	1:E:49:ASP:OD1	2.13	0.47
1:A:298:ALA:O	1:A:302:VAL:HG23	2.14	0.47
1:B:78:PHE:HE2	1:B:85:ARG:HD3	1.79	0.47
1:D:127:HIS:HD1	1:D:129:TYR:HH	1.58	0.47
2:E:404:LMD:H2	2:E:404:LMD:H8	1.56	0.47
1:B:298:ALA:O	1:B:302:VAL:HG23	2.13	0.47
3:B:402:PC1:H292	3:B:402:PC1:H342	1.97	0.47
1:D:5:VAL:CG2	1:D:6:SER:N	2.78	0.47
1:A:292:THR:O	1:A:296:ARG:HG3	2.14	0.47
3:A:402:PC1:H143	3:A:402:PC1:O14	2.15	0.47
1:D:7:PRO:O	1:D:51:ARG:NH1	2.48	0.47
1:B:119:TYR:CE2	1:B:246:LEU:HD11	2.49	0.47
1:D:297:ILE:O	1:D:301:VAL:HG23	2.15	0.47
1:A:14:GLU:OE1	1:A:14:GLU:N	2.48	0.46
1:A:48:LYS:HE2	1:A:48:LYS:HB3	1.78	0.46
1:A:8:PRO:HB3	1:A:49:ASP:OD1	2.14	0.46
1:B:16:LEU:HD11	1:B:47:TRP:HB2	1.97	0.46
1:B:135:VAL:HG12	1:B:136:ASP:H	1.80	0.46
2:C:402:LMD:H8	2:E:401:LMD:H25	1.97	0.46
1:A:82:GLU:HG3	1:A:109:ARG:HD3	1.97	0.46
3:A:403:PC1:H362	3:A:403:PC1:H282	1.97	0.46
3:C:404:PC1:H251	3:C:404:PC1:C3	2.35	0.46
3:B:401:PC1:H112	3:B:401:PC1:H152	1.70	0.46
1:D:119:TYR:CE2	1:D:246:LEU:HD11	2.51	0.46
1:B:211:ILE:HG22	1:B:227:LEU:HD21	1.98	0.46
1:E:142:LEU:O	1:E:171:PRO:HG3	2.16	0.46
1:A:142:LEU:O	1:A:171:PRO:HG3	2.15	0.46
1:A:305:LEU:HD22	1:A:305:LEU:HA	1.78	0.46
1:B:245:ASN:HD21	2:C:401:LMD:H49	1.79	0.46
1:C:118:ARG:O	1:C:121:PHE:N	2.38	0.46
1:D:55:ASP:HA	1:D:56:PRO:HD2	1.85	0.46
1:D:126:LEU:HB2	1:D:188:LEU:HB3	1.97	0.46
1:A:279:LEU:HB2	1:A:288:ALA:HB2	1.97	0.46
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.84	0.46
1:B:8:PRO:HB3	1:B:49:ASP:OD1	2.16	0.45
3:B:402:PC1:H252	3:B:402:PC1:H221	1.41	0.45
1:D:38:LYS:NZ	1:D:109:ARG:HD2	2.31	0.45
1:C:10:PRO:HB2	1:C:12:ALA:O	2.16	0.45
3:E:405:PC1:C25	3:E:405:PC1:H322	2.47	0.45
1:A:4:MET:O	1:A:72:TRP:HB2	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:HG3	1:B:109:ARG:HD3	1.99	0.45
1:C:8:PRO:CG	1:C:16:LEU:HD22	2.45	0.45
3:C:404:PC1:H251	3:C:404:PC1:H222	1.43	0.45
1:D:255:THR:O	1:D:259:ILE:HG13	2.15	0.45
3:D:503:PC1:H251	3:D:503:PC1:H221	1.42	0.45
3:E:406:PC1:H332	3:E:406:PC1:C23	2.46	0.45
1:A:285:PRO:HA	1:A:288:ALA:HB3	1.98	0.45
1:D:117:ARG:HG3	1:D:251:TYR:CE2	2.51	0.45
1:B:307:ASN:OD1	3:B:401:PC1:H392	2.17	0.45
3:B:402:PC1:H272	3:B:402:PC1:C34	2.46	0.45
3:C:403:PC1:H322	3:C:403:PC1:C26	2.46	0.45
1:E:310:LEU:HD23	1:E:310:LEU:HA	1.68	0.45
1:D:223:ALA:O	1:D:227:LEU:HB2	2.16	0.45
1:B:133:ARG:CZ	1:B:179:ARG:HB2	2.47	0.45
1:C:45:LEU:HB2	1:C:102:TYR:HB3	1.98	0.45
1:A:252:MET:N	3:A:403:PC1:H221	2.31	0.45
3:A:403:PC1:H322	3:A:403:PC1:H32	1.61	0.44
1:C:268:VAL:O	1:C:271:ILE:N	2.51	0.44
1:B:203:LEU:HA	1:B:203:LEU:HD23	1.63	0.44
1:D:252:MET:HB2	3:D:503:PC1:H242	2.00	0.44
2:E:401:LMD:H23	2:E:401:LMD:H16	1.62	0.44
1:D:310:LEU:HD23	1:D:310:LEU:HA	1.83	0.44
1:E:24:LEU:HB2	1:E:151:LYS:HB2	1.98	0.44
1:B:8:PRO:HA	1:B:9:PRO:HD3	1.63	0.44
1:E:176:LEU:HD12	1:E:177:GLN:HG3	2.00	0.44
1:E:289:ALA:O	1:E:293:ARG:HB2	2.18	0.44
1:B:16:LEU:HD12	1:B:17:THR:N	2.33	0.44
3:A:403:PC1:H32	3:A:403:PC1:H222	2.00	0.44
1:B:292:THR:O	1:B:296:ARG:HG3	2.17	0.44
1:C:223:ALA:HB2	1:D:222:GLU:HG3	2.00	0.44
1:D:37:PHE:CE1	1:D:110:VAL:HB	2.53	0.44
2:E:404:LMD:H18	2:E:404:LMD:H12	1.63	0.44
3:A:402:PC1:H152	3:A:402:PC1:H111	1.41	0.44
1:B:228:VAL:HG11	1:B:270:VAL:HG23	2.00	0.44
1:C:287:ARG:HA	1:C:287:ARG:HD2	1.84	0.44
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.72	0.44
3:B:401:PC1:H331	3:B:401:PC1:H361	1.87	0.43
1:D:187:GLN:OE1	1:D:189:ARG:NH2	2.51	0.43
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.61	0.43
1:B:38:LYS:NZ	1:B:109:ARG:HD2	2.32	0.43
1:C:119:TYR:CE2	1:C:246:LEU:HD11	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:SER:OG	1:D:99:THR:HB	2.18	0.43
1:B:76:ILE:HD13	1:B:132:VAL:HB	1.99	0.43
1:B:131:ILE:HD11	1:B:181:GLU:HB3	2.00	0.43
1:D:7:PRO:C	1:D:51:ARG:HH12	2.22	0.43
1:D:56:PRO:O	1:D:60:GLY:N	2.45	0.43
1:D:249:THR:HB	1:D:251:TYR:CE1	2.53	0.43
1:A:217:TRP:CH2	1:A:296:ARG:HB3	2.53	0.43
1:A:30:LEU:HD12	1:A:157:LEU:HD21	2.00	0.43
1:A:255:THR:O	1:A:259:ILE:HG13	2.18	0.43
1:B:255:THR:O	1:B:259:ILE:HG13	2.19	0.43
1:B:35:GLU:HG2	1:B:114:LEU:HG	1.99	0.43
1:B:43:LEU:HB3	1:B:104:GLU:CG	2.47	0.43
1:D:43:LEU:HB3	1:D:104:GLU:CG	2.48	0.43
1:D:119:TYR:HA	1:D:120:PRO:HA	1.67	0.43
3:E:405:PC1:H142	3:E:405:PC1:H112	1.87	0.43
1:B:119:TYR:HA	1:B:120:PRO:HA	1.69	0.43
1:D:315:PHE:CD1	1:D:315:PHE:N	2.87	0.43
1:B:26:GLU:HB2	1:B:40[B]:ASN:HB2	2.00	0.43
1:C:117:ARG:HG3	1:C:251:TYR:CE1	2.54	0.43
1:D:147:GLU:HB2	6:D:602:HOH:O	2.18	0.43
1:D:289:ALA:O	1:D:293:ARG:HB2	2.19	0.43
1:A:117:ARG:HG3	1:A:251:TYR:CE2	2.53	0.42
1:B:184:LEU:HA	1:B:184:LEU:HD23	1.81	0.42
1:B:217:TRP:CH2	1:B:296:ARG:HB3	2.54	0.42
1:C:278:TYR:O	1:C:281:VAL:HG12	2.18	0.42
2:C:401:LMD:OAW	2:C:402:LMD:H36	2.19	0.42
3:C:403:PC1:H242	3:C:403:PC1:O31	2.18	0.42
1:D:315:PHE:O	3:D:502:PC1:H122	2.19	0.42
1:D:24:LEU:HB2	1:D:151:LYS:HB2	2.00	0.42
1:E:205:MET:HE2	1:E:238:PHE:HB3	2.01	0.42
1:A:48:LYS:HD2	1:A:50:ARG:CZ	2.50	0.42
1:A:286:ALA:O	1:A:290:SER:HB3	2.19	0.42
1:B:284:GLN:N	1:B:285:PRO:HD3	2.34	0.42
1:C:20:THR:HG21	1:C:142:LEU:HD22	2.01	0.42
1:C:268:VAL:HG12	1:C:299:PHE:CZ	2.54	0.42
2:C:401:LMD:H5	2:C:401:LMD:H11	1.45	0.42
1:D:201:ILE:HG22	1:D:205:MET:HE3	2.01	0.42
1:E:284:GLN:N	1:E:285:PRO:HD3	2.34	0.42
1:A:37:PHE:CD1	1:A:126:LEU:HD13	2.54	0.42
1:A:119:TYR:HA	1:A:120:PRO:HA	1.72	0.42
1:C:130:LEU:HD23	1:C:130:LEU:HA	1.82	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:VAL:HG12	1:E:136:ASP:H	1.84	0.42
1:B:305:LEU:HD22	1:B:305:LEU:HA	1.87	0.42
1:A:43:LEU:HB3	1:A:104:GLU:CG	2.48	0.42
1:B:76:ILE:HG22	1:B:130:LEU:HD22	2.01	0.42
1:C:38:LYS:HZ3	1:C:109:ARG:HD2	1.84	0.42
1:D:260:PHE:O	1:D:263:TYR:HB2	2.20	0.42
3:D:502:PC1:H111	3:D:502:PC1:H152	1.72	0.42
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.86	0.42
2:E:401:LMD:H23	2:E:402:LMD:H14	2.01	0.42
3:A:403:PC1:H111	3:A:403:PC1:H142	1.56	0.42
1:B:315:PHE:HA	1:B:316:GLY:HA2	1.71	0.42
1:C:78:PHE:HE2	1:C:85:ARG:HD3	1.85	0.42
1:C:298:ALA:O	1:C:302:VAL:HG23	2.19	0.42
1:D:315:PHE:O	3:D:502:PC1:H143	2.20	0.42
1:E:26:GLU:HB2	1:E:40[A]:ASN:HB3	2.00	0.42
1:B:10:PRO:HD3	1:B:138:ARG:HD2	2.02	0.42
1:A:162:ILE:HA	1:A:190:ILE:HG22	2.02	0.42
1:B:25:ILE:HG21	1:B:105:ARG:HH21	1.85	0.42
1:D:8:PRO:HB3	1:D:49:ASP:HA	2.00	0.42
1:D:122:ASP:OD1	1:D:122:ASP:N	2.53	0.42
1:E:278:TYR:O	1:E:281:VAL:HG12	2.20	0.42
1:A:184:LEU:HD23	1:A:184:LEU:HA	1.75	0.41
1:C:55:ASP:HA	1:C:56:PRO:HD2	1.86	0.41
1:E:30:LEU:HD12	1:E:157:LEU:HD21	2.02	0.41
1:B:54:PHE:CZ	1:B:64:LYS:HG3	2.56	0.41
1:C:134:SER:HB3	1:C:139:ASN:HA	2.02	0.41
1:C:310:LEU:HD23	1:C:310:LEU:HA	1.67	0.41
1:D:116:PHE:O	1:D:253:THR:HG22	2.20	0.41
1:C:43:LEU:O	1:C:103:LEU:HD12	2.20	0.41
3:D:502:PC1:H2A1	3:D:502:PC1:H351	2.02	0.41
1:B:283:SER:C	1:B:285:PRO:HD3	2.40	0.41
1:E:213:TRP:HZ2	1:E:265:PHE:HD2	1.69	0.41
1:B:130:LEU:HA	1:B:130:LEU:HD23	1.77	0.41
3:B:401:PC1:H361	3:B:401:PC1:H282	2.02	0.41
1:C:9:PRO:HD3	1:C:51:ARG:HH11	1.85	0.41
2:C:401:LMD:H40	2:C:401:LMD:H33	1.76	0.41
1:B:4:MET:HG3	1:B:51:ARG:HH21	1.86	0.41
1:B:23:TYR:HA	1:B:150:GLY:O	2.20	0.41
1:C:30:LEU:HD23	1:C:31:ASP:N	2.36	0.41
1:C:43:LEU:HB3	1:C:104:GLU:CG	2.51	0.41
1:C:176:LEU:HD12	1:C:177:GLN:HG3	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:ALA:HB2	2:C:402:LMD:H6	2.03	0.41
1:C:267:PHE:O	1:C:271:ILE:HG12	2.20	0.41
3:C:404:PC1:H111	3:C:404:PC1:H152	1.64	0.41
1:E:20:THR:HA	1:E:44:SER:O	2.21	0.41
1:E:76:ILE:HG22	1:E:130:LEU:HD22	2.03	0.41
1:A:134:SER:HB3	1:A:139:ASN:HA	2.03	0.41
2:A:401:LMD:H3	2:A:401:LMD:H9	1.73	0.41
1:B:217:TRP:CE2	1:B:296:ARG:HD3	2.56	0.41
1:C:30:LEU:HD21	1:C:114:LEU:HD11	2.03	0.41
1:D:5:VAL:CG2	1:D:6:SER:H	2.33	0.40
3:E:405:PC1:H322	3:E:405:PC1:H251	2.03	0.40
1:E:285:PRO:HA	1:E:288:ALA:HB3	2.03	0.40
1:A:12:ALA:HB3	1:A:14:GLU:CD	2.41	0.40
3:B:402:PC1:H322	3:B:402:PC1:H272	2.03	0.40
1:E:249:THR:HB	1:E:251:TYR:CE2	2.56	0.40
1:A:41:ALA:HB3	1:A:106:PHE:CE1	2.55	0.40
1:B:119:TYR:HH	1:B:197:TYR:HE1	1.66	0.40
3:B:402:PC1:H251	3:B:402:PC1:C32	2.50	0.40
1:C:11:ILE:H	1:C:11:ILE:HG12	1.65	0.40
1:E:76:ILE:N	4:E:409:OXL:O2	2.34	0.40
2:E:401:LMD:H14	2:E:404:LMD:H21	2.04	0.40
1:A:237:ALA:CB	2:C:401:LMD:H3	2.50	0.40
1:C:8:PRO:HA	1:C:9:PRO:HD3	1.90	0.40
1:C:255:THR:O	1:C:259:ILE:HG13	2.20	0.40
1:C:283:SER:C	1:C:285:PRO:HD3	2.42	0.40
1:E:160:TRP:CE3	1:E:190:ILE:HD12	2.57	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	311/317 (98%)	302 (97%)	8 (3%)	1 (0%)	41	74
1	B	312/317 (98%)	303 (97%)	9 (3%)	0	100	100
1	C	310/317 (98%)	302 (97%)	7 (2%)	1 (0%)	41	74
1	D	312/317 (98%)	302 (97%)	9 (3%)	1 (0%)	41	74
1	E	311/317 (98%)	303 (97%)	8 (3%)	0	100	100
All	All	1556/1585 (98%)	1512 (97%)	41 (3%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ALA
1	C	10	PRO
1	D	6	SER

### 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	282/284 (99%)	263 (93%)	19 (7%)	16	50
1	B	282/284 (99%)	262 (93%)	20 (7%)	14	47
1	C	281/284 (99%)	265 (94%)	16 (6%)	20	56
1	D	282/284 (99%)	273 (97%)	9 (3%)	39	71
1	E	281/284 (99%)	270 (96%)	11 (4%)	32	67
All	All	1408/1420 (99%)	1333 (95%)	75 (5%)	22	58

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	44	SER
1	A	57	VAL
1	A	61	VAL
1	A	62	ARG

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	65	THR
1	A	69	GLU
1	A	86	ASP
1	A	97	ASP
1	A	100	VAL
1	A	135	VAL
1	A	140	ILE
1	A	178	ASN
1	A	181	GLU
1	A	222	GLU
1	A	229	VAL
1	A	273	VAL
1	A	281	VAL
1	A	305	LEU
1	B	17	THR
1	B	19	ASN
1	B	44	SER
1	B	57	VAL
1	B	62	ARG
1	B	65	THR
1	B	69	GLU
1	B	81	VAL
1	B	91	ASN
1	B	97	ASP
1	B	135	VAL
1	B	137	THR
1	B	194	TYR
1	B	229	VAL
1	B	243	GLU
1	B	245	ASN
1	B	270	VAL
1	B	281	VAL
1	B	304	LEU
1	B	305	LEU
1	C	17	THR
1	C	44	SER
1	C	57	VAL
1	C	61	VAL
1	C	65	THR
1	C	69	GLU
1	C	81	VAL
1	C	86	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	97	ASP
1	C	100	VAL
1	C	135	VAL
1	C	137	THR
1	C	140	ILE
1	C	229	VAL
1	C	304	LEU
1	C	305	LEU
1	D	17	THR
1	D	44	SER
1	D	57	VAL
1	D	81	VAL
1	D	135	VAL
1	D	136	ASP
1	D	137	THR
1	D	304	LEU
1	D	305	LEU
1	E	44	SER
1	E	57	VAL
1	E	61	VAL
1	E	63	VAL
1	E	81	VAL
1	E	135	VAL
1	E	212	SER
1	E	229	VAL
1	E	284	GLN
1	E	304	LEU
1	E	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	B	276	GLN
1	E	245	ASN

### 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](#)

43 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	ACT	E	412	-	3,3,3	0.77	0	3,3,3	1.40	0
5	ACT	D	508	-	3,3,3	0.72	0	3,3,3	1.43	0
3	PC1	C	404	-	31,31,53	1.24	6 (19%)	37,39,61	1.33	2 (5%)
4	OXL	A	405	-	5,5,5	1.67	0	6,6,6	1.26	0
5	ACT	C	408	-	3,3,3	0.82	0	3,3,3	1.46	0
5	ACT	A	408	-	3,3,3	0.83	0	3,3,3	1.55	1 (33%)
3	PC1	A	402	-	36,36,53	1.21	7 (19%)	42,44,61	1.16	3 (7%)
3	PC1	C	403	-	37,37,53	1.15	7 (18%)	43,45,61	1.18	4 (9%)
5	ACT	D	509	-	3,3,3	0.73	0	3,3,3	1.44	0
3	PC1	A	403	-	38,38,53	1.19	6 (15%)	44,46,61	1.31	7 (15%)
2	LMD	C	402	-	25,25,38	1.17	3 (12%)	28,29,49	1.66	3 (10%)
4	OXL	C	405	-	5,5,5	1.39	0	6,6,6	1.84	4 (66%)
3	PC1	E	406	-	37,37,53	1.16	7 (18%)	43,45,61	1.21	5 (11%)
3	PC1	B	401	-	38,38,53	1.15	7 (18%)	44,46,61	1.16	4 (9%)
4	OXL	C	406	-	5,5,5	1.30	0	6,6,6	2.01	4 (66%)
4	OXL	B	403	-	5,5,5	1.34	0	6,6,6	1.75	2 (33%)
4	OXL	D	506	-	5,5,5	1.32	0	6,6,6	2.00	4 (66%)
3	PC1	D	502	-	36,36,53	1.14	7 (19%)	42,44,61	1.22	2 (4%)
4	OXL	A	404	-	5,5,5	1.36	0	6,6,6	1.89	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OXL	E	409	-	5,5,5	1.44	0	6,6,6	1.52	1 (16%)
4	OXL	E	407	-	5,5,5	1.45	0	6,6,6	1.69	2 (33%)
2	LMD	A	401	-	38,38,38	1.05	1 (2%)	49,49,49	1.70	6 (12%)
4	OXL	E	408	-	5,5,5	1.35	0	6,6,6	2.12	4 (66%)
2	LMD	C	401	-	38,38,38	1.09	1 (2%)	49,49,49	1.72	11 (22%)
4	OXL	D	507	-	5,5,5	1.43	0	6,6,6	1.64	2 (33%)
5	ACT	E	411	-	3,3,3	0.81	0	3,3,3	1.25	0
2	LMD	E	402	-	26,26,38	0.97	1 (3%)	31,31,49	1.91	5 (16%)
4	OXL	D	505	-	5,5,5	1.45	0	6,6,6	1.63	2 (33%)
4	OXL	E	403	-	5,5,5	1.37	0	6,6,6	1.65	2 (33%)
3	PC1	B	402	-	37,37,53	1.16	6 (16%)	43,45,61	1.08	5 (11%)
2	LMD	E	404	-	38,38,38	1.16	1 (2%)	49,49,49	1.73	9 (18%)
5	ACT	C	407	-	3,3,3	0.85	0	3,3,3	1.33	0
5	ACT	B	405	-	3,3,3	0.77	0	3,3,3	1.29	0
4	OXL	B	404	-	5,5,5	1.42	0	6,6,6	1.59	2 (33%)
4	OXL	E	410	-	5,5,5	1.33	0	6,6,6	1.97	2 (33%)
5	ACT	A	407	-	3,3,3	0.80	0	3,3,3	1.18	0
3	PC1	E	405	-	37,37,53	1.16	7 (18%)	43,45,61	1.11	4 (9%)
4	OXL	A	406	-	5,5,5	1.45	0	6,6,6	1.57	2 (33%)
4	OXL	D	504	-	5,5,5	1.46	0	6,6,6	1.72	3 (50%)
2	LMD	E	401	-	21,21,38	0.92	0	21,22,49	1.25	2 (9%)
3	PC1	D	503	-	36,36,53	1.21	6 (16%)	42,44,61	1.08	3 (7%)
5	ACT	B	406	-	3,3,3	0.79	0	3,3,3	1.49	0
4	OXL	D	501	-	5,5,5	1.41	0	6,6,6	1.61	2 (33%)

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
3	PC1	C	404	-	-	20/35/35/57	-
4	OXL	A	405	-	-	4/4/4/4	-
3	PC1	A	402	-	-	20/40/40/57	-
3	PC1	C	403	-	-	22/41/41/57	-
3	PC1	A	403	-	-	18/42/42/57	-
2	LMD	C	402	-	-	8/17/33/63	0/1/1/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OXL	C	405	-	-	4/4/4/4	-
3	PC1	E	406	-	-	25/41/41/57	-
3	PC1	B	401	-	-	23/42/42/57	-
4	OXL	C	406	-	-	4/4/4/4	-
4	OXL	B	403	-	-	0/4/4/4	-
4	OXL	D	506	-	-	4/4/4/4	-
3	PC1	D	502	-	-	17/40/40/57	-
4	OXL	A	404	-	-	0/4/4/4	-
4	OXL	E	409	-	-	4/4/4/4	-
4	OXL	E	407	-	-	4/4/4/4	-
2	LMD	A	401	-	-	10/23/63/63	0/2/2/2
4	OXL	E	408	-	-	4/4/4/4	-
2	LMD	C	401	-	-	14/23/63/63	0/2/2/2
4	OXL	D	507	-	-	4/4/4/4	-
2	LMD	E	402	-	-	12/17/37/63	0/1/1/2
4	OXL	D	505	-	-	4/4/4/4	-
4	OXL	E	403	-	-	0/4/4/4	-
3	PC1	B	402	-	-	22/41/41/57	-
2	LMD	E	404	-	-	15/23/63/63	0/2/2/2
4	OXL	B	404	-	-	4/4/4/4	-
4	OXL	E	410	-	-	4/4/4/4	-
3	PC1	E	405	-	-	20/41/41/57	-
4	OXL	A	406	-	-	4/4/4/4	-
4	OXL	D	504	-	-	4/4/4/4	-
2	LMD	E	401	-	-	8/15/23/63	0/1/1/2
3	PC1	D	503	-	-	15/40/40/57	-
4	OXL	D	501	-	-	0/4/4/4	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	404	LMD	OAS-CAM	3.42	1.46	1.40
3	A	403	PC1	O31-C3	-3.24	1.37	1.45
3	D	503	PC1	O21-C2	-3.18	1.38	1.46
3	A	403	PC1	O21-C2	-3.16	1.38	1.46
3	E	405	PC1	O21-C2	-3.16	1.38	1.46
3	E	406	PC1	O21-C2	-3.08	1.38	1.46

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	PC1	O21-C2	-3.08	1.38	1.46
3	C	404	PC1	O31-C3	-3.01	1.38	1.45
2	A	401	LMD	OAS-CAM	3.00	1.45	1.40
2	C	401	LMD	OAS-CAM	2.99	1.45	1.40
3	B	402	PC1	O31-C3	-2.94	1.38	1.45
3	D	503	PC1	O31-C3	-2.90	1.38	1.45
2	C	402	LMD	OAS-CAM	2.90	1.45	1.40
3	A	402	PC1	O21-C2	-2.87	1.39	1.46
3	A	402	PC1	O31-C3	-2.87	1.38	1.45
3	B	402	PC1	O21-C2	-2.78	1.39	1.46
3	B	401	PC1	O31-C3	-2.78	1.38	1.45
2	E	402	LMD	OAS-CAM	2.74	1.44	1.40
3	B	401	PC1	O21-C2	-2.73	1.39	1.46
3	E	406	PC1	O31-C3	-2.72	1.39	1.45
2	C	402	LMD	CAO-CAN	2.64	1.56	1.52
3	D	502	PC1	O21-C2	-2.60	1.40	1.46
3	C	404	PC1	O21-C2	-2.56	1.40	1.46
3	D	502	PC1	O31-C3	-2.56	1.39	1.45
3	E	405	PC1	O31-C3	-2.56	1.39	1.45
3	C	403	PC1	O31-C3	-2.50	1.39	1.45
3	A	402	PC1	C12-N	-2.38	1.43	1.51
3	D	503	PC1	C12-N	-2.37	1.43	1.51
3	A	403	PC1	C15-N	-2.33	1.43	1.50
3	B	401	PC1	C12-N	-2.29	1.43	1.51
3	C	404	PC1	C12-N	-2.26	1.44	1.51
3	D	503	PC1	C15-N	-2.25	1.43	1.50
3	E	405	PC1	C13-N	-2.25	1.43	1.50
3	A	403	PC1	C12-N	-2.25	1.44	1.51
3	B	402	PC1	C14-N	-2.23	1.43	1.50
3	E	406	PC1	C13-N	-2.22	1.43	1.50
3	E	406	PC1	C12-N	-2.21	1.44	1.51
3	A	403	PC1	C14-N	-2.21	1.43	1.50
3	B	401	PC1	O31-C31	2.21	1.39	1.33
3	C	403	PC1	O31-C31	2.21	1.39	1.33
3	B	402	PC1	C12-N	-2.20	1.44	1.51
3	E	405	PC1	O31-C31	2.20	1.39	1.33
3	E	405	PC1	C15-N	-2.20	1.43	1.50
3	A	402	PC1	C13-N	-2.19	1.43	1.50
3	D	502	PC1	C15-N	-2.18	1.43	1.50
3	E	405	PC1	C12-N	-2.18	1.44	1.51
3	C	404	PC1	C15-N	-2.17	1.43	1.50
3	B	402	PC1	C13-N	-2.17	1.43	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	PC1	C14-N	-2.17	1.43	1.50
3	A	402	PC1	C15-N	-2.17	1.43	1.50
3	C	403	PC1	C14-N	-2.17	1.43	1.50
3	D	502	PC1	C14-N	-2.16	1.43	1.50
3	D	502	PC1	C13-N	-2.16	1.43	1.50
3	D	503	PC1	C14-N	-2.16	1.43	1.50
3	C	403	PC1	C13-N	-2.16	1.43	1.50
3	C	404	PC1	C14-N	-2.15	1.43	1.50
3	A	402	PC1	C14-N	-2.15	1.43	1.50
3	D	503	PC1	C13-N	-2.14	1.43	1.50
3	B	401	PC1	C15-N	-2.14	1.43	1.50
3	C	403	PC1	C12-N	-2.14	1.44	1.51
3	E	405	PC1	C14-N	-2.13	1.43	1.50
3	A	403	PC1	C13-N	-2.12	1.43	1.50
3	A	402	PC1	O31-C31	2.12	1.39	1.33
3	C	403	PC1	C15-N	-2.11	1.43	1.50
3	B	401	PC1	C13-N	-2.11	1.43	1.50
3	E	406	PC1	C15-N	-2.10	1.43	1.50
3	E	406	PC1	C14-N	-2.10	1.43	1.50
3	D	502	PC1	O31-C31	2.10	1.39	1.33
3	D	502	PC1	C12-N	-2.08	1.44	1.51
3	C	404	PC1	C13-N	-2.07	1.44	1.50
3	B	402	PC1	C15-N	-2.05	1.44	1.50
2	C	402	LMD	CAR-CAQ	2.02	1.56	1.51
3	E	406	PC1	O31-C31	2.00	1.39	1.33

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	LMD	OAS-CAM-CAN	8.07	120.90	108.30
2	E	402	LMD	OAS-CAM-CAN	6.96	119.17	108.30
2	C	401	LMD	OAS-CAM-CAN	6.77	118.87	108.30
2	C	402	LMD	OAS-CAM-CAN	6.76	118.86	108.30
2	E	404	LMD	OAS-CAM-CAN	5.94	117.58	108.30
3	C	404	PC1	O21-C21-C22	4.75	121.74	111.50
2	E	404	LMD	OAV-CAM-OAS	4.73	121.17	109.97
2	E	402	LMD	OAV-CAQ-CAP	4.49	117.85	109.69
3	A	403	PC1	O21-C21-C22	4.48	121.16	111.50
2	E	401	LMD	OAS-CAM-CAN	4.43	118.23	108.68
3	D	502	PC1	O21-C21-C22	4.07	120.27	111.50
2	E	402	LMD	CAM-OAV-CAQ	3.94	121.43	113.69
3	A	402	PC1	O21-C21-C22	3.86	119.81	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	PC1	O21-C21-C22	3.86	119.81	111.50
3	B	401	PC1	O21-C21-C22	3.85	119.79	111.50
3	E	406	PC1	O21-C21-C22	3.69	119.45	111.50
3	B	402	PC1	O21-C21-C22	3.42	118.88	111.50
3	C	403	PC1	O21-C21-C22	3.42	118.86	111.50
2	C	401	LMD	CAN-CAO-CAP	3.41	117.48	109.68
3	E	405	PC1	O21-C21-C22	3.37	118.77	111.50
2	E	404	LMD	O2-C2-C1	3.35	118.19	110.05
2	E	404	LMD	CAX-OAS-CAM	3.33	119.37	113.84
2	C	402	LMD	CAP-CAO-CAN	3.21	115.34	110.69
2	A	401	LMD	OAV-CAM-OAS	3.20	117.56	109.97
2	C	401	LMD	O1-C1-C2	3.20	116.38	108.10
2	E	404	LMD	CAN-CAO-CAP	3.06	116.67	109.68
4	E	408	OXL	O4-C2-C1	3.05	122.23	113.16
3	C	404	PC1	O31-C31-C32	2.96	121.19	111.91
3	E	406	PC1	O31-C31-C32	2.92	121.06	111.91
3	D	502	PC1	O31-C31-C32	2.91	121.04	111.91
2	C	401	LMD	OAT-CAN-CAO	-2.90	103.66	110.35
3	E	405	PC1	O31-C31-C32	2.87	120.93	111.91
4	E	410	OXL	O4-C2-C1	2.86	121.67	113.16
4	E	410	OXL	O3-C1-C2	2.82	121.54	113.16
4	D	506	OXL	O3-C1-C2	2.79	121.44	113.16
3	C	403	PC1	O31-C31-C32	2.78	120.63	111.91
4	D	506	OXL	O4-C2-C1	2.77	121.39	113.16
4	C	405	OXL	O3-C1-C2	2.77	121.39	113.16
3	B	401	PC1	O21-C21-O22	-2.75	117.04	123.70
4	E	403	OXL	O3-C1-C2	2.74	121.30	113.16
4	C	406	OXL	O4-C2-C1	2.73	121.27	113.16
2	A	401	LMD	OAV-CAM-CAN	-2.72	104.58	110.35
4	A	404	OXL	O4-C2-C1	2.71	121.22	113.16
3	A	403	PC1	C2-O21-C21	-2.70	111.14	117.79
3	E	406	PC1	C2-O21-C21	-2.68	111.19	117.79
4	E	409	OXL	O4-C2-C1	2.67	121.10	113.16
4	C	406	OXL	O3-C1-C2	2.66	121.06	113.16
4	D	505	OXL	O4-C2-C1	2.64	121.00	113.16
2	E	404	LMD	C1-O5-C5	2.61	118.82	113.69
2	C	402	LMD	OAV-CAM-OAS	2.60	116.14	109.97
4	E	408	OXL	O3-C1-C2	2.58	120.83	113.16
2	A	401	LMD	OAT-CAN-CAM	2.57	116.30	110.05
2	C	401	LMD	OAV-CAQ-CAP	2.57	115.18	109.75
3	C	403	PC1	C2-O21-C21	-2.56	111.49	117.79
4	B	403	OXL	O3-C1-C2	2.53	120.67	113.16

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	LMD	CAQ-OAV-CAM	2.52	118.34	111.21
2	E	402	LMD	OAT-CAN-CAM	2.52	116.16	110.05
2	E	404	LMD	O1-C1-C2	2.51	114.61	108.10
2	C	401	LMD	OAV-CAM-OAS	2.51	115.92	109.97
4	E	408	OXL	O3-C1-O1	-2.50	117.89	123.61
4	E	407	OXL	O3-C1-C2	2.48	120.54	113.16
2	C	401	LMD	O5-C1-C2	2.48	115.60	110.35
4	B	403	OXL	O4-C2-C1	2.48	120.52	113.16
3	A	403	PC1	O31-C31-C32	2.48	119.68	111.91
2	C	401	LMD	C1-O5-C5	2.47	118.54	113.69
2	A	401	LMD	O1-C1-C2	2.47	114.50	108.10
4	D	501	OXL	O3-C1-C2	2.45	120.43	113.16
3	A	402	PC1	O31-C31-C32	2.44	119.55	111.91
4	B	404	OXL	O3-C1-C2	2.43	120.39	113.16
4	D	507	OXL	O3-C1-C2	2.38	120.22	113.16
4	E	407	OXL	O4-C2-C1	2.36	120.18	113.16
4	A	404	OXL	O3-C1-C2	2.35	120.14	113.16
3	B	402	PC1	O31-C31-C32	2.34	119.24	111.91
2	E	404	LMD	C2-C3-C4	-2.34	106.74	110.82
3	B	401	PC1	O31-C31-C32	2.34	119.24	111.91
4	B	404	OXL	O4-C2-C1	2.33	120.09	113.16
4	A	406	OXL	O4-C2-C1	2.31	120.02	113.16
3	B	402	PC1	P-O13-C11	-2.29	110.30	121.59
2	C	401	LMD	OAT-CAN-CAM	2.27	115.57	110.05
4	D	501	OXL	O4-C2-C1	2.27	119.91	113.16
3	C	403	PC1	P-O13-C11	-2.26	110.47	121.59
2	C	401	LMD	CAM-OAV-CAQ	2.26	118.12	113.69
4	C	406	OXL	O3-C1-O1	-2.26	118.45	123.61
4	D	504	OXL	O3-C1-C2	2.26	119.86	113.16
3	E	406	PC1	P-O13-C11	-2.25	110.50	121.59
3	A	403	PC1	O31-C3-C2	2.24	114.95	108.43
4	D	507	OXL	O4-C2-C1	2.21	119.72	113.16
3	A	403	PC1	C3-O31-C31	-2.20	108.97	117.12
2	C	401	LMD	CAO-CAP-CAQ	2.18	115.93	110.93
2	A	401	LMD	OAV-CAQ-CAP	2.18	114.34	109.75
3	D	503	PC1	O31-C31-C32	2.17	118.71	111.91
4	D	505	OXL	O3-C1-C2	2.16	119.59	113.16
3	E	405	PC1	O21-C21-O22	-2.16	118.48	123.70
3	E	405	PC1	C2-O21-C21	-2.16	112.48	117.79
3	B	401	PC1	P-O13-C11	-2.15	110.98	121.59
4	D	504	OXL	O3-C1-O1	-2.15	118.69	123.61
4	C	406	OXL	O4-C2-O2	-2.14	118.72	123.61

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	PC1	P-O13-C11	-2.13	111.11	121.59
2	E	402	LMD	CAO-CAP-CAQ	2.11	114.00	110.24
4	A	404	OXL	O3-C1-O1	-2.11	118.78	123.61
3	B	402	PC1	C3-O31-C31	-2.08	109.41	117.12
4	D	506	OXL	O3-C1-O1	-2.08	118.85	123.61
4	A	406	OXL	O3-C1-C2	2.08	119.33	113.16
4	D	504	OXL	O4-C2-C1	2.08	119.33	113.16
3	A	403	PC1	P-O13-C11	-2.07	111.37	121.59
3	B	402	PC1	P-O11-C1	-2.07	109.52	121.68
4	E	408	OXL	O4-C2-O2	-2.07	118.87	123.61
4	C	405	OXL	O3-C1-O1	-2.06	118.90	123.61
3	A	402	PC1	P-O13-C11	-2.06	111.47	121.59
4	C	405	OXL	O4-C2-C1	2.05	119.26	113.16
3	E	406	PC1	O31-C3-C2	2.05	114.40	108.43
3	A	403	PC1	O31-C31-O32	-2.04	118.46	123.59
5	A	408	ACT	OXT-C-O	-2.03	114.56	122.05
2	E	404	LMD	C1-C2-C3	-2.03	105.76	110.00
4	E	403	OXL	O4-C2-C1	2.03	119.18	113.16
4	C	405	OXL	O4-C2-O2	-2.01	119.00	123.61
4	D	506	OXL	O4-C2-O2	-2.01	119.01	123.61

There are no chirality outliers.

All (321) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	LMD	CAN-CAM-OAS-CAX
2	C	401	LMD	OAV-CAM-OAS-CAX
2	C	402	LMD	OAV-CAQ-CAR-OAW
2	C	402	LMD	CAP-CAQ-CAR-OAW
2	E	401	LMD	CAN-CAM-OAS-CAX
2	E	401	LMD	OAV-CAM-OAS-CAX
2	E	402	LMD	CAN-CAM-OAS-CAX
2	E	402	LMD	OAV-CAM-OAS-CAX
2	E	404	LMD	CAN-CAM-OAS-CAX
3	A	402	PC1	C11-O13-P-O14
3	A	402	PC1	C1-O11-P-O14
3	A	402	PC1	C1-O11-P-O13
3	A	402	PC1	O13-C11-C12-N
3	A	402	PC1	O22-C21-O21-C2
3	A	402	PC1	C22-C21-O21-C2
3	A	403	PC1	C1-O11-P-O12
3	A	403	PC1	C1-O11-P-O14

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	403	PC1	O22-C21-O21-C2
3	A	403	PC1	C22-C21-O21-C2
3	A	403	PC1	O32-C31-O31-C3
3	B	401	PC1	C1-O11-P-O14
3	B	401	PC1	O13-C11-C12-N
3	B	401	PC1	O22-C21-O21-C2
3	B	401	PC1	C22-C21-O21-C2
3	B	402	PC1	C1-O11-P-O14
3	B	402	PC1	O13-C11-C12-N
3	C	403	PC1	C1-O11-P-O12
3	C	403	PC1	O11-C1-C2-O21
3	C	403	PC1	C22-C21-O21-C2
3	C	404	PC1	C1-O11-P-O12
3	C	404	PC1	C1-O11-P-O14
3	C	404	PC1	C1-O11-P-O13
3	C	404	PC1	O13-C11-C12-N
3	C	404	PC1	O11-C1-C2-O21
3	C	404	PC1	O22-C21-O21-C2
3	C	404	PC1	C22-C21-O21-C2
3	D	502	PC1	C22-C21-O21-C2
3	E	405	PC1	C1-O11-P-O12
3	E	405	PC1	C1-O11-P-O14
3	E	405	PC1	C1-O11-P-O13
3	E	405	PC1	O11-C1-C2-O21
3	E	406	PC1	C11-O13-P-O12
3	E	406	PC1	C1-O11-P-O12
3	E	406	PC1	C1-O11-P-O14
3	E	406	PC1	O13-C11-C12-N
3	E	406	PC1	O21-C2-C3-O31
4	A	405	OXL	O1-C1-C2-O2
4	A	405	OXL	O1-C1-C2-O4
4	A	405	OXL	O3-C1-C2-O2
4	A	405	OXL	O3-C1-C2-O4
4	D	506	OXL	O1-C1-C2-O2
4	D	506	OXL	O1-C1-C2-O4
4	D	506	OXL	O3-C1-C2-O2
4	D	506	OXL	O3-C1-C2-O4
4	D	507	OXL	O1-C1-C2-O2
4	D	507	OXL	O1-C1-C2-O4
4	D	507	OXL	O3-C1-C2-O2
4	D	507	OXL	O3-C1-C2-O4
4	E	410	OXL	O1-C1-C2-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	E	410	OXL	O3-C1-C2-O2
4	E	410	OXL	O3-C1-C2-O4
2	A	401	LMD	CAO-CAP-O1-C1
3	C	404	PC1	O32-C31-O31-C3
2	C	401	LMD	CAO-CAP-O1-C1
2	E	404	LMD	O5-C1-O1-CAP
3	B	401	PC1	C32-C31-O31-C3
3	B	401	PC1	O32-C31-O31-C3
3	C	403	PC1	O22-C21-O21-C2
3	D	502	PC1	O22-C21-O21-C2
3	A	403	PC1	C32-C31-O31-C3
3	C	404	PC1	C32-C31-O31-C3
3	E	405	PC1	C22-C21-O21-C2
2	E	404	LMD	CAP-CAQ-CAR-OAW
2	E	404	LMD	OAV-CAQ-CAR-OAW
3	E	405	PC1	O22-C21-O21-C2
3	D	503	PC1	C22-C23-C24-C25
2	E	404	LMD	O5-C5-C6-O6
3	B	402	PC1	C22-C23-C24-C25
2	A	401	LMD	OAV-CAQ-CAR-OAW
2	C	401	LMD	CBG-CBH-CBI-CBJ
2	E	404	LMD	CBC-CBD-CBE-CBF
4	D	505	OXL	O1-C1-C2-O2
4	E	410	OXL	O1-C1-C2-O2
4	D	505	OXL	O3-C1-C2-O4
4	E	407	OXL	O3-C1-C2-O4
3	D	502	PC1	C31-C32-C33-C34
2	C	401	LMD	CAN-CAM-OAS-CAX
2	E	402	LMD	CAP-CAQ-CAR-OAW
2	C	402	LMD	CBE-CBF-CBG-CBH
3	C	404	PC1	C22-C23-C24-C25
3	A	402	PC1	C21-C22-C23-C24
3	C	403	PC1	C21-C22-C23-C24
3	C	404	PC1	C31-C32-C33-C34
3	B	401	PC1	C22-C23-C24-C25
3	C	404	PC1	C21-C22-C23-C24
4	D	505	OXL	O1-C1-C2-O4
4	D	505	OXL	O3-C1-C2-O2
3	A	403	PC1	C1-O11-P-O13
3	B	401	PC1	C11-O13-P-O11
3	B	401	PC1	C1-O11-P-O13
3	C	403	PC1	C1-O11-P-O13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	E	406	PC1	C11-O13-P-O11
3	E	406	PC1	C1-O11-P-O13
3	B	401	PC1	C35-C36-C37-C38
2	E	401	LMD	CBA-CBB-CBC-CBD
3	A	402	PC1	C24-C25-C26-C27
3	A	403	PC1	C25-C26-C27-C28
3	B	402	PC1	C24-C25-C26-C27
2	C	402	LMD	CBD-CBE-CBF-CBG
3	A	402	PC1	C32-C33-C34-C35
3	D	503	PC1	C23-C24-C25-C26
3	A	403	PC1	C3-C2-O21-C21
3	C	404	PC1	C3-C2-O21-C21
4	E	407	OXL	O1-C1-C2-O2
3	E	405	PC1	C26-C27-C28-C29
2	E	402	LMD	CBG-CBH-CBI-CBJ
3	A	403	PC1	C36-C37-C38-C39
3	B	401	PC1	C27-C28-C29-C2A
3	A	402	PC1	C34-C35-C36-C37
2	E	404	LMD	CAZ-CBA-CBB-CBC
3	D	502	PC1	C32-C33-C34-C35
3	D	502	PC1	C34-C35-C36-C37
3	B	401	PC1	C26-C27-C28-C29
3	B	401	PC1	C34-C35-C36-C37
3	D	503	PC1	C24-C25-C26-C27
3	A	403	PC1	C34-C35-C36-C37
3	E	406	PC1	C32-C33-C34-C35
3	E	406	PC1	C24-C25-C26-C27
3	D	502	PC1	C21-C22-C23-C24
3	A	403	PC1	C26-C27-C28-C29
3	E	406	PC1	C33-C34-C35-C36
3	E	406	PC1	O22-C21-O21-C2
4	E	407	OXL	O1-C1-C2-O4
4	E	407	OXL	O3-C1-C2-O2
3	E	406	PC1	C22-C23-C24-C25
3	B	401	PC1	C24-C25-C26-C27
2	E	401	LMD	CBE-CBF-CBG-CBH
3	A	403	PC1	C23-C24-C25-C26
2	E	404	LMD	C4-C5-C6-O6
3	C	404	PC1	C33-C34-C35-C36
2	E	401	LMD	CBF-CBG-CBH-CBI
3	A	402	PC1	C26-C27-C28-C29
3	B	401	PC1	C33-C34-C35-C36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	E	406	PC1	C22-C21-O21-C2
3	E	406	PC1	C28-C29-C2A-C2B
3	A	403	PC1	C37-C38-C39-C3A
2	E	402	LMD	CAZ-CBA-CBB-CBC
3	D	502	PC1	C24-C25-C26-C27
3	E	405	PC1	C24-C25-C26-C27
2	E	402	LMD	OAS-CAX-CAY-CAZ
4	B	404	OXL	O1-C1-C2-O2
4	A	406	OXL	O3-C1-C2-O4
4	B	404	OXL	O3-C1-C2-O4
2	A	401	LMD	CBF-CBG-CBH-CBI
3	D	503	PC1	C26-C27-C28-C29
3	C	403	PC1	C35-C36-C37-C38
2	E	404	LMD	CBA-CBB-CBC-CBD
3	A	403	PC1	C32-C33-C34-C35
4	B	404	OXL	O1-C1-C2-O4
4	B	404	OXL	O3-C1-C2-O2
2	E	402	LMD	CAY-CAZ-CBA-CBB
3	B	401	PC1	C36-C37-C38-C39
2	C	401	LMD	CAP-CAQ-CAR-OAW
2	E	404	LMD	CBG-CBH-CBI-CBJ
2	E	402	LMD	CBA-CBB-CBC-CBD
2	E	404	LMD	CBD-CBE-CBF-CBG
3	A	403	PC1	C33-C34-C35-C36
3	B	402	PC1	C23-C24-C25-C26
3	E	405	PC1	C27-C28-C29-C2A
3	C	403	PC1	C1-C2-C3-O31
3	E	406	PC1	C1-C2-C3-O31
3	A	402	PC1	C28-C29-C2A-C2B
2	A	401	LMD	CAP-CAQ-CAR-OAW
3	B	402	PC1	C27-C28-C29-C2A
3	D	502	PC1	C28-C29-C2A-C2B
3	B	401	PC1	C3-C2-O21-C21
3	D	502	PC1	C1-C2-O21-C21
4	C	406	OXL	O1-C1-C2-O2
4	E	409	OXL	O1-C1-C2-O2
3	B	401	PC1	C25-C26-C27-C28
4	C	405	OXL	O3-C1-C2-O4
4	C	406	OXL	O3-C1-C2-O4
4	E	409	OXL	O3-C1-C2-O4
4	C	405	OXL	O1-C1-C2-O4
4	C	405	OXL	O3-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	C	406	OXL	O1-C1-C2-O4
4	C	406	OXL	O3-C1-C2-O2
4	E	409	OXL	O1-C1-C2-O4
4	E	409	OXL	O3-C1-C2-O2
3	E	406	PC1	O11-C1-C2-O21
3	E	406	PC1	C34-C35-C36-C37
2	E	401	LMD	OAS-CAX-CAY-CAZ
2	C	402	LMD	CBA-CBB-CBC-CBD
2	C	402	LMD	CBH-CBI-CBJ-CBK
3	D	503	PC1	C33-C34-C35-C36
2	C	401	LMD	CBH-CBI-CBJ-CBK
3	D	502	PC1	C22-C23-C24-C25
3	B	402	PC1	O11-C1-C2-C3
3	C	404	PC1	O11-C1-C2-C3
3	D	502	PC1	O11-C1-C2-C3
3	E	405	PC1	O11-C1-C2-C3
2	A	401	LMD	CAY-CAX-OAS-CAM
3	D	502	PC1	C26-C27-C28-C29
2	C	402	LMD	CBF-CBG-CBH-CBI
3	B	401	PC1	C1-C2-C3-O31
3	E	405	PC1	C34-C35-C36-C37
2	E	404	LMD	CAO-CAP-O1-C1
3	C	403	PC1	C22-C23-C24-C25
4	A	406	OXL	O1-C1-C2-O2
4	C	405	OXL	O1-C1-C2-O2
2	E	404	LMD	CBH-CBI-CBJ-CBK
2	C	401	LMD	CBC-CBD-CBE-CBF
3	C	403	PC1	C34-C35-C36-C37
3	D	502	PC1	O21-C2-C3-O31
2	C	401	LMD	CAQ-CAP-O1-C1
3	B	401	PC1	C28-C29-C2A-C2B
2	E	404	LMD	OAV-CAM-OAS-CAX
3	C	403	PC1	C26-C27-C28-C29
2	E	402	LMD	OAV-CAQ-CAR-OAW
3	D	503	PC1	C32-C33-C34-C35
3	E	405	PC1	C25-C26-C27-C28
3	E	405	PC1	C2-C1-O11-P
3	E	406	PC1	C2-C1-O11-P
3	A	402	PC1	C31-C32-C33-C34
2	E	402	LMD	CBH-CBI-CBJ-CBK
3	C	403	PC1	C33-C34-C35-C36
2	C	401	LMD	CBA-CBB-CBC-CBD

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	403	PC1	O11-C1-C2-C3
4	A	406	OXL	O1-C1-C2-O4
3	C	404	PC1	C32-C33-C34-C35
3	E	405	PC1	C3-C2-O21-C21
4	D	504	OXL	O1-C1-C2-O2
3	D	503	PC1	C31-C32-C33-C34
3	A	402	PC1	C22-C23-C24-C25
3	D	503	PC1	O11-C1-C2-O21
3	E	406	PC1	O31-C31-C32-C33
3	B	401	PC1	C23-C24-C25-C26
3	D	503	PC1	C21-C22-C23-C24
3	B	402	PC1	C32-C31-O31-C3
4	A	406	OXL	O3-C1-C2-O2
4	D	504	OXL	O3-C1-C2-O2
3	B	402	PC1	C21-C22-C23-C24
2	E	401	LMD	CAX-CAY-CAZ-CBA
3	A	402	PC1	C11-O13-P-O11
3	B	402	PC1	C1-O11-P-O13
3	D	503	PC1	C11-O13-P-O11
3	D	503	PC1	C1-O11-P-O13
3	C	403	PC1	C28-C29-C2A-C2B
3	B	401	PC1	C11-O13-P-O12
3	C	403	PC1	C1-O11-P-O14
3	E	406	PC1	C11-O13-P-O14
3	E	406	PC1	C21-C22-C23-C24
3	E	405	PC1	C22-C23-C24-C25
4	E	408	OXL	O1-C1-C2-O2
4	D	504	OXL	O3-C1-C2-O4
4	E	408	OXL	O3-C1-C2-O4
2	C	401	LMD	CBE-CBF-CBG-CBH
3	B	402	PC1	O11-C1-C2-O21
3	A	403	PC1	C27-C28-C29-C2A
2	C	401	LMD	C4-C5-C6-O6
3	C	403	PC1	O13-C11-C12-N
3	D	502	PC1	O13-C11-C12-N
3	D	503	PC1	O13-C11-C12-N
3	E	405	PC1	O13-C11-C12-N
4	D	504	OXL	O1-C1-C2-O4
4	E	408	OXL	O1-C1-C2-O4
3	B	401	PC1	O21-C2-C3-O31
3	B	402	PC1	C2-C1-O11-P
3	C	403	PC1	C36-C37-C38-C39

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	404	PC1	C23-C24-C25-C26
2	E	401	LMD	CBC-CBD-CBE-CBF
2	A	401	LMD	CAX-CAY-CAZ-CBA
3	E	405	PC1	O32-C31-O31-C3
3	E	405	PC1	O21-C21-C22-C23
4	E	408	OXL	O3-C1-C2-O2
3	B	402	PC1	C11-O13-P-O11
3	C	403	PC1	C11-O13-P-O11
3	C	404	PC1	C11-O13-P-O11
3	D	502	PC1	C11-O13-P-O11
3	E	405	PC1	C11-O13-P-O11
3	D	503	PC1	C27-C28-C29-C2A
3	B	402	PC1	C11-C12-N-C14
3	C	403	PC1	C2-C1-O11-P
3	D	503	PC1	O11-C1-C2-C3
3	E	406	PC1	O11-C1-C2-C3
2	A	401	LMD	CBH-CBI-CBJ-CBK
2	E	404	LMD	CAQ-CAP-O1-C1
3	E	406	PC1	C23-C24-C25-C26
3	D	502	PC1	C27-C28-C29-C2A
2	E	402	LMD	CBF-CBG-CBH-CBI
3	A	402	PC1	C1-C2-O21-C21
3	B	402	PC1	C3-C2-O21-C21
3	E	405	PC1	C28-C29-C2A-C2B
3	E	406	PC1	C36-C37-C38-C39
3	A	402	PC1	O11-C1-C2-C3
3	C	403	PC1	O21-C2-C3-O31
3	A	402	PC1	C25-C26-C27-C28
2	C	401	LMD	O5-C1-O1-CAP
3	B	402	PC1	C11-C12-N-C13
2	A	401	LMD	CAQ-CAP-O1-C1
3	D	503	PC1	C35-C36-C37-C38
3	C	403	PC1	C25-C26-C27-C28
2	C	402	LMD	CAZ-CBA-CBB-CBC
3	A	402	PC1	C11-C12-N-C15
3	B	402	PC1	C11-C12-N-C15
2	C	401	LMD	CAX-CAY-CAZ-CBA
2	A	401	LMD	CBB-CBC-CBD-CBE
3	A	403	PC1	C22-C23-C24-C25
3	B	402	PC1	C31-C32-C33-C34
3	A	402	PC1	O22-C21-C22-C23
2	C	401	LMD	O5-C5-C6-O6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	404	PC1	C34-C35-C36-C37
3	B	402	PC1	C11-O13-P-O14
3	C	404	PC1	C11-O13-P-O14
3	D	502	PC1	C11-O13-P-O14
3	B	402	PC1	O32-C31-C32-C33
3	C	403	PC1	O22-C21-C22-C23
3	E	406	PC1	C25-C26-C27-C28
2	E	402	LMD	CAX-CAY-CAZ-CBA
3	B	402	PC1	C34-C35-C36-C37
3	B	402	PC1	O31-C31-C32-C33

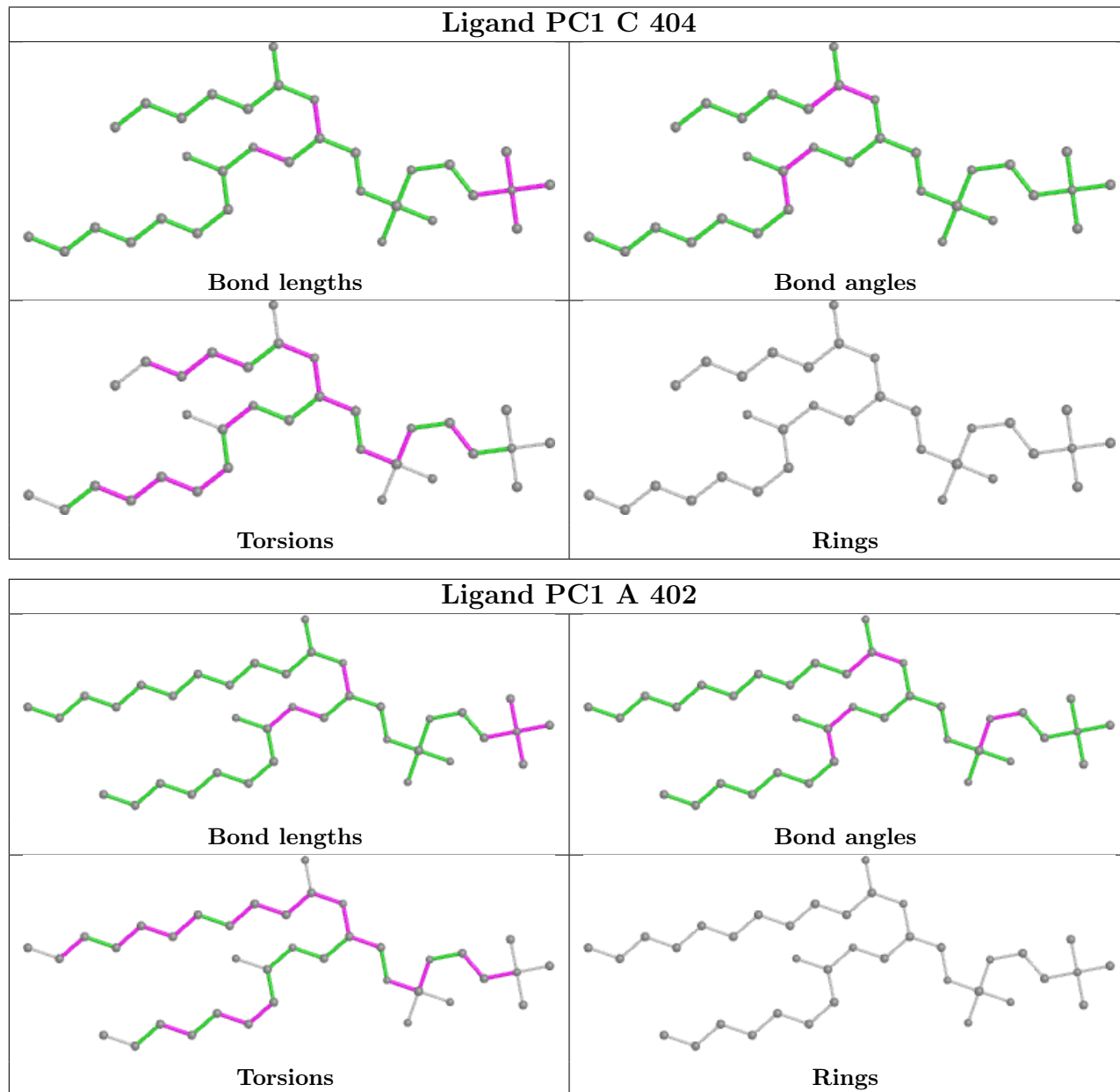
There are no ring outliers.

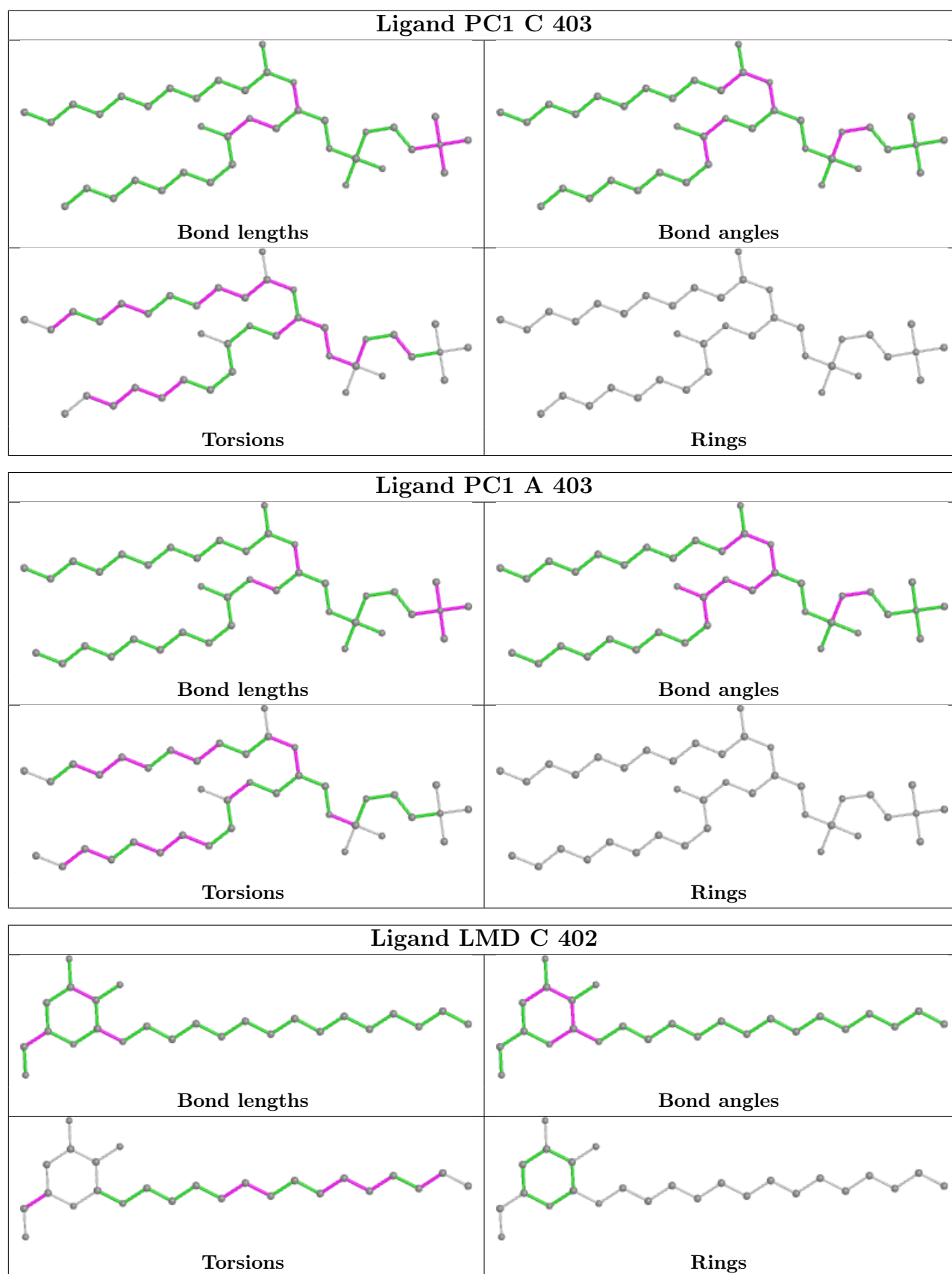
24 monomers are involved in 107 short contacts:

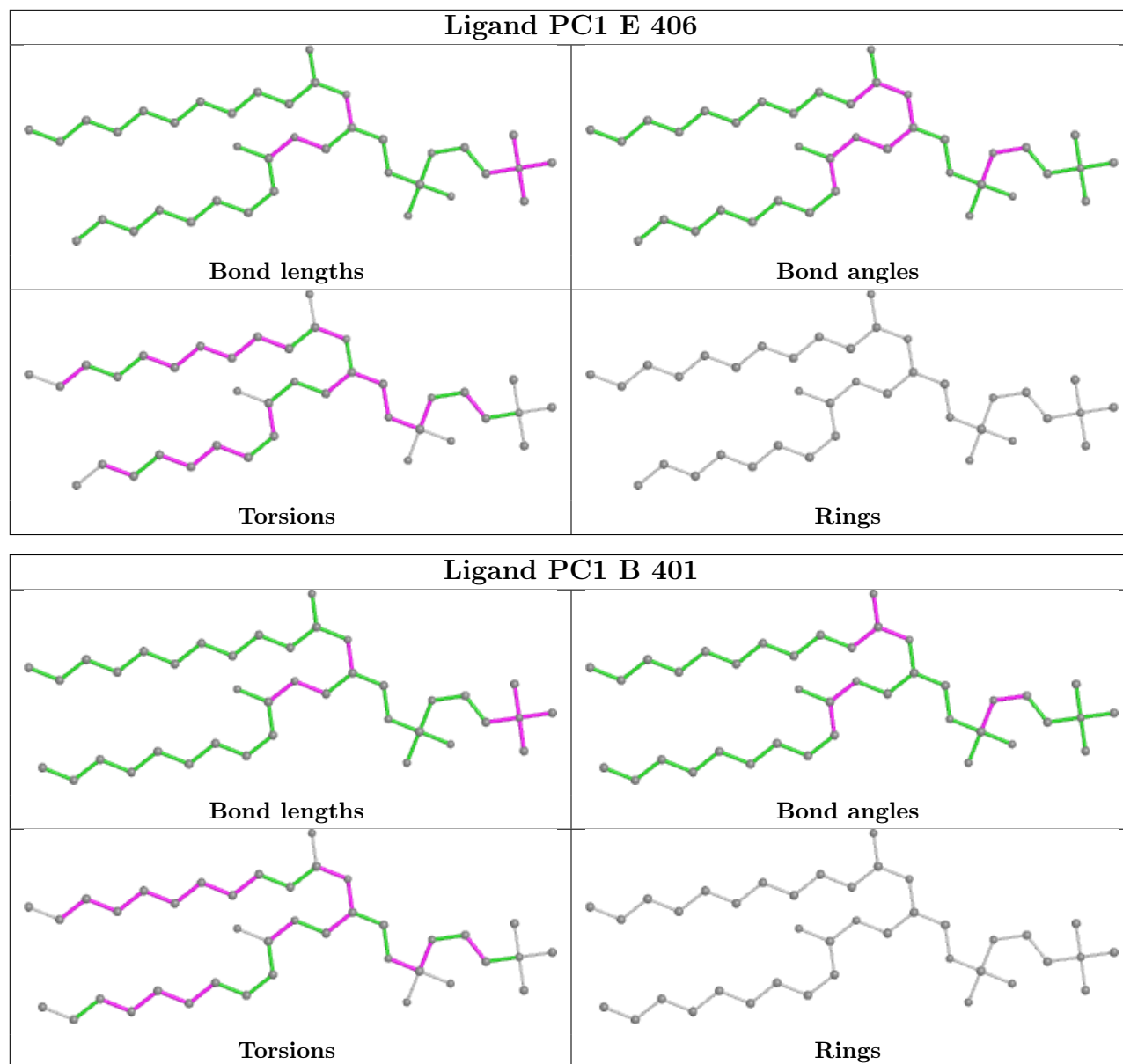
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	404	PC1	5	0
5	C	408	ACT	1	0
3	A	402	PC1	2	0
3	C	403	PC1	10	0
3	A	403	PC1	16	0
2	C	402	LMD	5	0
4	C	405	OXL	1	0
3	E	406	PC1	4	0
3	B	401	PC1	9	0
3	D	502	PC1	6	0
4	E	409	OXL	3	0
2	A	401	LMD	4	0
4	E	408	OXL	1	0
2	C	401	LMD	8	0
5	E	411	ACT	5	0
2	E	402	LMD	3	0
3	B	402	PC1	7	0
2	E	404	LMD	5	0
5	C	407	ACT	1	0
5	A	407	ACT	1	0
3	E	405	PC1	4	0
4	D	504	OXL	1	0
2	E	401	LMD	7	0
3	D	503	PC1	5	0

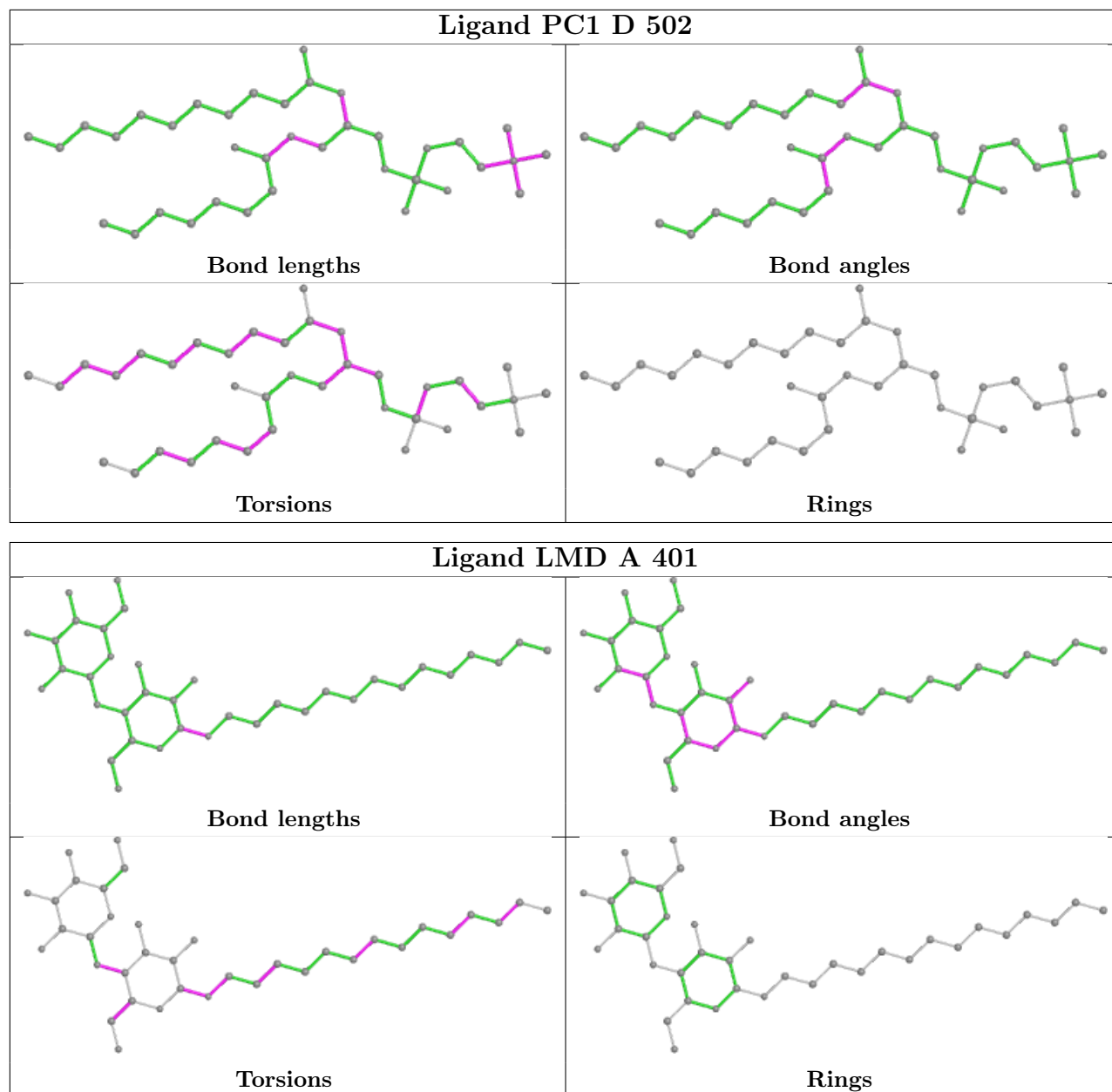
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

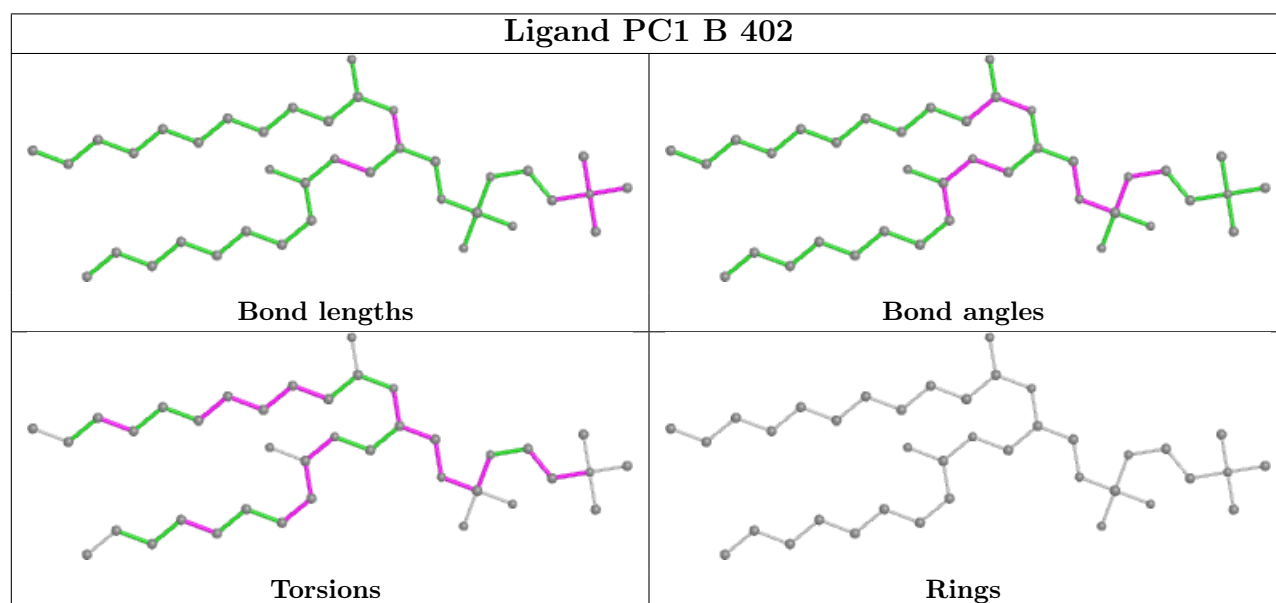
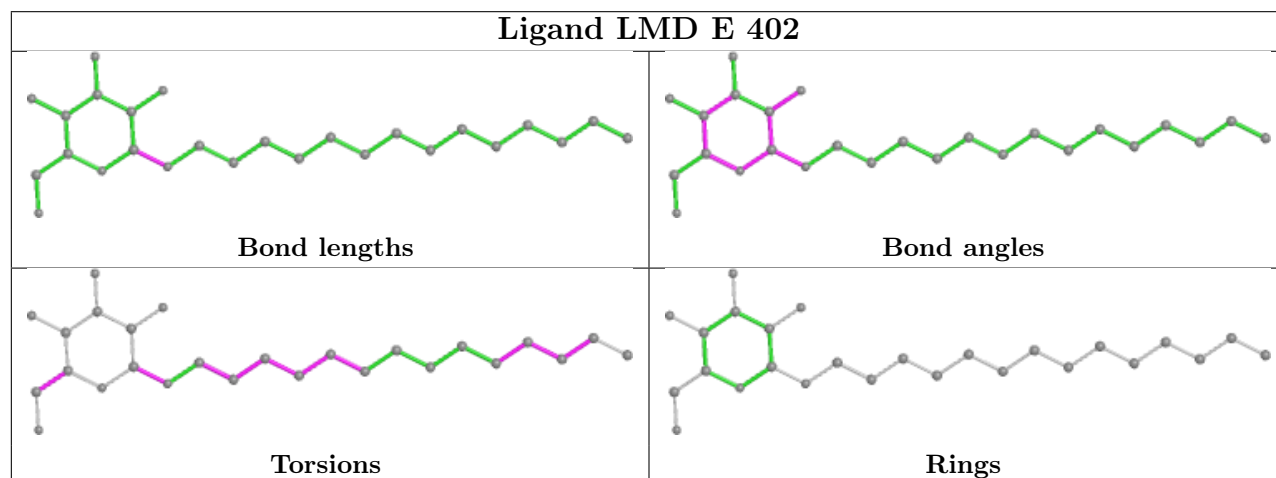
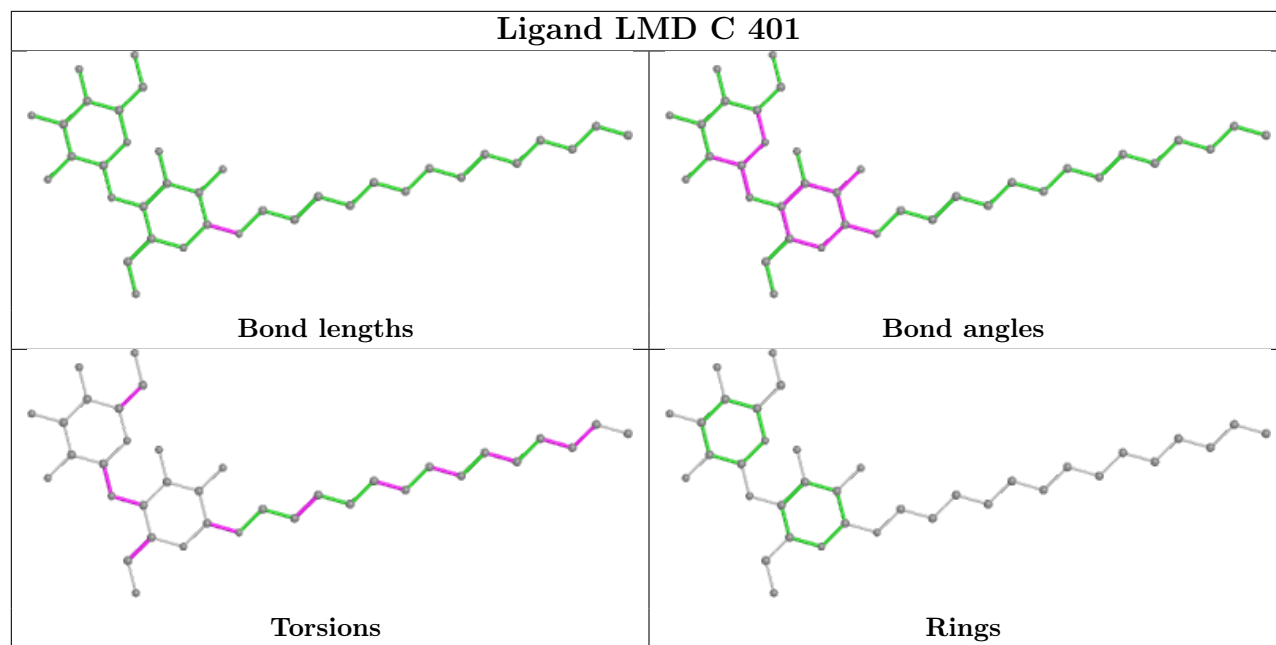
addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

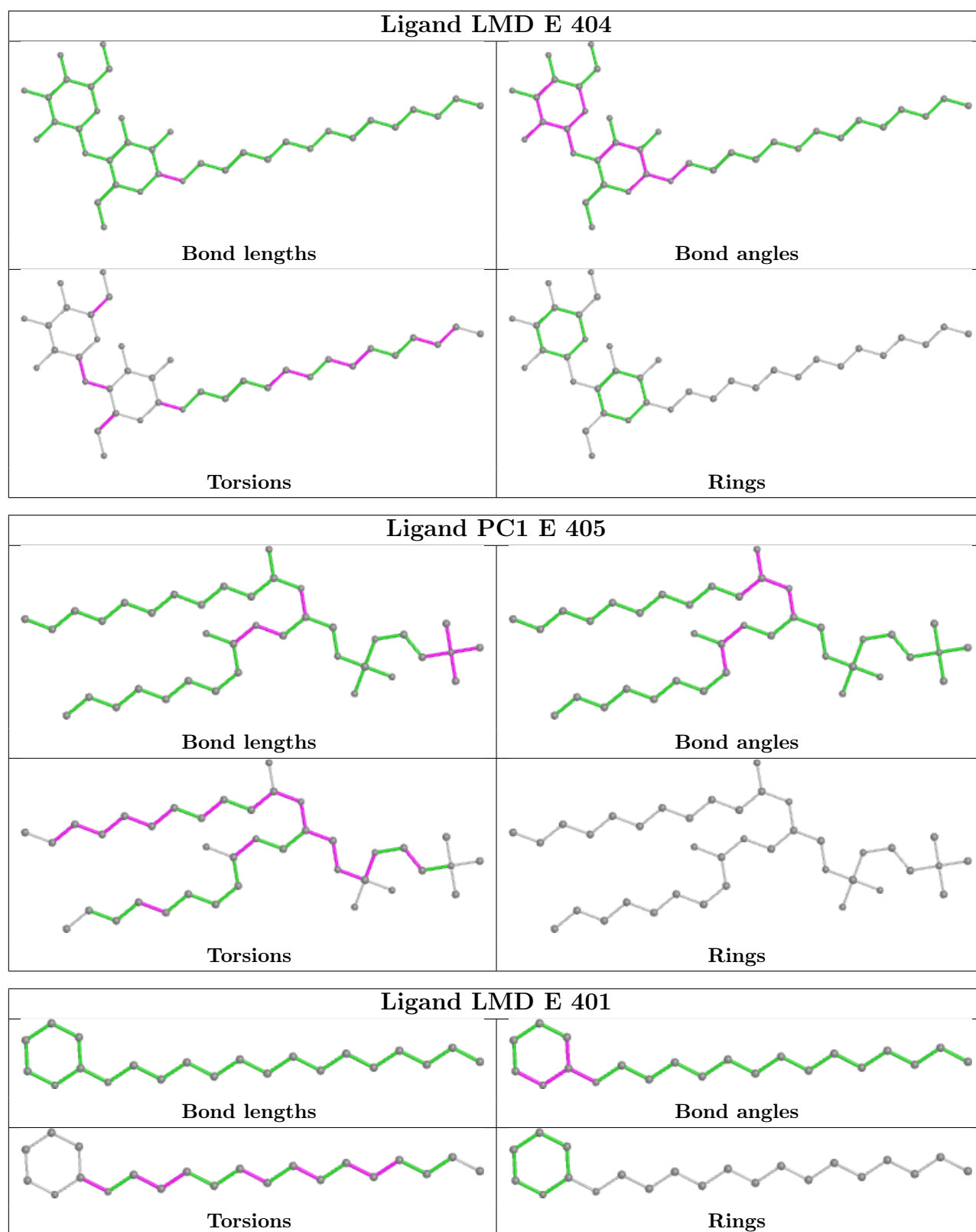




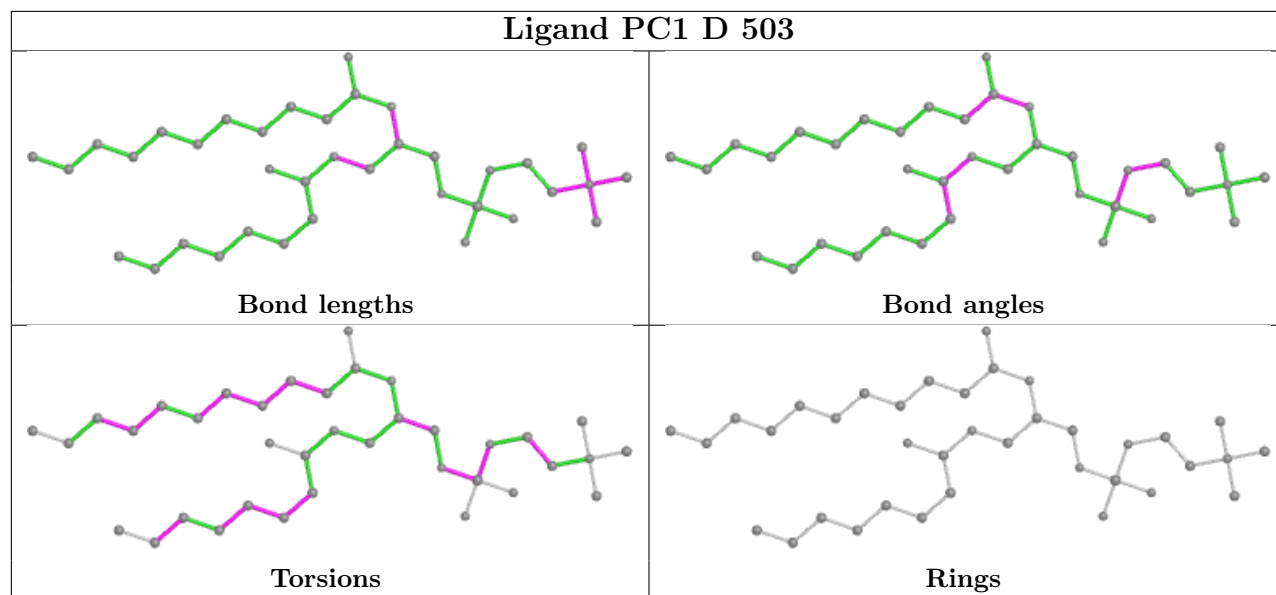












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	312/317 (98%)	-0.47	7 (2%) 62 48	61, 84, 120, 154	0
1	B	313/317 (98%)	-0.47	2 (0%) 89 83	59, 84, 118, 155	0
1	C	311/317 (98%)	-0.46	8 (2%) 56 40	58, 83, 121, 156	0
1	D	313/317 (98%)	-0.43	4 (1%) 77 65	61, 84, 121, 154	0
1	E	312/317 (98%)	-0.45	4 (1%) 77 65	60, 83, 120, 155	0
All	All	1561/1585 (98%)	-0.46	25 (1%) 72 59	58, 84, 121, 156	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	ASP	4.3
1	C	58	ARG	3.6
1	D	61	VAL	3.5
1	A	57	VAL	3.5
1	C	61	VAL	3.1
1	C	57	VAL	3.0
1	E	57	VAL	2.9
1	E	56	PRO	2.9
1	A	13	ASP	2.8
1	C	56	PRO	2.8
1	C	64	LYS	2.8
1	A	58	ARG	2.8
1	C	283	SER	2.7
1	E	58	ARG	2.7
1	B	136	ASP	2.5
1	D	13	ASP	2.4
1	D	64	LYS	2.4
1	A	56	PRO	2.4
1	D	4	MET	2.3
1	A	62	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	11	ILE	2.2
1	C	13	ASP	2.1
1	E	55	ASP	2.1
1	C	62	ARG	2.1
1	A	59	SER	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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
4	OXL	D	505	6/6	0.54	0.34	98,106,117,119	0
3	PC1	C	404	32/54	0.67	0.51	71,117,157,183	0
3	PC1	E	405	38/54	0.72	0.43	73,117,154,175	0
3	PC1	A	402	37/54	0.72	0.55	71,107,171,182	0
4	OXL	E	410	6/6	0.72	0.25	95,103,118,120	0
3	PC1	D	502	37/54	0.74	0.45	67,101,160,175	0
3	PC1	D	503	37/54	0.75	0.38	73,114,155,179	0
3	PC1	C	403	38/54	0.75	0.44	60,112,169,185	0
3	PC1	B	401	39/54	0.76	0.42	76,115,160,170	0
3	PC1	E	406	38/54	0.76	0.55	79,131,169,183	0
2	LMD	E	404	37/37	0.77	0.44	70,124,151,157	0
4	OXL	B	404	6/6	0.77	0.29	87,106,119,121	0
2	LMD	A	401	37/37	0.78	0.36	61,118,143,151	0
5	ACT	B	406	4/4	0.79	0.43	85,94,104,117	0
2	LMD	C	402	25/37	0.80	0.34	68,88,131,138	0
4	OXL	C	405	6/6	0.81	0.29	83,89,99,113	0
3	PC1	A	403	39/54	0.81	0.44	64,121,167,189	0
4	OXL	A	406	6/6	0.82	0.49	94,103,120,127	0

*Continued on next page...*

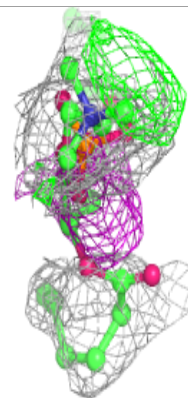
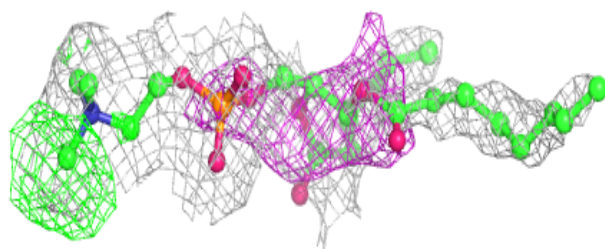
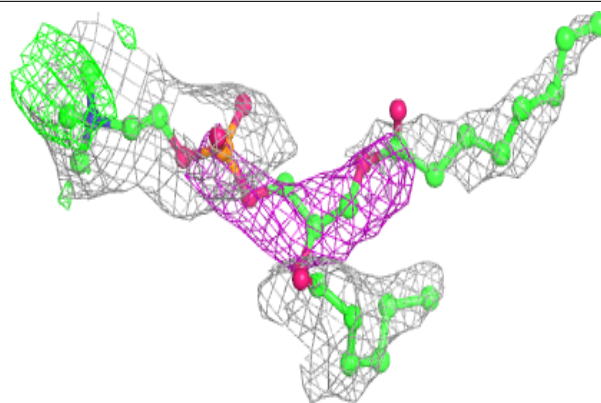
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LMD	E	402	26/37	0.82	0.41	65,102,134,139	0
4	OXL	E	409	6/6	0.83	0.29	92,106,110,110	0
2	LMD	C	401	37/37	0.83	0.30	63,111,144,154	0
4	OXL	E	407	6/6	0.83	0.17	84,105,114,123	0
5	ACT	E	412	4/4	0.83	0.51	80,114,116,131	0
4	OXL	A	404	6/6	0.86	0.18	77,88,107,111	0
4	OXL	D	506	6/6	0.86	0.33	89,101,114,118	0
4	OXL	D	507	6/6	0.86	0.41	103,113,117,119	0
3	PC1	B	402	38/54	0.86	0.44	75,133,158,162	0
4	OXL	C	406	6/6	0.87	0.42	91,95,112,115	0
5	ACT	A	408	4/4	0.88	0.27	79,90,100,106	0
4	OXL	D	501	6/6	0.88	0.14	78,97,108,113	0
4	OXL	E	408	6/6	0.88	0.23	81,88,106,114	0
4	OXL	B	403	6/6	0.89	0.12	89,97,104,110	0
4	OXL	D	504	6/6	0.89	0.26	74,83,88,106	0
5	ACT	C	408	4/4	0.90	0.58	91,95,116,122	0
4	OXL	E	403	6/6	0.90	0.13	71,97,108,114	0
2	LMD	E	401	21/37	0.91	0.30	60,84,105,126	0
5	ACT	D	508	4/4	0.94	0.23	82,98,104,107	0
5	ACT	D	509	4/4	0.94	0.41	93,97,100,102	0
4	OXL	A	405	6/6	0.94	0.24	64,84,92,100	0
5	ACT	C	407	4/4	0.95	0.36	72,88,93,102	0
5	ACT	E	411	4/4	0.96	0.15	85,92,99,104	0
5	ACT	A	407	4/4	0.98	0.13	78,89,91,100	0
5	ACT	B	405	4/4	0.99	0.16	68,93,95,97	0

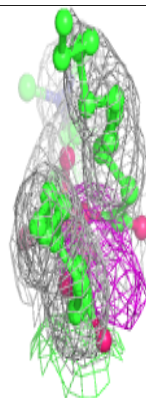
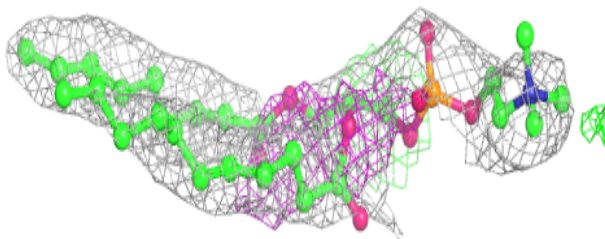
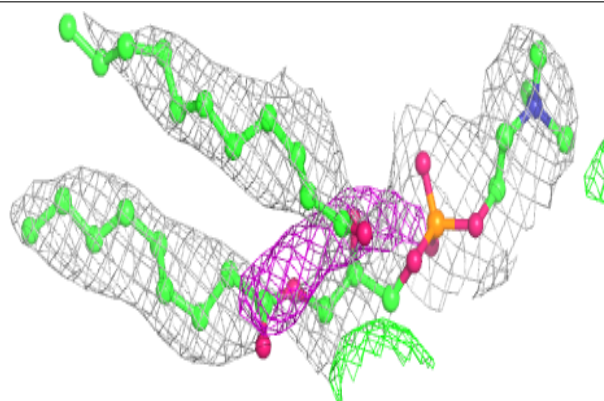
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around PC1 C 404:**

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

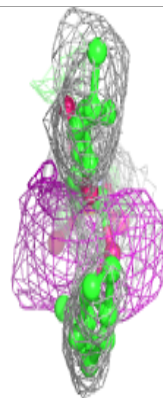
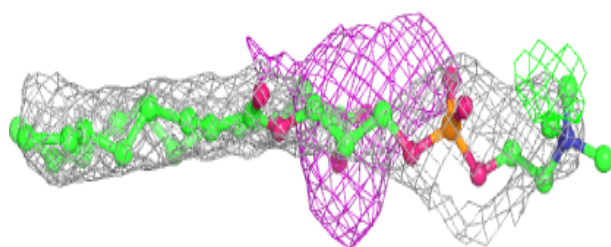
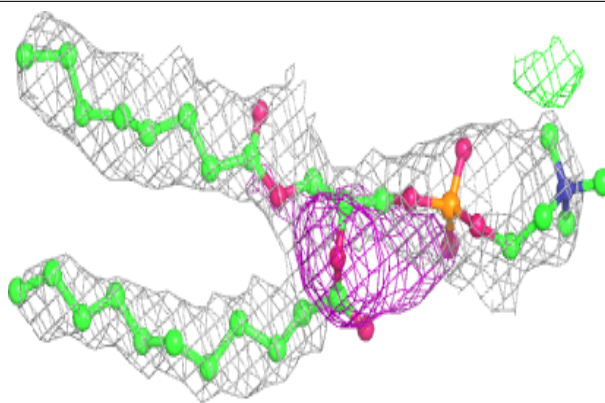
**Electron density around PC1 E 405:**

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

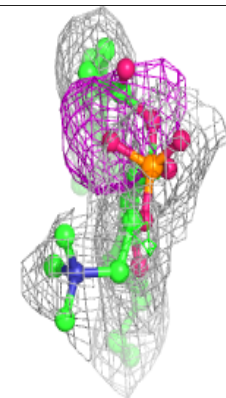
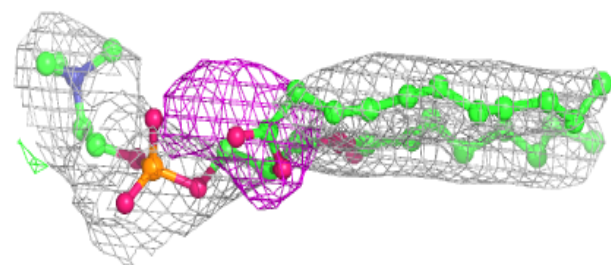
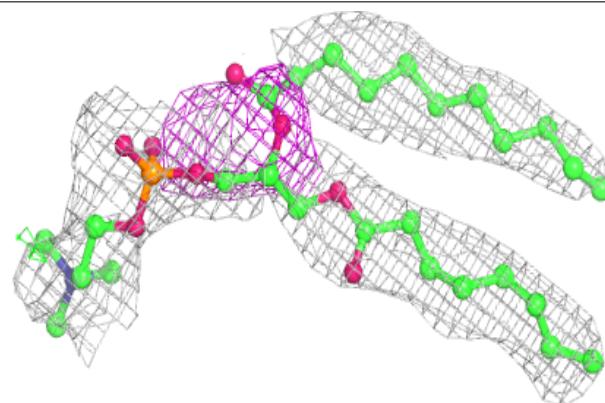


**Electron density around PC1 A 402:**

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

**Electron density around PC1 D 502:**

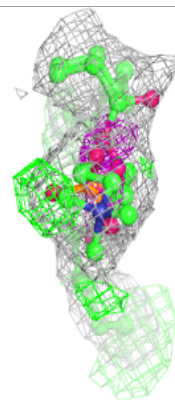
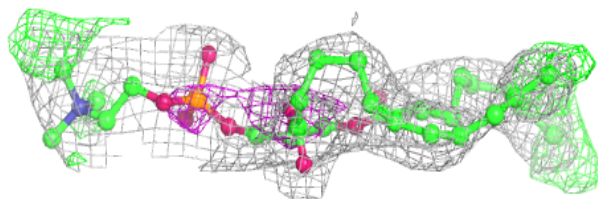
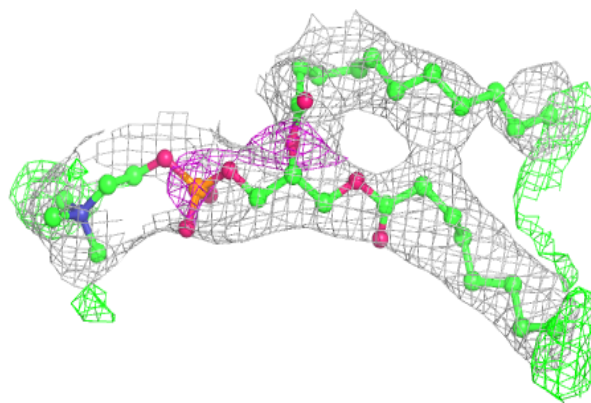
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



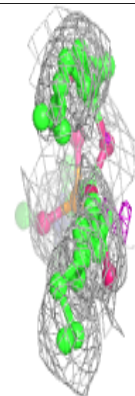
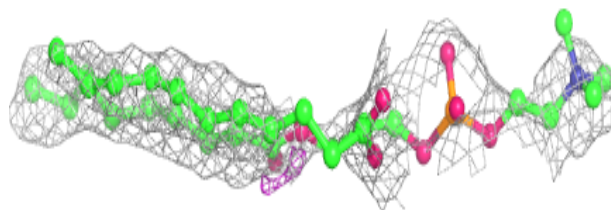
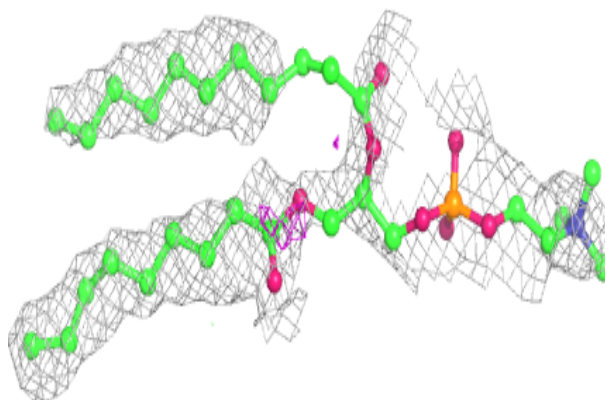


**Electron density around PC1 D 503:**

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

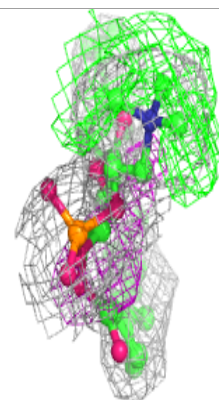
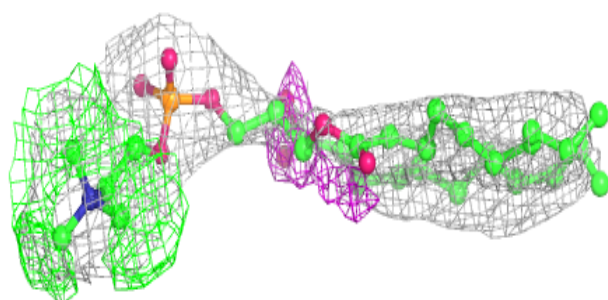
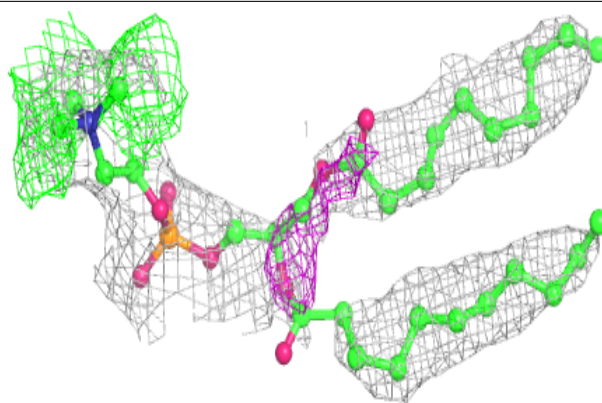
**Electron density around PC1 C 403:**

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

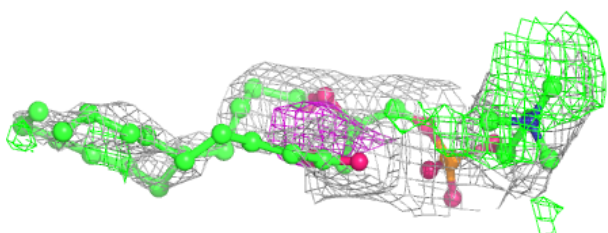
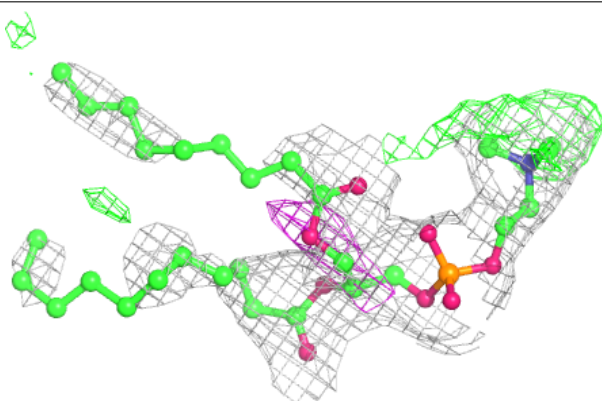


**Electron density around PC1 B 401:**

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

**Electron density around PC1 E 406:**

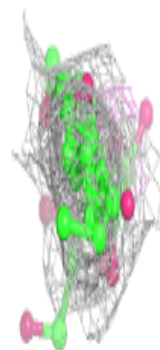
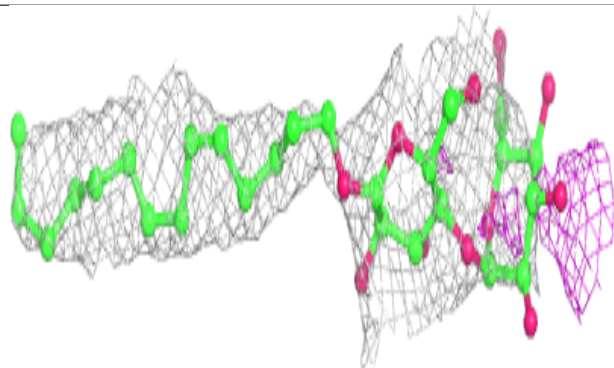
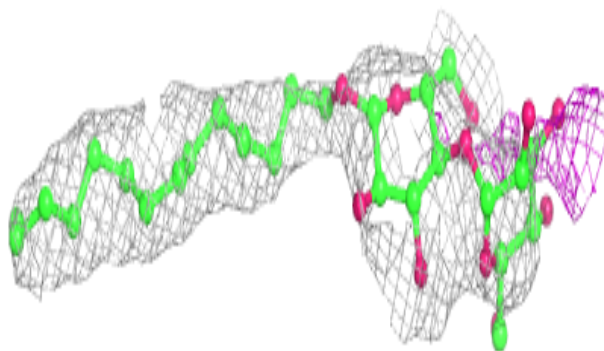
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



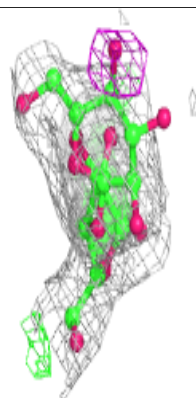
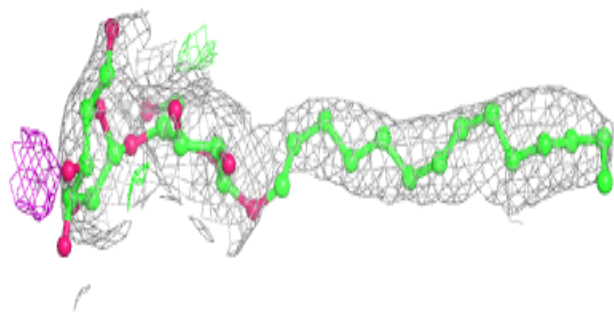
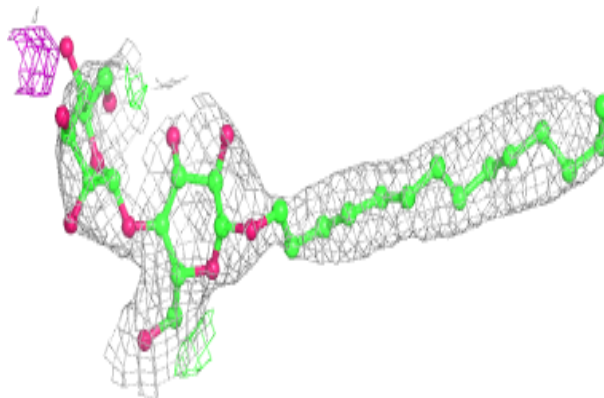


**Electron density around LMD E 404:**

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

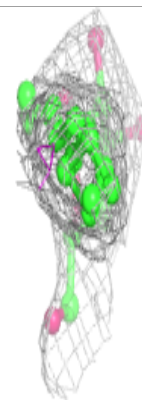
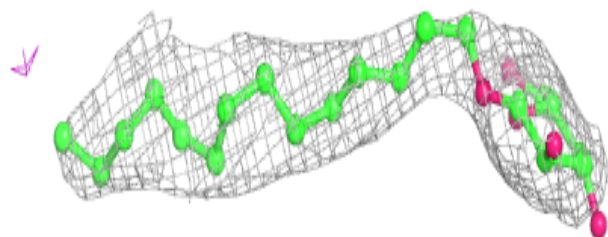
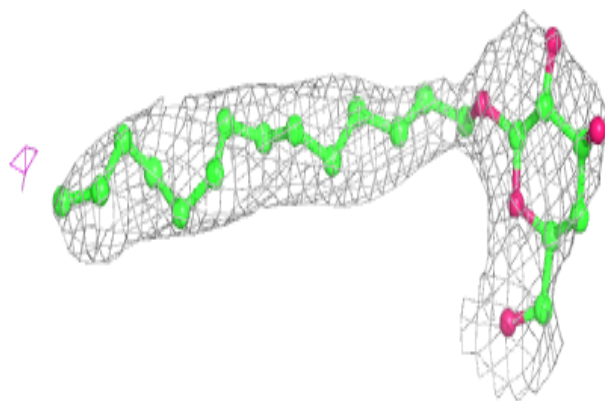
**Electron density around LMD A 401:**

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

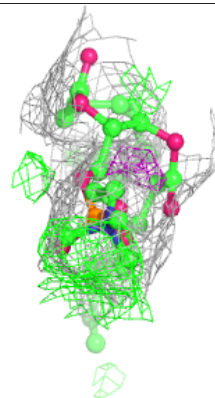
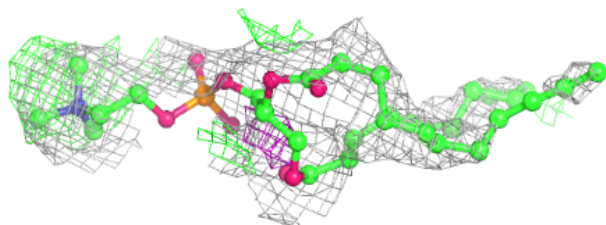
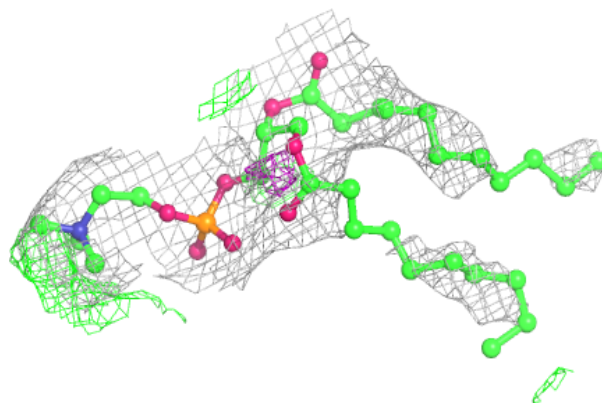


**Electron density around LMD C 402:**

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

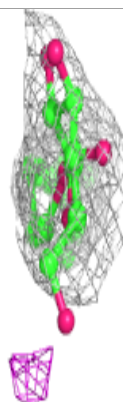
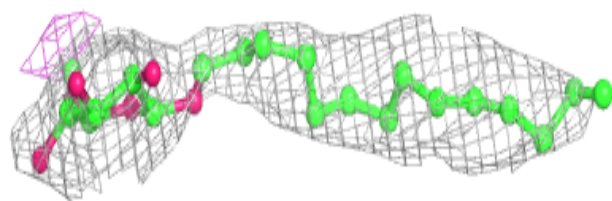
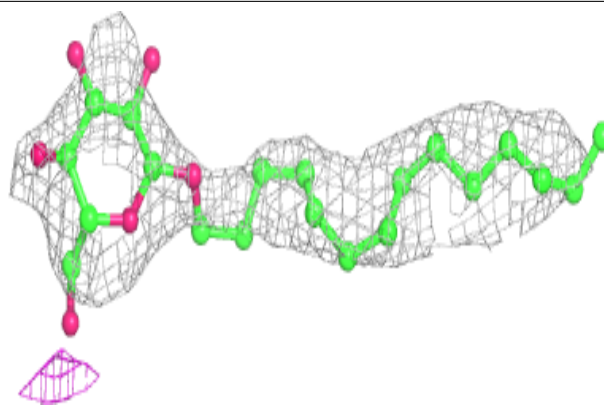
**Electron density around PC1 A 403:**

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

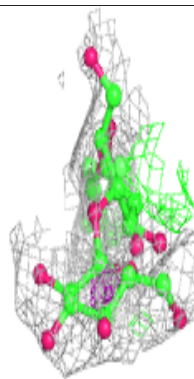
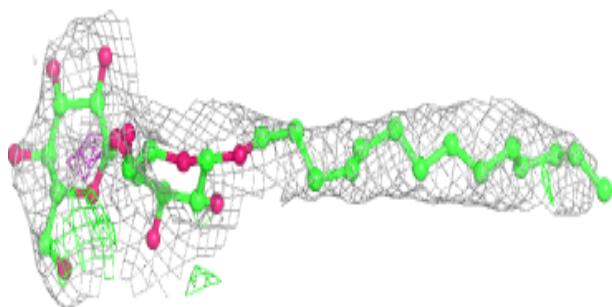
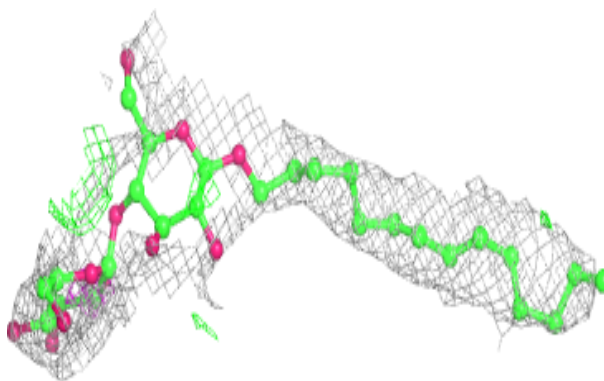


**Electron density around LMD E 402:**

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

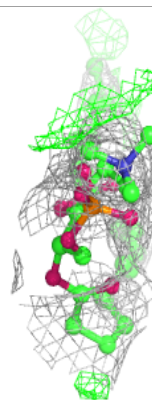
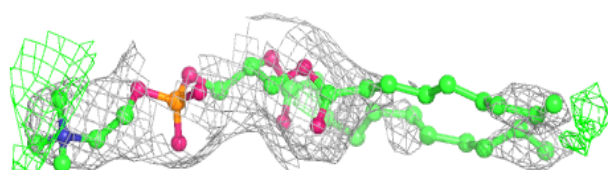
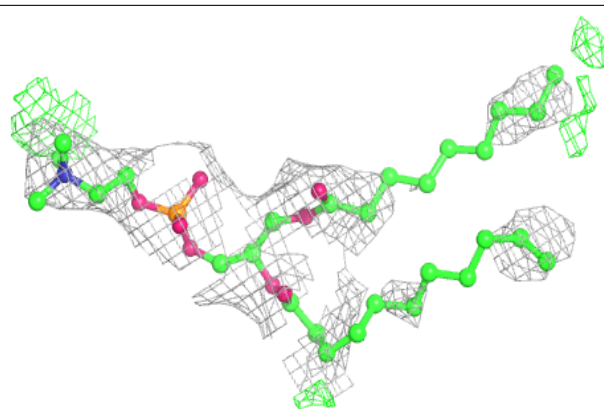
**Electron density around LMD C 401:**

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

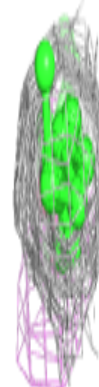
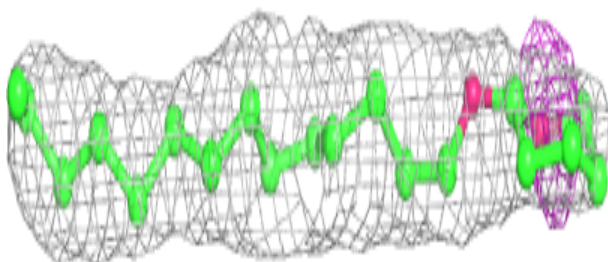
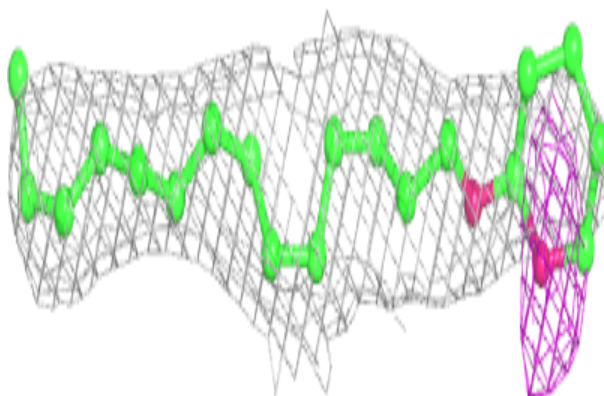


**Electron density around PC1 B 402:**

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

**Electron density around LMD E 401:**

$2mF_o-DF_c$  (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.