Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 11:11 PM EDT

PDB ID	:	3K5D
Title	:	Crystal Structure of BACE-1 in complex with AHM178
Authors	:	Rondeau, J.-M.
Deposited on	:	2009-10-07
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

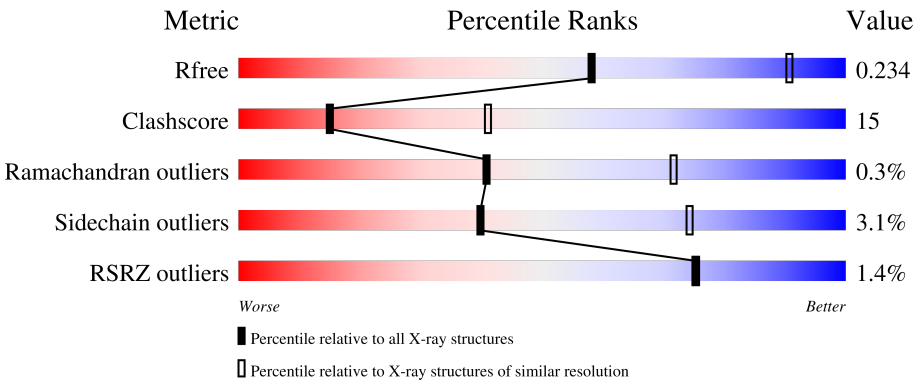
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	408	% 67% 23% • 8%
1	B	408	% 68% 23% • 8%
1	C	408	2% 68% 23% • 8%

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	XLI	A	393	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9049 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.

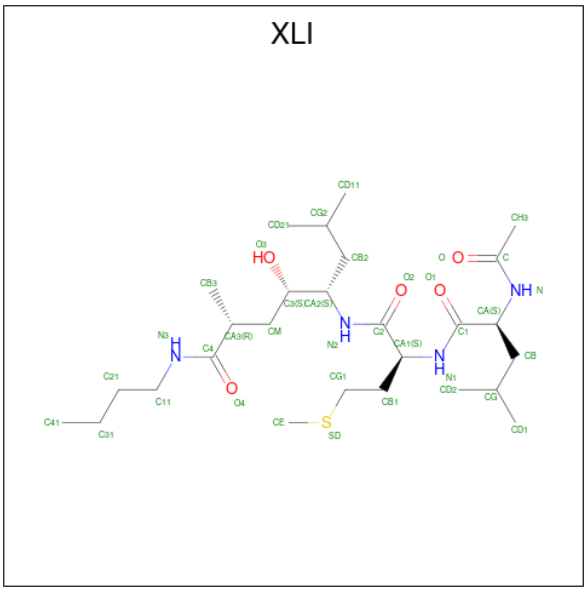
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	375	2953	1890	491	558	14	0	0	0
1	B	375	2953	1890	491	558	14	0	0	0
1	C	376	2961	1896	492	559	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33P	GLY	-	expression tag	UNP P56817
A	34P	PRO	-	expression tag	UNP P56817
B	33P	GLY	-	expression tag	UNP P56817
B	34P	PRO	-	expression tag	UNP P56817
C	33P	GLY	-	expression tag	UNP P56817
C	34P	PRO	-	expression tag	UNP P56817

- Molecule 2 is N-acetyl-L-leucyl-N-[(4S,5S,7R)-8-(butylamino)-5-hydroxy-2,7-dimethyl-8-oxo octan-4-yl]-L-methioninamide (three-letter code: XLI) (formula: $C_{27}H_{52}N_4O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	27	4	5	1		
2	B	1	Total	C	N	O	S	0	0
			37	27	4	5	1		
2	C	1	Total	C	N	O	S	0	0
			37	27	4	5	1		

- Molecule 3 is water.

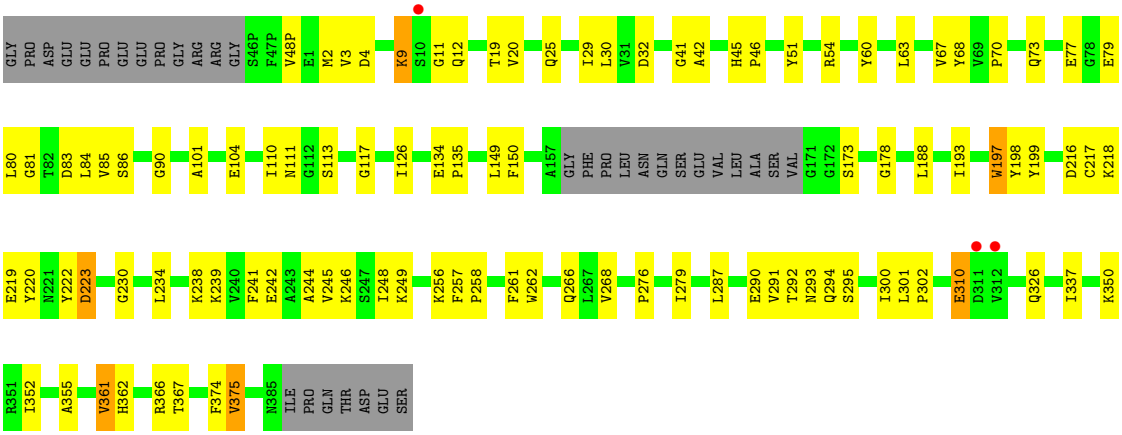
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	26	Total	O	0	0
			26	26		
3	C	20	Total	O	0	0
			20	20		

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.

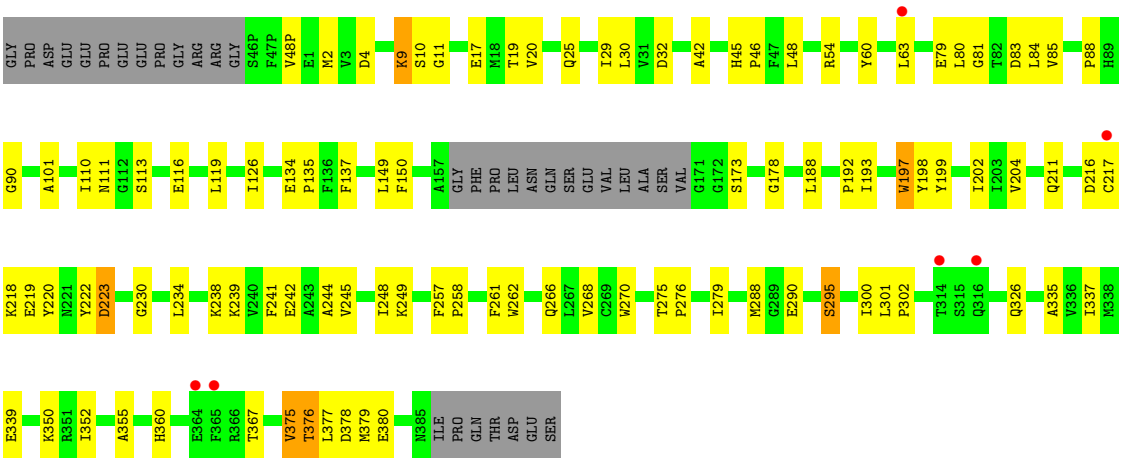
• Molecule 1: Beta-secretase 1

Chain A:



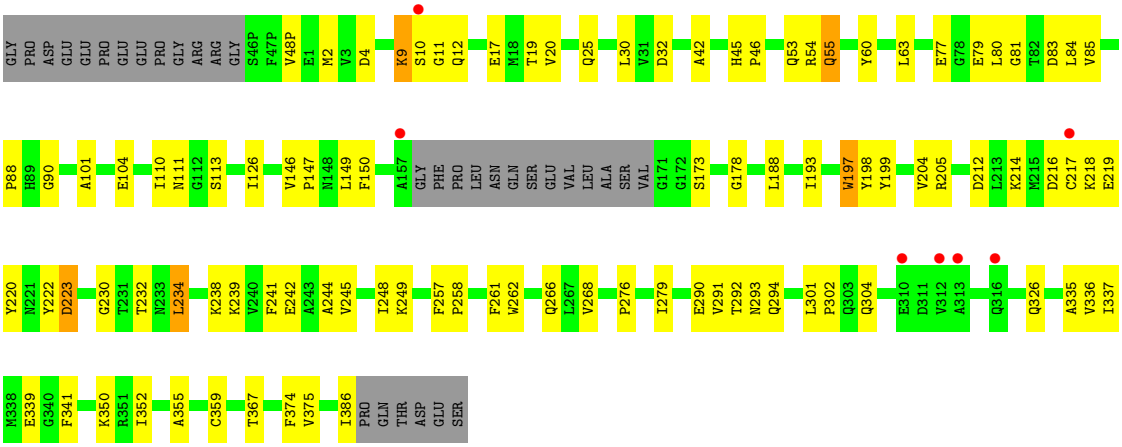
• Molecule 1: Beta-secretase 1

Chain B:



• Molecule 1: Beta-secretase 1

Chain C:


GLY PRO ASP GLU GLU PRO GLU GLU PRO GLY ARG ARG GLY S46P F47P V48P E1 M2 V3 D4 K9 S10 G11 Q12 E17 M18 T19 V20 Q25 L30 V31 D32 A42 H45 P46 Q53 R54 Q55 Y60 L63 E77 G78 E79 L80 G81 T82 D83 L84 V85
P88 H89 G90 A101 E104 I110 N111 G112 S113 I126 V146 P147 N148 L149 F150 A157 GLY PHE PRO LEU ASN GLN SER GLU VAL LEU ALA SER VAL G171 G172 S173 G178 L188 I193 W197 Y198 Y199 V204 R205 D212 L213 K214 M215 D216 C217 K218 E219
Y220 M221 Y222 D223 G230 T231 T232 N233 L234 K238 K239 V240 F241 E242 A243 A244 V245 I248 K249 F257 P258 F261 W262 Q266 L267 V268 P276 I279 E290 V291 T292 N293 Q294 L301 P302 Q303 Q304 E310 D311 V312 A313 Q316 Q326 A335 V336 I337
M338 E339 G340 F341 K350 R351 I352 A355 C359 T367 F374 V375 I386 PRO GLN THR ASP GLU SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.55Å 101.30Å 102.22Å 90.00° 104.16° 90.00°	Depositor
Resolution (Å)	71.39 – 2.90 80.04 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.39-2.90) 99.6 (80.04-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.91Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.202 , 0.238 0.196 , 0.234	Depositor DCC
R_{free} test set	3616 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9049	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: XLI

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	0.27	0/3028	0.48	0/4115
1	B	0.27	0/3028	0.47	0/4115
1	C	0.27	0/3036	0.47	0/4126
All	All	0.27	0/9092	0.48	0/12356

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	2953	0	2861	81	0
1	B	2953	0	2861	72	0
1	C	2961	0	2872	67	0
2	A	37	0	52	21	0
2	B	37	0	52	19	0
2	C	37	0	52	19	0
3	A	25	0	0	1	0
3	B	26	0	0	1	0
3	C	20	0	0	0	0
All	All	9049	0	8750	267	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 15.

All (267) 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)
2:C:393:XLI:CD11	2:C:393:XLI:HD15	0.97	1.15
2:C:393:XLI:CD21	2:C:393:XLI:HD26	0.97	1.15
2:B:393:XLI:HD15	2:B:393:XLI:CD11	0.97	1.12
1:A:375:VAL:HG22	1:B:375:VAL:HG22	1.29	1.11
2:B:393:XLI:HD25	2:B:393:XLI:CD21	0.97	1.11
2:A:393:XLI:CD21	2:A:393:XLI:HD25	0.97	1.10
2:A:393:XLI:CD11	2:A:393:XLI:HD14	0.97	1.10
2:C:393:XLI:CD21	2:C:393:XLI:HD25	0.97	1.09
1:B:4:ASP:H	1:B:173:SER:HB3	1.13	1.09
2:A:393:XLI:CD11	2:A:393:XLI:HD16	0.97	1.08
2:B:393:XLI:CD21	2:B:393:XLI:HD24	0.97	1.08
2:B:393:XLI:CD21	2:B:393:XLI:HD26	0.97	1.08
2:B:393:XLI:CD11	2:B:393:XLI:HD16	0.97	1.07
2:A:393:XLI:CD21	2:A:393:XLI:HD24	0.97	1.06
2:A:393:XLI:CD11	2:A:393:XLI:HD15	0.97	1.06
2:C:393:XLI:CD11	2:C:393:XLI:HD16	0.97	1.06
2:C:393:XLI:CD21	2:C:393:XLI:HD24	0.97	1.06
2:A:393:XLI:CD21	2:A:393:XLI:HD26	0.97	1.05
2:C:393:XLI:CD11	2:C:393:XLI:HD14	0.97	1.04
2:B:393:XLI:CD11	2:B:393:XLI:HD14	0.97	1.03
1:A:4:ASP:H	1:A:173:SER:HB3	1.32	0.94
1:B:20:VAL:HG12	1:B:85:VAL:HG22	1.54	0.89
2:A:393:XLI:HD25	2:A:393:XLI:HD24	1.58	0.85
2:C:393:XLI:HD26	2:C:393:XLI:HD24	1.58	0.85
2:C:393:XLI:HD25	2:C:393:XLI:HD24	1.58	0.85
2:B:393:XLI:HD24	2:B:393:XLI:HD26	1.58	0.85
2:A:393:XLI:HD14	2:A:393:XLI:HD15	1.58	0.85
2:C:393:XLI:HD16	2:C:393:XLI:HD14	1.58	0.85
2:B:393:XLI:HD15	2:B:393:XLI:HD16	1.58	0.85
2:B:393:XLI:HD25	2:B:393:XLI:HD26	1.58	0.85
2:C:393:XLI:HD15	2:C:393:XLI:HD14	1.58	0.85
1:A:291:VAL:HB	1:A:294:GLN:HG2	1.59	0.85
2:A:393:XLI:HD14	2:A:393:XLI:HD16	1.58	0.85
2:A:393:XLI:HD24	2:A:393:XLI:HD26	1.58	0.85
2:A:393:XLI:HD25	2:A:393:XLI:HD26	1.58	0.85
2:B:393:XLI:HD25	2:B:393:XLI:HD24	1.58	0.84
2:C:393:XLI:HD26	2:C:393:XLI:HD25	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:XLI:HD16	2:B:393:XLI:HD14	1.58	0.84
2:B:393:XLI:HD15	2:B:393:XLI:HD14	1.58	0.84
2:C:393:XLI:HD26	2:C:393:XLI:CG2	2.09	0.83
2:A:393:XLI:HD15	2:A:393:XLI:CG2	2.09	0.83
2:C:393:XLI:HD15	2:C:393:XLI:HD16	1.58	0.83
2:C:393:XLI:HD25	2:C:393:XLI:CG2	2.09	0.83
2:A:393:XLI:HD16	2:A:393:XLI:HD15	1.58	0.83
2:A:393:XLI:HD24	2:A:393:XLI:CG2	2.09	0.83
1:C:4:ASP:H	1:C:173:SER:HB3	1.44	0.83
2:A:393:XLI:HD25	2:A:393:XLI:CG2	2.09	0.82
2:B:393:XLI:HD25	2:B:393:XLI:CG2	2.09	0.82
2:B:393:XLI:HD24	2:B:393:XLI:CG2	2.09	0.82
2:B:393:XLI:HD26	2:B:393:XLI:CG2	2.09	0.82
2:A:393:XLI:HD14	2:A:393:XLI:CG2	2.09	0.82
2:B:393:XLI:HD14	2:B:393:XLI:CG2	2.09	0.82
1:A:20:VAL:HG12	1:A:85:VAL:HG22	1.62	0.82
2:C:393:XLI:HD15	2:C:393:XLI:CG2	2.09	0.81
2:A:393:XLI:HD16	2:A:393:XLI:CG2	2.09	0.81
2:B:393:XLI:HD15	2:B:393:XLI:CG2	2.09	0.81
2:C:393:XLI:HD16	2:C:393:XLI:CG2	2.09	0.81
2:C:393:XLI:HD24	2:C:393:XLI:CG2	2.09	0.81
2:B:393:XLI:HD16	2:B:393:XLI:CG2	2.09	0.81
2:A:393:XLI:HD26	2:A:393:XLI:CG2	2.09	0.81
2:C:393:XLI:HD14	2:C:393:XLI:CG2	2.09	0.80
1:B:4:ASP:N	1:B:173:SER:HB3	1.96	0.80
1:A:310:GLU:OE2	1:A:310:GLU:HA	1.83	0.77
1:C:10:SER:HB3	1:C:339:GLU:OE1	1.87	0.75
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.74	0.70
1:C:20:VAL:HG12	1:C:85:VAL:HG22	1.73	0.70
1:A:290:GLU:H	1:A:294:GLN:NE2	1.92	0.67
1:C:291:VAL:H	1:C:294:GLN:HE21	1.45	0.65
1:A:291:VAL:H	1:A:294:GLN:HE21	1.45	0.65
1:A:361:VAL:O	1:A:362:HIS:HB3	1.98	0.64
1:C:291:VAL:HB	1:C:294:GLN:HG2	1.78	0.64
1:A:77:GLU:HG3	1:C:48(P):VAL:HG12	1.78	0.64
1:B:110:ILE:HB	1:B:113:SER:HB3	1.80	0.64
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.79	0.63
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.80	0.62
1:A:110:ILE:HB	1:A:113:SER:HB3	1.80	0.62
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.29	0.62
1:C:9:LYS:HG2	1:C:11:GLY:H	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ILE:HB	1:C:113:SER:HB3	1.80	0.62
1:C:53:GLN:HB3	1:C:55:GLN:HE21	1.66	0.61
1:A:300:ILE:HD13	1:A:337:ILE:CD1	2.32	0.60
1:C:249:LYS:HE2	1:C:262:TRP:CD1	2.37	0.60
1:C:276:PRO:O	1:C:279:ILE:HG12	2.01	0.60
1:A:366:ARG:HA	1:B:211:GLN:HE22	1.66	0.60
1:B:249:LYS:HE2	1:B:262:TRP:CD1	2.37	0.60
1:C:232:THR:O	1:C:336:VAL:HG13	2.01	0.59
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.32	0.59
1:A:326:GLN:HG2	3:A:410:HOH:O	2.02	0.59
1:A:366:ARG:CA	1:B:211:GLN:HE22	2.15	0.59
1:A:249:LYS:HE2	1:A:262:TRP:CD1	2.37	0.59
1:B:380:GLU:O	1:B:380:GLU:HG2	2.03	0.59
1:A:219:GLU:OE1	1:A:239:LYS:HD3	2.02	0.59
1:A:4:ASP:N	1:A:173:SER:HB3	2.11	0.59
1:B:276:PRO:O	1:B:279:ILE:HG12	2.02	0.59
1:C:219:GLU:OE1	1:C:239:LYS:HD3	2.02	0.59
1:C:4:ASP:N	1:C:173:SER:HB3	2.16	0.58
1:A:276:PRO:O	1:A:279:ILE:HG12	2.04	0.58
1:B:376:THR:HG22	1:B:377:LEU:H	1.67	0.58
1:B:204:VAL:CG2	1:B:376:THR:HG21	2.35	0.57
1:B:219:GLU:OE1	1:B:239:LYS:HD3	2.04	0.57
1:B:258:PRO:HB2	1:B:266:GLN:OE1	2.05	0.57
1:C:258:PRO:HB2	1:C:266:GLN:OE1	2.04	0.56
1:A:73:GLN:HG3	2:A:393:XLI:CE	2.35	0.56
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.88	0.56
1:B:9:LYS:H	1:B:9:LYS:HD2	1.71	0.56
1:A:301:LEU:HB3	1:A:302:PRO:HD2	1.88	0.56
1:B:378:ASP:OD2	1:B:380:GLU:HB3	2.06	0.56
1:A:291:VAL:O	1:A:294:GLN:HG3	2.06	0.55
1:C:290:GLU:H	1:C:294:GLN:NE2	2.05	0.55
1:B:300:ILE:HD13	1:B:337:ILE:CD1	2.37	0.54
1:A:188:LEU:HD23	1:A:355:ALA:HB2	1.88	0.54
1:A:9:LYS:H	1:A:9:LYS:HD2	1.72	0.54
1:C:216:ASP:OD1	1:C:218:LYS:HB2	2.07	0.54
1:B:19:THR:HA	1:B:25:GLN:O	2.08	0.54
1:B:188:LEU:HD23	1:B:355:ALA:HB2	1.90	0.54
1:A:45:HIS:ND1	1:A:46:PRO:HD2	2.22	0.53
1:B:9:LYS:HG2	1:B:11:GLY:H	1.73	0.53
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.89	0.53
1:B:216:ASP:OD1	1:B:218:LYS:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:LEU:HD23	1:A:149:LEU:C	2.29	0.53
1:A:216:ASP:OD1	1:A:218:LYS:HB2	2.08	0.53
1:A:32:ASP:OD1	1:A:230:GLY:HA3	2.09	0.53
1:C:291:VAL:O	1:C:294:GLN:HG3	2.08	0.53
1:C:9:LYS:H	1:C:9:LYS:HD2	1.74	0.53
1:B:149:LEU:C	1:B:149:LEU:HD23	2.29	0.53
1:C:19:THR:HA	1:C:25:GLN:O	2.10	0.52
1:A:19:THR:HA	1:A:25:GLN:O	2.08	0.52
1:C:149:LEU:HD23	1:C:149:LEU:C	2.29	0.52
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.90	0.52
1:A:294:GLN:HA	1:A:374:PHE:O	2.10	0.52
1:B:32:ASP:OD1	1:B:230:GLY:HA3	2.09	0.52
1:A:242:GLU:O	1:A:246:LYS:HG2	2.09	0.52
1:C:32:ASP:OD1	1:C:230:GLY:HA3	2.10	0.52
1:B:45:HIS:ND1	1:B:46:PRO:HD2	2.25	0.52
1:A:241:PHE:O	1:A:245:VAL:HG23	2.10	0.51
1:A:367:THR:H	1:B:211:GLN:HE22	1.57	0.51
1:B:241:PHE:CG	1:B:326:GLN:HB3	2.46	0.51
1:A:217:CYS:HA	1:A:220:TYR:CD1	2.45	0.51
1:C:12:GLN:OE1	1:C:113:SER:HA	2.11	0.51
1:C:217:CYS:HA	1:C:220:TYR:CD1	2.45	0.51
2:A:393:XLI:HD12	2:A:393:XLI:H	1.75	0.51
1:A:9:LYS:HG2	1:A:11:GLY:H	1.75	0.50
1:A:238:LYS:O	1:A:242:GLU:HG2	2.11	0.50
1:B:241:PHE:O	1:B:245:VAL:HG23	2.10	0.50
1:B:238:LYS:O	1:B:242:GLU:HG2	2.11	0.50
2:B:393:XLI:HD12	2:B:393:XLI:H	1.76	0.50
1:B:137:PHE:HB2	3:B:403:HOH:O	2.11	0.50
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.47	0.50
1:A:222:TYR:O	1:A:223:ASP:CB	2.59	0.50
1:A:290:GLU:N	1:A:294:GLN:NE2	2.58	0.50
1:A:241:PHE:CG	1:A:326:GLN:HB3	2.47	0.50
1:B:17:GLU:O	1:B:88:PRO:HD2	2.12	0.50
1:C:241:PHE:O	1:C:245:VAL:HG23	2.11	0.49
1:B:288:MET:HA	1:B:295:SER:OG	2.12	0.49
2:C:393:XLI:HD12	2:C:393:XLI:H	1.78	0.49
1:C:244:ALA:O	1:C:248:ILE:HG13	2.12	0.49
1:C:193:ILE:O	1:C:350:LYS:HE2	2.12	0.49
1:C:238:LYS:O	1:C:242:GLU:HG2	2.12	0.49
1:C:241:PHE:CG	1:C:326:GLN:HB3	2.47	0.49
1:C:234:LEU:HB2	1:C:336:VAL:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:O	1:A:350:LYS:HE2	2.13	0.48
1:A:244:ALA:O	1:A:248:ILE:HG13	2.13	0.48
1:A:367:THR:H	1:B:211:GLN:NE2	2.10	0.48
1:B:63:LEU:HG	1:B:81:GLY:HA2	1.95	0.48
1:A:293:ASN:O	1:A:375:VAL:HA	2.13	0.48
1:A:366:ARG:HG2	1:B:211:GLN:OE1	2.14	0.48
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.49	0.48
1:A:29:ILE:HD12	1:A:117:GLY:HA3	1.96	0.47
1:B:54:ARG:HD2	1:B:60:TYR:CZ	2.49	0.47
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.50	0.47
1:A:54:ARG:HD2	1:A:60:TYR:CZ	2.50	0.47
1:B:193:ILE:O	1:B:350:LYS:HE2	2.13	0.47
1:A:3:VAL:O	1:A:4:ASP:HB2	2.15	0.47
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.50	0.47
1:C:63:LEU:HG	1:C:81:GLY:HA2	1.97	0.47
1:C:258:PRO:O	1:C:261:PHE:HB3	2.15	0.47
1:B:335:ALA:O	1:B:339:GLU:HG3	2.14	0.47
1:C:222:TYR:O	1:C:223:ASP:CB	2.62	0.46
1:C:83:ASP:OD1	1:C:84:LEU:N	2.48	0.46
1:B:244:ALA:O	1:B:248:ILE:HG13	2.16	0.46
1:C:54:ARG:HD2	1:C:60:TYR:CZ	2.50	0.46
1:B:10:SER:HB3	1:B:339:GLU:OE1	2.15	0.46
1:C:9:LYS:HE3	1:C:9:LYS:N	2.31	0.46
1:C:290:GLU:N	1:C:294:GLN:NE2	2.63	0.46
1:B:360:HIS:O	1:B:360:HIS:ND1	2.49	0.46
1:A:12:GLN:HE21	1:A:110:ILE:HG21	1.81	0.46
1:A:63:LEU:HG	1:A:81:GLY:HA2	1.97	0.46
1:A:149:LEU:HD23	1:A:150:PHE:N	2.31	0.46
1:B:197:TRP:N	1:B:197:TRP:CD1	2.83	0.46
1:A:77:GLU:HB2	1:A:104:GLU:HB2	1.99	0.45
1:A:366:ARG:HA	1:B:211:GLN:NE2	2.31	0.45
1:B:222:TYR:O	1:B:223:ASP:CB	2.63	0.45
1:A:287:LEU:O	1:A:295:SER:HB2	2.15	0.45
1:C:149:LEU:HD23	1:C:150:PHE:N	2.31	0.45
1:A:83:ASP:OD1	1:A:84:LEU:N	2.48	0.45
1:A:9:LYS:HE3	1:A:9:LYS:N	2.31	0.45
1:A:41:GLY:O	1:A:51:TYR:HB2	2.17	0.45
1:B:258:PRO:O	1:B:261:PHE:HB3	2.16	0.45
1:B:301:LEU:HD11	1:B:367:THR:HA	1.98	0.45
1:B:9:LYS:N	1:B:9:LYS:HE3	2.32	0.44
1:C:197:TRP:N	1:C:197:TRP:CD1	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLU:O	1:C:88:PRO:HD2	2.17	0.44
1:C:63:LEU:HD12	1:C:80:LEU:HB3	1.99	0.44
1:B:29:ILE:HG21	1:B:119:LEU:HB2	2.00	0.44
1:C:9:LYS:HG2	1:C:11:GLY:N	2.32	0.44
1:B:149:LEU:HD23	1:B:150:PHE:N	2.32	0.44
1:C:292:THR:O	1:C:293:ASN:HB2	2.16	0.44
1:A:301:LEU:HD11	1:A:367:THR:HA	1.99	0.44
1:A:258:PRO:O	1:A:261:PHE:HB3	2.17	0.44
1:C:45:HIS:ND1	1:C:46:PRO:HD2	2.33	0.44
1:A:258:PRO:HB2	1:A:266:GLN:OE1	2.17	0.44
1:B:83:ASP:OD1	1:B:84:LEU:N	2.49	0.44
1:B:202:ILE:HD12	1:B:379:MET:CE	2.47	0.43
1:C:204:VAL:O	1:C:205:ARG:HB2	2.17	0.43
1:A:73:GLN:HG3	2:A:393:XLI:HE3	2.00	0.43
1:A:246:LYS:HE2	1:A:246:LYS:HA	2.00	0.43
1:A:256:LYS:HA	1:A:256:LYS:HD2	1.61	0.43
1:C:301:LEU:HD11	1:C:367:THR:HA	1.98	0.43
1:A:45:HIS:CE1	1:A:46:PRO:HD2	2.53	0.43
1:C:197:TRP:CG	1:C:198:TYR:N	2.86	0.43
1:C:337:ILE:O	1:C:341:PHE:HD1	2.02	0.43
1:A:197:TRP:N	1:A:197:TRP:CD1	2.84	0.43
1:A:63:LEU:HD12	1:A:80:LEU:HB3	2.01	0.43
1:B:204:VAL:HG23	1:B:376:THR:HG21	2.00	0.43
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.86	0.43
1:B:63:LEU:HD12	1:B:80:LEU:HB3	2.01	0.43
1:B:197:TRP:CG	1:B:198:TYR:N	2.86	0.43
1:C:294:GLN:HA	1:C:374:PHE:O	2.19	0.43
1:A:197:TRP:CG	1:A:198:TYR:N	2.87	0.43
1:B:126:ILE:HG23	1:B:197:TRP:HB2	2.00	0.43
1:C:199:TYR:HB3	1:C:352:ILE:HD11	2.01	0.43
1:B:63:LEU:HD12	1:B:81:GLY:N	2.34	0.42
1:B:202:ILE:HD12	1:B:379:MET:HG2	2.01	0.42
1:C:63:LEU:HD12	1:C:81:GLY:N	2.33	0.42
1:A:367:THR:N	1:B:211:GLN:HE22	2.18	0.42
1:A:67:VAL:HG22	1:A:68:TYR:N	2.35	0.42
1:B:45:HIS:CE1	1:B:46:PRO:HD2	2.54	0.42
1:C:126:ILE:HG23	1:C:197:TRP:HB2	2.01	0.42
1:A:54:ARG:HH12	1:A:79:GLU:HG3	1.84	0.42
1:A:300:ILE:HD13	1:A:337:ILE:HD13	2.02	0.42
1:C:42:ALA:HB2	1:C:101:ALA:HB1	2.02	0.42
1:B:48:LEU:HD22	1:B:116:GLU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ILE:HG23	1:A:197:TRP:HB2	2.01	0.42
1:A:68:TYR:OH	1:A:70:PRO:HB3	2.20	0.41
1:B:149:LEU:HD22	1:B:178:GLY:HA2	2.02	0.41
1:C:146:VAL:HA	1:C:147:PRO:HD3	1.92	0.41
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.50	0.41
1:A:199:TYR:HB3	1:A:352:ILE:HD11	2.02	0.41
1:B:134:GLU:HA	1:B:135:PRO:HD3	1.86	0.41
1:B:199:TYR:HB3	1:B:352:ILE:HD11	2.01	0.41
1:B:204:VAL:HG21	1:B:376:THR:HG21	2.00	0.41
1:C:149:LEU:HD22	1:C:178:GLY:HA2	2.03	0.41
1:C:77:GLU:HB2	1:C:104:GLU:HB2	2.02	0.41
1:C:386:ILE:HG22	1:C:386:ILE:O	2.21	0.41
1:A:149:LEU:HD22	1:A:178:GLY:CA	2.51	0.41
1:A:291:VAL:HG12	1:A:292:THR:N	2.36	0.41
1:B:54:ARG:HH12	1:B:79:GLU:HG3	1.85	0.41
1:B:376:THR:HG22	1:B:377:LEU:N	2.35	0.41
1:A:63:LEU:HD12	1:A:81:GLY:N	2.36	0.41
1:A:149:LEU:HD22	1:A:178:GLY:HA2	2.03	0.41
1:C:335:ALA:O	1:C:339:GLU:HG3	2.21	0.40
1:B:192:PRO:HG3	1:B:290:GLU:HA	2.02	0.40
1:C:54:ARG:HH12	1:C:79:GLU:HG3	1.85	0.40
1:A:77:GLU:CG	1:C:48(P):VAL:HG12	2.46	0.40
1:B:270:TRP:CE3	1:B:275:THR:HG23	2.56	0.40
1:C:212:ASP:CG	1:C:214:LYS:H	2.25	0.40
1:C:359:CYS:O	1:C:359:CYS:SG	2.80	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	371/408 (91%)	350 (94%)	20 (5%)	1 (0%)	41 71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	371/408 (91%)	345 (93%)	25 (7%)	1 (0%)	41	71
1	C	372/408 (91%)	351 (94%)	20 (5%)	1 (0%)	41	71
All	All	1114/1224 (91%)	1046 (94%)	65 (6%)	3 (0%)	41	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	B	223	ASP
1	C	223	ASP

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	320/348 (92%)	309 (97%)	11 (3%)	37	71
1	B	320/348 (92%)	310 (97%)	10 (3%)	40	74
1	C	321/348 (92%)	312 (97%)	9 (3%)	43	76
All	All	961/1044 (92%)	931 (97%)	30 (3%)	40	74

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(P)	VAL
1	A	9	LYS
1	A	30	LEU
1	A	86	SER
1	A	111	ASN
1	A	197	TRP
1	A	234	LEU
1	A	257	PHE
1	A	310	GLU
1	A	361	VAL
1	A	375	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	48(P)	VAL
1	B	9	LYS
1	B	30	LEU
1	B	111	ASN
1	B	197	TRP
1	B	234	LEU
1	B	257	PHE
1	B	295	SER
1	B	375	VAL
1	B	376	THR
1	C	9	LYS
1	C	30	LEU
1	C	55	GLN
1	C	111	ASN
1	C	197	TRP
1	C	234	LEU
1	C	257	PHE
1	C	304	GLN
1	C	375	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	28	ASN
1	A	111	ASN
1	A	114	ASN
1	A	211	GLN
1	A	294	GLN
1	B	28	ASN
1	B	111	ASN
1	B	114	ASN
1	B	211	GLN
1	C	55	GLN
1	C	111	ASN
1	C	114	ASN
1	C	294	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)

3 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	$\#\|Z\| > 2$
2	XLI	A	393	-	36,36,36	0.91	1 (2%)	44,46,46	0.89	3 (6%)
2	XLI	B	393	-	36,36,36	0.91	1 (2%)	44,46,46	0.85	1 (2%)
2	XLI	C	393	-	36,36,36	0.90	0	44,46,46	0.87	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XLI	A	393	-	-	4/49/49/49	-
2	XLI	B	393	-	-	4/49/49/49	-
2	XLI	C	393	-	-	4/49/49/49	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	393	XLI	CB2-CA2	2.16	1.56	1.53
2	A	393	XLI	CB2-CA2	2.09	1.56	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	393	XLI	CB-CA-N	2.36	115.90	110.58
2	C	393	XLI	CB-CA-N	2.28	115.71	110.58
2	B	393	XLI	CB-CA-N	2.21	115.56	110.58
2	A	393	XLI	O-C-CH3	-2.12	118.28	122.05
2	A	393	XLI	CM-CA3-C4	2.10	113.87	109.84

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	393	XLI	O2-C2-CA1-N1
2	B	393	XLI	O2-C2-CA1-N1
2	C	393	XLI	O2-C2-CA1-N1
2	A	393	XLI	N2-C2-CA1-N1
2	B	393	XLI	N2-C2-CA1-N1
2	C	393	XLI	N2-C2-CA1-N1
2	B	393	XLI	O2-C2-CA1-CB1
2	A	393	XLI	O2-C2-CA1-CB1
2	C	393	XLI	O2-C2-CA1-CB1
2	A	393	XLI	N2-C2-CA1-CB1
2	B	393	XLI	N2-C2-CA1-CB1
2	C	393	XLI	N2-C2-CA1-CB1

There are no ring outliers.

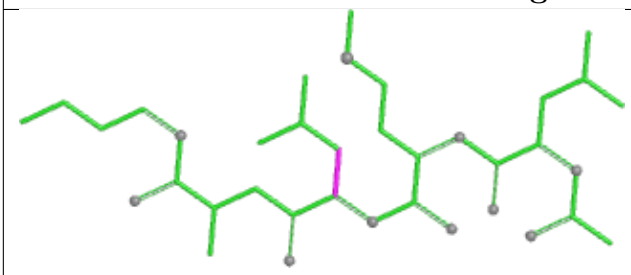
3 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	393	XLI	21	0
2	B	393	XLI	19	0
2	C	393	XLI	19	0

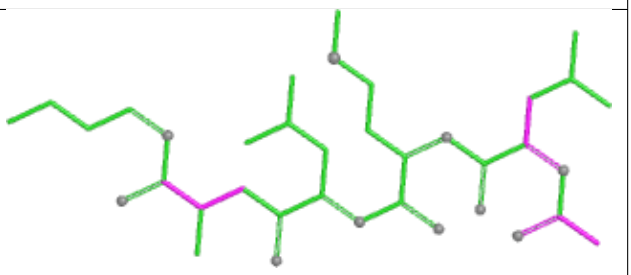
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

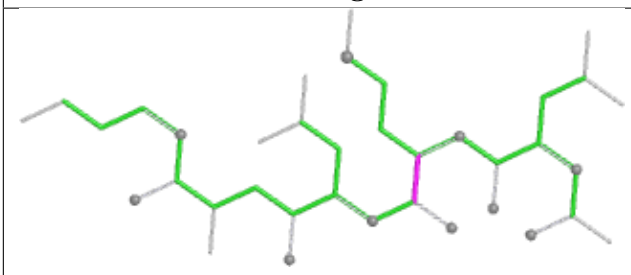
Ligand XLI A 393



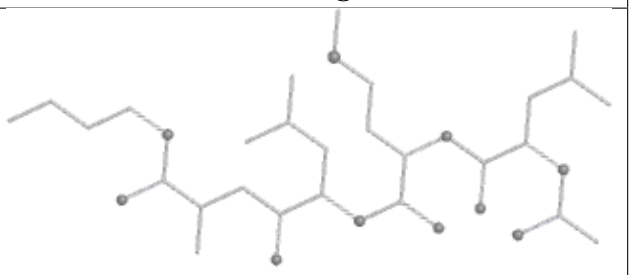
Bond lengths



Bond angles

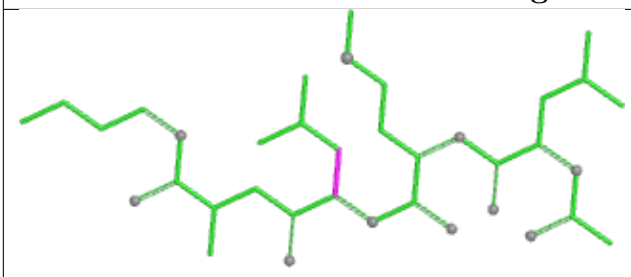


Torsions

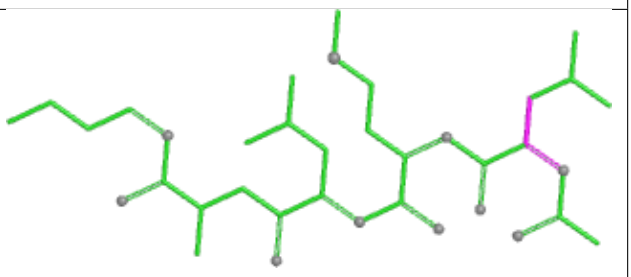


Rings

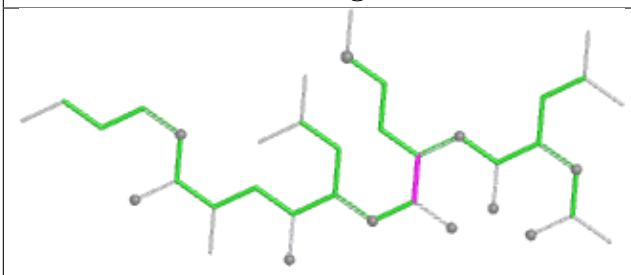
Ligand XLI B 393



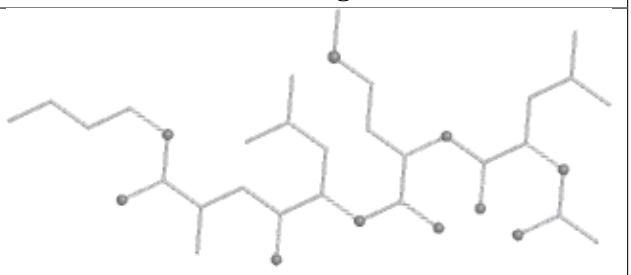
Bond lengths



Bond angles

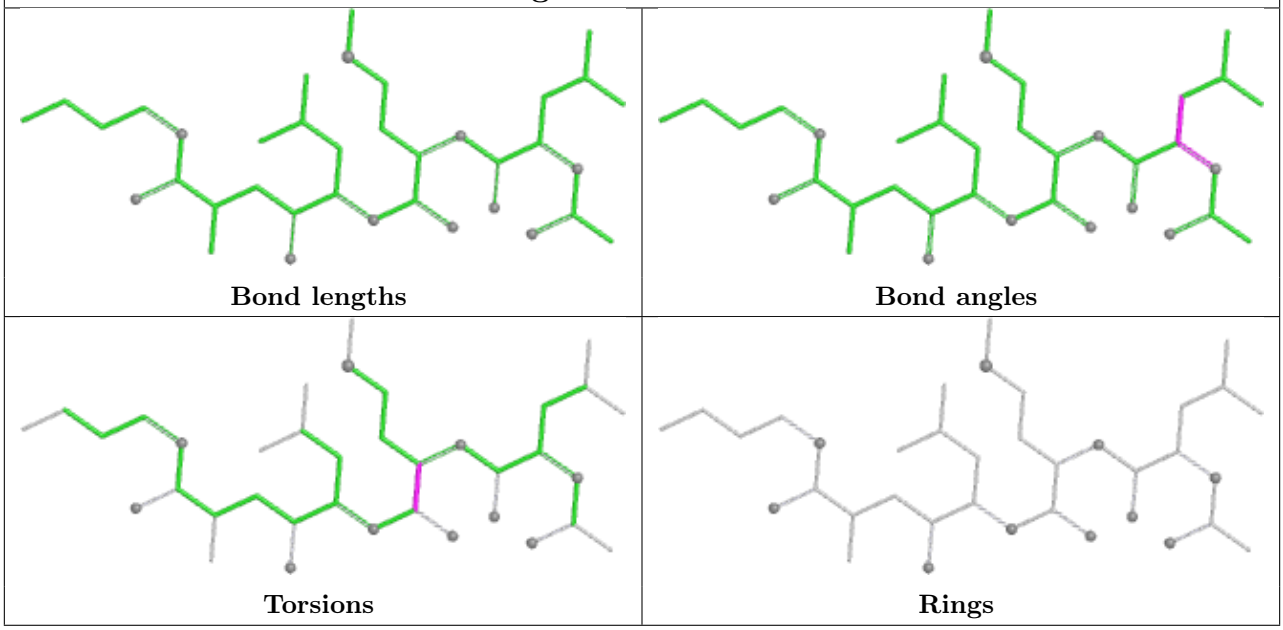


Torsions



Rings

Ligand XLI C 393



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	375/408 (91%)	0.17	3 (0%)	86	86	22, 47, 84, 118	0
1	B	375/408 (91%)	0.16	6 (1%)	72	71	24, 46, 84, 122	0
1	C	376/408 (92%)	0.18	7 (1%)	66	65	17, 49, 84, 121	0
All	All	1126/1224 (91%)	0.17	16 (1%)	75	75	17, 47, 84, 122	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10	SER	6.7
1	C	312	VAL	5.6
1	A	10	SER	4.5
1	B	217	CYS	3.2
1	B	364	GLU	2.9
1	C	316	GLN	2.9
1	A	312	VAL	2.8
1	B	314	THR	2.7
1	C	313	ALA	2.5
1	C	310	GLU	2.4
1	A	311	ASP	2.1
1	B	63	LEU	2.1
1	C	217	CYS	2.1
1	C	157	ALA	2.1
1	B	365	PHE	2.0
1	B	316	GLN	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)

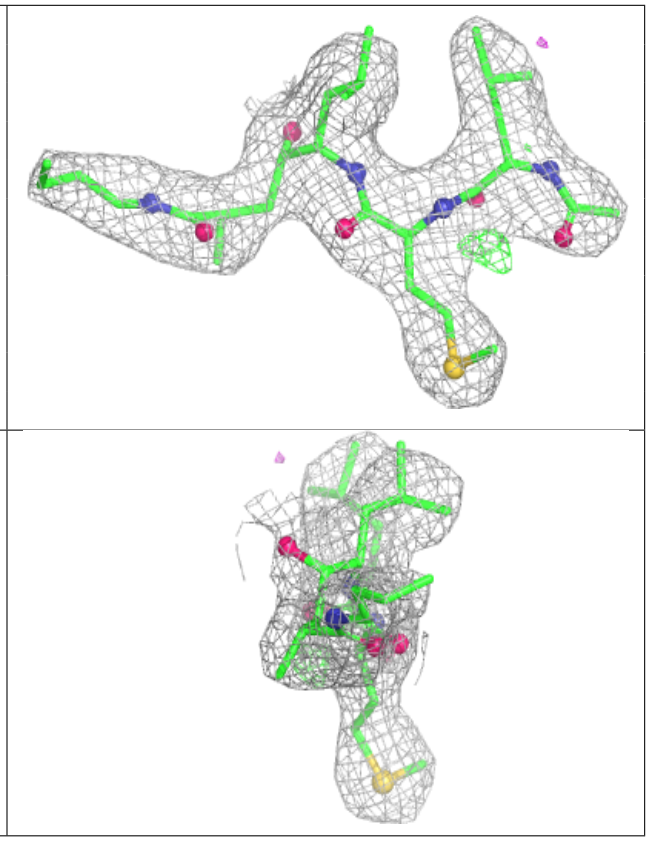
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XLI	A	393	37/37	0.96	0.27	21,41,52,54	0
2	XLI	B	393	37/37	0.97	0.26	30,41,51,55	0
2	XLI	C	393	37/37	0.97	0.29	22,39,57,62	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.

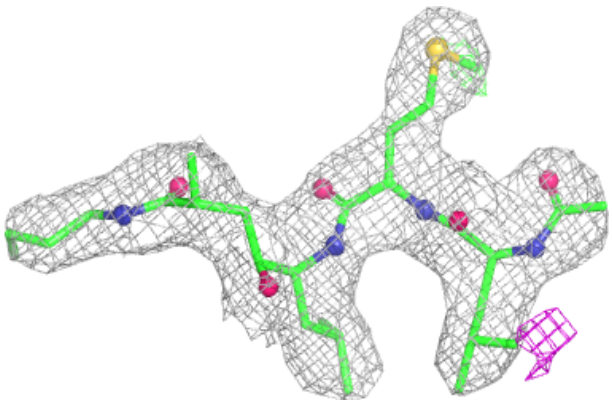
Electron density around XLI A 393:

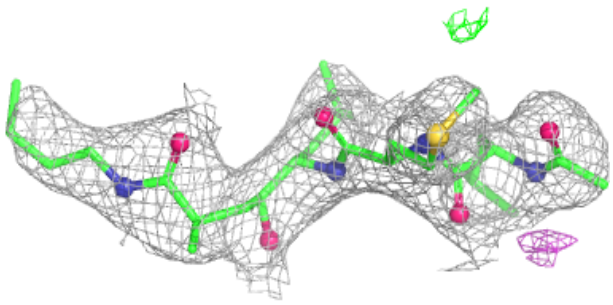
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

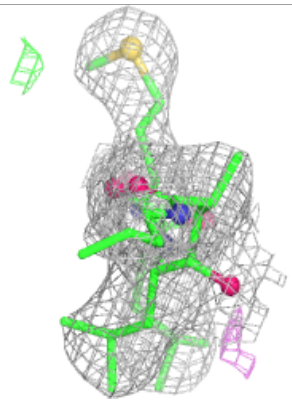


Electron density around XLI B 393:

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

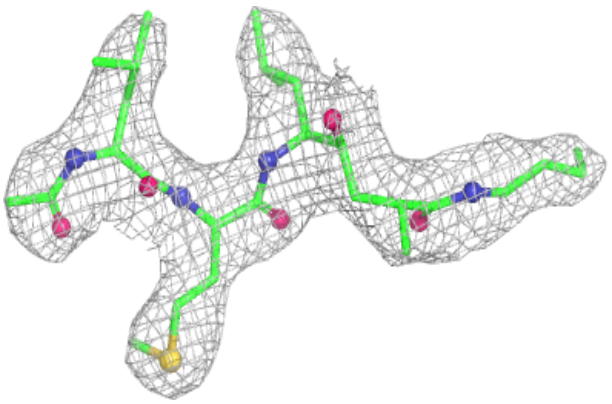


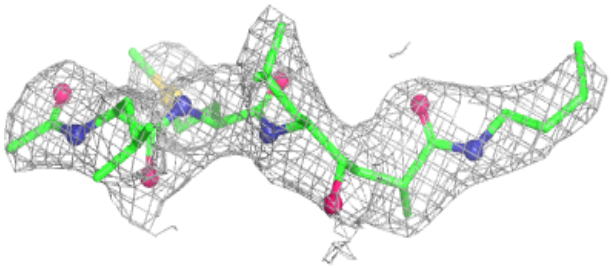


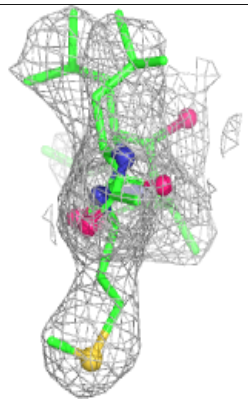


Electron density around XLI C 393:

$2mF_o$-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.