



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:08 am BST

PDB ID : 2HIZ  
Title : Crystal Structure of human beta-secretase (BACE) in the presence of an inhibitor  
Authors : Benson, T.E.; Prince, D.B.; Tomasselli, A.G.; Emmons, T.L.; Paddock, D.J.  
Deposited on : 2006-06-29  
Resolution : 2.50 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.

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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 : 2.11  
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) : 2.11

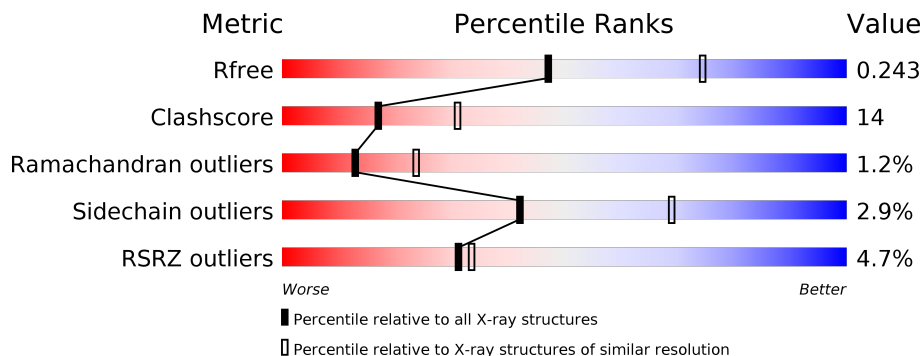
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

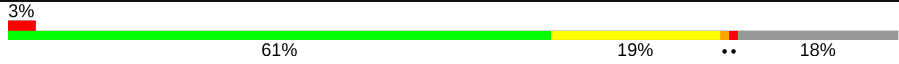


The reported resolution of this entry is 2.50 Å.

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	455	
1	B	455	
1	C	455	

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	PO4	A	703	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9176 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	371	2924	1874	487	549	14	0	0	0
1	B	372	2929	1879	487	549	14	0	0	0
1	C	373	2937	1883	488	552	14	0	0	0

There are 45 discrepancies between the modelled and reference sequences:

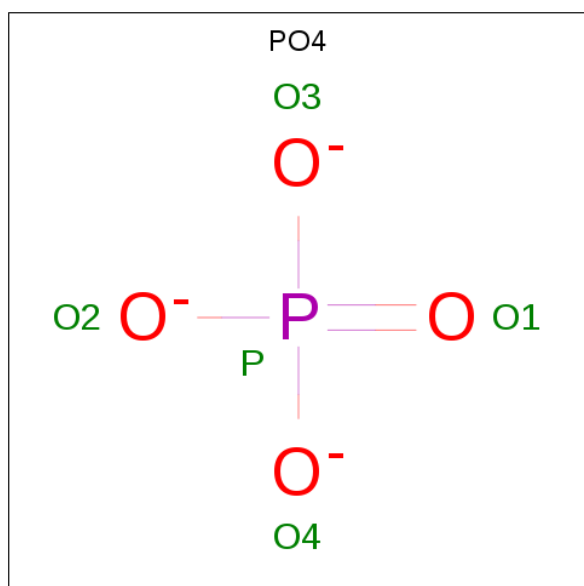
Chain	Residue	Modelled	Actual	Comment	Reference
A	1P	MET	-	CLONING ARTIFACT	UNP P56817
A	2P	ALA	-	CLONING ARTIFACT	UNP P56817
A	3P	SER	-	CLONING ARTIFACT	UNP P56817
A	4P	MET	-	CLONING ARTIFACT	UNP P56817
A	5P	THR	-	CLONING ARTIFACT	UNP P56817
A	6P	GLY	-	CLONING ARTIFACT	UNP P56817
A	7P	GLY	-	CLONING ARTIFACT	UNP P56817
A	8P	GLN	-	CLONING ARTIFACT	UNP P56817
A	9P	GLN	-	CLONING ARTIFACT	UNP P56817
A	10P	MET	-	CLONING ARTIFACT	UNP P56817
A	11P	GLY	-	CLONING ARTIFACT	UNP P56817
A	12P	ARG	-	CLONING ARTIFACT	UNP P56817
A	13P	GLY	-	CLONING ARTIFACT	UNP P56817
A	14P	SER	-	CLONING ARTIFACT	UNP P56817
A	15P	MET	-	CLONING ARTIFACT	UNP P56817
B	1P	MET	-	CLONING ARTIFACT	UNP P56817
B	2P	ALA	-	CLONING ARTIFACT	UNP P56817
B	3P	SER	-	CLONING ARTIFACT	UNP P56817
B	4P	MET	-	CLONING ARTIFACT	UNP P56817
B	5P	THR	-	CLONING ARTIFACT	UNP P56817
B	6P	GLY	-	CLONING ARTIFACT	UNP P56817
B	7P	GLY	-	CLONING ARTIFACT	UNP P56817
B	8P	GLN	-	CLONING ARTIFACT	UNP P56817

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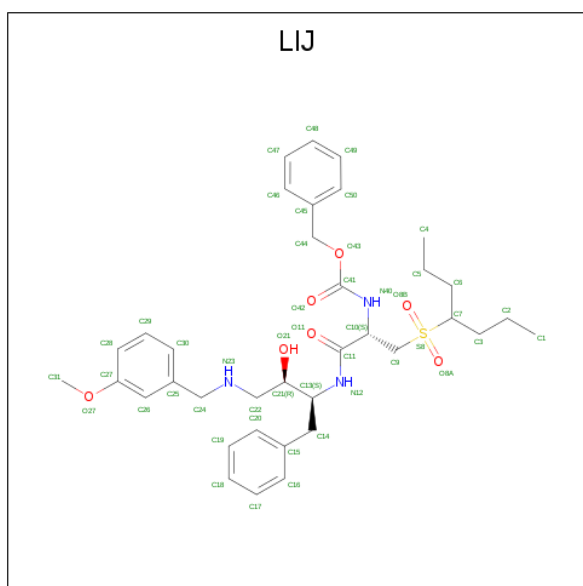
Chain	Residue	Modelled	Actual	Comment	Reference
B	9P	GLN	-	CLONING ARTIFACT	UNP P56817
B	10P	MET	-	CLONING ARTIFACT	UNP P56817
B	11P	GLY	-	CLONING ARTIFACT	UNP P56817
B	12P	ARG	-	CLONING ARTIFACT	UNP P56817
B	13P	GLY	-	CLONING ARTIFACT	UNP P56817
B	14P	SER	-	CLONING ARTIFACT	UNP P56817
B	15P	MET	-	CLONING ARTIFACT	UNP P56817
C	1P	MET	-	CLONING ARTIFACT	UNP P56817
C	2P	ALA	-	CLONING ARTIFACT	UNP P56817
C	3P	SER	-	CLONING ARTIFACT	UNP P56817
C	4P	MET	-	CLONING ARTIFACT	UNP P56817
C	5P	THR	-	CLONING ARTIFACT	UNP P56817
C	6P	GLY	-	CLONING ARTIFACT	UNP P56817
C	7P	GLY	-	CLONING ARTIFACT	UNP P56817
C	8P	GLN	-	CLONING ARTIFACT	UNP P56817
C	9P	GLN	-	CLONING ARTIFACT	UNP P56817
C	10P	MET	-	CLONING ARTIFACT	UNP P56817
C	11P	GLY	-	CLONING ARTIFACT	UNP P56817
C	12P	ARG	-	CLONING ARTIFACT	UNP P56817
C	13P	GLY	-	CLONING ARTIFACT	UNP P56817
C	14P	SER	-	CLONING ARTIFACT	UNP P56817
C	15P	MET	-	CLONING ARTIFACT	UNP P56817

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is BENZYL [(1S)-2-({(1S,2R)-1-BENZYL-2-HYDROXY-3-[(3-METHOXYBENZYL)AMINO]PROPYL}AMINO)-2-OXO-1-[(1-PROPYLBUTYL)SULFONYL]METHYL}ETHYL]CARBAMATE (three-letter code: LIJ) (formula: C<sub>36</sub>H<sub>49</sub>N<sub>3</sub>O<sub>7</sub>S).

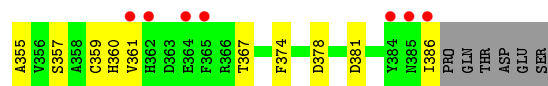


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 47 36 3 7 1	0	0
3	B	1	Total C N O S 47 36 3 7 1	0	0
3	C	1	Total C N O S 47 36 3 7 1	0	0

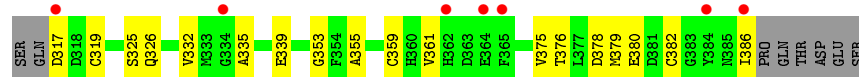
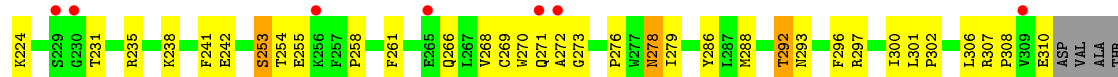
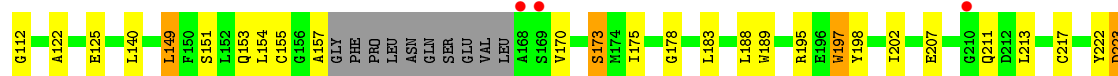
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	86	Total O 86 86	0	0
4	B	75	Total O 75 75	0	0
4	C	69	Total O 69 69	0	0





● Molecule 1: Beta-secretase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.24Å 104.09Å 100.95Å 90.00° 103.46° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 32.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.5 (20.00-2.50) 86.9 (32.73-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.14 (at 2.51Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.214 , 0.253 0.204 , 0.243	Depositor DCC
$R_{free}$ test set	5247 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.9	Xtrriage
Anisotropy	0.317	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9176	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: PO4, LIJ

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	0.36	0/2998	0.68	2/4072 (0.0%)
1	B	0.36	0/3003	0.66	2/4079 (0.0%)
1	C	0.37	0/3011	0.67	0/4090
All	All	0.36	0/9012	0.67	4/12241 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LEU	N-CA-C	-5.45	96.29	111.00
1	A	375	VAL	CB-CA-C	-5.31	101.31	111.40
1	B	198	TYR	N-CA-C	-5.27	96.78	111.00
1	B	234	LEU	N-CA-C	-5.11	97.20	111.00

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	2924	0	2844	74	0
1	B	2929	0	2854	76	0
1	C	2937	0	2858	97	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
3	A	47	0	49	2	0
3	B	47	0	49	0	0
3	C	47	0	49	2	0
4	A	86	0	0	2	0
4	B	75	0	0	1	0
4	C	69	0	0	1	0
All	All	9176	0	8703	238	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 (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:VAL:HG22	1:C:375:VAL:HG13	1.45	0.98
1:B:269:CYS:HG	1:B:319:CYS:HG	0.96	0.88
1:C:4:ASP:H	1:C:173:SER:HB3	1.40	0.86
1:A:375:VAL:CG2	1:C:375:VAL:HG13	2.11	0.81
1:B:276:PRO:O	1:B:279:ILE:HG12	1.86	0.75
1:C:155:CYS:HG	1:C:359:CYS:HG	0.78	0.75
1:C:269:CYS:HG	1:C:319:CYS:HG	0.77	0.74
1:B:20:VAL:HG12	1:B:85:VAL:HG22	1.70	0.74
1:C:288:MET:HE1	1:C:378:ASP:HA	1.69	0.73
1:A:149:LEU:HD23	1:A:150:PHE:N	2.02	0.73
1:A:155:CYS:HG	1:A:359:CYS:HG	0.87	0.72
1:A:375:VAL:HG22	1:C:375:VAL:CG1	2.19	0.72
1:C:217:CYS:HG	1:C:382:CYS:HG	0.75	0.72
1:A:258:PRO:HG3	1:A:266:GLN:NE2	2.06	0.70
1:B:258:PRO:HG3	1:B:266:GLN:NE2	2.07	0.69
1:C:202:ILE:CD1	1:C:379:MET:HG3	2.23	0.69
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.74	0.68
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.75	0.68
1:C:235:ARG:HB2	1:C:332:VAL:HB	1.76	0.68
1:A:258:PRO:HG3	1:A:266:GLN:HE21	1.60	0.67
1:A:61(P):SER:O	1:A:62(P):PHE:HB2	1.95	0.67
1:C:235:ARG:HG3	1:C:332:VAL:HB	1.77	0.67
1:B:170:VAL:HG12	1:B:171:GLY:N	2.10	0.67
1:B:155:CYS:O	1:B:170:VAL:HG13	1.96	0.66
1:B:234:LEU:HG	1:B:337:ILE:HD11	1.76	0.66
1:C:73:GLN:HB2	3:C:803:LIJ:H50	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:GLN:CD	1:C:271:GLN:H	1.99	0.65
1:A:61(P):SER:HB2	4:A:997:HOH:O	1.96	0.64
1:B:261:PHE:CD1	1:B:268:VAL:HG23	2.33	0.64
1:A:235:ARG:HG3	1:A:332:VAL:HB	1.79	0.64
1:B:155:CYS:O	1:B:170:VAL:CG1	2.46	0.64
1:A:276:PRO:O	1:A:279:ILE:HG12	1.97	0.64
1:C:4:ASP:N	1:C:173:SER:HB3	2.12	0.63
1:C:276:PRO:O	1:C:279:ILE:HG12	1.99	0.63
1:B:235:ARG:HG3	1:B:332:VAL:HB	1.81	0.62
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.82	0.62
1:B:244:ALA:O	1:B:248:ILE:HG13	1.99	0.62
1:B:378:ASP:HB3	1:B:381:ASP:OD2	1.99	0.62
1:A:300:ILE:HD12	1:A:300:ILE:N	2.16	0.61
1:A:367:THR:H	1:C:211:GLN:HE22	1.49	0.61
1:C:235:ARG:CG	1:C:332:VAL:HB	2.30	0.61
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.82	0.61
1:A:72:THR:HG22	3:A:801:LIJ:H46	1.82	0.61
1:A:155:CYS:O	1:A:170:VAL:CG1	2.49	0.61
1:B:309:VAL:HG21	1:B:321:LYS:HG3	1.83	0.60
1:B:188:LEU:HD23	1:B:355:ALA:HB2	1.83	0.60
1:C:61(P):SER:N	1:C:175:ILE:CG2	2.64	0.60
1:C:149:LEU:HD21	1:C:178:GLY:HA2	1.84	0.60
1:B:103:THR:O	1:B:104:GLU:HG3	2.02	0.59
1:C:149:LEU:O	1:C:149:LEU:HD23	2.02	0.59
1:B:303:GLN:HB2	1:B:361:VAL:CG1	2.33	0.59
1:A:269:CYS:HG	1:A:319:CYS:HG	0.74	0.59
1:A:19:THR:HA	1:A:25:GLN:O	2.03	0.59
1:A:125:GLU:HG3	1:A:125:GLU:O	2.02	0.59
1:C:271:GLN:CD	1:C:271:GLN:N	2.56	0.59
1:B:290:GLU:HG2	4:B:908:HOH:O	2.03	0.58
1:C:61(P):SER:N	1:C:175:ILE:HG23	2.19	0.58
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.39	0.57
1:B:245:VAL:HG12	1:B:249:LYS:HE3	1.86	0.57
1:B:271:GLN:HB2	1:B:274:THR:HG21	1.87	0.57
1:C:238:LYS:HE2	1:C:242:GLU:OE2	2.05	0.57
1:C:288:MET:CE	1:C:378:ASP:HA	2.33	0.57
1:C:155:CYS:HG	1:C:359:CYS:CB	2.16	0.57
1:C:63:LEU:HB2	1:C:80:LEU:O	2.05	0.57
1:C:9:LYS:HE2	1:C:112:GLY:O	2.05	0.57
1:A:363:ASP:HB3	1:A:366:ARG:O	2.05	0.56
1:A:9:LYS:HD2	1:A:12:GLN:OE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLN:HB2	1:B:361:VAL:HG11	1.87	0.56
1:C:235:ARG:CB	1:C:332:VAL:HB	2.36	0.56
1:A:254:THR:HG22	1:A:255:GLU:HG3	1.87	0.55
1:C:310:GLU:HG3	1:C:310:GLU:O	2.06	0.55
1:A:157:ALA:HB2	1:A:170:VAL:HG22	1.88	0.55
1:B:245:VAL:CG1	1:B:249:LYS:HE3	2.36	0.55
1:C:238:LYS:HG3	1:C:326:GLN:OE1	2.07	0.55
1:B:170:VAL:CG1	1:B:171:GLY:N	2.70	0.55
1:B:291:VAL:O	1:B:294:GLN:HG3	2.06	0.54
1:B:238:LYS:HE3	1:B:242:GLU:OE2	2.08	0.54
1:A:3:VAL:O	1:A:173:SER:OG	2.15	0.54
1:C:157:ALA:HB2	1:C:170:VAL:HG12	1.90	0.54
1:C:73:GLN:HB2	3:C:803:LIJ:C50	2.38	0.54
1:C:63(P):VAL:O	1:C:63(P):VAL:HG22	2.08	0.53
1:A:155:CYS:HG	1:A:359:CYS:CB	2.20	0.53
1:A:335:ALA:O	1:A:339:GLU:HG3	2.08	0.53
1:A:149:LEU:C	1:A:149:LEU:HD23	2.29	0.53
1:A:378:ASP:HB3	1:A:381:ASP:OD2	2.09	0.53
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.91	0.53
1:B:149:LEU:HD23	1:B:149:LEU:C	2.30	0.52
1:C:198:TYR:CE2	1:C:224:LYS:HE3	2.44	0.52
1:C:241:PHE:CD2	1:C:326:GLN:HB3	2.43	0.52
1:C:335:ALA:O	1:C:339:GLU:HG3	2.10	0.52
1:A:235:ARG:CG	1:A:332:VAL:HB	2.39	0.52
1:C:151:SER:OG	1:C:175:ILE:HB	2.10	0.52
1:C:3:VAL:O	1:C:4:ASP:HB3	2.08	0.52
1:A:91:PRO:HD3	1:A:176:ILE:HB	1.91	0.51
1:C:36:SER:OG	1:C:122:ALA:HB3	2.10	0.51
1:B:194:ARG:HB3	1:B:200:GLU:HG2	1.92	0.51
1:C:270:TRP:O	1:C:317:ASP:HB3	2.10	0.51
1:C:189:TRP:O	1:C:353:GLY:HA2	2.10	0.51
1:B:222:TYR:O	1:B:223:ASP:CB	2.59	0.50
1:C:222:TYR:O	1:C:223:ASP:CB	2.59	0.50
1:A:174:MET:CE	1:A:176:ILE:HD11	2.41	0.50
1:A:222:TYR:O	1:A:223:ASP:CB	2.59	0.50
1:A:365:PHE:CD1	1:A:366:ARG:HG3	2.46	0.50
1:C:63(P):VAL:CG2	1:C:63(P):VAL:O	2.60	0.50
1:B:126:ILE:HG23	1:B:197:TRP:HB2	1.94	0.49
1:A:209:ASN:ND2	1:A:281:PRO:HB3	2.27	0.49
1:A:278:ASN:OD1	1:C:254:THR:HG23	2.12	0.49
1:C:19:THR:HA	1:C:25:GLN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:SER:O	1:B:360:HIS:HB3	2.12	0.49
1:C:61(P):SER:HB3	1:C:178:GLY:HA3	1.94	0.49
1:C:376:THR:HB	4:C:950:HOH:O	2.11	0.49
1:B:303:GLN:N	1:B:303:GLN:OE1	2.36	0.49
1:A:125:GLU:HG2	1:A:197:TRP:HB3	1.94	0.49
1:C:4:ASP:H	1:C:173:SER:CB	2.20	0.49
1:A:375:VAL:HG22	1:C:375:VAL:HG22	1.95	0.48
1:C:302:PRO:O	1:C:306:LEU:HB2	2.13	0.48
1:B:77:GLU:HG2	1:B:104:GLU:HB2	1.95	0.48
1:B:154:LEU:O	1:B:339:GLU:HA	2.13	0.48
1:B:271:GLN:CD	1:B:271:GLN:H	2.16	0.48
1:B:301:LEU:HD11	1:B:367:THR:HA	1.95	0.48
1:B:155:CYS:CB	1:B:359:CYS:HG	2.22	0.48
1:A:234:LEU:HG	1:A:337:ILE:HD11	1.95	0.48
1:C:258:PRO:HB2	1:C:266:GLN:OE1	2.13	0.48
1:B:238:LYS:O	1:B:242:GLU:HG3	2.14	0.48
1:B:300:ILE:HG13	1:B:300:ILE:O	2.14	0.48
1:A:225:SER:OG	1:A:331:THR:HB	2.14	0.48
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.96	0.48
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.44	0.48
1:C:300:ILE:HG13	1:C:300:ILE:O	2.13	0.47
1:C:307:ARG:HA	1:C:308:PRO:HD3	1.68	0.47
1:B:302:PRO:O	1:B:306:LEU:HB2	2.15	0.47
1:A:45:HIS:ND1	1:A:46:PRO:HD2	2.29	0.47
1:C:63(P):VAL:HA	1:C:3:VAL:HG23	1.97	0.47
1:A:110:ILE:HB	1:A:113:SER:HB3	1.97	0.47
1:B:144:THR:OG1	1:B:146:VAL:HG23	2.14	0.47
1:B:268:VAL:HG12	1:B:269:CYS:N	2.30	0.47
1:C:8:GLY:O	1:C:170:VAL:HG22	2.15	0.47
1:C:95:VAL:HG11	1:C:140:LEU:HD12	1.95	0.47
1:A:300:ILE:HG12	1:A:337:ILE:HD12	1.96	0.47
1:B:302:PRO:HG2	1:B:303:GLN:OE1	2.15	0.47
1:B:212:ASP:O	1:B:214:LYS:HG3	2.15	0.46
1:B:205:ARG:NH1	1:B:212:ASP:OD2	2.48	0.46
1:C:59:THR:HG21	1:C:84:LEU:CD1	2.46	0.46
1:B:19:THR:HA	1:B:25:GLN:O	2.14	0.46
1:B:374:PHE:HD2	1:C:292:THR:HG22	1.80	0.46
1:A:54:ARG:HB3	1:A:60:TYR:CD2	2.50	0.46
1:C:125:GLU:CD	1:C:195:ARG:HH11	2.19	0.46
1:C:207:GLU:HA	1:C:211:GLN:O	2.15	0.46
1:C:241:PHE:CG	1:C:326:GLN:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:CYS:CB	1:A:319:CYS:HG	2.25	0.45
1:A:238:LYS:O	1:A:242:GLU:HG3	2.16	0.45
1:B:301:LEU:O	1:B:304:GLN:HB2	2.17	0.45
1:A:82:THR:HG22	1:A:98:ASN:HD22	1.80	0.45
1:C:213:LEU:HD12	1:C:213:LEU:HA	1.85	0.45
1:C:202:ILE:HD12	1:C:379:MET:HG3	1.97	0.45
1:B:222:TYR:O	1:B:223:ASP:HB3	2.17	0.45
1:A:205:ARG:HB3	1:A:286:TYR:HB2	1.98	0.45
1:A:271:GLN:O	1:A:272:ALA:C	2.55	0.45
1:A:241:PHE:CG	1:A:326:GLN:HB3	2.51	0.45
1:C:68:TYR:OH	1:C:70:PRO:HB3	2.17	0.45
1:C:76:TRP:HB2	1:C:102:ILE:HG23	1.99	0.45
1:B:125:GLU:O	1:B:125:GLU:HG3	2.17	0.45
1:A:198:TYR:CE2	1:A:224:LYS:HE3	2.52	0.44
1:A:14:TYR:CG	1:A:154:LEU:HD22	2.53	0.44
1:B:22:SER:HA	1:B:23:PRO:C	2.37	0.44
1:C:149:LEU:C	1:C:149:LEU:HD23	2.38	0.44
1:B:271:GLN:O	1:B:274:THR:HG23	2.17	0.44
1:C:380:GLU:H	1:C:380:GLU:CD	2.21	0.44
1:A:61(P):SER:O	1:A:62(P):PHE:CB	2.65	0.44
1:C:278:ASN:H	1:C:278:ASN:HD22	1.65	0.44
1:C:21:GLY:HA2	1:C:83:ASP:OD1	2.17	0.44
1:A:249:LYS:HE2	1:A:262:TRP:CD1	2.53	0.44
1:A:3:VAL:O	1:A:173:SER:CB	2.65	0.44
1:A:304:GLN:O	1:A:336:VAL:HB	2.18	0.44
1:A:70:PRO:HA	1:A:75:LYS:HB3	2.00	0.43
1:B:217:CYS:HA	1:B:220:TYR:CD1	2.53	0.43
1:C:19:THR:OG1	1:C:86:SER:HB2	2.17	0.43
1:A:189:TRP:CZ3	1:B:291:VAL:CG1	3.02	0.43
1:A:197:TRP:CG	1:A:198:TYR:N	2.86	0.43
1:C:197:TRP:CG	1:C:198:TYR:N	2.86	0.43
1:C:30:LEU:HD23	1:C:30:LEU:C	2.38	0.43
1:C:155:CYS:SG	1:C:359:CYS:CB	3.06	0.43
1:C:261:PHE:CD1	1:C:268:VAL:HG23	2.53	0.43
1:A:125:GLU:HG2	1:A:197:TRP:CB	2.48	0.43
1:A:375:VAL:CG2	1:C:375:VAL:HG22	2.48	0.43
1:C:54:ARG:HD2	1:C:60:TYR:CZ	2.54	0.43
1:A:179:ILE:HD11	1:A:344:VAL:HG11	1.99	0.43
1:C:293:ASN:CB	1:C:375:VAL:HG12	2.49	0.43
1:C:14:TYR:CG	1:C:154:LEU:HD22	2.54	0.42
1:C:153:GLN:OE1	1:C:183:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ASN:HA	1:C:375:VAL:HG12	2.01	0.42
1:A:9:LYS:HG3	1:A:12:GLN:HG3	2.01	0.42
1:A:241:PHE:CD2	1:A:326:GLN:HB3	2.55	0.42
1:B:271:GLN:O	1:B:272:ALA:C	2.57	0.42
1:B:199:TYR:HB3	1:B:352:ILE:HD11	2.01	0.42
1:B:149:LEU:HD12	1:B:346:ASP:HA	2.02	0.42
1:B:304:GLN:CG	1:B:361:VAL:HG21	2.50	0.42
1:C:293:ASN:HA	1:C:375:VAL:HA	2.01	0.42
1:A:213:LEU:HA	1:A:213:LEU:HD12	1.78	0.42
1:A:45:HIS:CE1	1:A:46:PRO:HD2	2.54	0.42
4:A:901:HOH:O	1:C:375:VAL:HG22	2.19	0.42
1:B:267:LEU:HD23	1:B:309:VAL:HG21	2.01	0.42
1:B:309:VAL:HG22	1:B:320:TYR:HA	2.00	0.42
1:B:91:PRO:HD3	1:B:176:ILE:HB	2.02	0.42
1:A:298:ILE:HA	1:A:369:ALA:O	2.20	0.41
1:C:271:GLN:O	1:C:273:GLY:N	2.53	0.41
1:C:231:THR:HG21	1:C:332:VAL:HG11	2.02	0.41
1:C:286:TYR:CD2	1:C:297:ARG:HB3	2.54	0.41
1:B:344:VAL:O	1:B:352:ILE:HA	2.19	0.41
1:B:34:GLY:HA3	1:B:228:ASP:OD1	2.20	0.41
1:B:36:SER:OG	1:B:122:ALA:HB3	2.20	0.41
1:C:111:ASN:HD22	1:C:112:GLY:N	2.17	0.41
1:A:287:LEU:O	1:A:295:SER:HB2	2.21	0.41
1:B:271:GLN:HB2	1:B:274:THR:CG2	2.49	0.41
1:B:298:ILE:HG13	1:B:298:ILE:O	2.20	0.41
1:C:189:TRP:HB3	1:C:296:PHE:CD2	2.56	0.41
1:B:219:GLU:OE2	1:B:239:LYS:HD3	2.21	0.41
1:C:68:TYR:OH	1:C:75:LYS:HD3	2.20	0.41
1:A:34:GLY:O	3:A:801:LIJ:H26	2.21	0.41
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.56	0.41
1:B:309:VAL:O	1:B:319:CYS:HB2	2.20	0.41
1:C:3:VAL:O	1:C:4:ASP:CB	2.67	0.41
1:B:9:LYS:O	1:B:10:SER:C	2.59	0.41
1:B:197:TRP:CG	1:B:198:TYR:N	2.89	0.41
1:B:267:LEU:HD23	1:B:309:VAL:CG2	2.51	0.41
1:A:188:LEU:HD23	1:A:355:ALA:HB2	2.03	0.40
1:C:149:LEU:HD21	1:C:178:GLY:CA	2.49	0.40
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.89	0.40
1:A:62(P):PHE:HD1	1:A:62(P):PHE:HA	1.81	0.40
1:C:268:VAL:O	1:C:319:CYS:HA	2.22	0.40
1:B:269:CYS:HG	1:B:319:CYS:CB	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLN:NE2	1:B:340:GLY:HA3	2.35	0.40
1:B:386:ILE:H	1:B:386:ILE:HG13	1.56	0.40
1:C:222:TYR:O	1:C:223:ASP:HB2	2.21	0.40
1:B:291:VAL:CG1	1:B:292:THR:N	2.84	0.40
1:C:17:GLU:HG2	1:C:88:PRO:HG2	2.03	0.40
1:A:307:ARG:HA	1:A:308:PRO:HD3	1.79	0.40
1:C:253:SER:C	1:C:255:GLU:H	2.23	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	365/455 (80%)	341 (93%)	21 (6%)	3 (1%)	19	35
1	B	366/455 (80%)	337 (92%)	24 (7%)	5 (1%)	11	20
1	C	367/455 (81%)	344 (94%)	18 (5%)	5 (1%)	11	20
All	All	1098/1365 (80%)	1022 (93%)	63 (6%)	13 (1%)	13	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62(P)	PHE
1	A	223	ASP
1	B	10	SER
1	B	223	ASP
1	C	223	ASP
1	C	272	ALA
1	C	10	SER
1	A	125	GLU
1	B	131	ASP
1	B	254	THR

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Mol	Chain	Res	Type
1	B	278	ASN
1	C	70	PRO
1	C	253	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	317/381 (83%)	310 (98%)	7 (2%)	52	77
1	B	317/381 (83%)	308 (97%)	9 (3%)	43	70
1	C	318/381 (84%)	306 (96%)	12 (4%)	33	58
All	All	952/1143 (83%)	924 (97%)	28 (3%)	42	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62(P)	PHE
1	A	173	SER
1	A	187	SER
1	A	197	TRP
1	A	234	LEU
1	A	254	THR
1	A	375	VAL
1	B	62(P)	PHE
1	B	111	ASN
1	B	149	LEU
1	B	197	TRP
1	B	209	ASN
1	B	213	LEU
1	B	234	LEU
1	B	267	LEU
1	B	294	GLN
1	C	1	GLU
1	C	55	GLN
1	C	64	ARG

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Mol	Chain	Res	Type
1	C	111	ASN
1	C	149	LEU
1	C	173	SER
1	C	197	TRP
1	C	278	ASN
1	C	292	THR
1	C	325	SER
1	C	361	VAL
1	C	386	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	73	GLN
1	A	98	ASN
1	A	111	ASN
1	A	266	GLN
1	A	271	GLN
1	B	92	ASN
1	B	98	ASN
1	B	111	ASN
1	B	209	ASN
1	C	73	GLN
1	C	98	ASN
1	C	111	ASN
1	C	211	GLN
1	C	278	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	PO4	C	701	-	4,4,4	1.55	0	6,6,6	0.43	0
3	LIJ	A	801	-	46,49,49	2.68	22 (47%)	55,64,64	1.39	10 (18%)
2	PO4	A	702	-	4,4,4	1.55	0	6,6,6	0.44	0
2	PO4	A	703	-	4,4,4	1.58	0	6,6,6	0.43	0
3	LIJ	B	802	-	46,49,49	2.73	23 (50%)	55,64,64	1.49	11 (20%)
3	LIJ	C	803	-	46,49,49	2.77	24 (52%)	55,64,64	1.56	11 (20%)

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	LIJ	C	803	-	-	14/50/50/50	0/3/3/3
3	LIJ	B	802	-	-	12/50/50/50	0/3/3/3
3	LIJ	A	801	-	-	14/50/50/50	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	803	LIJ	C26-C25	5.58	1.48	1.39
3	A	801	LIJ	C28-C27	5.49	1.49	1.38
3	C	803	LIJ	C26-C27	5.39	1.48	1.38
3	C	803	LIJ	C28-C27	5.37	1.49	1.38
3	B	802	LIJ	C26-C25	5.37	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	LIJ	C28-C27	5.32	1.49	1.38
3	A	801	LIJ	C26-C25	5.30	1.48	1.39
3	A	801	LIJ	C26-C27	4.98	1.47	1.38
3	B	802	LIJ	C26-C27	4.87	1.47	1.38
3	B	802	LIJ	C20-C15	4.79	1.49	1.38
3	A	801	LIJ	C20-C15	4.70	1.49	1.38
3	C	803	LIJ	C20-C15	4.48	1.48	1.38
3	A	801	LIJ	C16-C15	4.39	1.48	1.38
3	C	803	LIJ	C29-C30	4.36	1.48	1.38
3	B	802	LIJ	C16-C15	4.27	1.48	1.38
3	C	803	LIJ	C30-C25	4.25	1.48	1.38
3	A	801	LIJ	C30-C25	4.18	1.47	1.38
3	C	803	LIJ	C29-C28	4.17	1.47	1.38
3	B	802	LIJ	C50-C45	4.17	1.47	1.38
3	A	801	LIJ	C17-C16	4.16	1.47	1.38
3	B	802	LIJ	C29-C30	4.16	1.47	1.38
3	C	803	LIJ	C16-C15	4.15	1.47	1.38
3	C	803	LIJ	C50-C45	4.10	1.47	1.38
3	B	802	LIJ	C17-C16	4.09	1.47	1.38
3	A	801	LIJ	C29-C30	4.09	1.47	1.38
3	A	801	LIJ	C50-C45	4.07	1.47	1.38
3	A	801	LIJ	C29-C28	4.03	1.47	1.38
3	B	802	LIJ	C29-C28	3.96	1.47	1.38
3	C	803	LIJ	C17-C16	3.84	1.47	1.38
3	B	802	LIJ	C30-C25	3.67	1.46	1.38
3	A	801	LIJ	C18-C17	3.55	1.47	1.38
3	A	801	LIJ	C19-C20	3.54	1.46	1.38
3	B	802	LIJ	C46-C45	3.43	1.46	1.38
3	B	802	LIJ	C18-C17	3.37	1.47	1.38
3	C	803	LIJ	C18-C17	3.36	1.46	1.38
3	B	802	LIJ	C19-C20	3.36	1.46	1.38
3	C	803	LIJ	C46-C45	3.30	1.46	1.38
3	B	802	LIJ	C49-C50	3.27	1.45	1.38
3	C	803	LIJ	C49-C50	3.26	1.45	1.38
3	B	802	LIJ	C7-S8	3.20	1.86	1.80
3	B	802	LIJ	C19-C18	3.17	1.46	1.38
3	C	803	LIJ	C19-C20	3.15	1.45	1.38
3	C	803	LIJ	C47-C46	3.14	1.45	1.38
3	C	803	LIJ	C24-C25	3.14	1.58	1.51
3	A	801	LIJ	C7-S8	3.12	1.86	1.80
3	A	801	LIJ	C48-C47	3.07	1.46	1.38
3	A	801	LIJ	C19-C18	3.07	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	LIJ	C47-C46	3.06	1.45	1.38
3	A	801	LIJ	C46-C45	3.06	1.45	1.38
3	A	801	LIJ	C49-C50	3.01	1.45	1.38
3	B	802	LIJ	C48-C47	3.00	1.46	1.38
3	C	803	LIJ	C19-C18	2.98	1.45	1.38
3	C	803	LIJ	C48-C47	2.98	1.45	1.38
3	C	803	LIJ	C49-C48	2.90	1.45	1.38
3	B	802	LIJ	C24-C25	2.83	1.57	1.51
3	B	802	LIJ	C49-C48	2.83	1.45	1.38
3	C	803	LIJ	C7-S8	2.82	1.85	1.80
3	A	801	LIJ	C47-C46	2.77	1.44	1.38
3	A	801	LIJ	C49-C48	2.76	1.45	1.38
3	C	803	LIJ	O43-C41	2.58	1.40	1.35
3	C	803	LIJ	C41-N40	2.34	1.40	1.34
3	B	802	LIJ	C10-N40	-2.30	1.41	1.45
3	A	801	LIJ	C41-N40	2.28	1.40	1.34
3	B	802	LIJ	C41-N40	2.23	1.40	1.34
3	B	802	LIJ	C22-N23	2.22	1.50	1.47
3	C	803	LIJ	C22-N23	2.20	1.50	1.47
3	C	803	LIJ	C22-C21	-2.19	1.49	1.52
3	A	801	LIJ	C22-N23	2.16	1.50	1.47
3	A	801	LIJ	C24-C25	2.13	1.56	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803	LIJ	C13-N12-C11	4.10	130.32	123.07
3	C	803	LIJ	O8A-S8-O8B	-4.06	113.56	118.19
3	B	802	LIJ	C13-N12-C11	4.00	130.14	123.07
3	B	802	LIJ	C14-C13-N12	-3.97	104.28	110.07
3	A	801	LIJ	O8A-S8-O8B	-3.97	113.67	118.19
3	B	802	LIJ	O8A-S8-O8B	-3.92	113.72	118.19
3	C	803	LIJ	C14-C13-N12	-3.77	104.57	110.07
3	C	803	LIJ	C44-O43-C41	3.71	124.22	115.93
3	A	801	LIJ	C31-O27-C27	3.31	124.69	117.51
3	B	802	LIJ	C27-C26-C25	3.27	123.33	119.73
3	A	801	LIJ	C14-C13-N12	-3.24	105.35	110.07
3	A	801	LIJ	C25-C24-N23	-3.19	104.53	112.80
3	C	803	LIJ	C31-O27-C27	3.07	124.18	117.51
3	B	802	LIJ	C31-O27-C27	2.96	123.93	117.51
3	B	802	LIJ	C44-O43-C41	2.93	122.47	115.93
3	C	803	LIJ	C27-C26-C25	2.89	122.91	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	803	LIJ	C25-C24-N23	-2.81	105.51	112.80
3	A	801	LIJ	C27-C26-C25	2.78	122.80	119.73
3	B	802	LIJ	C25-C24-N23	-2.73	105.74	112.80
3	A	801	LIJ	O11-C11-C10	-2.70	114.77	120.45
3	C	803	LIJ	O11-C11-C10	-2.63	114.92	120.45
3	A	801	LIJ	C44-O43-C41	2.51	121.54	115.93
3	A	801	LIJ	C13-N12-C11	2.50	127.48	123.07
3	C	803	LIJ	C10-N40-C41	2.49	126.99	120.90
3	B	802	LIJ	O21-C21-C22	-2.47	104.70	109.69
3	C	803	LIJ	O21-C21-C22	-2.34	104.96	109.69
3	A	801	LIJ	C10-N40-C41	2.31	126.53	120.90
3	B	802	LIJ	O11-C11-C10	-2.22	115.79	120.45
3	B	802	LIJ	C28-C27-C26	-2.15	117.58	120.53
3	A	801	LIJ	C28-C27-C26	-2.14	117.59	120.53
3	B	802	LIJ	C11-C10-N40	2.12	116.94	111.16
3	C	803	LIJ	C28-C27-C26	-2.12	117.63	120.53

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	LIJ	C6-C7-S8-C9
3	A	801	LIJ	C3-C7-S8-O8B
3	A	801	LIJ	C3-C7-S8-O8A
3	A	801	LIJ	C3-C7-S8-C9
3	B	802	LIJ	C6-C7-S8-O8B
3	B	802	LIJ	C6-C7-S8-O8A
3	B	802	LIJ	C6-C7-S8-C9
3	B	802	LIJ	C3-C7-S8-O8B
3	B	802	LIJ	C3-C7-S8-O8A
3	B	802	LIJ	C3-C7-S8-C9
3	C	803	LIJ	C6-C7-S8-O8B
3	C	803	LIJ	C6-C7-S8-O8A
3	C	803	LIJ	C6-C7-S8-C9
3	C	803	LIJ	C3-C7-S8-O8A
3	C	803	LIJ	C3-C7-S8-C9
3	A	801	LIJ	C26-C27-O27-C31
3	A	801	LIJ	C28-C27-O27-C31
3	C	803	LIJ	C28-C27-O27-C31
3	C	803	LIJ	C26-C27-O27-C31
3	B	802	LIJ	N40-C10-C11-O11
3	A	801	LIJ	N40-C10-C11-O11

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Mol	Chain	Res	Type	Atoms
3	C	803	LIJ	N40-C10-C11-O11
3	B	802	LIJ	N40-C10-C11-N12
3	C	803	LIJ	C13-C14-C15-C20
3	A	801	LIJ	N40-C10-C11-N12
3	C	803	LIJ	C13-C14-C15-C16
3	C	803	LIJ	N40-C10-C11-N12
3	B	802	LIJ	C13-C14-C15-C20
3	A	801	LIJ	C13-C14-C15-C20
3	B	802	LIJ	C13-C14-C15-C16
3	A	801	LIJ	C13-C14-C15-C16
3	A	801	LIJ	C2-C3-C7-S8
3	A	801	LIJ	C6-C7-S8-O8B
3	A	801	LIJ	C6-C7-S8-O8A
3	C	803	LIJ	C3-C7-S8-O8B
3	A	801	LIJ	C2-C3-C7-C6
3	B	802	LIJ	C2-C3-C7-C6
3	C	803	LIJ	C2-C3-C7-C6
3	B	802	LIJ	C2-C3-C7-S8
3	C	803	LIJ	C2-C3-C7-S8

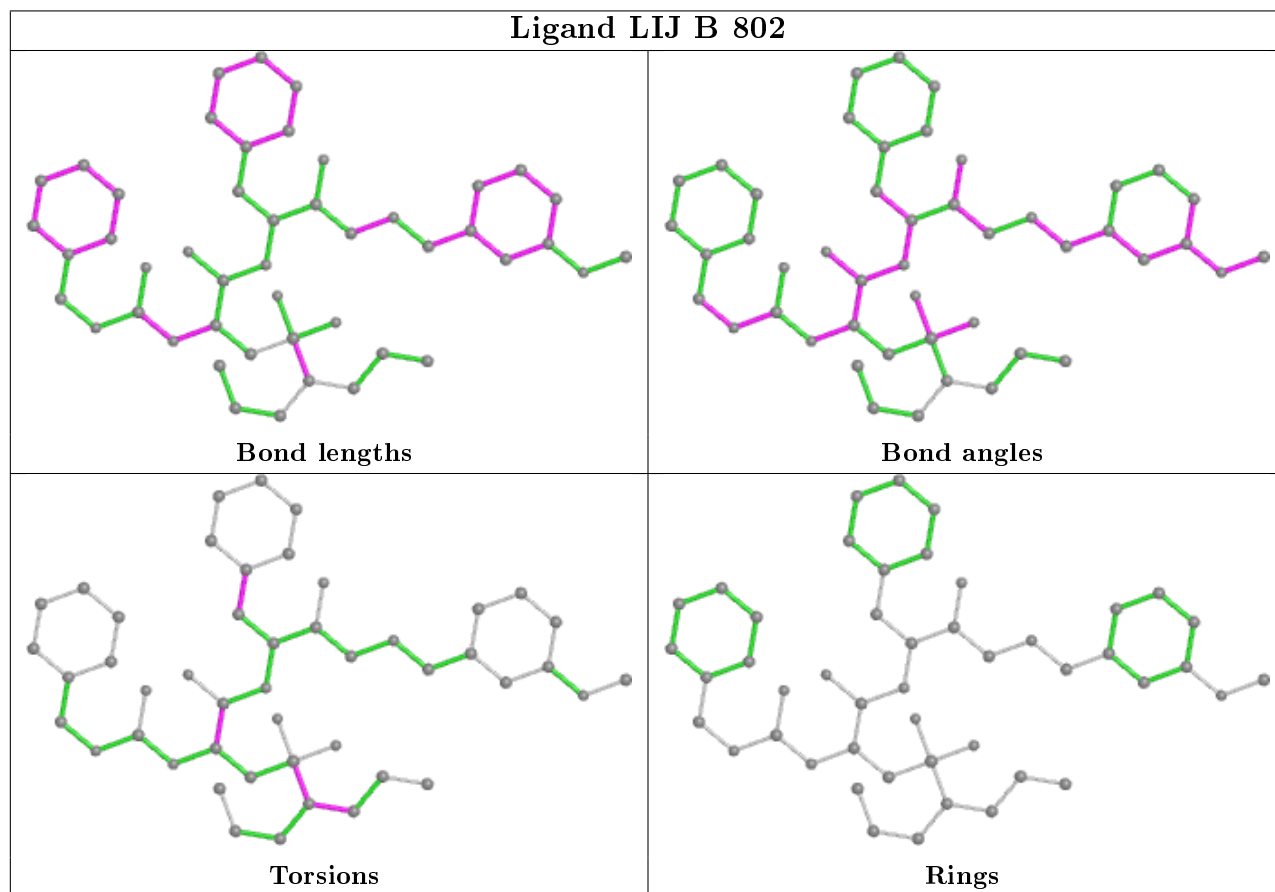
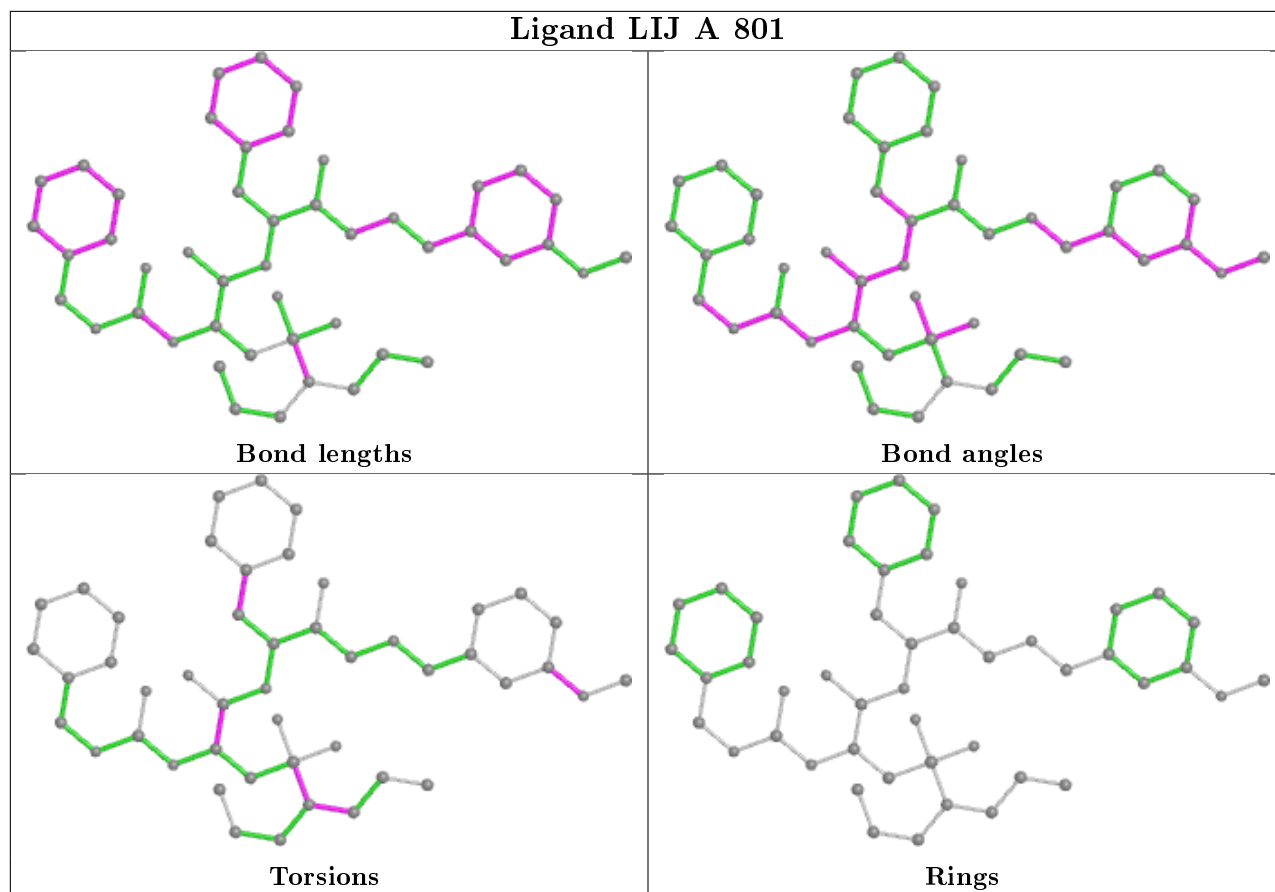
There are no ring outliers.

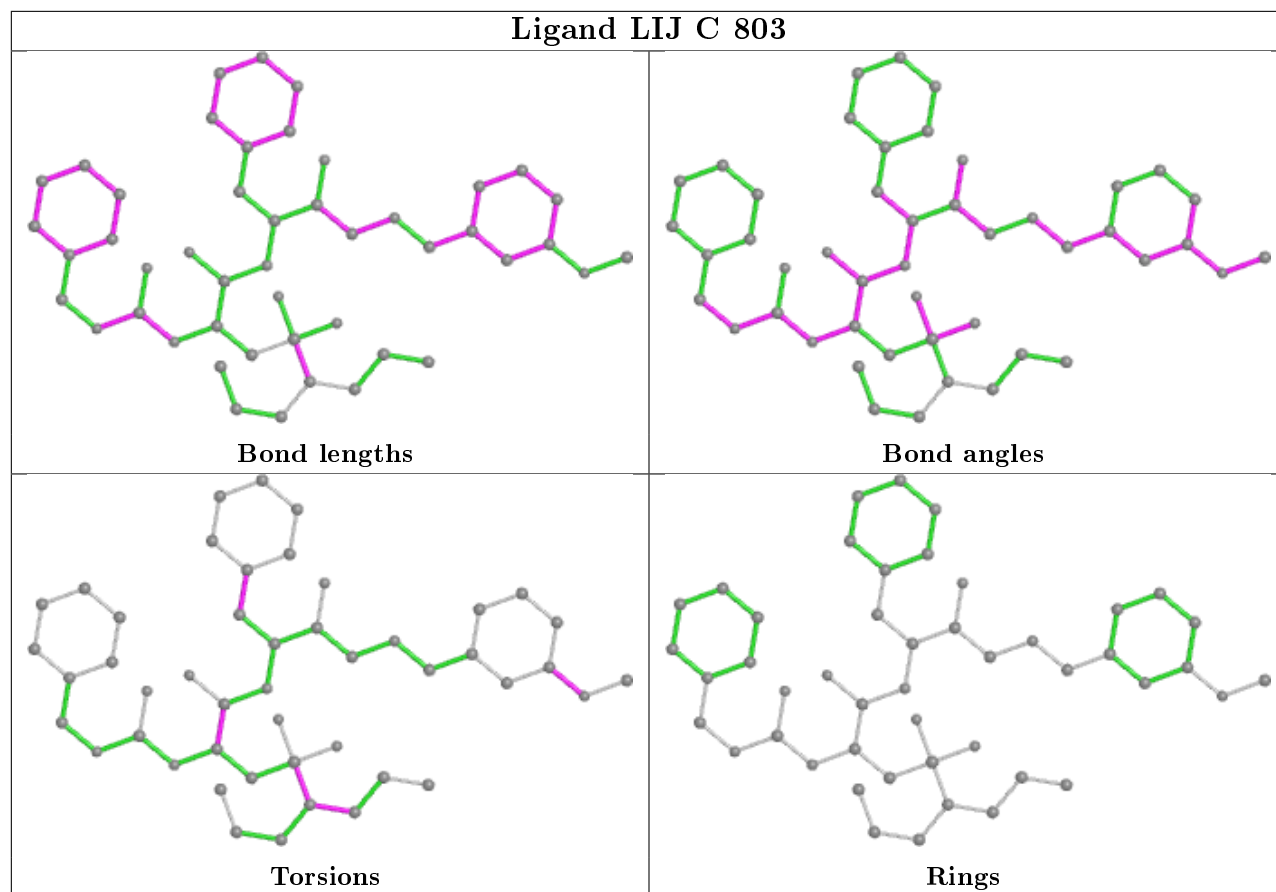
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	LIJ	2	0
3	C	803	LIJ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 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	371/455 (81%)	0.04	12 (3%) 47 51	23, 37, 62, 76	0
1	B	372/455 (81%)	0.15	22 (5%) 22 23	19, 40, 71, 85	0
1	C	373/455 (81%)	0.14	19 (5%) 28 29	22, 38, 64, 83	0
All	All	1116/1365 (81%)	0.11	53 (4%) 31 33	19, 38, 66, 85	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	ALA	6.8
1	C	386	ILE	5.8
1	C	168	ALA	5.0
1	B	309	VAL	4.7
1	A	169	SER	4.4
1	B	61(P)	SER	4.3
1	B	310	GLU	4.3
1	A	170	VAL	4.1
1	B	361	VAL	4.1
1	B	10	SER	4.1
1	C	364	GLU	4.0
1	C	62(P)	PHE	3.8
1	C	169	SER	3.8
1	C	61(P)	SER	3.7
1	B	386	ILE	3.7
1	A	61(P)	SER	3.5
1	C	365	PHE	3.3
1	B	385	ASN	3.1
1	C	362	HIS	3.1
1	B	362	HIS	3.0
1	B	272	ALA	2.9
1	B	169	SER	2.9
1	C	272	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	64	ARG	2.8
1	B	254	THR	2.8
1	A	362	HIS	2.7
1	B	365	PHE	2.6
1	C	317	ASP	2.5
1	A	364	GLU	2.5
1	B	364	GLU	2.5
1	B	256	LYS	2.5
1	B	320	TYR	2.4
1	B	271	GLN	2.4
1	B	337	ILE	2.3
1	C	256	LYS	2.3
1	C	271	GLN	2.3
1	A	9	LYS	2.3
1	C	309	VAL	2.2
1	B	234	LEU	2.2
1	C	210	GLY	2.2
1	A	64	ARG	2.2
1	A	7	ARG	2.2
1	C	334	GLY	2.2
1	C	229	SER	2.1
1	B	229	SER	2.1
1	B	384	TYR	2.1
1	C	384	TYR	2.1
1	A	365	PHE	2.1
1	A	157	ALA	2.0
1	A	271	GLN	2.0
1	C	230	GLY	2.0
1	C	265	GLU	2.0
1	A	55	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](#)

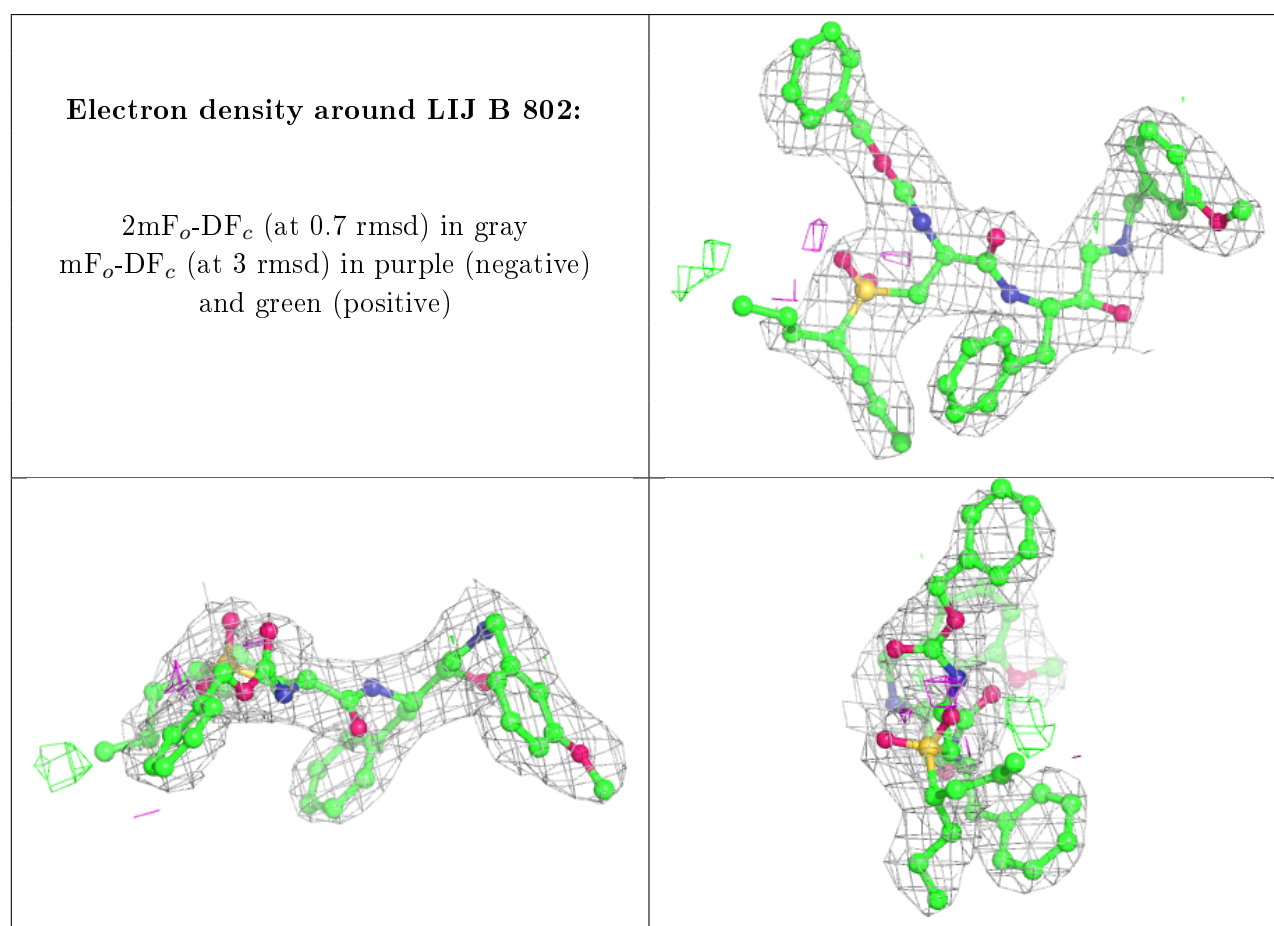
There are no carbohydrates in this entry.

## 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.

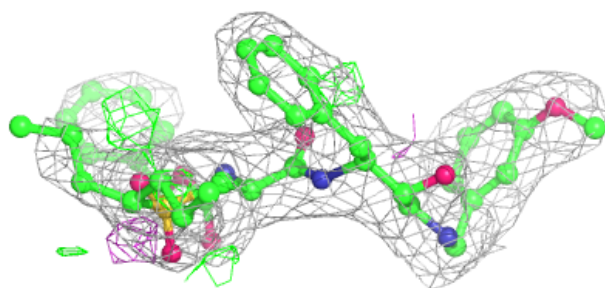
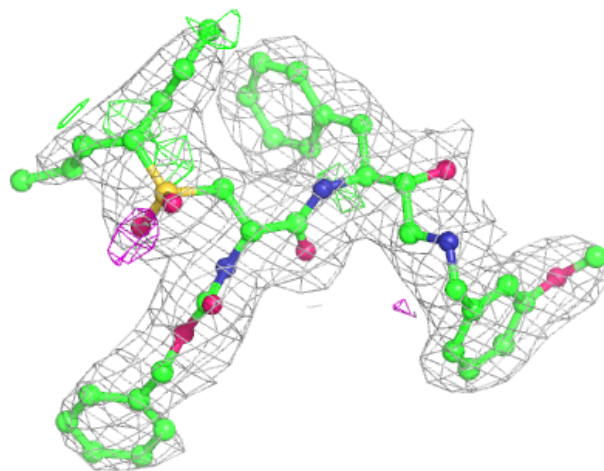
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	A	703	5/5	0.69	0.62	99,99,99,99	0
2	PO4	A	702	5/5	0.88	0.17	98,98,99,99	0
2	PO4	C	701	5/5	0.88	0.34	99,99,99,99	0
3	LIJ	B	802	47/47	0.91	0.23	31,48,62,64	0
3	LIJ	A	801	47/47	0.93	0.22	30,37,58,59	0
3	LIJ	C	803	47/47	0.93	0.22	23,40,64,66	0

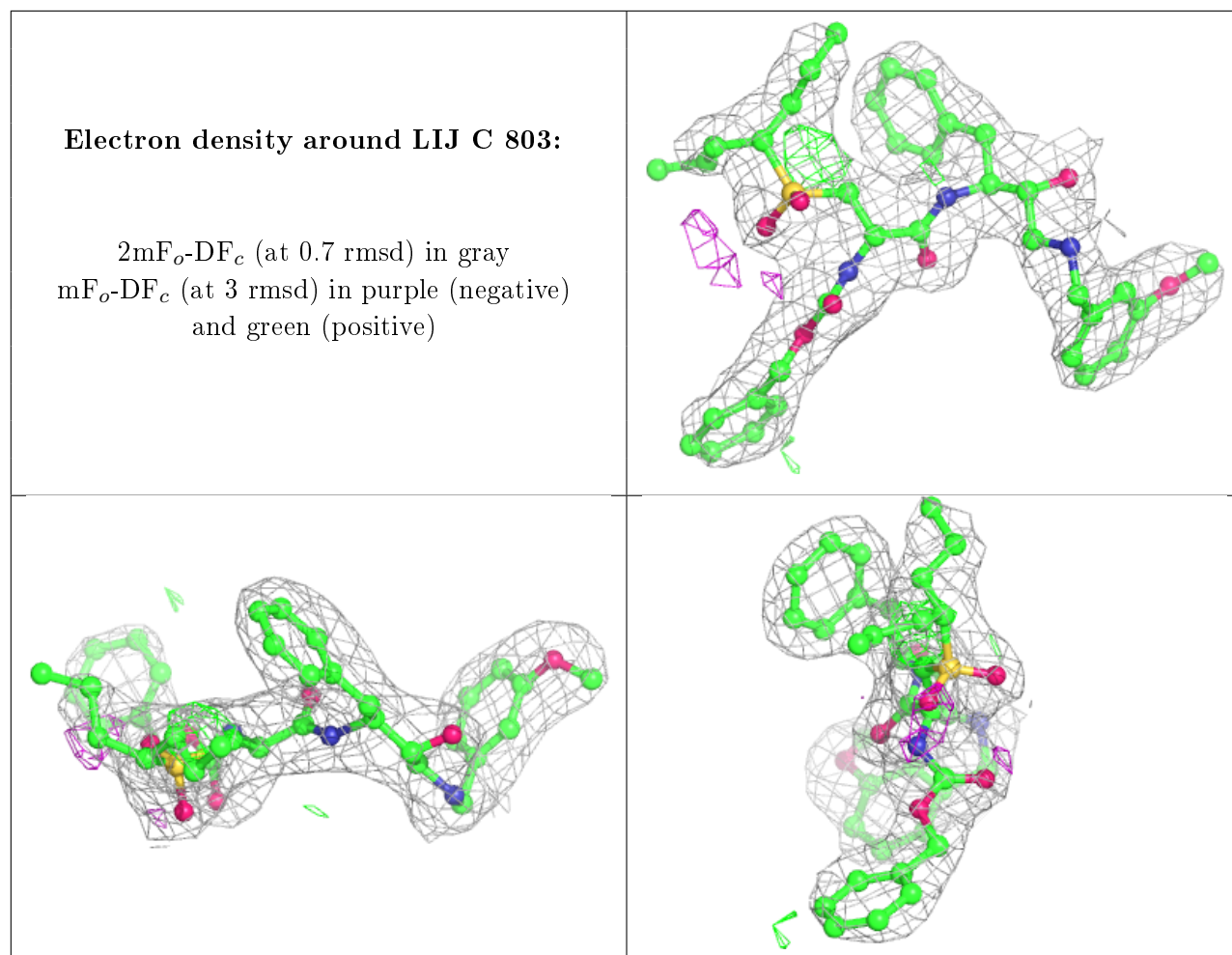
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around LIJ A 801:**

$2mF_o-DF_c$  (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.