Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 05:07 pm BST

PDB ID	:	3IVI
Title	:	Design and Synthesis of Potent BACE-1 Inhibitors with Cellular Activity: Structure-Activity Relationship of P1 Substituents
Authors	:	Pan, H.
Deposited on	:	2009-09-01
Resolution	:	2.20 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
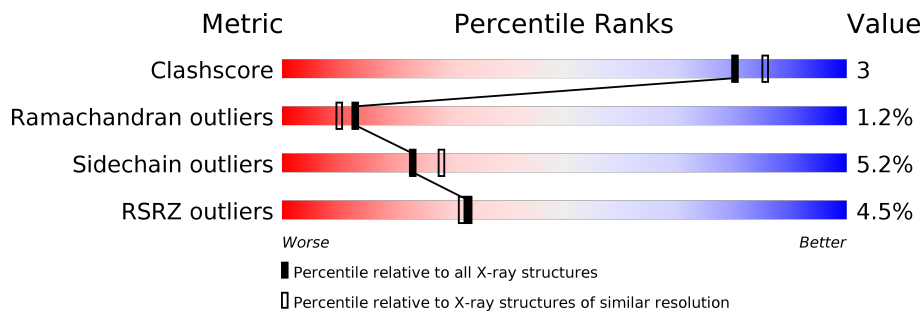with specific help available everywhere you see the (i) symbol.

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 2.20 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	Percentile Ranks	Value
Clashscore		3
Ramachandran outliers		1.2%
Sidechain outliers		5.2%
RSRZ outliers		4.5%

Worse .... *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	406	3% / 82% 9% • 6%
1	B	406	4% / 84% 8% • 7%
1	C	406	5% / 83% 8% • 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9299 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
1	A	380	Total 2991	C 1919	N 496	O 562	S 14	0	0	0
1	B	378	Total 2978	C 1910	N 494	O 560	S 14	0	0	0
1	C	373	Total 2936	C 1882	N 488	O 552	S 14	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	MET	-	expression tag	UNP P56817
A	454	ARG	-	expression tag	UNP P56817
A	455	SER	-	expression tag	UNP P56817
A	456	HIS	-	expression tag	UNP P56817
A	457	HIS	-	expression tag	UNP P56817
A	458	HIS	-	expression tag	UNP P56817
A	459	HIS	-	expression tag	UNP P56817
A	460	HIS	-	expression tag	UNP P56817
A	461	HIS	-	expression tag	UNP P56817
B	56	MET	-	expression tag	UNP P56817
B	454	ARG	-	expression tag	UNP P56817
B	455	SER	-	expression tag	UNP P56817
B	456	HIS	-	expression tag	UNP P56817
B	457	HIS	-	expression tag	UNP P56817
B	458	HIS	-	expression tag	UNP P56817
B	459	HIS	-	expression tag	UNP P56817
B	460	HIS	-	expression tag	UNP P56817
B	461	HIS	-	expression tag	UNP P56817
C	56	MET	-	expression tag	UNP P56817
C	454	ARG	-	expression tag	UNP P56817
C	455	SER	-	expression tag	UNP P56817
C	456	HIS	-	expression tag	UNP P56817
C	457	HIS	-	expression tag	UNP P56817

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	458	HIS	-	expression tag	UNP P56817
C	459	HIS	-	expression tag	UNP P56817
C	460	HIS	-	expression tag	UNP P56817
C	461	HIS	-	expression tag	UNP P56817

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
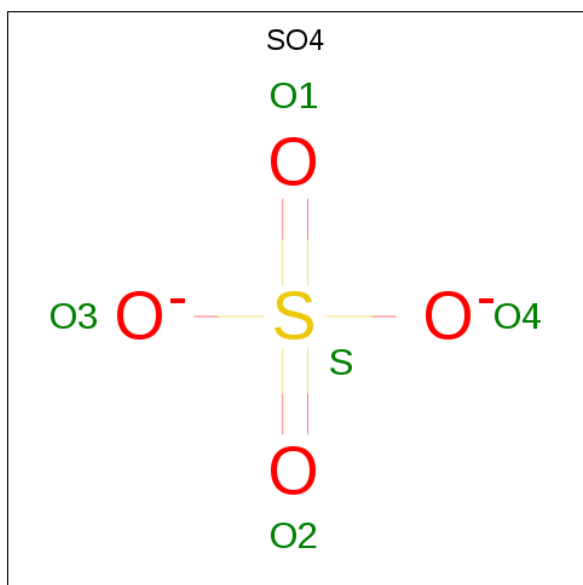
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0
2	C	1	Total 5	O 4	S 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0

- Molecule 4 is N-[(1S,2R)-3-{[(5S)-5-(3-tert-butylphenyl)-4,5,6,7-tetrahydro-1H-indazol-5-yl] amino}-1-(3,5-difluorobenzyl)-2-hydroxypropyl]acetamide (three-letter code: 2LI) (formula: $C_{29}H_{36}F_2N_4O_2$).

2LI
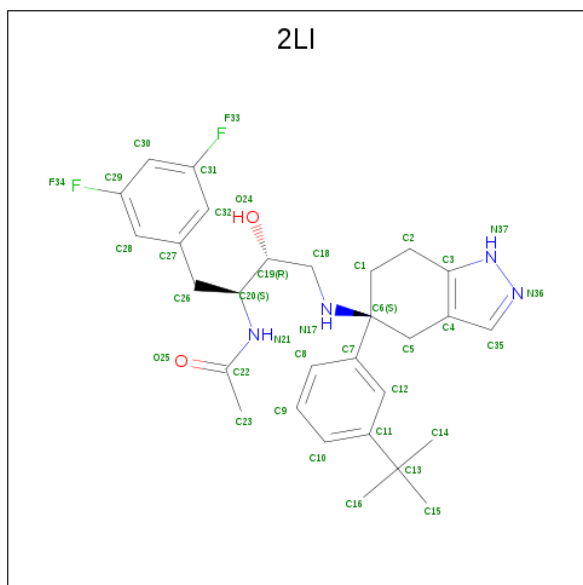
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 37	C 29	F 2	N 4	O 2	0	0
4	B	1	Total 37	C 29	F 2	N 4	O 2	0	0
4	C	1	Total 37	C 29	F 2	N 4	O 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total 91	O 91	0	0
5	B	82	Total 82	O 82	0	0
5	C	62	Total 62	O 62	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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
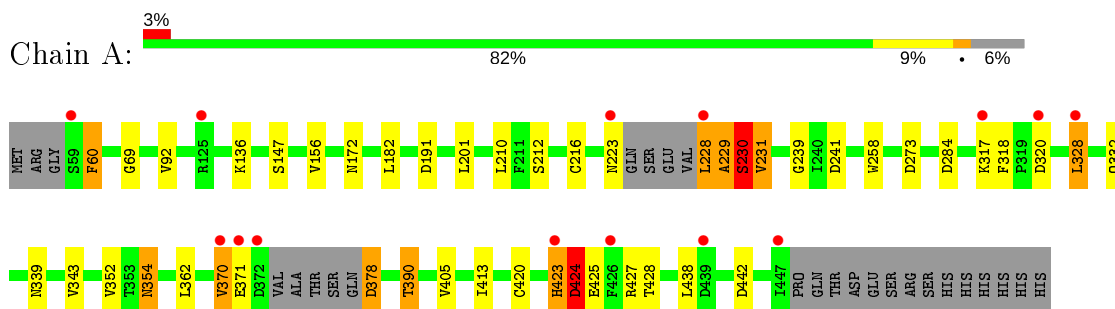
- Molecule 1: Beta-secretase 1
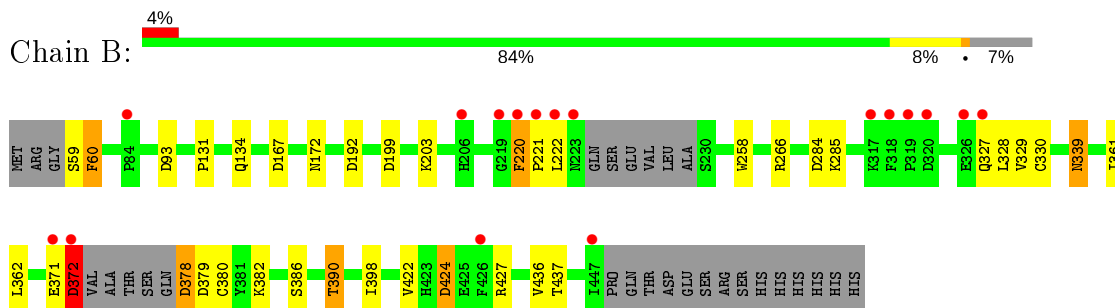
- Molecule 1: Beta-secretase 1

4 Data and refinement statistics (i)

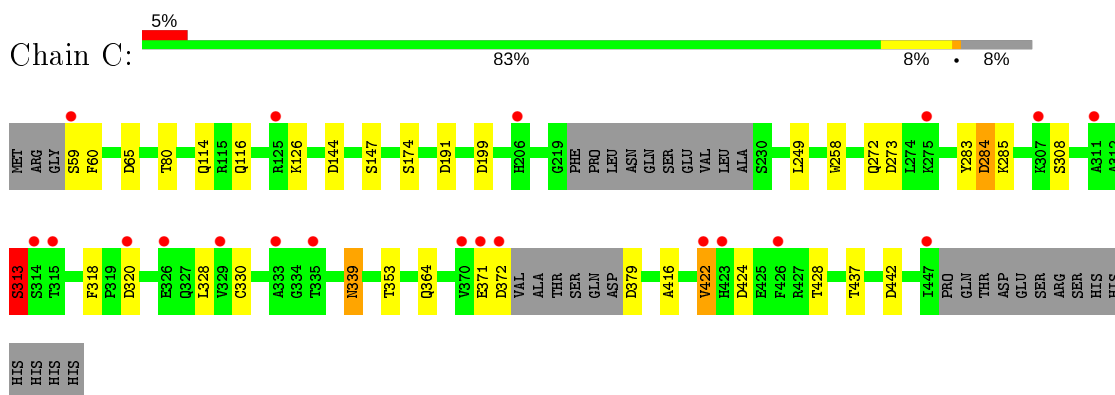| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.71Å 104.48Å 100.62Å 90.00° 104.83° 90.00°	Depositor
Resolution (Å)	95.35 – 2.20 55.22 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (95.35-2.20) 99.3 (55.22-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.25	Depositor
R, R_{free}	0.195 , 0.229 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: GOL, 2LI, SO4

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	0.47	0/3067	0.81	8/4167 (0.2%)
1	B	0.47	0/3054	0.81	8/4149 (0.2%)
1	C	0.49	1/3010 (0.0%)	0.79	9/4088 (0.2%)
All	All	0.48	1/9131 (0.0%)	0.80	25/12404 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	313	SER	CB-OG	6.00	1.50	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	ASP	CB-CG-OD2	7.88	125.40	118.30
1	B	199	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	378	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	442	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	167	ASP	CB-CG-OD2	6.16	123.84	118.30
1	C	191	ASP	CB-CG-OD2	6.13	123.82	118.30
1	C	144	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	424	ASP	CB-CG-OD2	5.79	123.52	118.30
1	A	423	HIS	N-CA-C	5.67	126.31	111.00
1	C	65	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	424	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	372	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	320	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	379	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	93	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	442	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	372	ASP	CB-CG-OD2	5.26	123.04	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	320	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	273	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	199	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	273	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	379	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	241	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	191	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	378	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2991	0	2909	18	0
1	B	2978	0	2891	16	0
1	C	2936	0	2854	10	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	37	0	36	1	0
4	B	37	0	36	2	0
4	C	37	0	36	1	0
5	A	91	0	0	0	0
5	B	82	0	0	0	0
5	C	62	0	0	0	0
All	All	9299	0	8786	44	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 3.

All (44) 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:69:GLY:O	1:A:230:SER:O	2.11	0.69
1:B:285:LYS:NZ	4:B:2:2LI:HN37	2.01	0.58
1:B:220:PHE:CB	1:B:221:PRO:CD	2.82	0.58
1:A:423:HIS:CG	1:A:424:ASP:H	2.27	0.52
1:C:364:GLN:NE2	1:C:424:ASP:OD2	2.42	0.52
1:A:423:HIS:CG	1:A:424:ASP:N	2.78	0.52
1:C:249:LEU:HD23	1:C:416:ALA:HB2	1.91	0.52
1:B:285:LYS:HZ1	4:B:2:2LI:HN37	1.57	0.52
1:A:390:THR:OG1	4:A:1:2LI:N36	2.39	0.51
1:A:216:CYS:HG	1:A:420:CYS:CB	2.22	0.51
1:B:220:PHE:CB	1:B:221:PRO:HD3	2.42	0.50
1:B:220:PHE:HB2	1:B:221:PRO:CD	2.43	0.49
1:A:328:LEU:CD2	1:A:370:VAL:HG21	2.43	0.49
1:B:266:ARG:NH2	1:B:437:THR:HG22	2.28	0.48
1:A:228:LEU:O	1:A:229:ALA:HB2	2.14	0.48
1:C:114:GLN:HE21	1:C:116:GLN:HE22	1.61	0.48
1:B:220:PHE:HB3	1:B:221:PRO:HD3	1.95	0.47
1:B:339:ASN:HD22	1:B:339:ASN:H	1.62	0.47
1:B:59:SER:OG	1:B:60:PHE:N	2.48	0.46
1:C:114:GLN:NE2	1:C:116:GLN:HE22	2.13	0.46
1:B:390:THR:O	1:B:390:THR:OG1	2.34	0.46
1:A:390:THR:O	1:A:390:THR:OG1	2.33	0.46
1:A:352:VAL:HG12	1:A:354:ASN:ND2	2.32	0.44
1:C:285:LYS:NZ	4:C:3:2LI:HN37	2.16	0.43
1:A:156:VAL:HG11	1:A:201:LEU:HA	1.99	0.43
1:C:339:ASN:HD22	1:C:339:ASN:N	2.16	0.43
1:C:80:THR:OG1	1:C:147:SER:HB2	2.17	0.43
1:C:313:SER:HG	1:C:318:PHE:HE1	1.65	0.43
1:A:60:PHE:CZ	1:A:239:GLY:HA3	2.54	0.42
1:B:371:GLU:O	1:B:372:ASP:C	2.57	0.42
1:C:364:GLN:HB3	1:C:422:VAL:HG11	2.01	0.42
1:B:362:LEU:HD12	1:B:422:VAL:HG23	2.02	0.41
1:B:330:CYS:SG	1:B:380:CYS:SG	3.01	0.41
1:A:405:VAL:O	1:A:413:ILE:HA	2.21	0.41
1:A:370:VAL:HG23	1:A:371:GLU:N	2.35	0.41
1:A:92:VAL:HG13	1:A:182:LEU:HD11	2.01	0.41
1:C:283:TYR:O	1:C:284:ASP:CB	2.67	0.41
1:A:230:SER:O	1:A:231:VAL:HG22	2.21	0.41
1:B:424:ASP:HB3	1:B:427:ARG:O	2.20	0.41
1:B:339:ASN:HD22	1:B:339:ASN:N	2.18	0.41
1:A:328:LEU:HD23	1:A:370:VAL:HG21	2.03	0.41
1:B:361:ILE:HD13	1:B:398:ILE:HD12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:HB3	1:A:427:ARG:O	2.21	0.40
1:A:343:VAL:HG12	1:A:362:LEU:HD22	2.04	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	374/406 (92%)	353 (94%)	14 (4%)	7 (2%)	8	5
1	B	372/406 (92%)	357 (96%)	11 (3%)	4 (1%)	14	12
1	C	367/406 (90%)	352 (96%)	13 (4%)	2 (0%)	29	31
All	All	1113/1218 (91%)	1062 (95%)	38 (3%)	13 (1%)	13	10

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	A	284	ASP
1	A	424	ASP
1	B	220	PHE
1	B	284	ASP
1	C	284	ASP
1	A	60	PHE
1	A	229	ALA
1	A	231	VAL
1	B	60	PHE
1	C	60	PHE
1	B	131	PRO
1	A	370	VAL

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	324/348 (93%)	304 (94%)	20 (6%)	18	21
1	B	323/348 (93%)	308 (95%)	15 (5%)	27	34
1	C	318/348 (91%)	303 (95%)	15 (5%)	26	33
All	All	965/1044 (92%)	915 (95%)	50 (5%)	23	28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LYS
1	A	147	SER
1	A	172	ASN
1	A	210	LEU
1	A	212	SER
1	A	223	ASN
1	A	228	LEU
1	A	230	SER
1	A	258	TRP
1	A	317	LYS
1	A	318	PHE
1	A	328	LEU
1	A	332	GLN
1	A	339	ASN
1	A	354	ASN
1	A	378	ASP
1	A	390	THR
1	A	425	GLU
1	A	428	THR
1	A	438	LEU
1	B	134	GLN
1	B	172	ASN
1	B	203	LYS
1	B	222	LEU
1	B	258	TRP
1	B	327	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	328	LEU
1	B	329	VAL
1	B	339	ASN
1	B	372	ASP
1	B	378	ASP
1	B	382	LYS
1	B	386	SER
1	B	390	THR
1	B	436	VAL
1	C	59	SER
1	C	126	LYS
1	C	174	SER
1	C	258	TRP
1	C	272	GLN
1	C	308	SER
1	C	313	SER
1	C	328	LEU
1	C	330	CYS
1	C	339	ASN
1	C	353	THR
1	C	371	GLU
1	C	422	VAL
1	C	428	THR
1	C	437	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	339	ASN
1	A	354	ASN
1	A	446	ASN
1	B	159	ASN
1	B	172	ASN
1	B	339	ASN
1	B	354	ASN
1	C	110	HIS
1	C	114	GLN
1	C	159	ASN
1	C	339	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	GOL	B	901	-	5,5,5	0.37	0	5,5,5	0.31	0
4	2LI	C	3	-	37,40,40	0.97	1 (2%)	44,59,59	1.51	6 (13%)
2	SO4	A	899	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	899	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	C	899	-	4,4,4	0.16	0	6,6,6	0.10	0
3	GOL	A	901	-	5,5,5	0.35	0	5,5,5	0.37	0
3	GOL	C	901	-	5,5,5	0.36	0	5,5,5	0.26	0
4	2LI	A	1	-	37,40,40	1.09	1 (2%)	44,59,59	1.54	7 (15%)
2	SO4	B	900	-	4,4,4	0.25	0	6,6,6	0.46	0
2	SO4	A	900	-	4,4,4	0.23	0	6,6,6	0.28	0
2	SO4	C	900	-	4,4,4	0.22	0	6,6,6	0.35	0
4	2LI	B	2	-	37,40,40	0.96	1 (2%)	44,59,59	1.41	5 (11%)

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	GOL	B	901	-	-	2/4/4/4	-
4	2LI	C	3	-	-	0/30/41/41	0/4/4/4
3	GOL	A	901	-	-	1/4/4/4	-
3	GOL	C	901	-	-	0/4/4/4	-
4	2LI	A	1	-	-	1/30/41/41	0/4/4/4
4	2LI	B	2	-	-	1/30/41/41	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	2LI	C4-C3	4.64	1.47	1.41
4	B	2	2LI	C4-C3	4.59	1.47	1.41
4	C	3	2LI	C4-C3	4.40	1.47	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3	2LI	C1-C2-C3	-6.56	106.66	112.95
4	B	2	2LI	C1-C2-C3	-4.85	108.29	112.95
4	A	1	2LI	C1-C2-C3	-4.66	108.48	112.95
4	B	2	2LI	C27-C26-C20	-3.19	107.79	113.33
4	A	1	2LI	C27-C32-C31	3.10	121.63	118.81
4	A	1	2LI	C19-C18-N17	2.90	114.72	110.74
4	A	1	2LI	C32-C31-C30	-2.76	120.03	123.52
4	C	3	2LI	C35-C4-C3	2.59	107.58	104.71
4	A	1	2LI	C7-C6-N17	2.47	111.13	106.33
4	A	1	2LI	C35-C4-C3	2.47	107.44	104.71
4	B	2	2LI	C30-C29-C28	-2.46	120.41	123.52
4	B	2	2LI	C32-C31-C30	-2.41	120.48	123.52
4	C	3	2LI	C19-C18-N17	2.35	113.96	110.74
4	C	3	2LI	C30-C29-C28	-2.24	120.69	123.52
4	C	3	2LI	C32-C31-C30	-2.16	120.79	123.52
4	B	2	2LI	C31-C30-C29	2.13	119.45	116.13
4	A	1	2LI	F33-C31-C30	2.06	121.20	118.25
4	C	3	2LI	C27-C26-C20	-2.06	109.75	113.33

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	901	GOL	O1-C1-C2-C3
3	B	901	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1	2LI	C5-C6-C7-C8
4	B	2	2LI	C5-C6-C7-C8
3	A	901	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3	2LI	1	0
4	A	1	2LI	1	0
4	B	2	2LI	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 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 2LI C 3

Bond lengths

Bond angles

Torsions

Rings

Ligand 2LI A 1

Bond lengths

Bond angles

Torsions

Rings

Ligand 2LI B 2

Bond lengths

Bond angles

Torsions

Rings
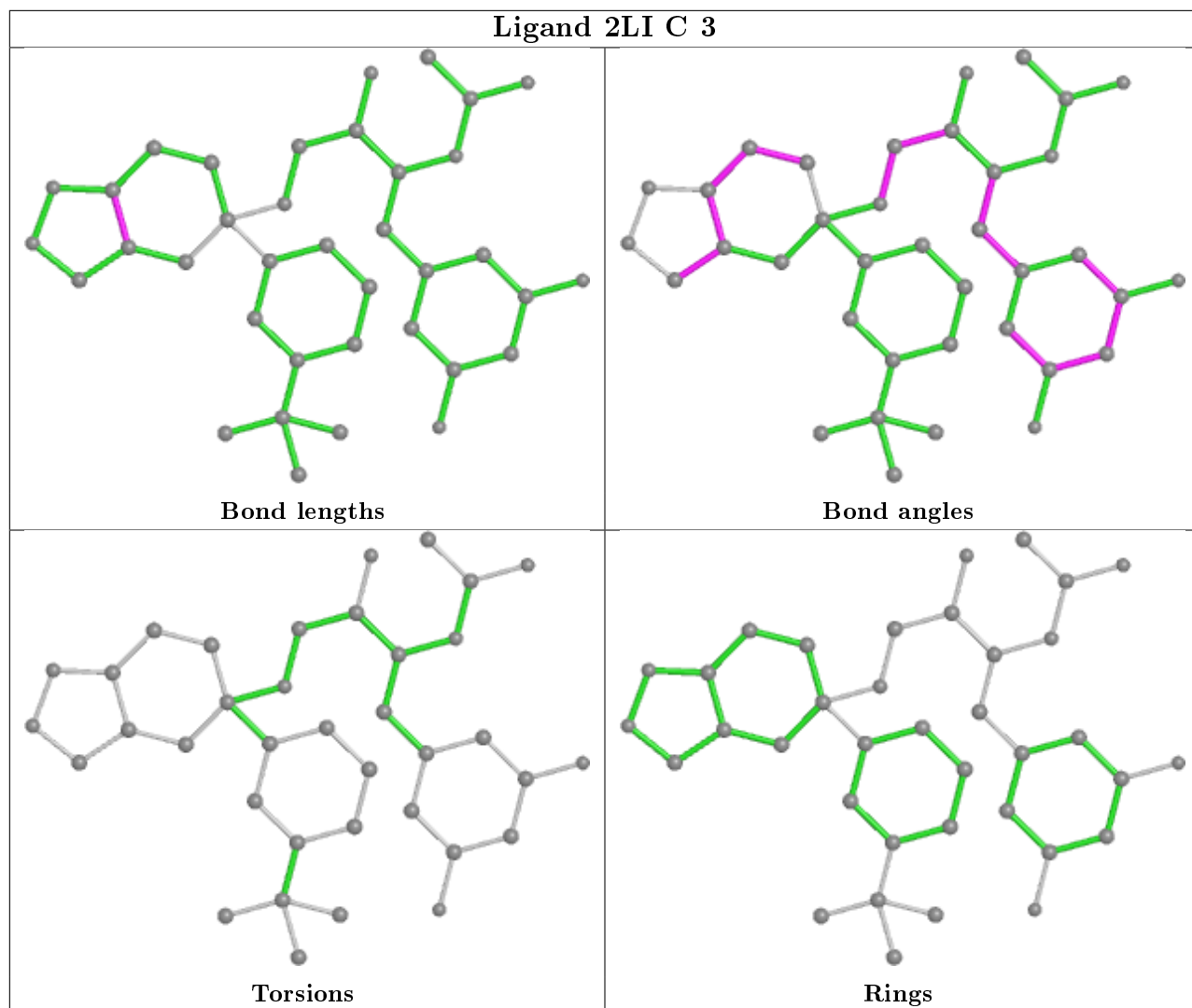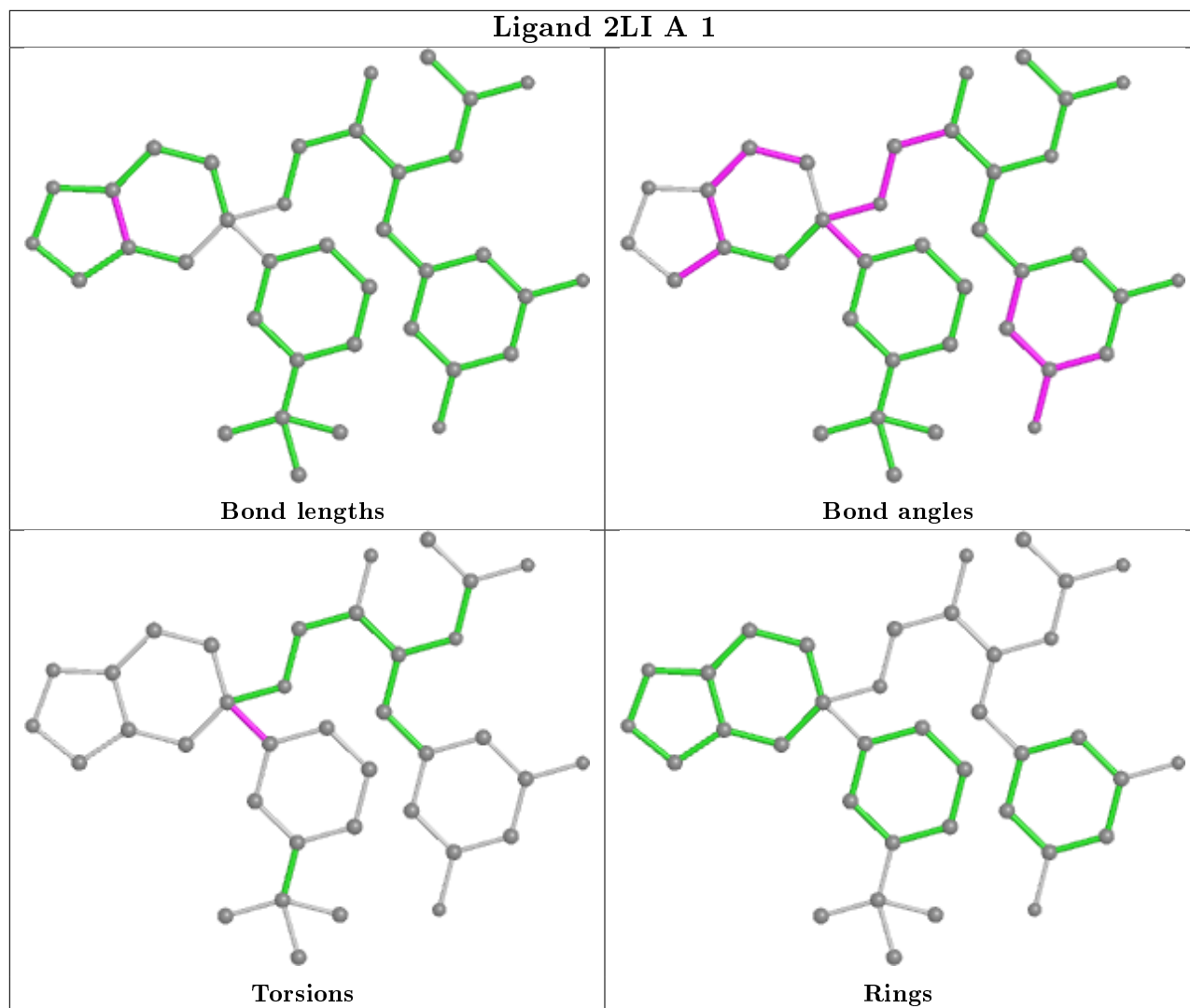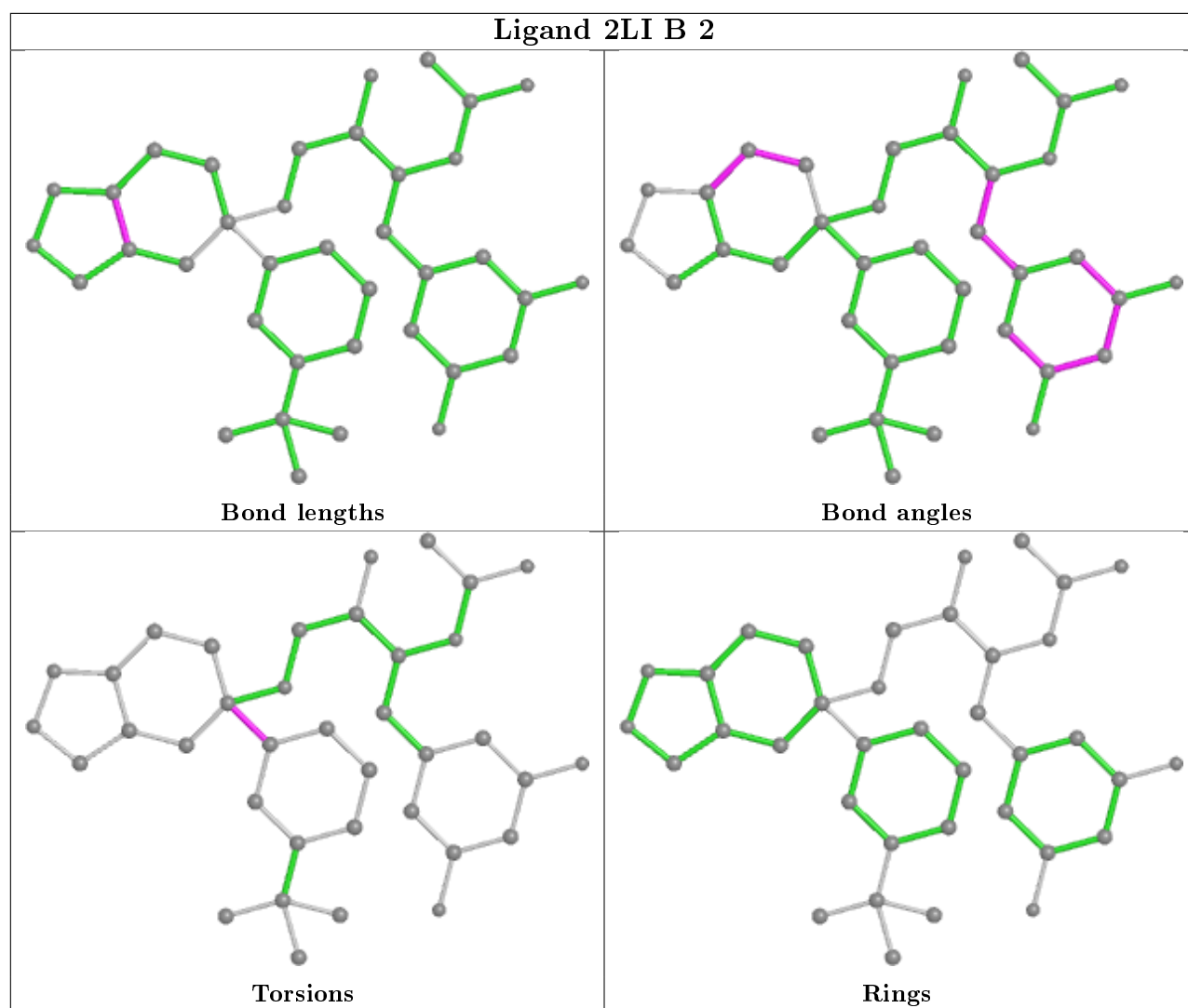
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	380/406 (93%)	0.11	14 (3%)	41	39	27, 35, 49, 58	0
1	B	378/406 (93%)	0.32	17 (4%)	33	32	26, 35, 48, 70	0
1	C	373/406 (91%)	0.25	20 (5%)	25	24	27, 36, 47, 64	0
All	All	1131/1218 (92%)	0.22	51 (4%)	33	32	26, 35, 48, 70	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	ILE	9.3
1	B	221	PRO	6.7
1	A	447	ILE	6.6
1	C	371	GLU	5.5
1	B	220	PHE	5.4
1	C	423	HIS	5.4
1	C	320	ASP	5.0
1	A	426	PHE	4.4
1	B	317	LYS	4.1
1	C	315	THR	4.0
1	B	372	ASP	3.9
1	B	219	GLY	3.7
1	B	371	GLU	3.6
1	C	370	VAL	3.6
1	A	423	HIS	3.5
1	A	59	SER	3.5
1	C	372	ASP	3.5
1	C	59	SER	3.4
1	B	222	LEU	3.2
1	A	371	GLU	3.1
1	C	311	ALA	3.0
1	A	228	LEU	2.9
1	B	327	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	426	PHE	2.7
1	C	206	HIS	2.6
1	B	326	GLU	2.5
1	C	426	PHE	2.5
1	C	275	LYS	2.5
1	C	422	VAL	2.5
1	B	318	PHE	2.4
1	C	447	ILE	2.3
1	B	84	PRO	2.3
1	B	319	PRO	2.3
1	C	125	ARG	2.3
1	C	329	VAL	2.3
1	A	372	ASP	2.3
1	B	223	ASN	2.3
1	C	307	LYS	2.2
1	C	333	ALA	2.2
1	A	320	ASP	2.2
1	C	326	GLU	2.1
1	B	320	ASP	2.1
1	C	314	SER	2.1
1	A	317	LYS	2.1
1	B	206	HIS	2.1
1	A	370	VAL	2.1
1	A	439	ASP	2.1
1	A	328	LEU	2.1
1	A	125	ARG	2.0
1	A	223	ASN	2.0
1	C	335	THR	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.

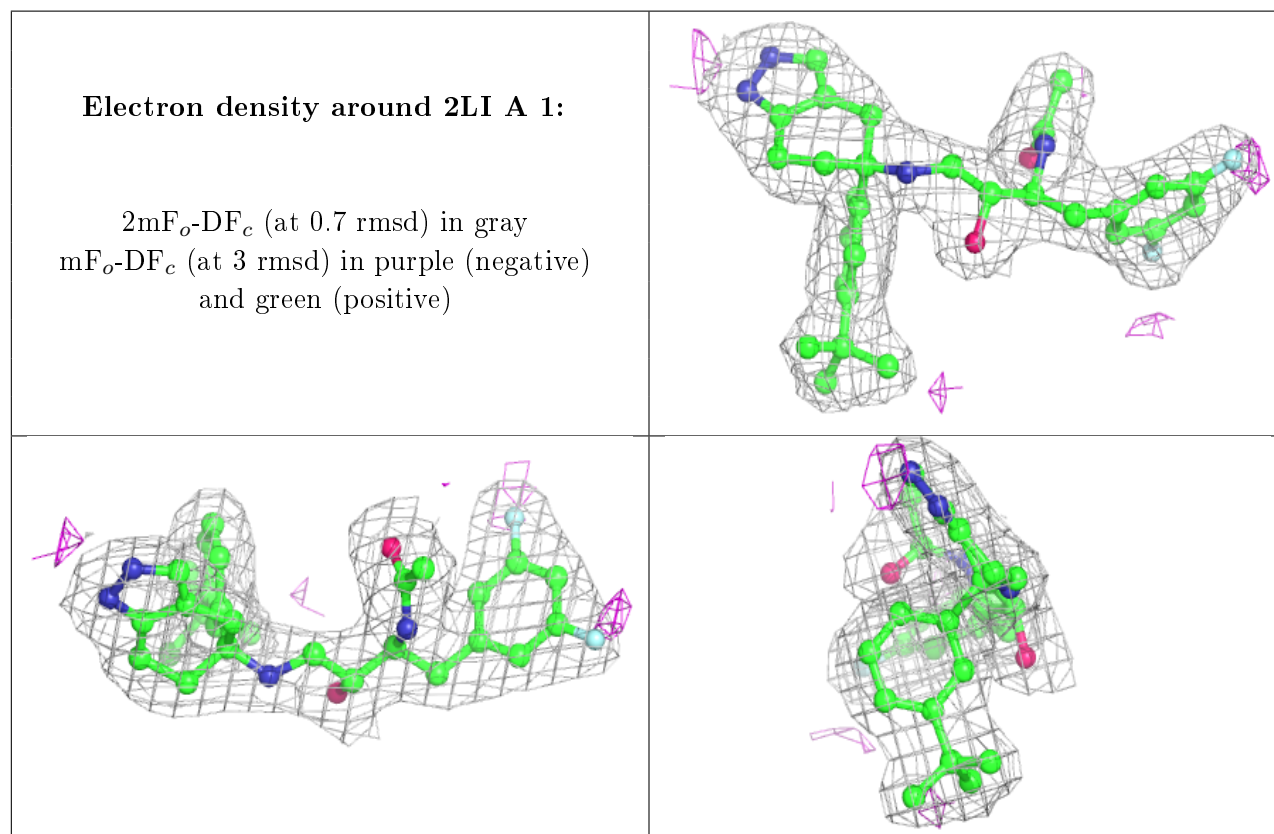## 6.3 Carbohydrates (i)

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, 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.
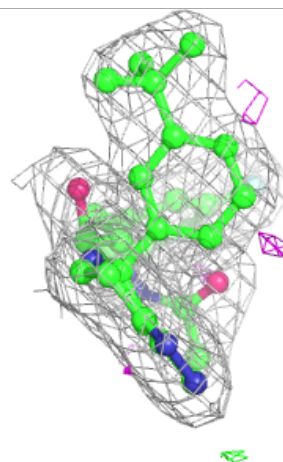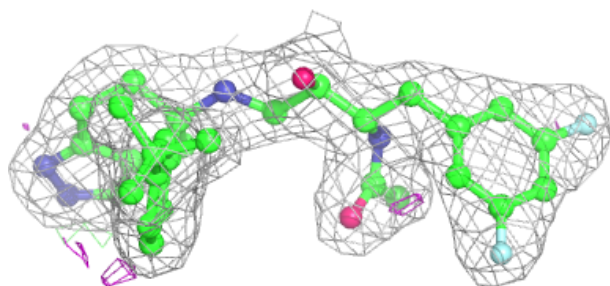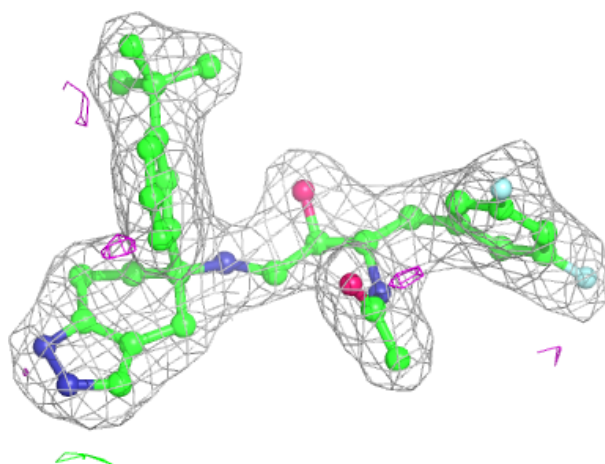
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	C	901	6/6	0.79	0.33	87,87,87,88	0
3	GOL	A	901	6/6	0.80	0.34	84,85,86,86	0
3	GOL	B	901	6/6	0.82	0.26	80,81,82,83	0
2	SO4	C	899	5/5	0.90	0.32	108,108,108,108	0
2	SO4	A	899	5/5	0.94	0.32	101,102,102,102	0
4	2LI	A	1	37/37	0.95	0.14	39,42,52,56	0
2	SO4	C	900	5/5	0.95	0.11	65,65,68,69	0
4	2LI	C	3	37/37	0.96	0.14	40,44,55,57	0
4	2LI	B	2	37/37	0.96	0.15	41,45,53,54	0
2	SO4	A	900	5/5	0.97	0.12	64,64,64,67	0
2	SO4	B	899	5/5	0.97	0.29	98,98,99,99	0
2	SO4	B	900	5/5	0.97	0.13	67,67,68,69	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.
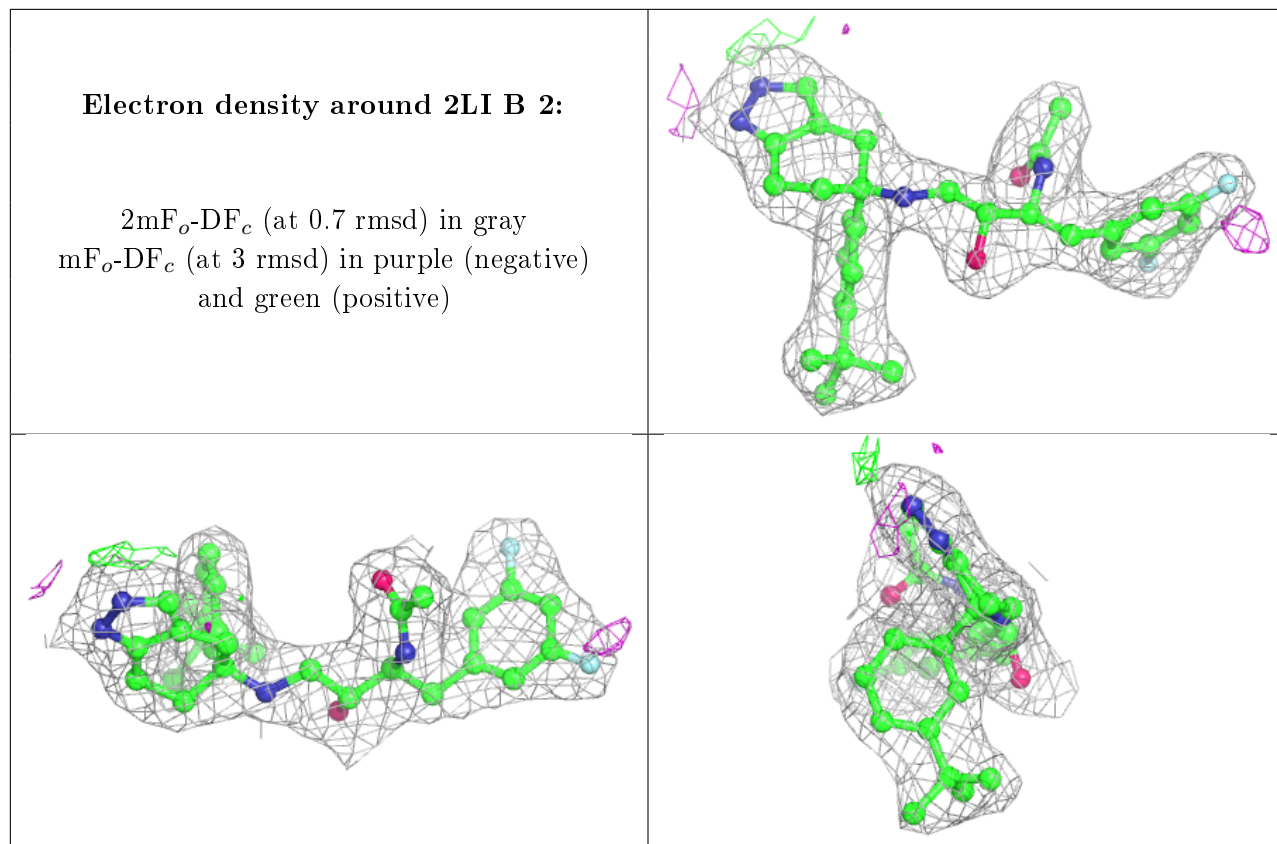

Electron density around 2LI A 1:

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

Electron density around 2LI C 3:

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

Electron density around 2LI B 2:

$2mF_o$-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.