



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:35 am BST

PDB ID : 2C0T
Title : Src family kinase Hck with bound inhibitor A-641359
Authors : Borhani, D.W.; Burchat, A.; Calderwood, D.J.; Hirst, G.C.; Li, B.; Loew, A.
Deposited on : 2005-09-07
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

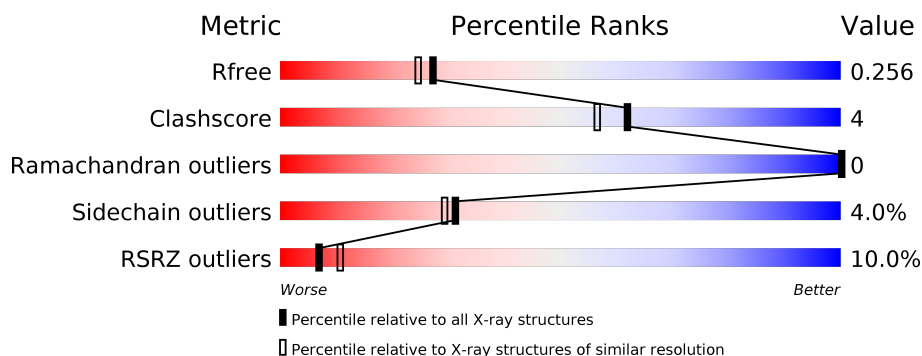
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 $\leq 5\%$. 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	454	<div> <div>7%</div> <div>85%</div> <div>9%</div> <div>6%</div> </div>
1	B	454	<div> <div>12%</div> <div>80%</div> <div>14%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7225 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.

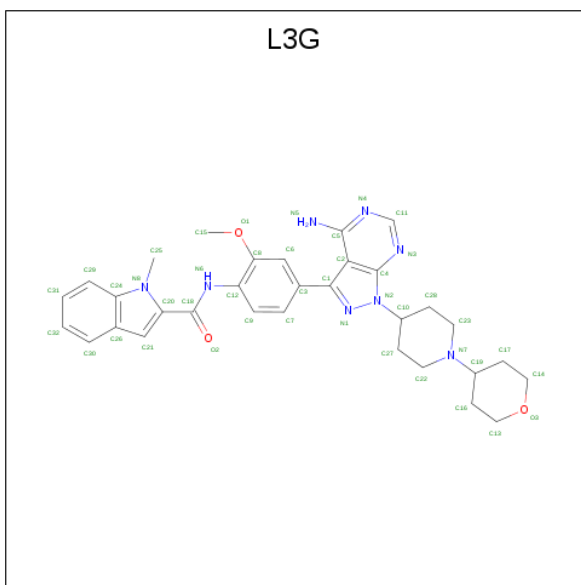
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE HCK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	P	S	0	1	0
			3467	2217	584	645	1	20			
1	B	430	Total	C	N	O	P	S	0	0	0
			3468	2217	583	647	1	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	GLU	GLN	engineered mutation	UNP P08631
A	503	GLU	GLN	engineered mutation	UNP P08631
A	504	ILE	GLN	engineered mutation	UNP P08631
B	502	GLU	GLN	engineered mutation	UNP P08631
B	503	GLU	GLN	engineered mutation	UNP P08631
B	504	ILE	GLN	engineered mutation	UNP P08631

- Molecule 2 is N-(4-{4-AMINO-1-[1-(TETRAHYDRO-2H-PYRAN-4-YL)PIPERIDIN-4-YL]-1H-PYRAZOLO[3,4-D]PYRIMIDIN-3-YL}-2-METHOXYPHENYL)-1-METHYL-1H-INDOLE-2-CARBOXAMIDE (three-letter code: L3G) (formula: C₃₂H₃₆N₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	32	8	3		
2	B	1	Total	C	N	O	0	0
			43	32	8	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	2	Total	Ca	0	0
			2	2		

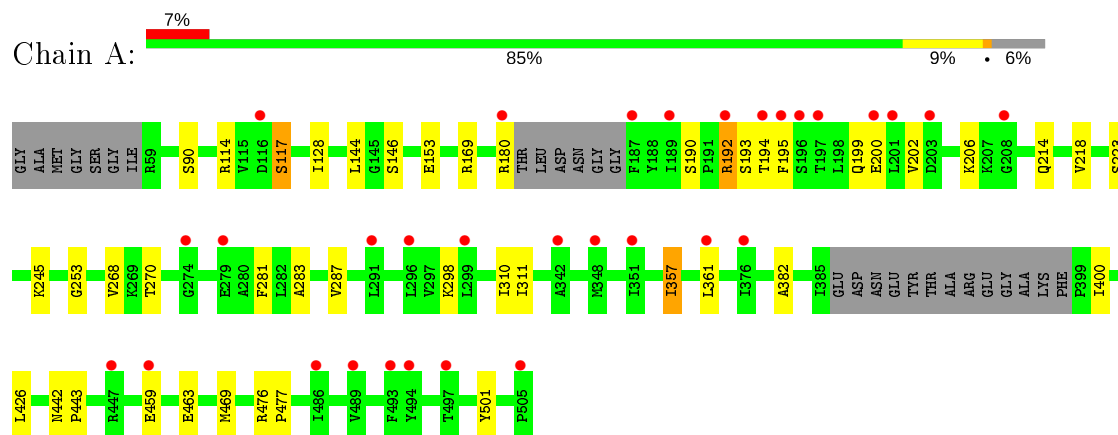
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	71	Total	O	0	0
			71	71		

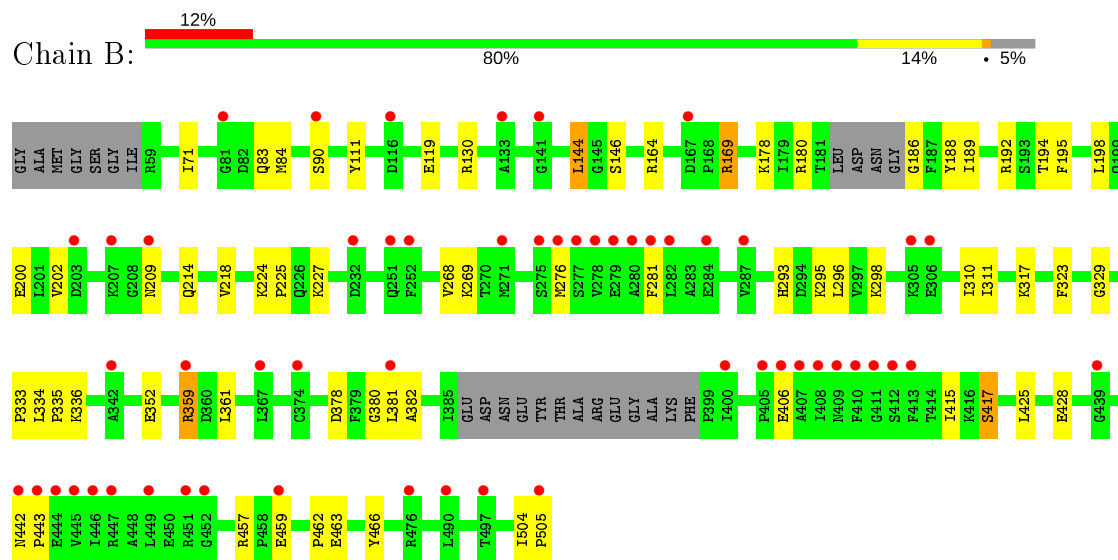
3 Residue-property plots [i](#)

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: TYROSINE-PROTEIN KINASE HCK



• Molecule 1: TYROSINE-PROTEIN KINASE HCK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.86Å 72.91Å 180.00Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 40.44 – 2.15	Depositor EDS
% Data completeness (in resolution range)	70.8 (20.00-2.15) 70.5 (40.44-2.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.253 0.196 , 0.256	Depositor DCC
R_{free} test set	2442 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7225	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L3G, CA, PTR

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	0.67	0/3533	0.70	0/4767
1	B	0.57	0/3532	0.65	0/4764
All	All	0.62	0/7065	0.68	0/9531

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

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	3467	0	3426	23	0
1	B	3468	0	3429	42	0
2	A	43	0	36	0	0
2	B	43	0	36	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	129	0	0	5	0
4	B	71	0	0	3	0
All	All	7225	0	6927	61	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 4.

All (61) 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:B:71:ILE:HD11	1:B:227:LYS:HE2	1.32	1.03
1:A:114:ARG:O	1:A:117:SER:HB2	1.83	0.79
1:A:214:GLN:NE2	4:A:2028:HOH:O	2.15	0.78
1:B:71:ILE:CD1	1:B:227:LYS:HE2	2.15	0.71
1:A:180:ARG:NH2	1:B:463:GLU:OE2	2.26	0.67
1:A:382:ALA:HB2	4:A:2083:HOH:O	1.98	0.63
1:B:352:GLU:HG3	1:B:415:ILE:HG12	1.80	0.63
1:A:180:ARG:HG2	4:A:2026:HOH:O	2.00	0.61
1:B:189:ILE:HG22	1:B:504:ILE:HG21	1.80	0.61
1:B:130:ARG:NH1	4:B:2063:HOH:O	2.34	0.60
1:A:195:PHE:HD2	1:A:200:GLU:HG2	1.65	0.60
1:A:463:GLU:OE2	1:B:180:ARG:NH2	2.36	0.59
1:B:195:PHE:HD2	1:B:200:GLU:HG2	1.69	0.56
1:B:281:PHE:HE2	1:B:310:ILE:HD11	1.71	0.56
1:B:417:SER:HB2	4:B:2044:HOH:O	2.06	0.55
1:A:190:SER:OG	1:A:192:ARG:HD2	2.07	0.55
1:A:463:GLU:OE2	1:B:180:ARG:NH1	2.41	0.54
1:B:425:LEU:O	1:B:428:GLU:HB2	2.08	0.54
1:A:268:VAL:HG22	1:A:311:ILE:HG13	1.90	0.54
1:B:359:ARG:HG2	1:B:382:ALA:CB	2.37	0.54
1:B:144:LEU:HD12	1:B:214:GLN:HG2	1.90	0.53
1:B:333:PRO:HB2	1:B:335:PRO:HD2	1.91	0.53
1:B:186:GLY:HA2	1:B:195:PHE:O	2.10	0.52
1:B:359:ARG:HG2	1:B:382:ALA:HB1	1.91	0.52
1:A:442:ASN:HB2	1:A:443:PRO:HD3	1.92	0.52
1:A:283:ALA:O	1:A:287:VAL:HG23	2.10	0.51
1:A:281:PHE:HE2	1:A:310:ILE:HD11	1.76	0.51
1:A:357:ILE:HD11	4:A:2089:HOH:O	2.10	0.51
1:B:146:SER:HA	1:B:218:VAL:O	2.10	0.51
1:B:281:PHE:CE2	1:B:310:ILE:HD11	2.46	0.50
1:B:378:ASP:OD1	2:B:1506:L3G:H9	2.11	0.50
1:B:195:PHE:CD2	1:B:200:GLU:HG2	2.48	0.49
1:B:293:HIS:HB3	1:B:296:LEU:HG	1.94	0.49
1:B:359:ARG:CG	1:B:382:ALA:HB1	2.43	0.49
1:A:253:GLY:HA3	1:A:270:THR:O	2.13	0.48
1:A:169:ARG:NH2	1:B:169:ARG:HH21	2.12	0.48
1:B:442:ASN:HB2	1:B:443:PRO:HD3	1.96	0.47
1:A:202:VAL:O	1:A:206:LYS:HG3	2.15	0.47
1:B:269:LYS:NZ	4:B:2023:HOH:O	2.10	0.46
1:B:209:ASN:O	1:B:209:ASN:CG	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:HD21	1:B:462:PRO:HD3	1.97	0.46
1:B:189:ILE:HG22	1:B:504:ILE:CG2	2.46	0.46
1:A:382:ALA:CB	4:A:2083:HOH:O	2.59	0.45
1:B:380:GLY:C	1:B:381:LEU:N	2.70	0.45
1:B:504:ILE:HA	1:B:505:PRO:HD3	1.76	0.45
1:B:198:LEU:O	1:B:202:VAL:HG13	2.17	0.45
1:B:295:LYS:HA	1:B:295:LYS:HD3	1.78	0.44
1:B:457:ARG:HG3	1:B:466:TYR:CG	2.52	0.44
1:B:323:PHE:O	1:B:329:GLY:HA3	2.18	0.44
1:B:268:VAL:HG22	1:B:311:ILE:HG13	1.99	0.44
1:B:180:ARG:HG3	1:B:188:TYR:CZ	2.53	0.44
1:B:83:GLN:C	1:B:84:MET:HG2	2.39	0.43
1:A:146:SER:HA	1:A:218:VAL:O	2.19	0.43
1:B:189:ILE:CG2	1:B:504:ILE:HG21	2.49	0.42
1:B:111:TYR:HE2	1:B:224:LYS:HE3	1.85	0.42
1:A:426:LEU:HD23	1:A:469:MET:HG2	2.00	0.42
1:A:192:ARG:HG2	1:A:193:SER:N	2.34	0.41
1:A:153:GLU:HB2	1:A:501:PTR:O2P	2.20	0.41
1:A:476:ARG:HA	1:A:477:PRO:HD3	1.93	0.41
1:B:224:LYS:HA	1:B:225:PRO:HD3	1.89	0.41
1:B:317:LYS:HG2	1:B:323:PHE:CD1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	422/454 (93%)	406 (96%)	16 (4%)	0	100	100
1	B	421/454 (93%)	401 (95%)	20 (5%)	0	100	100
All	All	843/908 (93%)	807 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	374/393 (95%)	360 (96%)	14 (4%)	34	32
1	B	374/393 (95%)	358 (96%)	16 (4%)	29	27
All	All	748/786 (95%)	718 (96%)	30 (4%)	31	29

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

Mol	Chain	Res	Type
1	A	90	SER
1	A	117	SER
1	A	128	ILE
1	A	144	LEU
1	A	192	ARG
1	A	194	THR
1	A	199	GLN
1	A	223	SER
1	A	245	LYS
1	A	298	LYS
1	A	357	ILE
1	A	361	LEU
1	A	400	ILE
1	A	459	GLU
1	B	90	SER
1	B	119	GLU
1	B	144	LEU
1	B	164	ARG
1	B	169	ARG
1	B	178	LYS
1	B	192	ARG
1	B	194	THR
1	B	276	MET
1	B	298	LYS
1	B	336	LYS

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Mol	Chain	Res	Type
1	B	359	ARG
1	B	361	LEU
1	B	406	GLU
1	B	417	SER
1	B	459	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	261	ASN
1	B	251	GLN
1	B	292	GLN
1	B	442	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	PTR	A	501	1,3	15,16,17	1.88	1 (6%)	19,22,24	0.95	1 (5%)
1	PTR	B	501	1,3	15,16,17	1.78	1 (6%)	19,22,24	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	501	1,3	-	2/10/11/13	0/1/1/1
1	PTR	B	501	1,3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	PTR	OH-CZ	-6.79	1.25	1.40
1	B	501	PTR	OH-CZ	-6.37	1.26	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	PTR	CG-CB-CA	-2.30	109.44	114.10

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	501	PTR	O-C-CA-CB
1	A	501	PTR	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	501	PTR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	L3G	A	1506	-	46,49,49	1.20	2 (4%)	53,71,71	1.96	12 (22%)
2	L3G	B	1506	-	46,49,49	0.81	1 (2%)	53,71,71	2.03	13 (24%)

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	L3G	A	1506	-	-	3/15/40/40	0/7/7/7
2	L3G	B	1506	-	-	6/15/40/40	0/7/7/7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1506	L3G	N1-N2	5.02	1.43	1.37
2	B	1506	L3G	N1-N2	2.12	1.40	1.37
2	A	1506	L3G	C9-C7	2.02	1.42	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1506	L3G	C23-N7-C22	6.34	120.66	109.08
2	B	1506	L3G	C21-C26-C24	5.75	111.29	106.27
2	A	1506	L3G	C21-C26-C24	5.72	111.26	106.27
2	B	1506	L3G	N3-C11-N4	-5.67	119.81	128.68
2	B	1506	L3G	C23-N7-C22	5.60	119.31	109.08
2	B	1506	L3G	C27-C22-N7	-5.16	103.52	111.43
2	A	1506	L3G	N3-C11-N4	-4.70	121.33	128.68
2	A	1506	L3G	C20-C21-C26	-3.61	102.05	106.55
2	A	1506	L3G	C26-C24-N8	-3.55	105.44	109.17
2	B	1506	L3G	C26-C24-N8	-3.32	105.68	109.17
2	B	1506	L3G	C20-C21-C26	-3.28	102.47	106.55
2	B	1506	L3G	O1-C8-C12	3.21	118.73	114.80
2	A	1506	L3G	O1-C8-C12	2.75	118.17	114.80
2	B	1506	L3G	C11-N4-C5	2.72	123.40	118.75
2	A	1506	L3G	C15-O1-C8	2.60	121.45	117.53
2	A	1506	L3G	C27-C22-N7	-2.59	107.46	111.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1506	L3G	C23-N7-C19	-2.42	105.84	112.64
2	B	1506	L3G	C28-C23-N7	-2.40	107.75	111.43
2	B	1506	L3G	C15-O1-C8	2.39	121.14	117.53
2	B	1506	L3G	C1-N1-N2	2.33	107.03	105.17
2	B	1506	L3G	C22-C27-C10	-2.32	108.62	110.44
2	A	1506	L3G	C11-N4-C5	2.19	122.51	118.75
2	A	1506	L3G	C1-N1-N2	2.18	106.91	105.17
2	B	1506	L3G	C8-C12-N6	2.09	120.41	116.66
2	A	1506	L3G	C17-C19-N7	2.06	117.87	112.52

There are no chirality outliers.

All (9) torsion outliers are listed below:

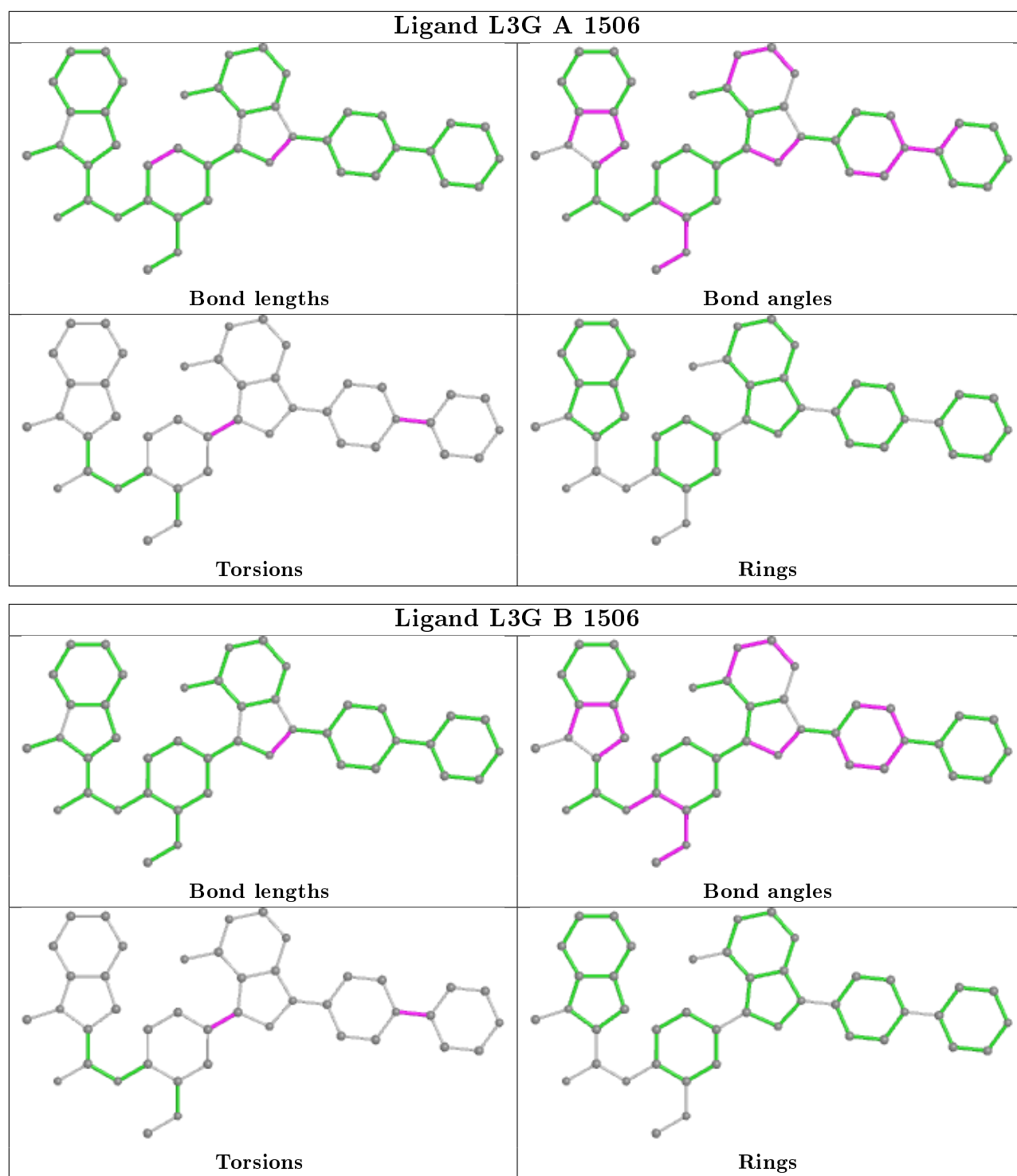
Mol	Chain	Res	Type	Atoms
2	A	1506	L3G	N1-C1-C3-C6
2	A	1506	L3G	N1-C1-C3-C7
2	B	1506	L3G	N1-C1-C3-C6
2	B	1506	L3G	N1-C1-C3-C7
2	B	1506	L3G	C16-C19-N7-C23
2	B	1506	L3G	C17-C19-N7-C23
2	B	1506	L3G	C16-C19-N7-C22
2	A	1506	L3G	C17-C19-N7-C23
2	B	1506	L3G	C17-C19-N7-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1506	L3G	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	380:GLY	C	381:LEU	N	2.70

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, 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	427/454 (94%)	0.85	31 (7%) 15 21	46, 61, 79, 87	0
1	B	429/454 (94%)	1.05	55 (12%) 3 5	51, 64, 82, 94	0
All	All	856/908 (94%)	0.95	86 (10%) 7 11	46, 63, 80, 94	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	VAL	9.1
1	B	439	GLY	7.1
1	B	449	LEU	5.8
1	B	271	MET	5.6
1	B	447	ARG	5.2
1	B	408	ILE	5.1
1	B	410	PHE	5.1
1	B	279	GLU	5.0
1	B	442	ASN	4.9
1	A	194	THR	4.7
1	B	276	MET	4.7
1	B	443	PRO	4.7
1	A	187	PHE	4.6
1	B	452	GLY	4.5
1	B	446	ILE	4.2
1	B	280	ALA	4.2
1	B	407	ALA	4.2
1	B	400	ILE	4.1
1	B	405	PRO	3.9
1	A	505	PRO	3.7
1	A	116	ASP	3.7
1	B	275	SER	3.7
1	B	90	SER	3.5
1	A	180	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	409	ASN	3.3
1	A	192	ARG	3.2
1	A	208	GLY	3.2
1	B	141	GLY	3.1
1	B	413	PHE	3.1
1	B	459	GLU	3.1
1	B	406	GLU	3.1
1	B	381	LEU	3.0
1	B	445	VAL	3.0
1	B	374	CYS	2.9
1	B	167	ASP	2.9
1	B	305	LYS	2.8
1	A	203	ASP	2.8
1	B	451	ARG	2.8
1	B	116	ASP	2.8
1	B	411	GLY	2.8
1	B	490	LEU	2.8
1	A	342	ALA	2.7
1	A	196	SER	2.7
1	B	359	ARG	2.7
1	A	195	PHE	2.7
1	B	497	THR	2.6
1	A	291	LEU	2.6
1	A	197	THR	2.6
1	B	282	LEU	2.6
1	B	277	SER	2.6
1	B	281	PHE	2.6
1	B	284	GLU	2.6
1	B	252	PHE	2.5
1	A	459	GLU	2.5
1	B	367	LEU	2.5
1	B	81	GLY	2.5
1	B	232	ASP	2.5
1	A	376	ILE	2.4
1	B	412	SER	2.4
1	A	351	ILE	2.4
1	B	444	GLU	2.4
1	A	299	LEU	2.3
1	B	209	ASN	2.3
1	B	342	ALA	2.2
1	B	476	ARG	2.2
1	A	447	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	505	PRO	2.2
1	A	497	THR	2.2
1	A	361	LEU	2.2
1	B	203	ASP	2.2
1	B	207	LYS	2.2
1	B	133	ALA	2.2
1	A	189	ILE	2.2
1	A	494	TYR	2.2
1	A	201	LEU	2.1
1	A	486	ILE	2.1
1	A	274	GLY	2.1
1	A	200	GLU	2.1
1	A	493	PHE	2.1
1	B	306	GLU	2.1
1	A	296	LEU	2.1
1	A	489	VAL	2.1
1	A	348	MET	2.0
1	B	287	VAL	2.0
1	A	279	GLU	2.0
1	B	251	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	A	501	16/17	0.96	0.16	63,66,67,68	0
1	PTR	B	501	16/17	0.96	0.16	55,58,60,62	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

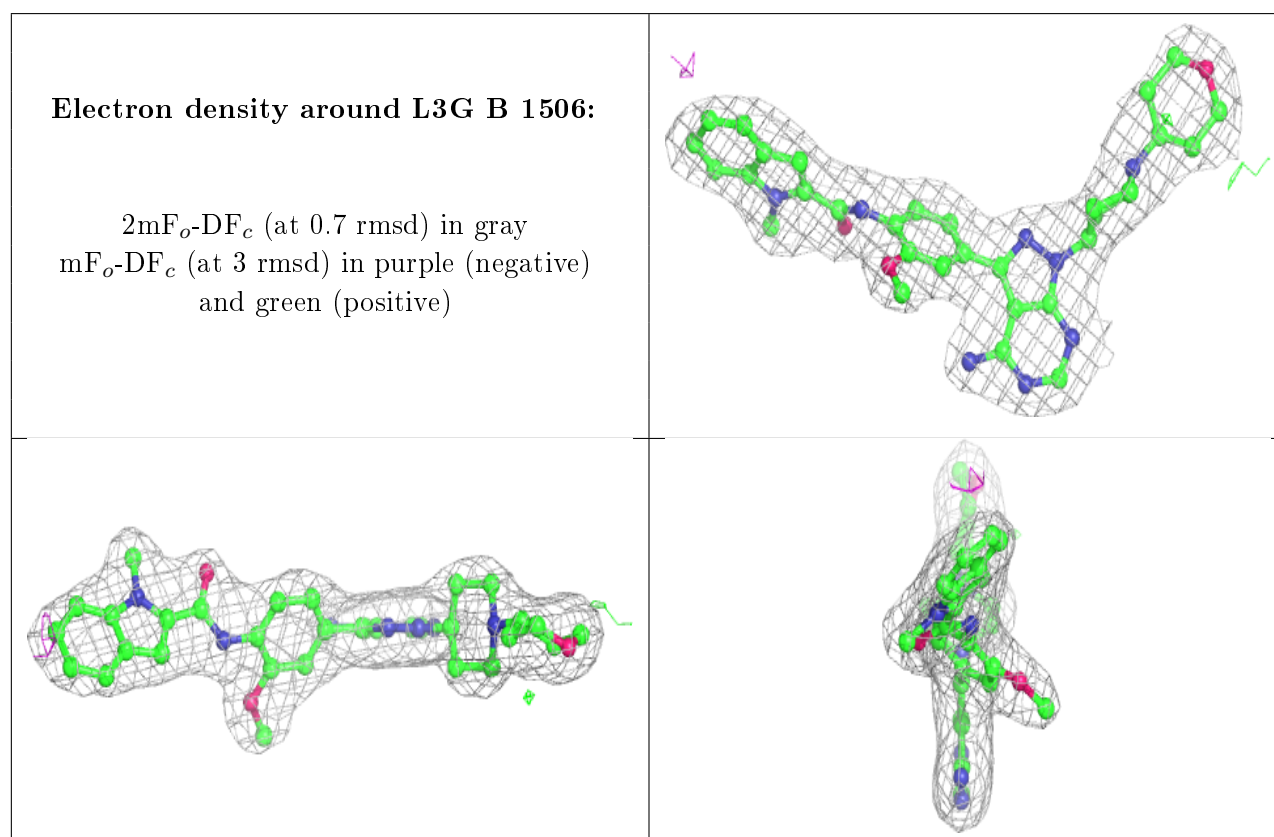
6.4 Ligands [i](#)

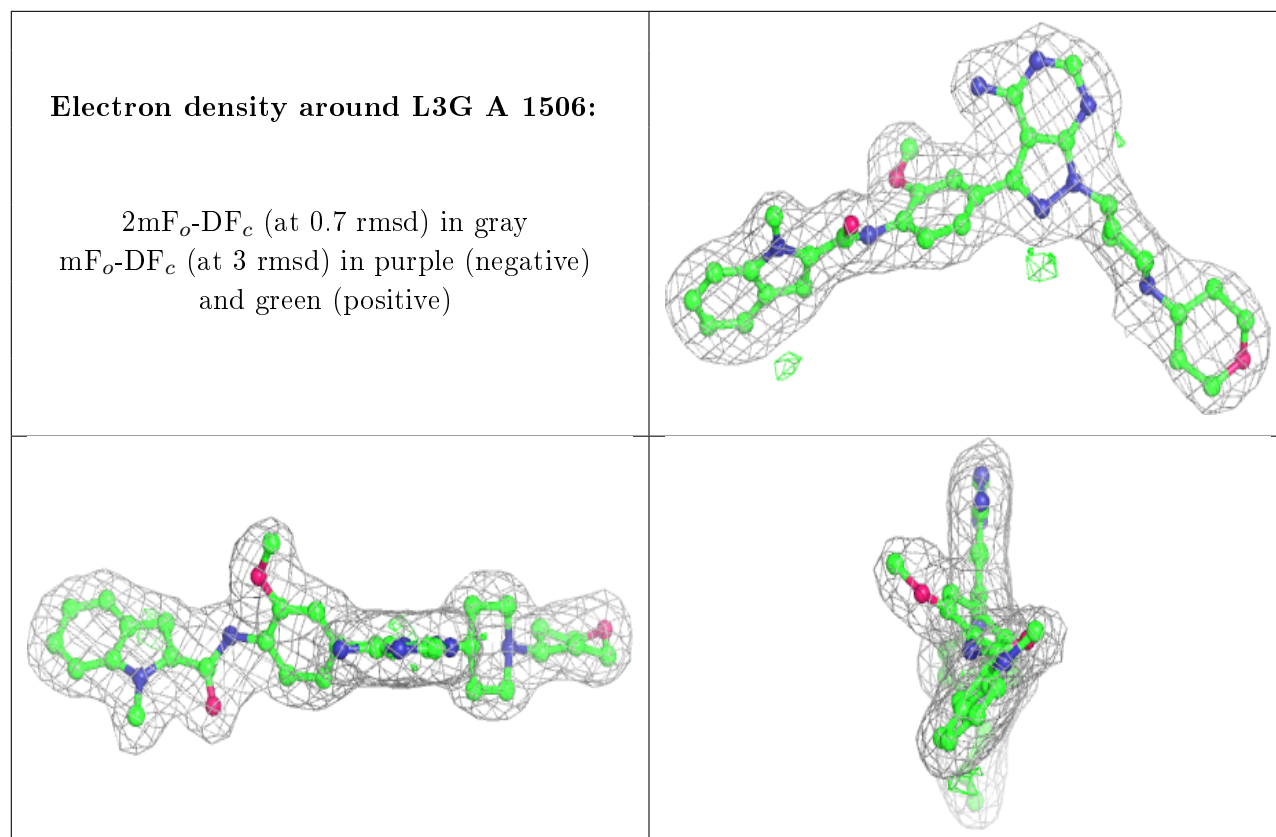
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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(\AA^2)	Q<0.9
2	L3G	B	1506	43/43	0.94	0.15	49,54,65,66	0
2	L3G	A	1506	43/43	0.96	0.15	40,46,59,63	0
3	CA	B	1507	1/1	0.98	0.15	53,53,53,53	0
3	CA	B	1508	1/1	0.98	0.04	74,74,74,74	0
3	CA	A	1508	1/1	0.99	0.07	66,66,66,66	0
3	CA	A	1507	1/1	0.99	0.14	52,52,52,52	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.