



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:12 AM UTC

PDB ID : 2C0T / pdb_00002c0t
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

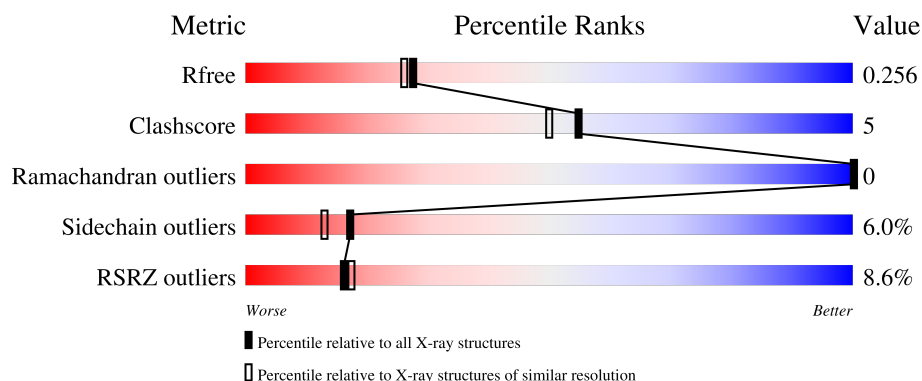
1 Overall quality at a glance

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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 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 $\leq 5\%$. 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	10% 83% 11% • 6%
1	B	454	7% 77% 16% • 5%

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.

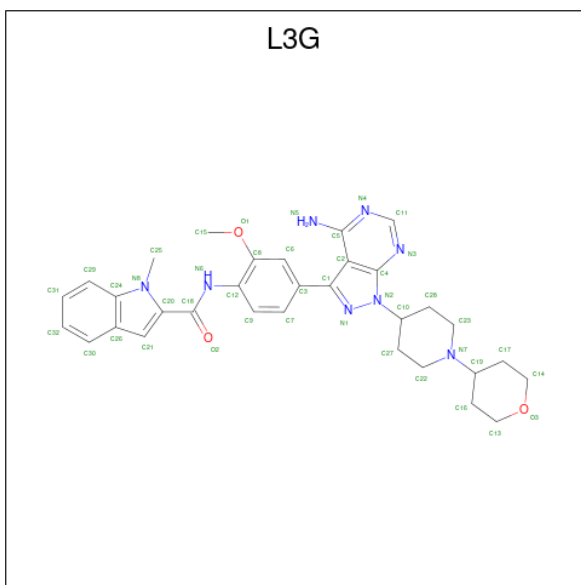
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE HCK.

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

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

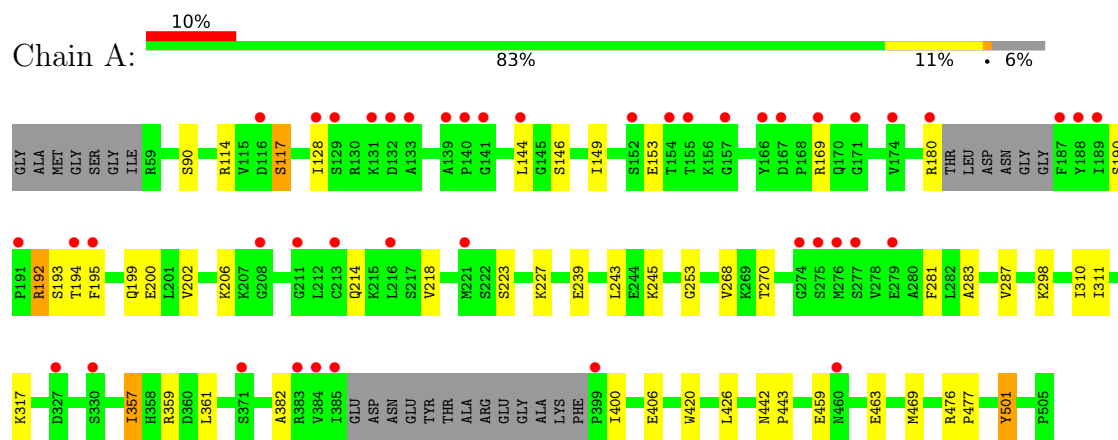
- Molecule 4 is water.

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

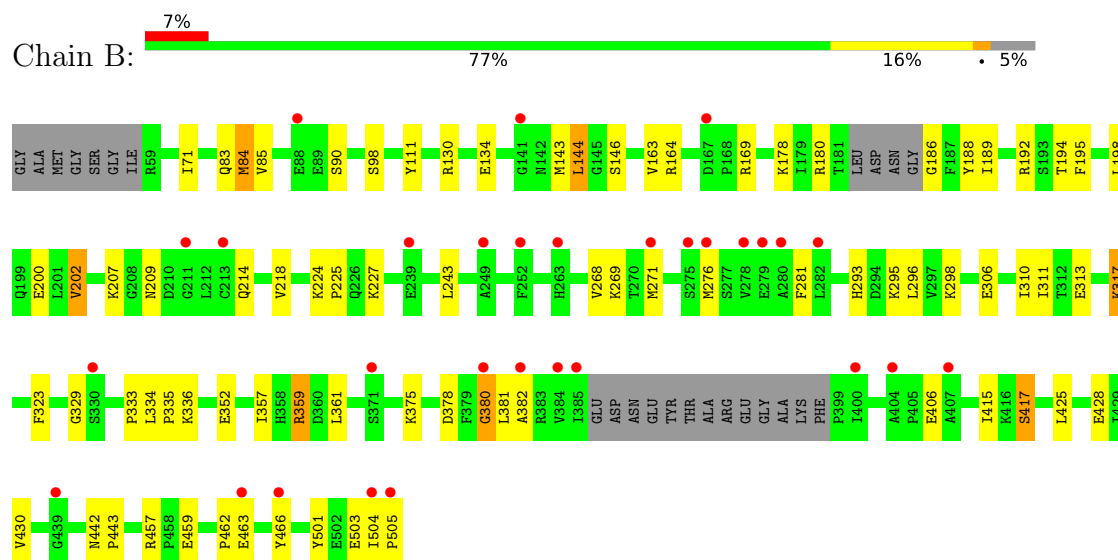
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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: 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 20.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	70.8 (20.00-2.15) 70.7 (20.00-2.15)	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 , 60.1	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.79	0/3533	0.93	3/4767 (0.1%)
1	B	0.68	0/3532	0.92	1/4764 (0.0%)
All	All	0.74	0/7065	0.93	4/9531 (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	359	ARG	N-CA-C	5.86	122.62	113.72
1	A	227	LYS	CA-C-N	-5.77	114.32	120.03
1	A	227	LYS	C-N-CA	-5.77	114.32	120.03
1	B	380	GLY	CA-C-O	5.32	125.18	119.06

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	3467	0	3426	25	0
1	B	3468	0	3429	46	0
2	A	43	0	36	0	0
2	B	43	0	36	1	0
3	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	67	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 5.

All (67) 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:B:269:LYS:NZ	4:B:2023:HOH:O	2.10	0.82
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:CE2	1:B:310:ILE:HD11	2.46	0.50
1:B:313:GLU:OE2	1:B:375:LYS:NZ	2.36	0.50
1:B:378:ASP:OD1	2:B:1506:L3G:H9	2.11	0.50
1:B:209:ASN:CG	1:B:209:ASN:O	2.54	0.50
1:B:380:GLY:C	1:B:381:LEU:N	2.70	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:83:GLN:C	1:B:84:MET:HG2	2.39	0.47
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: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: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:HD3	1:B:295:LYS:HA	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:A:420:TRP:C	1:A:420:TRP:CD1	2.97	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:B:271:MET:HE1	1:B:381:LEU:HD11	2.02	0.41
1:B:84:MET:HE3	1:B:98:SER:HB2	2.03	0.41
1:A:476:ARG:HA	1:A:477:PRO:HD3	1.93	0.41
1:B:84:MET:HB3	1:B:84:MET:HE2	1.89	0.41
1:B:224:LYS:HA	1:B:225:PRO:HD3	1.89	0.41
1:A:239:GLU:H	1:A:239:GLU:CD	2.28	0.40
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%)	356 (95%)	18 (5%)	23	20
1	B	374/393 (95%)	347 (93%)	27 (7%)	13	8
All	All	748/786 (95%)	703 (94%)	45 (6%)	17	13

All (45) 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	149	ILE
1	A	192	ARG
1	A	194	THR
1	A	199	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	223	SER
1	A	243	LEU
1	A	245	LYS
1	A	298	LYS
1	A	317	LYS
1	A	357	ILE
1	A	361	LEU
1	A	400	ILE
1	A	406	GLU
1	A	459	GLU
1	B	84	MET
1	B	85	VAL
1	B	90	SER
1	B	134	GLU
1	B	143	MET
1	B	144	LEU
1	B	163	VAL
1	B	164	ARG
1	B	178	LYS
1	B	192	ARG
1	B	194	THR
1	B	202	VAL
1	B	207	LYS
1	B	243	LEU
1	B	276	MET
1	B	298	LYS
1	B	306	GLU
1	B	317	LYS
1	B	336	LYS
1	B	357	ILE
1	B	359	ARG
1	B	361	LEU
1	B	406	GLU
1	B	417	SER
1	B	430	VAL
1	B	459	GLU
1	B	503	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	261	ASN
1	A	286	ASN
1	A	292	GLN
1	A	332	GLN
1	A	467	ASN
1	A	487	GLN
1	B	292	GLN
1	B	332	GLN

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	3,1	15,16,17	1.88	1 (6%)	17,22,24	0.74	0
1	PTR	B	501	3,1	15,16,17	1.81	1 (6%)	17,22,24	0.57	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	3,1	-	2/10/11/13	0/1/1/1
1	PTR	B	501	3,1	-	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	-6.85	1.25	1.40
1	B	501	PTR	OH-CZ	-6.43	1.26	1.40

There are no bond angle outliers.

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 oligosaccharides 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	B	1506	-	49,49,49	1.22	4 (8%)	69,71,71	2.17	20 (28%)
2	L3G	A	1506	-	49,49,49	1.44	10 (20%)	69,71,71	2.24	25 (36%)

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	B	1506	-	-	6/22/40/40	0/7/7/7
2	L3G	A	1506	-	-	3/22/40/40	0/7/7/7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1506	L3G	C4-N2	-5.05	1.30	1.36
2	A	1506	L3G	C4-N2	-4.10	1.31	1.36
2	A	1506	L3G	C2-C5	-3.64	1.38	1.42
2	A	1506	L3G	C1-N1	3.03	1.36	1.33
2	A	1506	L3G	N2-N1	2.96	1.43	1.38
2	B	1506	L3G	C2-C5	-2.71	1.39	1.42
2	A	1506	L3G	C24-N8	-2.46	1.35	1.39
2	B	1506	L3G	C1-N1	2.45	1.36	1.33
2	A	1506	L3G	C20-N8	-2.44	1.35	1.38
2	A	1506	L3G	C7-C3	2.41	1.43	1.39
2	A	1506	L3G	C9-C7	2.24	1.42	1.38
2	A	1506	L3G	C25-N8	2.22	1.50	1.46
2	A	1506	L3G	C26-C24	-2.13	1.38	1.41
2	B	1506	L3G	C24-N8	-2.09	1.35	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1506	L3G	C23-N7-C22	6.05	120.66	109.13
2	B	1506	L3G	N4-C11-N3	-5.79	119.81	128.58
2	A	1506	L3G	C4-C2-C1	5.51	108.58	104.74
2	A	1506	L3G	C26-C24-N8	-5.44	105.44	108.23
2	B	1506	L3G	C23-N7-C22	5.34	119.31	109.13
2	B	1506	L3G	C27-C22-N7	-5.13	103.52	111.42
2	B	1506	L3G	C2-C1-N1	-4.98	106.77	110.19
2	B	1506	L3G	C26-C24-N8	-4.97	105.68	108.23
2	A	1506	L3G	N4-C11-N3	-4.79	121.33	128.58
2	B	1506	L3G	C4-C2-C1	4.66	107.99	104.74
2	A	1506	L3G	C2-C1-N1	-4.65	107.00	110.19
2	A	1506	L3G	C28-C10-N2	-4.63	107.50	111.88
2	B	1506	L3G	C24-C26-C21	4.28	111.29	107.05
2	A	1506	L3G	C24-C26-C21	4.25	111.26	107.05
2	A	1506	L3G	C5-C2-C1	-4.17	134.85	139.07
2	B	1506	L3G	C2-C4-N3	-4.13	122.58	126.97
2	A	1506	L3G	C26-C21-C20	-3.52	102.05	107.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1506	L3G	C26-C21-C20	-3.24	102.47	107.31
2	B	1506	L3G	N3-C4-N2	3.24	130.27	126.05
2	A	1506	L3G	C2-C4-N3	-3.18	123.59	126.97
2	B	1506	L3G	O1-C8-C12	3.15	118.73	114.81
2	B	1506	L3G	C5-C2-C1	-3.14	135.90	139.07
2	A	1506	L3G	C27-C10-N2	-3.11	108.94	111.88
2	B	1506	L3G	C11-N3-C4	2.90	118.93	111.83
2	B	1506	L3G	C11-N4-C5	2.84	123.40	118.73
2	B	1506	L3G	C18-C20-N8	2.74	126.31	122.81
2	A	1506	L3G	C23-N7-C19	-2.73	105.84	112.79
2	A	1506	L3G	O1-C8-C12	2.70	118.17	114.81
2	A	1506	L3G	C3-C1-N1	2.68	122.40	118.91
2	A	1506	L3G	C15-O1-C8	2.68	121.45	117.51
2	A	1506	L3G	C27-C22-N7	-2.57	107.46	111.42
2	B	1506	L3G	C21-C20-C18	-2.49	123.28	129.48
2	B	1506	L3G	C15-O1-C8	2.47	121.14	117.51
2	A	1506	L3G	C24-N8-C20	2.41	110.80	108.10
2	A	1506	L3G	O3-C14-C17	-2.40	107.60	111.74
2	B	1506	L3G	C28-C23-N7	-2.39	107.75	111.42
2	A	1506	L3G	C11-N4-C5	2.30	122.51	118.73
2	A	1506	L3G	C21-C20-C18	-2.24	123.89	129.48
2	A	1506	L3G	C18-C20-N8	2.24	125.67	122.81
2	A	1506	L3G	N3-C4-N2	2.20	128.92	126.05
2	A	1506	L3G	C11-N3-C4	2.17	117.14	111.83
2	A	1506	L3G	C6-C3-C1	-2.16	116.91	120.34
2	B	1506	L3G	C29-C24-N8	2.10	134.21	129.88
2	B	1506	L3G	C3-C1-N1	2.06	121.59	118.91
2	A	1506	L3G	C17-C19-N7	2.03	117.87	112.66

There are no chirality outliers.

All (9) torsion outliers are listed below:

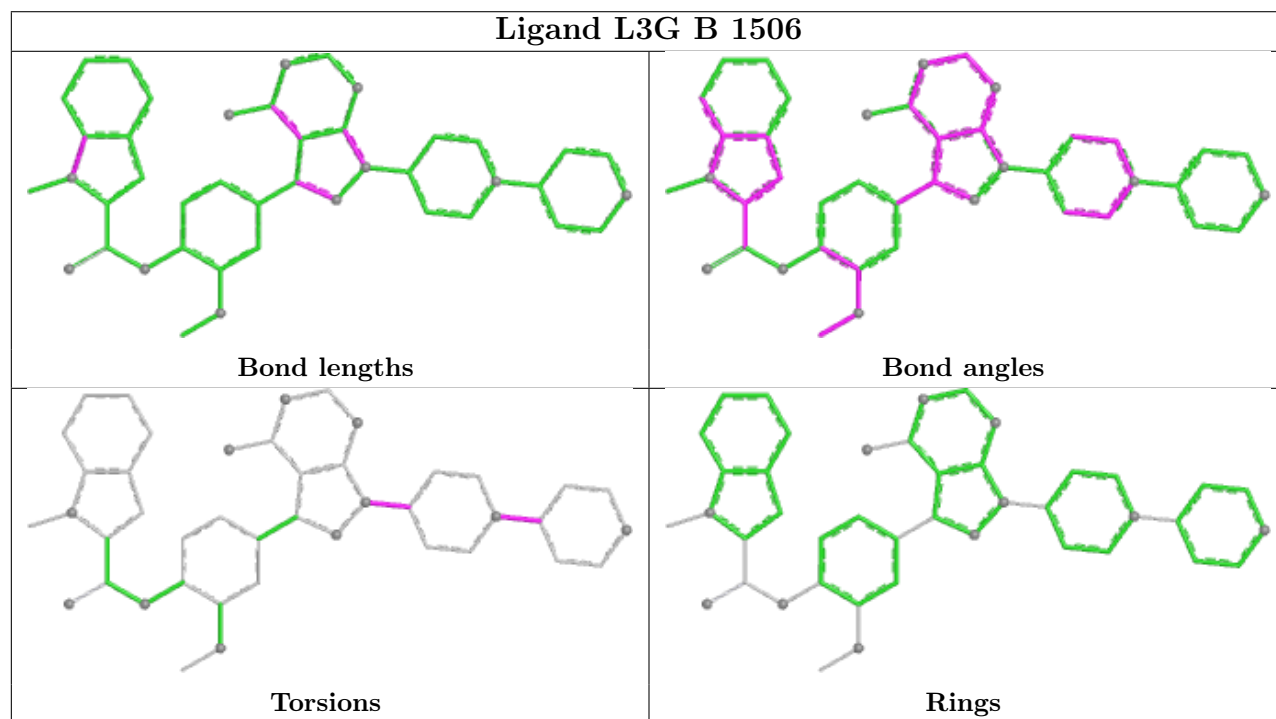
Mol	Chain	Res	Type	Atoms
2	B	1506	L3G	C16-C19-N7-C23
2	B	1506	L3G	C17-C19-N7-C23
2	B	1506	L3G	C16-C19-N7-C22
2	A	1506	L3G	C27-C10-N2-C4
2	B	1506	L3G	C27-C10-N2-C4
2	A	1506	L3G	C17-C19-N7-C23
2	B	1506	L3G	C17-C19-N7-C22
2	A	1506	L3G	C28-C10-N2-C4
2	B	1506	L3G	C28-C10-N2-C4

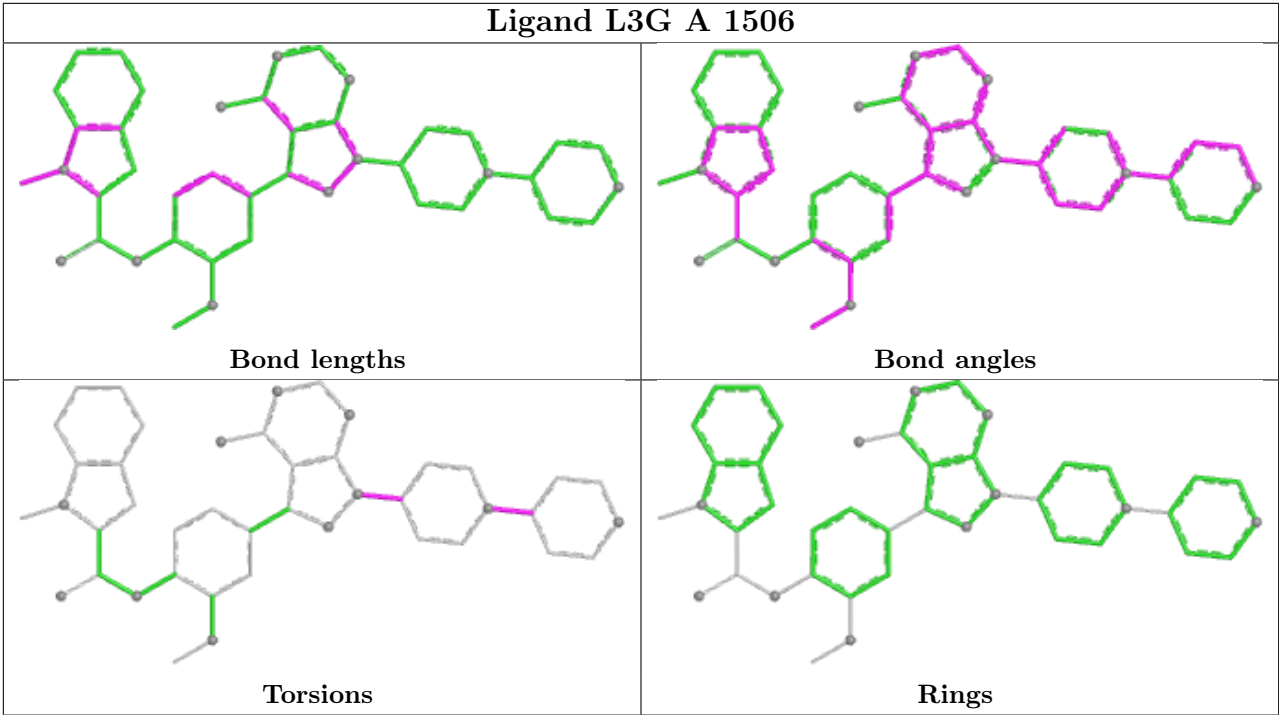
There are no ring outliers.

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%)	0.72	44 (10%) 12 13	27, 61, 79, 87	1 (0%)
1	B	429/454 (94%)	0.77	30 (6%) 22 25	51, 64, 82, 94	0
All	All	856/908 (94%)	0.74	74 (8%) 16 17	27, 63, 80, 94	1 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	PRO	4.1
1	A	187	PHE	4.1
1	A	276	MET	3.8
1	B	271	MET	3.5
1	A	189	ILE	3.4
1	B	280	ALA	3.4
1	A	194	THR	3.3
1	B	380	GLY	3.2
1	A	399	PRO	3.2
1	A	166	TYR	3.1
1	A	384	VAL	3.1
1	A	279	GLU	3.1
1	A	327	ASP	3.1
1	B	275	SER	3.1
1	B	167	ASP	3.0
1	A	274	GLY	3.0
1	B	211	GLY	3.0
1	A	221	MET	3.0
1	A	174	VAL	3.0
1	B	279	GLU	3.0
1	A	154	THR	3.0
1	B	371	SER	2.9
1	A	144	LEU	2.9
1	A	208	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	439	GLY	2.9
1	A	155	THR	2.9
1	A	140	PRO	2.7
1	B	278	VAL	2.7
1	B	276	MET	2.7
1	A	275	SER	2.7
1	A	460	ASN	2.6
1	B	213	CYS	2.6
1	A	141	GLY	2.6
1	B	141	GLY	2.6
1	B	282	LEU	2.6
1	A	330	SER	2.6
1	A	180	ARG	2.5
1	A	157	GLY	2.5
1	A	171	GLY	2.5
1	A	132	ASP	2.5
1	B	384	VAL	2.4
1	A	133	ALA	2.4
1	B	252	PHE	2.4
1	A	128	ILE	2.4
1	A	213	CYS	2.4
1	B	249	ALA	2.3
1	A	169	ARG	2.3
1	B	505	PRO	2.3
1	B	385	ILE	2.3
1	A	371	SER	2.3
1	B	463	GLU	2.2
1	A	116	ASP	2.2
1	A	139	ALA	2.2
1	B	330	SER	2.2
1	B	88	GLU	2.2
1	B	382	ALA	2.2
1	A	216	LEU	2.1
1	A	129	SER	2.1
1	B	504	ILE	2.1
1	A	167	ASP	2.1
1	A	211	GLY	2.1
1	B	400	ILE	2.1
1	B	239	GLU	2.0
1	B	407	ALA	2.1
1	A	383	ARG	2.0
1	B	263	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	131	LYS	2.0
1	A	188	TYR	2.0
1	A	385	ILE	2.0
1	A	195	PHE	2.0
1	A	152	SER	2.0
1	A	277	SER	2.0
1	B	404	ALA	2.0
1	B	466	TYR	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($\text{\AA}^2$)	Q<0.9
1	PTR	A	501	16/17	0.95	0.11	63,66,67,68	0
1	PTR	B	501	16/17	0.96	0.09	55,58,60,62	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

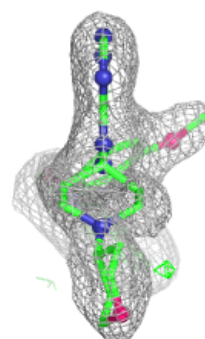
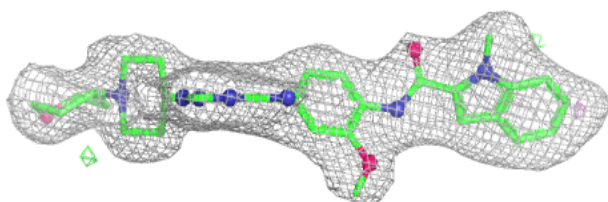
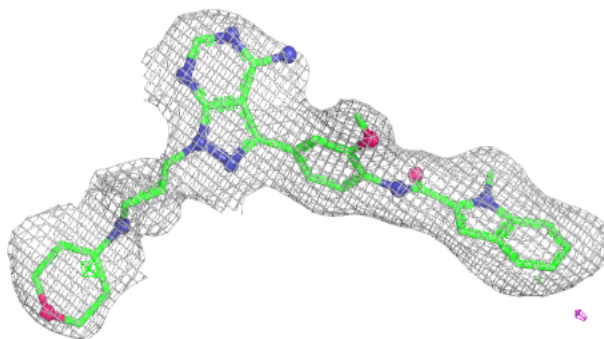
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	L3G	B	1506	43/43	0.94	0.09	49,54,65,66	0
2	L3G	A	1506	43/43	0.96	0.07	40,46,59,63	0
3	CA	B	1507	1/1	0.98	0.05	53,53,53,53	0
3	CA	A	1508	1/1	0.99	0.23	66,66,66,66	0
3	CA	A	1507	1/1	0.99	0.02	52,52,52,52	0
3	CA	B	1508	1/1	0.99	0.16	74,74,74,74	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.

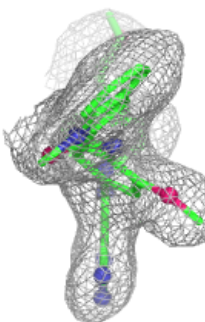
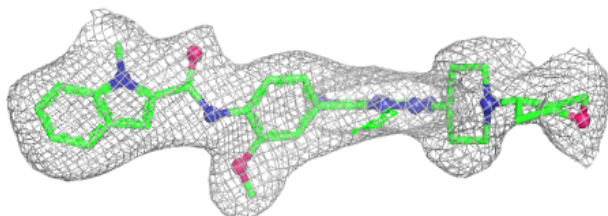
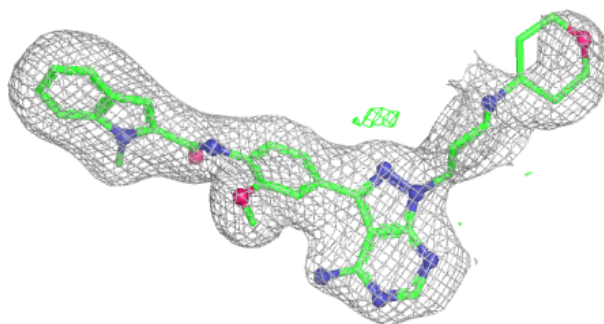
Electron density around L3G B 1506:

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



Electron density around L3G A 1506:

$2mF_o-DF_c$ (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.