



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:40 AM UTC

PDB ID : 2C0I / pdb_00002c0i
Title : Src family kinase Hck with bound inhibitor A-420983
Authors : Borhani, D.W.; Burchat, A.; Calderwood, D.J.; Hirst, G.C.; Li, B.; Loew, A.
Deposited on : 2005-09-03
Resolution : 2.30 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

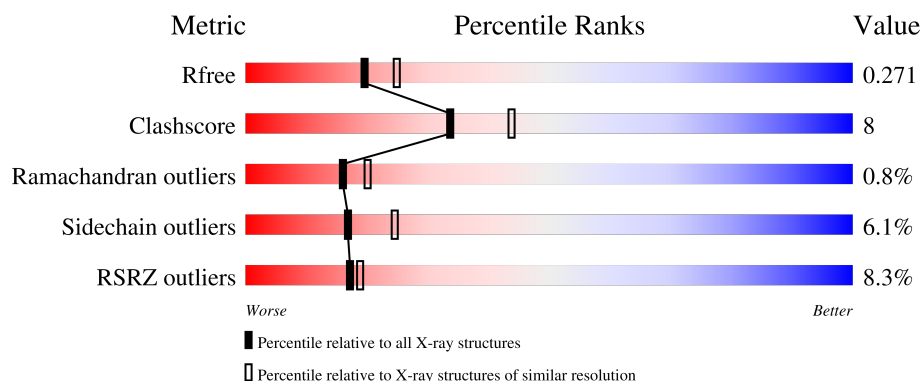
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	12% 73% 19% • •
1	B	454	4% 76% 18% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7383 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.

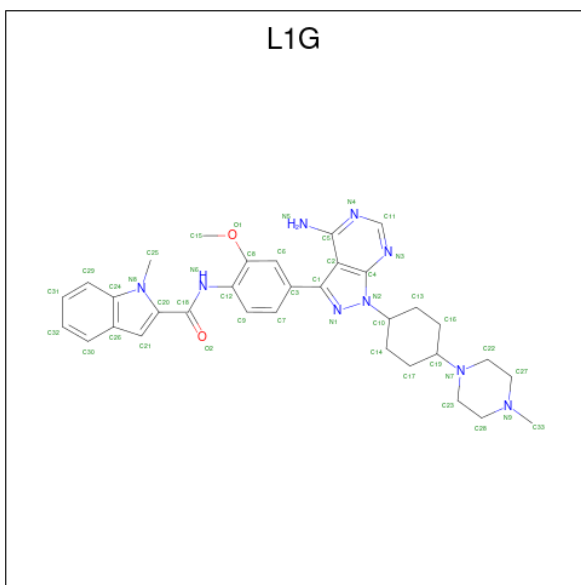
- Molecule 1 is a protein called TYROSINE-PROTEIN KINASE HCK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	P	S	0	1	0
			3506	2239	591	655	1	20			
1	B	434	Total	C	N	O	P	S	0	2	0
			3514	2243	593	657	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-[4-(4-METHYLPIPERAZIN-1-YL)-TRANS-CYCLOHEXYL]-1H-PYRAZOLO[3,4-D]PYRIMIDIN-3-YL}-2-METHOXYPHENYL)-1-METHYL-1H-INDOLE-2-CARBOXAMIDE (CCD ID: L1G) (formula: C₃₃H₃₉N₉O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	33	9	2		
2	B	1	Total	C	N	O	0	0
			44	33	9	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

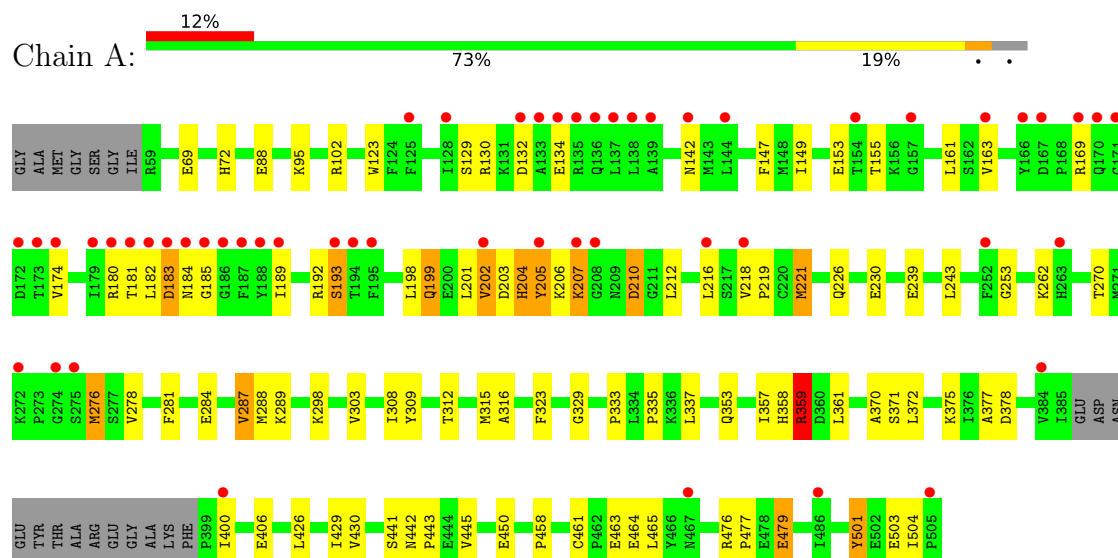
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	174	Total	O	0	0
			174	174		
4	B	99	Total	O	0	0
			99	99		

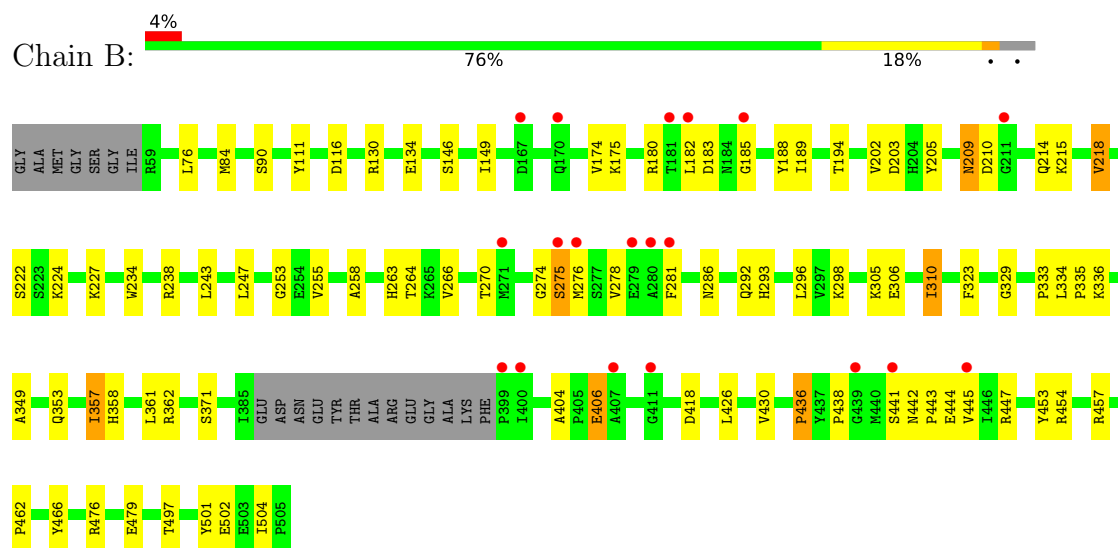
3 Residue-property plots [i](#)

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	49.08Å 73.12Å 179.49Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	19.96 – 2.30 19.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.9 (19.96-2.30) 89.7 (19.96-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.222 , 0.274 0.222 , 0.271	Depositor DCC
R_{free} test set	2515 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7383	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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: CA, PTR, L1G

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	1.00	21/3573 (0.6%)	0.98	6/4823 (0.1%)
1	B	0.66	4/3581 (0.1%)	0.86	0/4834
All	All	0.85	25/7154 (0.3%)	0.92	6/9657 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	LYS	CD-CE	14.80	1.96	1.52
1	A	203	ASP	CG-OD1	10.65	1.45	1.25
1	A	203	ASP	CG-OD2	10.59	1.45	1.25
1	A	210	ASP	CG-OD1	10.02	1.44	1.25
1	A	192	ARG	NE-CZ	9.46	1.43	1.33
1	B	447	ARG	NE-CZ	9.04	1.43	1.33
1	A	207	LYS	CE-NZ	8.13	1.73	1.49
1	A	204	HIS	ND1-CE1	8.07	1.40	1.32
1	B	447	ARG	CZ-NH1	7.92	1.43	1.32
1	A	204	HIS	CE1-NE2	7.82	1.40	1.32
1	A	210	ASP	CG-OD2	7.70	1.40	1.25
1	A	204	HIS	CD2-NE2	7.65	1.46	1.37
1	B	444	GLU	CD-OE1	7.62	1.39	1.25
1	A	204	HIS	CG-CD2	7.53	1.44	1.35
1	A	204	HIS	CB-CG	7.30	1.60	1.50
1	A	183	ASP	CG-OD1	7.13	1.38	1.25
1	A	204	HIS	CG-ND1	7.00	1.46	1.38
1	A	205	TYR	C-N	6.91	1.44	1.33
1	A	193	SER	CB-OG	6.57	1.55	1.42
1	A	207	LYS	CG-CD	6.09	1.70	1.52
1	B	444	GLU	CD-OE2	6.08	1.36	1.25
1	A	205	TYR	CG-CD1	5.88	1.51	1.39
1	A	205	TYR	CA-C	5.79	1.60	1.52
1	A	192	ARG	CZ-NH1	5.08	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	TYR	CE2-CZ	5.00	1.50	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	LEU	O-C-N	7.98	130.58	122.12
1	A	207	LYS	CG-CD-CE	-7.52	94.00	111.30
1	A	204	HIS	CA-CB-CG	-7.30	106.50	113.80
1	A	204	HIS	CB-CG-CD2	5.99	138.98	131.20
1	A	201	LEU	CA-C-O	-5.97	114.19	120.63
1	A	204	HIS	CB-CG-ND1	-5.48	114.48	122.70

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	3506	0	3461	62	0
1	B	3514	0	3466	51	0
2	A	44	0	39	1	0
2	B	44	0	39	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	174	0	0	3	1
4	B	99	0	0	4	0
All	All	7383	0	7005	109	1

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 8.

All (109) 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:207:LYS:CE	1:A:207:LYS:NZ	1.73	1.51
1:A:207:LYS:CE	1:A:207:LYS:CD	1.96	1.41
1:A:463:GLU:OE2	1:B:180:ARG:NH1	1.94	1.00
1:B:263[B]:HIS:HE1	4:B:2004:HOH:O	1.58	0.87
1:B:436:PRO:O	1:B:438:PRO:HD3	1.85	0.77
1:A:207:LYS:CE	1:A:207:LYS:CG	2.69	0.71
1:B:182:LEU:HG	1:B:183:ASP:H	1.54	0.71
1:B:263[B]:HIS:HD2	1:B:264:THR:OG1	1.74	0.70
1:A:476:ARG:HB2	1:A:479:GLU:HG3	1.78	0.66
1:B:130:ARG:NH1	4:B:2014:HOH:O	2.29	0.63
1:A:147:PHE:CD1	1:A:216:LEU:HB3	2.33	0.63
1:B:175:LYS:HD2	1:B:502:GLU:OE2	1.99	0.62
1:A:129:SER:HB2	1:A:153:GLU:OE1	2.00	0.62
1:A:358:HIS:O	1:A:359:ARG:HB2	2.00	0.61
1:B:333:PRO:HB2	1:B:335:PRO:HD2	1.81	0.61
1:B:234:TRP:HE1	1:B:286:ASN:HD21	1.48	0.60
1:A:183:ASP:C	1:A:185:GLY:H	2.10	0.59
1:B:183:ASP:C	1:B:185:GLY:H	2.10	0.59
1:B:180:ARG:HG3	1:B:188:TYR:CE2	2.38	0.59
1:B:358:HIS:O	1:B:418:ASP:OD1	2.22	0.58
1:B:189:ILE:HG22	1:B:504:ILE:HG21	1.85	0.57
1:B:453:TYR:O	1:B:454:ARG:HD2	2.04	0.57
1:A:189:ILE:HG22	1:A:504:ILE:HG21	1.87	0.56
1:B:476:ARG:HB2	1:B:479:GLU:HG3	1.87	0.56
1:B:357:ILE:HG22	1:B:418:ASP:OD2	2.05	0.56
1:A:253:GLY:HA3	1:A:270:THR:O	2.04	0.56
1:A:312:THR:OG1	2:A:1506:L1G:H153	2.05	0.56
1:A:463:GLU:OE2	1:B:180:ARG:CZ	2.52	0.55
1:A:134:GLU:HA	1:A:174:VAL:HG21	1.87	0.55
1:A:218:VAL:CG2	1:A:219:PRO:HD2	2.36	0.55
1:A:132:ASP:OD2	4:A:2038:HOH:O	2.18	0.54
1:B:441:SER:O	1:B:445:VAL:HG23	2.08	0.54
1:B:182:LEU:HG	1:B:183:ASP:N	2.22	0.54
1:A:426:LEU:O	1:A:430:VAL:HG23	2.08	0.54
1:B:234:TRP:HE1	1:B:286:ASN:ND2	2.06	0.54
1:B:253:GLY:HA3	1:B:270:THR:O	2.07	0.54
1:B:134:GLU:HA	1:B:174:VAL:HG21	1.92	0.52
1:A:226:GLN:NE2	4:A:2056:HOH:O	2.41	0.51
1:B:183:ASP:O	1:B:185:GLY:N	2.36	0.51
1:A:198:LEU:O	1:A:202:VAL:HG12	2.10	0.51
1:A:218:VAL:HG22	1:A:219:PRO:HD2	1.93	0.51
1:B:189:ILE:CG2	1:B:504:ILE:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLY:O	1:B:275:SER:HB2	2.10	0.50
1:B:281:PHE:CE2	1:B:310:ILE:HD11	2.46	0.50
1:A:278:VAL:HG13	1:A:308:ILE:HD11	1.93	0.50
1:A:130:ARG:HD3	1:A:501:PTR:CE2	2.42	0.50
1:A:426:LEU:HD11	1:A:465:LEU:HD11	1.94	0.49
1:B:205:TYR:HE1	1:B:210:ASP:HB2	1.77	0.49
1:A:123:TRP:HZ2	1:A:199:GLN:HG2	1.78	0.49
1:B:426:LEU:O	1:B:430:VAL:HG23	2.13	0.49
1:B:274:GLY:O	1:B:275:SER:CB	2.61	0.48
1:B:238:ARG:NH2	1:B:305:LYS:O	2.46	0.48
1:B:404:ALA:HB1	1:B:406:GLU:OE2	2.14	0.48
1:A:303:VAL:HB	1:A:309:TYR:HB2	1.96	0.48
1:B:457:ARG:HG3	1:B:466:TYR:CG	2.49	0.47
1:A:149:ILE:HD13	1:A:161:LEU:HD13	1.97	0.47
1:A:155:THR:HG21	1:A:180:ARG:HH12	1.79	0.47
1:A:442:ASN:HB2	1:A:443:PRO:HD3	1.97	0.47
1:A:463:GLU:OE2	1:B:180:ARG:NH2	2.47	0.47
1:A:315:MET:CE	1:A:375:LYS:HD2	2.44	0.47
1:A:504:ILE:HG23	1:A:504:ILE:O	2.14	0.47
1:B:247:LEU:HD12	1:B:255:VAL:HG12	1.97	0.46
1:B:263[B]:HIS:CE1	4:B:2004:HOH:O	2.47	0.46
1:A:284:GLU:O	1:A:288:MET:HG2	2.15	0.46
1:A:337:LEU:HB3	1:A:429:ILE:HG22	1.97	0.46
1:A:147:PHE:HB3	1:A:216:LEU:HD22	1.98	0.45
1:B:281:PHE:CZ	1:B:310:ILE:HD11	2.51	0.45
1:B:362:ARG:HD2	4:B:2057:HOH:O	2.15	0.45
1:A:123:TRP:HA	1:A:219:PRO:HB3	1.99	0.45
1:B:504:ILE:HG23	1:B:504:ILE:O	2.16	0.45
1:A:142:ASN:OD1	1:A:221:MET:HG2	2.16	0.45
1:A:102:ARG:HD3	4:A:2023:HOH:O	2.16	0.44
1:A:458:PRO:HG2	1:A:461:CYS:HB2	1.98	0.44
1:B:111:TYR:HE2	1:B:224:LYS:HE3	1.82	0.44
1:A:204:HIS:C	1:A:206:LYS:H	2.26	0.44
1:B:442:ASN:HB2	1:B:443:PRO:HD3	1.98	0.44
1:A:276:MET:HE2	1:A:281:PHE:CD1	2.53	0.44
1:B:76:LEU:HD12	1:B:84:MET:HE1	1.99	0.44
1:A:333:PRO:HB2	1:A:335:PRO:HD2	2.00	0.44
1:A:221:MET:HA	1:A:221:MET:HE2	2.00	0.43
1:A:287:VAL:HG13	1:A:288:MET:HE2	2.00	0.43
1:A:371:SER:O	1:A:372:LEU:HB2	2.19	0.43
1:A:180:ARG:HD3	1:A:180:ARG:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:HG22	1:A:155:THR:O	2.19	0.42
1:A:504:ILE:O	1:A:504:ILE:CG2	2.67	0.42
1:A:441:SER:O	1:A:445:VAL:HG23	2.19	0.42
1:A:72:HIS:CE1	1:A:230:GLU:HB2	2.53	0.42
1:A:464:GLU:HG2	1:B:497:THR:O	2.19	0.42
1:B:146:SER:HA	1:B:218:VAL:O	2.20	0.42
1:A:207:LYS:CE	1:A:207:LYS:HG2	2.48	0.42
1:A:284:GLU:O	1:A:287:VAL:HG12	2.19	0.42
1:B:334:LEU:HD21	1:B:462:PRO:CG	2.50	0.42
1:A:88:GLU:HB2	1:A:95:LYS:HB3	2.02	0.41
1:A:239:GLU:CD	1:A:239:GLU:H	2.27	0.41
1:A:323:PHE:O	1:A:329:GLY:HA3	2.20	0.41
1:A:476:ARG:HA	1:A:477:PRO:HD3	1.92	0.41
1:B:258:ALA:HB3	1:B:266:VAL:HG23	2.02	0.41
1:A:315:MET:HE1	1:A:375:LYS:HD2	2.01	0.41
1:A:316:ALA:HB3	1:A:370:ALA:HB2	2.03	0.41
1:B:183:ASP:C	1:B:185:GLY:N	2.77	0.41
1:B:323:PHE:O	1:B:329:GLY:HA3	2.21	0.41
1:A:218:VAL:HG23	1:A:219:PRO:HD2	2.03	0.41
1:B:292:GLN:HE21	1:B:292:GLN:HB2	1.63	0.41
1:B:209:ASN:HB3	1:B:214:GLN:C	2.47	0.40
1:A:183:ASP:C	1:A:185:GLY:N	2.77	0.40
1:A:377:ALA:O	1:A:378:ASP:HB2	2.20	0.40
1:B:293:HIS:HB3	1:B:296:LEU:HG	2.03	0.40
1:B:349:ALA:O	1:B:353:GLN:HB2	2.22	0.40
1:A:183:ASP:O	1:A:185:GLY:N	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2024:HOH:O	4:A:2079:HOH:O[2_555]	2.00	0.20

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	430/454 (95%)	404 (94%)	21 (5%)	5 (1%)	10	12
1	B	431/454 (95%)	406 (94%)	23 (5%)	2 (0%)	24	31
All	All	861/908 (95%)	810 (94%)	44 (5%)	7 (1%)	16	20

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	ASP
1	B	275	SER
1	B	436	PRO
1	A	205	TYR
1	A	359	ARG
1	A	182	LEU
1	A	184	ASN

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	378/393 (96%)	354 (94%)	24 (6%)	16	23
1	B	379/393 (96%)	357 (94%)	22 (6%)	18	26
All	All	757/786 (96%)	711 (94%)	46 (6%)	17	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	A	163	VAL
1	A	169	ARG
1	A	181	THR
1	A	193	SER
1	A	199	GLN

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Mol	Chain	Res	Type
1	A	202	VAL
1	A	212	LEU
1	A	221	MET
1	A	243	LEU
1	A	262	LYS
1	A	276	MET
1	A	287	VAL
1	A	289	LYS
1	A	298	LYS
1	A	353	GLN
1	A	357	ILE
1	A	359	ARG
1	A	361	LEU
1	A	400	ILE
1	A	406	GLU
1	A	450	GLU
1	A	479	GLU
1	A	503	GLU
1	B	90	SER
1	B	116	ASP
1	B	149	ILE
1	B	194	THR
1	B	202	VAL
1	B	203	ASP
1	B	209	ASN
1	B	215	LYS
1	B	218	VAL
1	B	222	SER
1	B	227	LYS
1	B	243	LEU
1	B	276	MET
1	B	278	VAL
1	B	298	LYS
1	B	306	GLU
1	B	310	ILE
1	B	336	LYS
1	B	357	ILE
1	B	361	LEU
1	B	371	SER
1	B	406	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	204	HIS
1	A	251	GLN
1	A	467	ASN
1	B	72	HIS
1	B	184	ASN
1	B	209	ASN
1	B	286	ASN
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	1.90	1 (6%)	17,22,24	0.86	1 (5%)
1	PTR	B	501	3,1	15,16,17	1.88	1 (6%)	17,22,24	0.47	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	-	1/10/11/13	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	-6.99	1.24	1.40
1	B	501	PTR	OH-CZ	-6.80	1.25	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	PTR	O2P-P-OH	2.35	112.25	105.32

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 4 ligands modelled in this entry, 2 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	L1G	B	1506	-	50,50,50	1.06	3 (6%)	73,73,73	1.80	18 (24%)
2	L1G	A	1506	-	50,50,50	1.07	3 (6%)	73,73,73	1.91	21 (28%)

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	L1G	B	1506	-	-	2/22/42/42	0/7/7/7
2	L1G	A	1506	-	-	3/22/42/42	0/7/7/7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1506	L1G	C4-N2	-3.36	1.32	1.36
2	A	1506	L1G	C10-N2	2.62	1.51	1.46
2	B	1506	L1G	C1-N1	2.61	1.36	1.33
2	A	1506	L1G	C1-N1	2.36	1.35	1.33
2	B	1506	L1G	C26-C24	-2.15	1.38	1.41
2	A	1506	L1G	C4-N2	-2.14	1.34	1.36

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1506	L1G	C26-C24-N8	-6.70	104.79	108.23
2	B	1506	L1G	C26-C24-N8	-5.45	105.43	108.23
2	B	1506	L1G	N4-C11-N3	-5.23	120.66	128.58
2	A	1506	L1G	N4-C11-N3	-5.09	120.87	128.58
2	A	1506	L1G	C2-C4-N3	-4.52	122.17	126.97
2	A	1506	L1G	C24-C26-C21	4.33	111.35	107.05
2	B	1506	L1G	C2-C4-N3	-4.24	122.47	126.97
2	B	1506	L1G	C24-C26-C21	4.18	111.20	107.05
2	B	1506	L1G	C4-C2-C1	3.53	107.20	104.74
2	A	1506	L1G	C5-C2-C1	-3.46	135.56	139.07
2	B	1506	L1G	O1-C8-C12	3.34	118.97	114.81
2	B	1506	L1G	N3-C4-N2	3.30	130.35	126.05
2	A	1506	L1G	C11-N4-C5	3.17	123.94	118.73
2	B	1506	L1G	C18-C20-N8	3.14	126.82	122.81
2	A	1506	L1G	C5-C2-C4	3.14	118.09	115.74
2	A	1506	L1G	C26-C21-C20	-3.07	102.72	107.31
2	B	1506	L1G	C26-C21-C20	-3.06	102.73	107.31
2	A	1506	L1G	N3-C4-N2	3.01	129.97	126.05
2	B	1506	L1G	C11-N3-C4	2.89	118.90	111.83
2	B	1506	L1G	C5-C2-C1	-2.69	136.35	139.07
2	A	1506	L1G	C11-N3-C4	2.60	118.17	111.83
2	A	1506	L1G	C20-C18-N6	2.54	118.59	114.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1506	L1G	C21-C20-C18	-2.53	123.17	129.48
2	B	1506	L1G	C2-C1-N1	-2.50	108.48	110.19
2	A	1506	L1G	C24-N8-C20	2.44	110.83	108.10
2	A	1506	L1G	C18-C20-N8	2.35	125.81	122.81
2	A	1506	L1G	C4-C2-C1	2.31	106.34	104.74
2	A	1506	L1G	C29-C24-N8	2.29	134.60	129.88
2	B	1506	L1G	C24-N8-C20	2.27	110.64	108.10
2	A	1506	L1G	C21-C20-C18	-2.26	123.83	129.48
2	B	1506	L1G	C11-N4-C5	2.24	122.41	118.73
2	B	1506	L1G	C14-C10-N2	-2.24	109.76	111.88
2	A	1506	L1G	C14-C10-N2	-2.22	109.78	111.88
2	B	1506	L1G	C29-C24-N8	2.21	134.44	129.88
2	B	1506	L1G	C1-N1-N2	-2.21	105.80	106.97
2	A	1506	L1G	C3-C1-N1	2.18	121.74	118.91
2	A	1506	L1G	C2-C5-N4	-2.10	116.75	118.64
2	A	1506	L1G	C9-C7-C3	-2.10	118.56	120.80
2	A	1506	L1G	C6-C3-C1	-2.10	117.02	120.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1506	L1G	C13-C10-N2-C4
2	B	1506	L1G	C13-C10-N2-C4
2	A	1506	L1G	N1-C1-C3-C6
2	A	1506	L1G	C14-C10-N2-C4
2	B	1506	L1G	C14-C10-N2-C4

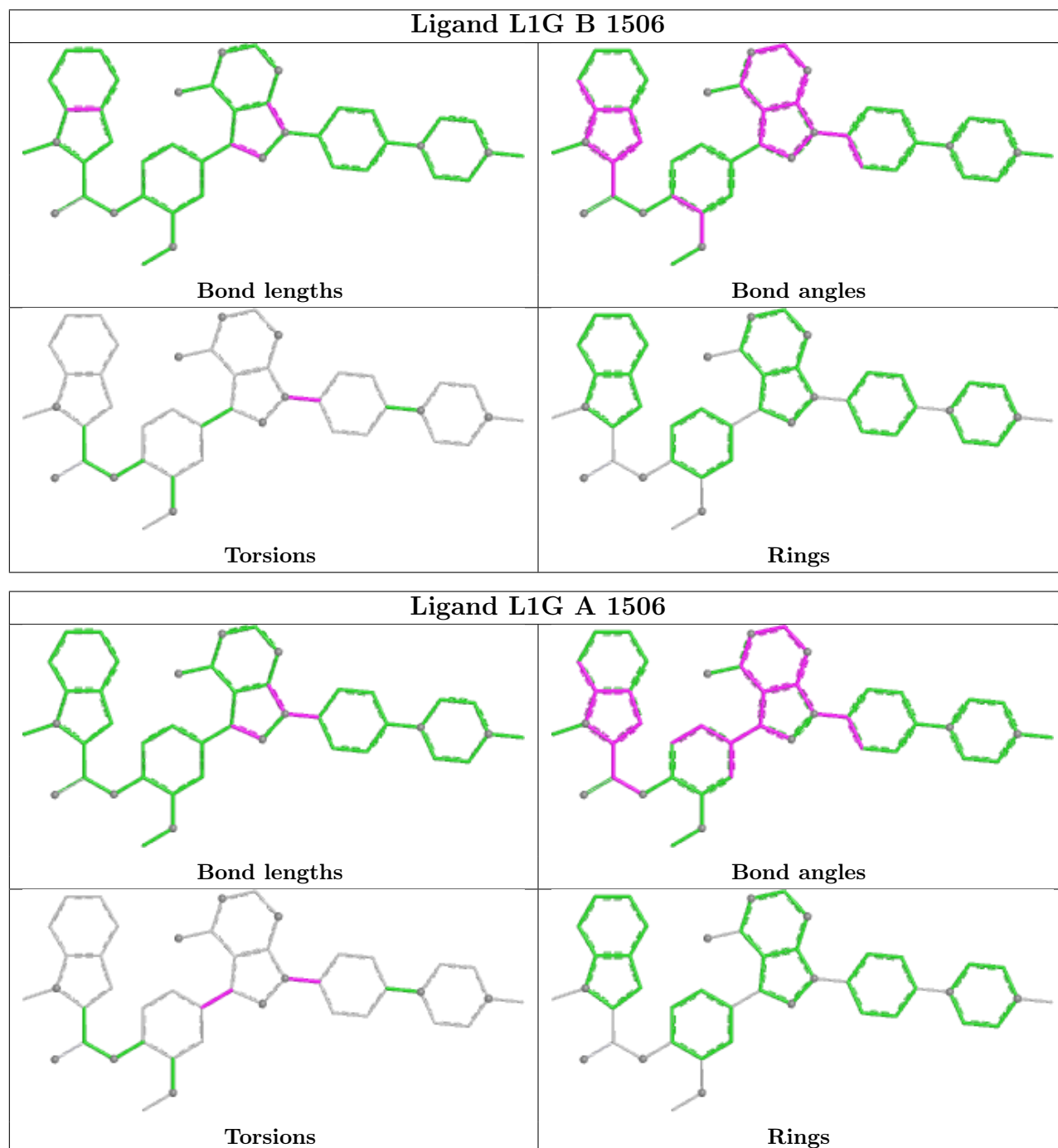
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1506	L1G	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 ⓘ

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, 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	433/454 (95%)	0.85	53 (12%) 8 9	21, 50, 63, 74	1 (0%)
1	B	433/454 (95%)	0.66	19 (4%) 39 41	22, 50, 63, 73	2 (0%)
All	All	866/908 (95%)	0.76	72 (8%) 17 19	21, 50, 63, 74	3 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	SER	4.6
1	B	181	THR	4.1
1	A	274	GLY	3.9
1	A	166	TYR	3.8
1	A	135	ARG	3.8
1	A	138	LEU	3.8
1	A	184	ASN	3.7
1	A	187	PHE	3.5
1	B	182	LEU	3.3
1	A	194	THR	3.3
1	B	411	GLY	3.2
1	A	125	PHE	3.1
1	A	208	GLY	3.1
1	B	170	GLN	3.1
1	A	142	ASN	3.0
1	A	186	GLY	3.0
1	B	439	GLY	3.0
1	A	505	PRO	2.9
1	A	133	ALA	2.9
1	A	170	GLN	2.9
1	A	154	THR	2.9
1	A	275	SER	2.8
1	A	185	GLY	2.8
1	A	137	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	174	VAL	2.8
1	A	181	THR	2.8
1	A	128	ILE	2.7
1	A	205	TYR	2.7
1	A	180	ARG	2.7
1	B	185	GLY	2.6
1	A	195	PHE	2.6
1	A	202	VAL	2.6
1	A	171	GLY	2.6
1	B	276	MET	2.6
1	B	399	PRO	2.6
1	A	272	LYS	2.6
1	B	407	ALA	2.6
1	A	134	GLU	2.5
1	A	182	LEU	2.5
1	A	167	ASP	2.5
1	A	139	ALA	2.5
1	A	172	ASP	2.5
1	B	167	ASP	2.5
1	A	263[A]	HIS	2.5
1	B	279	GLU	2.5
1	A	189	ILE	2.4
1	A	188	TYR	2.4
1	B	280	ALA	2.4
1	A	157	GLY	2.4
1	A	132	ASP	2.4
1	B	445	VAL	2.4
1	A	183	ASP	2.3
1	B	271	MET	2.3
1	B	400	ILE	2.3
1	A	207	LYS	2.3
1	A	384	VAL	2.3
1	A	169	ARG	2.3
1	A	163	VAL	2.2
1	A	136	GLN	2.2
1	A	467	ASN	2.2
1	A	173	THR	2.2
1	A	252	PHE	2.1
1	B	281	PHE	2.1
1	A	193	SER	2.1
1	B	441	SER	2.1
1	A	216	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	179	ILE	2.1
1	A	400	ILE	2.0
1	A	218	VAL	2.0
1	B	211	GLY	2.0
1	A	144	LEU	2.0
1	A	486	ILE	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	0.95	0.09	45,48,49,49	0
1	PTR	B	501	16/17	0.95	0.09	45,47,49,49	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

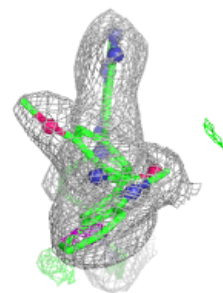
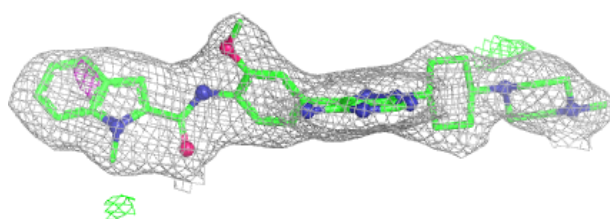
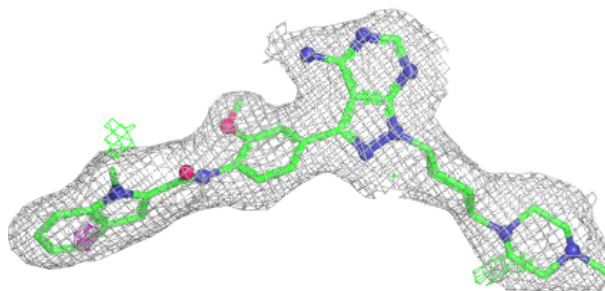
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	L1G	B	1506	44/44	0.93	0.09	39,41,44,46	0
2	L1G	A	1506	44/44	0.94	0.07	38,41,45,47	0
3	CA	A	1507	1/1	0.96	0.04	44,44,44,44	0
3	CA	B	1507	1/1	0.97	0.06	44,44,44,44	0

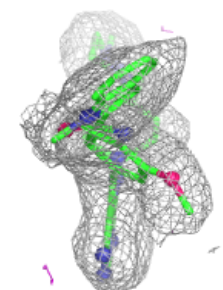
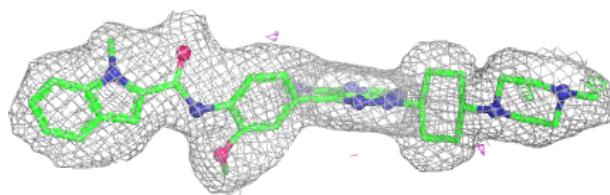
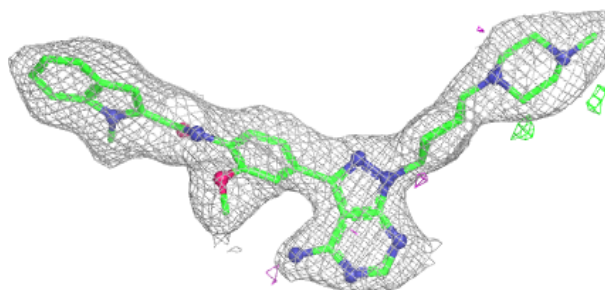
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around L1G 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 L1G 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.