



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:12 AM UTC

PDB ID : 7QG2 / pdb_00007qg2
Title : IRAK4 in complex with inhibitor
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Deposited on : 2021-12-07
Resolution : 3.03 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

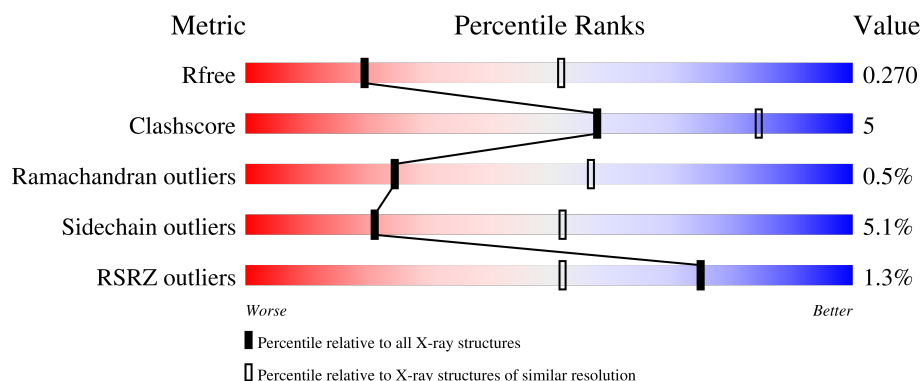
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	308	
1	B	308	
1	C	308	
1	D	308	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9096 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.

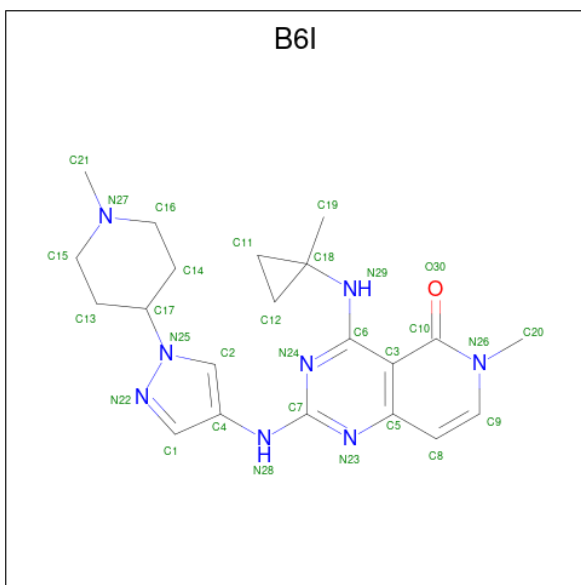
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	P	S	0	0	0
			2220	1394	375	435	2	14			
1	B	275	Total	C	N	O	P	S	0	1	0
			2182	1375	366	424	2	15			
1	C	284	Total	C	N	O	P	S	0	0	0
			2245	1410	378	441	2	14			
1	D	280	Total	C	N	O	P	S	0	0	0
			2214	1391	374	433	2	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 6-methyl-4-[(1-methylcyclopropyl)amino]-2-[[1-(1-methylpiperidin-4-yl)pyrazol-4-yl]amino]pyrido[4,3-d]pyrimidin-5-one (CCD ID: B6I) (formula: C₂₁H₂₈N₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	21	8	1		
2	B	1	Total	C	N	O	0	0
			30	21	8	1		
2	C	1	Total	C	N	O	0	0
			30	21	8	1		
2	D	1	Total	C	N	O	0	0
			30	21	8	1		

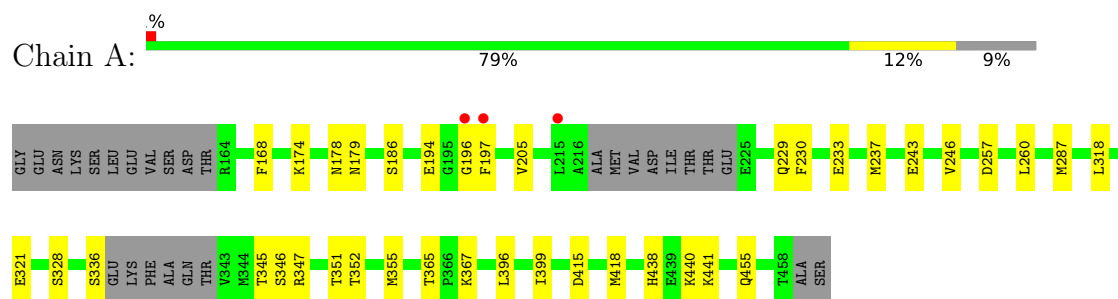
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	23	Total	O	0	0
			23	23		
3	C	28	Total	O	0	0
			28	28		
3	D	43	Total	O	0	0
			43	43		

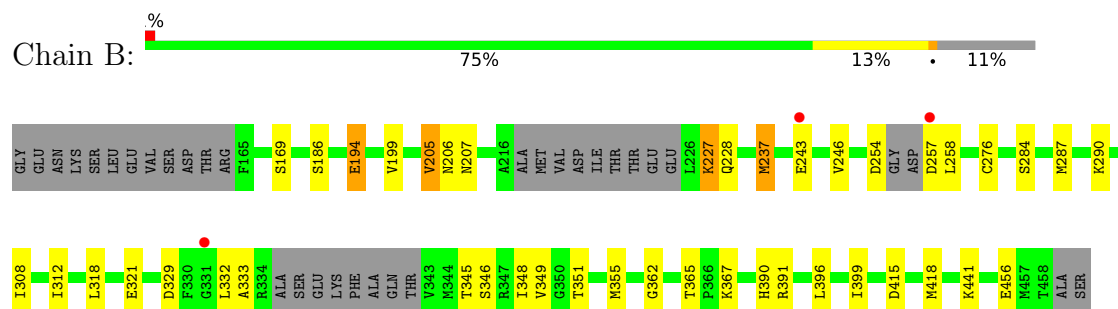
3 Residue-property plots [i](#)

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.

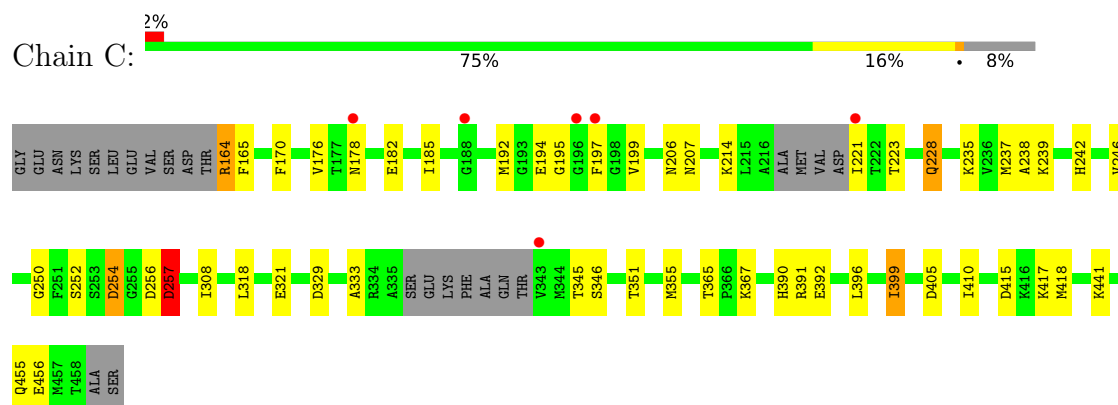
- Molecule 1: Interleukin-1 receptor-associated kinase 4



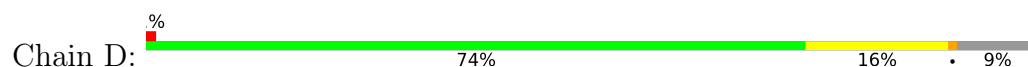
- Molecule 1: Interleukin-1 receptor-associated kinase 4

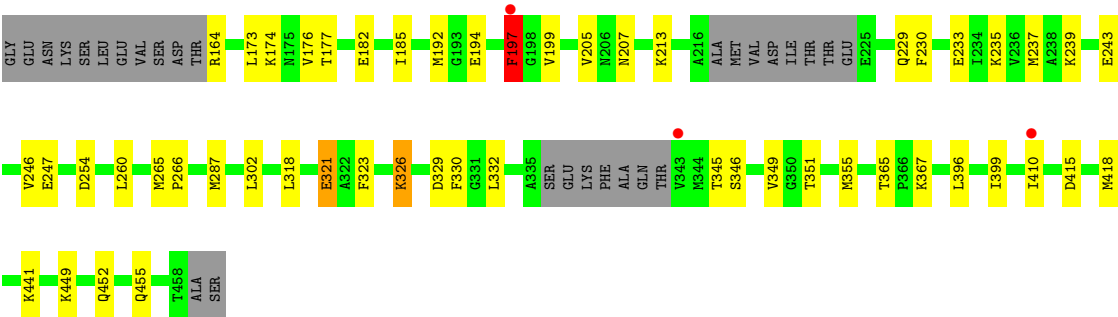


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.39Å 139.72Å 87.27Å 90.00° 123.62° 90.00°	Depositor
Resolution (Å)	72.67 – 3.03 72.67 – 3.03	Depositor EDS
% Data completeness (in resolution range)	97.0 (72.67-3.03) 97.0 (72.67-3.03)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.224 , 0.274 0.222 , 0.270	Depositor DCC
R_{free} test set	1312 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9096	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2701e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TPO, SEP, B6I

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	0.71	0/2235	1.07	2/3009 (0.1%)
1	B	0.72	1/2199 (0.0%)	1.07	7/2959 (0.2%)
1	C	0.72	0/2260	1.10	7/3044 (0.2%)
1	D	0.73	0/2229	1.10	4/3001 (0.1%)
All	All	0.72	1/8923 (0.0%)	1.09	20/12013 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	312	ILE	CG1-CD1	-6.66	1.25	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	197	PHE	CA-CB-CG	10.28	124.08	113.80
1	B	207	ASN	CA-C-N	7.52	132.26	121.50
1	B	207	ASN	C-N-CA	7.52	132.26	121.50
1	C	178	ASN	CA-C-N	6.33	131.35	122.36
1	C	178	ASN	C-N-CA	6.33	131.35	122.36
1	D	230	PHE	CA-CB-CG	6.05	119.85	113.80
1	D	174	LYS	N-CA-C	-5.62	105.07	111.14
1	C	405	ASP	CA-C-N	5.41	130.03	122.08
1	C	405	ASP	C-N-CA	5.41	130.03	122.08
1	B	227	LYS	CA-C-N	5.40	127.83	120.54
1	B	227	LYS	C-N-CA	5.40	127.83	120.54
1	D	254	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	456	GLU	CA-C-N	5.18	127.74	120.28
1	B	456	GLU	C-N-CA	5.18	127.74	120.28
1	A	230	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	254	ASP	CA-CB-CG	5.12	117.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ASN	CA-CB-CG	5.10	117.70	112.60
1	C	321	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	456	GLU	CA-C-N	5.05	127.55	120.28
1	C	456	GLU	C-N-CA	5.05	127.55	120.28

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	2220	0	2188	14	0
1	B	2182	0	2160	19	0
1	C	2245	0	2214	27	0
1	D	2214	0	2183	25	0
2	A	30	0	0	1	0
2	B	30	0	0	1	0
2	C	30	0	0	1	0
2	D	30	0	0	1	0
3	A	21	0	0	0	0
3	B	23	0	0	0	0
3	C	28	0	0	0	0
3	D	43	0	0	0	0
All	All	9096	0	8745	80	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 (80) 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:237:MET:HE1	1:A:246:VAL:HG23	1.46	0.97
1:D:185:ILE:HD11	1:D:192:MET:HG2	1.50	0.94
1:C:256:ASP:O	1:C:257:ASP:HB2	1.88	0.73
1:A:237:MET:CE	1:A:246:VAL:HG23	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:MET:HE2	1:D:323:PHE:HB2	1.76	0.68
1:D:266:PRO:HG2	1:D:321:GLU:HG3	1.76	0.66
1:C:235:LYS:HE3	1:C:239:LYS:NZ	2.13	0.63
1:C:396:LEU:HD12	1:C:399:ILE:HD13	1.80	0.62
1:D:246:VAL:HG11	1:D:318:LEU:HD12	1.81	0.62
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.83	0.61
1:D:449:LYS:NZ	1:D:452:GLN:HE22	1.99	0.61
1:C:246:VAL:HG11	1:C:318:LEU:HD12	1.84	0.59
1:C:194:GLU:HG3	1:C:199:VAL:HG22	1.84	0.59
1:D:237:MET:HE1	1:D:246:VAL:HG23	1.84	0.58
1:A:321:GLU:HG3	1:C:242:HIS:CD2	2.39	0.57
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.87	0.57
1:C:237:MET:HE1	1:C:246:VAL:HG23	1.86	0.57
1:B:194:GLU:HG3	1:B:199:VAL:HG22	1.87	0.56
1:C:164:ARG:HE	1:C:238:ALA:HA	1.70	0.56
1:C:194:GLU:HG2	1:C:195:GLY:H	1.73	0.54
1:D:321:GLU:H	1:D:321:GLU:CD	2.15	0.54
1:D:235:LYS:HE2	1:D:239:LYS:NZ	2.23	0.53
1:C:367:LYS:HD2	1:C:441:LYS:HD2	1.90	0.53
2:A:501:B6I:C1	2:A:501:B6I:N24	2.72	0.53
1:A:367:LYS:HD2	1:A:441:LYS:HD2	1.92	0.52
1:B:367:LYS:HD2	1:B:441:LYS:HD2	1.92	0.51
1:D:367:LYS:HD2	1:D:441:LYS:HD2	1.93	0.51
1:B:391:ARG:HA	1:C:390:HIS:O	2.11	0.51
1:D:302:LEU:HD11	1:D:330:PHE:HE1	1.76	0.51
1:A:174:LYS:HE2	1:A:179:ASN:HD22	1.75	0.50
1:D:287:MET:HE2	1:D:323:PHE:CB	2.40	0.50
1:D:173:LEU:HA	1:D:176:VAL:HG12	1.94	0.50
2:C:501:B6I:N24	2:C:501:B6I:C1	2.72	0.50
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.97	0.47
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.97	0.47
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.97	0.47
1:B:351:THR:O	1:B:355:MET:HG3	2.15	0.47
1:D:396:LEU:O	1:D:399:ILE:HG12	2.15	0.47
1:A:351:THR:O	1:A:355:MET:HG3	2.14	0.47
1:C:235:LYS:HE3	1:C:239:LYS:HZ1	1.79	0.47
1:B:237:MET:HE1	1:B:246:VAL:O	2.15	0.47
1:D:415:ASP:HB3	1:D:418:MET:HE2	1.98	0.46
1:B:284:SER:H	1:B:287[B]:MET:HE3	1.81	0.46
1:B:290:LYS:HZ1	1:D:247:GLU:CD	2.25	0.45
1:B:396:LEU:O	1:B:399:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:B6I:C1	2:B:501:B6I:N24	2.78	0.45
1:D:197:PHE:HE2	1:D:213:LYS:NZ	2.14	0.45
1:C:256:ASP:O	1:C:257:ASP:CB	2.62	0.45
1:D:265:MET:HE1	1:D:326:LYS:HE3	1.99	0.45
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.99	0.45
1:D:449:LYS:HZ2	1:D:452:GLN:HE22	1.64	0.45
1:D:351:THR:O	1:D:355:MET:HG3	2.17	0.44
1:B:308:ILE:O	1:B:333:ALA:HA	2.18	0.44
1:A:233:GLU:HG2	1:A:260:LEU:HD13	1.99	0.44
1:C:185:ILE:HD11	1:C:192:MET:HG2	1.99	0.44
1:A:438:HIS:HE1	1:A:440:LYS:HD2	1.83	0.43
1:D:233:GLU:HG2	1:D:260:LEU:HD13	1.99	0.43
1:D:235:LYS:HE2	1:D:239:LYS:HZ2	1.82	0.43
1:C:206:ASN:HB3	1:C:207:ASN:H	1.73	0.43
1:C:308:ILE:O	1:C:333:ALA:HA	2.18	0.43
1:D:452:GLN:O	1:D:455:GLN:HG3	2.19	0.43
1:A:396:LEU:O	1:A:399:ILE:HG12	2.19	0.42
1:D:176:VAL:HG13	1:D:177:THR:HG23	2.01	0.42
2:D:501:B6I:O30	2:D:501:B6I:N29	2.51	0.42
1:B:205:VAL:O	1:B:206:ASN:HB2	2.18	0.42
1:A:321:GLU:CG	1:C:242:HIS:CD2	3.03	0.42
1:A:321:GLU:HG3	1:C:242:HIS:HD2	1.85	0.42
1:B:332:LEU:HD22	1:B:349:VAL:HG21	2.02	0.42
1:B:276:CYS:HB2	1:C:417:LYS:HD2	2.01	0.42
1:A:168:PHE:HE1	1:A:205:VAL:HG11	1.85	0.41
1:B:390:HIS:HB3	1:C:392:GLU:H	1.85	0.41
1:C:235:LYS:HE3	1:C:239:LYS:HZ2	1.83	0.41
1:D:332:LEU:HD22	1:D:349:VAL:HG21	2.03	0.41
1:B:348:ILE:HG12	1:B:362:GLY:HA2	2.02	0.41
1:C:228:GLN:HE21	1:C:228:GLN:HA	1.85	0.41
1:B:227:LYS:HG2	1:B:258:LEU:HD11	2.03	0.41
1:C:351:THR:O	1:C:355:MET:HG3	2.21	0.41
1:B:390:HIS:O	1:C:391:ARG:HA	2.21	0.40
1:B:321:GLU:O	1:D:243:GLU:HB3	2.21	0.40
1:C:170:PHE:HB2	1:C:254:ASP:OD1	2.21	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	273/308 (89%)	264 (97%)	8 (3%)	1 (0%)	30	61
1	B	266/308 (86%)	256 (96%)	9 (3%)	1 (0%)	30	61
1	C	276/308 (90%)	263 (95%)	11 (4%)	2 (1%)	18	49
1	D	272/308 (88%)	265 (97%)	6 (2%)	1 (0%)	30	61
All	All	1087/1232 (88%)	1048 (96%)	34 (3%)	5 (0%)	24	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	257	ASP
1	A	196	GLY
1	C	329	ASP
1	D	329	ASP
1	B	329	ASP

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	243/266 (91%)	230 (95%)	13 (5%)	20	51
1	B	240/266 (90%)	231 (96%)	9 (4%)	29	60
1	C	246/266 (92%)	231 (94%)	15 (6%)	17	46
1	D	242/266 (91%)	230 (95%)	12 (5%)	22	53
All	All	971/1064 (91%)	922 (95%)	49 (5%)	21	53

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	SER
1	A	194	GLU
1	A	197	PHE
1	A	229	GLN
1	A	243	GLU
1	A	257	ASP
1	A	287	MET
1	A	328	SER
1	A	336	SER
1	A	347	ARG
1	A	352	THR
1	A	365	THR
1	A	455	GLN
1	B	169	SER
1	B	186	SER
1	B	194	GLU
1	B	205	VAL
1	B	228	GLN
1	B	237	MET
1	B	243	GLU
1	B	257	ASP
1	B	365	THR
1	C	164	ARG
1	C	176	VAL
1	C	182	GLU
1	C	197	PHE
1	C	214	LYS
1	C	221	ILE
1	C	223	THR
1	C	228	GLN
1	C	252	SER
1	C	254	ASP
1	C	257	ASP
1	C	365	THR
1	C	399	ILE
1	C	410	ILE
1	C	455	GLN
1	D	164	ARG
1	D	182	GLU
1	D	194	GLU
1	D	197	PHE
1	D	199	VAL

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Mol	Chain	Res	Type
1	D	205	VAL
1	D	207	ASN
1	D	229	GLN
1	D	321	GLU
1	D	326	LYS
1	D	365	THR
1	D	410	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	179	ASN
1	A	293	GLN
1	A	297	ASN
1	A	390	HIS
1	A	394	GLN
1	A	435	GLN
1	A	451	GLN
1	B	293	GLN
1	B	297	ASN
1	B	390	HIS
1	B	451	GLN
1	C	166	HIS
1	C	228	GLN
1	C	232	GLN
1	C	286	HIS
1	C	297	ASN
1	C	307	HIS
1	C	390	HIS
1	C	394	GLN
1	C	435	GLN
1	C	451	GLN
1	D	179	ASN
1	D	286	HIS
1	D	297	ASN
1	D	390	HIS
1	D	435	GLN
1	D	451	GLN
1	D	452	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	SEP	A	346	1	8,9,10	0.74	0	7,12,14	1.30	1 (14%)
1	TPO	A	345	1	8,10,11	1.10	0	10,14,16	1.15	1 (10%)
1	SEP	D	346	1	8,9,10	1.09	1 (12%)	7,12,14	0.92	0
1	TPO	D	345	1	8,10,11	0.90	0	10,14,16	1.04	1 (10%)
1	TPO	B	345	1	8,10,11	1.00	1 (12%)	10,14,16	0.87	0
1	TPO	C	345	1	8,10,11	0.89	0	10,14,16	1.10	1 (10%)
1	SEP	B	346	1	8,9,10	0.96	0	7,12,14	1.41	2 (28%)
1	SEP	C	346	1	8,9,10	0.85	0	7,12,14	1.11	1 (14%)

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	SEP	A	346	1	-	3/6/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	2/9/11/13	-
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	B	346	1	-	2/6/8/10	-
1	SEP	C	346	1	-	3/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	346	SEP	P-OG	-2.15	1.53	1.60
1	B	345	TPO	P-OG1	-2.08	1.55	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-P-O1P	2.84	114.12	106.44
1	C	346	SEP	O3P-P-OG	2.41	112.97	106.67
1	A	346	SEP	O3P-P-OG	2.35	112.80	106.67
1	A	345	TPO	O3P-P-OG1	2.29	114.78	105.85
1	B	346	SEP	OG-CB-CA	2.10	110.19	108.14
1	C	345	TPO	O3P-P-OG1	2.08	113.96	105.85
1	D	345	TPO	O3P-P-OG1	2.06	113.88	105.85

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	346	SEP	CB-OG-P-O1P
1	A	346	SEP	CB-OG-P-O2P
1	B	345	TPO	N-CA-CB-OG1
1	B	346	SEP	CB-OG-P-O2P
1	B	346	SEP	CB-OG-P-O3P
1	C	345	TPO	N-CA-CB-OG1
1	C	346	SEP	CB-OG-P-O1P
1	C	346	SEP	CB-OG-P-O2P
1	D	345	TPO	N-CA-CB-OG1
1	A	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O1P
1	A	346	SEP	CB-OG-P-O3P
1	C	346	SEP	CB-OG-P-O3P
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	O-C-CA-CB
1	D	345	TPO	CB-OG1-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	B6I	C	501	-	31,34,34	0.93	1 (3%)	34,51,51	1.40	5 (14%)
2	B6I	D	501	-	31,34,34	0.89	2 (6%)	34,51,51	1.39	5 (14%)
2	B6I	B	501	-	31,34,34	0.95	3 (9%)	34,51,51	2.07	10 (29%)
2	B6I	A	501	-	31,34,34	0.96	1 (3%)	34,51,51	2.23	11 (32%)

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	B6I	C	501	-	-	1/12/27/27	0/5/5/5
2	B6I	D	501	-	-	1/12/27/27	0/5/5/5
2	B6I	B	501	-	-	1/12/27/27	0/5/5/5
2	B6I	A	501	-	-	1/12/27/27	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	B6I	C19-C18	-2.60	1.48	1.53
2	C	501	B6I	C19-C18	-2.42	1.49	1.53
2	D	501	B6I	C3-C6	-2.22	1.37	1.42
2	B	501	B6I	C19-C18	-2.19	1.49	1.53
2	B	501	B6I	C3-C6	-2.13	1.37	1.42
2	A	501	B6I	C19-C18	-2.05	1.49	1.53
2	B	501	B6I	C17-N25	-2.03	1.44	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	B6I	C13-C17-N25	5.68	118.74	110.95
2	A	501	B6I	C14-C17-N25	5.55	118.56	110.95
2	A	501	B6I	C2-N25-N22	5.47	116.14	112.45
2	B	501	B6I	C2-N25-N22	4.22	115.30	112.45
2	A	501	B6I	C17-N25-N22	-4.02	114.92	120.41
2	C	501	B6I	C2-N25-N22	3.84	115.04	112.45
2	B	501	B6I	C14-C17-N25	3.79	116.15	110.95
2	A	501	B6I	C11-C18-N29	3.56	120.42	115.60
2	D	501	B6I	C21-N27-C16	-3.33	104.29	110.63
2	D	501	B6I	C21-N27-C15	-3.30	104.34	110.63
2	A	501	B6I	C13-C17-N25	3.17	115.30	110.95
2	B	501	B6I	C11-C18-N29	3.13	119.84	115.60
2	A	501	B6I	C21-N27-C15	-3.10	104.72	110.63
2	B	501	B6I	O30-C10-N26	3.00	123.74	119.70
2	C	501	B6I	C17-N25-N22	-2.94	116.39	120.41
2	A	501	B6I	C1-N22-N25	-2.84	102.68	104.14
2	B	501	B6I	C15-C13-C17	-2.77	105.71	110.78
2	B	501	B6I	C9-N26-C10	2.73	124.88	122.72
2	D	501	B6I	O30-C10-N26	2.72	123.37	119.70
2	B	501	B6I	C1-N22-N25	-2.65	102.78	104.14
2	A	501	B6I	C12-C18-N29	2.61	119.14	115.60
2	B	501	B6I	C21-N27-C15	-2.46	105.95	110.63
2	A	501	B6I	O30-C10-N26	2.45	123.00	119.70
2	D	501	B6I	C2-N25-N22	2.40	114.07	112.45
2	C	501	B6I	C14-C16-N27	-2.39	108.11	111.20
2	C	501	B6I	C21-N27-C15	-2.32	106.22	110.63
2	B	501	B6I	C17-N25-N22	-2.29	117.28	120.41
2	D	501	B6I	C11-C18-N29	2.29	118.70	115.60
2	C	501	B6I	C13-C17-N25	2.08	113.80	110.95
2	A	501	B6I	C16-N27-C15	2.03	112.77	109.54
2	A	501	B6I	C15-C13-C17	-2.02	107.08	110.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

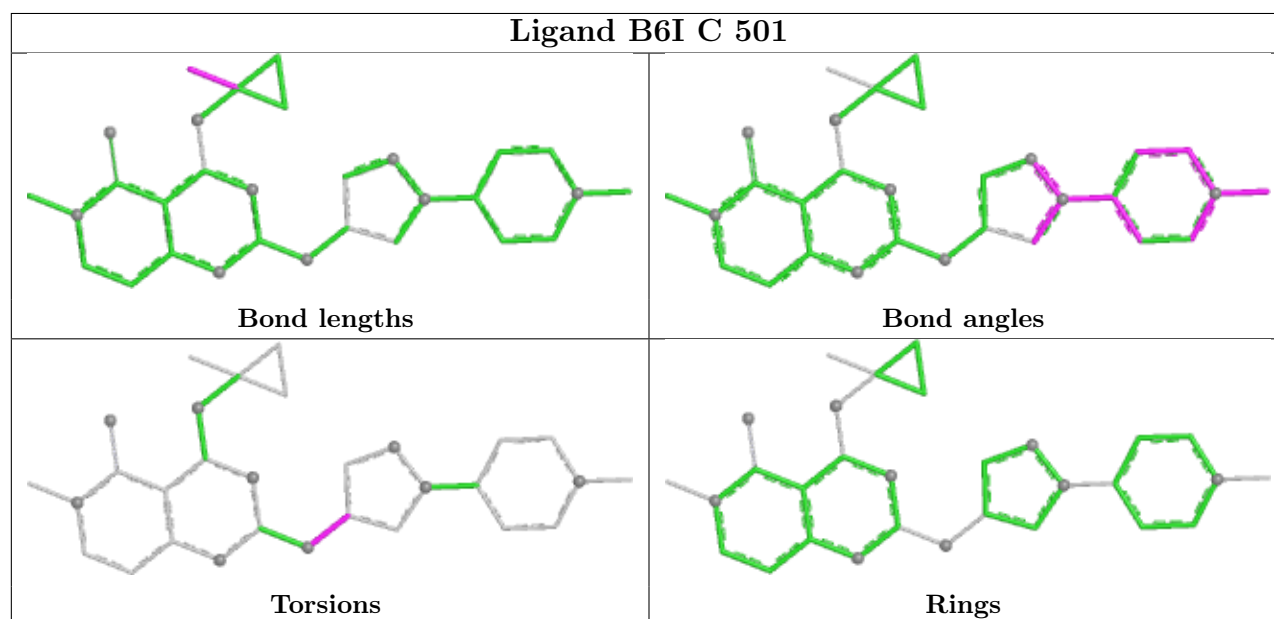
Mol	Chain	Res	Type	Atoms
2	A	501	B6I	C2-C4-N28-C7
2	B	501	B6I	C2-C4-N28-C7
2	C	501	B6I	C2-C4-N28-C7
2	D	501	B6I	C2-C4-N28-C7

There are no ring outliers.

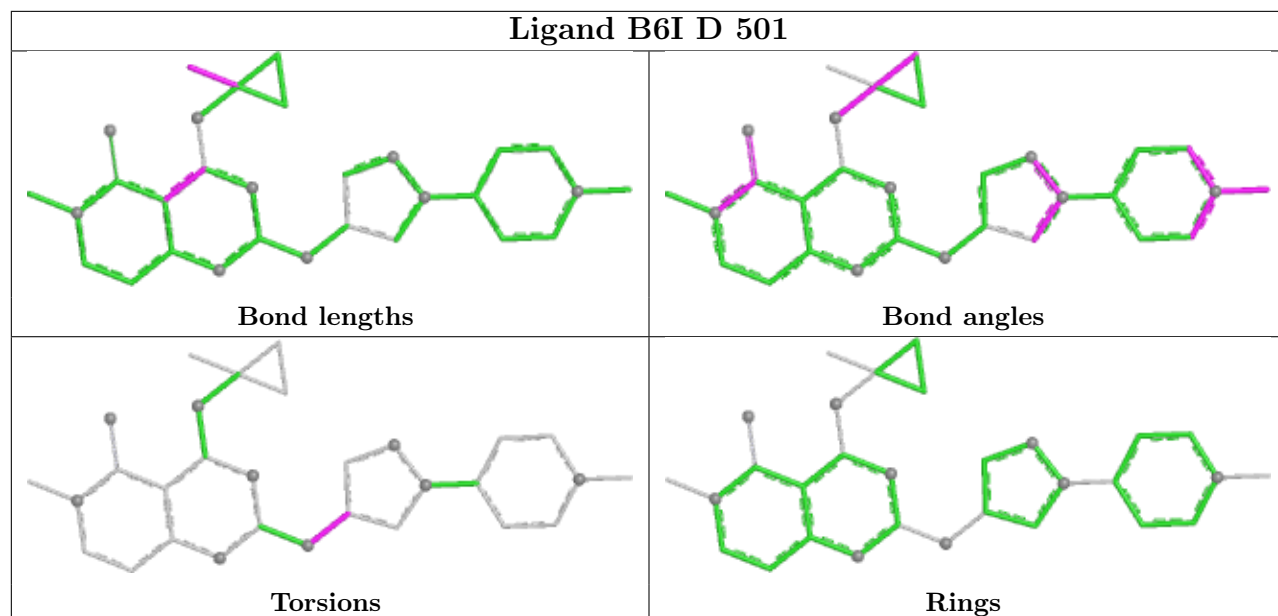
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	B6I	1	0
2	D	501	B6I	1	0
2	B	501	B6I	1	0
2	A	501	B6I	1	0

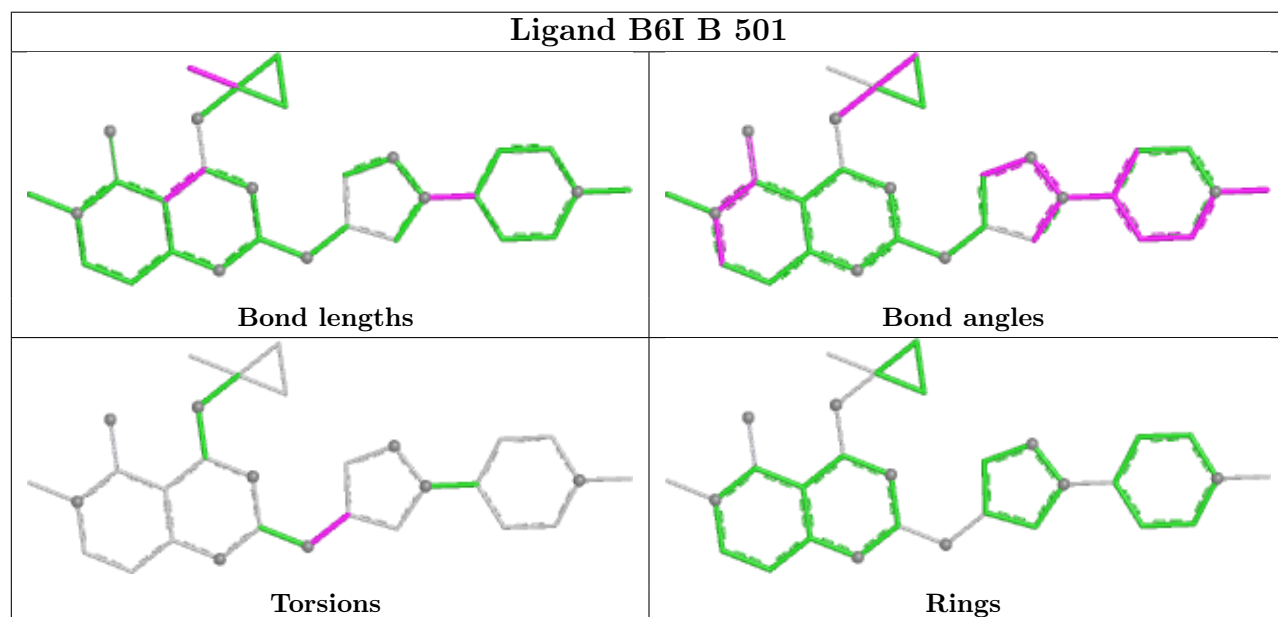
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

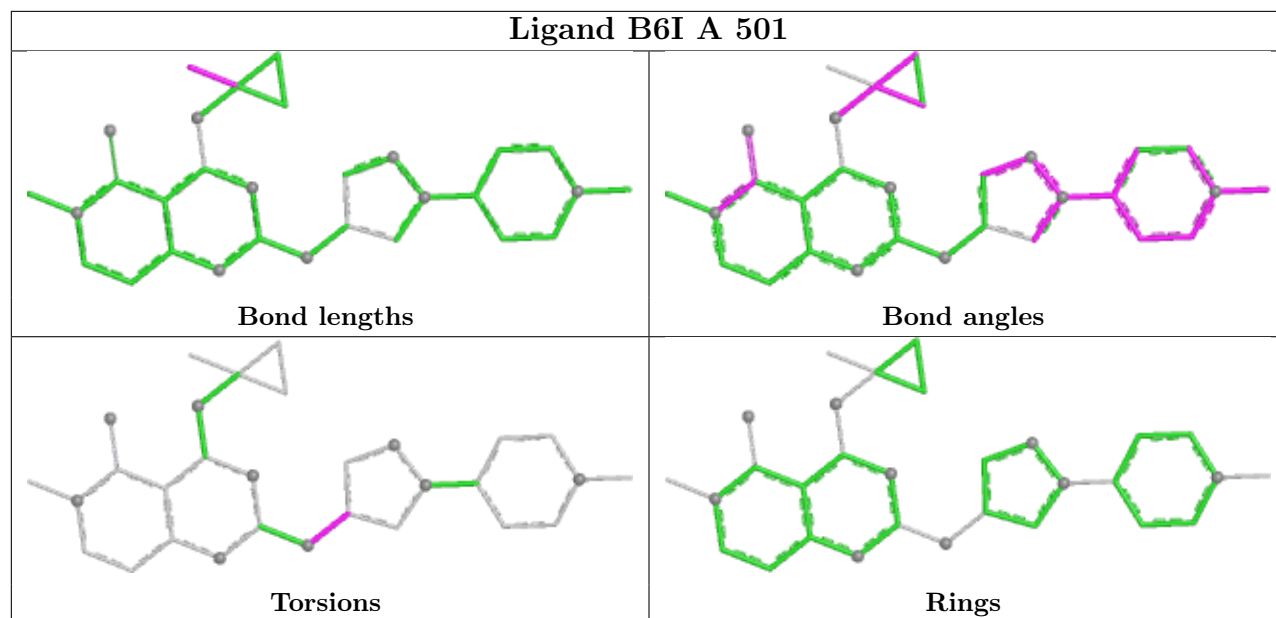


Ligand B6I D 501



Ligand B6I B 501





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(Å ²)	Q<0.9
1	A	279/308 (90%)	0.06	3 (1%) 78 56	40, 68, 95, 104	0
1	B	273/308 (88%)	0.07	3 (1%) 78 56	29, 65, 90, 100	1 (0%)
1	C	282/308 (91%)	0.02	6 (2%) 63 39	37, 60, 89, 101	1 (0%)
1	D	278/308 (90%)	-0.02	3 (1%) 78 56	38, 61, 85, 106	0
All	All	1112/1232 (90%)	0.03	15 (1%) 75 52	29, 63, 90, 106	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	PHE	2.6
1	B	331	GLY	2.6
1	C	343	VAL	2.5
1	A	197	PHE	2.5
1	C	221	ILE	2.4
1	C	178	ASN	2.4
1	A	196	GLY	2.3
1	B	243	GLU	2.3
1	D	410	ILE	2.3
1	C	196	GLY	2.2
1	C	188	GLY	2.1
1	C	197	PHE	2.1
1	B	257	ASP	2.1
1	D	343	VAL	2.0
1	A	215	LEU	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	SEP	C	346	10/11	0.67	0.13	86,92,135,138	0
1	SEP	B	346	10/11	0.72	0.11	95,99,120,131	0
1	SEP	D	346	10/11	0.74	0.10	84,88,115,121	0
1	SEP	A	346	10/11	0.75	0.10	84,87,121,131	0
1	TPO	A	345	11/12	0.83	0.11	77,83,88,88	0
1	TPO	D	345	11/12	0.86	0.10	80,85,101,102	0
1	TPO	B	345	11/12	0.87	0.09	96,96,104,104	0
1	TPO	C	345	11/12	0.89	0.10	81,88,94,95	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

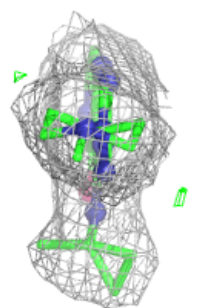
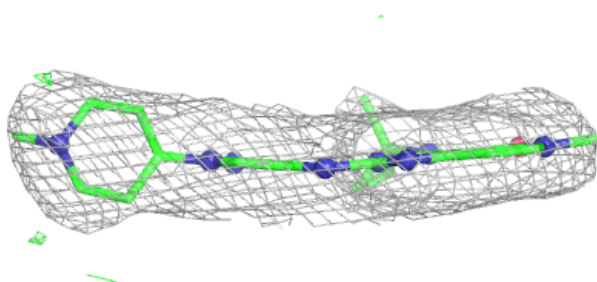
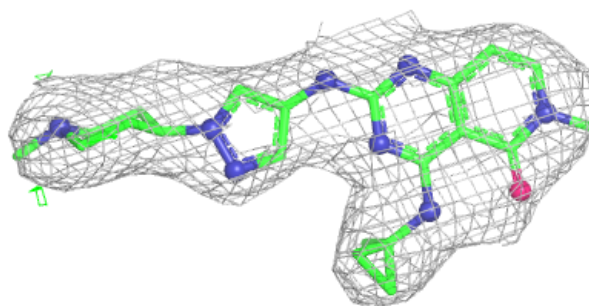
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B6I	B	501	30/30	0.95	0.09	53,53,54,54	0
2	B6I	C	501	30/30	0.95	0.09	48,51,52,53	0
2	B6I	A	501	30/30	0.96	0.07	50,52,53,53	0
2	B6I	D	501	30/30	0.96	0.07	35,38,42,43	0

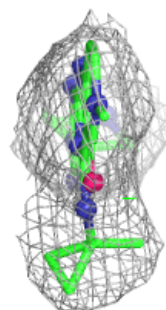
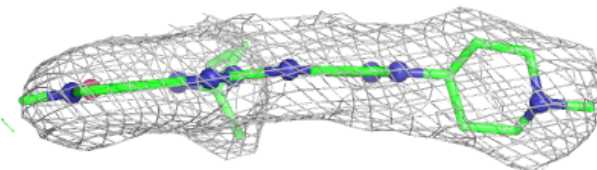
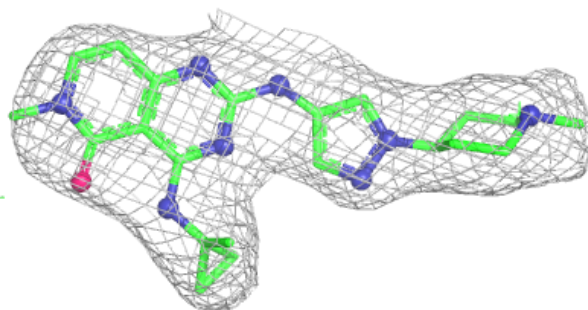
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B6I B 501:

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

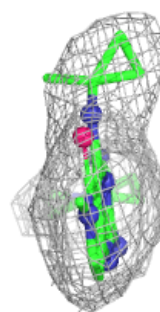
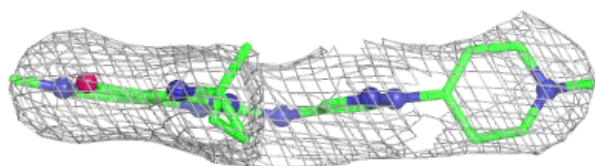
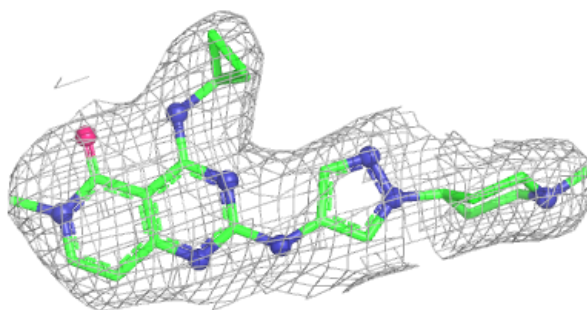
**Electron density around B6I C 501:**

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

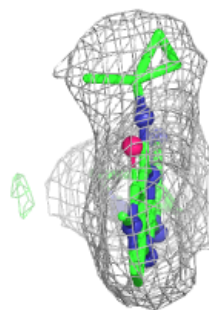
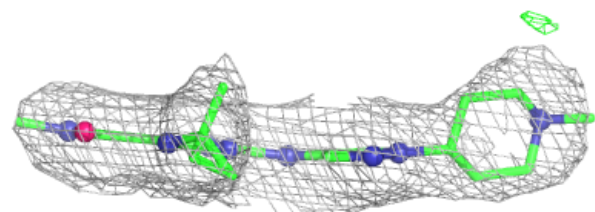
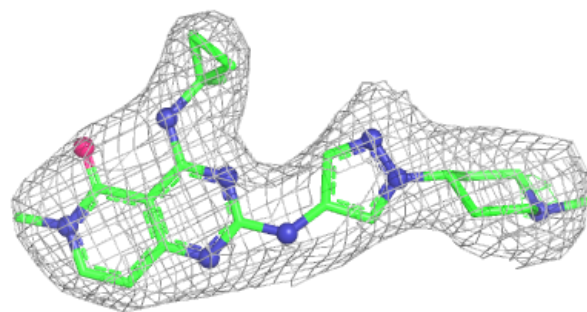


Electron density around B6I A 501:

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

**Electron density around B6I D 501:**

$2mF_o-DF_c$ (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.