



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 04:41 AM EDT

PDB ID : 6EIP
Title : DYRK1A in complex with XMD8-62e
Authors : Rothweiler, U.
Deposited on : 2017-09-19
Resolution : 2.56 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

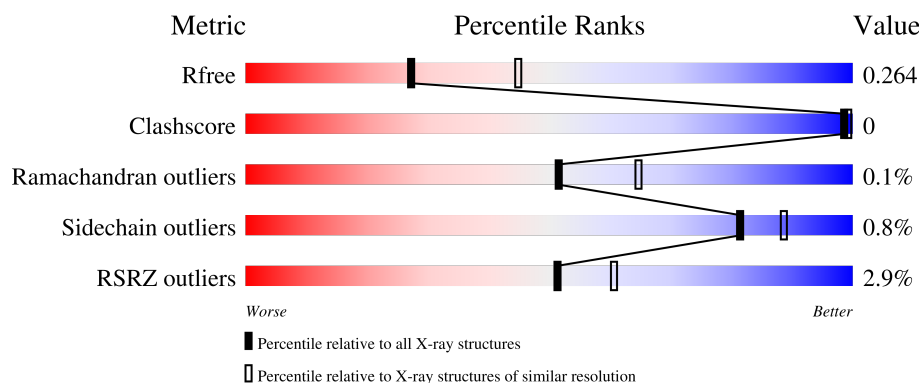
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	368	<div> <div>0%</div> <div>90%</div> <div>7%</div> </div>
1	B	368	<div> <div>2%</div> <div>91%</div> <div>8%</div> </div>
1	C	368	<div> <div>6%</div> <div>91%</div> <div>8%</div> </div>
1	D	368	<div> <div>2%</div> <div>87%</div> <div>10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11243 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.

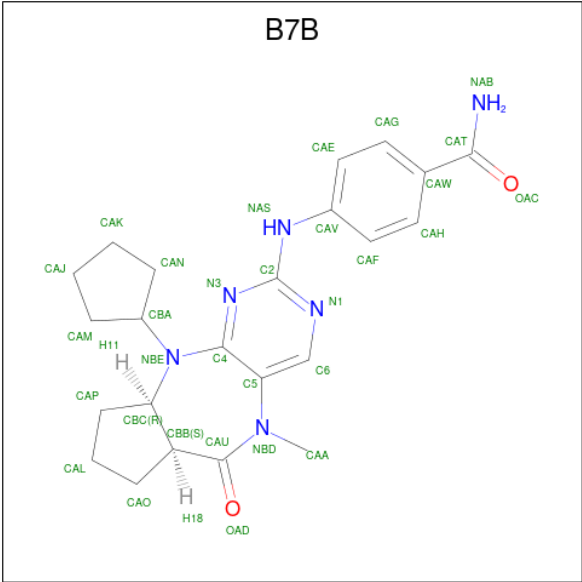
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	P	S	0	0	0
			2794	1798	477	501	1	17			
1	B	340	Total	C	N	O	P	S	0	0	0
			2761	1777	471	495	1	17			
1	C	339	Total	C	N	O	P	S	0	0	0
			2715	1747	455	495	1	17			
1	D	333	Total	C	N	O	P	S	0	0	0
			2711	1752	455	486	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q13627
A	124	ALA	-	expression tag	UNP Q13627
A	125	SER	-	expression tag	UNP Q13627
B	123	GLY	-	expression tag	UNP Q13627
B	124	ALA	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
C	123	GLY	-	expression tag	UNP Q13627
C	124	ALA	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
D	123	GLY	-	expression tag	UNP Q13627
D	124	ALA	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627

- Molecule 2 is 4-[[[(3 {R},7 {S})-2-cyclopentyl-9-methyl-8-oxidanylidene-2,9,12,14-tetrazatri cyclo[8.4.0.0[^]{3,7}]tetradeca-1(14),10,12-trien-13-yl]amino]benzamide (three-letter code: B7B) (formula: C₂₃H₂₈N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	23	6	2		
2	B	1	Total	C	N	O	0	0
			31	23	6	2		
2	C	1	Total	C	N	O	0	0
			31	23	6	2		
2	D	1	Total	C	N	O	0	0
			31	23	6	2		

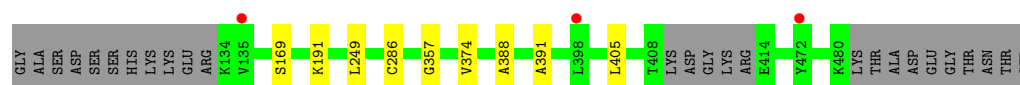
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		
3	B	32	Total	O	0	0
			32	32		
3	C	22	Total	O	0	0
			22	22		
3	D	38	Total	O	0	0
			38	38		

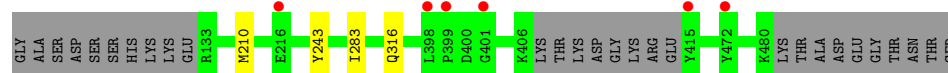
3 Residue-property plots [i](#)

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.

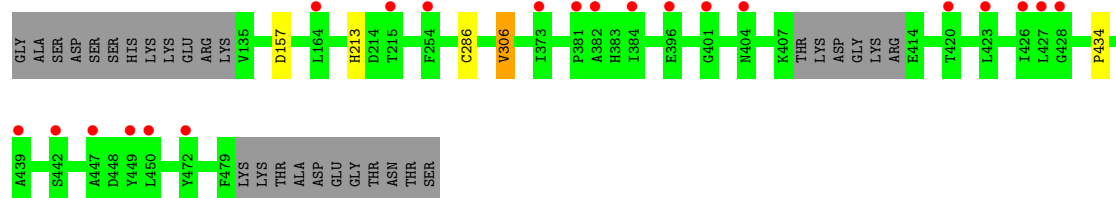
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



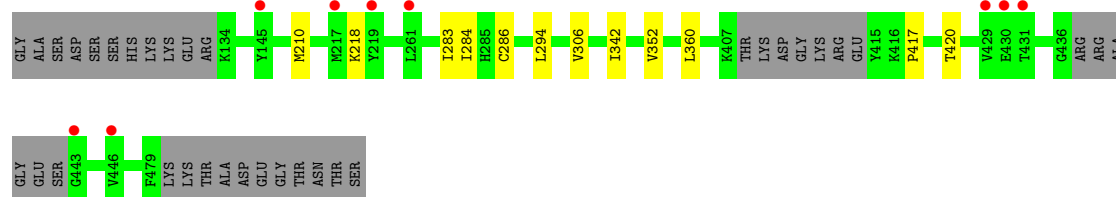
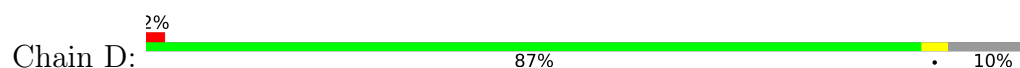
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.95Å 88.37Å 229.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.30 – 2.56 48.30 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.30-2.56) 97.5 (48.30-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.241 , 0.266 0.241 , 0.264	Depositor DCC
R_{free} test set	2793 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 6.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.067 for k,h,-l	Xtriage
Reported twinning fraction	0.878 for H, K, L 0.122 for K, H, -L	Depositor
Outliers	0 of 57731 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11243	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: B7B, 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	0.38	0/2842	0.57	0/3833
1	B	0.37	0/2808	0.58	0/3789
1	C	0.38	0/2763	0.55	0/3743
1	D	0.38	0/2758	0.55	0/3723
All	All	0.38	0/11171	0.56	0/15088

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 [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	2794	0	2787	4	0
1	B	2761	0	2745	1	0
1	C	2715	0	2629	1	0
1	D	2711	0	2693	5	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	C	31	0	0	1	0
2	D	31	0	0	0	0
3	A	46	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	0	0	0
3	C	22	0	0	0	0
3	D	38	0	0	0	0
All	All	11243	0	10854	11	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 0.

All (11) 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:388:ALA:HB3	1:A:391:ALA:HB2	1.99	0.44
1:D:352:VAL:HG11	1:D:360:LEU:HD13	2.01	0.43
1:B:210:MET:CE	1:B:283:ILE:HG21	2.49	0.43
1:A:249:LEU:HD22	1:A:357:GLY:HA2	1.99	0.42
1:C:306:VAL:HG22	2:C:501:B7B:CAH	2.49	0.42
1:D:210:MET:HE3	1:D:283:ILE:HD13	2.01	0.42
1:A:169:SER:O	1:A:191:LYS:NZ	2.43	0.41
1:D:294:LEU:HD13	1:D:306:VAL:HG21	2.03	0.41
1:D:284:ILE:HG21	1:D:342:ILE:HD11	2.02	0.41
1:D:417:PRO:HG2	1:D:420:THR:HG21	2.02	0.41
1:A:374:VAL:HG11	1:A:405:LEU:HD11	2.02	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	337/368 (92%)	323 (96%)	14 (4%)	0	100	100
1	B	335/368 (91%)	316 (94%)	19 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/368 (91%)	315 (94%)	18 (5%)	1 (0%)	41	50
1	D	326/368 (89%)	308 (94%)	18 (6%)	0	100	100
All	All	1332/1472 (90%)	1262 (95%)	69 (5%)	1 (0%)	51	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	434	PRO

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	301/324 (93%)	300 (100%)	1 (0%)	92	96
1	B	296/324 (91%)	294 (99%)	2 (1%)	84	90
1	C	286/324 (88%)	282 (99%)	4 (1%)	67	78
1	D	292/324 (90%)	290 (99%)	2 (1%)	84	90
All	All	1175/1296 (91%)	1166 (99%)	9 (1%)	81	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	CYS
1	B	243	TYR
1	B	316	GLN
1	C	157	ASP
1	C	213	HIS
1	C	286	CYS
1	C	306	VAL
1	D	218	LYS
1	D	286	CYS

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

Mol	Chain	Res	Type
1	B	144	ASN
1	C	192	ASN
1	C	260	ASN
1	C	320	GLN
1	D	172	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	D	321	1	15,16,17	0.78	0	19,22,24	0.81	0
1	PTR	A	321	1	15,16,17	0.85	0	19,22,24	0.79	0
1	PTR	C	321	1	15,16,17	0.79	0	19,22,24	0.86	0
1	PTR	B	321	1	15,16,17	0.81	0	19,22,24	0.76	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	D	321	1	-	0/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1
1	PTR	C	321	1	-	0/10/11/13	0/1/1/1
1	PTR	B	321	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321	PTR	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	B7B	A	501	-	32,35,35	1.76	7 (21%)	37,51,51	2.54	14 (37%)
2	B7B	B	501	-	32,35,35	1.77	6 (18%)	37,51,51	2.53	9 (24%)
2	B7B	D	501	-	32,35,35	1.71	5 (15%)	37,51,51	3.05	13 (35%)
2	B7B	C	501	-	32,35,35	1.66	5 (15%)	37,51,51	3.03	13 (35%)

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	B7B	A	501	-	-	1/8/49/49	0/5/5/5
2	B7B	B	501	-	-	6/8/49/49	0/5/5/5
2	B7B	D	501	-	-	2/8/49/49	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B7B	C	501	-	-	5/8/49/49	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	B7B	CAW-CAT	-6.79	1.40	1.50
2	C	501	B7B	CAW-CAT	-6.45	1.40	1.50
2	A	501	B7B	CAW-CAT	-6.38	1.41	1.50
2	D	501	B7B	CAW-CAT	-6.31	1.41	1.50
2	C	501	B7B	CAA-NBD	3.68	1.52	1.46
2	D	501	B7B	CAA-NBD	3.42	1.52	1.46
2	B	501	B7B	CBC-NBE	3.24	1.53	1.48
2	C	501	B7B	C6-N1	3.10	1.41	1.34
2	B	501	B7B	CAA-NBD	3.06	1.51	1.46
2	A	501	B7B	CAO-CBB	-3.03	1.48	1.54
2	A	501	B7B	CAA-NBD	2.96	1.51	1.46
2	D	501	B7B	C6-N1	2.90	1.40	1.34
2	B	501	B7B	C6-N1	2.89	1.40	1.34
2	A	501	B7B	C6-N1	2.87	1.40	1.34
2	B	501	B7B	CAV-NAS	-2.86	1.34	1.40
2	A	501	B7B	CAV-NAS	-2.70	1.34	1.40
2	C	501	B7B	CAV-NAS	-2.69	1.34	1.40
2	D	501	B7B	CAV-NAS	-2.63	1.34	1.40
2	D	501	B7B	CBC-NBE	2.55	1.52	1.48
2	A	501	B7B	CBC-NBE	2.43	1.52	1.48
2	B	501	B7B	C5-NBD	-2.27	1.36	1.42
2	A	501	B7B	C5-NBD	-2.25	1.36	1.42
2	C	501	B7B	C6-C5	2.03	1.42	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	B7B	N1-C2-N3	-9.47	117.58	126.55
2	D	501	B7B	N1-C2-N3	-9.37	117.67	126.55
2	B	501	B7B	N1-C2-N3	-8.39	118.60	126.55
2	A	501	B7B	N1-C2-N3	-8.29	118.69	126.55
2	D	501	B7B	C5-C4-NBE	7.93	130.15	120.41
2	D	501	B7B	C4-C5-NBD	7.33	129.02	121.69
2	B	501	B7B	C5-C4-NBE	7.01	129.02	120.41
2	C	501	B7B	C4-C5-NBD	6.99	128.68	121.69
2	C	501	B7B	C5-C4-NBE	6.86	128.84	120.41
2	B	501	B7B	C4-C5-NBD	6.04	127.72	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	B7B	OAD-CAU-NBD	-5.90	114.47	121.95
2	A	501	B7B	C4-C5-NBD	5.77	127.46	121.69
2	D	501	B7B	OAD-CAU-NBD	-5.75	114.65	121.95
2	C	501	B7B	CAO-CBB-CBC	-5.56	94.59	104.47
2	A	501	B7B	C5-C4-NBE	5.40	127.04	120.41
2	B	501	B7B	OAD-CAU-NBD	-4.58	116.14	121.95
2	A	501	B7B	OAD-CAU-NBD	-4.26	116.55	121.95
2	D	501	B7B	CAO-CBB-CBC	-4.17	97.07	104.47
2	D	501	B7B	C5-C4-N3	-3.81	118.05	123.67
2	B	501	B7B	C5-C4-N3	-3.65	118.29	123.67
2	D	501	B7B	CAA-NBD-CAU	-3.64	113.04	117.36
2	C	501	B7B	C4-NBE-CBA	3.44	119.12	116.29
2	D	501	B7B	C2-N3-C4	3.40	126.08	114.34
2	C	501	B7B	C5-NBD-CAU	3.36	127.45	123.27
2	A	501	B7B	C5-C4-N3	-3.29	118.82	123.67
2	C	501	B7B	CAV-NAS-C2	-3.26	119.76	129.23
2	A	501	B7B	C6-N1-C2	3.18	120.68	115.88
2	C	501	B7B	C2-N3-C4	3.15	125.20	114.34
2	B	501	B7B	C2-N3-C4	3.07	124.94	114.34
2	C	501	B7B	C6-N1-C2	3.06	120.50	115.88
2	B	501	B7B	CAV-NAS-C2	-2.99	120.56	129.23
2	C	501	B7B	CAJ-CAM-CBA	-2.96	97.78	104.68
2	D	501	B7B	C5-NBD-CAU	2.88	126.85	123.27
2	D	501	B7B	C6-N1-C2	2.86	120.19	115.88
2	A	501	B7B	CAJ-CAM-CBA	-2.85	98.04	104.68
2	C	501	B7B	CAA-NBD-CAU	-2.83	114.00	117.36
2	B	501	B7B	C6-N1-C2	2.79	120.08	115.88
2	A	501	B7B	C2-N3-C4	2.78	123.94	114.34
2	D	501	B7B	CAJ-CAM-CBA	-2.73	98.33	104.68
2	A	501	B7B	CAO-CAL-CAP	-2.60	98.91	105.79
2	A	501	B7B	CAN-CBA-CAM	-2.58	98.51	104.72
2	A	501	B7B	CAV-NAS-C2	-2.51	121.95	129.23
2	A	501	B7B	CAL-CAP-CBC	2.49	108.35	104.16
2	C	501	B7B	C5-C4-N3	-2.47	120.02	123.67
2	D	501	B7B	CAV-NAS-C2	-2.45	122.13	129.23
2	A	501	B7B	NAS-C2-N3	2.35	124.90	116.92
2	D	501	B7B	NAS-C2-N3	2.33	124.83	116.92
2	B	501	B7B	C4-NBE-CBA	-2.17	114.51	116.29
2	A	501	B7B	C5-NBD-CAU	2.17	125.97	123.27

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	B7B	NAB-CAT-CAW-CAH
2	B	501	B7B	NAB-CAT-CAW-CAG
2	C	501	B7B	NAB-CAT-CAW-CAH
2	B	501	B7B	OAC-CAT-CAW-CAH
2	B	501	B7B	OAC-CAT-CAW-CAG
2	C	501	B7B	CAE-CAV-NAS-C2
2	C	501	B7B	CAF-CAV-NAS-C2
2	C	501	B7B	NAB-CAT-CAW-CAG
2	B	501	B7B	CAF-CAV-NAS-C2
2	B	501	B7B	CAE-CAV-NAS-C2
2	D	501	B7B	CAF-CAV-NAS-C2
2	D	501	B7B	CAE-CAV-NAS-C2
2	C	501	B7B	OAC-CAT-CAW-CAH
2	A	501	B7B	CAE-CAV-NAS-C2

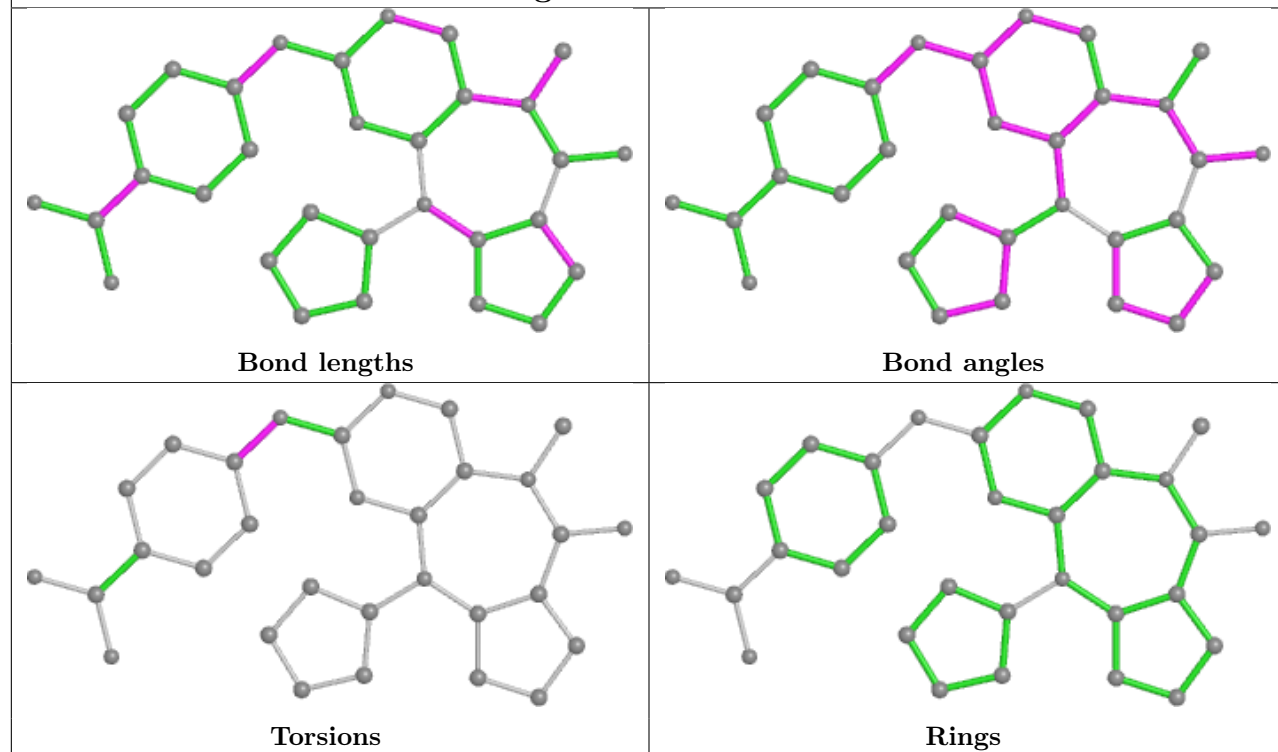
There are no ring outliers.

1 monomer is involved in 1 short contact:

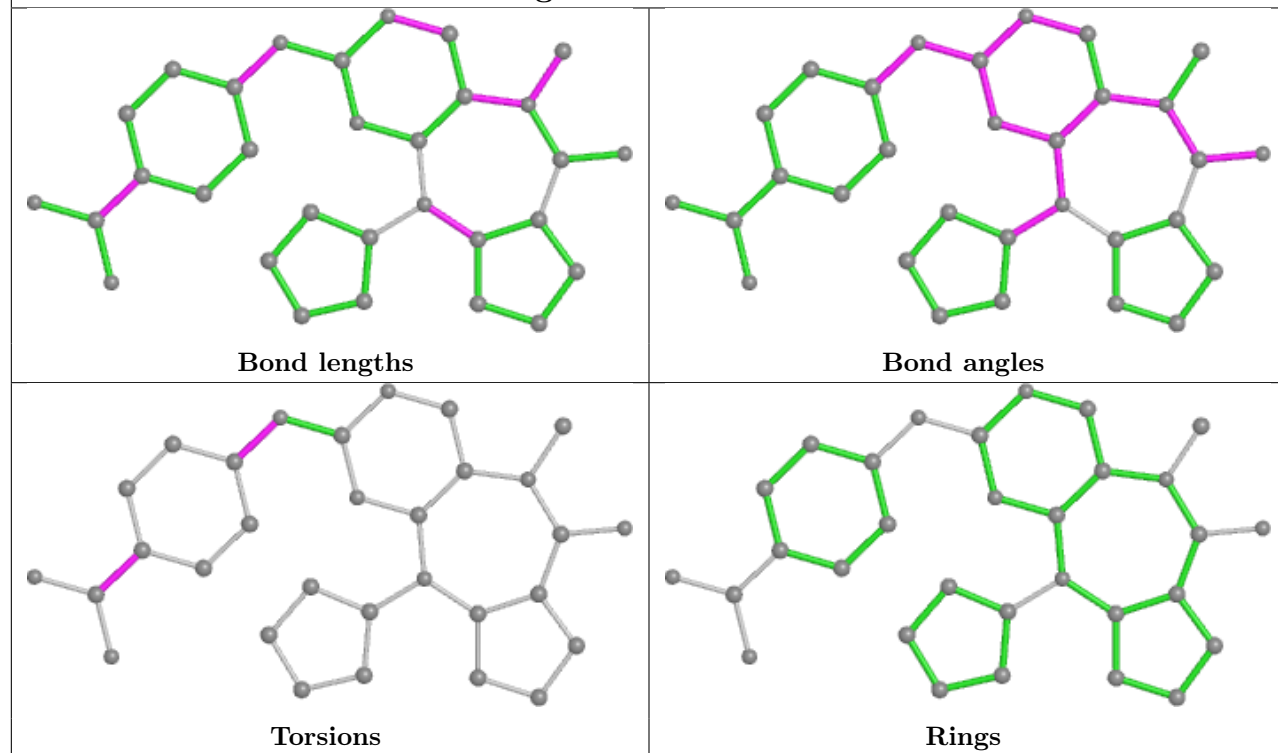
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	B7B	1	0

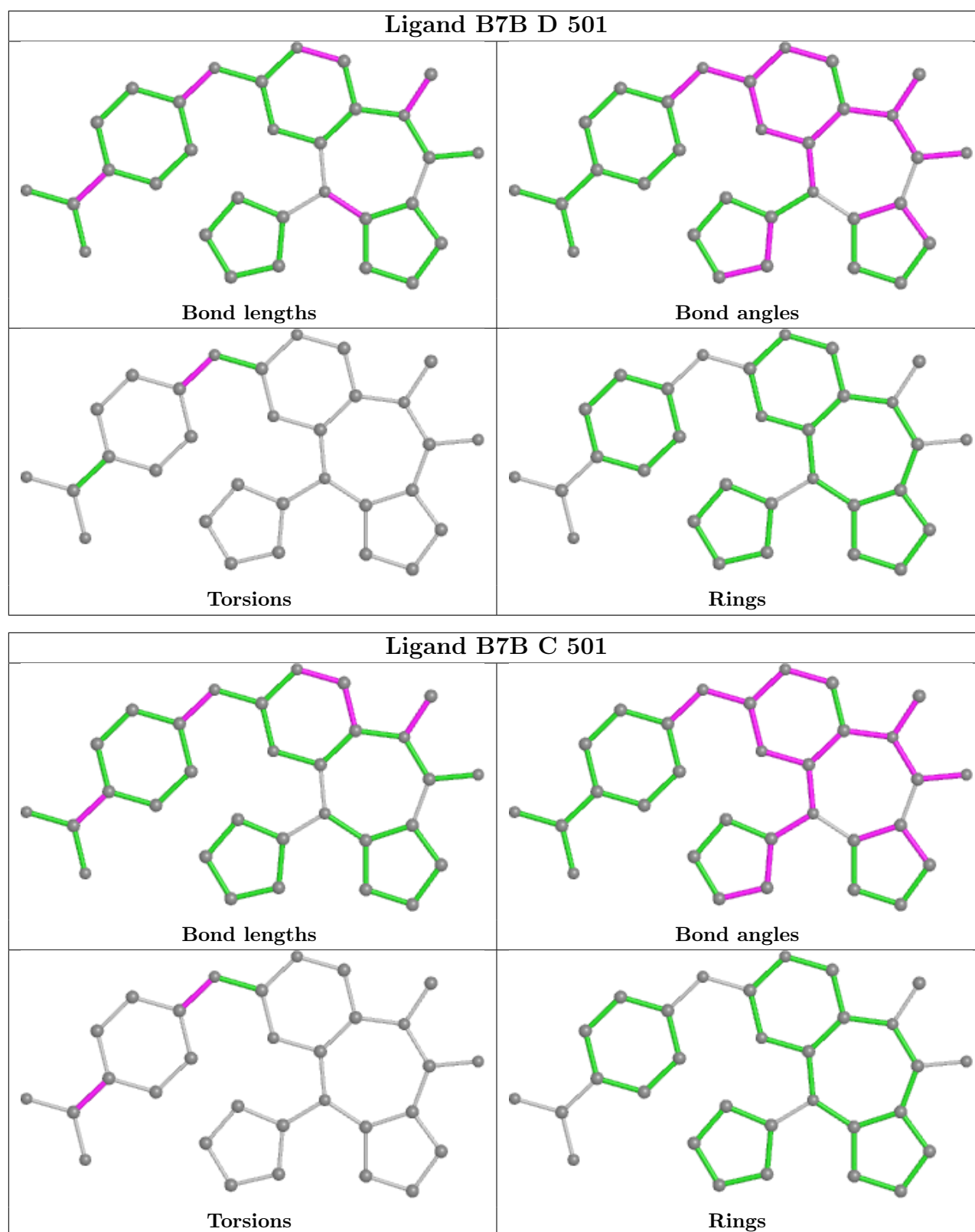
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 B7B A 501



Ligand B7B B 501





5.7 Other polymers [i](#)

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	341/368 (92%)	0.02	3 (0%) 84 89	29, 42, 59, 70	0
1	B	339/368 (92%)	0.21	6 (1%) 68 75	34, 49, 76, 116	0
1	C	338/368 (91%)	0.49	21 (6%) 20 25	36, 60, 93, 100	0
1	D	332/368 (90%)	0.24	9 (2%) 54 63	35, 54, 82, 92	0
All	All	1350/1472 (91%)	0.24	39 (2%) 51 61	29, 50, 87, 116	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	THR	6.4
1	B	398	LEU	6.3
1	B	399	PRO	6.0
1	D	446	VAL	5.0
1	C	423	LEU	4.3
1	C	404	ASN	4.3
1	C	472	TYR	4.0
1	C	447	ALA	3.9
1	D	430	GLU	3.9
1	C	420	THR	3.8
1	D	443	GLY	3.6
1	B	216	GLU	3.5
1	A	472	TYR	3.3
1	B	401	GLY	3.3
1	D	431	THR	3.2
1	C	427	LEU	3.1
1	C	450	LEU	3.0
1	D	429	VAL	2.9
1	D	145	TYR	2.9
1	C	254	PHE	2.9
1	D	217	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	398	LEU	2.6
1	D	261	LEU	2.6
1	B	472	TYR	2.6
1	D	219	TYR	2.6
1	C	373	ILE	2.6
1	C	384	ILE	2.5
1	C	428	GLY	2.5
1	C	381	PRO	2.5
1	C	382	ALA	2.5
1	B	415	TYR	2.4
1	C	396	GLU	2.4
1	A	135	VAL	2.4
1	C	442	SER	2.2
1	C	439	ALA	2.2
1	C	426	ILE	2.1
1	C	164	LEU	2.1
1	C	401	GLY	2.1
1	C	449	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(Å ²)	Q<0.9
1	PTR	B	321	16/17	0.95	0.14	47,50,51,51	0
1	PTR	A	321	16/17	0.96	0.15	35,36,37,38	0
1	PTR	C	321	16/17	0.96	0.12	48,50,51,52	0
1	PTR	D	321	16/17	0.96	0.13	40,42,44,45	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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,

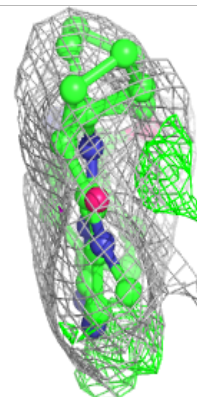
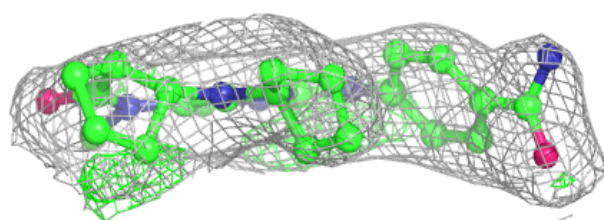
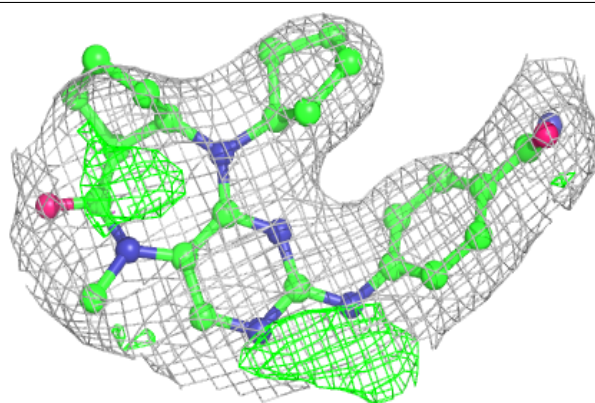
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	B7B	D	501	31/31	0.81	0.23	57,66,70,70	0
2	B7B	A	501	31/31	0.82	0.22	51,57,60,61	0
2	B7B	C	501	31/31	0.87	0.23	61,69,71,71	0
2	B7B	B	501	31/31	0.88	0.19	51,59,63,64	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.

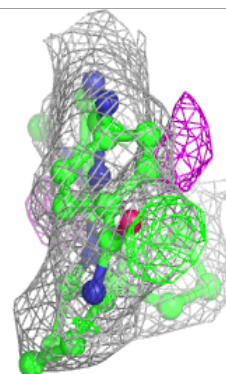
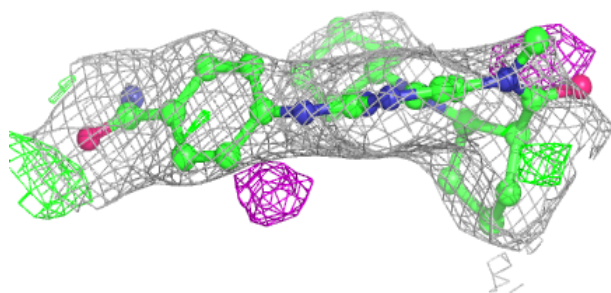
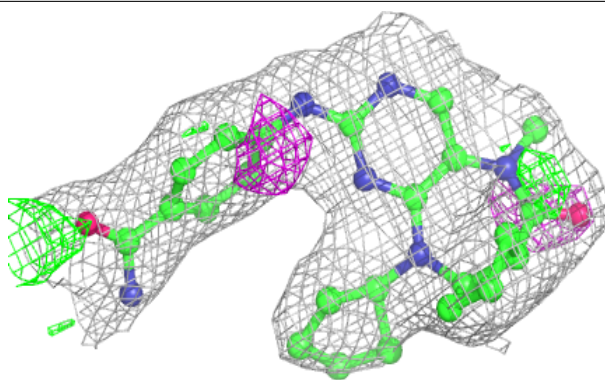
Electron density around B7B D 501:

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

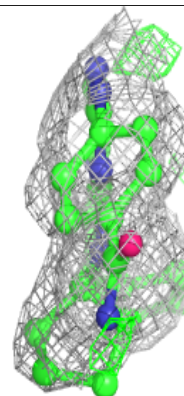
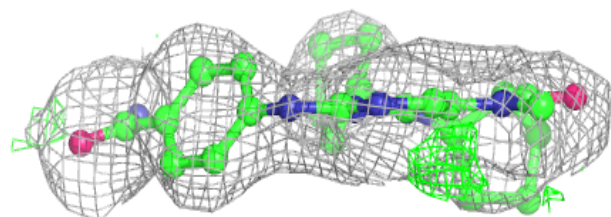
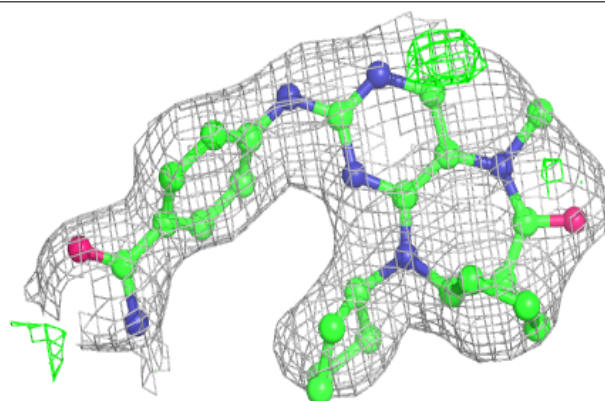


Electron density around B7B A 501:

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

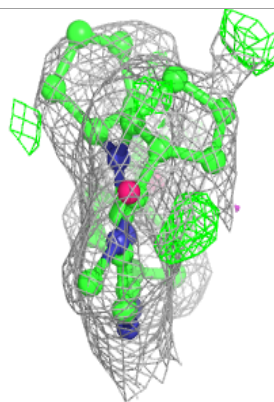
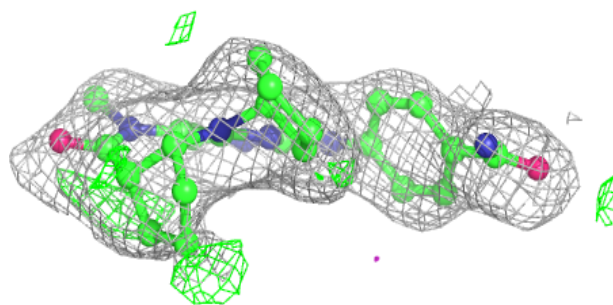
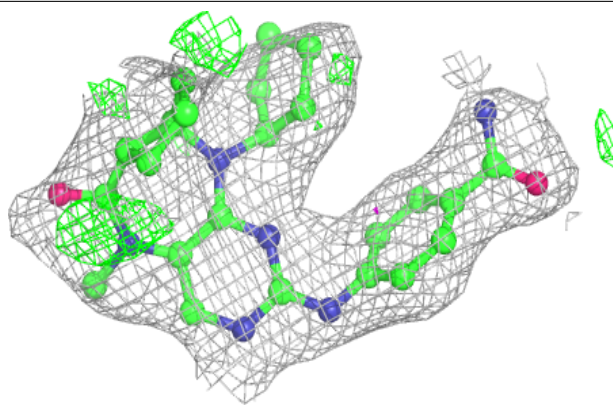
**Electron density around B7B C 501:**

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



Electron density around B7B 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.