



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:10 AM UTC

PDB ID : 6EIQ / pdb_00006eiq
Title : DYRK1A in complex with XMD14-124
Authors : Rothweiler, U.
Deposited on : 2017-09-19
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

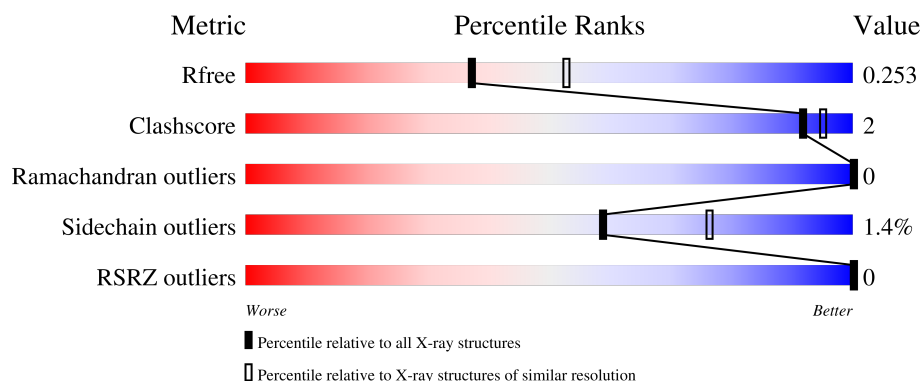
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

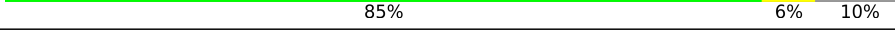
The reported resolution of this entry is 2.30 Å.

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	368	 86% 7% 7%
1	B	368	 86% 6% 8%
1	C	368	 87% • 10%
1	D	368	 85% 6% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11312 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.

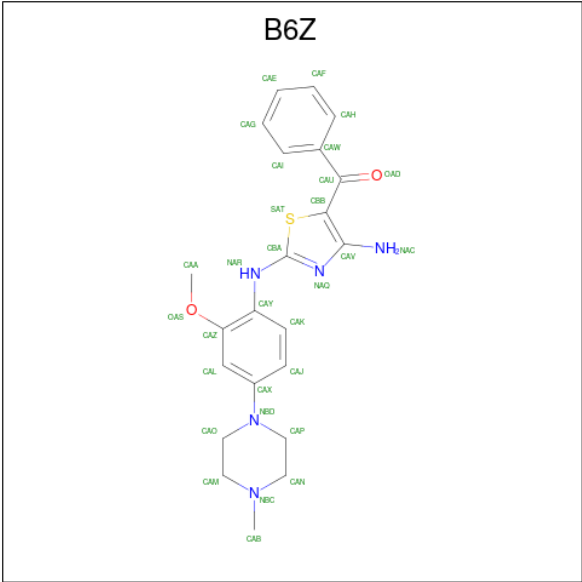
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

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
			2765	1780	472	495	1	17			
1	C	333	Total	C	N	O	P	S	0	0	0
			2678	1724	452	484	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-azanyl-2-[[2-methoxy-4-(4-methylpiperazin-1-yl)phenyl]amino]-1,3-thiazol-5-yl]-phenyl-methanone (CCD ID: B6Z) (formula: C₂₂H₂₅N₅O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	22	5	2	1		
2	B	1	Total	C	N	O	S	0	0
			30	22	5	2	1		
2	C	1	Total	C	N	O	S	0	0
			30	22	5	2	1		
2	D	1	Total	C	N	O	S	0	0
			30	22	5	2	1		

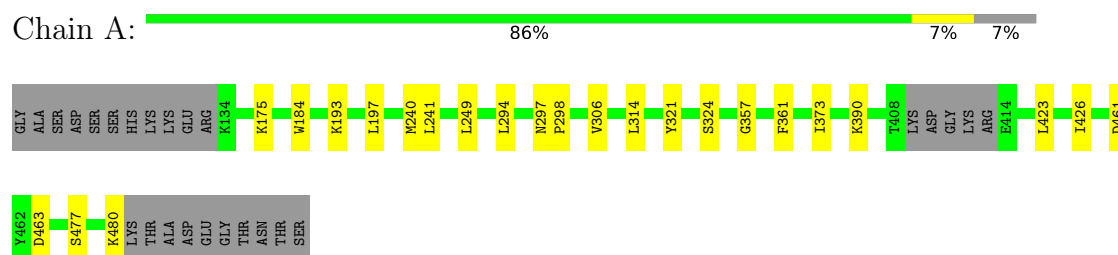
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	82	Total	O	0	0
			82	82		
3	B	52	Total	O	0	0
			52	52		
3	C	47	Total	O	0	0
			47	47		
3	D	63	Total	O	0	0
			63	63		

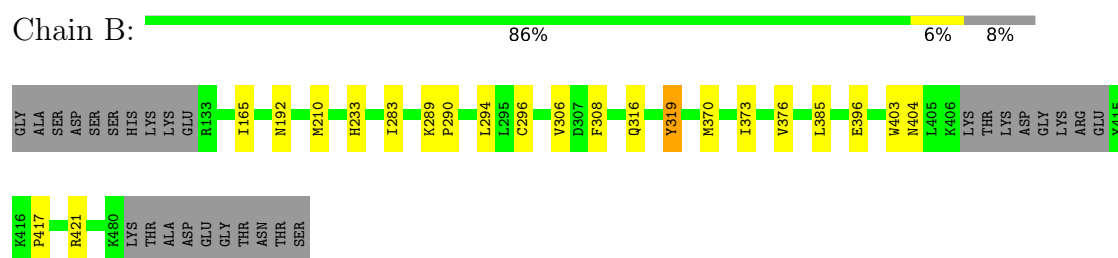
3 Residue-property plots

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.

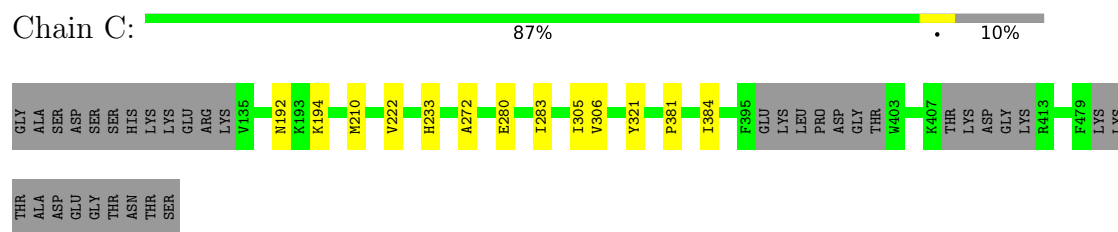
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



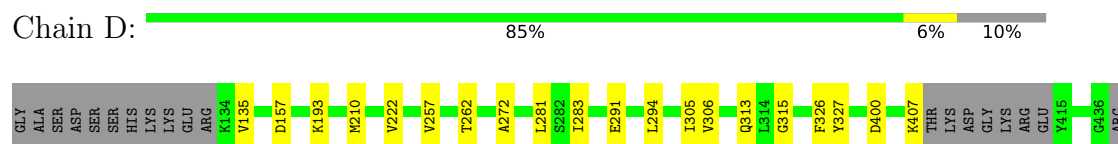
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



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



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



ARG	ALA	GLY	GLU	SER	G443	R488	F479	LYS	LYS	THR	ALA	ASP	GLU	GLY	THR	ASN	THR	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.56Å 87.60Å 229.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 2.30 48.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.10-2.30) 97.2 (48.10-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.218 , 0.252 (Not available) , 0.253	Depositor DCC
R_{free} test set	3846 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.206 for k,h,-l	Xtriage
Reported twinning fraction	0.751 for H, K, L 0.249 for K, H, -L	Depositor
Outliers	0 of 77070 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11312	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, B6Z

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	0.58	0/2842	0.83	3/3833 (0.1%)
1	B	0.58	0/2812	0.85	1/3793 (0.0%)
1	C	0.56	0/2724	0.81	0/3686
1	D	0.57	0/2758	0.82	0/3723
All	All	0.57	0/11136	0.83	4/15035 (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	298	PRO	N-CA-C	5.43	123.65	112.47
1	A	297	ASN	CA-C-N	5.15	126.28	119.84
1	A	297	ASN	C-N-CA	5.15	126.28	119.84
1	B	417	PRO	N-CA-C	5.01	115.28	110.47

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	2794	0	2787	14	0
1	B	2765	0	2756	10	0
1	C	2678	0	2599	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2711	0	2693	8	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
3	A	82	0	0	0	0
3	B	52	0	0	0	0
3	C	47	0	0	0	0
3	D	63	0	0	0	0
All	All	11312	0	10835	35	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 2.

All (35) 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:175:LYS:CD	1:A:240:MET:HE1	2.05	0.87
1:A:175:LYS:HD2	1:A:240:MET:HE1	1.59	0.84
1:D:294:LEU:HD22	1:D:306:VAL:HG11	1.65	0.76
1:A:175:LYS:CE	1:A:240:MET:HE1	2.28	0.63
1:A:294:LEU:HD22	1:A:306:VAL:HG11	1.80	0.61
1:A:197:LEU:HD23	1:B:319:TYR:HD2	1.72	0.55
1:A:241:LEU:HB2	1:A:294:LEU:HD23	1.89	0.54
1:B:294:LEU:HD22	1:B:306:VAL:HG11	1.89	0.53
1:D:222:VAL:HB	1:D:306:VAL:HG12	1.94	0.49
1:A:249:LEU:HD22	1:A:357:GLY:HA2	1.95	0.48
1:B:192:ASN:HB2	1:B:233:HIS:CE1	2.49	0.48
1:B:210:MET:HE1	1:B:308:PHE:CE2	2.49	0.47
1:A:294:LEU:HD13	1:A:306:VAL:HG21	1.97	0.47
1:C:381:PRO:HG2	1:C:384:ILE:HD12	1.97	0.47
1:C:192:ASN:HB2	1:C:233:HIS:CE1	2.51	0.46
1:A:314:LEU:O	1:D:315:GLY:HA2	2.15	0.46
1:A:361:PHE:CE1	1:A:373:ILE:HA	2.52	0.44
1:A:423:LEU:HA	1:A:426:ILE:HD12	1.98	0.44
1:A:477:SER:HA	1:A:480:LYS:HG2	1.99	0.44
1:C:222:VAL:HG11	1:C:306:VAL:HG23	1.99	0.44
1:A:184:TRP:HB3	1:A:240:MET:SD	2.58	0.43
1:A:461:ASP:OD1	1:A:463:ASP:N	2.50	0.43
1:B:210:MET:HE3	1:B:283:ILE:HD13	2.00	0.43
1:B:385:LEU:HD23	1:B:403:TRP:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:HB2	1:B:290:PRO:HD2	2.00	0.42
1:D:210:MET:HE3	1:D:283:ILE:HD13	2.02	0.42
1:D:257:VAL:HG23	1:D:262:THR:HG23	2.00	0.42
1:B:376:VAL:HA	1:B:421:ARG:O	2.20	0.42
1:C:272:ALA:HB1	1:C:305:ILE:HD12	2.02	0.41
1:B:396:GLU:N	1:B:404:ASN:O	2.52	0.41
1:C:210:MET:HE2	1:C:283:ILE:HD13	2.03	0.41
1:D:326:PHE:HB2	1:D:327:TYR:CE1	2.56	0.41
1:D:272:ALA:HB1	1:D:305:ILE:HD12	2.02	0.40
1:B:370:MET:HE3	1:B:373:ILE:HB	2.03	0.40
1:D:281:LEU:O	1:D:313:GLN:NE2	2.53	0.40

There are no symmetry-related clashes.

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	337/368 (92%)	319 (95%)	18 (5%)	0	100	100
1	B	335/368 (91%)	315 (94%)	20 (6%)	0	100	100
1	C	326/368 (89%)	300 (92%)	26 (8%)	0	100	100
1	D	326/368 (89%)	304 (93%)	22 (7%)	0	100	100
All	All	1324/1472 (90%)	1238 (94%)	86 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	298 (99%)	3 (1%)	68	82
1	B	297/324 (92%)	293 (99%)	4 (1%)	61	77
1	C	282/324 (87%)	280 (99%)	2 (1%)	76	87
1	D	292/324 (90%)	285 (98%)	7 (2%)	43	62
All	All	1172/1296 (90%)	1156 (99%)	16 (1%)	59	76

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LYS
1	A	324	SER
1	A	390	LYS
1	B	165	ILE
1	B	296	CYS
1	B	316	GLN
1	B	319	TYR
1	C	194	LYS
1	C	280	GLU
1	D	135	VAL
1	D	157	ASP
1	D	193	LYS
1	D	291	GLU
1	D	400	ASP
1	D	407	LYS
1	D	458	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	HIS
1	A	232	ASN
1	B	172	GLN
1	B	227	HIS
1	B	424	HIS
1	C	211	ASN
1	C	371	ASN
1	C	387	GLN
1	D	232	ASN

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Mol	Chain	Res	Type
1	D	371	ASN
1	D	444	HIS

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	A	321	1	15,16,17	0.79	0	17,22,24	0.84	1 (5%)
1	PTR	B	321	1	15,16,17	0.77	0	17,22,24	0.83	0
1	PTR	C	321	1	15,16,17	0.81	0	17,22,24	0.95	1 (5%)
1	PTR	D	321	1	15,16,17	0.70	0	17,22,24	0.77	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	321	1	-	0/10/11/13	0/1/1/1
1	PTR	B	321	1	-	0/10/11/13	0/1/1/1
1	PTR	C	321	1	-	1/10/11/13	0/1/1/1
1	PTR	D	321	1	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	PTR	O3P-P-O2P	2.06	115.52	107.80
1	A	321	PTR	OH-P-O1P	-2.00	102.80	109.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	321	PTR	O-C-CA-CB
1	D	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 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	B6Z	B	501	-	32,33,33	1.79	7 (21%)	44,46,46	2.99	8 (18%)
2	B6Z	A	501	-	32,33,33	1.67	4 (12%)	44,46,46	2.52	10 (22%)
2	B6Z	C	501	-	32,33,33	1.49	4 (12%)	44,46,46	2.23	9 (20%)
2	B6Z	D	501	-	32,33,33	1.62	5 (15%)	44,46,46	2.81	8 (18%)

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	B6Z	B	501	-	-	2/18/28/28	0/4/4/4
2	B6Z	A	501	-	-	7/18/28/28	0/4/4/4
2	B6Z	C	501	-	-	2/18/28/28	0/4/4/4
2	B6Z	D	501	-	-	4/18/28/28	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	B6Z	CBA-SAT	-5.00	1.65	1.73
2	A	501	B6Z	CAW-CAU	-4.45	1.40	1.49
2	D	501	B6Z	CAW-CAU	-4.38	1.40	1.49
2	C	501	B6Z	CAW-CAU	-4.27	1.40	1.49
2	B	501	B6Z	CAW-CAU	-4.16	1.40	1.49
2	A	501	B6Z	CBB-CAU	-4.11	1.35	1.47
2	B	501	B6Z	CBB-CAU	-3.98	1.35	1.47
2	A	501	B6Z	CBA-SAT	-3.95	1.67	1.73
2	D	501	B6Z	CBB-CAU	-3.91	1.36	1.47
2	C	501	B6Z	CBB-CAU	-3.84	1.36	1.47
2	A	501	B6Z	CAY-NAR	-3.25	1.35	1.41
2	B	501	B6Z	CAY-NAR	-3.19	1.35	1.41
2	B	501	B6Z	CBB-SAT	-3.17	1.67	1.74
2	C	501	B6Z	CAY-NAR	-3.12	1.35	1.41
2	D	501	B6Z	CBB-SAT	-2.94	1.68	1.74
2	D	501	B6Z	CAY-NAR	-2.80	1.36	1.41
2	D	501	B6Z	CBA-SAT	-2.75	1.69	1.73
2	B	501	B6Z	CAP-NBD	2.43	1.50	1.46
2	C	501	B6Z	CAO-NBD	2.19	1.50	1.46
2	B	501	B6Z	CAO-NBD	2.07	1.50	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	B6Z	CBA-SAT-CBB	14.21	96.33	88.34
2	D	501	B6Z	CBA-SAT-CBB	13.01	95.66	88.34
2	A	501	B6Z	CBA-SAT-CBB	10.53	94.26	88.34
2	D	501	B6Z	SAT-CBA-NAQ	-9.83	106.98	115.78
2	B	501	B6Z	SAT-CBA-NAQ	-9.46	107.31	115.78
2	C	501	B6Z	SAT-CBA-NAQ	-8.32	108.34	115.78
2	C	501	B6Z	CBA-SAT-CBB	8.05	92.87	88.34
2	A	501	B6Z	SAT-CBA-NAQ	-8.04	108.59	115.78
2	B	501	B6Z	CAP-NBD-CAO	5.06	122.94	111.57
2	A	501	B6Z	CAN-NBC-CAM	5.04	117.56	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	B6Z	CAN-NBC-CAM	4.74	117.09	109.54
2	D	501	B6Z	CAN-NBC-CAM	4.27	116.33	109.54
2	B	501	B6Z	CBB-CAV-NAQ	-4.20	114.13	117.84
2	A	501	B6Z	CBB-CAV-NAQ	-4.04	114.27	117.84
2	D	501	B6Z	CBB-CAV-NAQ	-3.53	114.72	117.84
2	C	501	B6Z	CBB-CAV-NAQ	-3.30	114.93	117.84
2	A	501	B6Z	CAM-CAO-NBD	-3.05	104.36	110.78
2	B	501	B6Z	CAA-OAS-CAZ	-2.94	113.20	117.51
2	A	501	B6Z	CAU-CBB-SAT	2.59	129.28	117.41
2	A	501	B6Z	CAP-NBD-CAO	2.57	117.34	111.57
2	B	501	B6Z	OAS-CAZ-CAY	2.53	117.96	114.81
2	D	501	B6Z	CAP-NBD-CAO	2.51	117.21	111.57
2	B	501	B6Z	CAN-CAP-NBD	2.50	116.05	110.78
2	C	501	B6Z	CAP-NBD-CAO	2.49	117.16	111.57
2	B	501	B6Z	CAU-CBB-SAT	2.48	128.76	117.41
2	C	501	B6Z	CAU-CBB-SAT	2.44	128.60	117.41
2	A	501	B6Z	CAO-CAM-NBC	-2.36	107.06	110.86
2	D	501	B6Z	OAS-CAZ-CAY	2.35	117.74	114.81
2	D	501	B6Z	CAU-CBB-SAT	2.32	128.02	117.41
2	C	501	B6Z	SAT-CBA-NAR	2.30	130.85	122.19
2	A	501	B6Z	SAT-CBA-NAR	2.24	130.65	122.19
2	A	501	B6Z	CAL-CAX-NBD	-2.20	118.95	121.33
2	C	501	B6Z	NAC-CAV-NAQ	-2.19	117.41	121.03
2	D	501	B6Z	SAT-CBA-NAR	2.15	130.31	122.19
2	C	501	B6Z	CAA-OAS-CAZ	-2.01	114.56	117.51

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	B6Z	CAY-CAZ-OAS-CAA
2	A	501	B6Z	CAY-CAZ-OAS-CAA
2	D	501	B6Z	CAY-CAZ-OAS-CAA
2	C	501	B6Z	CAY-CAZ-OAS-CAA
2	B	501	B6Z	CAL-CAZ-OAS-CAA
2	C	501	B6Z	CAL-CAZ-OAS-CAA
2	A	501	B6Z	CAL-CAZ-OAS-CAA
2	D	501	B6Z	CAL-CAZ-OAS-CAA
2	A	501	B6Z	CAL-CAX-NBD-CAP
2	A	501	B6Z	CAJ-CAX-NBD-CAO
2	A	501	B6Z	CAJ-CAX-NBD-CAP
2	D	501	B6Z	OAD-CAU-CAW-CAI

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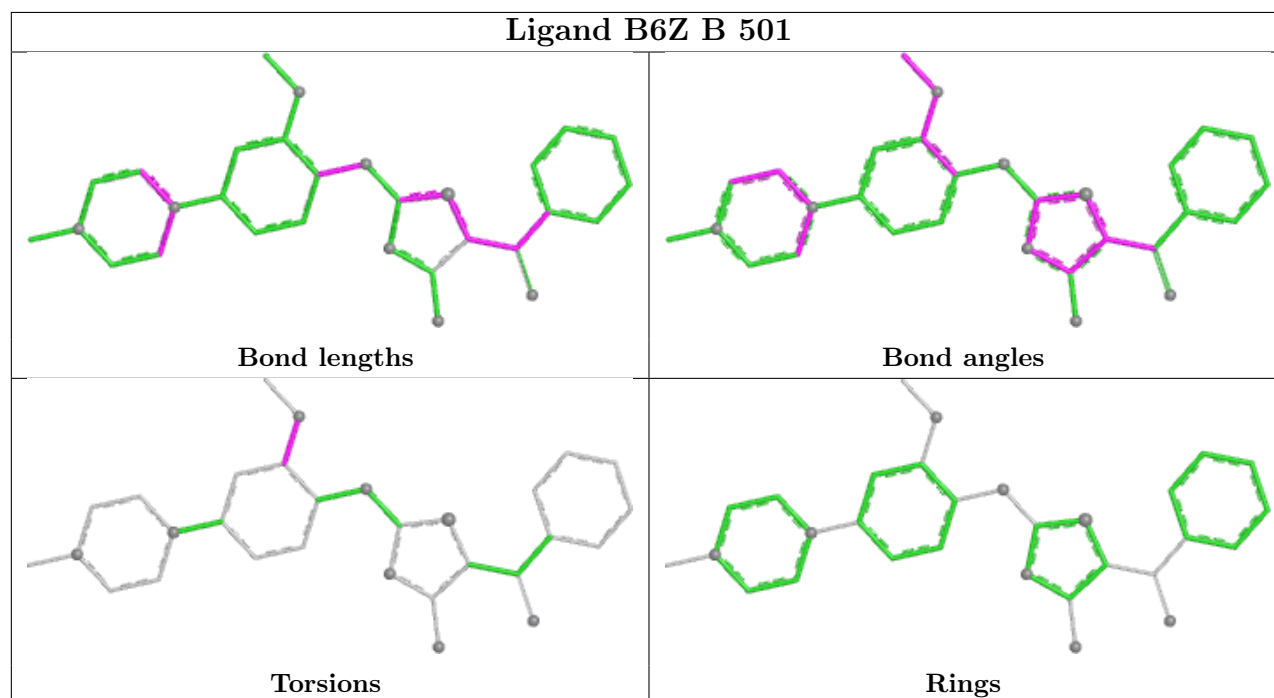
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Mol	Chain	Res	Type	Atoms
2	A	501	B6Z	CAL-CAX-NBD-CAO
2	D	501	B6Z	OAD-CAU-CAW-CAH
2	A	501	B6Z	OAD-CAU-CAW-CAI

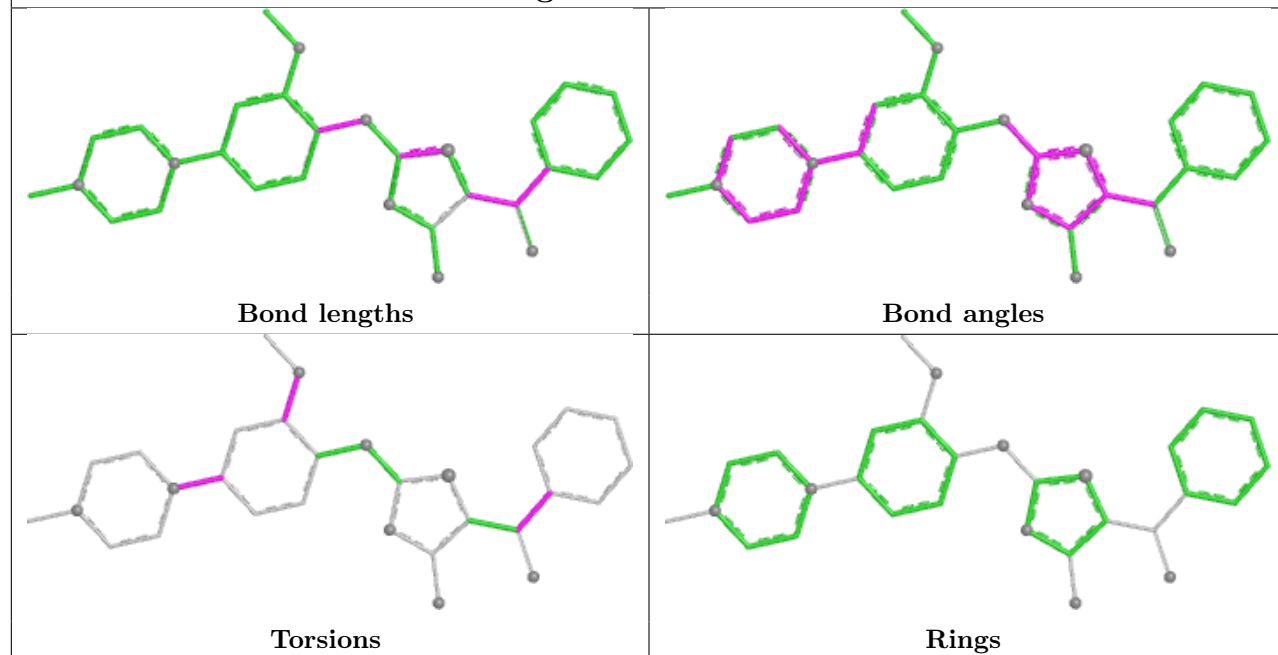
There are no ring outliers.

No monomer is involved in short contacts.

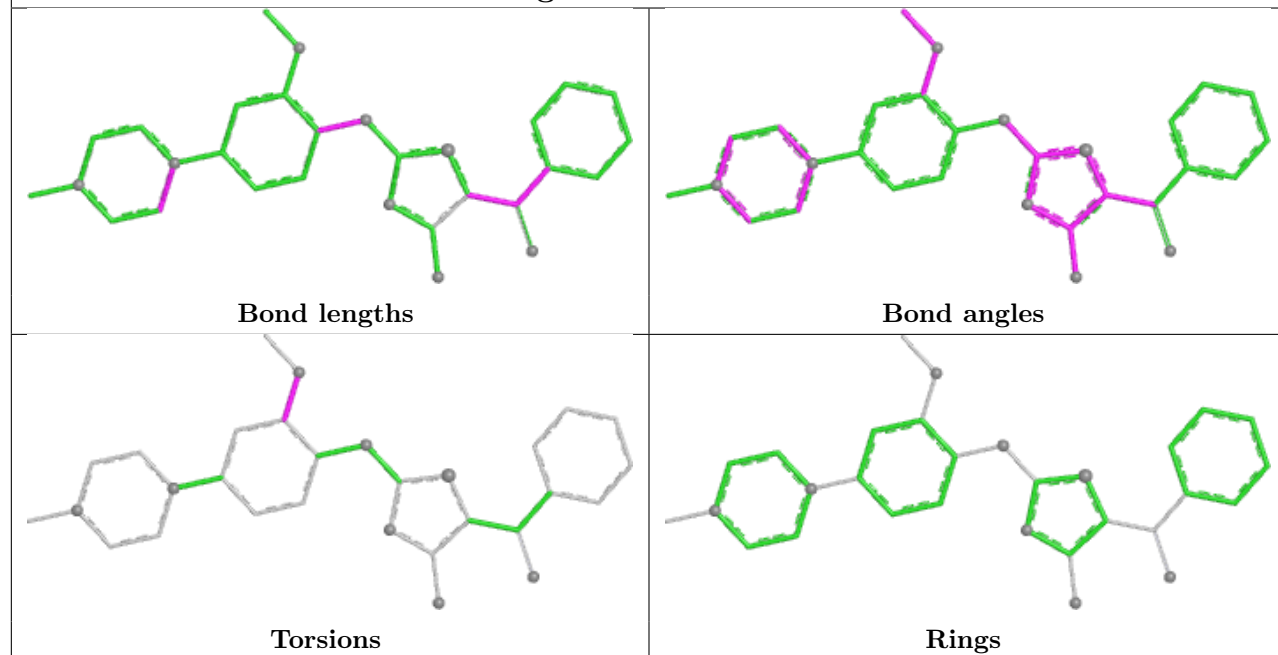
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

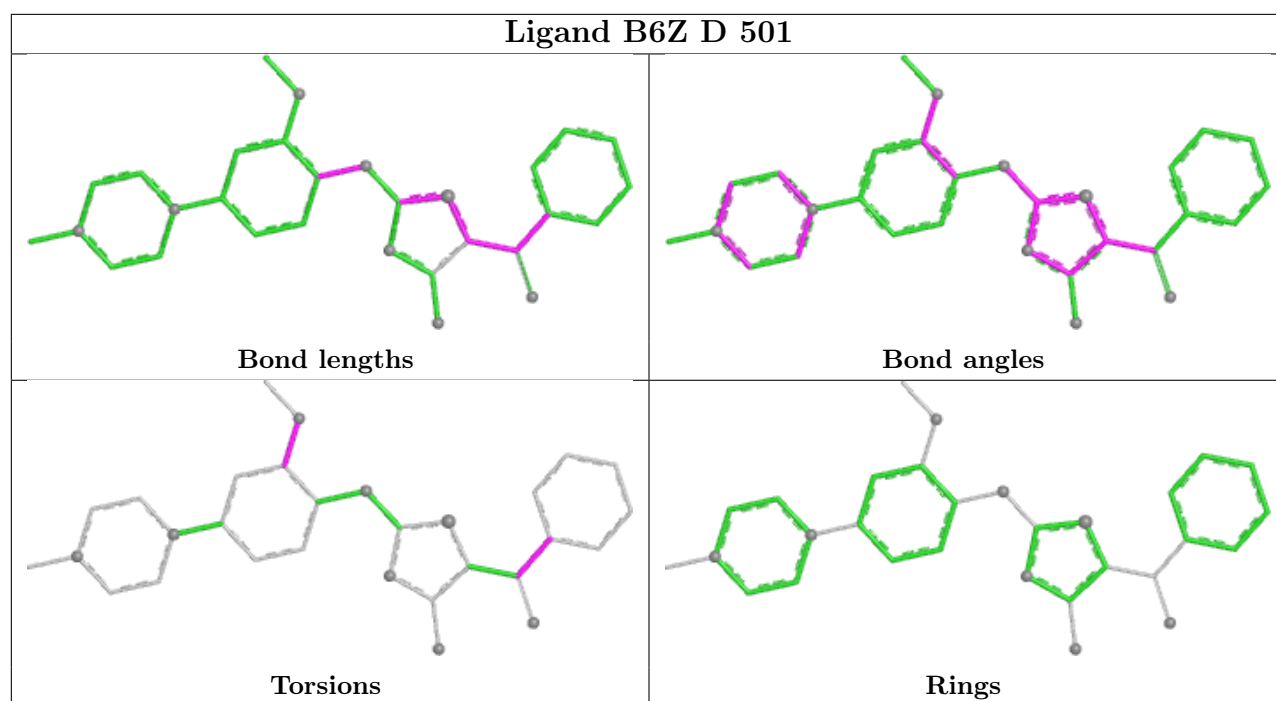


Ligand B6Z A 501



Ligand B6Z C 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	341/368 (92%)	-0.95	0 100 100	28, 44, 61, 80	0
1	B	339/368 (92%)	-0.76	0 100 100	38, 61, 86, 121	0
1	C	332/368 (90%)	-0.83	0 100 100	35, 62, 86, 96	0
1	D	332/368 (90%)	-0.85	0 100 100	34, 54, 81, 96	0
All	All	1344/1472 (91%)	-0.85	0 100 100	28, 55, 84, 121	0

There are no RSRZ outliers to report.

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	321	16/17	0.99	0.04	37,39,40,40	0
1	PTR	B	321	16/17	0.99	0.05	56,60,60,61	0
1	PTR	C	321	16/17	0.99	0.05	54,59,60,60	0
1	PTR	D	321	16/17	0.99	0.04	37,42,46,46	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

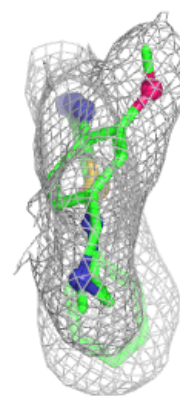
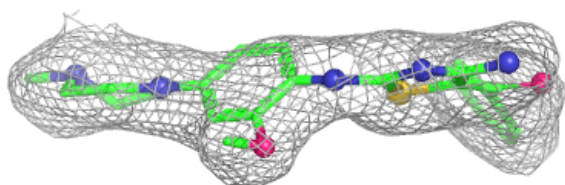
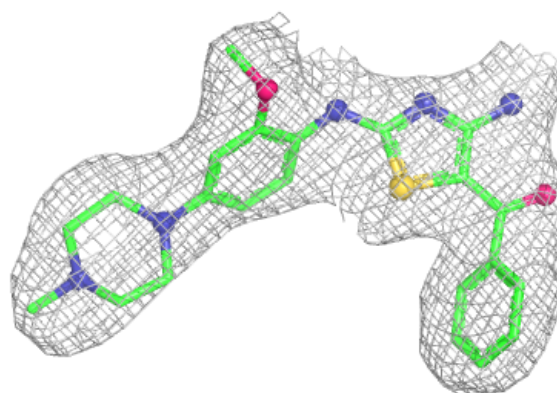
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	B6Z	B	501	30/30	0.98	0.05	37,49,54,55	0
2	B6Z	C	501	30/30	0.98	0.05	46,49,51,54	0
2	B6Z	D	501	30/30	0.98	0.05	45,49,57,57	0
2	B6Z	A	501	30/30	0.99	0.05	46,48,51,51	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.

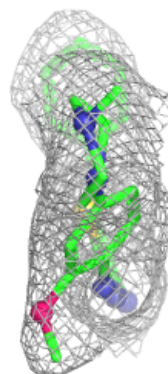
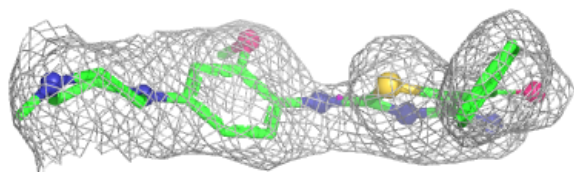
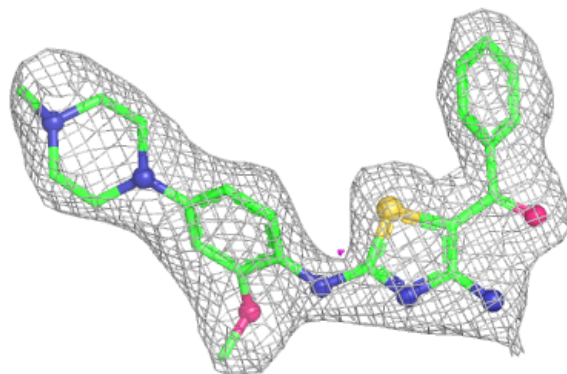
Electron density around B6Z B 501:

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



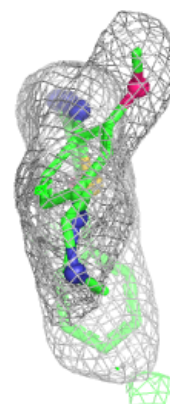
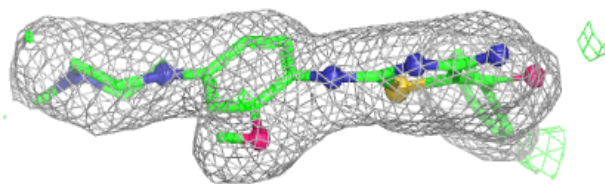
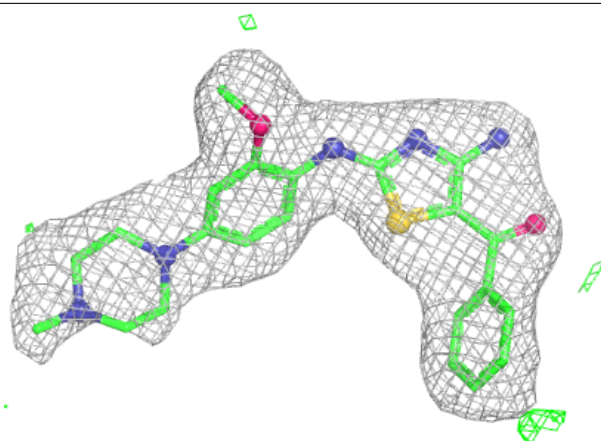
Electron density around B6Z C 501:

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

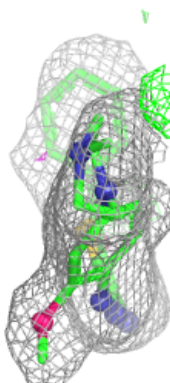
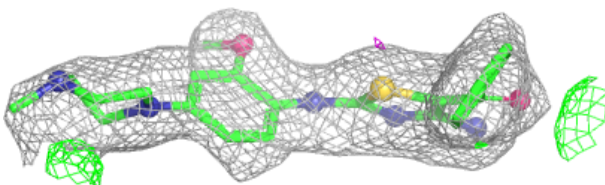
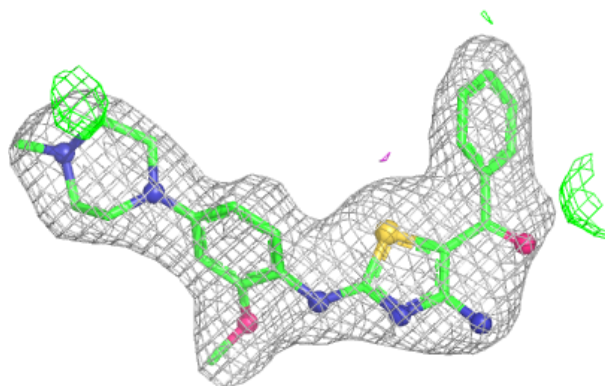


Electron density around B6Z D 501:

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

**Electron density around B6Z 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.