Full wwPDB X-ray Structure Validation Report (i)

Jun 29, 2021 – 08:08 AM BST

PDB ID	:	6EIR
Title	:	DYRK1A in complex with XMD15-27-2
Authors	:	Rothweiler, U.
Deposited on	:	2017-09-19
Resolution	:	2.40 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 (i) symbol.

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

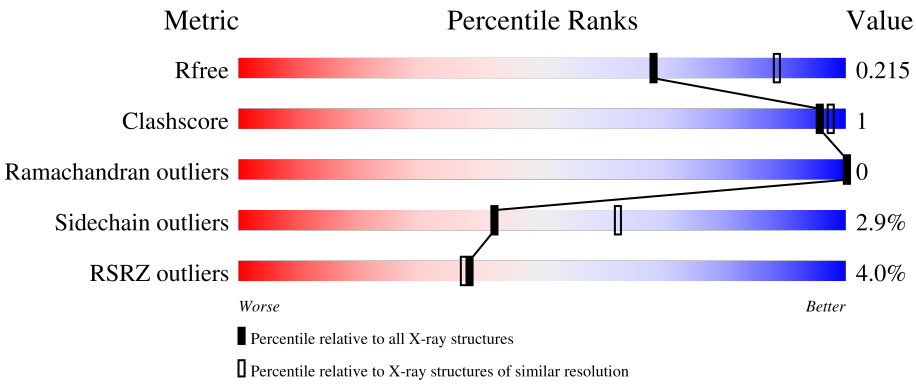
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	% 89% • 7%
1	B	368	3% 86% 5% 9%
1	C	368	6% 86% • 10%
1	D	368	5% 83% 7% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11161 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.

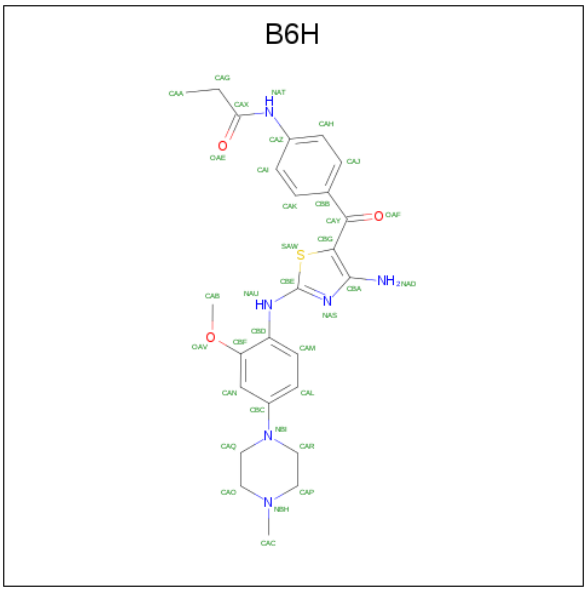
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	342	2794	1798	477	501	1	17	0	0	0
1	B	335	2721	1751	464	488	1	17	0	0	0
1	C	333	2684	1727	455	484	1	17	0	0	0
1	D	333	2711	1752	455	486	1	17	0	0	0

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 {N}-[4-[[4-azanyl-2-[[2-methoxy-4-(4-methylpiperazin-1-yl)phenyl]amino]-1,3-thiazol-5-yl]carbonyl]phenyl]propanamide (three-letter code: B6H) (formula: $C_{25}H_{30}N_6O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	25	6	3	1		
2	B	1	Total	C	N	O	S	0	0
			35	25	6	3	1		
2	C	1	Total	C	N	O	S	0	0
			35	25	6	3	1		
2	D	1	Total	C	N	O	S	0	0
			35	25	6	3	1		

- Molecule 3 is water.

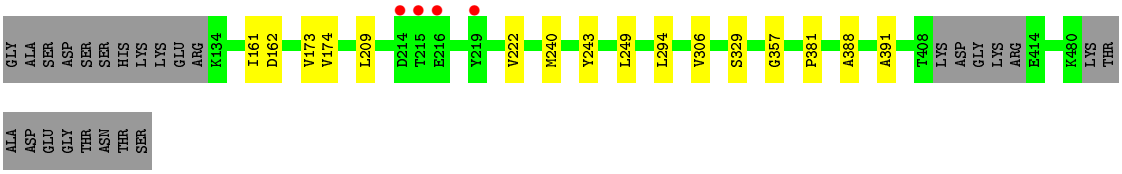
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	14	Total	O	0	0
			14	14		
3	C	20	Total	O	0	0
			20	20		
3	D	35	Total	O	0	0
			35	35		

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.

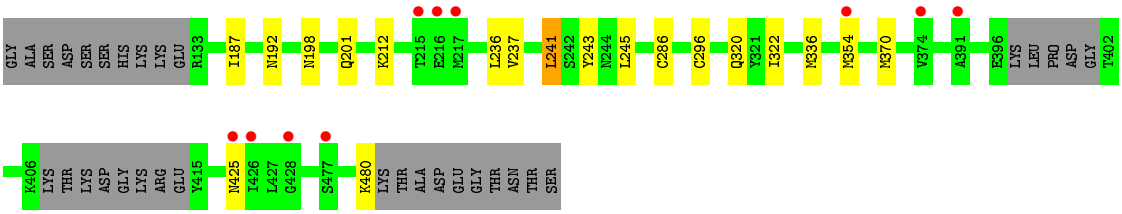
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain A:



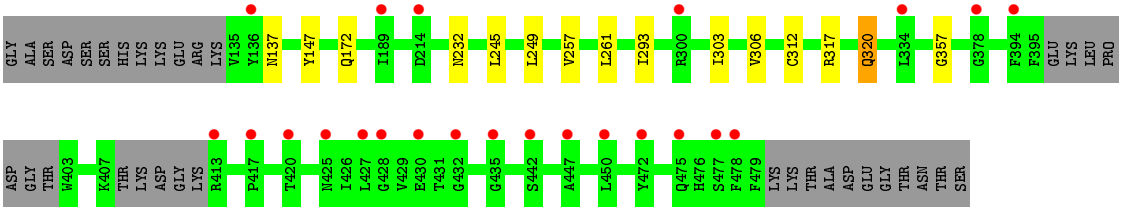
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

Chain B:



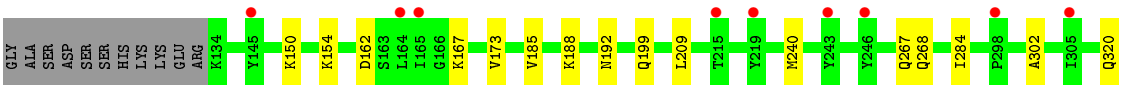
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

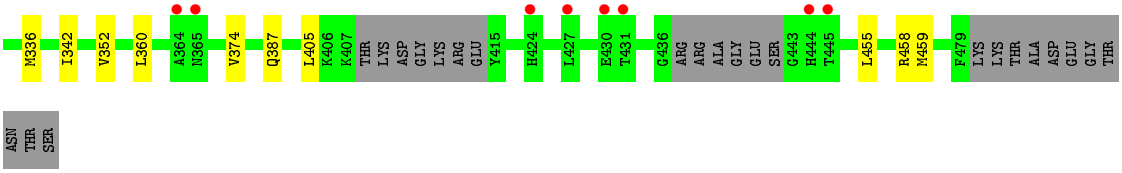
Chain C:



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

Chain D:




ASN
THR
SER
M336
I342
V352
L360
A364
N365
V374
Q387
L405
K406
K407
THR
LYS
ASP
GLY
LYS
ARG
GLU
Y415
H424
L427
E430
T431
G436
ARG
ARG
ALA
GLY
GLU
SER
G443
H444
T445
L455
R458
M459
F479
LYS
LYS
THR
ALA
ASP
GLU
GLY
THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.69Å 87.49Å 229.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.94 – 2.40 47.91 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (47.94-2.40) 92.0 (47.91-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.72 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.234 , 0.258 0.218 , 0.215	Depositor DCC
R_{free} test set	2100 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å^2)	41.7	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 12.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	0.356 for k,h,-l	Xtriage
Reported twinning fraction	0.615 for H, K, L 0.385 for K, H, -L	Depositor
Outliers	0 of 66701 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11161	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 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: B6H, 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	0.37	0/2842	0.55	0/3833
1	B	0.37	0/2766	0.55	0/3732
1	C	0.37	0/2730	0.54	0/3693
1	D	0.37	0/2758	0.55	0/3723
All	All	0.37	0/11096	0.55	0/14981

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	7	0
1	B	2721	0	2695	5	0
1	C	2684	0	2612	7	0
1	D	2711	0	2693	6	0
2	A	35	0	0	1	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
2	D	35	0	0	0	0
3	A	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	0	0	0
3	C	20	0	0	0	0
3	D	35	0	0	0	0
All	All	11161	0	10787	25	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 1.

All (25) 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:C:137:ASN:HD21	1:C:232:ASN:HD22	1.29	0.80
1:B:245:LEU:HD12	1:B:354:MET:SD	2.48	0.54
1:A:222:VAL:CG2	1:A:306:VAL:HG12	2.39	0.53
1:D:268:GLN:HE22	1:D:302:ALA:HA	1.75	0.51
1:B:286:CYS:SG	1:B:322:ILE:HD11	2.51	0.51
1:D:284:ILE:HG21	1:D:342:ILE:HD11	1.94	0.50
1:C:293:ILE:HD11	1:C:303:ILE:HG23	1.95	0.49
1:D:374:VAL:HG11	1:D:405:LEU:HD11	1.95	0.49
1:C:257:VAL:CG1	1:C:261:LEU:HD23	2.43	0.48
1:A:294:LEU:HG	1:A:306:VAL:HG11	1.96	0.48
1:A:161:ILE:HG23	1:A:174:VAL:HG11	1.95	0.48
1:C:320:GLN:HA	1:C:320:GLN:HE21	1.79	0.47
1:D:173:VAL:HG12	1:D:188:LYS:HA	1.96	0.47
1:C:249:LEU:HD22	1:C:357:GLY:HA2	1.95	0.47
1:C:245:LEU:HD11	1:C:303:ILE:HD11	1.98	0.45
1:B:241:LEU:HD13	1:B:296:CYS:HA	1.99	0.45
1:B:187:ILE:CD1	1:B:237:VAL:HG22	2.48	0.44
1:B:198:ASN:HA	1:B:201:GLN:HE21	1.82	0.44
1:C:147:TYR:O	1:C:172:GLN:NE2	2.50	0.44
1:D:455:LEU:HD13	1:D:459:MET:CE	2.47	0.44
1:A:173:VAL:HG21	2:A:501:B6H:CAH	2.48	0.43
1:A:222:VAL:HG21	1:A:306:VAL:HG12	1.98	0.43
1:D:352:VAL:HG11	1:D:360:LEU:HD13	2.01	0.43
1:A:249:LEU:HD22	1:A:357:GLY:HA2	2.00	0.43
1:A:388:ALA:HB3	1:A:391:ALA:HB2	2.02	0.42

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%)	328 (97%)	9 (3%)	0	100	100
1	B	328/368 (89%)	310 (94%)	18 (6%)	0	100	100
1	C	326/368 (89%)	311 (95%)	15 (5%)	0	100	100
1	D	326/368 (89%)	312 (96%)	14 (4%)	0	100	100
All	All	1317/1472 (90%)	1261 (96%)	56 (4%)	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%)	295 (98%)	6 (2%)	55	74
1	B	291/324 (90%)	281 (97%)	10 (3%)	37	56
1	C	283/324 (87%)	279 (99%)	4 (1%)	67	82
1	D	292/324 (90%)	278 (95%)	14 (5%)	25	41
All	All	1167/1296 (90%)	1133 (97%)	34 (3%)	42	62

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	209	LEU

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Mol	Chain	Res	Type
1	A	240	MET
1	A	243	TYR
1	A	329	SER
1	A	381	PRO
1	B	192	ASN
1	B	212	LYS
1	B	236	LEU
1	B	241	LEU
1	B	243	TYR
1	B	320	GLN
1	B	336	MET
1	B	370	MET
1	B	425	ASN
1	B	480	LYS
1	C	306	VAL
1	C	312	CYS
1	C	317	ARG
1	C	320	GLN
1	D	150	LYS
1	D	154	LYS
1	D	162	ASP
1	D	167	LYS
1	D	185	VAL
1	D	192	ASN
1	D	199	GLN
1	D	209	LEU
1	D	240	MET
1	D	267	GLN
1	D	320	GLN
1	D	336	MET
1	D	387	GLN
1	D	458	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	A	369	GLN
1	B	201	GLN
1	B	211	ASN
1	B	268	GLN
1	B	425	ASN

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Mol	Chain	Res	Type
1	C	137	ASN
1	C	260	ASN
1	C	320	GLN
1	D	192	ASN
1	D	199	GLN
1	D	260	ASN
1	D	268	GLN
1	D	320	GLN
1	D	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	C	321	1	15,16,17	0.83	0	19,22,24	0.76	0
1	PTR	B	321	1	15,16,17	0.81	0	19,22,24	0.74	0
1	PTR	A	321	1	15,16,17	0.79	0	19,22,24	0.78	0
1	PTR	D	321	1	15,16,17	0.79	0	19,22,24	0.74	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	C	321	1	-	1/10/11/13	0/1/1/1
1	PTR	B	321	1	-	1/10/11/13	0/1/1/1
1	PTR	A	321	1	-	1/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	D	321	1	-	1/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	321	PTR	O-C-CA-CB
1	B	321	PTR	O-C-CA-CB
1	D	321	PTR	O-C-CA-CB
1	C	321	PTR	N-CA-CB-CG

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	B6H	D	501	-	33,38,38	1.79	5 (15%)	43,53,53	1.79	11 (25%)
2	B6H	A	501	-	33,38,38	1.73	4 (12%)	43,53,53	1.70	8 (18%)
2	B6H	C	501	-	33,38,38	1.70	3 (9%)	43,53,53	1.88	12 (27%)
2	B6H	B	501	-	33,38,38	1.74	4 (12%)	43,53,53	1.72	7 (16%)

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	B6H	D	501	-	-	6/18/34/34	0/4/4/4
2	B6H	A	501	-	-	10/18/34/34	0/4/4/4
2	B6H	C	501	-	-	12/18/34/34	0/4/4/4
2	B6H	B	501	-	-	4/18/34/34	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	B6H	CBG-CAY	-6.24	1.35	1.50
2	A	501	B6H	CBG-CAY	-6.14	1.35	1.50
2	B	501	B6H	CBG-CAY	-6.09	1.35	1.50
2	C	501	B6H	CBG-CAY	-6.02	1.35	1.50
2	A	501	B6H	CBB-CAY	-5.04	1.40	1.49
2	D	501	B6H	CBB-CAY	-5.04	1.40	1.49
2	B	501	B6H	CBB-CAY	-4.90	1.41	1.49
2	C	501	B6H	CBB-CAY	-4.82	1.41	1.49
2	D	501	B6H	CAZ-NAT	-3.75	1.34	1.41
2	B	501	B6H	CAZ-NAT	-3.72	1.34	1.41
2	A	501	B6H	CAZ-NAT	-3.46	1.34	1.41
2	C	501	B6H	CAZ-NAT	-3.39	1.34	1.41
2	B	501	B6H	CAQ-NBI	2.62	1.50	1.46
2	A	501	B6H	CAQ-NBI	2.37	1.50	1.46
2	D	501	B6H	CAR-NBI	2.18	1.50	1.46
2	D	501	B6H	CAQ-NBI	2.12	1.50	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	B6H	CAP-NBH-CAO	5.48	117.19	109.52
2	B	501	B6H	CAZ-NAT-CAX	-5.35	118.14	127.50
2	D	501	B6H	CAZ-NAT-CAX	-5.15	118.49	127.50
2	B	501	B6H	CAR-CAP-NBH	-5.14	105.00	110.80
2	D	501	B6H	CAR-NBI-CAQ	5.05	122.66	111.52
2	A	501	B6H	CAR-NBI-CAQ	4.98	122.52	111.52
2	A	501	B6H	CAR-CAP-NBH	-4.84	105.33	110.80
2	C	501	B6H	CAO-CAQ-NBI	-4.74	101.48	110.70
2	C	501	B6H	CBD-NAU-CBE	-4.65	117.66	129.60
2	D	501	B6H	CBD-NAU-CBE	-4.14	118.95	129.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	B6H	CBD-NAU-CBE	-3.94	119.48	129.60
2	A	501	B6H	CAZ-NAT-CAX	-3.76	120.92	127.50
2	A	501	B6H	CBD-NAU-CBE	-3.75	119.97	129.60
2	B	501	B6H	CAR-NBI-CAQ	3.54	119.34	111.52
2	C	501	B6H	CAZ-NAT-CAX	-3.43	121.49	127.50
2	A	501	B6H	NAD-CBA-NAS	-3.36	118.83	123.19
2	D	501	B6H	NAD-CBA-NAS	-3.29	118.93	123.19
2	C	501	B6H	CAB-OAV-CBF	-3.28	112.58	117.53
2	D	501	B6H	CAB-OAV-CBF	-3.26	112.60	117.53
2	A	501	B6H	CAB-OAV-CBF	-3.25	112.62	117.53
2	D	501	B6H	CAQ-CAO-NBH	-3.24	107.15	110.80
2	B	501	B6H	NAD-CBA-NAS	-3.20	119.03	123.19
2	C	501	B6H	NAD-CBA-NAS	-3.20	119.05	123.19
2	B	501	B6H	OAV-CBF-CBD	2.54	117.92	114.80
2	D	501	B6H	CAP-CAR-NBI	2.48	115.53	110.70
2	C	501	B6H	CAR-NBI-CBC	2.46	124.73	118.09
2	C	501	B6H	OAV-CBF-CBD	2.40	117.75	114.80
2	C	501	B6H	CAR-NBI-CAQ	2.34	116.69	111.52
2	D	501	B6H	CAC-NBH-CAP	-2.33	107.18	110.66
2	C	501	B6H	CAQ-CAO-NBH	-2.33	108.18	110.80
2	C	501	B6H	CAA-CAG-CAX	2.31	120.63	113.30
2	A	501	B6H	CAA-CAG-CAX	2.30	120.59	113.30
2	D	501	B6H	OAV-CBF-CBD	2.28	117.60	114.80
2	D	501	B6H	CAA-CAG-CAX	2.26	120.47	113.30
2	B	501	B6H	CAA-CAG-CAX	2.24	120.42	113.30
2	C	501	B6H	CAL-CBC-NBI	-2.15	118.41	121.38
2	A	501	B6H	OAV-CBF-CBD	2.11	117.39	114.80
2	D	501	B6H	CAP-NBH-CAO	2.10	112.46	109.52

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	B6H	CAN-CBC-NBI-CAR
2	A	501	B6H	CBD-CBF-OAV-CAB
2	B	501	B6H	CBD-CBF-OAV-CAB
2	C	501	B6H	CAL-CBC-NBI-CAR
2	C	501	B6H	CAN-CBC-NBI-CAQ
2	C	501	B6H	CAL-CBC-NBI-CAQ
2	C	501	B6H	CBD-CBF-OAV-CAB
2	D	501	B6H	CBD-CBF-OAV-CAB
2	B	501	B6H	CAN-CBF-OAV-CAB

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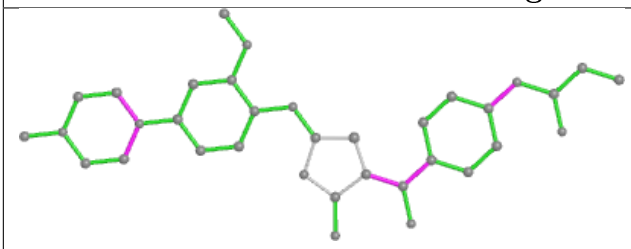
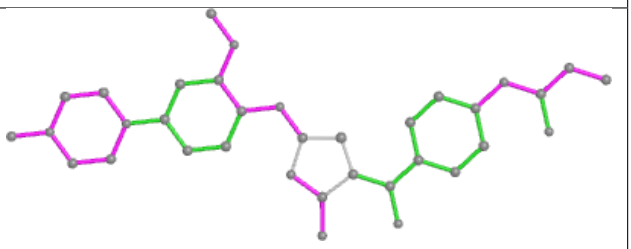
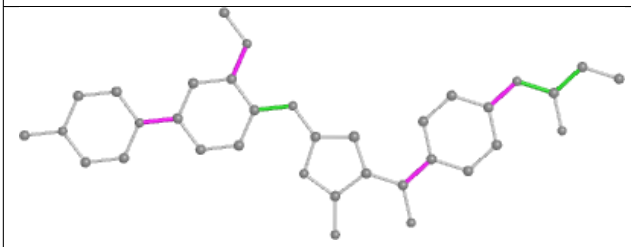
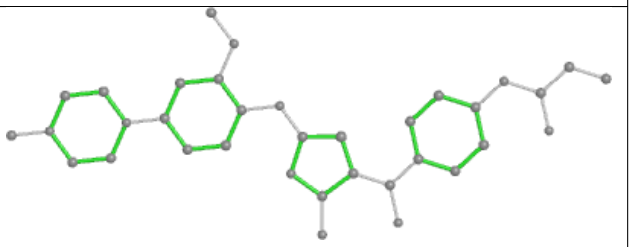
Mol	Chain	Res	Type	Atoms
2	C	501	B6H	CAN-CBF-OAV-CAB
2	D	501	B6H	CAN-CBF-OAV-CAB
2	A	501	B6H	CAN-CBF-OAV-CAB
2	B	501	B6H	CAI-CAZ-NAT-CAX
2	B	501	B6H	CAH-CAZ-NAT-CAX
2	D	501	B6H	CAI-CAZ-NAT-CAX
2	D	501	B6H	CAH-CAZ-NAT-CAX
2	C	501	B6H	OAF-CAY-CBB-CAJ
2	C	501	B6H	CBG-CAY-CBB-CAJ
2	C	501	B6H	OAF-CAY-CBB-CAK
2	A	501	B6H	CAI-CAZ-NAT-CAX
2	A	501	B6H	CAH-CAZ-NAT-CAX
2	C	501	B6H	CBG-CAY-CBB-CAK
2	A	501	B6H	OAF-CAY-CBB-CAK
2	A	501	B6H	CAL-CBC-NBI-CAR
2	A	501	B6H	OAF-CAY-CBB-CAJ
2	C	501	B6H	CAI-CAZ-NAT-CAX
2	C	501	B6H	CAH-CAZ-NAT-CAX
2	A	501	B6H	CAN-CBC-NBI-CAQ
2	D	501	B6H	CAL-CBC-NBI-CAR
2	A	501	B6H	CAN-CBC-NBI-CAR
2	A	501	B6H	CBG-CAY-CBB-CAJ
2	D	501	B6H	OAF-CAY-CBB-CAK

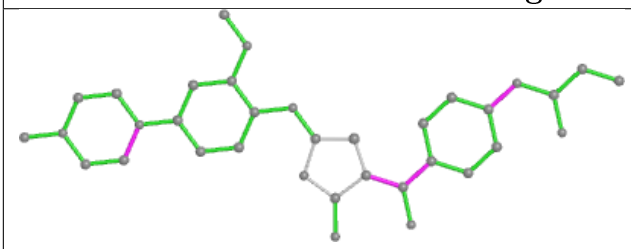
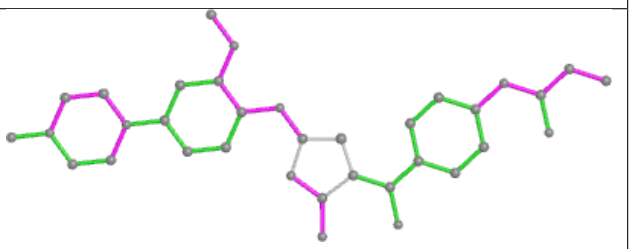
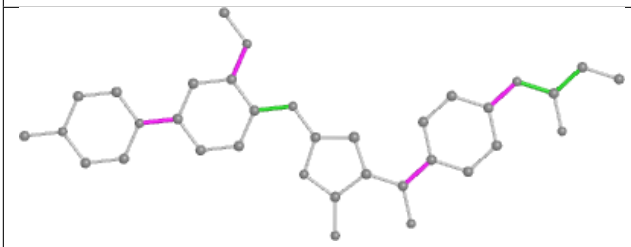
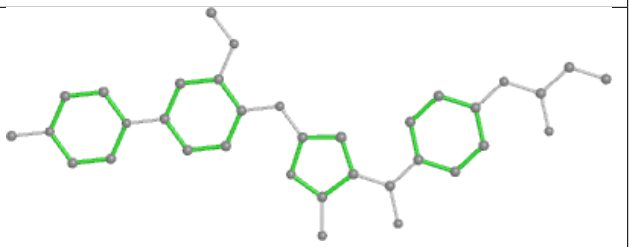
There are no ring outliers.

1 monomer is involved in 1 short contact:

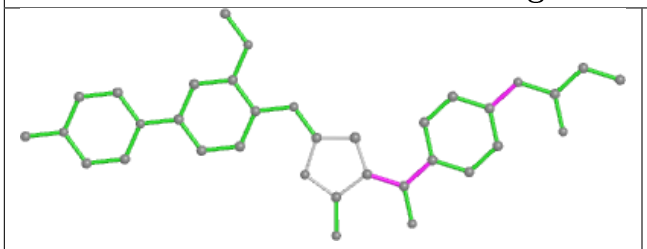
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	B6H	1	0

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 then 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.

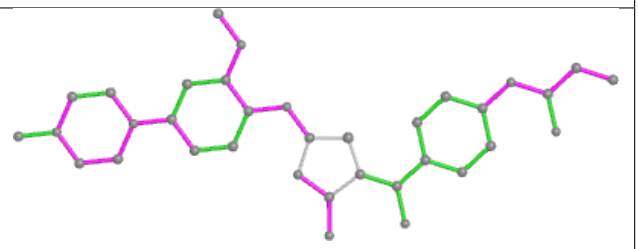
Ligand B6H D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand B6H A 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

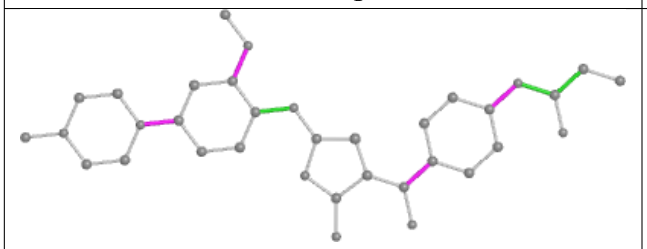
Ligand B6H C 501



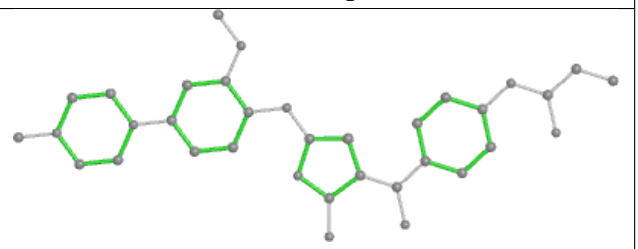
Bond lengths



Bond angles

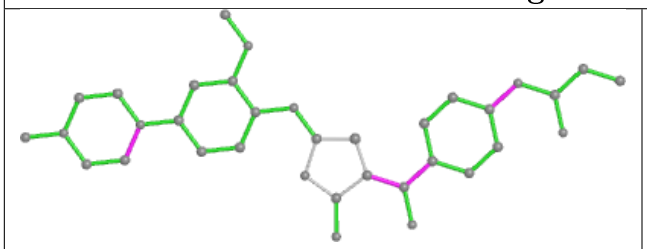


Torsions

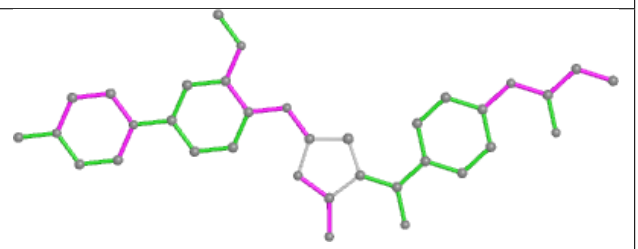


Rings

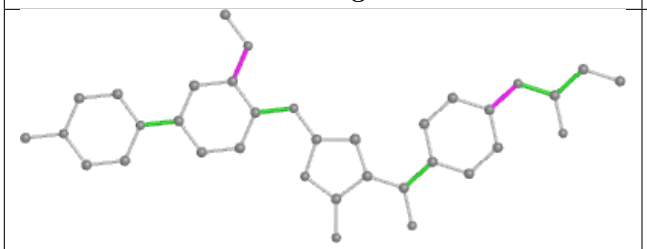
Ligand B6H B 501



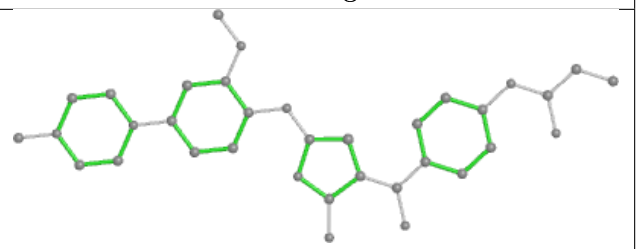
Bond lengths



Bond angles



Torsions



Rings

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%)	0.17	4 (1%)	79	77	30, 40, 53, 66	0
1	B	334/368 (90%)	0.46	10 (2%)	50	49	34, 51, 72, 90	0
1	C	332/368 (90%)	0.57	23 (6%)	16	15	35, 54, 83, 89	0
1	D	332/368 (90%)	0.32	17 (5%)	28	26	31, 47, 68, 88	0
All	All	1339/1472 (90%)	0.38	54 (4%)	38	37	30, 48, 76, 90	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	472	TYR	6.1
1	C	442	SER	5.3
1	D	145	TYR	5.3
1	C	413	ARG	4.7
1	B	217	MET	4.4
1	C	435	GLY	3.7
1	D	243	TYR	3.7
1	B	216	GLU	3.7
1	D	444	HIS	3.4
1	D	215	THR	3.3
1	A	214	ASP	3.3
1	B	215	THR	3.1
1	B	374	VAL	3.1
1	C	450	LEU	3.1
1	A	219	TYR	3.0
1	C	428	GLY	3.0
1	C	427	LEU	3.0
1	C	432	GLY	3.0
1	A	215	THR	2.9
1	C	478	PHE	2.9
1	D	365	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	378	GLY	2.8
1	C	425	ASN	2.8
1	D	424	HIS	2.7
1	C	334	LEU	2.7
1	C	430	GLU	2.6
1	C	447	ALA	2.6
1	D	427	LEU	2.6
1	C	136	TYR	2.6
1	D	430	GLU	2.5
1	A	216	GLU	2.5
1	B	391	ALA	2.4
1	C	300	ARG	2.4
1	D	445	THR	2.3
1	D	219	TYR	2.3
1	C	420	THR	2.3
1	D	165	ILE	2.2
1	B	425	ASN	2.2
1	C	417	PRO	2.2
1	D	305	ILE	2.2
1	B	428	GLY	2.2
1	D	431	THR	2.1
1	C	475	GLN	2.1
1	C	477	SER	2.1
1	D	164	LEU	2.1
1	B	477	SER	2.1
1	C	214	ASP	2.1
1	D	246	TYR	2.1
1	D	364	ALA	2.1
1	C	189	ILE	2.1
1	B	354	MET	2.0
1	D	298	PRO	2.0
1	B	426	ILE	2.0
1	C	394	PHE	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	C	321	16/17	0.90	0.16	53,55,56,56	0
1	PTR	B	321	16/17	0.91	0.13	47,49,50,51	0
1	PTR	D	321	16/17	0.95	0.13	37,38,38,38	0
1	PTR	A	321	16/17	0.97	0.14	31,32,32,33	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

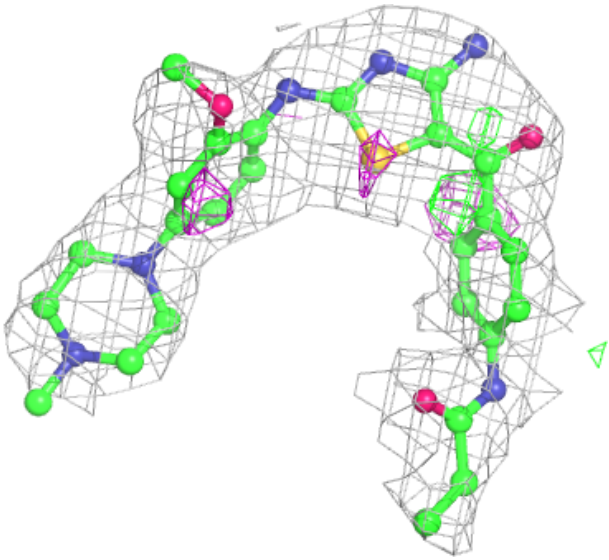
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

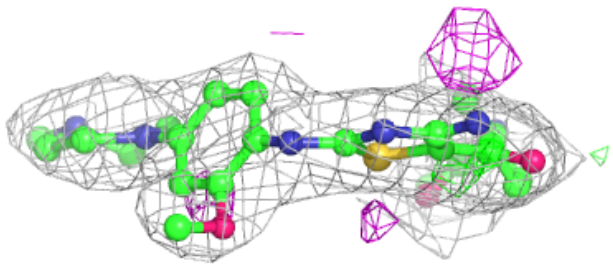
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	B6H	D	501	35/35	0.83	0.24	65,69,73,73	0
2	B6H	B	501	35/35	0.84	0.21	71,72,73,74	0
2	B6H	A	501	35/35	0.84	0.24	66,70,74,75	0
2	B6H	C	501	35/35	0.85	0.19	71,74,76,77	0

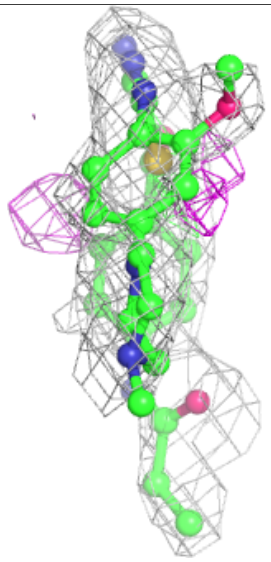
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B6H 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)

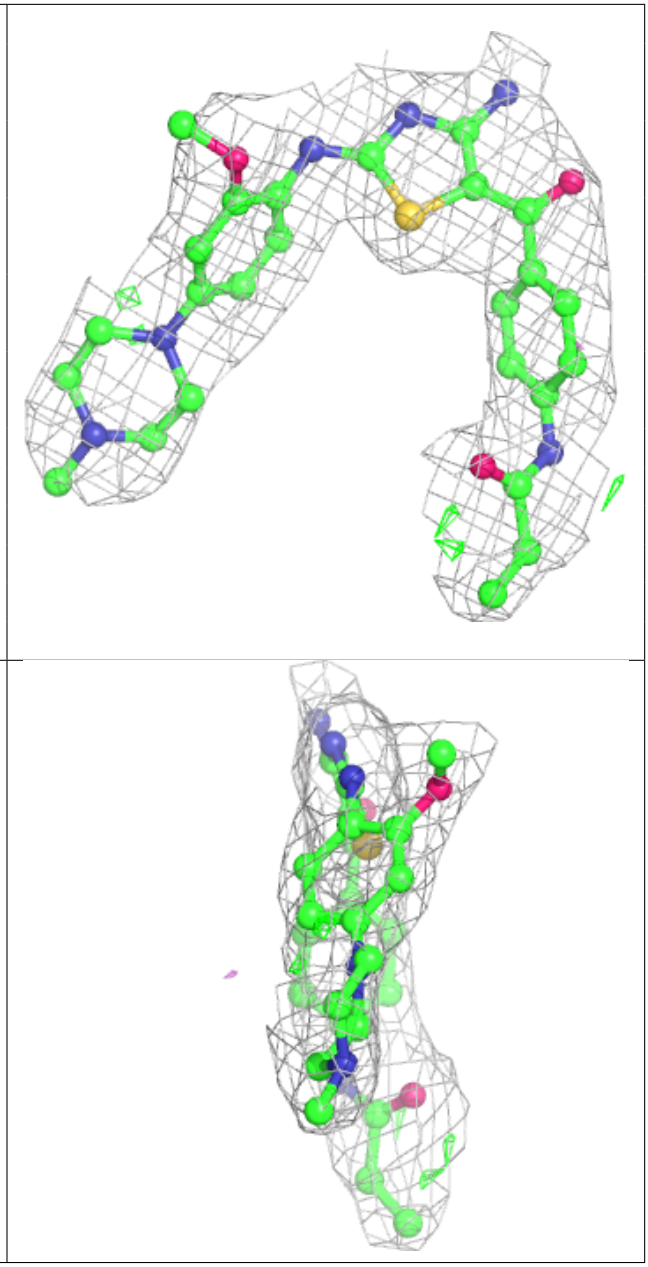






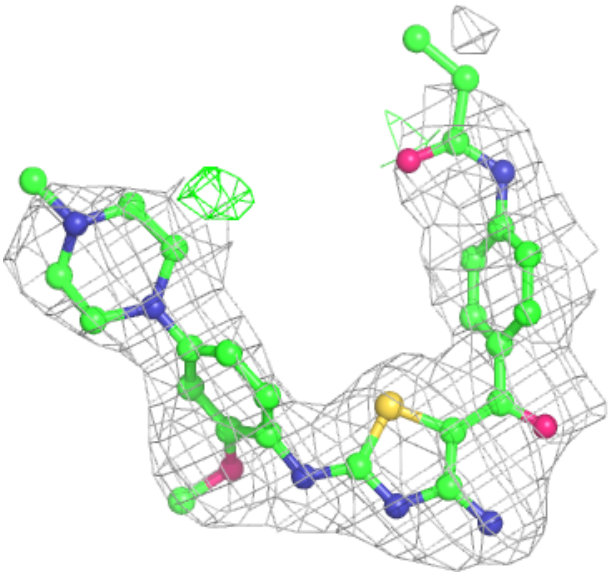
Electron density around B6H B 501:

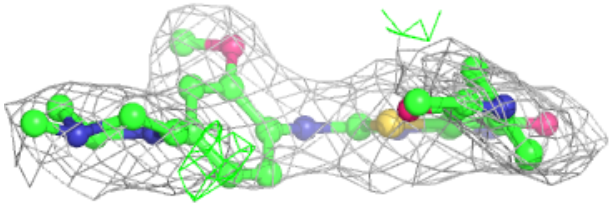
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around B6H 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 B6H C 501:

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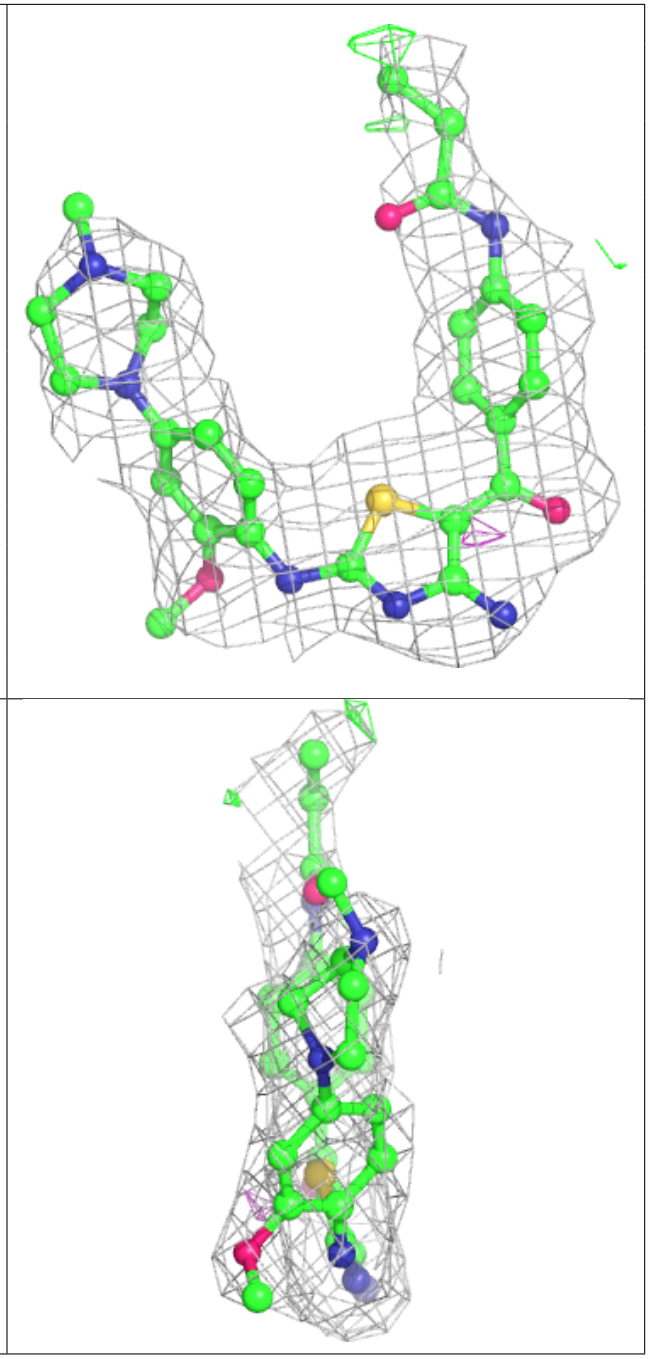
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.