Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 09:57 AM EDT

PDB ID	:	6HZV
Title	:	HUMAN JAK3 IN COMPLEX WITH LASW959 PROTEIN IN COMPLEX WITH LIGAND
Authors	:	Lozoya, E.; Segarra, V.; Bach, J.; Jestel, A.; Lammens, A.; Blaesse, M.
Deposited on	:	2018-10-24
Resolution	:	2.46 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

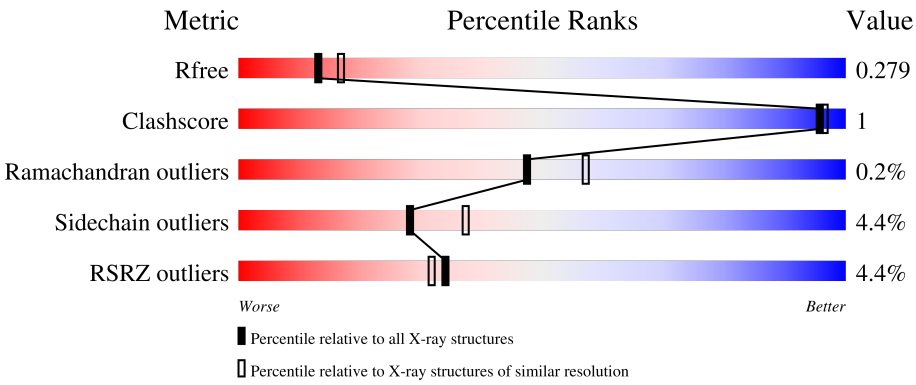
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	285	4% 87% 7% 7%
1	B	285	6% 85% 7% • 6%
1	C	285	2% 87% 6% 7%
1	D	285	4% 85% 6% 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8789 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

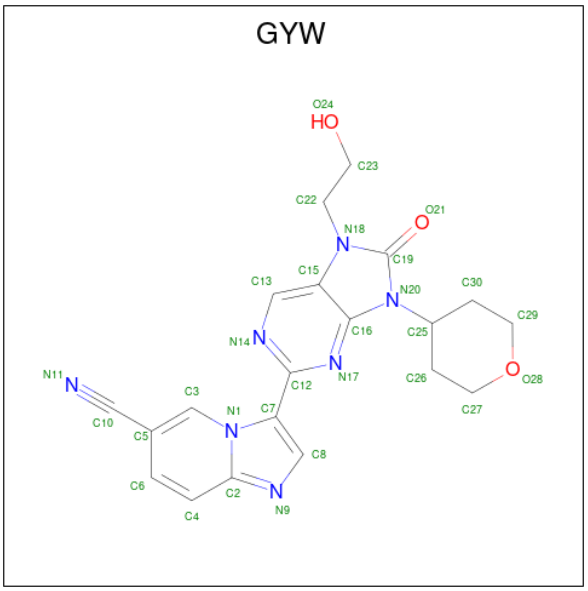
- Molecule 1 is a protein called Tyrosine-protein kinase JAK3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	266	2148	1368	373	392	2	13	0	0	0
1	B	269	2177	1388	377	397	2	13	0	0	0
1	C	265	2153	1371	375	392	2	13	0	2	0
1	D	259	2084	1326	359	385	2	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1048	SER	CYS	conflict	UNP P52333
B	1048	SER	CYS	conflict	UNP P52333
C	1048	SER	CYS	conflict	UNP P52333
D	1048	SER	CYS	conflict	UNP P52333

- Molecule 2 is 3-[7-(2-hydroxyethyl)-9-(oxan-4-yl)-8-oxidanylidene-purin-2-yl]imidazo[1,2-a]pyridine-6-carbonitrile (three-letter code: GYW) (formula: $C_{20}H_{19}N_7O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	20	7	3	0	0
			Total	C	N	O		
2	B	1	30	20	7	3	0	0
			Total	C	N	O		
2	C	1	30	20	7	3	0	0
			Total	C	N	O		
2	D	1	30	20	7	3	0	0

- Molecule 3 is water.

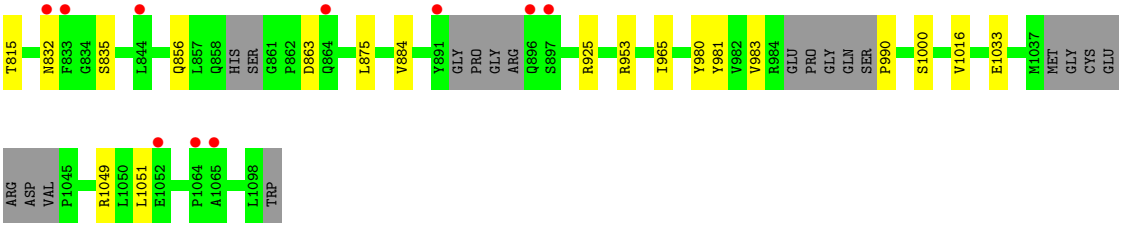
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	29	29	29	0	0
			Total	O		
3	B	27	27	27	0	0
			Total	O		
3	C	28	28	28	0	0
			Total	O		
3	D	23	23	23	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

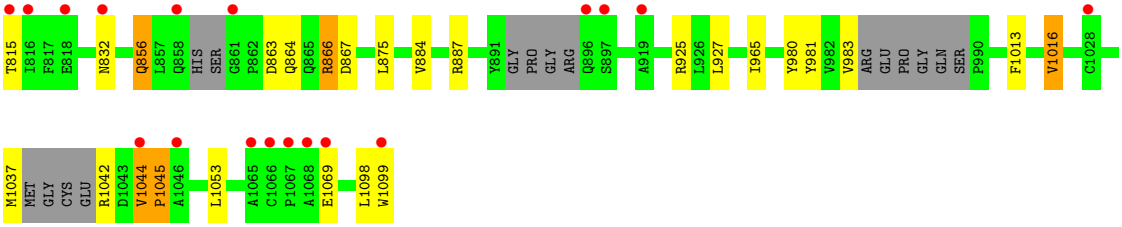
• Molecule 1: Tyrosine-protein kinase JAK3

Chain A:



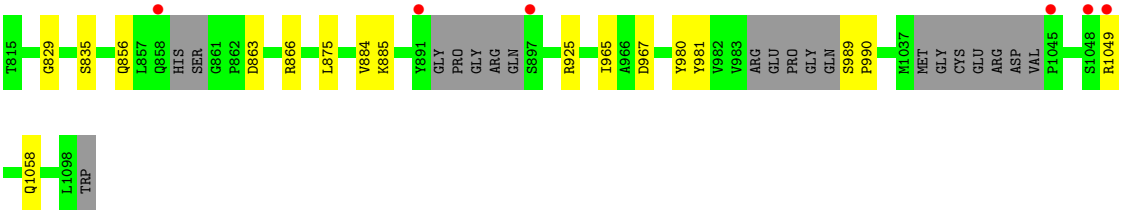
• Molecule 1: Tyrosine-protein kinase JAK3

Chain B:



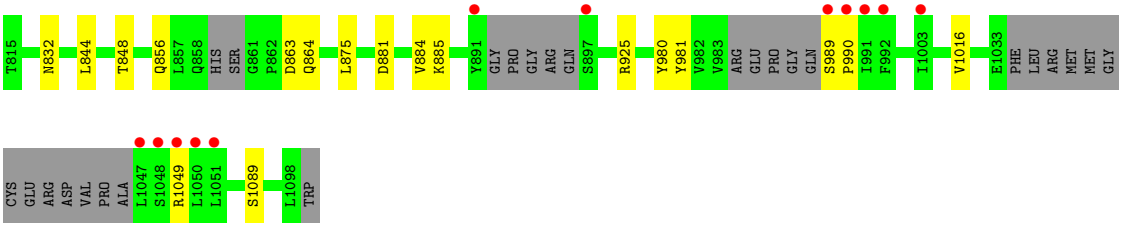
• Molecule 1: Tyrosine-protein kinase JAK3

Chain C:



• Molecule 1: Tyrosine-protein kinase JAK3

Chain D:


T815
N832
L844
T848
Q856
L857
Q858
HIS
SER
G861
P862
D863
Q864
L875
D881
V884
K885
Y891
GLY
PRO
GLY
ARG
GLN
S897
R925
Y980
Y981
V982
V983
ARG
GLU
PRO
GLY
GLN
S989
P990
I991
F992
I1003
V1016
E1033
PHE
LEU
ARG
MET
MET
GLY
CYS
GLU
ARG
ASP
VAL
PRO
ALA
L1047
S1048
R1049
L1050
L1051
S1089
L1098
TRP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.07Å 112.81Å 104.47Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	43.23 – 2.46 43.23 – 2.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.23-2.46) 99.6 (43.23-2.46)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.223 , 0.275 0.232 , 0.279	Depositor DCC
R_{free} test set	1000 reflections (2.11%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8789	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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: PTR, GYW

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	0.33	0/2160	0.51	0/2911
1	B	0.33	0/2191	0.51	0/2956
1	C	0.33	0/2168	0.51	0/2922
1	D	0.33	0/2094	0.50	0/2825
All	All	0.33	0/8613	0.51	0/11614

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	832	ASN	Peptide
1	B	832	ASN	Peptide
1	D	832	ASN	Peptide

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	2148	0	2132	3	0
1	B	2177	0	2155	11	0
1	C	2153	0	2140	5	0
1	D	2084	0	2060	2	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	29	0	0	0	0
3	B	27	0	0	0	0
3	C	28	0	0	0	0
3	D	23	0	0	0	0
All	All	8789	0	8487	18	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 (18) 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:B:1044:VAL:HB	1:B:1045:PRO:HD2	1.75	0.67
1:B:927:LEU:HD12	1:B:1099:TRP:CZ3	2.40	0.57
1:C:866:ARG:HG3	1:D:1089:SER:OG	2.06	0.56
1:B:1069:GLU:HB3	1:B:1098:LEU:HD11	1.87	0.56
1:C:884:VAL:HG23	1:C:965:ILE:O	2.07	0.55
1:B:884:VAL:HG23	1:B:965:ILE:O	2.07	0.54
1:B:1044:VAL:CB	1:B:1045:PRO:HD2	2.39	0.52
1:B:1042:ARG:HD3	1:C:829:GLY:HA2	1.92	0.51
1:B:866:ARG:HG2	1:B:867:ASP:N	2.31	0.46
1:B:1013:PHE:HA	1:B:1016:VAL:HG13	1.98	0.45
1:B:856:GLN:HE21	1:B:856:GLN:C	2.22	0.42
1:D:989:SER:N	1:D:990:PRO:CD	2.83	0.42
1:C:989:SER:N	1:C:990:PRO:CD	2.82	0.42
1:A:1000:SER:HB3	1:A:1051:LEU:HD21	2.03	0.41
1:A:953:ARG:NH1	1:A:990:PRO:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1042:ARG:CD	1:C:829:GLY:HA2	2.51	0.41
1:A:884:VAL:HG23	1:A:965:ILE:O	2.21	0.41
1:B:1037:MET:HB3	1:B:1053:LEU:HD21	2.03	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	254/285 (89%)	246 (97%)	8 (3%)	0	100	100
1	B	257/285 (90%)	249 (97%)	7 (3%)	1 (0%)	34	41
1	C	255/285 (90%)	250 (98%)	4 (2%)	1 (0%)	34	41
1	D	247/285 (87%)	239 (97%)	8 (3%)	0	100	100
All	All	1013/1140 (89%)	984 (97%)	27 (3%)	2 (0%)	47	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	967	ASP
1	B	1045	PRO

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	232/247 (94%)	222 (96%)	10 (4%)	29	38
1	B	235/247 (95%)	224 (95%)	11 (5%)	26	34
1	C	233/247 (94%)	225 (97%)	8 (3%)	37	48
1	D	226/247 (92%)	214 (95%)	12 (5%)	22	29
All	All	926/988 (94%)	885 (96%)	41 (4%)	28	37

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	815	THR
1	A	835	SER
1	A	856	GLN
1	A	863	ASP
1	A	875	LEU
1	A	925	ARG
1	A	983	VAL
1	A	1016	VAL
1	A	1033	GLU
1	A	1049	ARG
1	B	815	THR
1	B	856	GLN
1	B	863	ASP
1	B	864	GLN
1	B	866	ARG
1	B	875	LEU
1	B	887	ARG
1	B	925	ARG
1	B	983	VAL
1	B	1016	VAL
1	B	1044	VAL
1	C	835	SER
1	C	856	GLN
1	C	863	ASP
1	C	875	LEU
1	C	885	LYS
1	C	925	ARG
1	C	1049	ARG
1	C	1058	GLN
1	D	844	LEU
1	D	848	THR
1	D	856	GLN
1	D	863	ASP

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Mol	Chain	Res	Type
1	D	864	GLN
1	D	875	LEU
1	D	881	ASP
1	D	884	VAL
1	D	885	LYS
1	D	925	ARG
1	D	1016	VAL
1	D	1049	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	827	GLN
1	A	832	ASN
1	A	856	GLN
1	A	873	GLN
1	A	915	GLN
1	A	1058	GLN
1	B	873	GLN
1	B	915	GLN
1	B	1058	GLN
1	C	869	GLN
1	C	873	GLN
1	C	915	GLN
1	C	1058	GLN
1	D	915	GLN
1	D	1058	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	B	980	1	15,16,17	2.02	1 (6%)	19,22,24	0.55	0
1	PTR	D	980	1	15,16,17	2.05	1 (6%)	19,22,24	0.49	0
1	PTR	C	980	1	15,16,17	2.00	1 (6%)	19,22,24	0.63	0
1	PTR	D	981	1	15,16,17	1.95	1 (6%)	19,22,24	0.84	0
1	PTR	A	980	1	15,16,17	2.03	1 (6%)	19,22,24	0.56	0
1	PTR	C	981	1	15,16,17	2.05	1 (6%)	19,22,24	0.55	0
1	PTR	A	981	1	15,16,17	2.00	1 (6%)	19,22,24	0.57	0
1	PTR	B	981	1	15,16,17	1.98	1 (6%)	19,22,24	0.55	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	B	980	1	-	0/10/11/13	0/1/1/1
1	PTR	D	980	1	-	1/10/11/13	0/1/1/1
1	PTR	C	980	1	-	0/10/11/13	0/1/1/1
1	PTR	D	981	1	-	0/10/11/13	0/1/1/1
1	PTR	A	980	1	-	0/10/11/13	0/1/1/1
1	PTR	C	981	1	-	0/10/11/13	0/1/1/1
1	PTR	A	981	1	-	1/10/11/13	0/1/1/1
1	PTR	B	981	1	-	0/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	981	PTR	OH-CZ	-7.54	1.23	1.40
1	A	981	PTR	OH-CZ	-7.51	1.23	1.40
1	C	980	PTR	OH-CZ	-7.48	1.23	1.40
1	D	980	PTR	OH-CZ	-7.46	1.23	1.40
1	B	981	PTR	OH-CZ	-7.40	1.23	1.40
1	B	980	PTR	OH-CZ	-7.25	1.24	1.40
1	D	981	PTR	OH-CZ	-7.24	1.24	1.40
1	A	980	PTR	OH-CZ	-7.24	1.24	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	981	PTR	CZ-OH-P-O1P
1	D	980	PTR	CZ-OH-P-O2P

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	GYW	A	1101	-	31,34,34	1.24	4 (12%)	32,49,49	3.22	13 (40%)
2	GYW	B	1101	-	31,34,34	1.18	3 (9%)	32,49,49	3.34	13 (40%)
2	GYW	C	1101	-	31,34,34	1.27	4 (12%)	32,49,49	3.27	12 (37%)
2	GYW	D	1101	-	31,34,34	1.31	5 (16%)	32,49,49	3.32	11 (34%)

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	GYW	A	1101	-	-	2/9/21/21	0/5/5/5
2	GYW	B	1101	-	-	2/9/21/21	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GYW	C	1101	-	-	2/9/21/21	0/5/5/5
2	GYW	D	1101	-	-	2/9/21/21	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	GYW	C12-N14	3.40	1.39	1.34
2	A	1101	GYW	C12-N14	3.39	1.39	1.34
2	D	1101	GYW	C16-N17	3.26	1.38	1.34
2	C	1101	GYW	C12-N14	3.24	1.39	1.34
2	A	1101	GYW	C16-N17	3.05	1.38	1.34
2	C	1101	GYW	C16-N17	3.04	1.38	1.34
2	B	1101	GYW	C12-N14	3.01	1.39	1.34
2	B	1101	GYW	C16-N17	2.98	1.38	1.34
2	C	1101	GYW	C13-N14	2.60	1.39	1.34
2	D	1101	GYW	C13-N14	2.38	1.39	1.34
2	A	1101	GYW	C13-N14	2.25	1.39	1.34
2	D	1101	GYW	C16-N20	2.22	1.41	1.38
2	D	1101	GYW	C12-N17	2.22	1.39	1.34
2	A	1101	GYW	C12-N17	2.17	1.39	1.34
2	B	1101	GYW	C13-N14	2.14	1.38	1.34
2	C	1101	GYW	C12-N17	2.13	1.39	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	GYW	N20-C19-N18	11.08	114.92	106.89
2	D	1101	GYW	N20-C19-N18	10.83	114.74	106.89
2	C	1101	GYW	N20-C19-N18	10.43	114.46	106.89
2	A	1101	GYW	N20-C19-N18	10.36	114.40	106.89
2	B	1101	GYW	C15-N18-C19	-7.35	102.41	110.05
2	A	1101	GYW	C15-N18-C19	-7.19	102.58	110.05
2	D	1101	GYW	C15-N18-C19	-7.12	102.65	110.05
2	C	1101	GYW	C15-N18-C19	-6.96	102.82	110.05
2	D	1101	GYW	C15-C16-N17	-6.54	121.71	126.51
2	D	1101	GYW	N14-C12-N17	-6.51	118.87	125.25
2	C	1101	GYW	N14-C12-N17	-6.43	118.95	125.25
2	C	1101	GYW	C15-C16-N17	-6.24	121.93	126.51
2	B	1101	GYW	C15-C16-N17	-6.14	122.00	126.51
2	A	1101	GYW	C15-C16-N17	-6.01	122.10	126.51
2	A	1101	GYW	N14-C12-N17	-5.83	119.54	125.25
2	B	1101	GYW	N14-C12-N17	-5.56	119.81	125.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	GYW	C16-N20-C25	4.60	134.86	125.40
2	C	1101	GYW	O21-C19-N18	-4.55	122.32	126.92
2	B	1101	GYW	C13-N14-C12	3.89	121.36	116.22
2	C	1101	GYW	C13-N14-C12	3.80	121.24	116.22
2	D	1101	GYW	O21-C19-N18	-3.78	123.10	126.92
2	A	1101	GYW	C13-N14-C12	3.77	121.20	116.22
2	B	1101	GYW	O21-C19-N18	-3.75	123.13	126.92
2	D	1101	GYW	C13-N14-C12	3.74	121.17	116.22
2	A	1101	GYW	C16-N20-C25	3.73	133.07	125.40
2	D	1101	GYW	C22-N18-C15	3.73	132.20	124.56
2	B	1101	GYW	C22-N18-C15	3.66	132.06	124.56
2	A	1101	GYW	O21-C19-N18	-3.65	123.23	126.92
2	C	1101	GYW	C7-C12-N14	3.64	122.37	116.88
2	C	1101	GYW	C22-N18-C15	3.55	131.82	124.56
2	D	1101	GYW	C16-N20-C25	3.37	132.33	125.40
2	A	1101	GYW	C22-N18-C15	3.16	131.04	124.56
2	D	1101	GYW	C7-C12-N14	3.06	121.50	116.88
2	B	1101	GYW	O21-C19-N20	-3.02	121.95	126.89
2	A	1101	GYW	C22-N18-C19	2.98	126.36	122.30
2	B	1101	GYW	C7-C12-N14	2.91	121.28	116.88
2	D	1101	GYW	O21-C19-N20	-2.90	122.15	126.89
2	A	1101	GYW	O21-C19-N20	-2.77	122.37	126.89
2	C	1101	GYW	C16-N20-C25	2.77	131.09	125.40
2	A	1101	GYW	C7-C12-N14	2.69	120.94	116.88
2	B	1101	GYW	C22-N18-C19	2.36	125.52	122.30
2	A	1101	GYW	C16-C15-N18	2.32	110.07	106.91
2	B	1101	GYW	C15-C13-N14	-2.27	118.37	121.22
2	C	1101	GYW	O21-C19-N20	-2.25	123.22	126.89
2	C	1101	GYW	C22-N18-C19	2.23	125.34	122.30
2	B	1101	GYW	C16-C15-N18	2.19	109.89	106.91
2	C	1101	GYW	C25-N20-C19	2.15	126.51	122.62
2	A	1101	GYW	C15-C13-N14	-2.14	118.53	121.22
2	D	1101	GYW	C22-N18-C19	2.09	125.14	122.30

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	GYW	C23-C22-N18-C19
2	B	1101	GYW	C23-C22-N18-C15
2	B	1101	GYW	C23-C22-N18-C19
2	C	1101	GYW	C23-C22-N18-C15

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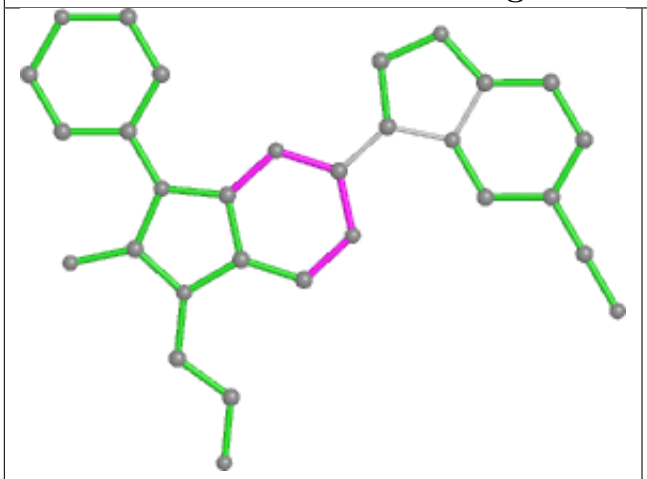
Mol	Chain	Res	Type	Atoms
2	C	1101	GYW	C23-C22-N18-C19
2	D	1101	GYW	C23-C22-N18-C15
2	D	1101	GYW	C23-C22-N18-C19
2	A	1101	GYW	C23-C22-N18-C15

There are no ring outliers.

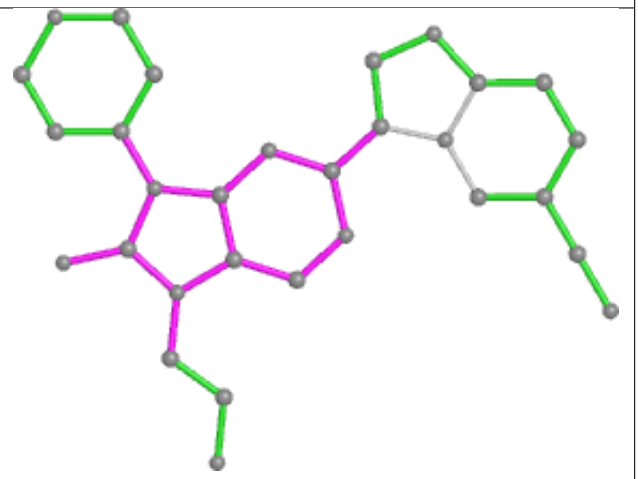
No monomer is involved in short contacts.

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 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.

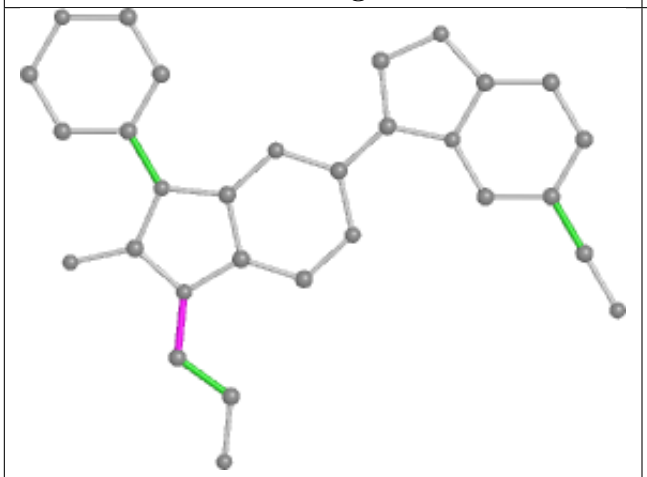
Ligand GYW A 1101



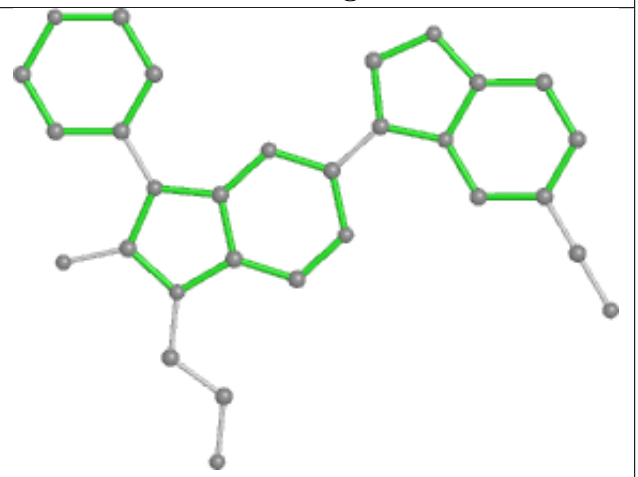
Bond lengths



Bond angles

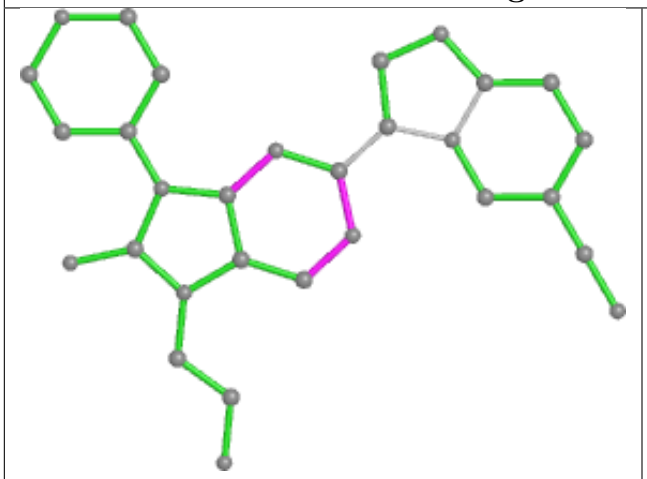


Torsions

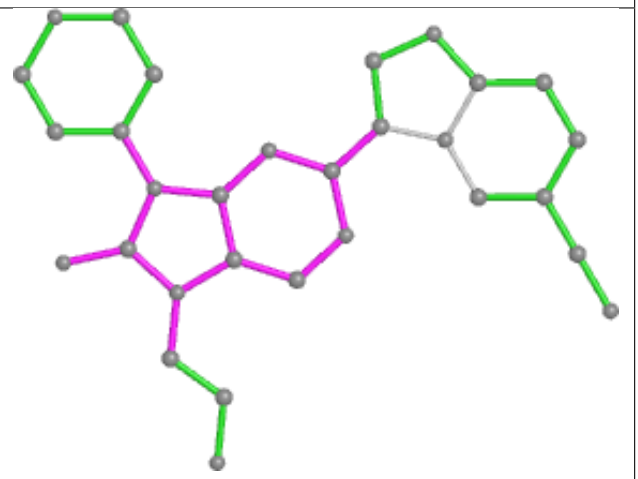


Rings

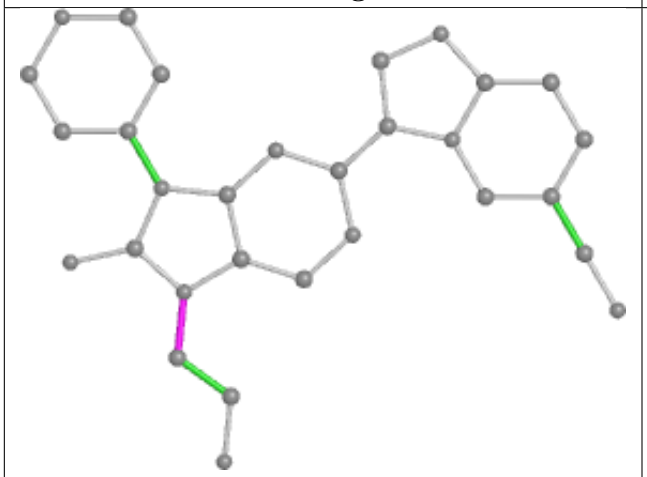
Ligand GYW B 1101



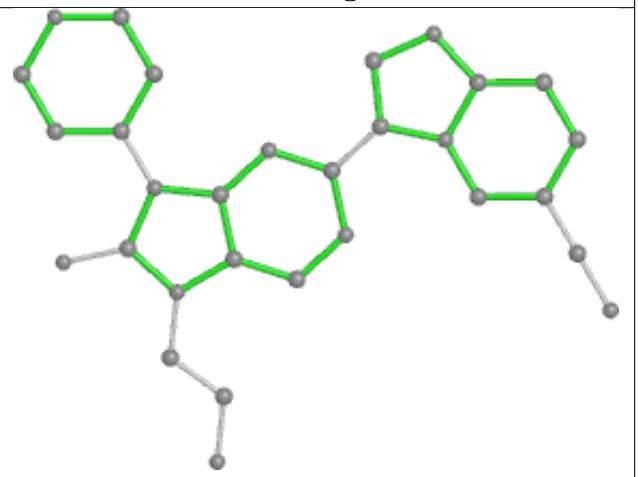
Bond lengths



Bond angles

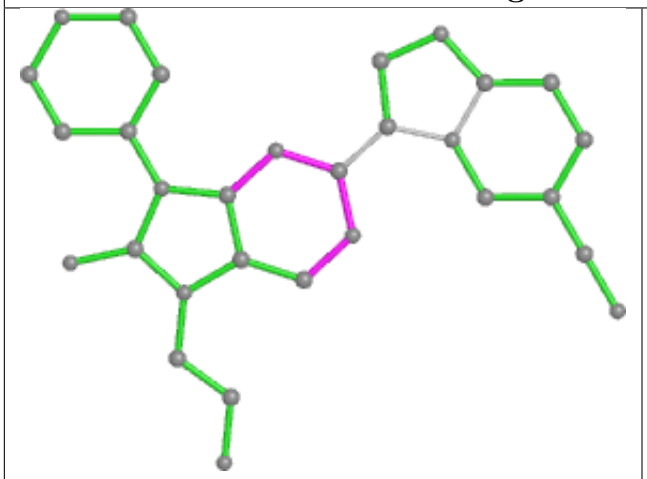


Torsions

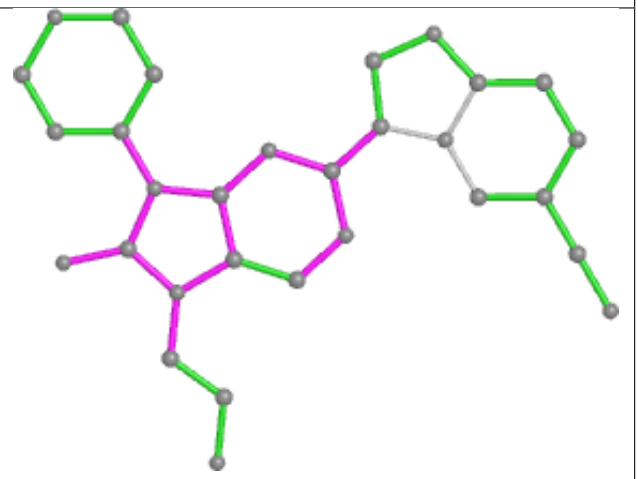


Rings

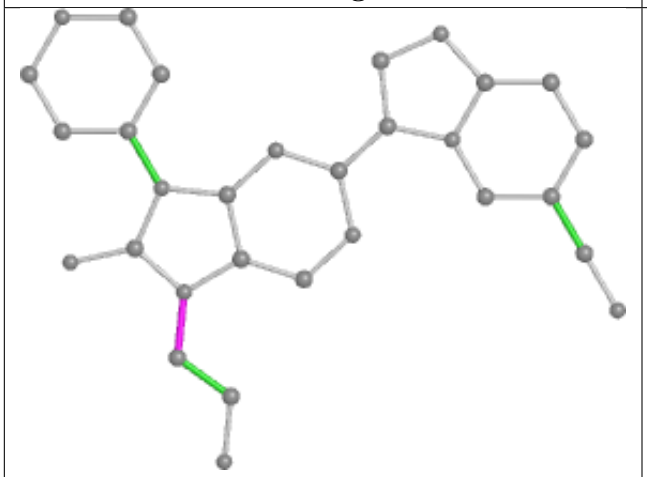
Ligand GYW C 1101



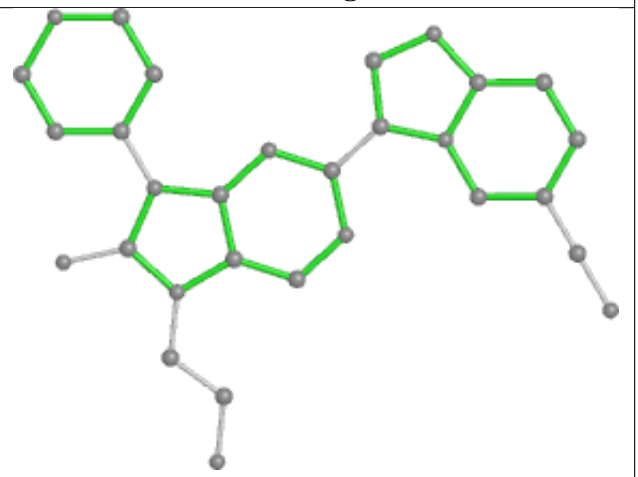
Bond lengths



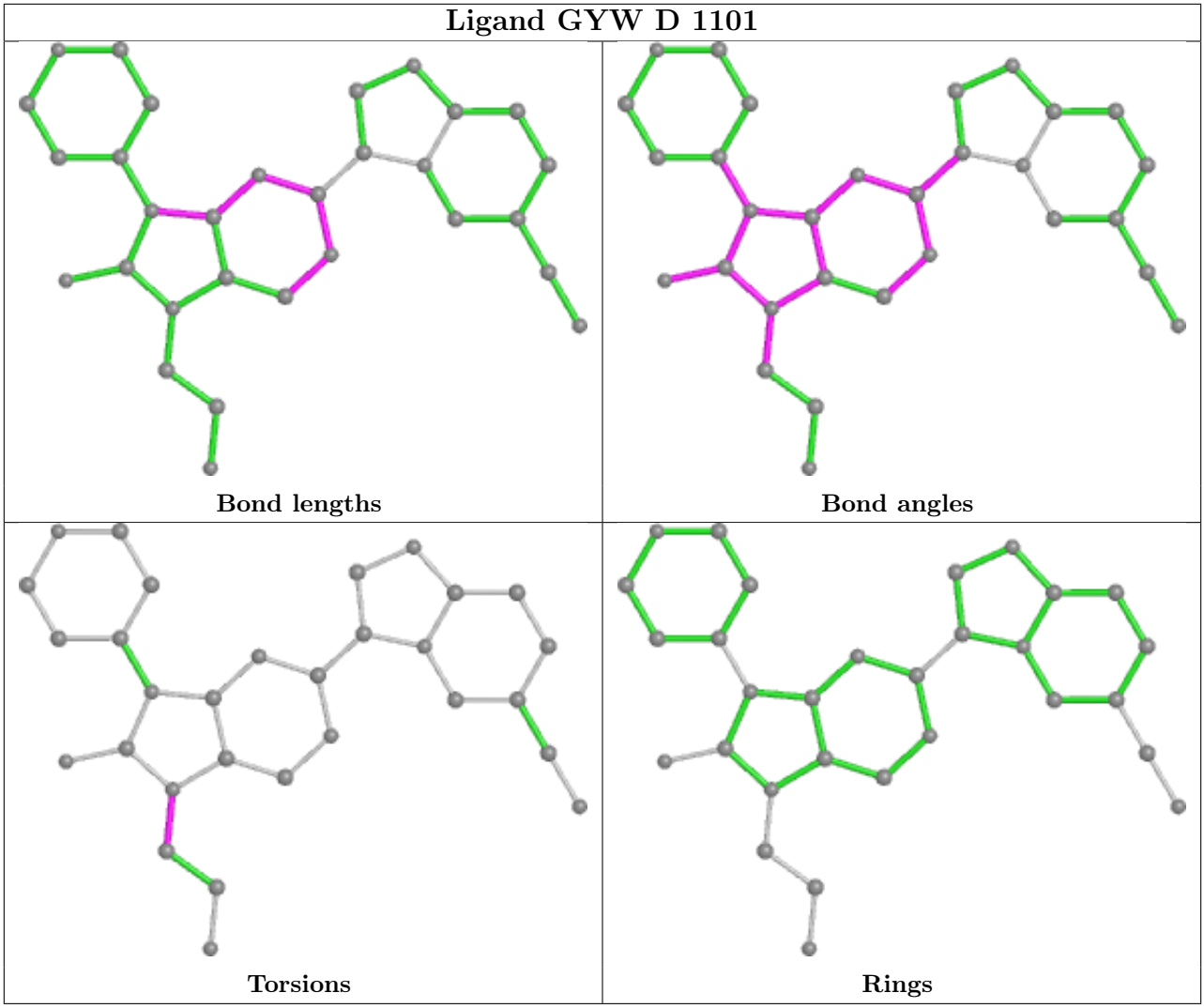
Bond angles



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	264/285 (92%)	0.27	10 (3%)	40	37	28, 43, 72, 88	1 (0%)
1	B	267/285 (93%)	0.33	18 (6%)	17	14	28, 44, 69, 108	0
1	C	263/285 (92%)	0.12	6 (2%)	60	56	27, 41, 62, 70	0
1	D	257/285 (90%)	0.32	12 (4%)	31	29	29, 46, 75, 104	0
All	All	1051/1140 (92%)	0.26	46 (4%)	34	32	27, 44, 70, 108	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	896	GLN	5.5
1	A	897	SER	5.1
1	A	833	PHE	4.5
1	B	1065	ALA	4.0
1	A	891	TYR	3.7
1	B	832	ASN	3.7
1	D	989	SER	3.5
1	D	1050	LEU	3.5
1	D	1048	SER	3.5
1	B	1099	TRP	3.4
1	B	1068	ALA	3.4
1	B	896	GLN	3.4
1	B	1046	ALA	3.3
1	C	897	SER	3.3
1	D	1049	ARG	3.3
1	B	816	ILE	3.2
1	C	891	TYR	3.2
1	D	1003	ILE	3.0
1	B	1028	CYS	2.9
1	C	858	GLN	2.9
1	B	1067	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	897	SER	2.7
1	B	1066	CYS	2.7
1	C	1045	PRO	2.7
1	B	919	ALA	2.6
1	A	864	GLN	2.6
1	B	1044	VAL	2.5
1	B	818	GLU	2.5
1	A	844	LEU	2.4
1	D	992	PHE	2.4
1	B	861	GLY	2.3
1	D	991	ILE	2.3
1	D	1047	LEU	2.3
1	B	858	GLN	2.3
1	B	815	THR	2.3
1	A	832	ASN	2.2
1	D	1051	LEU	2.2
1	A	1064	PRO	2.2
1	B	897	SER	2.1
1	A	1052	GLU	2.1
1	D	990	PRO	2.1
1	C	1048	SER	2.1
1	C	1049	ARG	2.1
1	D	891	TYR	2.0
1	B	1069	GLU	2.0
1	A	1065	ALA	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	980	16/17	0.80	0.22	55,59,77,77	0
1	PTR	A	981	16/17	0.85	0.18	57,67,72,73	0
1	PTR	A	980	16/17	0.86	0.17	55,60,78,79	0
1	PTR	D	980	16/17	0.89	0.17	57,66,85,86	0
1	PTR	C	981	16/17	0.90	0.17	51,60,64,65	0
1	PTR	B	981	16/17	0.90	0.19	57,66,71,71	0
1	PTR	D	981	16/17	0.90	0.20	61,72,79,79	0
1	PTR	C	980	16/17	0.91	0.14	50,53,70,72	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

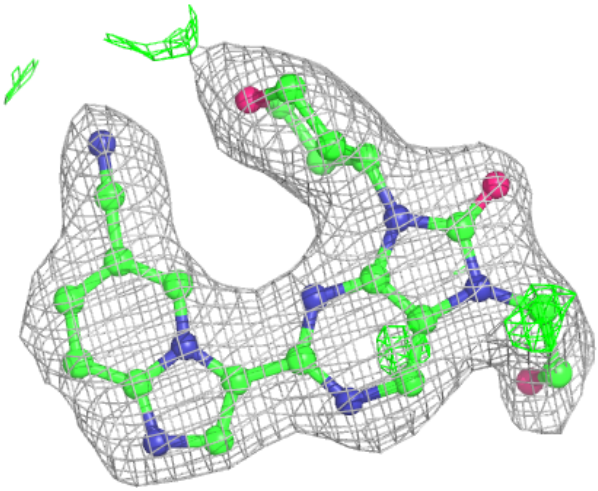
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

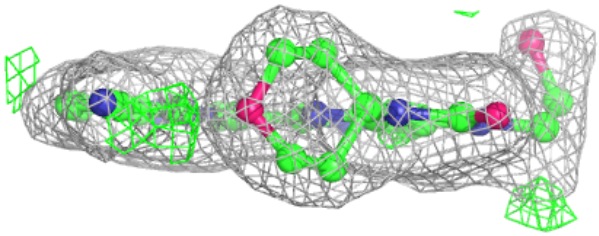
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GYW	D	1101	30/30	0.93	0.14	35,38,43,45	0
2	GYW	B	1101	30/30	0.94	0.18	34,36,41,43	0
2	GYW	C	1101	30/30	0.94	0.15	31,35,42,45	0
2	GYW	A	1101	30/30	0.94	0.15	32,34,39,43	0

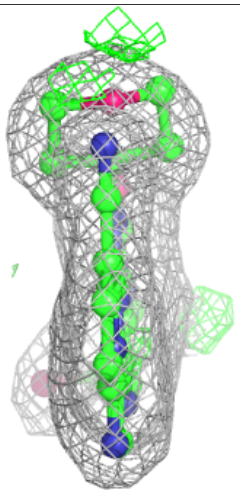
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GYW D 1101:

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

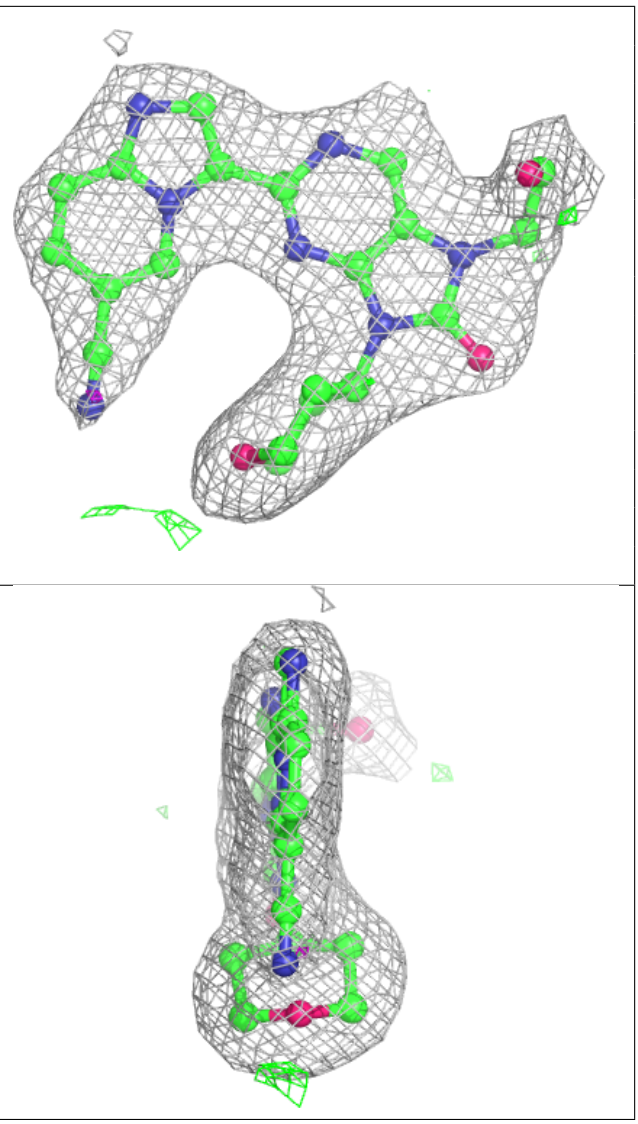






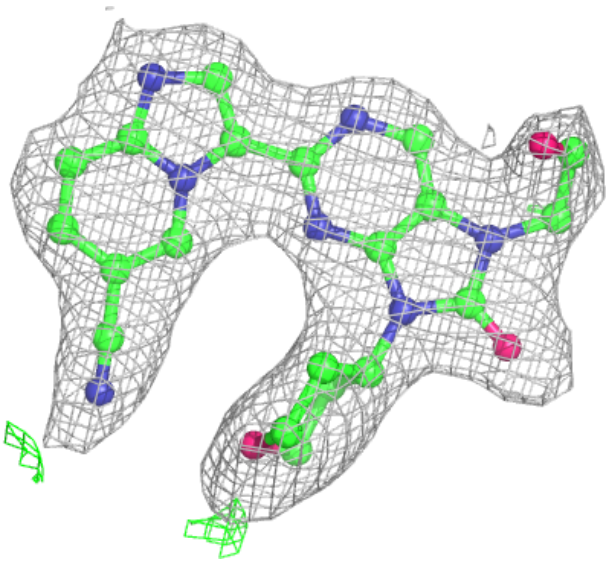
Electron density around GYW B 1101:

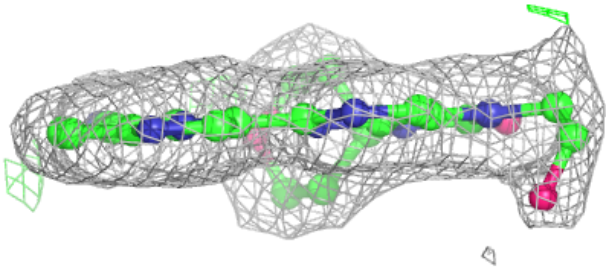
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

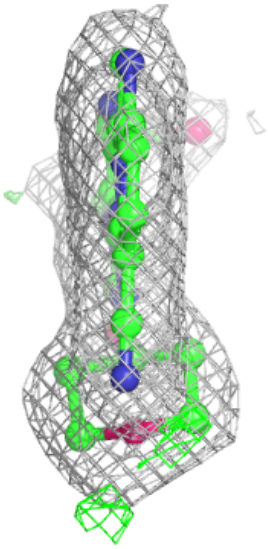


Electron density around GYW C 1101:

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

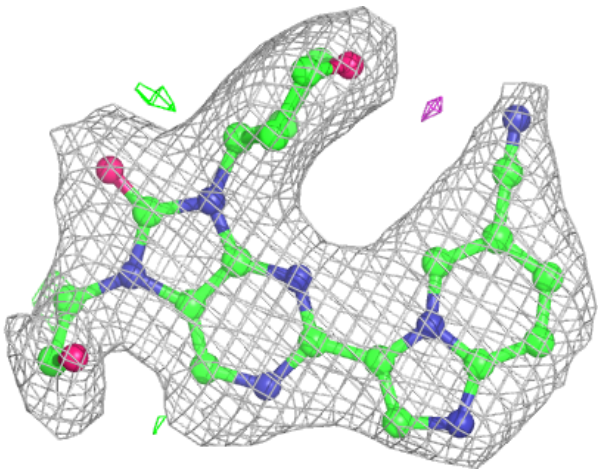


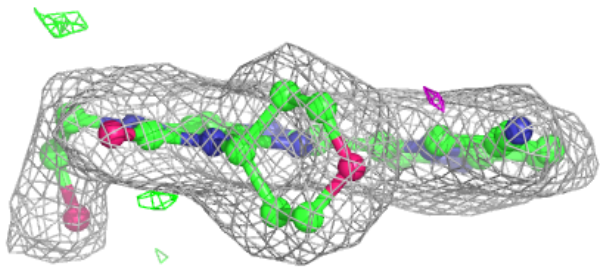


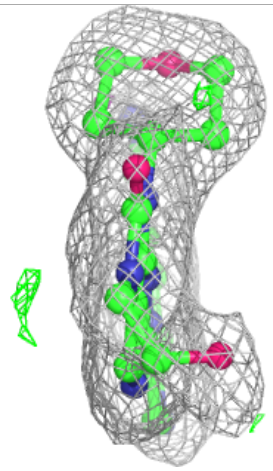


Electron density around GYW A 1101:

$2mF_o$-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.