Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 03:12 am BST

PDB ID	:	5WNG
Title	:	X-RAY CO-STRUCTURE OF RHO-ASSOCIATED PROTEIN KINASE (ROCK1) WITH A HIGHLY SELECTIVE INHIBITOR
Authors	:	Li, X.
Deposited on	:	2017-07-31
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

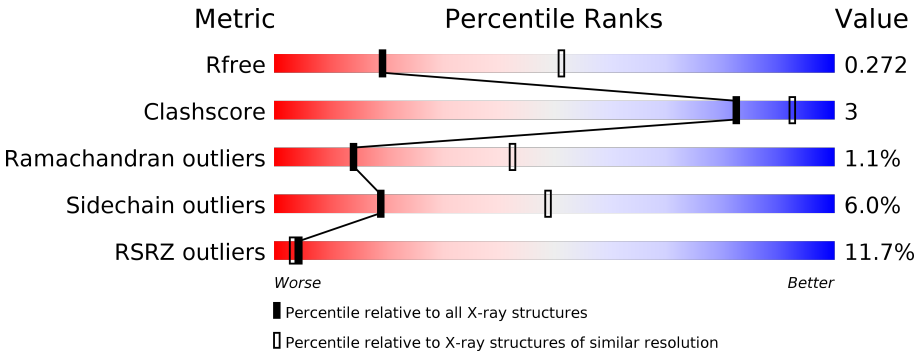
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	415	5% 83% 11% • 5%
1	B	415	23% 77% 10% • 12%
1	C	415	13% 81% 12% 7%
1	D	415	2% 84% 11% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12813 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.

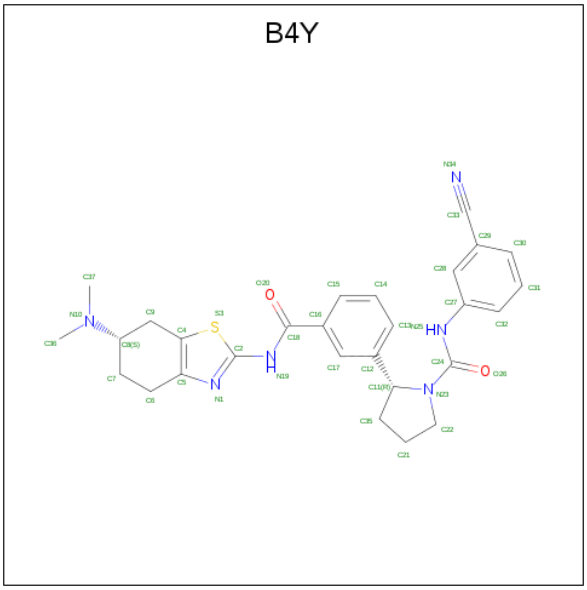
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3214	2055	530	608	21			
1	B	365	Total	C	N	O	S	0	0	0
			2984	1923	489	551	21			
1	C	387	Total	C	N	O	S	0	0	0
			3149	2021	515	591	22			
1	D	396	Total	C	N	O	S	0	0	0
			3222	2059	532	610	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q13464
A	2	SER	-	expression tag	UNP Q13464
A	3	LEU	-	expression tag	UNP Q13464
A	4	HIS	-	expression tag	UNP Q13464
A	5	MET	-	expression tag	UNP Q13464
B	1	GLY	-	expression tag	UNP Q13464
B	2	SER	-	expression tag	UNP Q13464
B	3	LEU	-	expression tag	UNP Q13464
B	4	HIS	-	expression tag	UNP Q13464
B	5	MET	-	expression tag	UNP Q13464
C	1	GLY	-	expression tag	UNP Q13464
C	2	SER	-	expression tag	UNP Q13464
C	3	LEU	-	expression tag	UNP Q13464
C	4	HIS	-	expression tag	UNP Q13464
C	5	MET	-	expression tag	UNP Q13464
D	1	GLY	-	expression tag	UNP Q13464
D	2	SER	-	expression tag	UNP Q13464
D	3	LEU	-	expression tag	UNP Q13464
D	4	HIS	-	expression tag	UNP Q13464
D	5	MET	-	expression tag	UNP Q13464

- Molecule 2 is (2R)-N-(3-cyanophenyl)-2-(3-{[(6S)-6-(dimethylamino)-4,5,6,7-tetrahydro-1,3-benzothiazol-2-yl]carbamoyl}phenyl)pyrrolidine-1-carboxamide (three-letter code: B4Y) (formula: $C_{28}H_{30}N_6O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	28	6	2	1		
2	B	1	Total	C	N	O	S	0	0
			37	28	6	2	1		
2	C	1	Total	C	N	O	S	0	0
			37	28	6	2	1		
2	D	1	Total	C	N	O	S	0	0
			37	28	6	2	1		

- Molecule 3 is water.

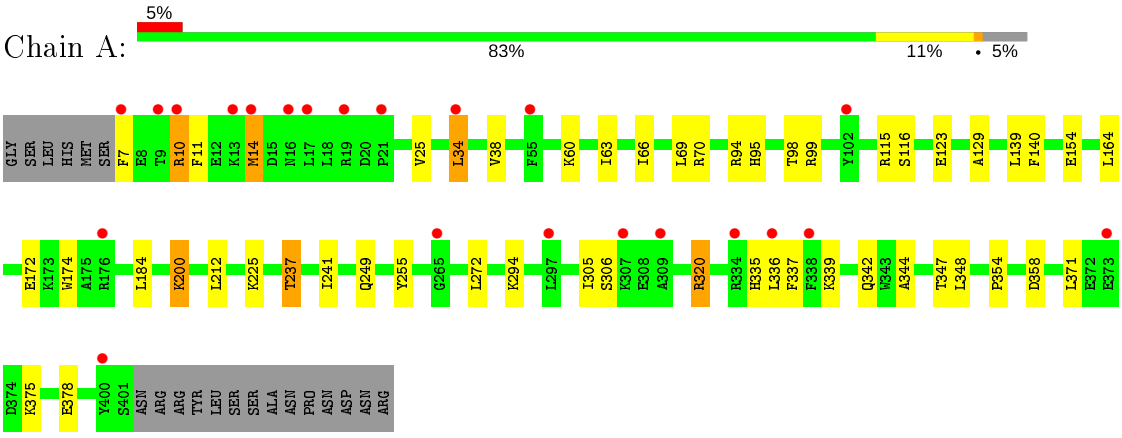
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	17	Total	O	0	0
			17	17		
3	C	18	Total	O	0	0
			18	18		
3	D	29	Total	O	0	0
			29	29		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

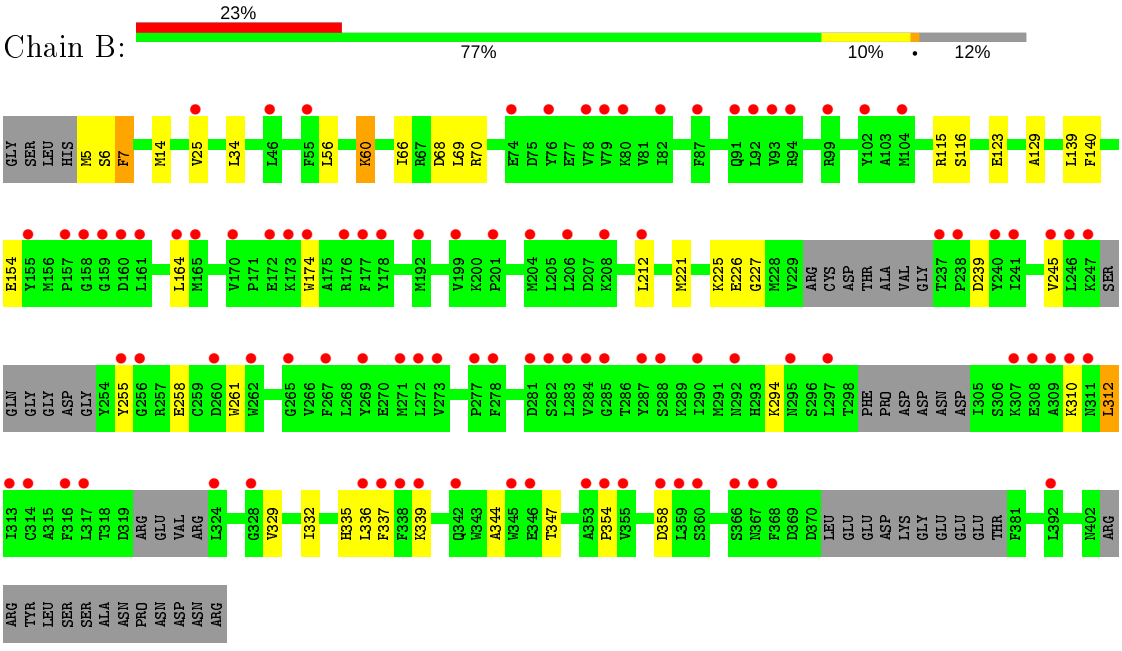
- Molecule 1: Rho-associated protein kinase 1

Chain A:



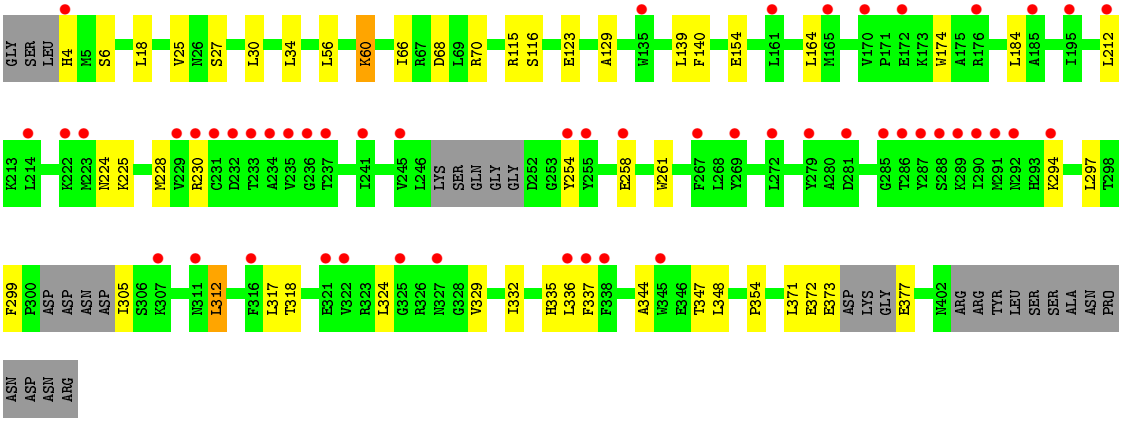
- Molecule 1: Rho-associated protein kinase 1

Chain B:



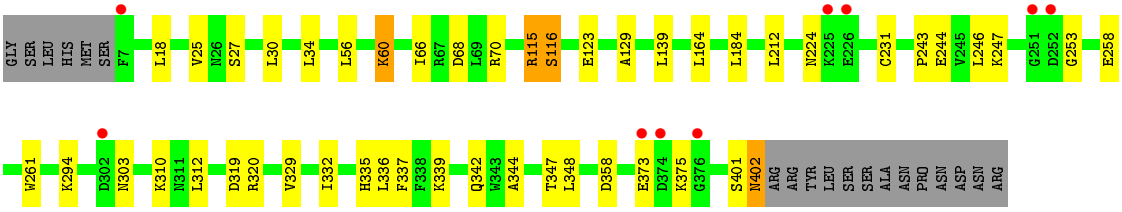
- Molecule 1: Rho-associated protein kinase 1

Chain C:



- Molecule 1: Rho-associated protein kinase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	160.92Å 81.42Å 168.89Å 90.00° 115.10° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 44.58 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.90) 99.8 (44.58-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.230 , 0.250 0.247 , 0.272	Depositor DCC
R_{free} test set	2125 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	91.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 77.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12813	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B4Y

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.38	0/3291	0.61	0/4446
1	B	0.38	0/3054	0.59	0/4119
1	C	0.38	0/3224	0.59	0/4355
1	D	0.38	0/3299	0.59	0/4457
All	All	0.38	0/12868	0.59	0/17377

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

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	3214	0	3114	21	0
1	B	2984	0	2914	16	0
1	C	3149	0	3046	20	0
1	D	3222	0	3120	16	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
2	C	37	0	0	0	0
2	D	37	0	0	0	0
3	A	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	0	0	0
3	C	18	0	0	0	0
3	D	29	0	0	0	0
All	All	12813	0	12194	63	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 3.

All (63) 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:66:ILE:HD11	1:D:25:VAL:HG21	1.70	0.72
1:A:95:HIS:HD2	1:A:98:THR:H	1.38	0.68
1:A:69:LEU:HB3	1:B:14:MET:HG2	1.79	0.64
1:C:297:LEU:HD12	1:C:317:LEU:CD2	2.29	0.63
1:C:297:LEU:HD12	1:C:317:LEU:HD23	1.82	0.62
1:D:243:PRO:O	1:D:247:LYS:HB2	2.00	0.60
1:A:14:MET:HG3	1:B:69:LEU:HB3	1.86	0.58
1:C:372:GLU:HB3	1:C:373:GLU:HA	1.86	0.58
1:B:56:LEU:O	1:B:60:LYS:HB2	2.04	0.57
1:C:56:LEU:O	1:C:60:LYS:HB2	2.05	0.57
1:A:25:VAL:HG21	1:B:66:ILE:HD11	1.87	0.56
1:D:56:LEU:O	1:D:60:LYS:HB2	2.06	0.56
1:A:272:LEU:HB3	1:A:305:ILE:HG21	1.87	0.56
1:B:335:HIS:HD2	1:B:337:PHE:H	1.54	0.56
1:C:335:HIS:HD2	1:C:337:PHE:H	1.54	0.55
1:D:335:HIS:HD2	1:D:337:PHE:H	1.54	0.54
1:A:335:HIS:HD2	1:A:337:PHE:H	1.55	0.54
1:B:129:ALA:HB2	1:B:139:LEU:HD23	1.90	0.54
1:D:129:ALA:HB2	1:D:139:LEU:HD23	1.89	0.54
1:A:66:ILE:HD11	1:B:25:VAL:HG21	1.90	0.52
1:C:129:ALA:HB2	1:C:139:LEU:HD23	1.92	0.52
1:A:94:ARG:HD3	1:A:99:ARG:HE	1.75	0.52
1:A:34:LEU:HD12	1:A:63:ILE:HD13	1.92	0.52
1:A:129:ALA:HB2	1:A:139:LEU:HD23	1.92	0.51
1:C:25:VAL:HG21	1:D:66:ILE:HD11	1.94	0.50
1:A:38:VAL:HG11	1:A:63:ILE:HG21	1.95	0.49
1:A:38:VAL:HG21	1:A:63:ILE:HG21	1.96	0.48
1:D:329:VAL:HA	1:D:332:ILE:HD12	1.96	0.48
1:C:140:PHE:HE2	1:C:154:GLU:HB3	1.79	0.47
1:D:244:GLU:HB2	1:D:320:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HG3	1:B:69:LEU:HA	1.95	0.47
1:A:344:ALA:HB3	1:A:347:THR:HG22	1.98	0.46
1:B:329:VAL:HA	1:B:332:ILE:HD12	1.97	0.46
1:B:344:ALA:HB3	1:B:347:THR:HG22	1.98	0.45
1:A:255:TYR:HA	1:A:320:ARG:HH12	1.81	0.45
1:C:329:VAL:HA	1:C:332:ILE:HD12	1.97	0.45
1:C:297:LEU:HD12	1:C:317:LEU:HD22	1.98	0.45
1:D:344:ALA:HB3	1:D:347:THR:HG22	1.98	0.45
1:B:5:MET:HA	1:B:6:SER:HA	1.80	0.45
1:D:401:SER:HA	1:D:402:ASN:HA	1.72	0.45
1:C:344:ALA:HB3	1:C:347:THR:HG22	1.97	0.44
1:C:174:TRP:CD1	1:C:354:PRO:HB3	2.53	0.44
1:B:258:GLU:HA	1:B:261:TRP:HD1	1.83	0.44
1:D:258:GLU:HA	1:D:261:TRP:HD1	1.83	0.44
1:B:174:TRP:CD1	1:B:354:PRO:HB3	2.53	0.43
1:A:174:TRP:CD1	1:A:354:PRO:HB3	2.54	0.43
1:C:18:LEU:HD22	1:D:27:SER:HB3	2.00	0.42
1:C:335:HIS:CD2	1:C:337:PHE:H	2.37	0.42
1:B:312:LEU:HG	1:B:335:HIS:CD2	2.54	0.42
1:B:140:PHE:HE2	1:B:154:GLU:HB3	1.83	0.42
1:C:30:LEU:HB3	1:D:30:LEU:HB3	2.01	0.42
1:C:312:LEU:HG	1:C:335:HIS:CD2	2.55	0.42
1:B:245:VAL:HG22	1:B:255:TYR:CZ	2.55	0.41
1:C:258:GLU:HA	1:C:261:TRP:HD1	1.84	0.41
1:A:140:PHE:HE2	1:A:154:GLU:HB3	1.84	0.41
1:A:184:LEU:HD12	1:A:348:LEU:HD23	2.02	0.41
1:C:184:LEU:HD12	1:C:348:LEU:HD23	2.03	0.41
1:A:335:HIS:CD2	1:A:337:PHE:H	2.38	0.41
1:D:115:ARG:HB2	1:D:116:SER:H	1.69	0.41
1:D:184:LEU:HD12	1:D:348:LEU:HD23	2.03	0.41
1:A:200:LYS:NZ	1:A:237:THR:HG21	2.36	0.41
1:A:172:GLU:OE2	1:A:306:SER:HB3	2.21	0.40
1:C:27:SER:HB3	1:D:18:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/415 (95%)	374 (95%)	15 (4%)	4 (1%)	15	45
1	B	353/415 (85%)	335 (95%)	14 (4%)	4 (1%)	14	42
1	C	379/415 (91%)	356 (94%)	19 (5%)	4 (1%)	14	42
1	D	394/415 (95%)	368 (93%)	22 (6%)	4 (1%)	15	45
All	All	1519/1660 (92%)	1433 (94%)	70 (5%)	16 (1%)	14	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	PHE
1	A	11	PHE
1	D	253	GLY
1	B	116	SER
1	C	116	SER
1	D	116	SER
1	A	115	ARG
1	A	116	SER
1	B	115	ARG
1	C	6	SER
1	C	115	ARG
1	C	324	LEU
1	D	115	ARG
1	D	373	GLU
1	A	320	ARG
1	B	227	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/369 (95%)	329 (94%)	22 (6%)	18	46
1	B	327/369 (89%)	309 (94%)	18 (6%)	21	53
1	C	344/369 (93%)	323 (94%)	21 (6%)	18	48
1	D	352/369 (95%)	331 (94%)	21 (6%)	19	49
All	All	1374/1476 (93%)	1292 (94%)	82 (6%)	19	49

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	10	ARG
1	A	14	MET
1	A	34	LEU
1	A	60	LYS
1	A	70	ARG
1	A	123	GLU
1	A	164	LEU
1	A	200	LYS
1	A	212	LEU
1	A	225	LYS
1	A	237	THR
1	A	241	ILE
1	A	249	GLN
1	A	294	LYS
1	A	336	LEU
1	A	339	LYS
1	A	342	GLN
1	A	358	ASP
1	A	371	LEU
1	A	375	LYS
1	A	378	GLU
1	B	7	PHE
1	B	34	LEU
1	B	60	LYS
1	B	68	ASP
1	B	70	ARG
1	B	123	GLU
1	B	164	LEU
1	B	212	LEU

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Mol	Chain	Res	Type
1	B	221	MET
1	B	225	LYS
1	B	226	GLU
1	B	239	ASP
1	B	294	LYS
1	B	310	LYS
1	B	312	LEU
1	B	336	LEU
1	B	339	LYS
1	B	358	ASP
1	C	4	HIS
1	C	34	LEU
1	C	60	LYS
1	C	68	ASP
1	C	70	ARG
1	C	123	GLU
1	C	164	LEU
1	C	212	LEU
1	C	224	ASN
1	C	225	LYS
1	C	228	MET
1	C	230	ARG
1	C	254	TYR
1	C	294	LYS
1	C	299	PHE
1	C	305	ILE
1	C	312	LEU
1	C	318	THR
1	C	336	LEU
1	C	371	LEU
1	C	377	GLU
1	D	34	LEU
1	D	60	LYS
1	D	68	ASP
1	D	70	ARG
1	D	123	GLU
1	D	164	LEU
1	D	212	LEU
1	D	224	ASN
1	D	231	CYS
1	D	246	LEU
1	D	294	LYS

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Mol	Chain	Res	Type
1	D	303	ASN
1	D	310	LYS
1	D	312	LEU
1	D	319	ASP
1	D	336	LEU
1	D	339	LYS
1	D	342	GLN
1	D	358	ASP
1	D	375	LYS
1	D	402	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	335	HIS
1	B	26	ASN
1	B	190	HIS
1	B	335	HIS
1	C	224	ASN
1	C	335	HIS
1	D	190	HIS
1	D	335	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates 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	B4Y	B	900	-	37,41,41	1.01	2 (5%)	43,58,58	1.34	5 (11%)
2	B4Y	A	900	-	37,41,41	1.02	2 (5%)	43,58,58	1.22	5 (11%)
2	B4Y	D	900	-	37,41,41	0.98	2 (5%)	43,58,58	1.37	5 (11%)
2	B4Y	C	900	-	37,41,41	1.01	3 (8%)	43,58,58	1.26	4 (9%)

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	B4Y	B	900	-	-	0/24/45/45	0/5/5/5
2	B4Y	A	900	-	-	0/24/45/45	0/5/5/5
2	B4Y	D	900	-	-	0/24/45/45	0/5/5/5
2	B4Y	C	900	-	-	0/24/45/45	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	B4Y	C4-C5	-3.57	1.35	1.42
2	A	900	B4Y	C4-C5	-3.55	1.35	1.42
2	D	900	B4Y	C4-C5	-3.46	1.35	1.42
2	C	900	B4Y	C4-C5	-3.40	1.35	1.42
2	B	900	B4Y	C9-C4	2.27	1.52	1.50
2	C	900	B4Y	C9-C4	2.26	1.52	1.50
2	D	900	B4Y	C9-C4	2.25	1.52	1.50
2	A	900	B4Y	C9-C4	2.15	1.52	1.50
2	C	900	B4Y	C2-N19	2.03	1.40	1.36

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	900	B4Y	C35-C11-N23	4.44	107.04	101.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	B4Y	C35-C11-N23	4.24	106.81	101.94
2	D	900	B4Y	C22-N23-C11	-4.02	107.16	111.83
2	C	900	B4Y	C35-C11-N23	4.00	106.53	101.94
2	A	900	B4Y	C35-C11-N23	3.93	106.45	101.94
2	B	900	B4Y	C22-N23-C11	-3.77	107.46	111.83
2	C	900	B4Y	C22-N23-C11	-3.34	107.95	111.83
2	A	900	B4Y	C22-N23-C11	-3.23	108.08	111.83
2	C	900	B4Y	C36-N10-C8	3.12	117.76	112.39
2	B	900	B4Y	C36-N10-C8	3.09	117.69	112.39
2	A	900	B4Y	C36-N10-C8	2.92	117.42	112.39
2	D	900	B4Y	C21-C22-N23	2.79	108.15	103.25
2	D	900	B4Y	C36-N10-C8	2.76	117.13	112.39
2	B	900	B4Y	C21-C22-N23	2.74	108.06	103.25
2	C	900	B4Y	C21-C22-N23	2.56	107.73	103.25
2	A	900	B4Y	C21-C22-N23	2.47	107.58	103.25
2	D	900	B4Y	C4-C9-C8	-2.27	109.72	112.57
2	B	900	B4Y	C4-C9-C8	-2.19	109.82	112.57
2	A	900	B4Y	C4-C9-C8	-2.03	110.01	112.57

There are no chirality outliers.

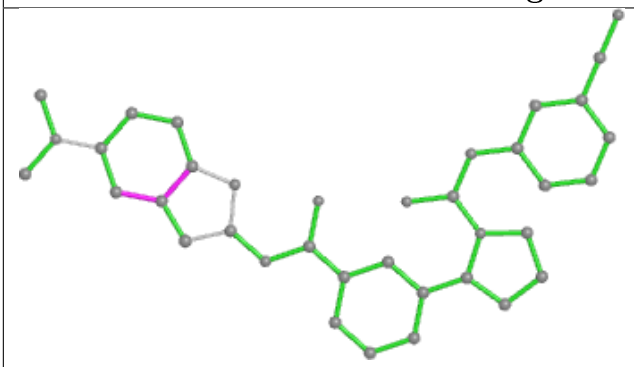
There are no torsion outliers.

There are no ring outliers.

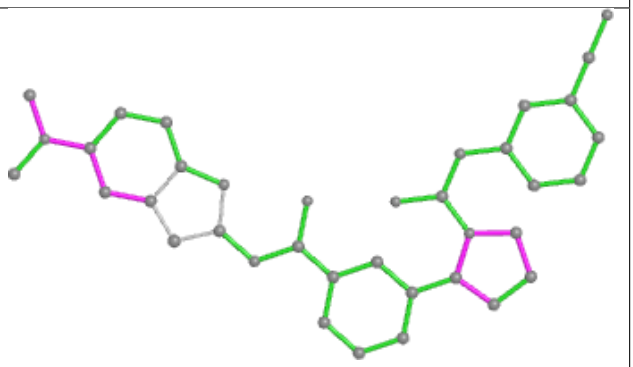
No monomer is involved in short contacts.

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.

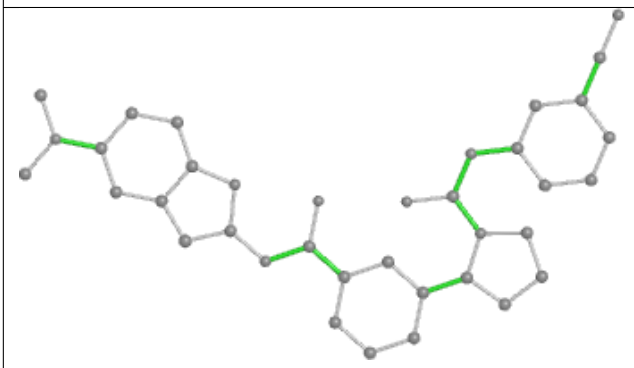
Ligand B4Y B 900



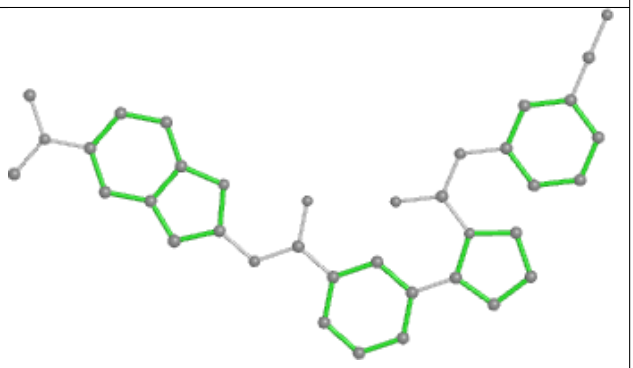
Bond lengths



Bond angles

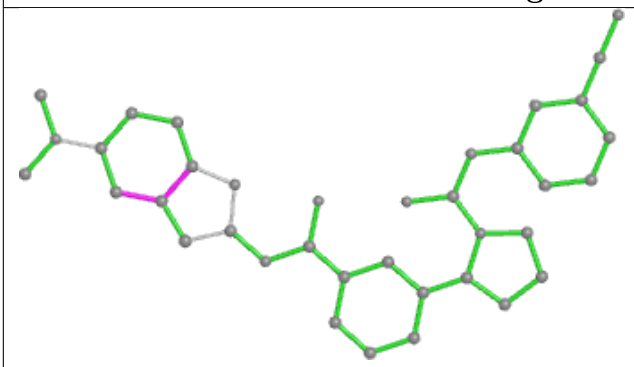


Torsions

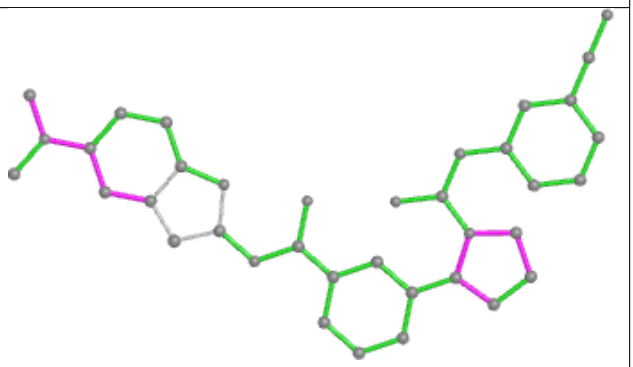


Rings

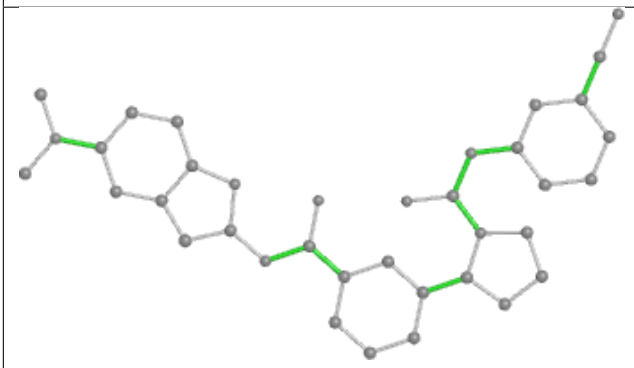
Ligand B4Y A 900



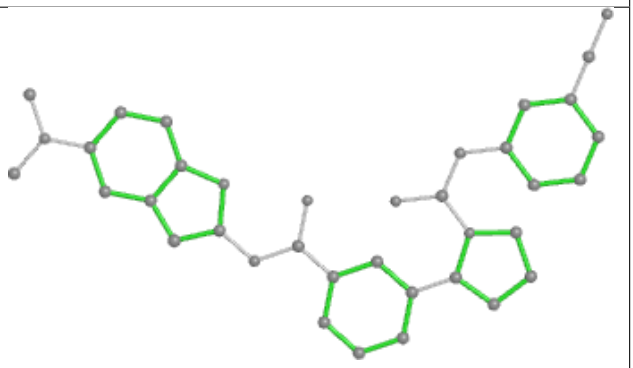
Bond lengths



Bond angles

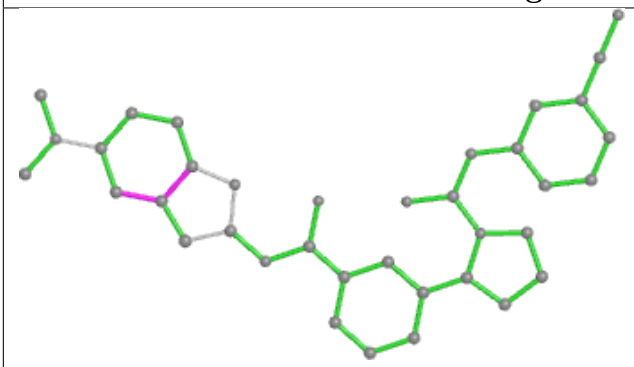


Torsions

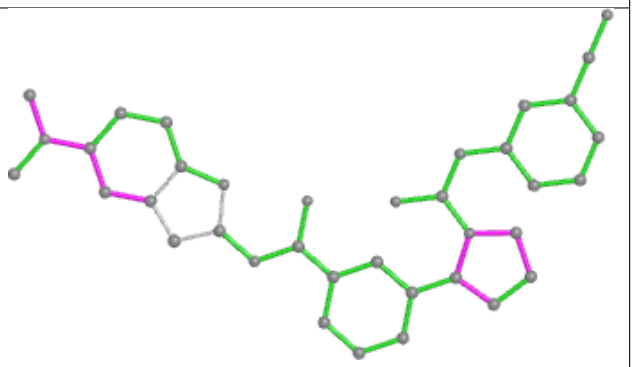


Rings

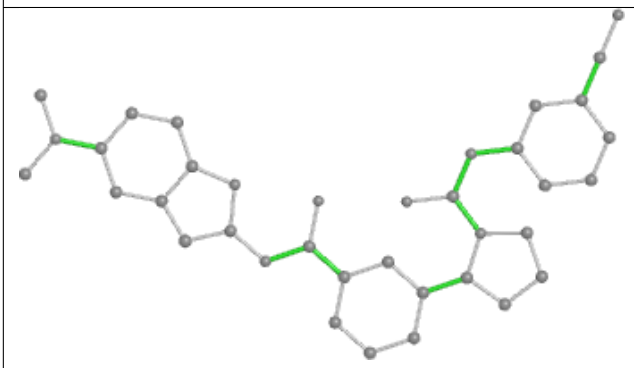
Ligand B4Y D 900



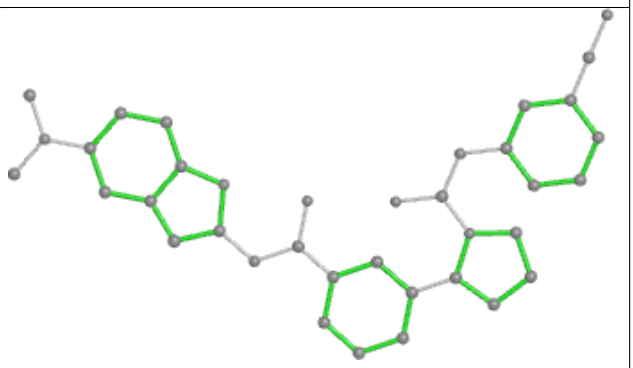
Bond lengths



Bond angles

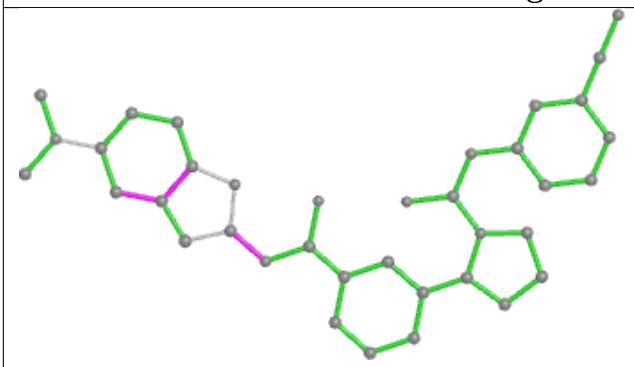


Torsions

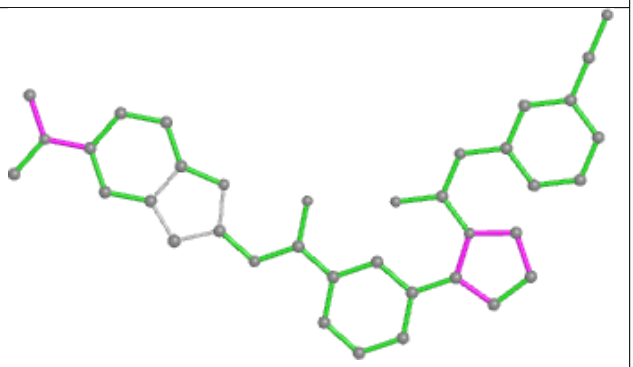


Rings

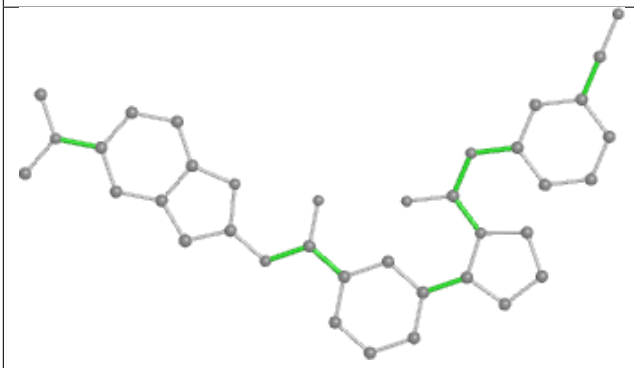
Ligand B4Y C 900



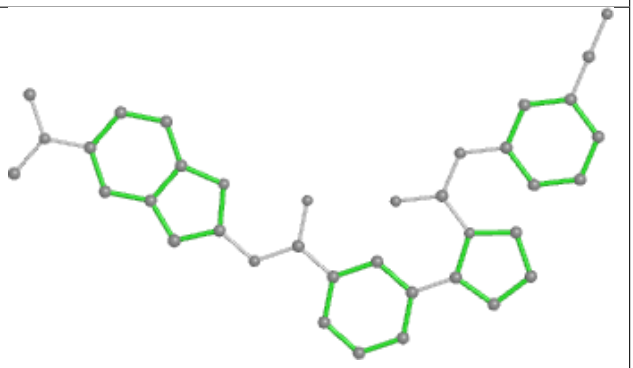
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	395/415 (95%)	0.51	22 (5%) 24 20	76, 103, 153, 197	0
1	B	365/415 (87%)	1.38	97 (26%) 0 0	89, 156, 216, 243	0
1	C	387/415 (93%)	0.97	52 (13%) 3 2	74, 123, 214, 243	0
1	D	396/415 (95%)	0.42	9 (2%) 60 58	68, 100, 143, 157	0
All	All	1543/1660 (92%)	0.81	180 (11%) 4 3	68, 114, 204, 243	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	291	MET	10.5
1	B	336	LEU	10.1
1	C	232	ASP	9.6
1	B	79	VAL	9.3
1	B	278	PHE	8.2
1	B	309	ALA	7.9
1	C	288	SER	7.8
1	B	314	CYS	7.4
1	C	281	ASP	7.4
1	C	287	TYR	7.2
1	C	290	ILE	7.0
1	C	316	PHE	6.7
1	C	236	GLY	6.4
1	B	338	PHE	6.2
1	B	337	PHE	6.2
1	C	338	PHE	5.8
1	B	265	GLY	5.7
1	C	230	ARG	5.6
1	B	241	ILE	5.5
1	C	272	LEU	5.4
1	D	225	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	297	LEU	5.2
1	B	287	TYR	5.1
1	B	245	VAL	5.0
1	B	307	LYS	4.9
1	B	272	LEU	4.9
1	B	290	ILE	4.9
1	C	233	THR	4.8
1	B	246	LEU	4.7
1	C	325	GLY	4.7
1	B	269	TYR	4.6
1	B	271	MET	4.5
1	B	165	MET	4.4
1	D	376	GLY	4.4
1	B	199	VAL	4.4
1	B	159	GLY	4.4
1	B	155	TYR	4.3
1	C	245	VAL	4.3
1	B	76	TYR	4.3
1	B	313	ILE	4.1
1	D	373	GLU	4.1
1	C	234	ALA	4.1
1	C	337	PHE	4.0
1	B	92	LEU	4.0
1	B	237	THR	4.0
1	B	281	ASP	4.0
1	B	288	SER	3.9
1	B	93	VAL	3.9
1	C	222	LYS	3.9
1	B	355	VAL	3.8
1	B	240	TYR	3.8
1	C	172	GLU	3.7
1	A	13	LYS	3.7
1	B	316	PHE	3.6
1	B	345	TRP	3.6
1	C	286	THR	3.6
1	A	10	ARG	3.6
1	C	223	MET	3.6
1	A	400	TYR	3.6
1	C	321	GLU	3.6
1	B	238	PRO	3.6
1	C	345	TRP	3.5
1	B	359	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	226	GLU	3.5
1	D	251	GLY	3.4
1	C	135	TRP	3.4
1	C	231	CYS	3.4
1	A	338	PHE	3.3
1	C	292	ASN	3.3
1	B	172	GLU	3.3
1	B	178	TYR	3.2
1	A	19	ARG	3.2
1	C	235	VAL	3.2
1	B	80	LYS	3.1
1	C	241	ILE	3.1
1	B	204	MET	3.1
1	B	247	LYS	3.1
1	A	307	LYS	3.1
1	C	336	LEU	3.1
1	B	87	PHE	3.0
1	B	368	PHE	3.0
1	B	311	ASN	3.0
1	C	327	ASN	3.0
1	A	373	GLU	3.0
1	C	229	VAL	2.9
1	C	255	TYR	2.9
1	A	14	MET	2.9
1	B	367	ASN	2.9
1	B	273	VAL	2.9
1	B	324	LEU	2.9
1	C	285	GLY	2.8
1	C	269	TYR	2.8
1	B	360	SER	2.8
1	B	176	ARG	2.8
1	C	195	ILE	2.8
1	B	310	LYS	2.7
1	B	260	ASP	2.7
1	B	170	VAL	2.7
1	B	255	TYR	2.7
1	C	170	VAL	2.7
1	B	285	GLY	2.7
1	C	165	MET	2.7
1	A	297	LEU	2.7
1	C	214	LEU	2.6
1	B	158	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	174	TRP	2.6
1	D	252	ASP	2.6
1	C	267	PHE	2.6
1	B	295	ASN	2.6
1	B	206	LEU	2.6
1	C	294	LYS	2.5
1	B	157	PRO	2.5
1	A	334	ARG	2.5
1	B	342	GLN	2.5
1	B	25	VAL	2.5
1	B	317	LEU	2.5
1	C	307	LYS	2.4
1	A	309	ALA	2.4
1	B	94	ARG	2.4
1	C	237	THR	2.4
1	A	21	PRO	2.4
1	B	99	ARG	2.4
1	B	160	ASP	2.4
1	D	374	ASP	2.4
1	A	16	ASN	2.4
1	B	282	SER	2.4
1	B	346	GLU	2.3
1	A	102	TYR	2.3
1	B	339	LYS	2.3
1	B	277	PRO	2.3
1	B	392	LEU	2.3
1	C	212	LEU	2.3
1	B	262	TRP	2.3
1	C	4	HIS	2.3
1	B	292	ASN	2.3
1	C	322	VAL	2.3
1	B	358	ASP	2.3
1	C	161	LEU	2.3
1	C	185	ALA	2.3
1	A	7	PHE	2.3
1	B	267	PHE	2.3
1	C	311	ASN	2.3
1	B	328	GLY	2.3
1	B	353	ALA	2.3
1	A	34	LEU	2.2
1	A	265	GLY	2.2
1	A	336	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	201	PRO	2.2
1	B	308	GLU	2.2
1	D	7	PHE	2.2
1	A	9	THR	2.2
1	A	55	PHE	2.2
1	C	254	TYR	2.2
1	B	74	GLU	2.2
1	B	164	LEU	2.2
1	B	256	GLY	2.2
1	B	82	ILE	2.2
1	B	91	GLN	2.2
1	B	354	PRO	2.2
1	C	289	LYS	2.2
1	B	161	LEU	2.1
1	B	177	PHE	2.1
1	B	208	LYS	2.1
1	C	258	GLU	2.1
1	B	283	LEU	2.1
1	B	366	SER	2.1
1	C	176	ARG	2.1
1	B	173	LYS	2.1
1	B	104	MET	2.1
1	A	176	ARG	2.1
1	B	212	LEU	2.1
1	C	279	TYR	2.1
1	B	78	VAL	2.1
1	B	192	MET	2.1
1	B	55	PHE	2.1
1	A	17	LEU	2.1
1	B	46	LEU	2.1
1	D	302	ASP	2.1
1	B	102	TYR	2.0
1	B	284	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

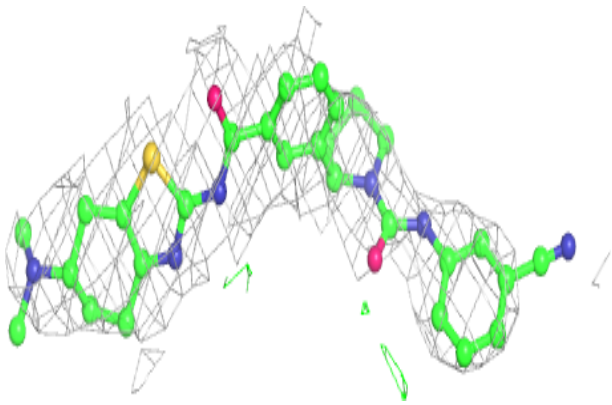
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

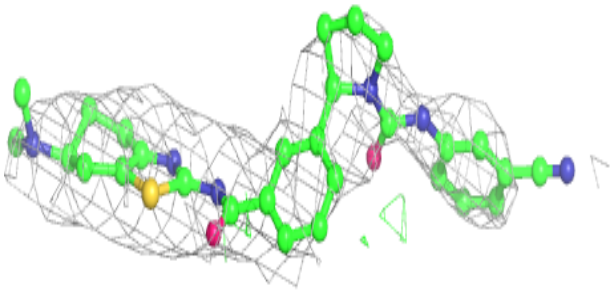
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	B4Y	B	900	37/37	0.90	0.32	135,147,160,163	0
2	B4Y	C	900	37/37	0.92	0.26	96,98,103,104	0
2	B4Y	A	900	37/37	0.94	0.25	82,86,90,92	0
2	B4Y	D	900	37/37	0.95	0.27	75,77,81,82	0

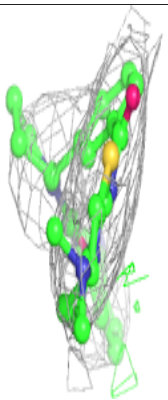
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B4Y B 900:

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

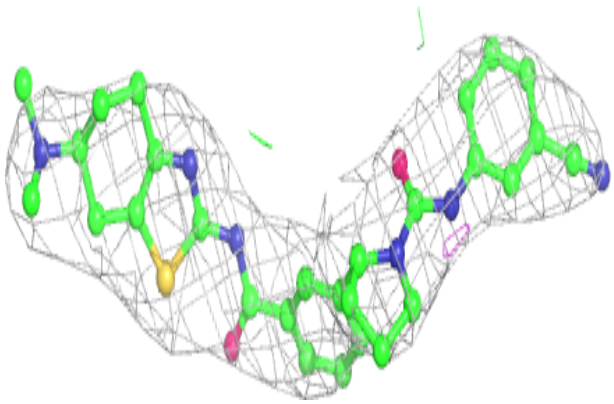


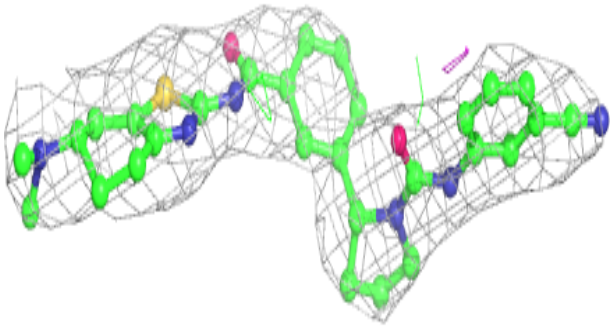


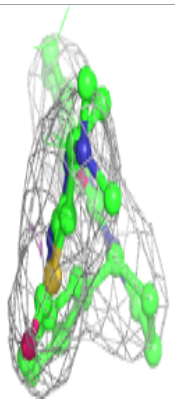


Electron density around B4Y C 900:

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

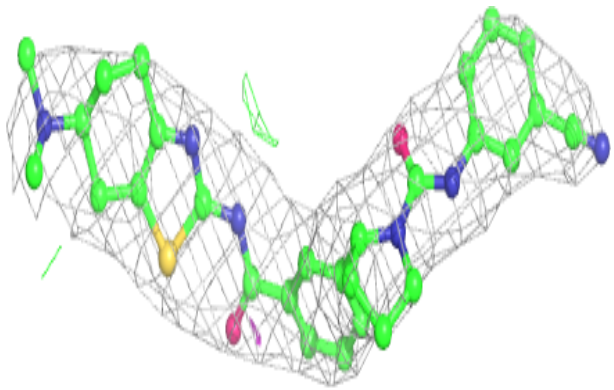


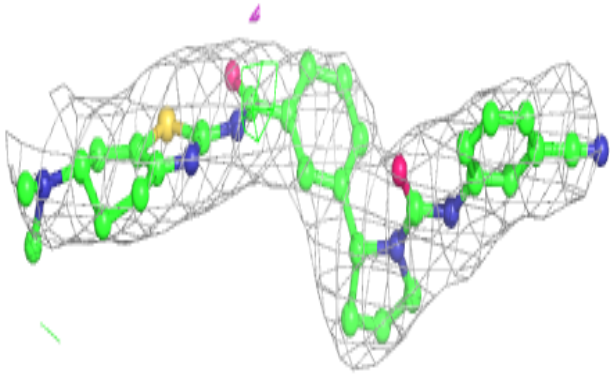




Electron density around B4Y A 900:

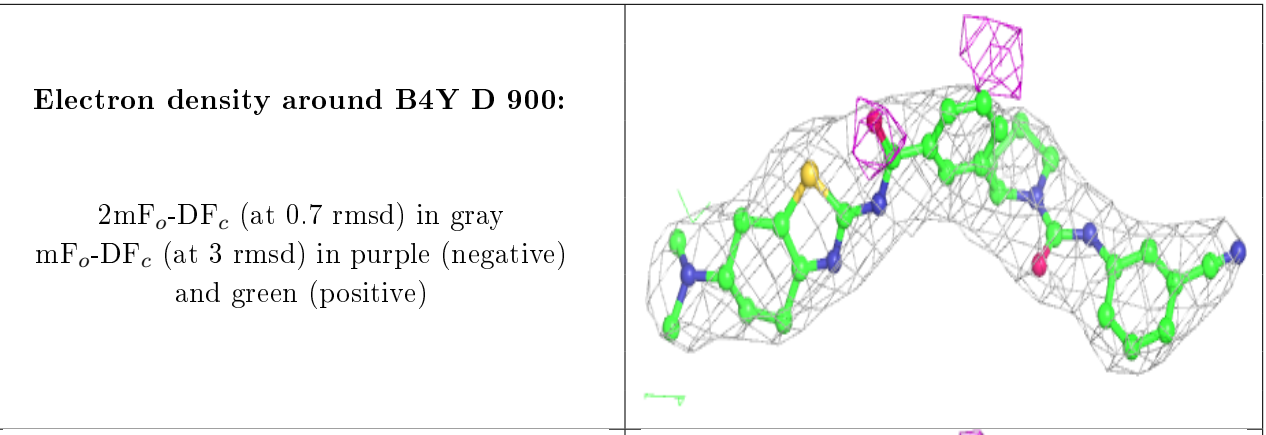
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

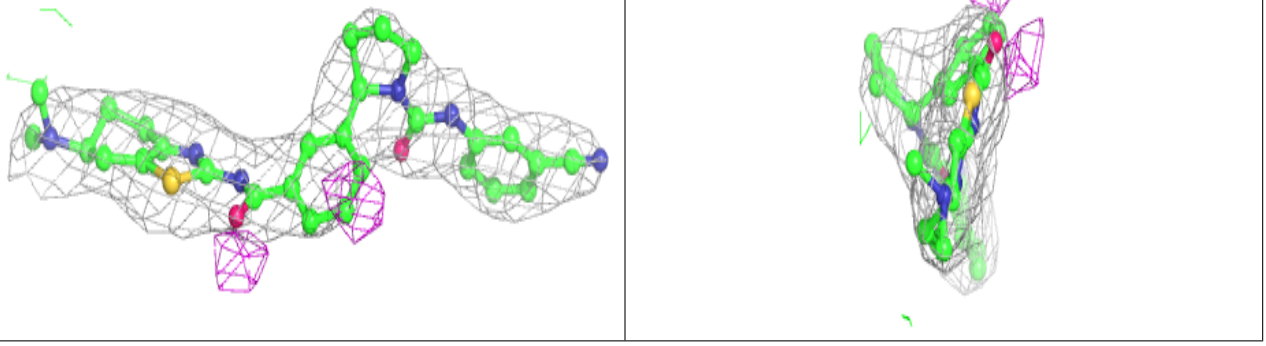




Electron density around B4Y D 900:

$2mF_o$-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

There are no such residues in this entry.