



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 09:09 am BST

PDB ID : 4YP8
Title : Irak4-inhibitor co-structure
Authors : Fischmann, T.O.
Deposited on : 2015-03-12
Resolution : 2.64 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

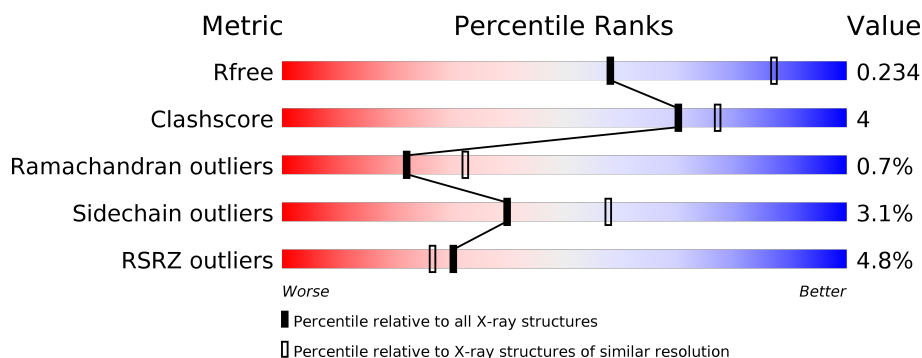
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	<div> <div>8%</div> <div>85% 9% • 5%</div> </div>
1	B	301	<div> <div>8%</div> <div>80% 12% • 7%</div> </div>
1	C	301	<div> <div>%</div> <div>84% 12% •</div> </div>
1	D	301	<div> <div>%</div> <div>83% 13% •</div> </div>

2 Entry composition [i](#)

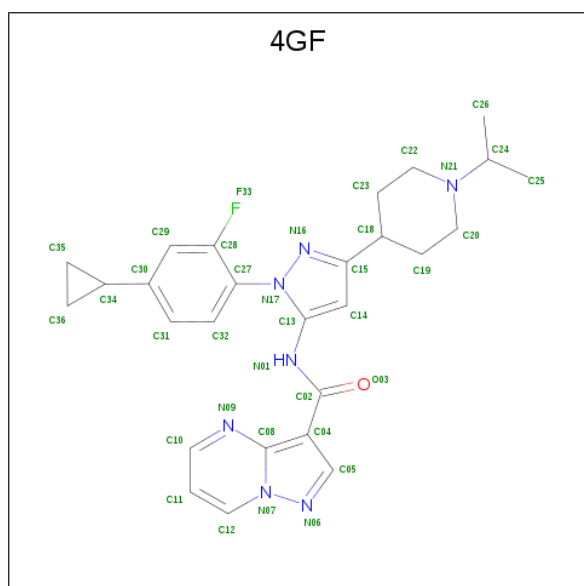
There are 3 unique types of molecules in this entry. The entry contains 9177 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	P	S	0	0	3
			2243	1405	376	445	3	14			
1	B	281	Total	C	N	O	P	S	0	0	2
			2207	1382	372	436	3	14			
1	C	290	Total	C	N	O	P	S	0	0	3
			2260	1415	379	449	3	14			
1	D	288	Total	C	N	O	P	S	0	0	3
			2260	1414	382	447	3	14			

- Molecule 2 is N-{1-(4-cyclopropyl-2-fluorophenyl)-3-[1-(propan-2-yl)piperidin-4-yl]-1H-pyrazol-5-yl}pyrazolo[1,5-a]pyrimidine-3-carboxamide (three-letter code: 4GF) (formula: C₂₇H₃₀FN₇O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			36	27	1	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			36	27	1	7	1		
2	C	1	Total	C	F	N	O	0	0
			36	27	1	7	1		
2	D	1	Total	C	F	N	O	0	0
			36	27	1	7	1		

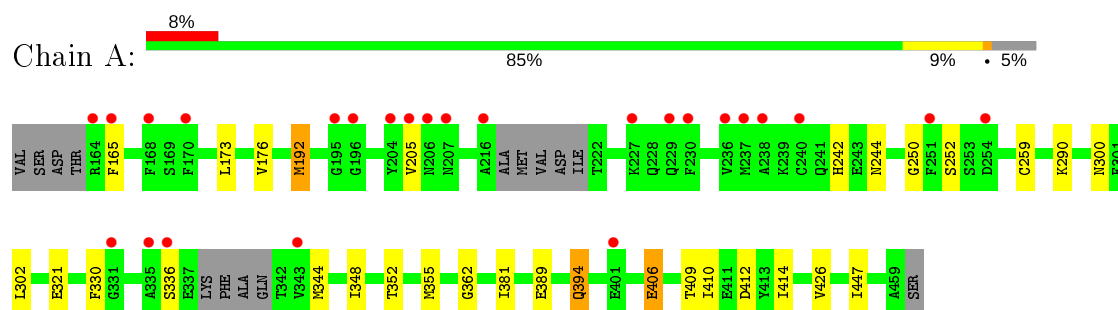
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	12	Total	O	0	0
			12	12		
3	C	22	Total	O	0	0
			22	22		
3	D	19	Total	O	0	0
			19	19		

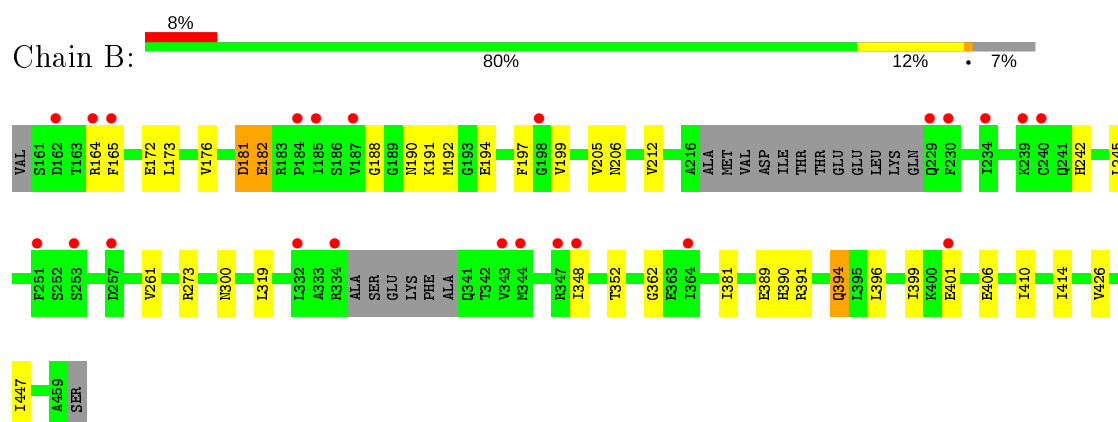
3 Residue-property plots [i](#)

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.

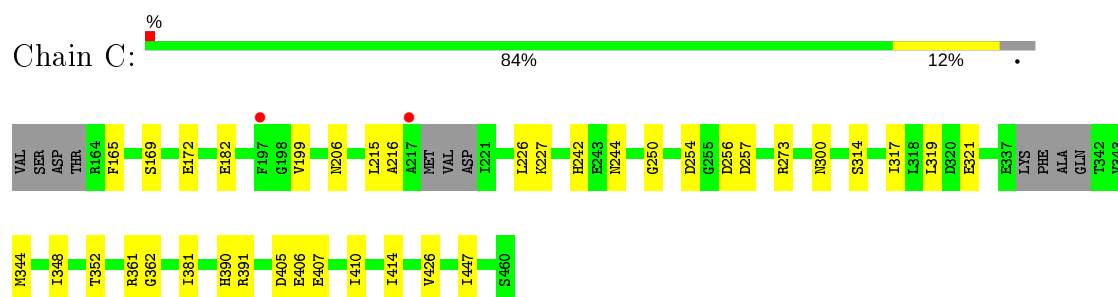
- Molecule 1: Interleukin-1 receptor-associated kinase 4



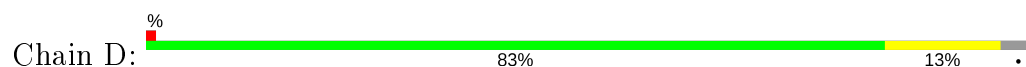
- Molecule 1: Interleukin-1 receptor-associated kinase 4

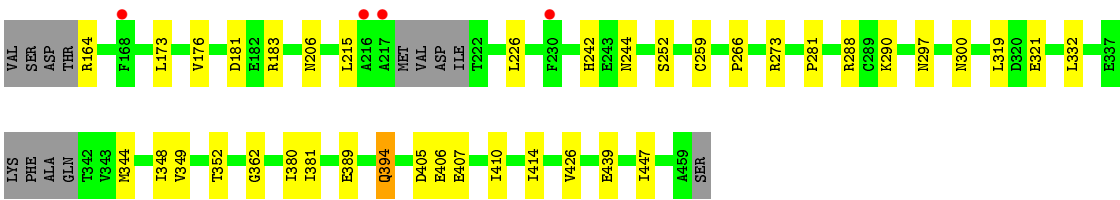


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.01Å 138.19Å 88.08Å 90.00° 124.72° 90.00°	Depositor
Resolution (Å)	47.27 – 2.64 47.27 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.27-2.64) 99.0 (47.27-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.192 , 0.219 0.204 , 0.234	Depositor DCC
R_{free} test set	2095 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.105 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9177	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, 4GF, SEP

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	0.49	0/2247	0.68	0/3027
1	B	0.50	0/2210	0.69	0/2976
1	C	0.52	0/2264	0.72	0/3051
1	D	0.53	0/2264	0.69	0/3050
All	All	0.51	0/8985	0.70	0/12104

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	2243	0	2195	15	1
1	B	2207	0	2158	18	0
1	C	2260	0	2212	17	1
1	D	2260	0	2218	19	0
2	A	36	0	29	1	0
2	B	36	0	29	0	0
2	C	36	0	29	0	0
2	D	36	0	29	0	0
3	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	0	0	0
3	C	22	0	0	0	0
3	D	19	0	0	1	0
All	All	9177	0	8899	64	1

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 4.

All (64) 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:D:266:PRO:HG2	1:D:321:GLU:HG3	1.75	0.66
1:A:409:THR:HG22	1:A:412:ASP:OD1	1.98	0.63
1:C:321:GLU:HG3	1:D:281:PRO:HD3	1.81	0.62
1:B:391:ARG:HA	1:C:390:HIS:HB3	1.82	0.61
1:B:390:HIS:HB3	1:C:391:ARG:HA	1.84	0.59
1:A:242:HIS:HD2	1:A:244:ASN:H	1.49	0.58
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.86	0.58
1:B:389:GLU:HA	1:B:394:GLN:NE2	2.19	0.57
1:B:205:VAL:HG12	1:B:206:ASN:HD22	1.69	0.56
1:A:242:HIS:CD2	1:A:244:ASN:H	2.24	0.56
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.88	0.56
1:A:389:GLU:HA	1:A:394:GLN:NE2	2.22	0.55
1:A:252:SER:HB3	1:A:259:CYS:HB2	1.88	0.54
1:D:439:GLU:CD	1:D:439:GLU:H	2.11	0.52
1:A:192:MET:HB3	2:A:501:4GF:H26	1.91	0.51
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.92	0.51
1:A:414:ILE:HG12	1:A:426:VAL:HG11	1.92	0.50
1:D:389:GLU:HA	1:D:394:GLN:NE2	2.26	0.50
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.94	0.50
1:D:273:ARG:HG3	1:D:319:LEU:HD12	1.93	0.50
1:C:215:LEU:HD23	1:C:226:LEU:HG	1.95	0.49
1:D:252:SER:HB3	1:D:259:CYS:HB2	1.95	0.48
1:B:242:HIS:HB3	1:B:245:LEU:HG	1.96	0.48
1:D:242:HIS:CD2	1:D:244:ASN:H	2.30	0.48
1:B:173:LEU:HA	1:B:176:VAL:HG22	1.96	0.48
1:C:242:HIS:CD2	1:C:244:ASN:H	2.32	0.48
1:B:194:GLU:HG3	1:B:199:VAL:HG22	1.96	0.48
1:B:172:GLU:O	1:B:176:VAL:HG13	2.13	0.47
1:B:212:VAL:HG22	1:B:261:VAL:HG22	1.95	0.47
1:C:165:PHE:HB3	1:C:250:GLY:HA2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:HB2	1:C:242:HIS:CE1	2.50	0.47
1:D:181:ASP:OD1	1:D:183:ARG:HG2	2.15	0.46
1:B:396:LEU:O	1:B:399:ILE:HG12	2.14	0.46
1:D:414:ILE:HG12	1:D:426:VAL:HG11	1.98	0.46
1:A:381:ILE:HG21	1:A:410:ILE:HD11	1.98	0.46
1:D:290:LYS:HD3	3:D:605:HOH:O	2.15	0.46
1:B:273:ARG:HG3	1:B:319:LEU:HD12	1.99	0.45
1:C:414:ILE:HG12	1:C:426:VAL:HG11	1.98	0.45
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.99	0.45
1:B:348:ILE:HG12	1:B:362:GLY:HA2	1.99	0.44
1:B:181:ASP:HB3	1:B:190:ASN:HB2	1.98	0.44
1:A:165:PHE:HB3	1:A:250:GLY:HA2	1.98	0.44
1:C:169:SER:HB3	1:C:172:GLU:HG3	2.00	0.44
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.99	0.44
1:D:381:ILE:HG21	1:D:410:ILE:HD11	2.00	0.44
1:B:381:ILE:HG21	1:B:410:ILE:HD11	2.00	0.43
1:B:390:HIS:O	1:C:390:HIS:O	2.37	0.43
1:A:348:ILE:HG12	1:A:362:GLY:HA2	2.00	0.43
1:C:381:ILE:HG21	1:C:410:ILE:HD11	2.02	0.42
1:C:314:SER:HA	1:C:317:ILE:HD12	2.01	0.42
1:A:394:GLN:HE21	1:A:394:GLN:HB3	1.69	0.42
1:D:348:ILE:HG12	1:D:362:GLY:HA2	2.02	0.42
1:D:394:GLN:HB3	1:D:394:GLN:HE21	1.70	0.42
1:D:215:LEU:HD23	1:D:226:LEU:HG	2.02	0.42
1:B:182:GLU:HA	1:B:191:LYS:HB2	2.03	0.41
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.03	0.41
1:C:348:ILE:HG12	1:C:362:GLY:HA2	2.03	0.41
1:C:405:ASP:O	1:C:407:GLU:N	2.54	0.41
1:C:273:ARG:HG3	1:C:319:LEU:HD12	2.03	0.40
1:C:300:ASN:HA	1:C:447:ILE:CG2	2.51	0.40
1:D:288:ARG:HB3	1:D:380:ILE:HG23	2.03	0.40
1:D:332:LEU:HD22	1:D:349:VAL:HG21	2.04	0.40
1:A:302:LEU:HD11	1:A:330:PHE:HE1	1.87	0.40
1:D:405:ASP:O	1:D:407:GLU:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:O	1:C:361:ARG:NH1[4_555]	2.17	0.03

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	279/301 (93%)	270 (97%)	8 (3%)	1 (0%)	34	48
1	B	272/301 (90%)	254 (93%)	15 (6%)	3 (1%)	14	20
1	C	282/301 (94%)	268 (95%)	11 (4%)	3 (1%)	14	20
1	D	280/301 (93%)	267 (95%)	12 (4%)	1 (0%)	34	48
All	All	1113/1204 (92%)	1059 (95%)	46 (4%)	8 (1%)	22	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	C	254	ASP
1	C	406	GLU
1	D	406	GLU
1	C	216	ALA
1	B	188	GLY
1	B	181	ASP

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	244/259 (94%)	236 (97%)	8 (3%)	38	55
1	B	241/259 (93%)	233 (97%)	8 (3%)	38	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	245/259 (95%)	237 (97%)	8 (3%)	38	55
1	D	246/259 (95%)	240 (98%)	6 (2%)	49	67
All	All	976/1036 (94%)	946 (97%)	30 (3%)	40	58

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	MET
1	A	205	VAL
1	A	290	LYS
1	A	336	SER
1	A	344	MET
1	A	352	THR
1	A	394	GLN
1	A	406	GLU
1	B	164	ARG
1	B	165	PHE
1	B	182	GLU
1	B	192	MET
1	B	197	PHE
1	B	352	THR
1	B	394	GLN
1	B	401	GLU
1	C	182	GLU
1	C	199	VAL
1	C	206	ASN
1	C	227	LYS
1	C	256	ASP
1	C	257	ASP
1	C	344	MET
1	C	352	THR
1	D	164	ARG
1	D	206	ASN
1	D	297	ASN
1	D	344	MET
1	D	352	THR
1	D	394	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	297	ASN
1	A	394	GLN
1	A	451	GLN
1	B	242	HIS
1	B	297	ASN
1	B	394	GLN
1	B	451	GLN
1	C	166	HIS
1	C	242	HIS
1	C	297	ASN
1	C	451	GLN
1	D	166	HIS
1	D	229	GLN
1	D	242	HIS
1	D	297	ASN
1	D	394	GLN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	TPO	B	342	1	8,10,11	0.74	0	10,14,16	1.38	3 (30%)
1	TPO	A	342	1	8,10,11	0.90	0	10,14,16	1.35	2 (20%)
1	SEP	D	346	1	8,9,10	0.91	0	8,12,14	1.94	2 (25%)
1	TPO	A	345	1	8,10,11	1.47	1 (12%)	10,14,16	1.66	1 (10%)
1	SEP	A	346	1	8,9,10	0.89	0	8,12,14	2.37	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	D	342	1	8,10,11	0.83	0	10,14,16	1.26	1 (10%)
1	TPO	D	345	1	8,10,11	0.78	0	10,14,16	1.04	0
1	SEP	B	346	1	8,9,10	0.98	0	8,12,14	2.16	2 (25%)
1	SEP	C	346	1	8,9,10	1.00	0	8,12,14	1.92	2 (25%)
1	TPO	B	345	1	8,10,11	1.16	1 (12%)	10,14,16	1.07	0
1	TPO	C	345	1	8,10,11	1.14	0	10,14,16	1.03	1 (10%)
1	TPO	C	342	1	8,10,11	0.70	0	10,14,16	1.26	1 (10%)

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	TPO	B	342	1	-	1/9/11/13	-
1	TPO	A	342	1	-	2/9/11/13	-
1	SEP	D	346	1	-	1/5/8/10	-
1	TPO	A	345	1	-	2/9/11/13	-
1	SEP	A	346	1	-	1/5/8/10	-
1	TPO	D	342	1	-	2/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	SEP	B	346	1	-	1/5/8/10	-
1	SEP	C	346	1	-	1/5/8/10	-
1	TPO	B	345	1	-	4/9/11/13	-
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	C	342	1	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	P-OG1	-3.10	1.53	1.59
1	B	345	TPO	P-OG1	-2.27	1.55	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	SEP	OG-CB-CA	5.40	113.40	108.14
1	B	346	SEP	OG-CB-CA	5.19	113.20	108.14
1	D	346	SEP	OG-CB-CA	4.61	112.63	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	OG-CB-CA	4.10	112.13	108.14
1	A	346	SEP	P-OG-CB	-3.27	109.29	118.30
1	A	345	TPO	P-OG1-CB	-3.03	114.06	123.21
1	B	346	SEP	P-OG-CB	-2.84	110.47	118.30
1	C	346	SEP	P-OG-CB	-2.61	111.11	118.30
1	A	342	TPO	P-OG1-CB	-2.40	115.97	123.21
1	B	342	TPO	P-OG1-CB	-2.38	116.02	123.21
1	D	346	SEP	P-OG-CB	-2.16	112.36	118.30
1	B	342	TPO	CG2-CB-CA	-2.15	108.92	113.16
1	D	342	TPO	P-OG1-CB	-2.13	116.77	123.21
1	C	342	TPO	P-OG1-CB	-2.13	116.78	123.21
1	A	342	TPO	O3P-P-OG1	2.09	115.34	105.99
1	B	342	TPO	O2P-P-OG1	2.02	115.06	105.99
1	C	345	TPO	P-OG1-CB	-2.01	117.14	123.21

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	342	TPO	CB-OG1-P-O1P
1	A	345	TPO	N-CA-CB-OG1
1	A	346	SEP	N-CA-CB-OG
1	D	342	TPO	CB-OG1-P-O1P
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	345	TPO	CB-OG1-P-O1P
1	B	346	SEP	N-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	N-CA-CB-OG1
1	A	342	TPO	CB-OG1-P-O1P
1	C	342	TPO	CB-OG1-P-O1P
1	D	346	SEP	N-CA-CB-OG
1	C	346	SEP	N-CA-CB-OG
1	D	342	TPO	CB-OG1-P-O3P
1	D	345	TPO	CB-OG1-P-O3P
1	B	345	TPO	CB-OG1-P-O3P
1	C	345	TPO	CB-OG1-P-O2P
1	A	342	TPO	O-C-CA-CB
1	A	345	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

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	4GF	D	501	-	34,41,41	1.06	5 (14%)	43,60,60	1.46	5 (11%)
2	4GF	B	501	-	34,41,41	1.47	5 (14%)	43,60,60	1.48	7 (16%)
2	4GF	C	501	-	34,41,41	1.22	5 (14%)	43,60,60	1.69	9 (20%)
2	4GF	A	501	-	34,41,41	1.23	6 (17%)	43,60,60	1.51	5 (11%)

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	4GF	D	501	-	-	1/20/36/36	0/6/6/6
2	4GF	B	501	-	-	3/20/36/36	0/6/6/6
2	4GF	C	501	-	-	6/20/36/36	0/6/6/6
2	4GF	A	501	-	-	6/20/36/36	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4GF	C08-N09	4.22	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	4GF	C13-N17	4.19	1.41	1.37
2	A	501	4GF	C08-N09	4.14	1.41	1.35
2	C	501	4GF	C08-N09	4.12	1.41	1.35
2	B	501	4GF	C15-N16	3.46	1.38	1.33
2	B	501	4GF	C04-C02	-3.22	1.45	1.50
2	A	501	4GF	C13-N17	3.10	1.40	1.37
2	D	501	4GF	C15-N16	2.97	1.37	1.33
2	B	501	4GF	C14-C15	2.85	1.45	1.39
2	C	501	4GF	C15-N16	2.79	1.37	1.33
2	C	501	4GF	C14-C15	2.78	1.45	1.39
2	D	501	4GF	C08-N09	2.44	1.39	1.35
2	A	501	4GF	C15-N16	2.44	1.37	1.33
2	D	501	4GF	C14-C15	2.38	1.44	1.39
2	C	501	4GF	C13-N17	2.36	1.39	1.37
2	D	501	4GF	C10-N09	2.19	1.36	1.32
2	D	501	4GF	C13-N17	2.16	1.39	1.37
2	C	501	4GF	C10-N09	2.13	1.36	1.32
2	A	501	4GF	C10-N09	2.12	1.36	1.32
2	A	501	4GF	C04-C02	-2.12	1.46	1.50
2	A	501	4GF	C14-C15	2.09	1.43	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	4GF	C28-C27-N17	6.36	123.72	117.86
2	B	501	4GF	C28-C27-N17	5.57	122.98	117.86
2	D	501	4GF	C28-C27-N17	5.31	122.75	117.86
2	A	501	4GF	C28-C27-N17	5.21	122.66	117.86
2	A	501	4GF	C36-C34-C30	-5.03	116.26	121.64
2	D	501	4GF	F33-C28-C27	-4.06	117.90	121.04
2	A	501	4GF	F33-C28-C27	-3.84	118.07	121.04
2	D	501	4GF	C36-C34-C30	-3.80	117.57	121.64
2	B	501	4GF	F33-C28-C27	-3.75	118.14	121.04
2	C	501	4GF	F33-C28-C27	-3.61	118.25	121.04
2	C	501	4GF	C12-C11-C10	3.48	121.70	117.27
2	A	501	4GF	C12-C11-C10	3.20	121.34	117.27
2	B	501	4GF	C12-C11-C10	2.93	121.00	117.27
2	C	501	4GF	C23-C18-C15	2.78	116.56	111.49
2	C	501	4GF	C35-C34-C30	-2.75	118.70	121.64
2	D	501	4GF	C12-C11-C10	2.67	120.67	117.27
2	C	501	4GF	C20-C19-C18	-2.47	108.12	111.04
2	B	501	4GF	C29-C28-C27	2.46	123.42	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	4GF	C29-C28-C27	2.43	123.39	121.44
2	A	501	4GF	C29-C28-C27	2.37	123.34	121.44
2	C	501	4GF	C29-C28-C27	2.24	123.24	121.44
2	C	501	4GF	C19-C18-C15	2.17	115.44	111.49
2	B	501	4GF	C18-C15-N16	-2.16	117.05	120.23
2	B	501	4GF	C35-C34-C30	-2.08	119.42	121.64
2	B	501	4GF	C23-C18-C15	2.07	115.26	111.49
2	C	501	4GF	C18-C15-N16	-2.06	117.19	120.23

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	4GF	C25-C24-N21-C20
2	C	501	4GF	C26-C24-N21-C20
2	A	501	4GF	C14-C15-C18-C23
2	A	501	4GF	N16-C15-C18-C23
2	B	501	4GF	C29-C30-C34-C35
2	B	501	4GF	C31-C30-C34-C35
2	A	501	4GF	C29-C30-C34-C36
2	A	501	4GF	C31-C30-C34-C36
2	B	501	4GF	C32-C27-N17-N16
2	C	501	4GF	C32-C27-N17-N16
2	A	501	4GF	C32-C27-N17-N16
2	C	501	4GF	N16-C15-C18-C19
2	C	501	4GF	C26-C24-N21-C22
2	A	501	4GF	C25-C24-N21-C22
2	D	501	4GF	C14-C15-C18-C23
2	C	501	4GF	C14-C15-C18-C19

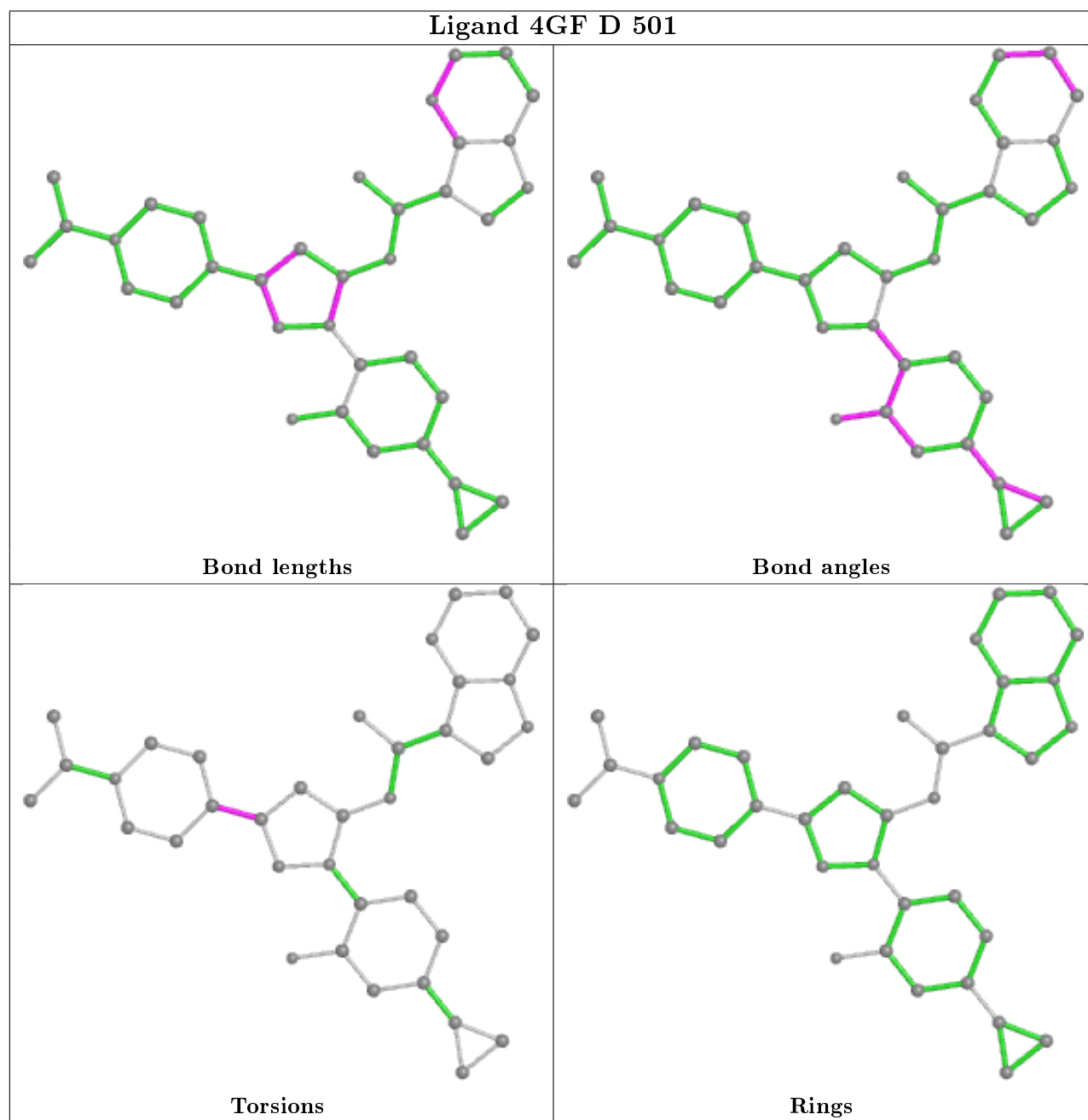
There are no ring outliers.

1 monomer is involved in 1 short contact:

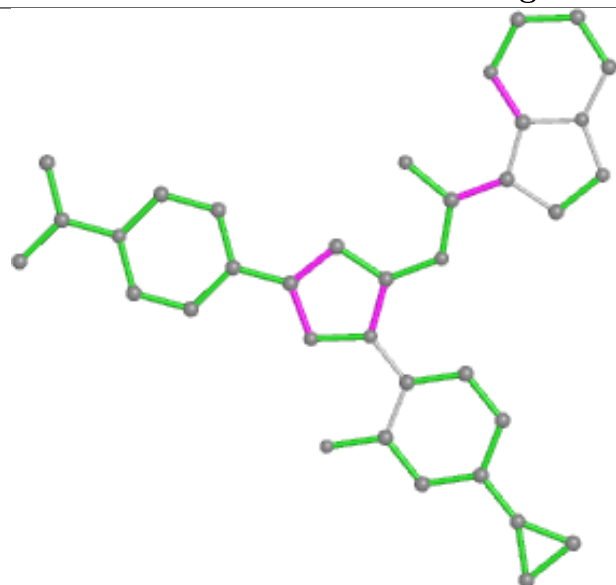
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	4GF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

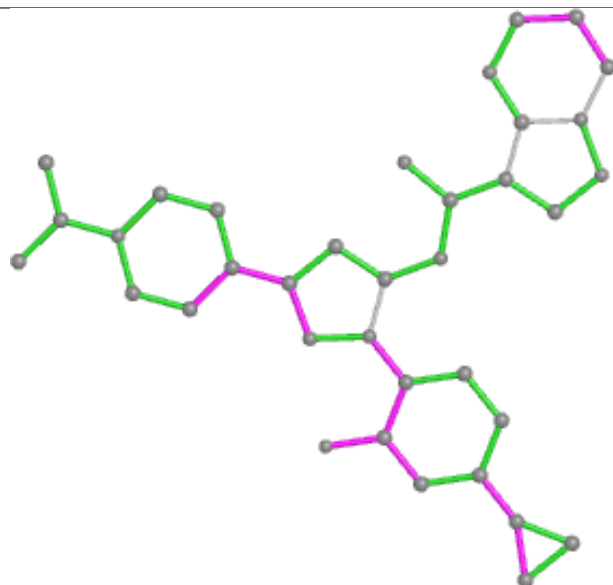
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



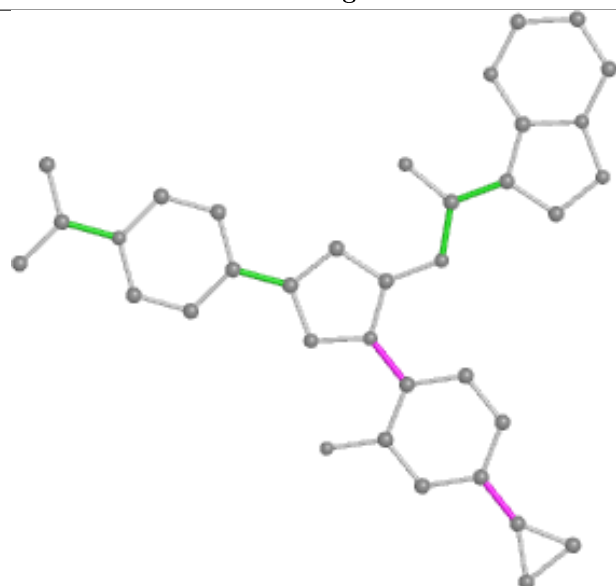
Ligand 4GF B 501



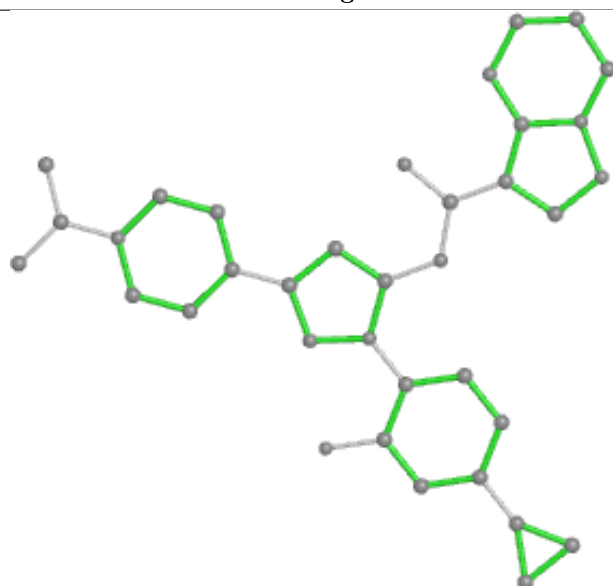
Bond lengths



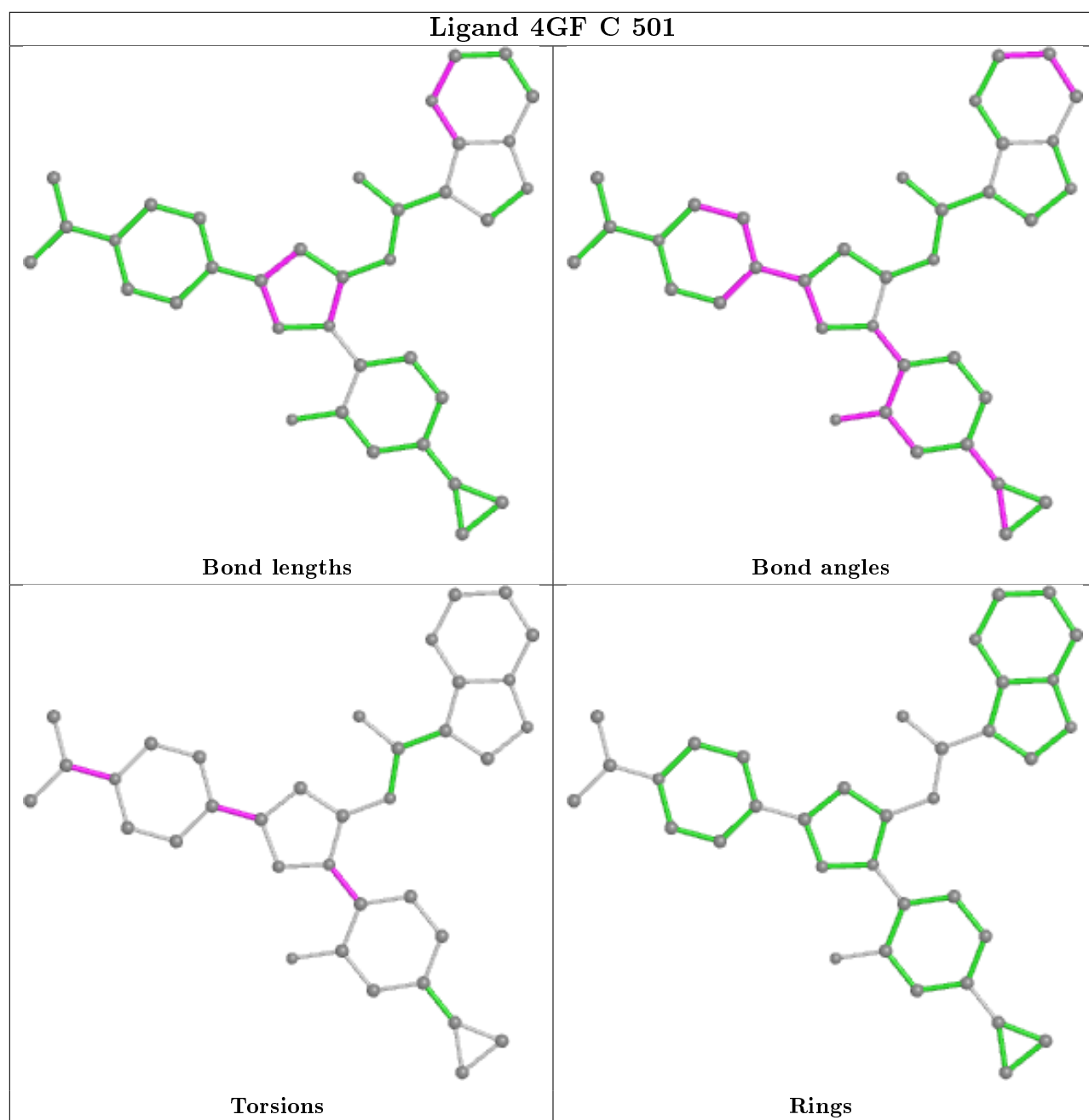
Bond angles

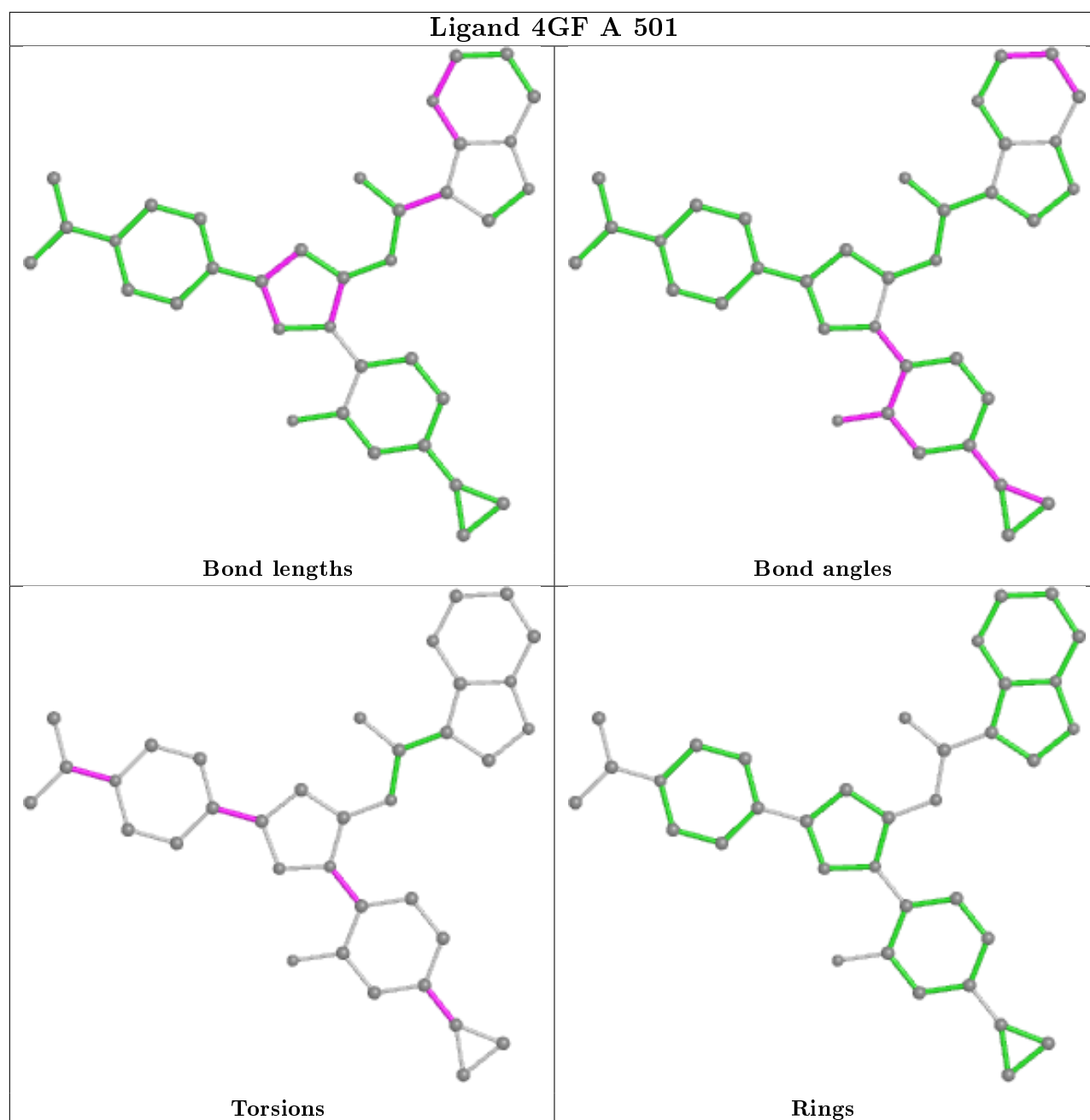


Torsions



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/301 (94%)	0.55	25 (8%) 10 7	42, 81, 119, 131	0
1	B	278/301 (92%)	0.49	23 (8%) 11 9	35, 77, 123, 142	0
1	C	287/301 (95%)	0.04	2 (0%) 87 86	35, 61, 93, 110	0
1	D	285/301 (94%)	0.07	4 (1%) 75 73	36, 61, 98, 116	0
All	All	1134/1204 (94%)	0.28	54 (4%) 30 26	35, 67, 113, 142	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	240	CYS	6.5
1	B	240	CYS	6.4
1	B	230	PHE	5.1
1	A	204	TYR	5.0
1	A	196	GLY	4.6
1	B	257	ASP	4.5
1	A	164	ARG	4.0
1	A	168	PHE	3.6
1	A	238	ALA	3.6
1	A	254	ASP	3.4
1	B	334	ARG	3.3
1	A	195	GLY	3.2
1	B	253	SER	3.1
1	B	187	VAL	3.1
1	B	239	LYS	3.1
1	B	343	VAL	3.0
1	D	230	PHE	3.0
1	B	164	ARG	3.0
1	B	347	ARG	3.0
1	A	230	PHE	2.9
1	C	197	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	227	LYS	2.8
1	A	401	GLU	2.7
1	B	332	LEU	2.7
1	B	348	ILE	2.7
1	A	251	PHE	2.6
1	A	165	PHE	2.6
1	B	229	GLN	2.6
1	A	205	VAL	2.5
1	B	251	PHE	2.5
1	A	236	VAL	2.4
1	A	343	VAL	2.4
1	B	165	PHE	2.4
1	B	184	PRO	2.4
1	B	198	GLY	2.4
1	A	229	GLN	2.3
1	B	234	ILE	2.3
1	D	217	ALA	2.2
1	A	207	ASN	2.2
1	D	216	ALA	2.2
1	A	206	ASN	2.2
1	A	237	MET	2.2
1	D	168	PHE	2.2
1	A	336	SER	2.1
1	B	364	ILE	2.1
1	A	331	GLY	2.1
1	A	170	PHE	2.1
1	B	162	ASP	2.1
1	A	335	ALA	2.1
1	C	217	ALA	2.1
1	B	185	ILE	2.1
1	A	216	ALA	2.1
1	B	401	GLU	2.1
1	B	344	MET	2.0

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

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(\AA^2)	Q<0.9
1	TPO	A	342	11/12	0.68	0.30	136,137,143,143	0
1	TPO	B	342	11/12	0.79	0.24	129,130,136,137	0
1	TPO	D	342	11/12	0.80	0.16	106,110,117,118	0
1	TPO	C	342	11/12	0.83	0.17	99,104,111,112	0
1	SEP	D	346	10/11	0.85	0.14	103,107,113,113	0
1	SEP	B	346	10/11	0.85	0.15	116,119,124,124	0
1	SEP	A	346	10/11	0.85	0.19	120,123,128,129	0
1	TPO	B	345	11/12	0.86	0.24	116,117,120,120	0
1	TPO	A	345	11/12	0.88	0.15	122,123,124,125	0
1	TPO	D	345	11/12	0.91	0.12	97,102,105,105	0
1	SEP	C	346	10/11	0.91	0.10	88,93,99,100	0
1	TPO	C	345	11/12	0.96	0.13	81,84,90,90	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

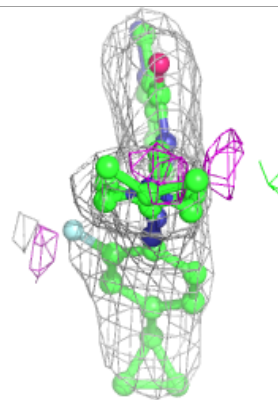
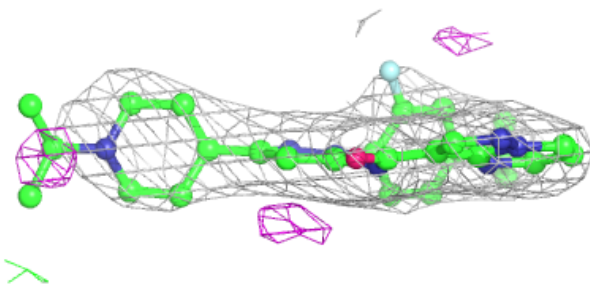
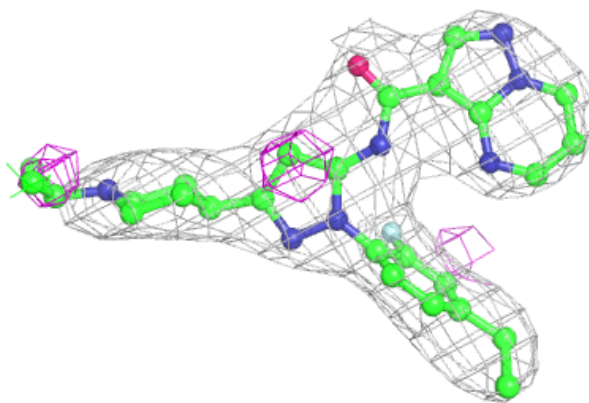
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	4GF	B	501	36/36	0.93	0.25	59,70,87,89	0
2	4GF	A	501	36/36	0.95	0.23	57,74,84,85	0
2	4GF	D	501	36/36	0.96	0.21	49,59,68,71	0
2	4GF	C	501	36/36	0.97	0.20	43,55,69,69	0

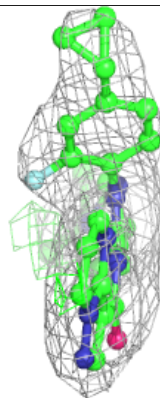
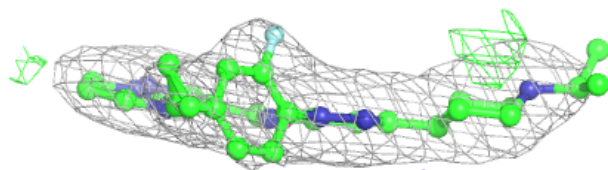
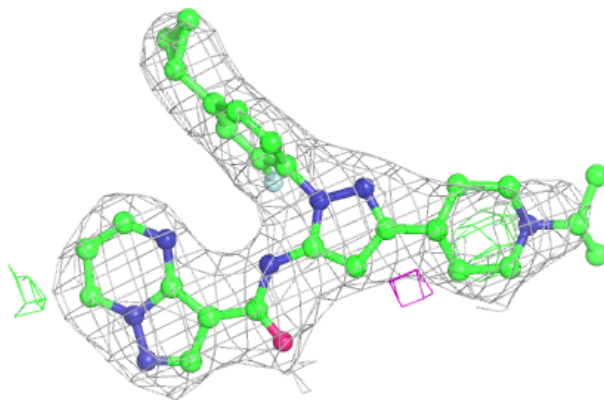
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4GF 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)

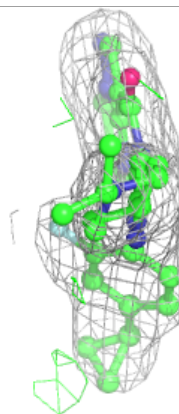
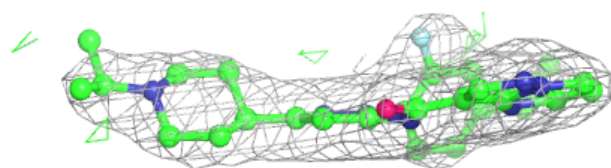
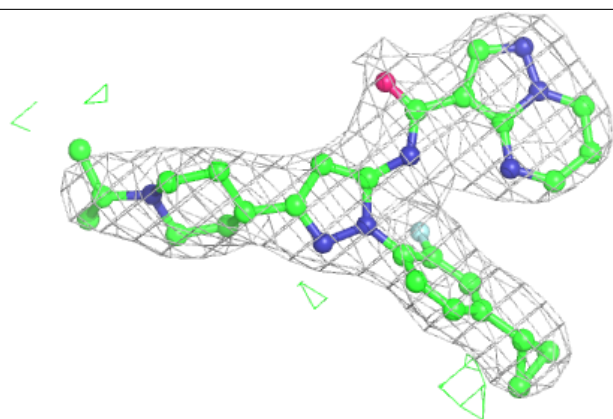
**Electron density around 4GF A 501:**

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

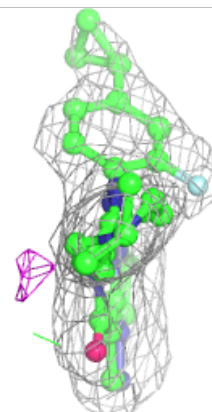
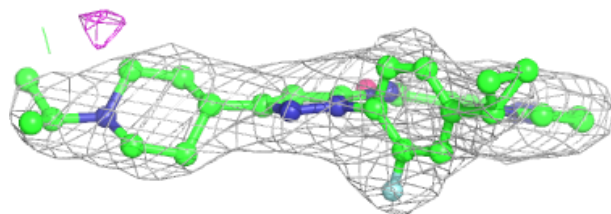
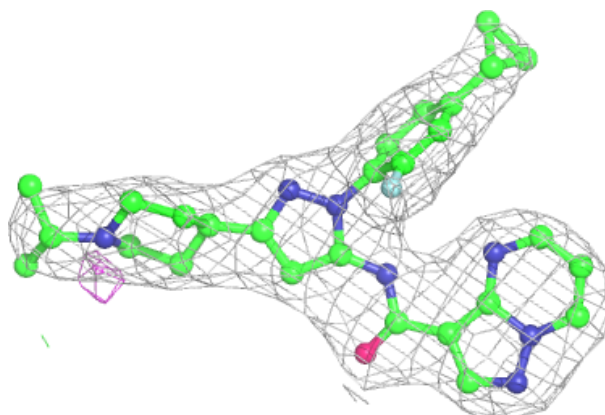


Electron density around 4GF D 501:

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

**Electron density around 4GF C 501:**

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



6.5 Other polymers

There are no such residues in this entry.