



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2025 – 05:34 am BST

PDB ID : 9R9K / pdb\_00009r9k  
Title : IRAK4 in complex with inhibitor  
Authors : Xue, Y.; Terstiege, I.; Aagaard, A.  
Deposited on : 2025-05-20  
Resolution : 1.87 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

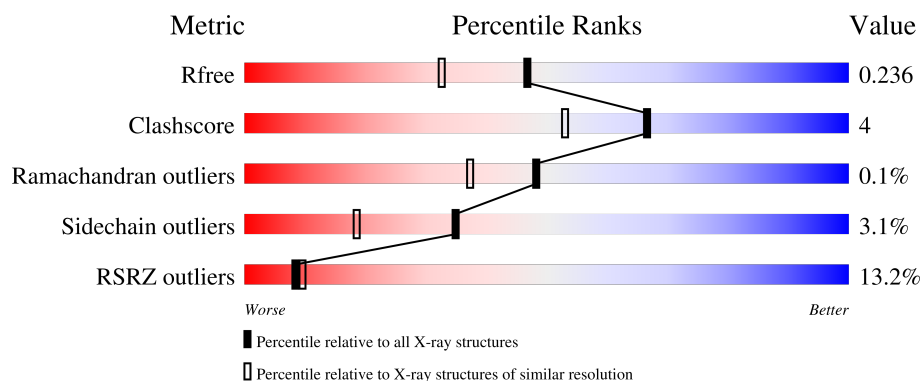
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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))
$R_{free}$	164625	1090 (1.88-1.88)
Clashscore	180529	1144 (1.88-1.88)
Ramachandran outliers	177936	1135 (1.88-1.88)
Sidechain outliers	177891	1135 (1.88-1.88)
RSRZ outliers	164620	1090 (1.88-1.88)

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  $\geq 3$ , 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	308	<div> <div>14%</div> <div>82% 10% 7%</div> </div>
1	B	308	<div> <div>13%</div> <div>86% 8% 6%</div> </div>
1	C	308	<div> <div>12%</div> <div>79% 13% 7%</div> </div>
1	D	308	<div> <div>11%</div> <div>86% 6% 7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9831 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.

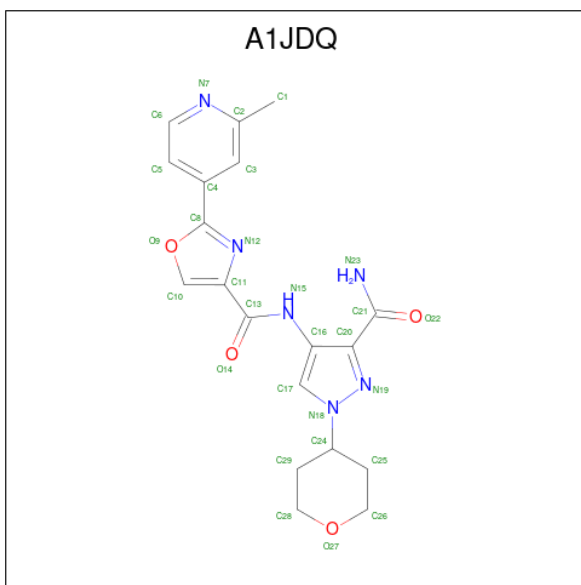
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	0
			2256	1414	380	446	2	14			
1	B	290	Total	C	N	O	P	S	0	0	0
			2286	1433	384	453	2	14			
1	C	287	Total	C	N	O	P	S	0	0	0
			2264	1419	382	447	2	14			
1	D	287	Total	C	N	O	P	S	0	0	0
			2266	1422	382	446	2	14			

There are 4 discrepancies between the modelled and reference sequences:

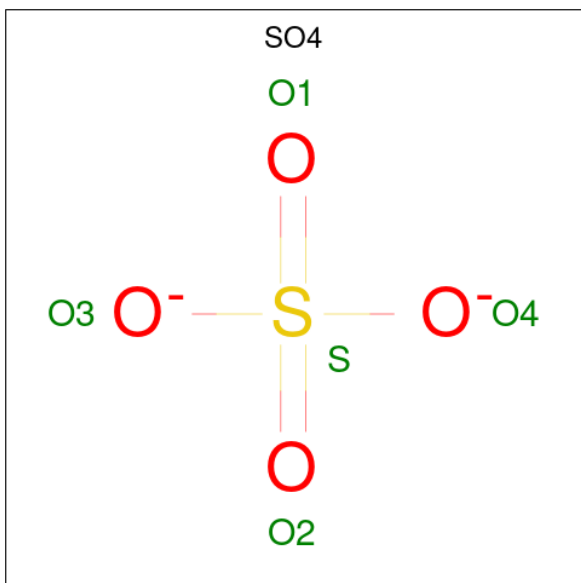
Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is {N}-[3-aminocarbonyl-1-(oxan-4-yl)pyrazol-4-yl]-2-(2-methylpyridin-4-yl)-1,3-oxazole-4-carboxamide (CCD ID: A1JDQ) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 29	C 19	N 6	O 4	0	0
2	B	1	Total 29	C 19	N 6	O 4	0	0
2	C	1	Total 29	C 19	N 6	O 4	0	0
2	D	1	Total 29	C 19	N 6	O 4	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula:  $\text{O}_4\text{S}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

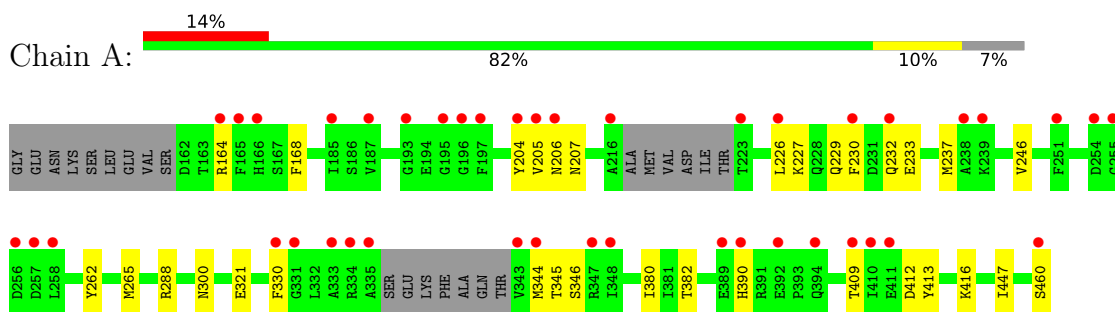
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		
4	B	152	Total	O	0	0
			152	152		
4	C	162	Total	O	0	0
			162	162		
4	D	185	Total	O	0	0
			185	185		

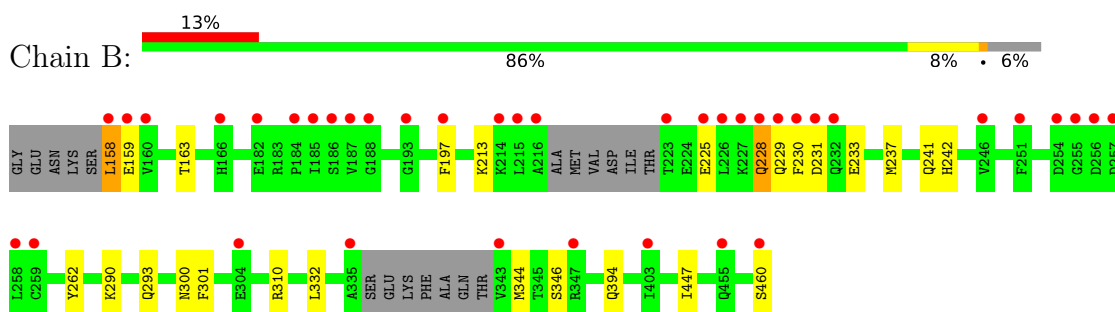
### 3 Residue-property plots [i](#)

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.

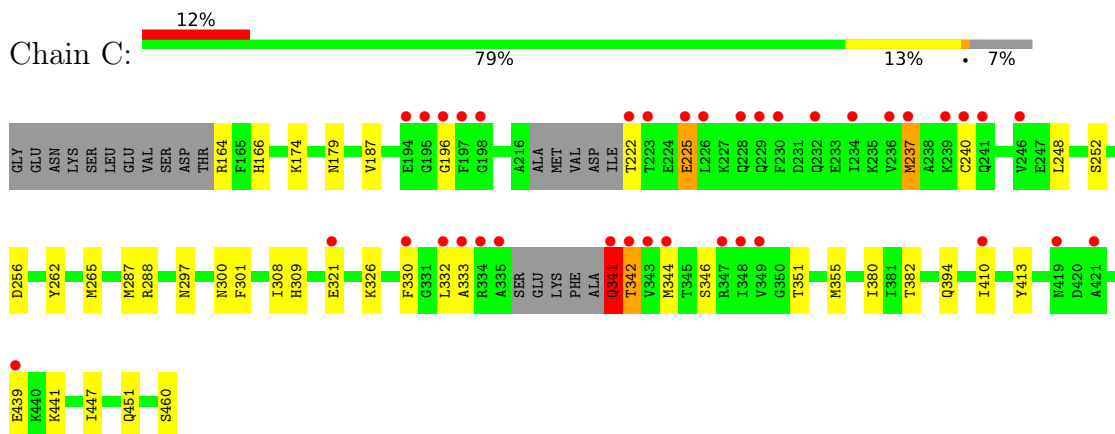
- Molecule 1: Interleukin-1 receptor-associated kinase 4



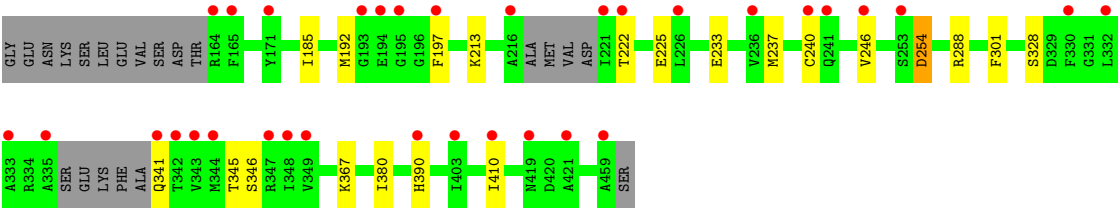
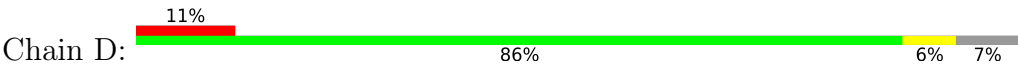
- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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, $\alpha$ , $\beta$ , $\gamma$	142.32Å 140.50Å 88.40Å 90.00° 123.50° 90.00°	Depositor
Resolution (Å)	90.66 – 1.87 90.66 – 1.87	Depositor EDS
% Data completeness (in resolution range)	68.5 (90.66-1.87) 68.5 (90.66-1.87)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.87Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, $R_{free}$	0.215 , 0.242 0.209 , 0.236	Depositor DCC
$R_{free}$ test set	4082 reflections (3.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, TPO, A1JDQ, 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	0.72	1/2271 (0.0%)	1.03	1/3059 (0.0%)
1	B	0.73	0/2301	1.06	1/3100 (0.0%)
1	C	0.78	0/2279	1.06	4/3070 (0.1%)
1	D	0.76	0/2281	1.02	1/3073 (0.0%)
All	All	0.75	1/9132 (0.0%)	1.04	7/12302 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	MET	SD-CE	-6.41	1.63	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	PHE	CA-CB-CG	5.94	119.74	113.80
1	C	341	GLN	CA-C-N	5.51	132.06	121.54
1	C	341	GLN	C-N-CA	5.51	132.06	121.54
1	C	196	GLY	CA-C-N	5.19	127.19	120.44
1	C	196	GLY	C-N-CA	5.19	127.19	120.44
1	A	230	PHE	CA-CB-CG	5.16	118.96	113.80
1	D	254	ASP	CA-CB-CG	5.13	117.73	112.60

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	2256	0	2216	15	0
1	B	2286	0	2247	14	0
1	C	2264	0	2227	22	0
1	D	2266	0	2233	15	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
3	A	5	0	0	0	0
4	A	139	0	0	2	0
4	B	152	0	0	2	0
4	C	162	0	0	1	0
4	D	185	0	0	0	0
All	All	9831	0	8923	65	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 4.

All (65) 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:222:THR:HB	1:C:225:GLU:HB3	1.41	1.03
1:B:158:LEU:HD22	1:B:242:HIS:HD2	1.46	0.80
1:B:310:ARG:HD3	1:B:332:LEU:O	1.81	0.80
1:A:390:HIS:O	1:D:390:HIS:O	2.02	0.77
1:C:341:GLN:HB2	1:C:441:LYS:NZ	2.01	0.76
1:D:341:GLN:HB3	1:D:367:LYS:HZ2	1.54	0.71
1:A:168:PHE:HE1	1:A:205:VAL:HG11	1.57	0.70
1:C:222:THR:HB	1:C:225:GLU:CB	2.18	0.70
1:A:168:PHE:CE1	1:A:205:VAL:HG11	2.28	0.68
1:D:341:GLN:CD	1:D:367:LYS:HZ2	2.02	0.68
1:B:233:GLU:O	1:B:237:MET:HG2	1.95	0.67
1:B:158:LEU:HD22	1:B:242:HIS:CD2	2.30	0.65
1:C:297:ASN:ND2	1:C:451:GLN:HE21	1.95	0.65
1:D:233:GLU:O	1:D:237:MET:HG2	1.97	0.64
1:D:341:GLN:HB3	1:D:367:LYS:NZ	2.17	0.60
1:C:237:MET:HG2	1:C:248:LEU:HB2	1.84	0.60
1:C:341:GLN:HB2	1:C:441:LYS:HZ2	1.66	0.59
1:D:341:GLN:CB	1:D:367:LYS:HZ2	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:ASN:ND2	4:C:602:HOH:O	2.38	0.56
1:C:297:ASN:HD22	1:C:451:GLN:HE21	1.52	0.56
1:B:237:MET:HE2	1:B:262:TYR:HE2	1.71	0.55
1:D:246:VAL:HG21	1:D:328:SER:HB3	1.90	0.53
1:C:174:LYS:HG3	1:C:179:ASN:OD1	2.11	0.51
1:C:187:VAL:HG12	1:C:187:VAL:O	2.10	0.51
1:C:240:CYS:HA	1:C:301:PHE:HE2	1.76	0.51
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.93	0.51
1:A:321:GLU:H	1:A:321:GLU:CD	2.19	0.50
1:C:288:ARG:HB3	1:C:380:ILE:HG23	1.93	0.49
1:D:288:ARG:HB3	1:D:380:ILE:HG23	1.93	0.49
1:B:310:ARG:CD	1:B:332:LEU:O	2.57	0.49
1:D:341:GLN:CG	1:D:367:LYS:HZ2	2.26	0.48
1:B:290:LYS:HG2	4:B:601:HOH:O	2.12	0.48
1:D:185:ILE:HD11	1:D:192:MET:HG2	1.95	0.48
1:A:237:MET:SD	1:A:330:PHE:CD2	3.07	0.47
1:B:197:PHE:CD1	1:B:213:LYS:HD2	2.50	0.47
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.96	0.47
4:A:604:HOH:O	1:C:166:HIS:HD2	1.98	0.46
1:C:237:MET:HE2	1:C:262:TYR:HE1	1.80	0.46
1:B:158:LEU:HB3	1:B:301:PHE:CD1	2.52	0.45
1:C:309:HIS:CD2	1:C:330:PHE:HB3	2.52	0.45
1:D:222:THR:HB	1:D:225:GLU:HG3	1.99	0.45
1:D:240:CYS:HA	1:D:301:PHE:HE2	1.81	0.44
1:C:308:ILE:O	1:C:333:ALA:HA	2.17	0.44
1:C:265:MET:SD	1:C:326:LYS:HG3	2.58	0.43
1:B:163:THR:OG1	1:B:241:GLN:NE2	2.52	0.43
1:B:293:GLN:NE2	4:B:609:HOH:O	2.51	0.43
1:B:225:GLU:HA	1:B:228:GLN:HG3	2.00	0.43
1:A:409:THR:HG23	1:A:412:ASP:H	1.84	0.42
1:A:382:THR:HG22	1:A:413:TYR:HB3	2.01	0.42
1:A:237:MET:HE1	1:A:246:VAL:HG23	2.02	0.42
1:A:226:LEU:HA	1:A:229:GLN:HG2	2.02	0.42
1:D:197:PHE:CD2	1:D:213:LYS:HD2	2.54	0.42
1:A:288:ARG:HB3	1:A:380:ILE:CG2	2.49	0.42
1:C:287:MET:HA	1:C:287:MET:HE2	2.02	0.42
1:C:351:THR:O	1:C:355:MET:HG3	2.20	0.41
1:A:416:LYS:NZ	4:A:612:HOH:O	2.53	0.41
1:D:246:VAL:CG2	1:D:328:SER:HB3	2.50	0.41
1:A:204:TYR:CZ	1:A:207:ASN:HA	2.55	0.41
1:A:300:ASN:HA	1:A:447:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ARG:HB3	1:C:380:ILE:CG2	2.51	0.41
1:D:222:THR:HB	1:D:225:GLU:CG	2.51	0.41
1:A:237:MET:HE2	1:A:262:TYR:HE2	1.85	0.40
1:C:382:THR:HG22	1:C:413:TYR:HB3	2.03	0.40
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.03	0.40
1:B:225:GLU:HA	1:B:228:GLN:CG	2.51	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	278/308 (90%)	271 (98%)	7 (2%)	0	100	100
1	B	282/308 (92%)	274 (97%)	8 (3%)	0	100	100
1	C	279/308 (91%)	272 (98%)	6 (2%)	1 (0%)	30	18
1	D	279/308 (91%)	270 (97%)	9 (3%)	0	100	100
All	All	1118/1232 (91%)	1087 (97%)	30 (3%)	1 (0%)	48	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	342	THR

### 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	247/266 (93%)	240 (97%)	7 (3%)	38	22
1	B	251/266 (94%)	243 (97%)	8 (3%)	34	17
1	C	248/266 (93%)	234 (94%)	14 (6%)	17	5
1	D	248/266 (93%)	246 (99%)	2 (1%)	79	74
All	All	994/1064 (93%)	963 (97%)	31 (3%)	35	18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	206	ASN
1	A	227	LYS
1	A	232	GLN
1	A	233	GLU
1	A	344	MET
1	A	460	SER
1	B	158	LEU
1	B	159	GLU
1	B	228	GLN
1	B	229	GLN
1	B	231	ASP
1	B	344	MET
1	B	394	GLN
1	B	460	SER
1	C	164	ARG
1	C	225	GLU
1	C	237	MET
1	C	252	SER
1	C	256	ASP
1	C	321	GLU
1	C	332	LEU
1	C	341	GLN
1	C	342	THR
1	C	344	MET
1	C	394	GLN
1	C	410	ILE
1	C	439	GLU
1	C	460	SER
1	D	254	ASP
1	D	410	ILE

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

Mol	Chain	Res	Type
1	A	166	HIS
1	A	179	ASN
1	A	307	HIS
1	A	390	HIS
1	A	394	GLN
1	B	232	GLN
1	B	241	GLN
1	B	307	HIS
1	B	390	HIS
1	B	394	GLN
1	B	435	GLN
1	B	451	GLN
1	C	166	HIS
1	C	297	ASN
1	C	306	HIS
1	C	394	GLN
1	D	390	HIS
1	D	394	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	TPO	D	345	1	8,10,11	1.18	1 (12%)	10,14,16	1.02	0
1	TPO	A	345	1	8,10,11	1.23	1 (12%)	10,14,16	1.13	1 (10%)
1	SEP	D	346	1	8,9,10	0.75	0	8,12,14	1.43	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TPO	C	345	1	8,10,11	1.16	0	10,14,16	1.02	0
1	SEP	B	346	1	8,9,10	0.89	1 (12%)	8,12,14	1.29	2 (25%)
1	SEP	A	346	1	8,9,10	0.83	0	8,12,14	1.06	1 (12%)
1	TPO	B	345	1	8,10,11	1.05	0	10,14,16	1.04	0
1	SEP	C	346	1	8,9,10	0.86	0	8,12,14	1.41	2 (25%)

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	D	345	1	-	5/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	SEP	D	346	1	-	0/5/8/10	-
1	TPO	C	345	1	-	4/9/11/13	-
1	SEP	B	346	1	-	0/5/8/10	-
1	SEP	A	346	1	-	0/5/8/10	-
1	TPO	B	345	1	-	5/9/11/13	-
1	SEP	C	346	1	-	0/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	TPO	CB-CA	2.18	1.58	1.53
1	D	345	TPO	CB-CA	2.17	1.58	1.53
1	B	346	SEP	P-OG	-2.10	1.53	1.60

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	P-OG-CB	-2.91	110.27	118.30
1	C	346	SEP	P-OG-CB	-2.87	110.38	118.30
1	B	346	SEP	P-OG-CB	-2.56	111.25	118.30
1	A	346	SEP	P-OG-CB	-2.29	112.00	118.30
1	D	346	SEP	O3P-P-OG	2.19	112.55	106.73
1	A	345	TPO	O3P-P-OG1	2.15	115.60	105.99
1	C	346	SEP	O3P-P-OG	2.09	112.28	106.73
1	B	346	SEP	O3P-P-OG	2.04	112.17	106.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

5 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	A1JDQ	B	501	-	26,32,32	1.30	5 (19%)	28,45,45	2.15	6 (21%)
2	A1JDQ	A	501	-	26,32,32	1.17	5 (19%)	28,45,45	2.02	8 (28%)
3	SO4	A	502	-	4,4,4	0.17	0	6,6,6	0.66	0
2	A1JDQ	C	501	-	26,32,32	1.24	4 (15%)	28,45,45	2.17	7 (25%)
2	A1JDQ	D	501	-	26,32,32	1.32	5 (19%)	28,45,45	2.07	7 (25%)

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	A1JDQ	B	501	-	-	0/4/28/28	0/4/4/4
2	A1JDQ	A	501	-	-	0/4/28/28	0/4/4/4
2	A1JDQ	C	501	-	-	0/4/28/28	0/4/4/4
2	A1JDQ	D	501	-	-	0/4/28/28	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1JDQ	C20-N19	-2.94	1.33	1.35
2	D	501	A1JDQ	C11-C13	-2.92	1.43	1.50
2	D	501	A1JDQ	C21-N23	2.80	1.38	1.33
2	B	501	A1JDQ	C11-C13	-2.72	1.44	1.50
2	B	501	A1JDQ	C20-C21	-2.70	1.43	1.51
2	C	501	A1JDQ	C11-C13	-2.65	1.44	1.50
2	C	501	A1JDQ	C20-C21	-2.61	1.43	1.51
2	D	501	A1JDQ	C20-C21	-2.60	1.43	1.51
2	C	501	A1JDQ	C21-N23	2.58	1.37	1.33
2	A	501	A1JDQ	C20-C21	-2.58	1.44	1.51
2	A	501	A1JDQ	C11-C13	-2.42	1.44	1.50
2	C	501	A1JDQ	C20-N19	-2.32	1.33	1.35
2	D	501	A1JDQ	C24-N18	-2.26	1.45	1.49
2	D	501	A1JDQ	C20-N19	-2.19	1.33	1.35
2	B	501	A1JDQ	C24-N18	-2.13	1.46	1.49
2	A	501	A1JDQ	C20-N19	-2.11	1.33	1.35
2	A	501	A1JDQ	C21-N23	2.11	1.37	1.33
2	B	501	A1JDQ	C21-N23	2.08	1.36	1.33
2	A	501	A1JDQ	C16-N15	-2.03	1.37	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	A1JDQ	C17-N18-N19	6.20	115.40	111.70
2	C	501	A1JDQ	C17-N18-C24	6.02	130.81	125.48
2	D	501	A1JDQ	C17-N18-C24	5.19	130.08	125.48
2	A	501	A1JDQ	C17-N18-N19	4.88	114.61	111.70
2	C	501	A1JDQ	C4-C3-C2	-4.83	118.07	120.23
2	D	501	A1JDQ	C17-N18-N19	4.82	114.58	111.70
2	A	501	A1JDQ	C17-N18-C24	4.58	129.54	125.48
2	D	501	A1JDQ	C4-C3-C2	-4.36	118.28	120.23
2	A	501	A1JDQ	C4-C3-C2	-4.21	118.34	120.23
2	C	501	A1JDQ	C17-N18-N19	3.99	114.08	111.70
2	B	501	A1JDQ	C4-C3-C2	-3.93	118.47	120.23
2	B	501	A1JDQ	C17-N18-C24	3.70	128.76	125.48
2	B	501	A1JDQ	C16-C17-N18	-3.60	103.25	107.59
2	C	501	A1JDQ	O22-C21-N23	3.57	127.65	122.58
2	A	501	A1JDQ	C16-C17-N18	-3.07	103.89	107.59
2	D	501	A1JDQ	C16-C17-N18	-2.84	104.17	107.59
2	C	501	A1JDQ	C20-C21-N23	-2.77	111.38	115.75
2	D	501	A1JDQ	O22-C21-N23	2.66	126.36	122.58
2	A	501	A1JDQ	C4-C8-N12	2.48	126.89	123.56
2	B	501	A1JDQ	C4-C8-N12	2.45	126.84	123.56
2	C	501	A1JDQ	C4-C8-N12	2.34	126.70	123.56
2	D	501	A1JDQ	C4-C8-N12	2.29	126.64	123.56
2	C	501	A1JDQ	C16-C17-N18	-2.27	104.85	107.59
2	B	501	A1JDQ	C20-N19-N18	-2.27	102.61	105.26
2	D	501	A1JDQ	C6-C5-C4	-2.10	116.45	119.57
2	A	501	A1JDQ	C28-O27-C26	2.09	116.87	109.89
2	A	501	A1JDQ	C3-C2-N7	2.02	123.63	121.66
2	A	501	A1JDQ	O14-C13-C11	2.00	125.45	121.08

There are no chirality outliers.

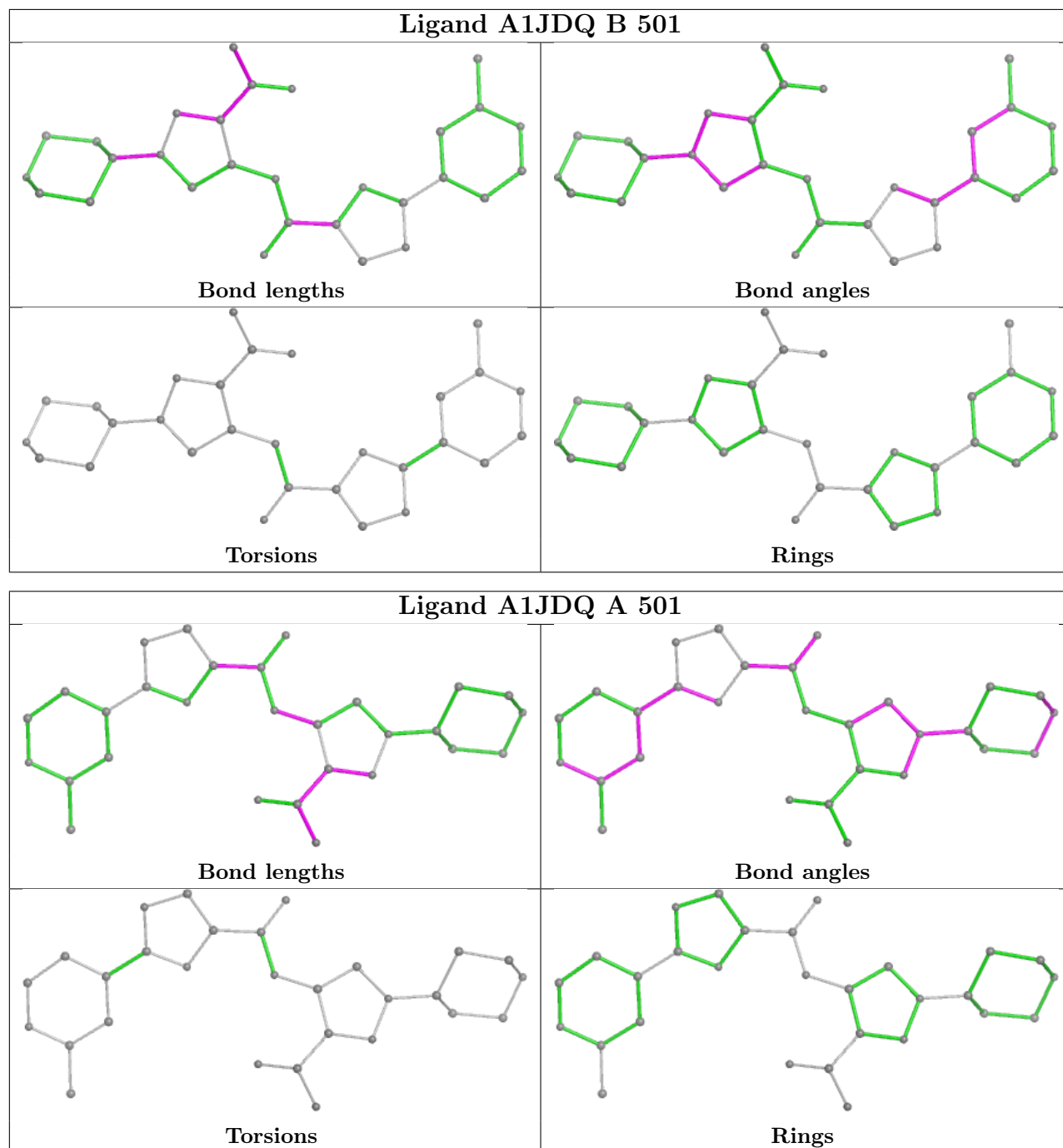
There are no torsion outliers.

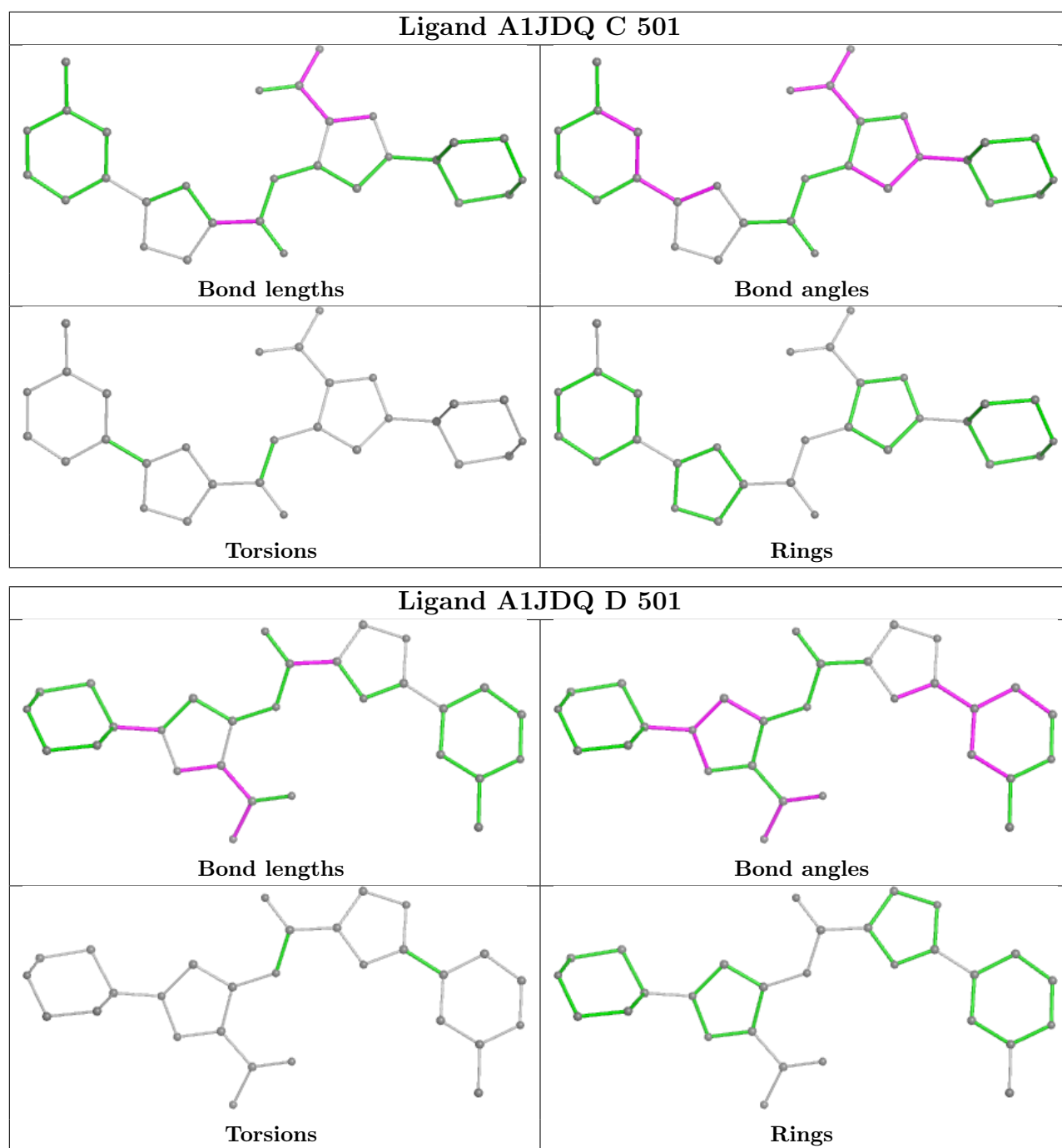
There are no ring outliers.

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 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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	284/308 (92%)	0.84	42 (14%) <b>7</b> <b>7</b>	20, 38, 67, 89	0
1	B	288/308 (93%)	0.76	39 (13%) <b>8</b> <b>9</b>	21, 39, 68, 87	0
1	C	285/308 (92%)	0.71	37 (12%) <b>9</b> <b>10</b>	21, 33, 67, 85	0
1	D	285/308 (92%)	0.68	33 (11%) <b>11</b> <b>12</b>	19, 36, 61, 79	0
All	All	1142/1232 (92%)	0.75	151 (13%) <b>8</b> <b>9</b>	19, 36, 67, 89	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	221	ILE	7.6
1	C	197	PHE	5.9
1	C	335	ALA	5.3
1	C	195	GLY	5.2
1	C	240	CYS	5.1
1	B	223	THR	4.8
1	C	342	THR	4.8
1	A	226	LEU	4.8
1	D	343	VAL	4.7
1	C	222	THR	4.7
1	C	223	THR	4.7
1	B	257	ASP	4.4
1	C	333	ALA	4.3
1	B	343	VAL	4.2
1	C	343	VAL	4.2
1	A	256	ASP	4.2
1	D	342	THR	4.1
1	C	349	VAL	4.1
1	B	460	SER	4.0
1	A	223	THR	4.0
1	B	254	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	256	ASP	3.9
1	A	216	ALA	3.9
1	A	204	TYR	3.8
1	A	343	VAL	3.8
1	C	198	GLY	3.8
1	C	332	LEU	3.7
1	D	419	ASN	3.7
1	D	197	PHE	3.7
1	D	333	ALA	3.7
1	B	158	LEU	3.6
1	C	348	ILE	3.6
1	D	410	ILE	3.6
1	B	215	LEU	3.6
1	D	330	PHE	3.6
1	C	341	GLN	3.5
1	A	205	VAL	3.5
1	B	216	ALA	3.5
1	A	335	ALA	3.5
1	C	226	LEU	3.5
1	B	187	VAL	3.4
1	D	344	MET	3.4
1	D	335	ALA	3.4
1	C	225	GLU	3.3
1	A	333	ALA	3.3
1	D	332	LEU	3.3
1	A	230	PHE	3.3
1	C	246	VAL	3.2
1	C	410	ILE	3.2
1	A	330	PHE	3.2
1	C	236	VAL	3.1
1	A	197	PHE	3.1
1	A	196	GLY	3.1
1	A	392	GLU	3.0
1	C	419	ASN	3.0
1	B	185	ILE	3.0
1	C	421	ALA	3.0
1	C	230	PHE	3.0
1	C	194	GLU	3.0
1	A	460	SER	3.0
1	A	251	PHE	3.0
1	A	255	GLY	3.0
1	D	171	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	459	ALA	2.9
1	B	160	VAL	2.9
1	C	334	ARG	2.9
1	C	347	ARG	2.9
1	C	229	GLN	2.9
1	A	232	GLN	2.9
1	C	232	GLN	2.9
1	D	253	SER	2.9
1	C	330	PHE	2.8
1	D	240	CYS	2.8
1	B	335	ALA	2.8
1	D	403	ILE	2.8
1	B	226	LEU	2.8
1	B	184	PRO	2.8
1	A	187	VAL	2.8
1	A	238	ALA	2.8
1	B	304	GLU	2.8
1	C	196	GLY	2.7
1	D	348	ILE	2.7
1	B	231	ASP	2.7
1	B	228	GLN	2.6
1	C	241	GLN	2.6
1	A	185	ILE	2.6
1	C	239	LYS	2.6
1	D	216	ALA	2.6
1	A	344	MET	2.6
1	B	182	GLU	2.6
1	D	390	HIS	2.6
1	A	347	ARG	2.6
1	B	232	GLN	2.6
1	C	321	GLU	2.6
1	B	251	PHE	2.5
1	B	229	GLN	2.5
1	C	228	GLN	2.5
1	A	331	GLY	2.5
1	A	410	ILE	2.5
1	B	166	HIS	2.5
1	D	341	GLN	2.5
1	A	195	GLY	2.5
1	D	164	ARG	2.5
1	B	225	GLU	2.5
1	A	193	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	206	ASN	2.4
1	D	421	ALA	2.4
1	A	258	LEU	2.4
1	C	234	ILE	2.4
1	B	227	LYS	2.4
1	C	237	MET	2.3
1	B	197	PHE	2.3
1	A	409	THR	2.3
1	A	411	GLU	2.3
1	A	254	ASP	2.3
1	D	194	GLU	2.3
1	A	164	ARG	2.2
1	A	334	ARG	2.2
1	B	255	GLY	2.2
1	D	193	GLY	2.2
1	A	165	PHE	2.2
1	D	165	PHE	2.2
1	C	439	GLU	2.2
1	A	257	ASP	2.2
1	A	394	GLN	2.2
1	B	186	SER	2.2
1	B	259	CYS	2.2
1	C	344	MET	2.2
1	B	230	PHE	2.1
1	D	347	ARG	2.1
1	B	403	ILE	2.1
1	D	222	THR	2.1
1	B	455	GLN	2.1
1	B	188	GLY	2.1
1	B	193	GLY	2.1
1	D	246	VAL	2.1
1	A	389	GLU	2.1
1	A	166	HIS	2.1
1	B	347	ARG	2.1
1	D	349	VAL	2.1
1	B	258	LEU	2.1
1	A	348	ILE	2.1
1	B	159	GLU	2.1
1	A	390	HIS	2.0
1	D	195	GLY	2.1
1	D	236	VAL	2.0
1	A	239	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	214	LYS	2.0
1	B	246	VAL	2.0
1	D	241	GLN	2.0
1	D	226	LEU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	SEP	D	346	10/11	0.66	0.20	63,66,97,99	0
1	SEP	C	346	10/11	0.68	0.12	68,72,105,111	0
1	SEP	A	346	10/11	0.73	0.14	64,68,100,104	0
1	SEP	B	346	10/11	0.75	0.13	61,64,102,105	0
1	TPO	A	345	11/12	0.91	0.10	62,67,71,71	0
1	TPO	B	345	11/12	0.92	0.11	55,60,62,64	0
1	TPO	C	345	11/12	0.93	0.11	66,69,71,74	0
1	TPO	D	345	11/12	0.94	0.09	53,62,63,64	0

## 6.3 Carbohydrates [i](#)

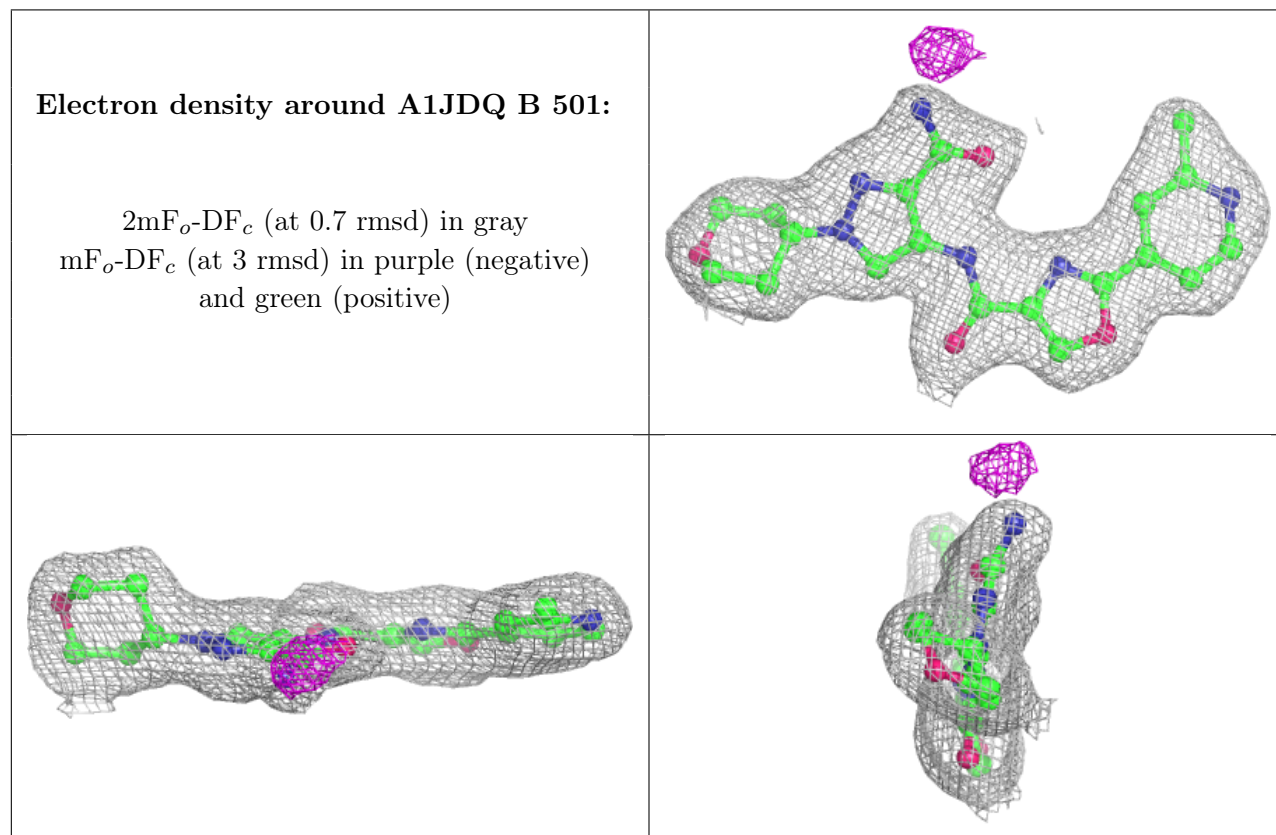
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

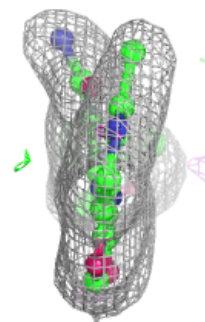
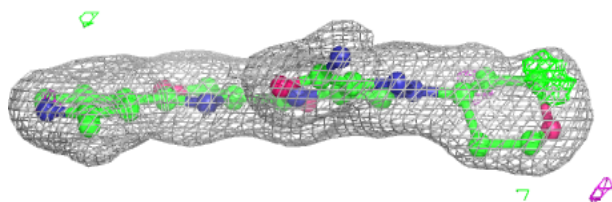
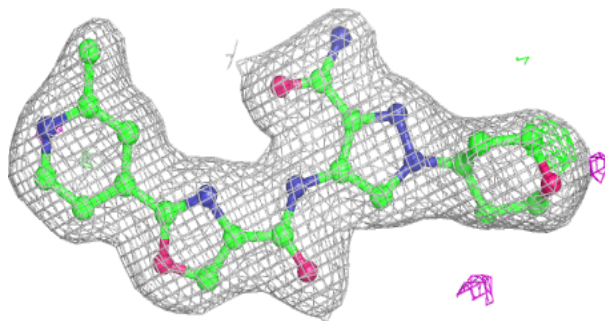
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	502	5/5	0.92	0.09	67,67,67,67	0
2	A1JDQ	B	501	29/29	0.93	0.09	25,28,33,34	0
2	A1JDQ	D	501	29/29	0.94	0.08	20,25,33,33	0
2	A1JDQ	C	501	29/29	0.94	0.07	22,24,30,30	0
2	A1JDQ	A	501	29/29	0.95	0.07	26,29,32,32	0

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.

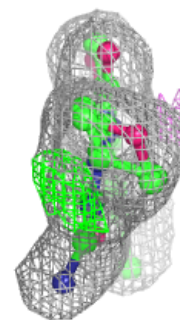
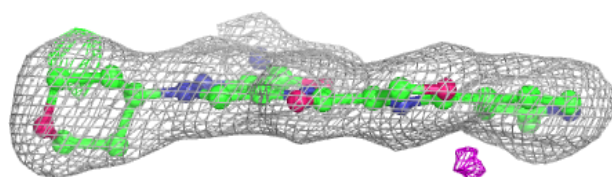
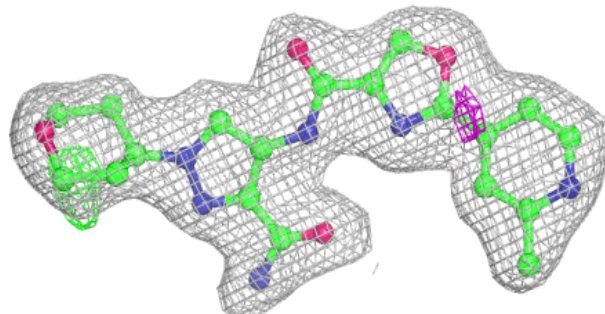


**Electron density around A1JDQ D 501:**

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

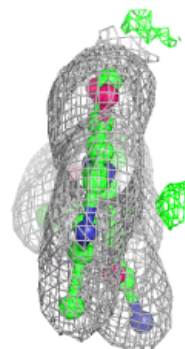
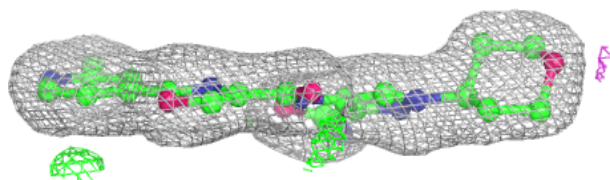
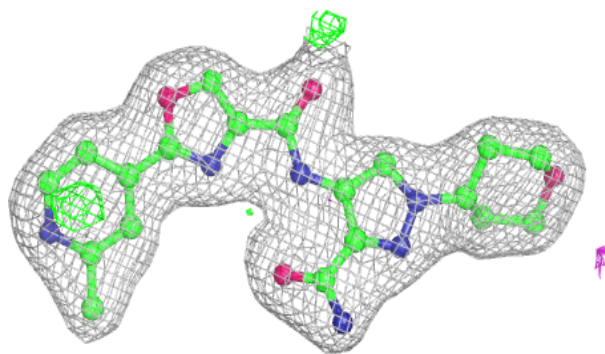
**Electron density around A1JDQ C 501:**

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



**Electron density around A1JDQ A 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.