



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2025 – 01:38 am BST

PDB ID : 9R9J / pdb_00009r9j
Title : IRAK4 in complex with inhibitor
Authors : Xue, Y.; Terstiege, I.; Aagaard, A.
Deposited on : 2025-05-20
Resolution : 2.39 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 types of validation reports are described at

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

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

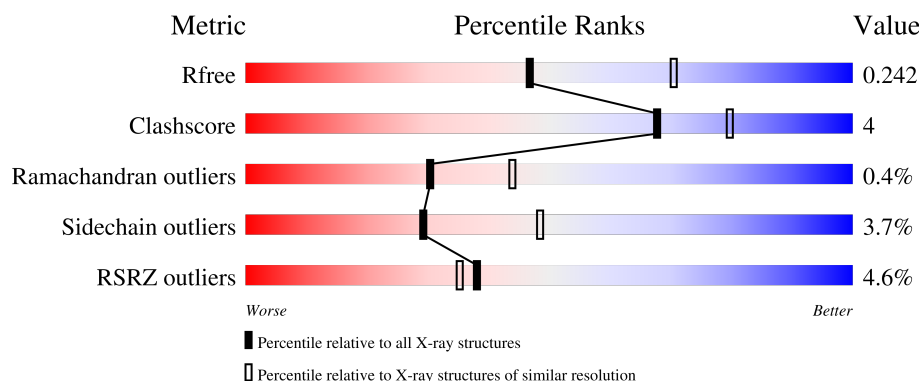
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 4% 79% 13% • 7%
1	B	308	 4% 79% 13% • 6%
1	C	308	 5% 78% 13% • 7%
1	D	308	 4% 82% 9% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9583 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.

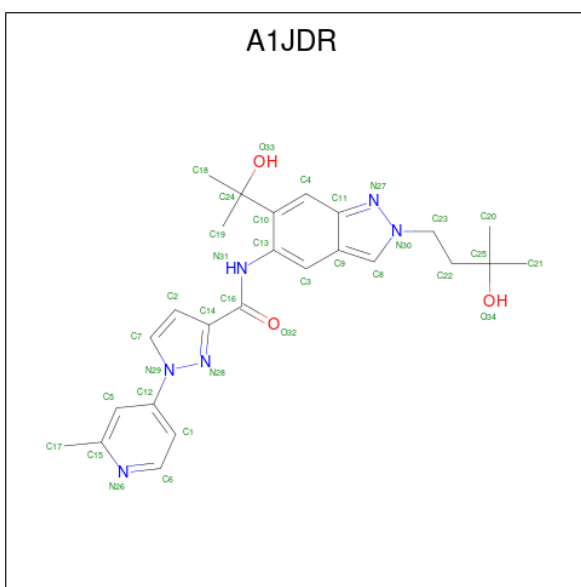
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	P	S	0	0	0
			2253	1412	380	445	2	14			
1	B	288	Total	C	N	O	P	S	0	0	0
			2273	1424	382	451	2	14			
1	C	286	Total	C	N	O	P	S	0	0	0
			2259	1416	380	447	2	14			
1	D	281	Total	C	N	O	P	S	0	0	0
			2220	1394	375	435	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}-[2-(3-methyl-3-oxidanyl-butyl)-6-(2-oxidanylpropan-2-yl)indazol-5-yl]-1-(2-methylpyridin-4-yl)pyrazole-3-carboxamide (CCD ID: A1JDR) (formula: C₂₅H₃₀N₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	25	6	3		
2	B	1	Total	C	N	O	0	0
			34	25	6	3		
2	C	1	Total	C	N	O	0	0
			34	25	6	3		
2	D	1	Total	C	N	O	0	0
			34	25	6	3		

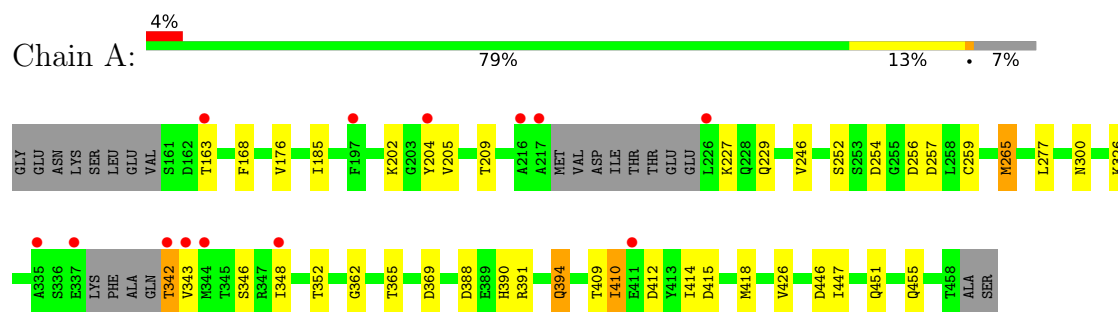
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	89	Total	O	0	0
			89	89		
3	B	136	Total	O	0	0
			136	136		
3	C	119	Total	O	0	0
			119	119		
3	D	98	Total	O	0	0
			98	98		

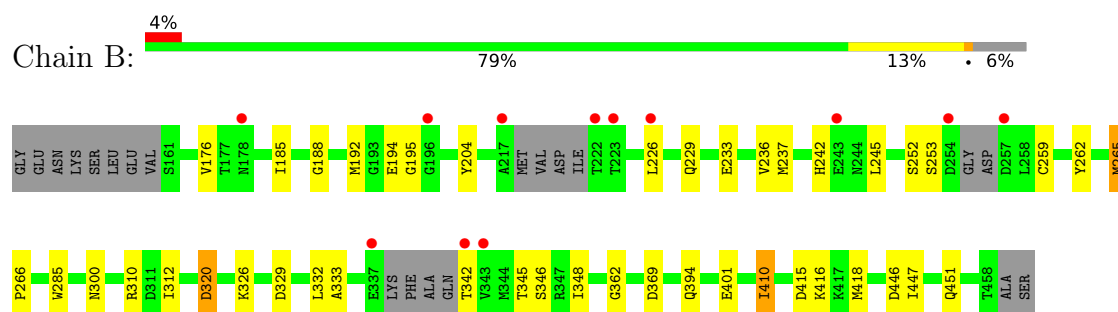
3 Residue-property plots [i](#)

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.

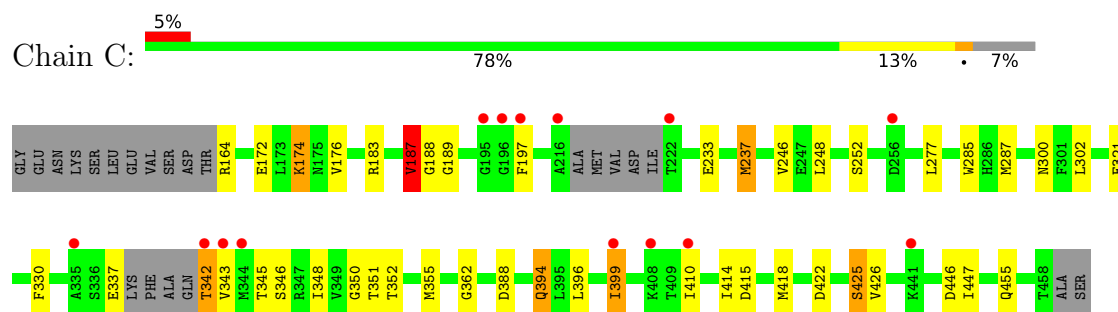
- Molecule 1: Interleukin-1 receptor-associated kinase 4



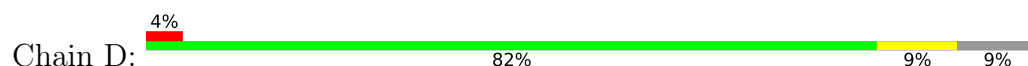
- Molecule 1: Interleukin-1 receptor-associated kinase 4

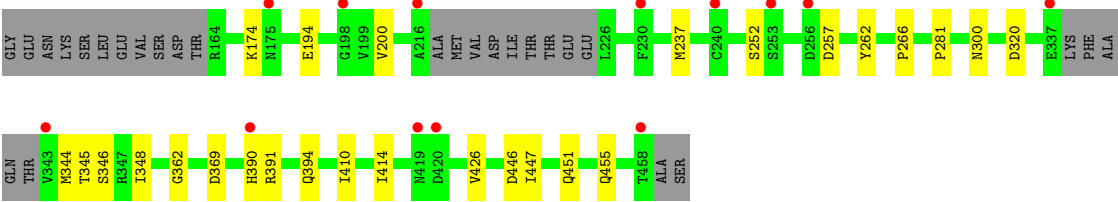


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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, α , β , γ	143.29Å 140.24Å 88.80Å 90.00° 124.06° 90.00°	Depositor
Resolution (Å)	90.00 – 2.39 90.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.1 (90.00-2.39) 99.1 (90.00-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.40Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.221 , 0.263 0.206 , 0.242	Depositor DCC
R_{free} test set	2780 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9583	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.4800e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO, A1JDR

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	0.84	1/2268 (0.0%)	1.32	10/3055 (0.3%)
1	B	0.86	2/2287 (0.1%)	1.35	11/3080 (0.4%)
1	C	0.88	2/2274 (0.1%)	1.36	8/3063 (0.3%)
1	D	0.85	0/2235	1.31	4/3009 (0.1%)
All	All	0.86	5/9064 (0.1%)	1.34	33/12207 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	187	VAL	CA-C	10.33	1.62	1.52
1	B	265	MET	SD-CE	-7.56	1.60	1.79
1	A	265	MET	SD-CE	-6.80	1.62	1.79
1	C	237	MET	SD-CE	-5.81	1.65	1.79
1	B	312	ILE	CG1-CD1	-5.64	1.29	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	VAL	N-CA-C	8.95	121.79	113.20
1	C	187	VAL	N-CA-CB	-7.47	101.24	112.67
1	A	369	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	451	GLN	CA-C-N	5.88	128.08	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	451	GLN	C-N-CA	5.88	128.08	120.44
1	C	342	THR	CA-C-N	5.70	129.11	120.95
1	C	342	THR	C-N-CA	5.70	129.11	120.95
1	C	174	LYS	N-CA-C	-5.68	105.17	111.36
1	D	369	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	369	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	285	TRP	CA-C-N	5.45	127.53	120.44
1	B	285	TRP	C-N-CA	5.45	127.53	120.44
1	D	451	GLN	CB-CG-CD	-5.45	103.34	112.60
1	C	187	VAL	CA-C-N	5.45	131.50	121.70
1	C	187	VAL	C-N-CA	5.45	131.50	121.70
1	A	446	ASP	CA-CB-CG	5.34	117.94	112.60
1	D	446	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	256	ASP	CA-C-N	5.25	131.56	121.54
1	A	256	ASP	C-N-CA	5.25	131.56	121.54
1	B	320	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	342	THR	CA-C-N	5.20	129.93	122.45
1	A	342	THR	C-N-CA	5.20	129.93	122.45
1	A	410	ILE	CA-C-N	5.16	127.44	120.38
1	A	410	ILE	C-N-CA	5.16	127.44	120.38
1	B	229	GLN	CA-C-N	5.10	127.07	120.44
1	B	229	GLN	C-N-CA	5.10	127.07	120.44
1	D	174	LYS	N-CA-C	-5.08	105.82	111.36
1	C	446	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	451	GLN	CA-C-N	5.06	127.01	120.44
1	B	451	GLN	C-N-CA	5.06	127.01	120.44
1	B	446	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	410	ILE	CA-C-N	5.02	127.25	120.38
1	B	410	ILE	C-N-CA	5.02	127.25	120.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	394	GLN	Sidechain

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	2253	0	2215	18	0
1	B	2273	0	2233	16	0
1	C	2259	0	2220	25	0
1	D	2220	0	2187	10	0
2	A	34	0	0	0	0
2	B	34	0	0	1	0
2	C	34	0	0	0	0
2	D	34	0	0	0	0
3	A	89	0	0	0	0
3	B	136	0	0	0	0
3	C	119	0	0	1	0
3	D	98	0	0	0	0
All	All	9583	0	8855	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 4.

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:A:390:HIS:O	1:D:390:HIS:O	1.75	1.04
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.57	0.86
1:A:265:MET:HE1	1:A:326:LYS:HG3	1.58	0.85
1:A:390:HIS:HB3	1:D:391:ARG:HA	1.58	0.85
1:A:265:MET:CE	1:A:326:LYS:HG3	2.14	0.78
1:C:285:TRP:HE1	1:C:425:SER:HB3	1.50	0.77
1:B:265:MET:CE	1:B:326:LYS:HG3	2.15	0.76
1:C:350:GLY:C	1:C:355:MET:HE2	2.20	0.66
1:A:342:THR:HG23	1:A:343:VAL:HG23	1.81	0.62
1:C:396:LEU:HD12	1:C:399:ILE:HD13	1.82	0.62
1:B:237:MET:HE1	1:B:262:TYR:HE2	1.64	0.62
1:A:168:PHE:CE1	1:A:205:VAL:HG11	2.40	0.56
1:C:172:GLU:O	1:C:176:VAL:HG13	2.04	0.56
1:A:168:PHE:HE1	1:A:205:VAL:HG11	1.71	0.56
1:B:242:HIS:HB3	1:B:245:LEU:HG	1.90	0.53
1:B:237:MET:HE1	1:B:262:TYR:CE2	2.44	0.53
1:A:390:HIS:C	1:D:390:HIS:O	2.49	0.52
1:B:176:VAL:HB	1:B:204:TYR:H	1.76	0.51
1:D:237:MET:HE3	1:D:262:TYR:HE2	1.76	0.51
1:C:302:LEU:HD11	1:C:330:PHE:HE1	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:LEU:O	1:C:399:ILE:HB	2.11	0.50
1:C:183:ARG:HB2	1:C:189:GLY:HA3	1.93	0.49
1:C:237:MET:HE3	1:C:248:LEU:HB2	1.94	0.49
1:C:187:VAL:H	1:C:188:GLY:HA2	1.77	0.49
1:C:321:GLU:HG3	1:D:281:PRO:HD3	1.92	0.49
1:A:202:LYS:HE3	1:A:209:THR:HG21	1.93	0.49
1:A:409:THR:HG22	1:A:412:ASP:OD2	2.13	0.48
1:B:310:ARG:HD3	1:B:332:LEU:O	2.13	0.48
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.96	0.48
1:C:287:MET:HG2	3:C:719:HOH:O	2.14	0.48
1:C:285:TRP:NE1	1:C:425:SER:HB3	2.26	0.48
1:C:187:VAL:N	1:C:188:GLY:HA2	2.29	0.47
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.97	0.46
1:C:342:THR:HG23	1:C:343:VAL:HG23	1.97	0.46
1:C:233:GLU:O	1:C:237:MET:HG2	2.15	0.46
1:C:414:ILE:HG12	1:C:426:VAL:HG11	1.97	0.46
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.96	0.46
1:B:236:VAL:HG21	1:B:333:ALA:HB3	1.97	0.45
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.98	0.45
1:C:237:MET:HE1	1:C:246:VAL:HG23	1.99	0.44
1:A:415:ASP:HB3	1:A:418:MET:HE2	2.00	0.44
1:C:351:THR:O	1:C:355:MET:HG3	2.17	0.44
1:C:300:ASN:HA	1:C:447:ILE:HG21	1.99	0.43
1:A:388:ASP:O	1:A:394:GLN:HG3	2.18	0.43
1:C:352:THR:HA	1:C:355:MET:HE3	2.00	0.43
1:D:414:ILE:HG12	1:D:426:VAL:HG11	2.00	0.43
1:A:348:ILE:HG12	1:A:362:GLY:HA2	2.01	0.42
1:B:348:ILE:HG12	1:B:362:GLY:HA2	2.00	0.42
1:C:348:ILE:HG12	1:C:362:GLY:HA2	2.02	0.42
1:B:416:LYS:HB3	1:C:277:LEU:HD12	2.00	0.42
1:B:415:ASP:HB3	1:B:418:MET:HE2	2.02	0.42
1:A:176:VAL:HB	1:A:204:TYR:H	1.85	0.42
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.01	0.42
1:D:348:ILE:HG12	1:D:362:GLY:HA2	2.02	0.42
1:B:195:GLY:HA3	2:B:501:A1JDR:C17	2.50	0.41
1:C:415:ASP:HB3	1:C:418:MET:HE2	2.01	0.41
1:B:185:ILE:HD13	1:B:192:MET:HG2	2.02	0.41
1:C:422:ASP:OD1	1:C:425:SER:HB2	2.20	0.41
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.02	0.41
1:A:391:ARG:HA	1:D:390:HIS:HB3	2.02	0.41
1:C:388:ASP:O	1:C:394:GLN:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:PRO:HD2	1:D:320:ASP:HA	2.04	0.40
1:B:266:PRO:HD2	1:B:320:ASP:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/308 (90%)	267 (96%)	9 (3%)	2 (1%)	19	29
1	B	278/308 (90%)	267 (96%)	9 (3%)	2 (1%)	19	29
1	C	278/308 (90%)	270 (97%)	8 (3%)	0	100	100
1	D	273/308 (89%)	262 (96%)	11 (4%)	0	100	100
All	All	1107/1232 (90%)	1066 (96%)	37 (3%)	4 (0%)	30	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	ASP
1	A	254	ASP
1	B	188	GLY
1	B	329	ASP

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%)	236 (96%)	11 (4%)	23	40
1	B	250/266 (94%)	243 (97%)	7 (3%)	38	59
1	C	248/266 (93%)	237 (96%)	11 (4%)	24	41
1	D	243/266 (91%)	235 (97%)	8 (3%)	33	53
All	All	988/1064 (93%)	951 (96%)	37 (4%)	29	48

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	THR
1	A	185	ILE
1	A	227	LYS
1	A	229	GLN
1	A	246	VAL
1	A	277	LEU
1	A	352	THR
1	A	365	THR
1	A	394	GLN
1	A	410	ILE
1	A	455	GLN
1	B	194	GLU
1	B	226	LEU
1	B	233	GLU
1	B	253	SER
1	B	342	THR
1	B	401	GLU
1	B	410	ILE
1	C	164	ARG
1	C	174	LYS
1	C	187	VAL
1	C	197	PHE
1	C	252	SER
1	C	337	GLU
1	C	394	GLN
1	C	399	ILE
1	C	410	ILE
1	C	425	SER
1	C	455	GLN
1	D	194	GLU
1	D	200	VAL
1	D	252	SER
1	D	257	ASP

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Mol	Chain	Res	Type
1	D	344	MET
1	D	394	GLN
1	D	410	ILE
1	D	455	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	229	GLN
1	A	306	HIS
1	A	307	HIS
1	A	435	GLN
1	A	452	GLN
1	B	229	GLN
1	B	241	GLN
1	B	306	HIS
1	B	435	GLN
1	B	451	GLN
1	B	452	GLN
1	C	179	ASN
1	C	207	ASN
1	C	228	GLN
1	C	297	ASN
1	C	306	HIS
1	C	307	HIS
1	C	390	HIS
1	C	435	GLN
1	C	451	GLN
1	C	452	GLN
1	C	455	GLN
1	D	175	ASN
1	D	307	HIS
1	D	435	GLN
1	D	455	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	SEP	D	346	1	8,9,10	0.98	0	8,12,14	1.82	1 (12%)
1	TPO	B	345	1	8,10,11	1.07	1 (12%)	10,14,16	1.19	1 (10%)
1	TPO	A	345	1	8,10,11	1.30	0	10,14,16	1.05	0
1	TPO	D	345	1	8,10,11	1.16	1 (12%)	10,14,16	1.32	1 (10%)
1	SEP	B	346	1	8,9,10	0.93	1 (12%)	8,12,14	2.08	3 (37%)
1	SEP	C	346	1	8,9,10	0.93	0	8,12,14	1.99	1 (12%)
1	TPO	C	345	1	8,10,11	1.22	1 (12%)	10,14,16	1.24	1 (10%)
1	SEP	A	346	1	8,9,10	0.86	0	8,12,14	1.87	1 (12%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	345	TPO	CB-CA	2.15	1.58	1.53
1	D	345	TPO	CB-CA	2.12	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	346	SEP	P-O1P	2.03	1.57	1.50
1	B	345	TPO	CB-CA	2.03	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	SEP	OG-CB-CA	4.69	112.71	108.14
1	B	346	SEP	OG-CB-CA	4.67	112.69	108.14
1	D	346	SEP	OG-CB-CA	4.38	112.41	108.14
1	A	346	SEP	OG-CB-CA	4.37	112.40	108.14
1	D	345	TPO	O3P-P-OG1	2.39	116.70	105.99
1	B	345	TPO	O3P-P-OG1	2.23	116.00	105.99
1	C	345	TPO	O3P-P-OG1	2.23	115.97	105.99
1	B	346	SEP	P-OG-CB	-2.09	112.54	118.30
1	B	346	SEP	OG-P-O1P	2.05	112.22	106.47

There are no chirality outliers.

All (22) 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	A	346	SEP	N-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	346	SEP	N-CA-CB-OG
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	C	346	SEP	N-CA-CB-OG
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	346	SEP	N-CA-CB-OG
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	B	345	TPO	CB-OG1-P-O3P
1	C	345	TPO	CB-OG1-P-O2P
1	C	345	TPO	CB-OG1-P-O3P
1	D	345	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	A1JDR	A	501	-	34,37,37	1.22	4 (11%)	42,56,56	1.99	11 (26%)
2	A1JDR	B	501	-	34,37,37	1.12	4 (11%)	42,56,56	1.98	11 (26%)
2	A1JDR	D	501	-	34,37,37	1.18	4 (11%)	42,56,56	1.94	11 (26%)
2	A1JDR	C	501	-	34,37,37	1.29	5 (14%)	42,56,56	1.87	8 (19%)

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	A1JDR	A	501	-	-	6/21/24/24	0/4/4/4
2	A1JDR	B	501	-	-	2/21/24/24	0/4/4/4
2	A1JDR	D	501	-	-	2/21/24/24	0/4/4/4
2	A1JDR	C	501	-	-	2/21/24/24	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1JDR	C14-C16	-3.34	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	A1JDR	C24-C10	-3.34	1.51	1.54
2	A	501	A1JDR	C24-C10	-2.97	1.51	1.54
2	D	501	A1JDR	C14-C16	-2.84	1.43	1.50
2	C	501	A1JDR	N28-N29	-2.64	1.34	1.39
2	B	501	A1JDR	N28-N29	-2.57	1.34	1.39
2	C	501	A1JDR	C14-C16	-2.57	1.44	1.50
2	B	501	A1JDR	C24-C10	-2.55	1.52	1.54
2	C	501	A1JDR	C4-C11	-2.46	1.38	1.41
2	A	501	A1JDR	N28-N29	-2.42	1.34	1.39
2	B	501	A1JDR	C14-C16	-2.41	1.44	1.50
2	D	501	A1JDR	N28-N29	-2.35	1.35	1.39
2	B	501	A1JDR	C4-C11	-2.18	1.38	1.41
2	D	501	A1JDR	O33-C24	-2.15	1.41	1.44
2	C	501	A1JDR	O33-C24	-2.15	1.41	1.44
2	A	501	A1JDR	C4-C11	-2.11	1.38	1.41
2	D	501	A1JDR	C4-C11	-2.09	1.38	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	A1JDR	C13-C3-C9	-5.61	111.19	120.23
2	A	501	A1JDR	C13-C3-C9	-5.53	111.33	120.23
2	B	501	A1JDR	C3-C9-C11	5.46	127.49	119.87
2	D	501	A1JDR	C13-C3-C9	-5.38	111.56	120.23
2	A	501	A1JDR	C3-C9-C11	5.28	127.23	119.87
2	C	501	A1JDR	C3-C9-C11	5.27	127.22	119.87
2	C	501	A1JDR	C13-C3-C9	-5.23	111.81	120.23
2	A	501	A1JDR	C8-C9-C3	-5.00	124.91	134.80
2	B	501	A1JDR	C8-C9-C3	-4.92	125.07	134.80
2	C	501	A1JDR	C8-C9-C3	-4.85	125.20	134.80
2	D	501	A1JDR	C3-C9-C11	4.60	126.30	119.87
2	D	501	A1JDR	C8-C9-C3	-4.47	125.96	134.80
2	D	501	A1JDR	C10-C13-N31	-3.79	116.80	120.54
2	C	501	A1JDR	C10-C4-C11	-3.45	115.20	119.79
2	C	501	A1JDR	C4-C10-C13	3.35	122.94	118.72
2	D	501	A1JDR	C8-N30-N27	3.31	114.04	111.45
2	D	501	A1JDR	C3-C13-C10	3.28	124.24	120.09
2	B	501	A1JDR	C10-C4-C11	-3.21	115.51	119.79
2	B	501	A1JDR	C10-C13-N31	-3.08	117.50	120.54
2	A	501	A1JDR	C10-C4-C11	-3.08	115.69	119.79
2	B	501	A1JDR	C4-C10-C13	3.02	122.52	118.72
2	D	501	A1JDR	C10-C4-C11	-3.01	115.78	119.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1JDR	C3-C13-C10	2.96	123.83	120.09
2	C	501	A1JDR	O33-C24-C18	-2.94	101.17	107.08
2	B	501	A1JDR	C3-C13-C10	2.79	123.61	120.09
2	B	501	A1JDR	C5-C15-N26	2.67	124.25	121.66
2	A	501	A1JDR	C8-N30-N27	2.54	113.44	111.45
2	A	501	A1JDR	C4-C10-C13	2.53	121.91	118.72
2	B	501	A1JDR	C8-N30-N27	2.50	113.40	111.45
2	D	501	A1JDR	C17-C15-C5	-2.50	118.00	121.81
2	A	501	A1JDR	C10-C13-N31	-2.47	118.10	120.54
2	D	501	A1JDR	C5-C15-N26	2.33	123.92	121.66
2	A	501	A1JDR	O33-C24-C18	-2.31	102.44	107.08
2	D	501	A1JDR	C1-C12-N29	2.29	121.15	119.15
2	C	501	A1JDR	C3-C13-C10	2.24	122.92	120.09
2	B	501	A1JDR	C18-C24-C19	-2.20	107.79	110.49
2	B	501	A1JDR	C17-C15-C5	-2.19	118.47	121.81
2	A	501	A1JDR	C18-C24-C10	2.15	114.97	111.55
2	C	501	A1JDR	C8-N30-N27	2.14	113.12	111.45
2	D	501	A1JDR	C4-C10-C13	2.10	121.37	118.72
2	A	501	A1JDR	C5-C15-N26	2.01	123.61	121.66

There are no chirality outliers.

All (12) torsion outliers are listed below:

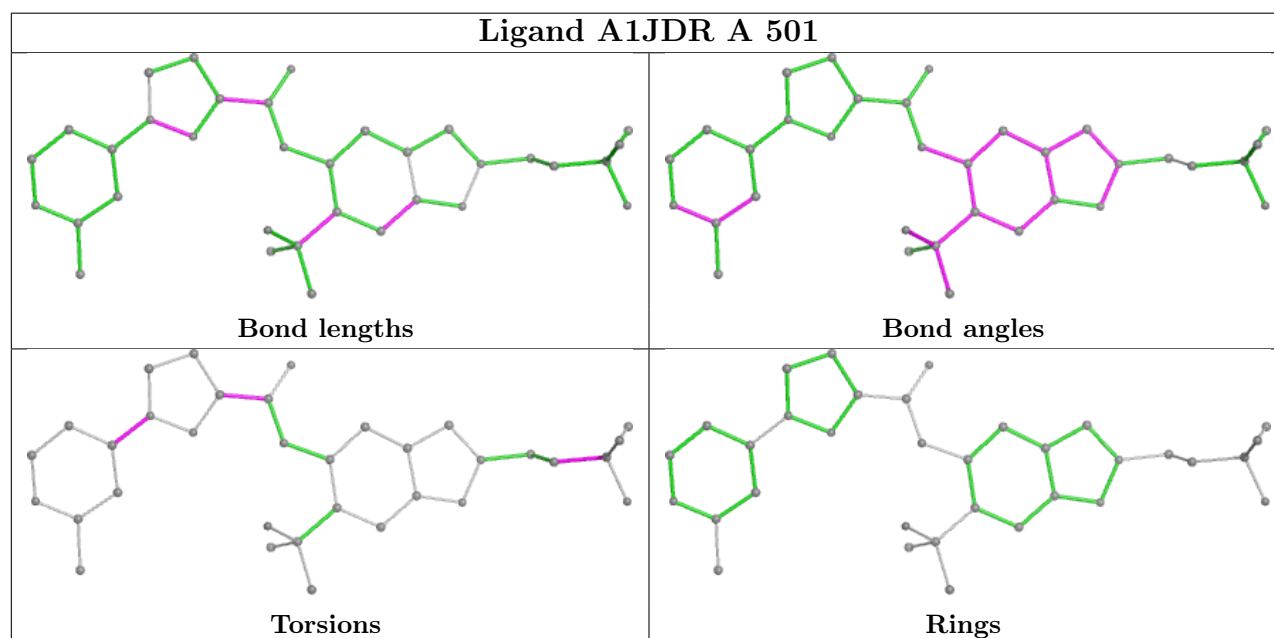
Mol	Chain	Res	Type	Atoms
2	A	501	A1JDR	C23-C22-C25-O34
2	A	501	A1JDR	C23-C22-C25-C20
2	A	501	A1JDR	C23-C22-C25-C21
2	A	501	A1JDR	C1-C12-N29-C7
2	B	501	A1JDR	C1-C12-N29-C7
2	B	501	A1JDR	C5-C12-N29-C7
2	C	501	A1JDR	C1-C12-N29-C7
2	C	501	A1JDR	C5-C12-N29-C7
2	D	501	A1JDR	C5-C12-N29-C7
2	A	501	A1JDR	C5-C12-N29-C7
2	D	501	A1JDR	C1-C12-N29-C7
2	A	501	A1JDR	C2-C14-C16-O32

There are no ring outliers.

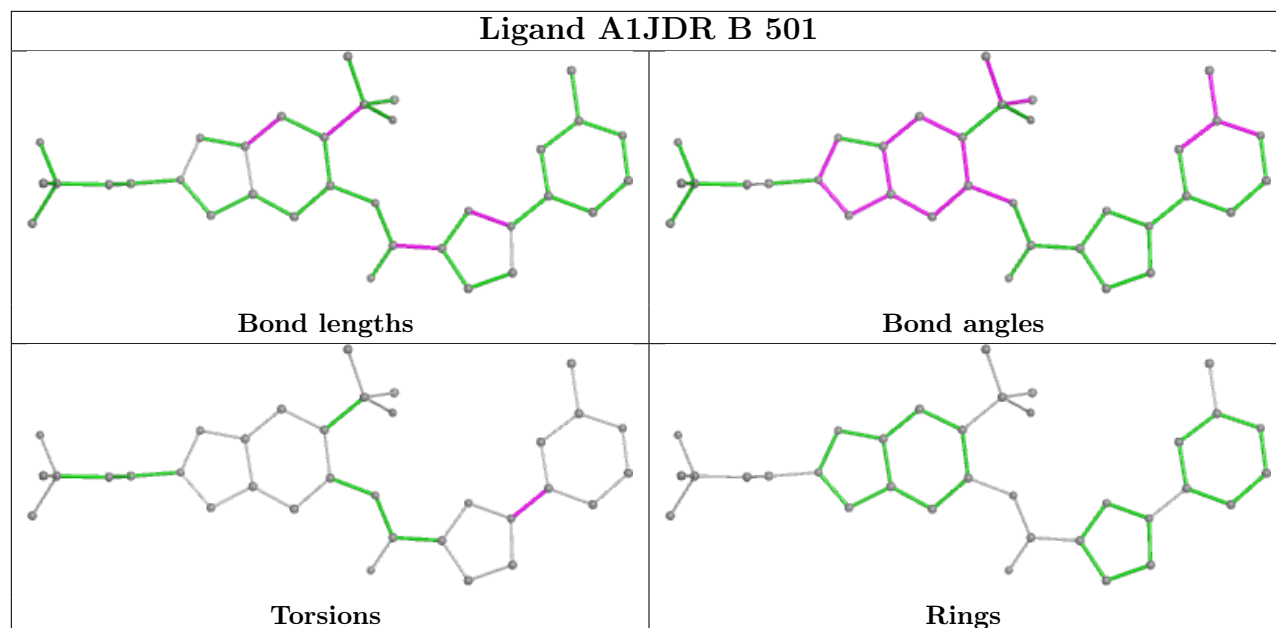
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	A1JDR	1	0

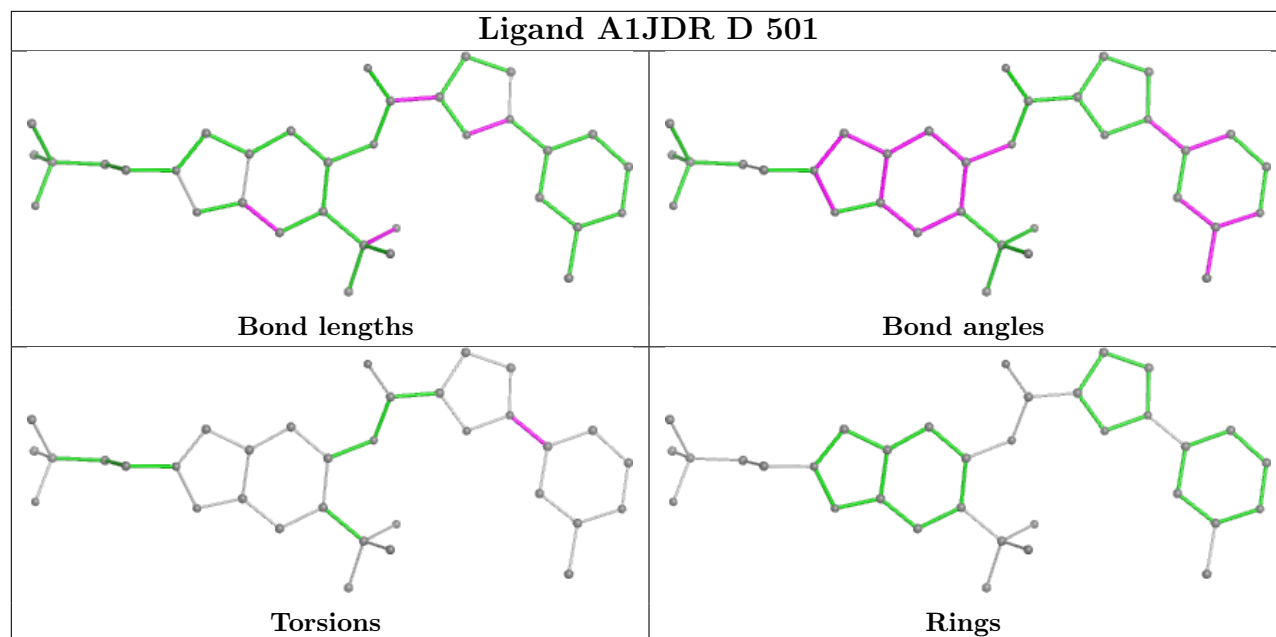
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

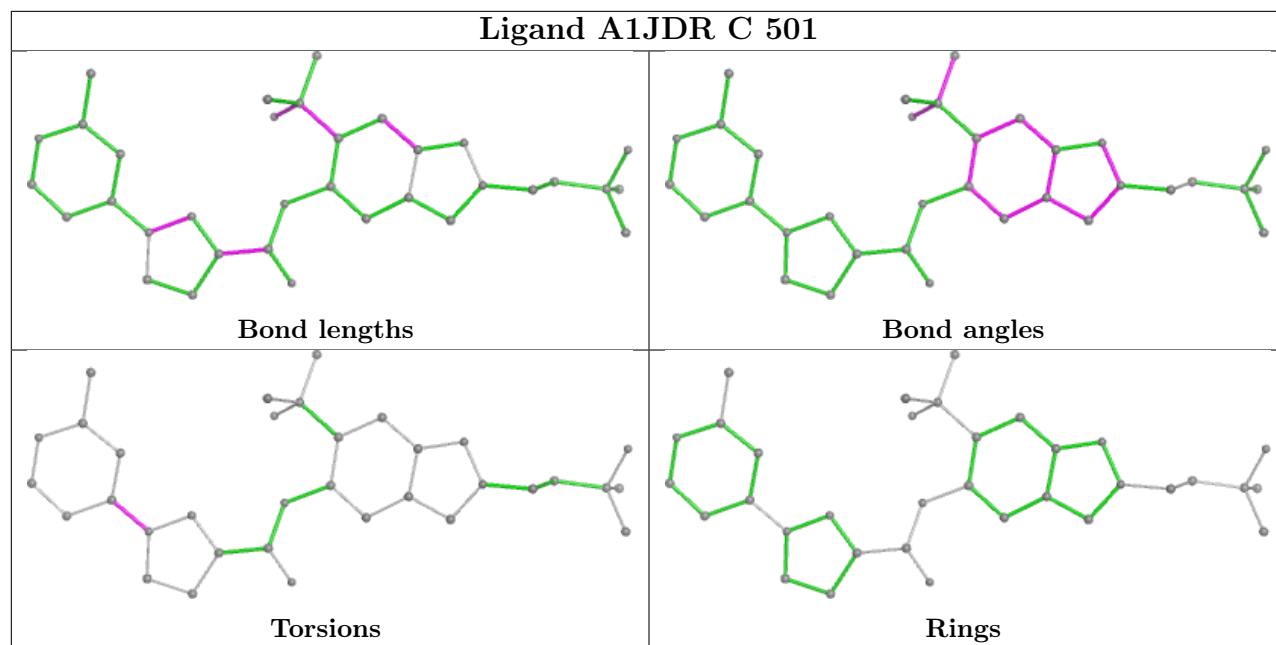


Ligand A1JDR B 501



Ligand A1JDR D 501





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	284/308 (92%)	0.35	13 (4%) 38 35	28, 50, 87, 126	0
1	B	286/308 (92%)	0.22	12 (4%) 41 38	30, 47, 79, 118	0
1	C	284/308 (92%)	0.31	14 (4%) 36 33	29, 50, 89, 112	0
1	D	279/308 (90%)	0.32	13 (4%) 37 34	26, 49, 87, 120	0
All	All	1133/1232 (91%)	0.30	52 (4%) 38 35	26, 49, 88, 126	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	342	THR	4.5
1	D	343	VAL	4.2
1	B	342	THR	4.1
1	C	342	THR	3.9
1	D	216	ALA	3.7
1	A	226	LEU	3.6
1	C	410	ILE	3.5
1	C	343	VAL	3.5
1	A	343	VAL	3.5
1	B	226	LEU	3.4
1	A	335	ALA	3.3
1	C	216	ALA	3.3
1	D	175	ASN	3.2
1	B	217	ALA	3.2
1	C	197	PHE	3.1
1	D	337	GLU	3.1
1	D	420	ASP	3.0
1	A	197	PHE	2.9
1	A	204	TYR	2.9
1	B	343	VAL	2.7
1	A	163	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	217	ALA	2.6
1	A	348	ILE	2.5
1	D	253	SER	2.5
1	D	458	THR	2.5
1	B	196	GLY	2.5
1	C	222	THR	2.5
1	C	256	ASP	2.4
1	C	195	GLY	2.4
1	D	198	GLY	2.4
1	B	222	THR	2.4
1	C	408	LYS	2.3
1	D	390	HIS	2.3
1	A	216	ALA	2.3
1	B	257	ASP	2.3
1	D	256	ASP	2.3
1	C	399	ILE	2.3
1	C	196	GLY	2.2
1	A	337	GLU	2.2
1	D	240	CYS	2.2
1	B	337	GLU	2.2
1	C	335	ALA	2.2
1	D	230	PHE	2.2
1	B	254	ASP	2.2
1	A	344	MET	2.2
1	C	441	LYS	2.2
1	B	223	THR	2.1
1	C	344	MET	2.1
1	B	243	GLU	2.1
1	B	178	ASN	2.1
1	D	419	ASN	2.1
1	A	411	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	D	346	10/11	0.74	0.13	78,84,90,91	0
1	SEP	C	346	10/11	0.77	0.14	82,87,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	A	346	10/11	0.78	0.10	84,88,94,94	0
1	SEP	B	346	10/11	0.82	0.10	70,75,82,83	0
1	TPO	D	345	11/12	0.90	0.10	69,71,77,78	0
1	TPO	C	345	11/12	0.91	0.10	77,78,83,83	0
1	TPO	A	345	11/12	0.92	0.09	77,78,85,85	0
1	TPO	B	345	11/12	0.96	0.07	62,63,71,71	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

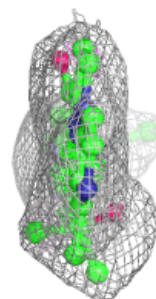
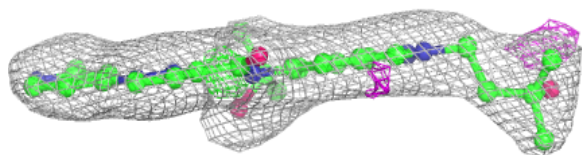
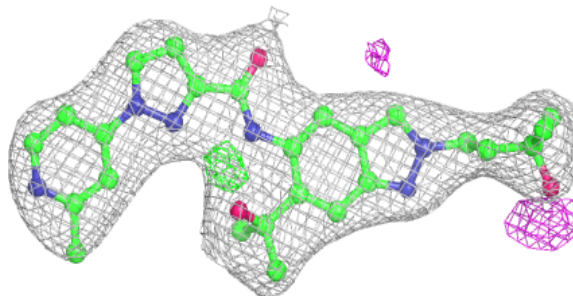
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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	A1JDR	A	501	34/34	0.93	0.08	28,33,43,45	0
2	A1JDR	D	501	34/34	0.93	0.08	31,36,45,46	0
2	A1JDR	B	501	34/34	0.95	0.07	33,37,43,47	0
2	A1JDR	C	501	34/34	0.96	0.07	26,34,44,46	0

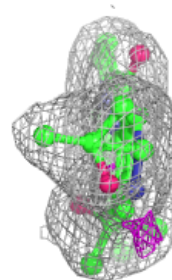
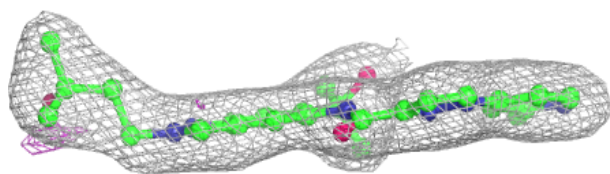
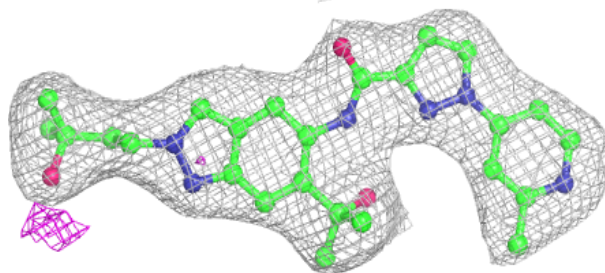
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JDR 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)

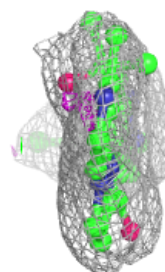
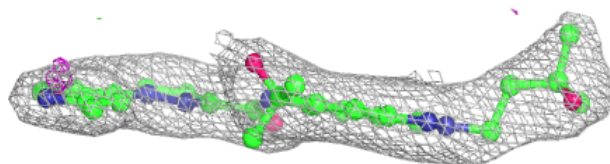
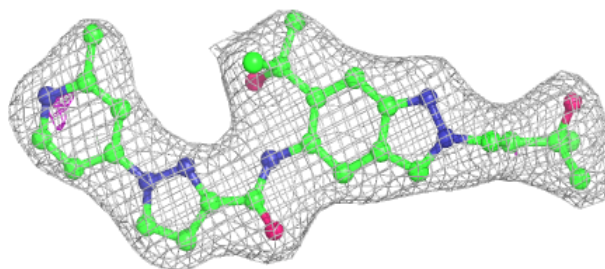
**Electron density around A1JDR D 501:**

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

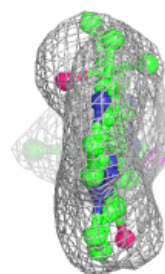
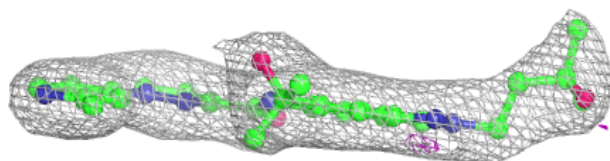
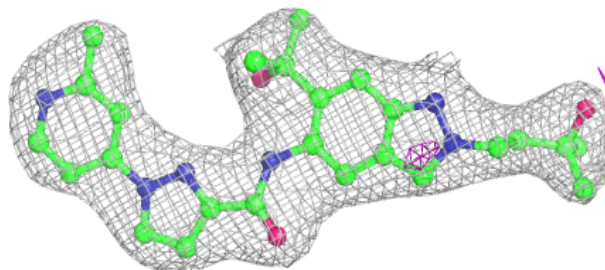


Electron density around A1JDR B 501:

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

**Electron density around A1JDR 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 [i](#)

There are no such residues in this entry.