



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 8V2F / pdb_00008v2f
Title : Crystal structure of IRAK4 kinase domain with compound 9
Authors : Weiss, M.M.; Zheng, X.; Browne, C.M.; Campbell, V.; Chen, D.; Enerson, B.;
Fei, X.; Huang, X.; Klaus, C.R.; Li, H.; Mayo, M.; McDonald, A.A.; Paul, A.;
Sharma, K.; Shi, Y.; Slavin, A.; Walter, D.M.; Yuan, K.; Zhang, Y.; Zhu, X.;
Kelleher, J.; Ji, N.; Walker, D.; Mainolfi, N.
Deposited on : 2023-11-22
Resolution : 2.09 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

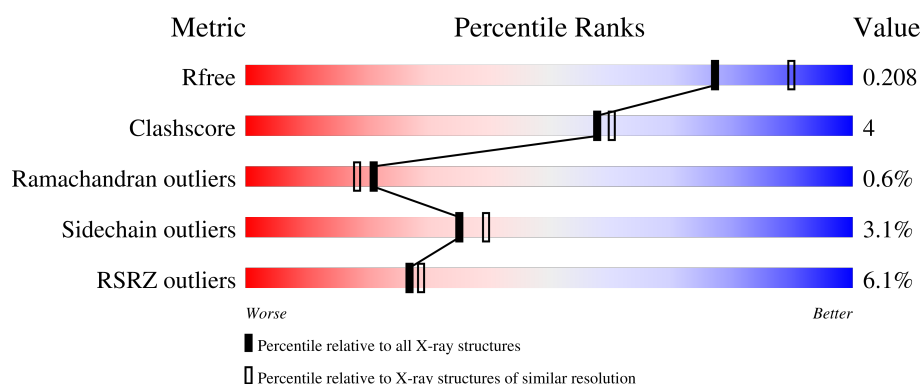
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	327	3% 83% 7% • 9%
1	B	327	5% 81% 9% • 9%
1	C	327	7% 80% 11% • 8%
1	D	327	7% 80% 9% • 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10225 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	297	Total	C	N	O	P	S	0	2	0
			2353	1475	393	466	3	16			
1	B	298	Total	C	N	O	P	S	0	1	0
			2358	1477	394	468	3	16			
1	C	302	Total	C	N	O	P	S	0	3	0
			2392	1500	398	474	3	17			
1	D	294	Total	C	N	O	P	S	0	2	0
			2328	1458	389	462	3	16			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	-	initiating methionine	UNP Q9NWZ3
A	135	SER	-	expression tag	UNP Q9NWZ3
A	136	TYR	-	expression tag	UNP Q9NWZ3
A	137	TYR	-	expression tag	UNP Q9NWZ3
A	138	HIS	-	expression tag	UNP Q9NWZ3
A	139	HIS	-	expression tag	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	ASP	-	expression tag	UNP Q9NWZ3
A	145	TYR	-	expression tag	UNP Q9NWZ3
A	146	ASP	-	expression tag	UNP Q9NWZ3
A	147	ILE	-	expression tag	UNP Q9NWZ3
A	148	PRO	-	expression tag	UNP Q9NWZ3
A	149	THR	-	expression tag	UNP Q9NWZ3
A	150	THR	-	expression tag	UNP Q9NWZ3
A	151	GLU	-	expression tag	UNP Q9NWZ3
A	152	ASN	-	expression tag	UNP Q9NWZ3
A	153	LEU	-	expression tag	UNP Q9NWZ3
A	154	TYR	-	expression tag	UNP Q9NWZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	PHE	-	expression tag	UNP Q9NWZ3
A	156	GLN	-	expression tag	UNP Q9NWZ3
A	157	SER	-	expression tag	UNP Q9NWZ3
A	158	ILE	-	expression tag	UNP Q9NWZ3
A	159	ALA	-	expression tag	UNP Q9NWZ3
B	134	MET	-	initiating methionine	UNP Q9NWZ3
B	135	SER	-	expression tag	UNP Q9NWZ3
B	136	TYR	-	expression tag	UNP Q9NWZ3
B	137	TYR	-	expression tag	UNP Q9NWZ3
B	138	HIS	-	expression tag	UNP Q9NWZ3
B	139	HIS	-	expression tag	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	ASP	-	expression tag	UNP Q9NWZ3
B	145	TYR	-	expression tag	UNP Q9NWZ3
B	146	ASP	-	expression tag	UNP Q9NWZ3
B	147	ILE	-	expression tag	UNP Q9NWZ3
B	148	PRO	-	expression tag	UNP Q9NWZ3
B	149	THR	-	expression tag	UNP Q9NWZ3
B	150	THR	-	expression tag	UNP Q9NWZ3
B	151	GLU	-	expression tag	UNP Q9NWZ3
B	152	ASN	-	expression tag	UNP Q9NWZ3
B	153	LEU	-	expression tag	UNP Q9NWZ3
B	154	TYR	-	expression tag	UNP Q9NWZ3
B	155	PHE	-	expression tag	UNP Q9NWZ3
B	156	GLN	-	expression tag	UNP Q9NWZ3
B	157	SER	-	expression tag	UNP Q9NWZ3
B	158	ILE	-	expression tag	UNP Q9NWZ3
B	159	ALA	-	expression tag	UNP Q9NWZ3
C	134	MET	-	initiating methionine	UNP Q9NWZ3
C	135	SER	-	expression tag	UNP Q9NWZ3
C	136	TYR	-	expression tag	UNP Q9NWZ3
C	137	TYR	-	expression tag	UNP Q9NWZ3
C	138	HIS	-	expression tag	UNP Q9NWZ3
C	139	HIS	-	expression tag	UNP Q9NWZ3
C	140	HIS	-	expression tag	UNP Q9NWZ3
C	141	HIS	-	expression tag	UNP Q9NWZ3
C	142	HIS	-	expression tag	UNP Q9NWZ3
C	143	HIS	-	expression tag	UNP Q9NWZ3
C	144	ASP	-	expression tag	UNP Q9NWZ3

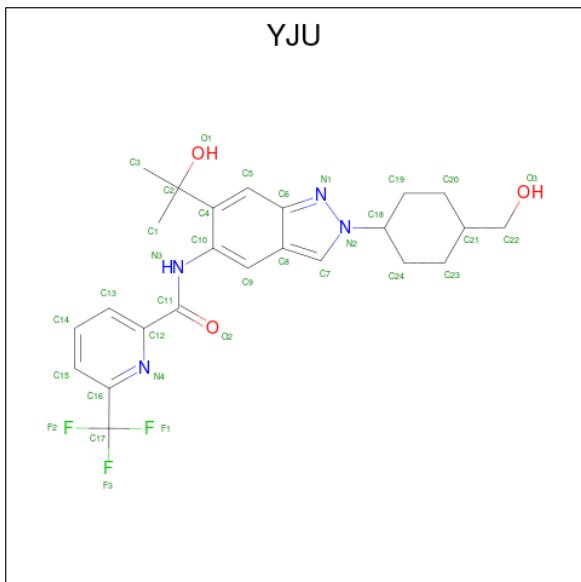
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	145	TYR	-	expression tag	UNP Q9NWZ3
C	146	ASP	-	expression tag	UNP Q9NWZ3
C	147	ILE	-	expression tag	UNP Q9NWZ3
C	148	PRO	-	expression tag	UNP Q9NWZ3
C	149	THR	-	expression tag	UNP Q9NWZ3
C	150	THR	-	expression tag	UNP Q9NWZ3
C	151	GLU	-	expression tag	UNP Q9NWZ3
C	152	ASN	-	expression tag	UNP Q9NWZ3
C	153	LEU	-	expression tag	UNP Q9NWZ3
C	154	TYR	-	expression tag	UNP Q9NWZ3
C	155	PHE	-	expression tag	UNP Q9NWZ3
C	156	GLN	-	expression tag	UNP Q9NWZ3
C	157	SER	-	expression tag	UNP Q9NWZ3
C	158	ILE	-	expression tag	UNP Q9NWZ3
C	159	ALA	-	expression tag	UNP Q9NWZ3
D	134	MET	-	initiating methionine	UNP Q9NWZ3
D	135	SER	-	expression tag	UNP Q9NWZ3
D	136	TYR	-	expression tag	UNP Q9NWZ3
D	137	TYR	-	expression tag	UNP Q9NWZ3
D	138	HIS	-	expression tag	UNP Q9NWZ3
D	139	HIS	-	expression tag	UNP Q9NWZ3
D	140	HIS	-	expression tag	UNP Q9NWZ3
D	141	HIS	-	expression tag	UNP Q9NWZ3
D	142	HIS	-	expression tag	UNP Q9NWZ3
D	143	HIS	-	expression tag	UNP Q9NWZ3
D	144	ASP	-	expression tag	UNP Q9NWZ3
D	145	TYR	-	expression tag	UNP Q9NWZ3
D	146	ASP	-	expression tag	UNP Q9NWZ3
D	147	ILE	-	expression tag	UNP Q9NWZ3
D	148	PRO	-	expression tag	UNP Q9NWZ3
D	149	THR	-	expression tag	UNP Q9NWZ3
D	150	THR	-	expression tag	UNP Q9NWZ3
D	151	GLU	-	expression tag	UNP Q9NWZ3
D	152	ASN	-	expression tag	UNP Q9NWZ3
D	153	LEU	-	expression tag	UNP Q9NWZ3
D	154	TYR	-	expression tag	UNP Q9NWZ3
D	155	PHE	-	expression tag	UNP Q9NWZ3
D	156	GLN	-	expression tag	UNP Q9NWZ3
D	157	SER	-	expression tag	UNP Q9NWZ3
D	158	ILE	-	expression tag	UNP Q9NWZ3
D	159	ALA	-	expression tag	UNP Q9NWZ3

- Molecule 2 is N-{2-[(1r,4r)-4-(hydroxymethyl)cyclohexyl]-6-(2-hydroxypropan-2-yl)-2

H-indazol-5-yl}-6-(trifluoromethyl)pyridine-2-carboxamide (CCD ID: YJU) (formula: $C_{24}H_{27}F_3N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			34	24	3	4	3		
2	B	1	Total	C	F	N	O	0	0
			34	24	3	4	3		
2	C	1	Total	C	F	N	O	0	0
			34	24	3	4	3		
2	D	1	Total	C	F	N	O	0	0
			34	24	3	4	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

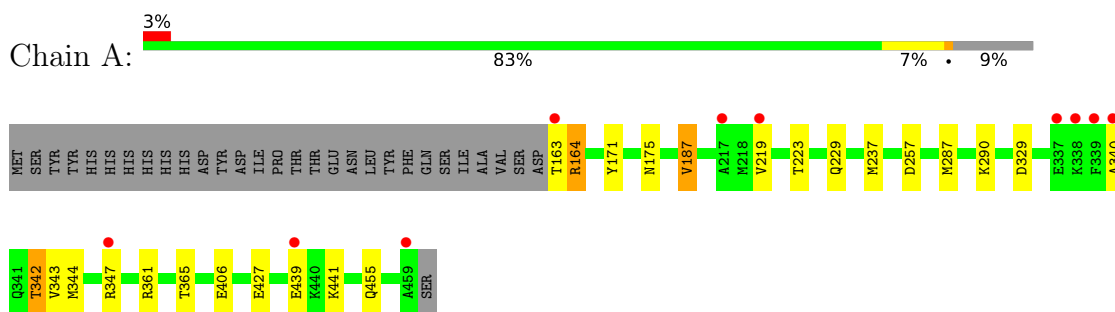
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	176	Total	O	0	0
			176	176		
5	B	139	Total	O	0	0
			139	139		
5	C	149	Total	O	0	0
			149	149		
5	D	155	Total	O	0	0
			155	155		

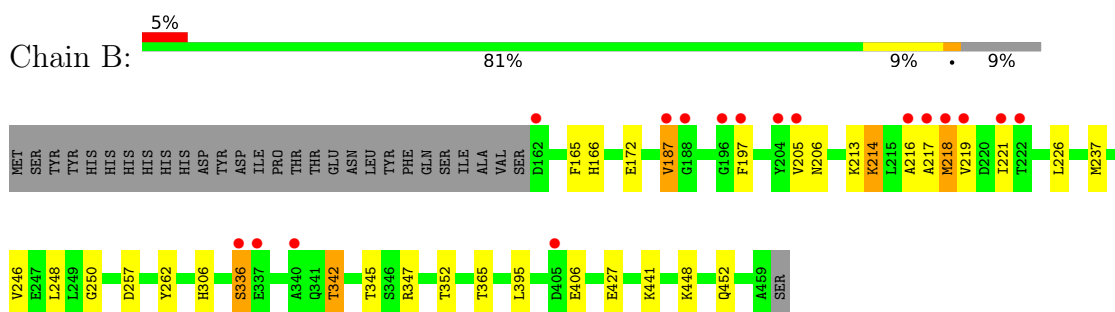
3 Residue-property plots [i](#)

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.

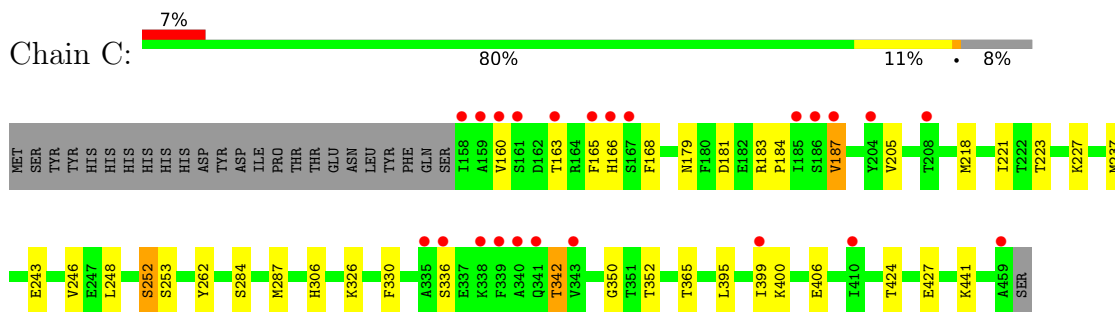
- Molecule 1: Interleukin-1 receptor-associated kinase 4



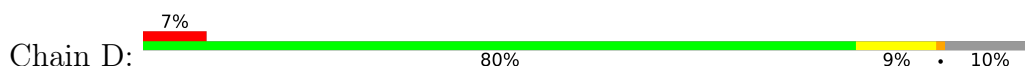
- Molecule 1: Interleukin-1 receptor-associated kinase 4

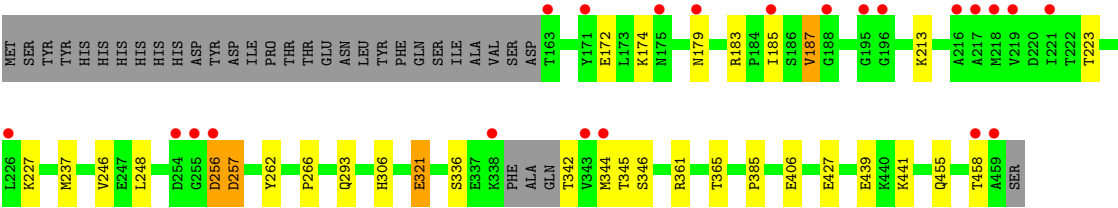


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- 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	142.87Å 140.68Å 89.02Å 90.00° 124.00° 90.00°	Depositor
Resolution (Å)	49.14 – 2.09 49.14 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.14-2.09) 99.9 (49.14-2.09)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.168 , 0.208 (Not available) , 0.208	Depositor DCC
R_{free} test set	4334 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.6	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	0.96	EDS
Total number of atoms	10225	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 19.92 % 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 9.7314e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, YJU, TPO, 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	1.04	0/2364	1.30	1/3183 (0.0%)
1	B	1.04	0/2367	1.30	0/3189
1	C	1.05	0/2407	1.32	2/3243 (0.1%)
1	D	1.04	0/2339	1.33	3/3151 (0.1%)
All	All	1.04	0/9477	1.31	6/12766 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	439	GLU	CB-CG-CD	5.60	122.12	112.60
1	A	257	ASP	CB-CA-C	5.44	118.69	109.50
1	C	350	GLY	CA-C-O	-5.29	117.15	121.76
1	D	385	PRO	CA-C-N	5.14	127.42	120.38
1	D	385	PRO	C-N-CA	5.14	127.42	120.38
1	C	166	HIS	CA-CB-CG	5.02	118.82	113.80

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	2353	0	2320	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2358	0	2319	26	0
1	C	2392	0	2363	24	1
1	D	2328	0	2299	21	2
2	A	34	0	0	0	0
2	B	34	0	0	0	0
2	C	34	0	0	0	0
2	D	34	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	12	0	16	1	0
4	B	12	0	16	1	0
4	C	6	0	8	2	0
4	D	6	0	8	0	0
5	A	176	0	0	5	2
5	B	139	0	0	4	0
5	C	149	0	0	5	1
5	D	155	0	0	4	0
All	All	10225	0	9349	85	3

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 (85) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:HB2	1:B:226:LEU:HD22	1.43	1.01
1:C:284:SER:H	1:C:287[A]:MET:HE3	1.26	1.00
1:B:237[A]:MET:HE1	1:B:246:VAL:HG23	1.54	0.89
1:C:237[B]:MET:HE1	1:C:246:VAL:HG23	1.54	0.89
1:D:237[A]:MET:HE1	1:D:246:VAL:HG23	1.58	0.86
1:D:361:ARG:NH1	5:D:601:HOH:O	2.07	0.85
1:D:293:GLN:HE22	1:D:458:THR:HG21	1.44	0.82
1:C:179:ASN:HB2	5:C:606:HOH:O	1.81	0.81
1:C:306:HIS:HB3	1:C:336:SER:O	1.89	0.73
1:B:217:ALA:HB2	1:B:226:LEU:CD2	2.18	0.73
1:D:266:PRO:HG2	1:D:321:GLU:HG3	1.71	0.71
1:C:237[A]:MET:HA	1:C:237[A]:MET:HE2	1.76	0.68
1:A:237:MET:HA	1:A:237:MET:HE2	1.77	0.66
1:D:237[B]:MET:HA	1:D:237[B]:MET:HE2	1.79	0.65
1:B:172:GLU:OE2	5:B:601:HOH:O	2.14	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237[B]:MET:HA	1:B:237[B]:MET:HE2	1.81	0.63
1:C:168:PHE:O	1:C:252:SER:HB2	1.97	0.63
1:D:213:LYS:NZ	5:D:602:HOH:O	2.32	0.62
1:A:347:ARG:NH1	5:A:603:HOH:O	2.33	0.61
4:C:503:GOL:O2	5:C:601:HOH:O	2.15	0.60
1:D:293:GLN:HE22	1:D:458:THR:CG2	2.13	0.60
1:C:237[B]:MET:HE3	1:C:248:LEU:HB2	1.83	0.60
1:A:171:TYR:OH	5:A:601:HOH:O	2.16	0.59
1:D:257:ASP:N	1:D:257:ASP:OD1	2.36	0.59
1:D:237[A]:MET:CE	1:D:262:TYR:HE2	2.17	0.58
1:B:197:PHE:CD1	1:B:221:ILE:CD1	2.87	0.57
1:D:342:TPO:O3P	1:D:441:LYS:NZ	2.37	0.57
1:D:237[A]:MET:HE3	1:D:248:LEU:HB2	1.87	0.57
1:D:174:LYS:HE2	1:D:179:ASN:HD21	1.71	0.55
1:C:342:TPO:O3P	1:C:441:LYS:NZ	2.39	0.55
1:B:347:ARG:HD2	5:B:617:HOH:O	2.06	0.55
1:A:439:GLU:HG2	5:A:602:HOH:O	2.06	0.55
1:A:340:ALA:HB3	5:A:620:HOH:O	2.06	0.54
1:B:342:TPO:O3P	1:B:441:LYS:NZ	2.40	0.54
1:A:342:TPO:O3P	1:A:441:LYS:NZ	2.41	0.53
1:A:287:MET:HE3	1:A:290:LYS:HB2	1.89	0.53
1:B:395:LEU:HG	1:D:344:MET:HE1	1.91	0.53
1:B:197:PHE:HD1	1:B:221:ILE:CD1	2.21	0.53
1:B:237[A]:MET:CE	1:B:262:TYR:HE2	2.21	0.53
1:A:329:ASP:OD1	4:A:504:GOL:H12	2.09	0.53
1:C:237[B]:MET:CE	1:C:262:TYR:HE2	2.21	0.53
1:B:217:ALA:O	1:B:218:MET:C	2.52	0.53
1:C:237[B]:MET:HE2	1:C:262:TYR:HE2	1.73	0.53
1:B:197:PHE:CE1	1:B:221:ILE:HD11	2.44	0.52
4:C:503:GOL:O1	4:C:503:GOL:O3	2.15	0.51
1:B:237[A]:MET:HE3	1:B:248:LEU:HB2	1.91	0.51
1:B:306:HIS:HB3	1:B:336:SER:O	2.10	0.51
1:B:166:HIS:HD2	5:B:720:HOH:O	1.93	0.50
1:A:361:ARG:HA	1:C:352:THR:CG2	2.42	0.49
1:D:321:GLU:H	1:D:321:GLU:CD	2.21	0.49
1:D:183:ARG:NH1	5:D:606:HOH:O	2.43	0.48
1:C:184:PRO:HB3	5:C:707:HOH:O	2.14	0.48
1:B:214:LYS:HE2	1:B:257:ASP:OD2	2.14	0.47
1:C:160:VAL:O	1:C:163:THR:HB	2.14	0.47
1:D:256:ASP:HB3	1:D:257:ASP:OD1	2.15	0.47
1:C:218:MET:HE2	1:C:218:MET:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:GLN:HG3	5:D:686:HOH:O	2.14	0.46
1:B:197:PHE:CD1	1:B:221:ILE:HD13	2.51	0.46
1:D:306:HIS:HB3	1:D:336:SER:O	2.16	0.45
1:B:187:VAL:O	1:B:187:VAL:CG1	2.65	0.44
1:A:229:GLN:NE2	5:A:605:HOH:O	2.37	0.44
1:A:344[B]:MET:HE1	1:C:395:LEU:HD11	1.99	0.44
1:D:237[A]:MET:CE	1:D:262:TYR:CE2	3.01	0.44
1:A:163:THR:O	1:A:164:ARG:HB3	2.18	0.43
1:B:352:THR:CG2	1:D:361:ARG:HA	2.48	0.43
1:B:197:PHE:HE1	1:B:221:ILE:HD11	1.83	0.43
1:B:216:ALA:O	1:B:217:ALA:HB3	2.18	0.43
1:B:448:LYS:O	1:B:452:GLN:HG3	2.18	0.43
1:C:165:PHE:CE2	1:C:248:LEU:HD23	2.53	0.43
1:A:187:VAL:O	1:A:187:VAL:CG1	2.67	0.42
1:A:175:ASN:HD22	1:A:175:ASN:HA	1.66	0.42
1:B:165:PHE:HB3	1:B:250:GLY:HA2	2.02	0.42
1:C:400:LYS:NZ	5:C:616:HOH:O	2.52	0.42
1:C:187:VAL:O	1:C:187:VAL:CG1	2.68	0.41
1:C:326:LYS:NZ	5:C:619:HOH:O	2.53	0.41
4:B:504:GOL:H11	5:B:700:HOH:O	2.19	0.41
1:C:168:PHE:HE2	1:C:205:VAL:HG11	1.84	0.41
1:A:163:THR:O	1:A:164:ARG:CB	2.69	0.41
1:C:284:SER:OG	1:C:287[B]:MET:HG3	2.20	0.41
1:B:205:VAL:HG12	1:B:206:ASN:ND2	2.35	0.41
1:B:237[A]:MET:CE	1:B:246:VAL:HG23	2.37	0.41
1:C:237[A]:MET:HE3	1:C:330:PHE:CE2	2.56	0.40
1:C:181:ASP:OD2	1:C:183:ARG:NH1	2.54	0.40
1:D:187:VAL:O	1:D:187:VAL:CG1	2.69	0.40
1:A:344[B]:MET:CE	1:C:395:LEU:HD11	2.52	0.40

All (3) 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:C:424:THR:OG1	1:D:256:ASP:OD2[2_556]	1.94	0.26
1:D:172:GLU:OE1	5:A:601:HOH:O[3_555]	2.18	0.02
5:A:696:HOH:O	5:C:732:HOH:O[4_446]	2.18	0.02

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	294/327 (90%)	283 (96%)	9 (3%)	2 (1%)	18	15
1	B	294/327 (90%)	285 (97%)	7 (2%)	2 (1%)	18	15
1	C	300/327 (92%)	291 (97%)	8 (3%)	1 (0%)	36	36
1	D	290/327 (89%)	279 (96%)	9 (3%)	2 (1%)	18	15
All	All	1178/1308 (90%)	1138 (97%)	33 (3%)	7 (1%)	21	18

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLU
1	B	406	GLU
1	D	406	GLU
1	B	218	MET
1	C	406	GLU
1	D	256	ASP
1	A	164	ARG

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	257/284 (90%)	250 (97%)	7 (3%)	39	45
1	B	257/284 (90%)	250 (97%)	7 (3%)	39	45
1	C	262/284 (92%)	252 (96%)	10 (4%)	29	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	255/284 (90%)	247 (97%)	8 (3%)	35	39
All	All	1031/1136 (91%)	999 (97%)	32 (3%)	35	39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	VAL
1	A	219	VAL
1	A	223	THR
1	A	343	VAL
1	A	365	THR
1	A	427	GLU
1	A	455	GLN
1	B	187	VAL
1	B	213	LYS
1	B	214	LYS
1	B	219	VAL
1	B	336	SER
1	B	365	THR
1	B	427	GLU
1	C	187	VAL
1	C	221	ILE
1	C	223	THR
1	C	227	LYS
1	C	243	GLU
1	C	252	SER
1	C	253	SER
1	C	365	THR
1	C	399	ILE
1	C	427	GLU
1	D	185	ILE
1	D	187	VAL
1	D	223	THR
1	D	227	LYS
1	D	257	ASP
1	D	321	GLU
1	D	365	THR
1	D	427	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	ASN
1	A	178	ASN
1	A	435	GLN
1	B	175	ASN
1	B	206	ASN
1	B	228	GLN
1	B	306	HIS
1	B	341	GLN
1	C	206	ASN
1	C	435	GLN
1	D	175	ASN
1	D	179	ASN
1	D	286	HIS
1	D	293	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	C	345	1	8,10,11	0.94	0	10,14,16	0.90	0
1	TPO	D	345	1	8,10,11	1.03	1 (12%)	10,14,16	0.95	0
1	TPO	B	345	1	8,10,11	0.87	0	10,14,16	1.03	1 (10%)
1	SEP	A	346	1	8,9,10	0.57	0	7,12,14	0.84	0
1	TPO	D	342	1	8,10,11	0.66	0	10,14,16	0.94	0
1	SEP	D	346	1	8,9,10	0.48	0	7,12,14	1.21	1 (14%)
1	TPO	A	345	1	8,10,11	0.99	0	10,14,16	0.94	0
1	TPO	A	342	1	8,10,11	0.50	0	10,14,16	1.10	1 (10%)
1	SEP	B	346	1	8,9,10	0.70	0	7,12,14	0.86	0

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	1.00	1 (12%)	10,14,16	1.22	1 (10%)
1	TPO	C	342	1	8,10,11	0.65	0	10,14,16	1.25	1 (10%)
1	SEP	C	346	1	8,9,10	0.56	0	7,12,14	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	C	345	1	-	3/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	D	342	1	-	1/9/11/13	-
1	SEP	D	346	1	-	3/6/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	B	342	1	-	1/9/11/13	-
1	TPO	C	342	1	-	0/9/11/13	-
1	SEP	C	346	1	-	0/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	TPO	P-OG1	2.42	1.63	1.59
1	D	345	TPO	P-OG1	2.24	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	342	TPO	P-OG1-CB	-2.83	115.63	123.33
1	D	346	SEP	OG-P-O1P	-2.31	100.19	106.44
1	A	342	TPO	O3P-P-O2P	2.29	116.39	107.80
1	B	345	TPO	O3P-P-O2P	2.25	116.23	107.80
1	C	342	TPO	OG1-P-O1P	-2.23	101.37	109.33

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	342	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	D	346	SEP	CB-OG-P-O1P
1	D	346	SEP	CB-OG-P-O2P
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	346	SEP	CB-OG-P-O3P
1	D	345	TPO	CB-OG1-P-O3P
1	A	342	TPO	O-C-CA-CB
1	D	342	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	342	TPO	1	0
1	A	342	TPO	1	0
1	B	342	TPO	1	0
1	C	342	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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	$\# Z > 2$
4	GOL	A	504	-	5,5,5	0.11	0	5,5,5	0.37	0
4	GOL	A	503	-	5,5,5	0.16	0	5,5,5	0.27	0
2	YJU	B	501	-	35,37,37	1.47	6 (17%)	47,56,56	2.04	12 (25%)
4	GOL	C	503	-	5,5,5	0.12	0	5,5,5	0.29	0
4	GOL	B	503	-	5,5,5	0.13	0	5,5,5	0.28	0
4	GOL	B	504	-	5,5,5	0.17	0	5,5,5	0.38	0
2	YJU	A	501	-	35,37,37	1.49	7 (20%)	47,56,56	2.00	10 (21%)
4	GOL	D	502	-	5,5,5	0.10	0	5,5,5	0.30	0
2	YJU	D	501	-	35,37,37	1.75	7 (20%)	47,56,56	2.19	14 (29%)
2	YJU	C	501	-	35,37,37	2.17	9 (25%)	47,56,56	2.64	16 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	504	-	-	4/4/4/4	-
4	GOL	A	503	-	-	3/4/4/4	-
2	YJU	B	501	-	-	2/26/36/36	0/4/4/4
4	GOL	C	503	-	-	4/4/4/4	-
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
2	YJU	A	501	-	-	4/26/36/36	0/4/4/4
4	GOL	D	502	-	-	2/4/4/4	-
2	YJU	D	501	-	-	2/26/36/36	0/4/4/4
2	YJU	C	501	-	-	2/26/36/36	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	YJU	C6-N1	-6.55	1.24	1.33
2	C	501	YJU	C2-C4	-4.92	1.50	1.54
2	C	501	YJU	C9-C10	-4.66	1.35	1.40
2	D	501	YJU	C3-C2	-4.55	1.47	1.52
2	B	501	YJU	C16-N4	-4.42	1.28	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	YJU	C6-N1	-4.26	1.27	1.33
2	C	501	YJU	C10-C4	3.99	1.44	1.40
2	A	501	YJU	C9-C10	-3.82	1.36	1.40
2	C	501	YJU	C7-N2	-3.56	1.31	1.35
2	C	501	YJU	C5-C4	-3.29	1.33	1.39
2	D	501	YJU	C9-C10	-3.23	1.36	1.40
2	D	501	YJU	C10-C4	3.20	1.43	1.40
2	A	501	YJU	C16-N4	-3.11	1.30	1.34
2	C	501	YJU	C5-C6	-3.01	1.37	1.40
2	D	501	YJU	C5-C4	-2.95	1.34	1.39
2	A	501	YJU	C5-C4	-2.93	1.34	1.39
2	C	501	YJU	C6-C8	2.60	1.47	1.43
2	B	501	YJU	C9-C10	-2.47	1.37	1.40
2	B	501	YJU	C6-C8	2.37	1.47	1.43
2	A	501	YJU	C12-N4	-2.31	1.31	1.34
2	A	501	YJU	C6-N1	-2.27	1.30	1.33
2	B	501	YJU	C12-N4	-2.24	1.31	1.34
2	A	501	YJU	C10-C4	2.22	1.42	1.40
2	B	501	YJU	C15-C16	-2.18	1.34	1.39
2	A	501	YJU	C2-C4	-2.17	1.52	1.54
2	D	501	YJU	C6-C8	2.07	1.46	1.43
2	B	501	YJU	C18-N2	-2.02	1.44	1.47
2	C	501	YJU	F1-C17	2.01	1.40	1.33
2	D	501	YJU	C16-N4	-2.01	1.31	1.34

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	YJU	C6-N1-N2	10.35	109.44	104.44
2	B	501	YJU	C6-N1-N2	8.64	108.62	104.44
2	C	501	YJU	C18-N2-N1	-8.11	110.25	119.76
2	A	501	YJU	C6-N1-N2	7.40	108.02	104.44
2	D	501	YJU	C3-C2-C1	-6.33	102.80	110.53
2	A	501	YJU	C24-C18-N2	-6.02	102.72	110.95
2	D	501	YJU	C6-N1-N2	5.91	107.30	104.44
2	C	501	YJU	C18-N2-C7	4.94	136.96	128.77
2	D	501	YJU	C18-N2-N1	-4.47	114.52	119.76
2	D	501	YJU	C13-C12-N4	-4.25	117.96	122.92
2	C	501	YJU	C23-C21-C20	4.20	119.56	109.29
2	B	501	YJU	C24-C18-N2	-4.03	105.44	110.95
2	D	501	YJU	C19-C20-C21	-3.92	104.96	112.36
2	A	501	YJU	O1-C2-C1	-3.76	99.30	107.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	YJU	C1-C2-C4	3.60	117.38	111.52
2	C	501	YJU	F1-C17-C16	-3.49	106.29	112.43
2	B	501	YJU	C18-N2-N1	-3.48	115.68	119.76
2	C	501	YJU	C4-C10-N3	-3.47	116.74	120.42
2	B	501	YJU	C4-C10-N3	-3.22	117.01	120.42
2	D	501	YJU	C12-N4-C16	3.21	123.01	118.78
2	A	501	YJU	C12-N4-C16	3.20	122.99	118.78
2	C	501	YJU	C19-C18-N2	2.97	115.02	110.95
2	A	501	YJU	C4-C10-N3	-2.94	117.30	120.42
2	D	501	YJU	C4-C10-N3	-2.91	117.34	120.42
2	D	501	YJU	C19-C18-N2	2.77	114.74	110.95
2	C	501	YJU	C12-N4-C16	2.76	122.41	118.78
2	B	501	YJU	C20-C19-C18	-2.75	104.67	109.98
2	C	501	YJU	C13-C12-N4	-2.71	119.76	122.92
2	C	501	YJU	C19-C20-C21	-2.67	107.33	112.36
2	A	501	YJU	C5-C4-C10	2.65	122.12	118.80
2	B	501	YJU	C3-C2-C1	-2.56	107.40	110.53
2	D	501	YJU	C18-N2-C7	2.48	132.88	128.77
2	B	501	YJU	F1-C17-C16	-2.48	108.06	112.43
2	B	501	YJU	C18-N2-C7	2.47	132.85	128.77
2	B	501	YJU	C3-C2-C4	2.37	115.39	111.52
2	C	501	YJU	C19-C18-C24	2.33	116.44	111.17
2	B	501	YJU	C19-C18-N2	2.30	114.10	110.95
2	A	501	YJU	C7-N2-N1	-2.29	110.69	113.14
2	C	501	YJU	C17-C16-N4	2.28	117.32	114.60
2	C	501	YJU	C20-C21-C22	-2.25	104.56	112.31
2	C	501	YJU	F2-C17-C16	2.23	116.36	112.43
2	D	501	YJU	F3-C17-F2	2.17	113.61	105.77
2	D	501	YJU	C20-C19-C18	-2.12	105.89	109.98
2	A	501	YJU	C17-C16-N4	2.12	117.12	114.60
2	C	501	YJU	C20-C19-C18	-2.10	105.92	109.98
2	B	501	YJU	C5-C4-C10	2.10	121.43	118.80
2	A	501	YJU	C13-C12-N4	-2.09	120.48	122.92
2	B	501	YJU	C23-C24-C18	2.07	113.98	109.98
2	D	501	YJU	C5-C4-C10	2.06	121.39	118.80
2	A	501	YJU	C1-C2-C4	2.06	114.87	111.52
2	D	501	YJU	C24-C18-N2	-2.01	108.19	110.95
2	C	501	YJU	C24-C18-N2	-2.01	108.20	110.95

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	YJU	C23-C21-C22-O3
2	D	501	YJU	C20-C21-C22-O3
2	D	501	YJU	C23-C21-C22-O3
4	A	504	GOL	C1-C2-C3-O3
4	B	504	GOL	C1-C2-C3-O3
4	D	502	GOL	O1-C1-C2-C3
4	A	503	GOL	O1-C1-C2-C3
4	A	503	GOL	C1-C2-C3-O3
4	C	503	GOL	O1-C1-C2-C3
4	C	503	GOL	C1-C2-C3-O3
4	A	504	GOL	O2-C2-C3-O3
4	B	504	GOL	O2-C2-C3-O3
4	C	503	GOL	O1-C1-C2-O2
4	D	502	GOL	O1-C1-C2-O2
2	A	501	YJU	C20-C21-C22-O3
2	A	501	YJU	C23-C21-C22-O3
2	B	501	YJU	C20-C21-C22-O3
2	C	501	YJU	C20-C21-C22-O3
4	A	503	GOL	O2-C2-C3-O3
4	B	503	GOL	O2-C2-C3-O3
4	A	504	GOL	O1-C1-C2-C3
2	A	501	YJU	C19-C18-N2-C7
4	C	503	GOL	O2-C2-C3-O3
2	B	501	YJU	C23-C21-C22-O3
4	B	503	GOL	C1-C2-C3-O3
4	A	504	GOL	O1-C1-C2-O2
2	A	501	YJU	C19-C18-N2-N1

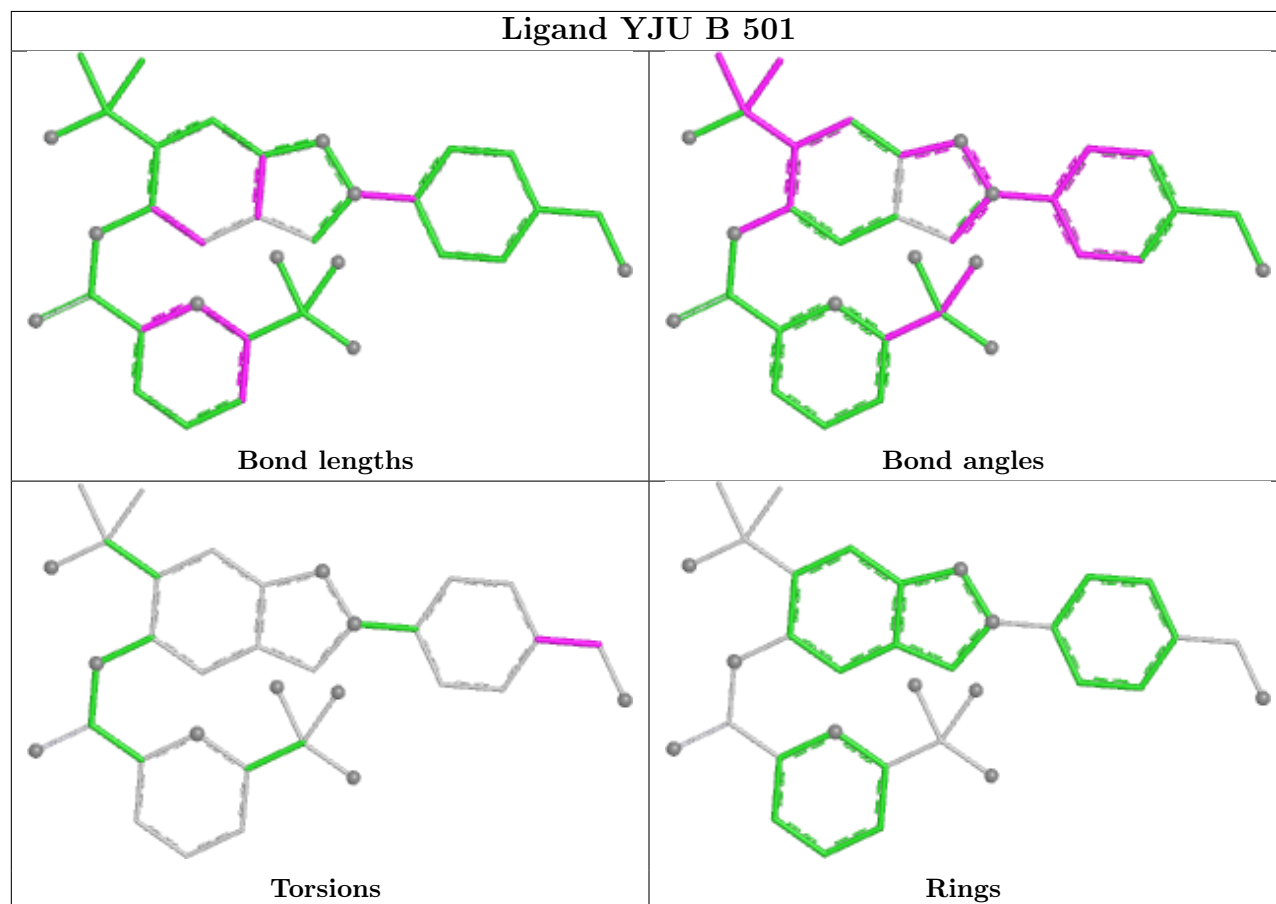
There are no ring outliers.

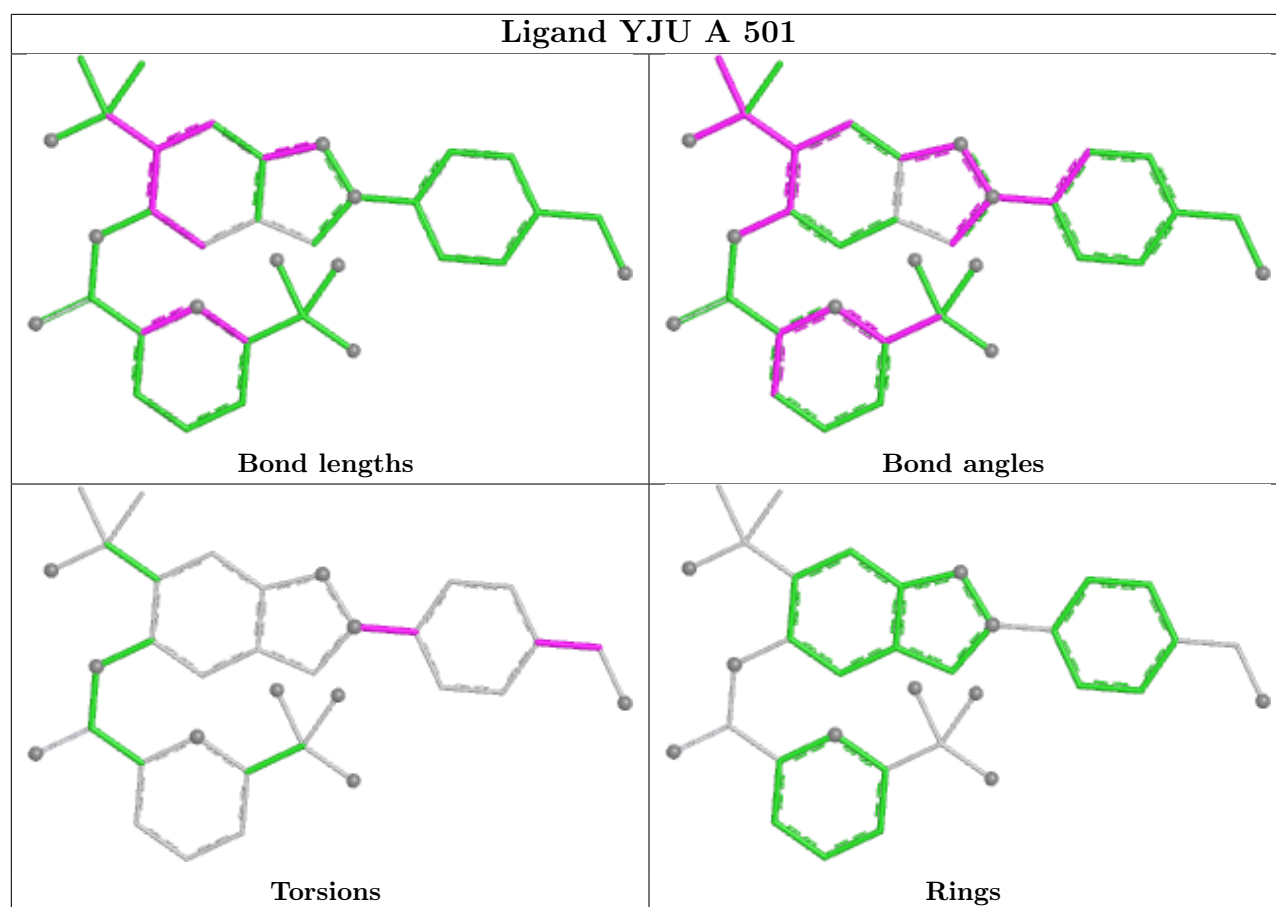
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	GOL	1	0
4	C	503	GOL	2	0
4	B	504	GOL	1	0

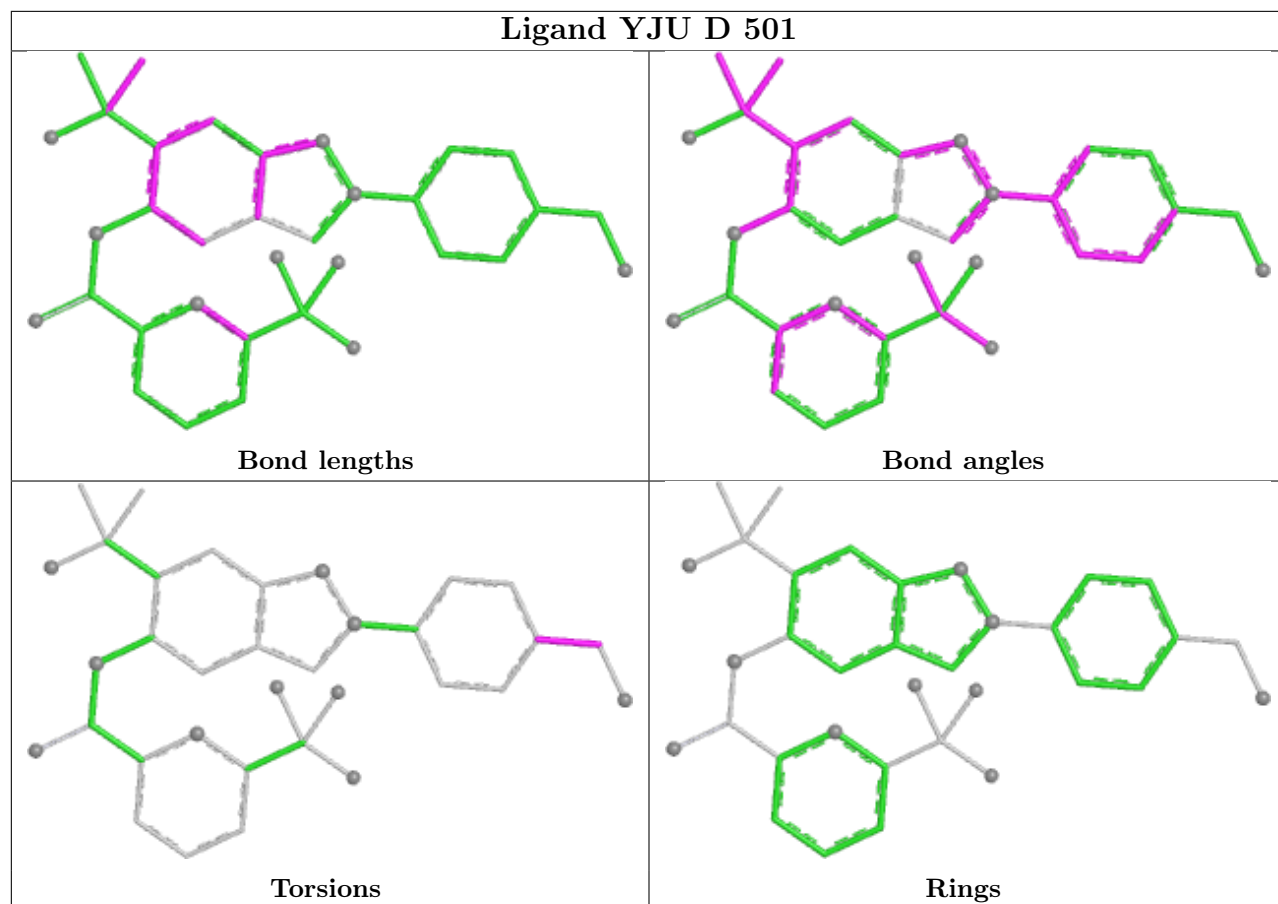
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

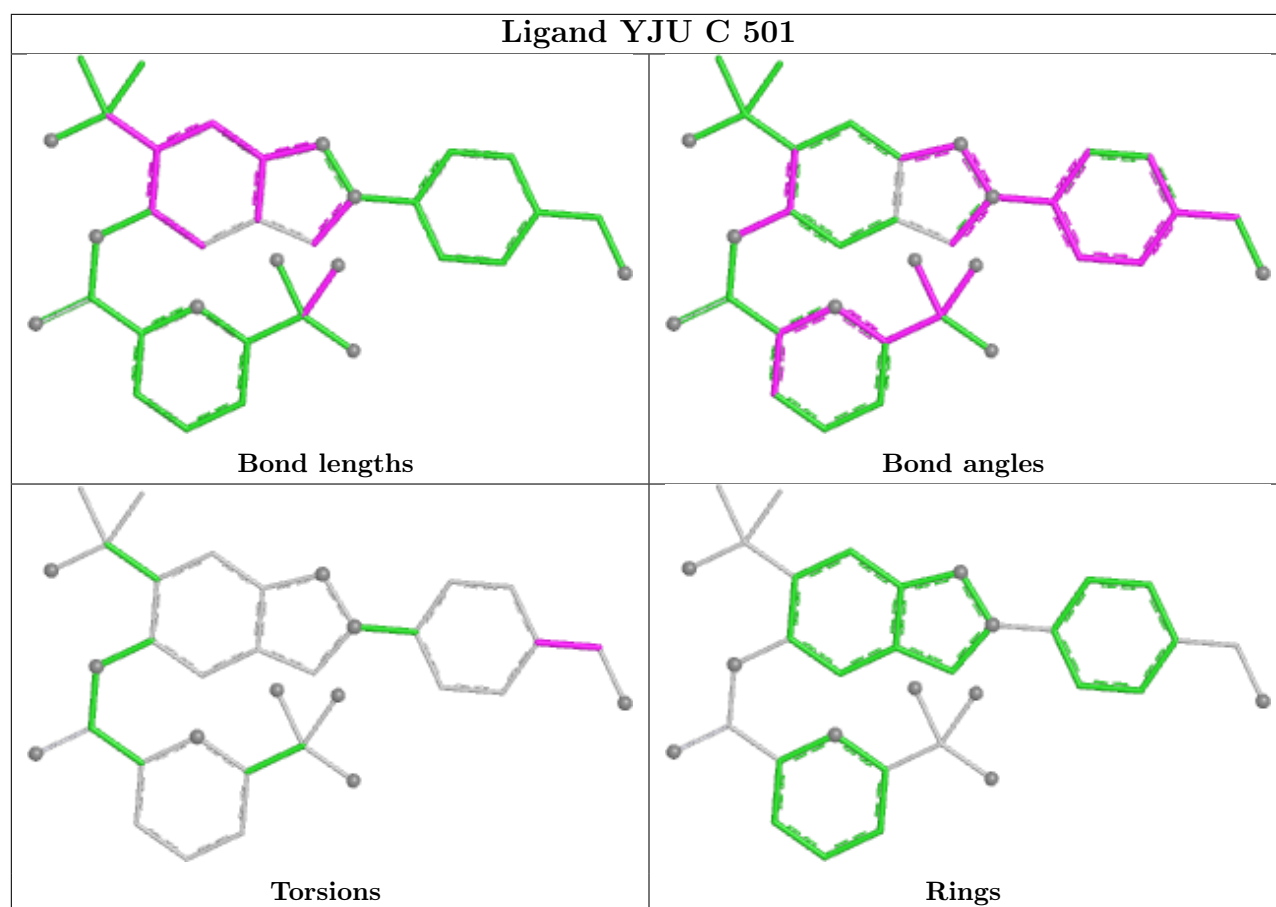
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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





Ligand YJU 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	294/327 (89%)	0.16	10 (3%)	48 50	25, 36, 78, 165	2 (0%)
1	B	295/327 (90%)	0.30	17 (5%)	29 30	25, 43, 88, 140	1 (0%)
1	C	299/327 (91%)	0.36	23 (7%)	19 21	20, 43, 90, 147	3 (1%)
1	D	291/327 (88%)	0.35	22 (7%)	20 21	21, 41, 86, 136	2 (0%)
All	All	1179/1308 (90%)	0.29	72 (6%)	27 29	20, 40, 86, 165	8 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	PHE	6.6
1	C	340	ALA	5.0
1	A	340	ALA	4.8
1	B	340	ALA	4.8
1	D	195	GLY	4.8
1	C	165	PHE	4.5
1	C	339	PHE	4.5
1	C	158	ILE	4.4
1	B	219	VAL	4.1
1	A	217	ALA	4.1
1	D	185	ILE	3.7
1	C	343	VAL	3.7
1	C	204	TYR	3.6
1	D	343	VAL	3.6
1	A	459	ALA	3.6
1	A	338	LYS	3.5
1	D	219	VAL	3.4
1	B	221	ILE	3.4
1	C	336	SER	3.1
1	D	217	ALA	3.1
1	C	166	HIS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	405	ASP	3.1
1	A	219	VAL	3.0
1	B	218	MET	3.0
1	D	171	TYR	3.0
1	B	217	ALA	2.9
1	C	399	ILE	2.8
1	D	255	GLY	2.7
1	A	439	GLU	2.7
1	B	205	VAL	2.6
1	A	163	THR	2.6
1	C	338	LYS	2.6
1	D	179	ASN	2.6
1	D	459	ALA	2.6
1	B	188	GLY	2.6
1	C	186	SER	2.6
1	C	341	GLN	2.5
1	B	187	VAL	2.5
1	B	216	ALA	2.5
1	D	188	GLY	2.5
1	B	204	TYR	2.5
1	D	344	MET	2.4
1	D	196	GLY	2.4
1	B	337	GLU	2.4
1	D	221	ILE	2.4
1	C	163	THR	2.4
1	B	336	SER	2.4
1	D	216	ALA	2.4
1	C	185	ILE	2.4
1	C	167	SER	2.4
1	A	337	GLU	2.3
1	B	196	GLY	2.3
1	C	161	SER	2.3
1	C	459	ALA	2.3
1	C	159	ALA	2.3
1	A	347	ARG	2.2
1	D	163	THR	2.2
1	D	338	LYS	2.2
1	B	197	PHE	2.2
1	D	458	THR	2.1
1	C	410	ILE	2.1
1	C	160	VAL	2.1
1	D	226	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	218	MET	2.1
1	C	335	ALA	2.1
1	D	175	ASN	2.1
1	D	256	ASP	2.1
1	B	222	THR	2.1
1	B	162	ASP	2.0
1	D	254	ASP	2.0
1	C	187	VAL	2.0
1	C	208	THR	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	0.79	0.10	52,70,93,100	0
1	TPO	D	342	11/12	0.83	0.13	70,74,90,93	0
1	SEP	B	346	10/11	0.85	0.11	46,60,83,88	0
1	SEP	A	346	10/11	0.87	0.11	42,58,78,85	0
1	SEP	C	346	10/11	0.87	0.09	49,61,89,91	0
1	TPO	C	342	11/12	0.90	0.11	54,64,75,83	0
1	TPO	A	342	11/12	0.90	0.12	54,65,78,83	0
1	TPO	B	342	11/12	0.91	0.11	56,62,74,78	0
1	TPO	B	345	11/12	0.95	0.08	44,47,52,62	0
1	TPO	C	345	11/12	0.96	0.08	42,46,51,62	0
1	TPO	D	345	11/12	0.96	0.09	41,47,51,56	0
1	TPO	A	345	11/12	0.96	0.08	38,43,48,53	0

6.3 Carbohydrates [i](#)

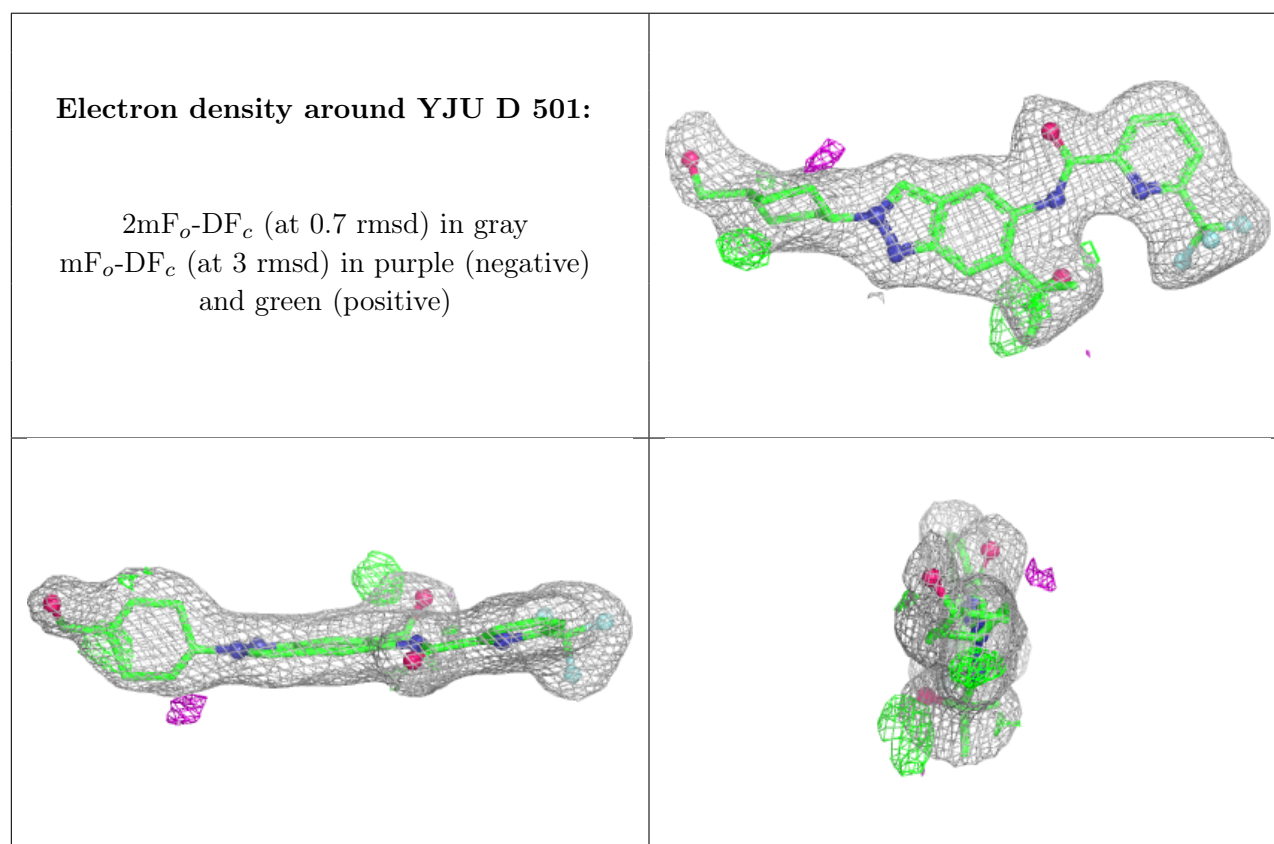
There are no oligosaccharides in this entry.

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.

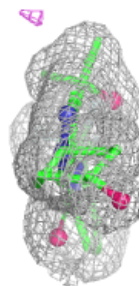
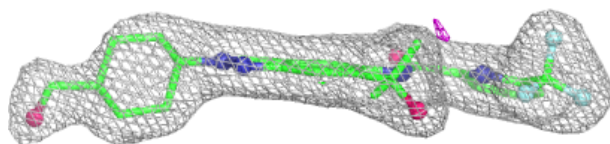
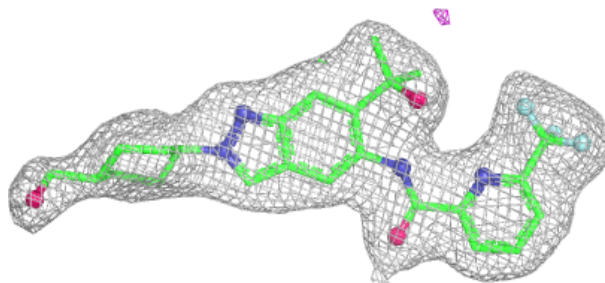
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	502	1/1	0.85	0.16	84,84,84,84	0
4	GOL	B	504	6/6	0.90	0.10	45,51,57,58	0
4	GOL	C	503	6/6	0.90	0.12	64,71,74,81	0
4	GOL	A	504	6/6	0.91	0.12	56,61,67,68	0
4	GOL	D	502	6/6	0.91	0.10	55,58,62,66	0
4	GOL	B	503	6/6	0.92	0.10	57,62,68,77	0
4	GOL	A	503	6/6	0.92	0.14	56,63,68,75	0
3	CL	C	502	1/1	0.93	0.14	83,83,83,83	0
2	YJU	D	501	34/34	0.95	0.07	27,34,56,61	0
3	CL	A	502	1/1	0.95	0.12	69,69,69,69	0
2	YJU	B	501	34/34	0.96	0.07	29,34,50,51	0
2	YJU	C	501	34/34	0.96	0.06	26,30,48,50	0
2	YJU	A	501	34/34	0.96	0.06	26,29,49,57	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.

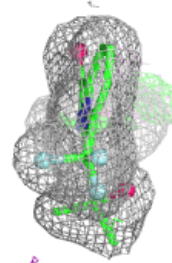
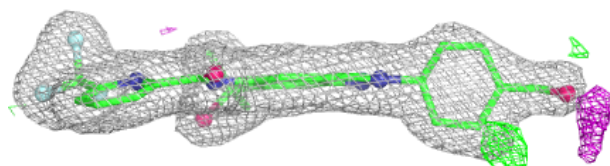
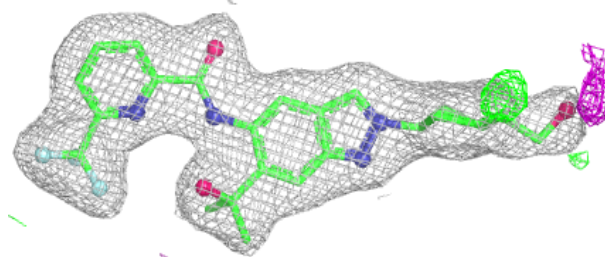


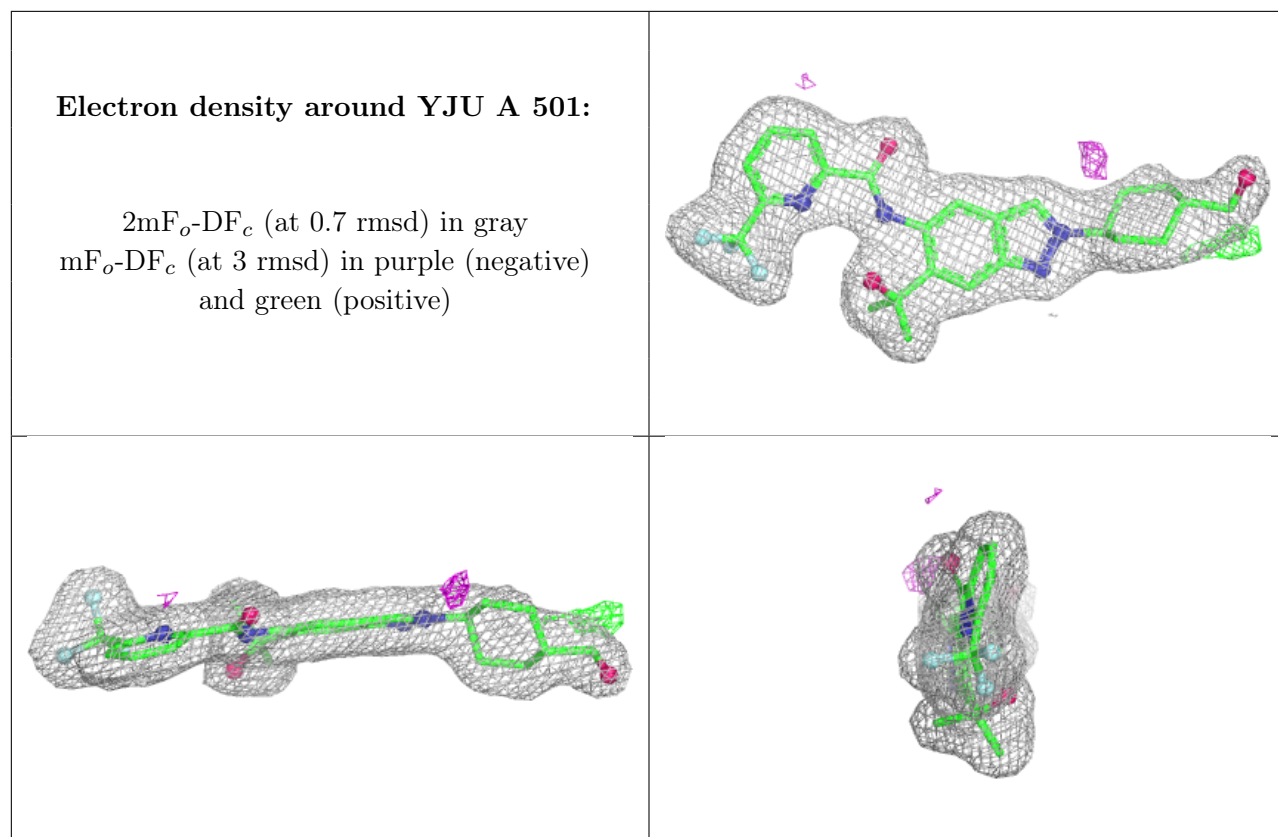
Electron density around YJU B 501:

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

**Electron density around YJU 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.