Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:41 PM UTC

PDB ID	:	9S64 / pdb_00009s64
Title	:	Human TEAD1 in complex with 2-(4-chloro-3-{3-methyl-5-[4-(trifluoromethyl)phenoxy]phenyl}-1H-pyrrolo[3,2-c]pyridin-1-yl)ethan-1-ol
Authors	:	Musil, D.; Freire, F.
Deposited on	:	2025-07-30
Resolution	:	1.85 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:

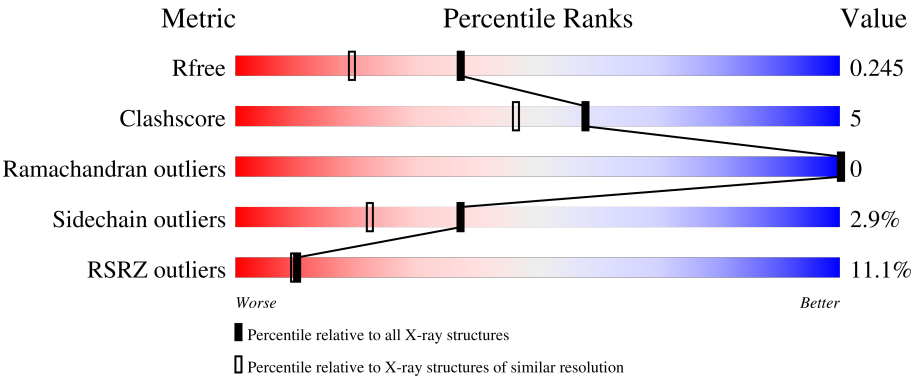
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 <=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	220	6% 81% 12% 7%
1	B	220	9% 78% 12% • 8%
1	C	220	8% 82% 10% • 8%
1	D	220	17% 71% 11% 17%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6932 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.

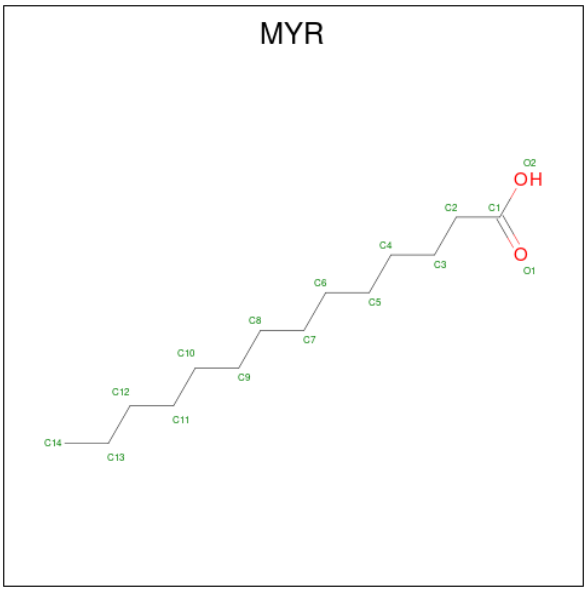
- Molecule 1 is a protein called Transcriptional enhancer factor TEF-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	13	8	0
			1727	1109	291	315	12			
1	B	202	Total	C	N	O	S	4	3	0
			1661	1068	282	299	12			
1	C	203	Total	C	N	O	S	7	7	0
			1707	1093	289	313	12			
1	D	182	Total	C	N	O	S	14	3	0
			1498	968	251	266	13			

There are 8 discrepancies between the modelled and reference sequences:

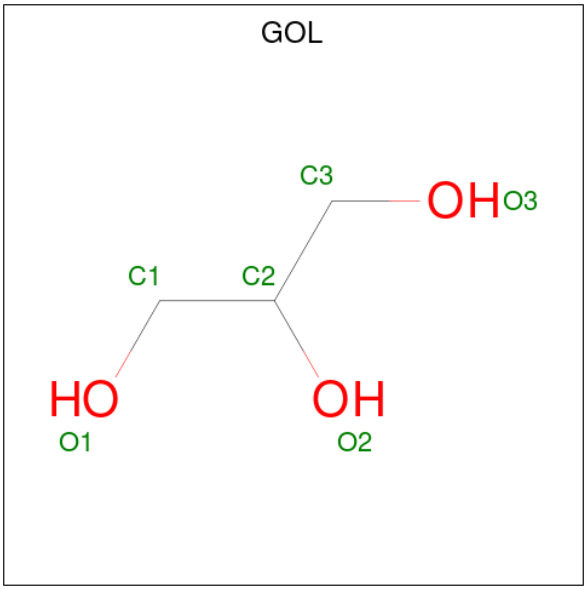
Chain	Residue	Modelled	Actual	Comment	Reference
A	207	GLY	-	expression tag	UNP P28347
A	208	PRO	-	expression tag	UNP P28347
B	207	GLY	-	expression tag	UNP P28347
B	208	PRO	-	expression tag	UNP P28347
C	207	GLY	-	expression tag	UNP P28347
C	208	PRO	-	expression tag	UNP P28347
D	207	GLY	-	expression tag	UNP P28347
D	208	PRO	-	expression tag	UNP P28347

- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 15 14 1	0	0
2	B	1	Total C O 15 14 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

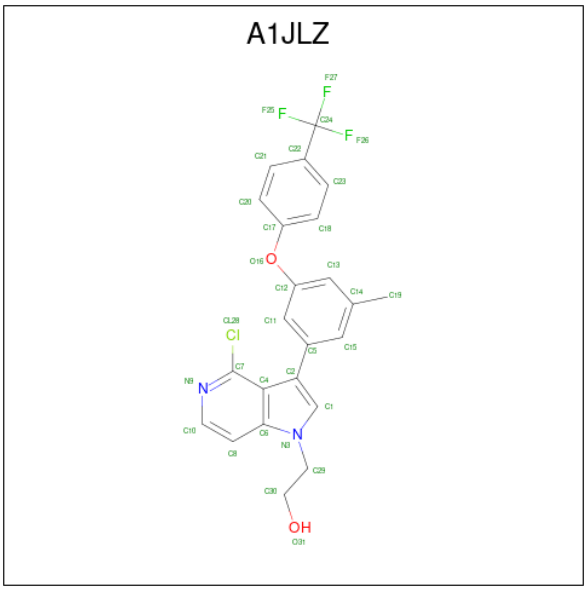


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is 2-[4-chloranyl-3-[3-methyl-5-[4-(trifluoromethyl)phenoxy]phenyl]pyrrolo[3,2-c]pyridin-1-yl]ethanol (CCD ID: A1JLZ) (formula: $C_{23}H_{18}ClF_3N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C Cl F N O 31 23 1 3 2 2	0	0
5	D	1	Total C Cl F N O 31 23 1 3 2 2	0	0

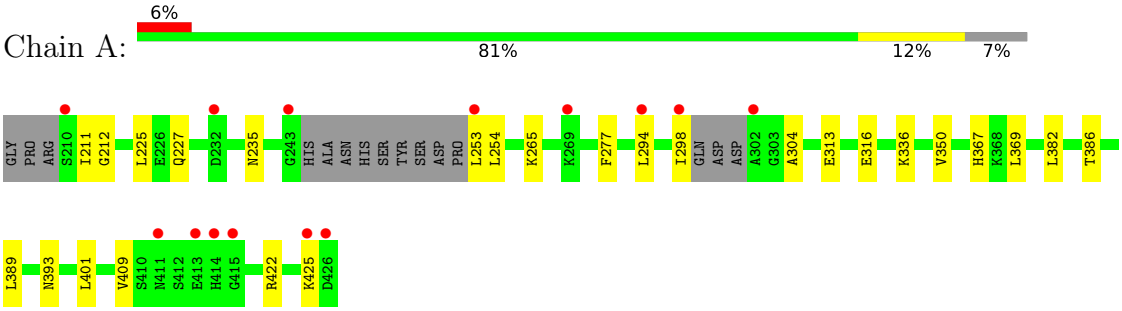
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	79	Total O 79 79	0	0
6	B	67	Total O 67 67	0	0
6	C	56	Total O 56 56	0	0
6	D	38	Total O 38 38	0	0

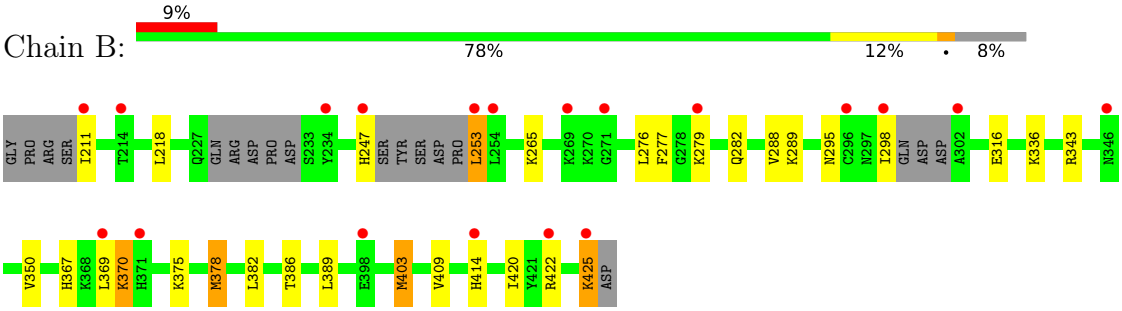
3 Residue-property plots (i)

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.

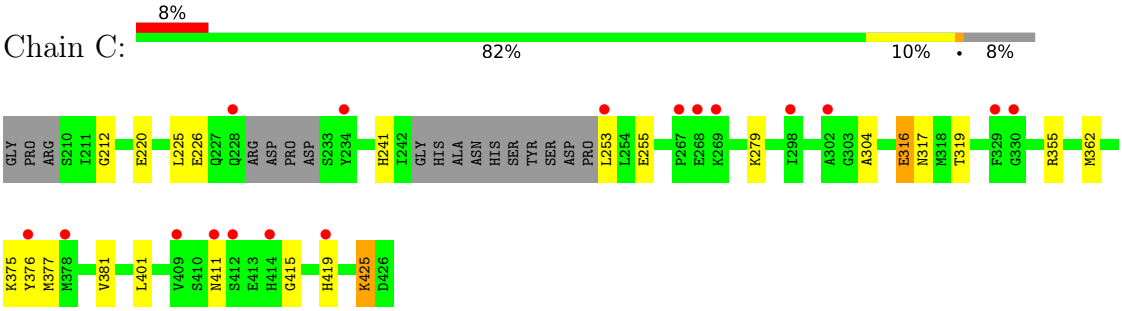
• Molecule 1: Transcriptional enhancer factor TEF-1



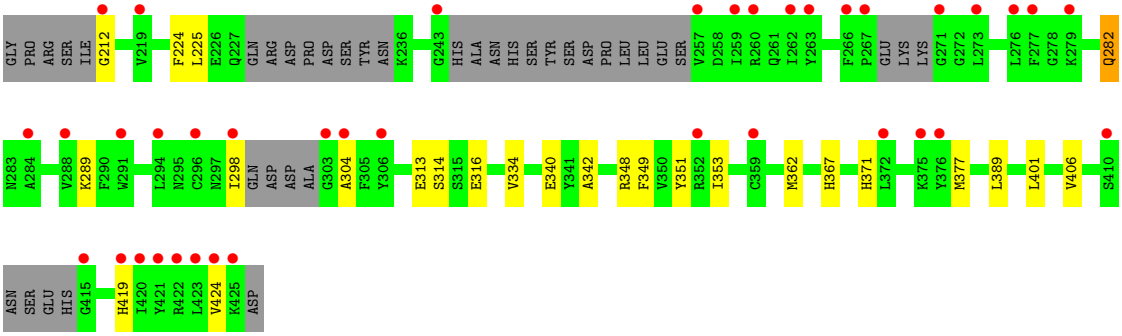
• Molecule 1: Transcriptional enhancer factor TEF-1



• Molecule 1: Transcriptional enhancer factor TEF-1



• Molecule 1: Transcriptional enhancer factor TEF-1


GLY PRO ARG SER ILE G212 V219 F224 L225 E226 Q227 GLN ARG ASP PRO ASP SER TYR ASN K236 G243 HIS ALA ASN HIS SER TYR SER ASP PRO LEU LEU GLU SER V257 D258 I259 R260 Q261 I262 Y263 F266 P267 GLU LYS LYS G271 G272 L273 L276 F277 G278 K279 Q282
N283 A284 V288 K289 F290 W291 L294 N295 C296 N297 I298 GLN ASP ASP ALA G303 A304 F305 Y306 E313 S314 S315 E316 V334 E340 Y341 A342 R348 F349 V350 Y351 R352 I353 C359 M362 H367 H371 L372 K375 Y376 M377 L389 L401 V406 S410
ASN SER GLU HIS G415 H419 I420 Y421 R422 L423 V424 K425 ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.71Å 81.88Å 76.60Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	36.55 – 1.85 36.55 – 1.85	Depositor EDS
% Data completeness (in resolution range)	60.2 (36.55-1.85) 60.1 (36.55-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.85Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.215 , 0.255 0.207 , 0.245	Depositor DCC
R_{free} test set	2172 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6932	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, GOL, CL, A1JLZ

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	0.76	0/1778	0.96	1/2390 (0.0%)
1	B	0.78	2/1702 (0.1%)	1.00	0/2288
1	C	0.71	0/1755	1.03	6/2359 (0.3%)
1	D	0.65	0/1530	0.96	1/2053 (0.0%)
All	All	0.73	2/6765 (0.0%)	0.99	8/9090 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	403	MET	SD-CE	8.41	2.00	1.79
1	B	378	MET	SD-CE	-5.43	1.66	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	425	LYS	CA-C-N	6.35	133.13	121.70
1	C	425	LYS	C-N-CA	6.35	133.13	121.70
1	C	411	ASN	CA-C-N	5.39	128.37	120.71
1	C	411	ASN	C-N-CA	5.39	128.37	120.71
1	C	415	GLY	N-CA-C	5.25	122.44	112.62
1	A	393	ASN	N-CA-C	-5.19	100.63	108.67
1	C	319	THR	N-CA-C	-5.11	100.19	108.52
1	D	224	PHE	N-CA-C	5.10	116.75	109.14

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	1727	0	1715	12	0
1	B	1661	0	1642	19	0
1	C	1707	0	1682	12	0
1	D	1498	0	1489	15	0
2	A	15	0	27	1	0
2	B	15	0	27	0	0
3	B	6	0	8	1	0
4	C	1	0	0	0	0
5	C	31	0	0	4	0
5	D	31	0	0	2	0
6	A	79	0	0	0	0
6	B	67	0	0	1	0
6	C	56	0	0	0	0
6	D	38	0	0	0	0
All	All	6932	0	6590	60	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 5.

All (60) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:MET:HE3	5:D:501:A1JLZ:CL28	2.03	0.95
1:C:362:MET:HE3	5:C:502:A1JLZ:CL28	2.06	0.92
1:B:247:HIS:CE1	1:B:420:ILE:HD12	2.05	0.91
1:A:254:LEU:HB2	1:A:422:ARG:HD2	1.67	0.77
1:D:289:LYS:HD3	1:D:406:VAL:HG23	1.69	0.73
1:D:298:ILE:HD12	1:D:367:HIS:CD2	2.26	0.71
1:C:225:LEU:HD11	1:C:304:ALA:HB1	1.74	0.69
1:C:381:VAL:HG22	1:D:377:MET:HE1	1.78	0.66
1:A:313[A]:GLU:HG2	1:A:350:VAL:HG22	1.81	0.63
1:A:212:GLY:HA2	1:A:401[B]:LEU:HD21	1.83	0.60
5:C:502:A1JLZ:CL28	5:C:502:A1JLZ:C11	2.87	0.59
1:D:282:GLN:H	1:D:282:GLN:HE21	1.53	0.55
1:D:212:GLY:HA2	1:D:401:LEU:HD21	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLU:OE2	1:C:355:ARG:NH1	2.41	0.54
1:B:265:LYS:HB3	1:B:386:THR:HG21	1.91	0.53
1:B:288:VAL:HG21	1:B:403:MET:HE3	1.90	0.53
1:A:277:PHE:HE2	1:A:425:LYS:HB2	1.74	0.52
1:C:376:TYR:CD1	1:D:371:HIS:ND1	2.78	0.52
1:B:375:LYS:HA	1:B:378:MET:HE2	1.92	0.51
1:A:211:ILE:HG22	1:A:401[A]:LEU:HD11	1.94	0.50
1:C:255:GLU:OE2	1:C:419[B]:HIS:HE1	1.95	0.50
1:B:277:PHE:CZ	1:B:282:GLN:HG2	2.47	0.50
1:B:276:LEU:HD23	1:B:279:LYS:HE2	1.94	0.49
1:D:282:GLN:H	1:D:282:GLN:NE2	2.11	0.48
1:B:295:ASN:HD22	1:B:414:HIS:CE1	2.31	0.48
1:D:340:GLU:HG3	1:D:353:ILE:HG12	1.96	0.47
1:D:342:ALA:HB1	1:D:349:PHE:HB3	1.96	0.47
1:B:298:ILE:HD13	1:B:367:HIS:CD2	2.50	0.47
1:B:343:ARG:HD2	1:B:350:VAL:O	2.15	0.46
1:D:298:ILE:HD12	1:D:367:HIS:HD2	1.79	0.46
1:C:212:GLY:HA2	1:C:401:LEU:HD21	1.97	0.46
1:A:227:GLN:O	1:A:235:ASN:HB2	2.15	0.46
5:D:501:A1JLZ:CL28	5:D:501:A1JLZ:C11	3.01	0.46
1:D:313:GLU:OE1	1:D:348:ARG:HD2	2.16	0.45
1:C:377:MET:O	1:C:381:VAL:HG23	2.17	0.45
1:B:378:MET:HE3	1:B:409:VAL:HG21	1.98	0.44
1:C:316:GLU:HG3	1:C:317:ASN:N	2.31	0.44
1:B:425:LYS:HD3	1:B:425:LYS:H	1.81	0.44
1:A:294:LEU:HD13	1:A:409:VAL:HG22	1.99	0.44
1:B:218:LEU:HD22	1:B:403:MET:SD	2.58	0.44
3:B:502:GOL:H12	6:B:613:HOH:O	2.17	0.44
1:C:362:MET:HG2	5:C:502:A1JLZ:CL28	2.55	0.43
1:D:314:SER:OG	1:D:316:GLU:O	2.37	0.43
1:A:225:LEU:HD11	1:A:304:ALA:HB1	2.00	0.43
1:D:225:LEU:HD11	1:D:304:ALA:HB1	2.02	0.42
2:A:501:MYR:H131	2:A:501:MYR:H101	1.92	0.42
1:B:369:LEU:HD11	1:B:382:LEU:HD21	2.01	0.42
1:D:342:ALA:HB2	1:D:351:TYR:CE2	2.55	0.41
1:A:369:LEU:HD11	1:A:382:LEU:HD21	2.03	0.41
1:B:253:LEU:HD22	1:B:422:ARG:HH21	1.86	0.41
1:B:295:ASN:ND2	1:B:414:HIS:CE1	2.88	0.41
1:A:211:ILE:CG2	1:A:401[A]:LEU:HD11	2.51	0.41
1:B:370:LYS:HE3	1:B:370:LYS:HB3	1.91	0.41
1:C:220[B]:GLU:OE2	1:C:241[B]:HIS:HE1	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:H	1:B:425:LYS:CD	2.34	0.41
1:C:362:MET:CE	5:C:502:A1JLZ:CL28	2.93	0.41
1:B:211:ILE:HD12	1:B:218:LEU:HD23	2.03	0.40
1:A:265:LYS:HB3	1:A:386:THR:HG21	2.03	0.40
1:A:298:ILE:HD11	1:A:367:HIS:HA	2.03	0.40
1:B:279:LYS:HE3	1:B:279:LYS:HB3	1.97	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	207/220 (94%)	204 (99%)	3 (1%)	0	100	100
1	B	196/220 (89%)	195 (100%)	1 (0%)	0	100	100
1	C	204/220 (93%)	200 (98%)	4 (2%)	0	100	100
1	D	173/220 (79%)	173 (100%)	0	0	100	100
All	All	780/880 (89%)	772 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	194/199 (98%)	189 (97%)	5 (3%)	40	25
1	B	185/199 (93%)	177 (96%)	8 (4%)	26	11
1	C	192/199 (96%)	187 (97%)	5 (3%)	40	25
1	D	167/199 (84%)	162 (97%)	5 (3%)	36	21
All	All	738/796 (93%)	715 (97%)	23 (3%)	37	20

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	LEU
1	A	316	GLU
1	A	336	LYS
1	A	389[A]	LEU
1	A	389[B]	LEU
1	B	253	LEU
1	B	289	LYS
1	B	316	GLU
1	B	336	LYS
1	B	370	LYS
1	B	389[A]	LEU
1	B	389[B]	LEU
1	B	425	LYS
1	C	253	LEU
1	C	279	LYS
1	C	316	GLU
1	C	375	LYS
1	C	425	LYS
1	D	282	GLN
1	D	334	VAL
1	D	389	LEU
1	D	419	HIS
1	D	424	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	B	295	ASN
1	B	297	ASN
1	B	317	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	354	ASN
1	B	364	ASN
1	B	414	HIS
1	B	417	GLN
1	C	235	ASN
1	C	354	ASN
1	C	397	GLN
1	C	414	HIS
1	D	282	GLN
1	D	332	GLN
1	D	397	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
2	MYR	A	501	1	13,14,15	0.25	0	12,13,15	0.30	0
2	MYR	B	501	1	13,14,15	0.29	0	12,13,15	0.36	0
5	A1JLZ	C	502	-	34,34,34	0.28	0	47,50,50	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	A1JLZ	D	501	-	34,34,34	0.26	0	47,50,50	0.61	1 (2%)
3	GOL	B	502	-	5,5,5	0.13	0	5,5,5	0.26	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
2	MYR	A	501	1	-	8/12/12/13	-
2	MYR	B	501	1	-	8/12/12/13	-
5	A1JLZ	C	502	-	-	0/17/17/17	0/4/4/4
5	A1JLZ	D	501	-	-	0/17/17/17	0/4/4/4
3	GOL	B	502	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	501	A1JLZ	C17-O16-C12	2.14	123.66	118.78

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MYR	O1-C1-C2-C3
2	B	501	MYR	O1-C1-C2-C3
2	B	501	MYR	C6-C7-C8-C9
2	A	501	MYR	C6-C7-C8-C9
2	B	501	MYR	C4-C5-C6-C7
2	A	501	MYR	C4-C5-C6-C7
2	B	501	MYR	C2-C3-C4-C5
2	A	501	MYR	C2-C3-C4-C5
2	A	501	MYR	C10-C11-C12-C13
2	B	501	MYR	C7-C8-C9-C10
2	A	501	MYR	C3-C4-C5-C6
2	A	501	MYR	C7-C8-C9-C10
2	B	501	MYR	C9-C10-C11-C12
2	A	501	MYR	C9-C10-C11-C12
2	B	501	MYR	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	501	MYR	C3-C4-C5-C6

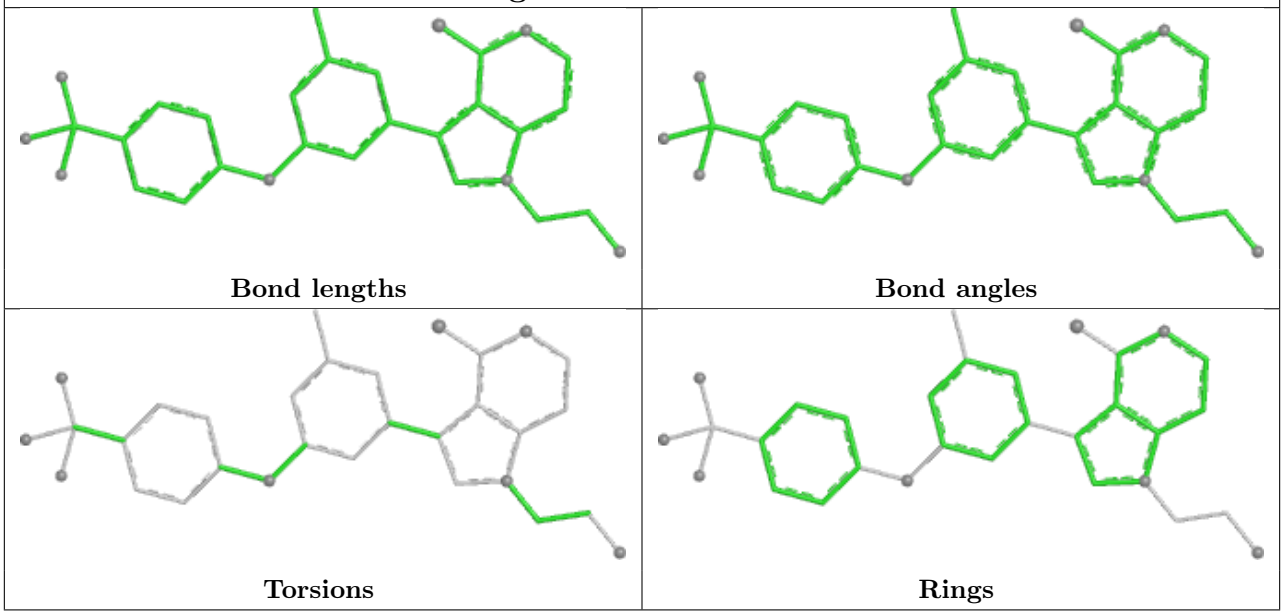
There are no ring outliers.

4 monomers are involved in 8 short contacts:

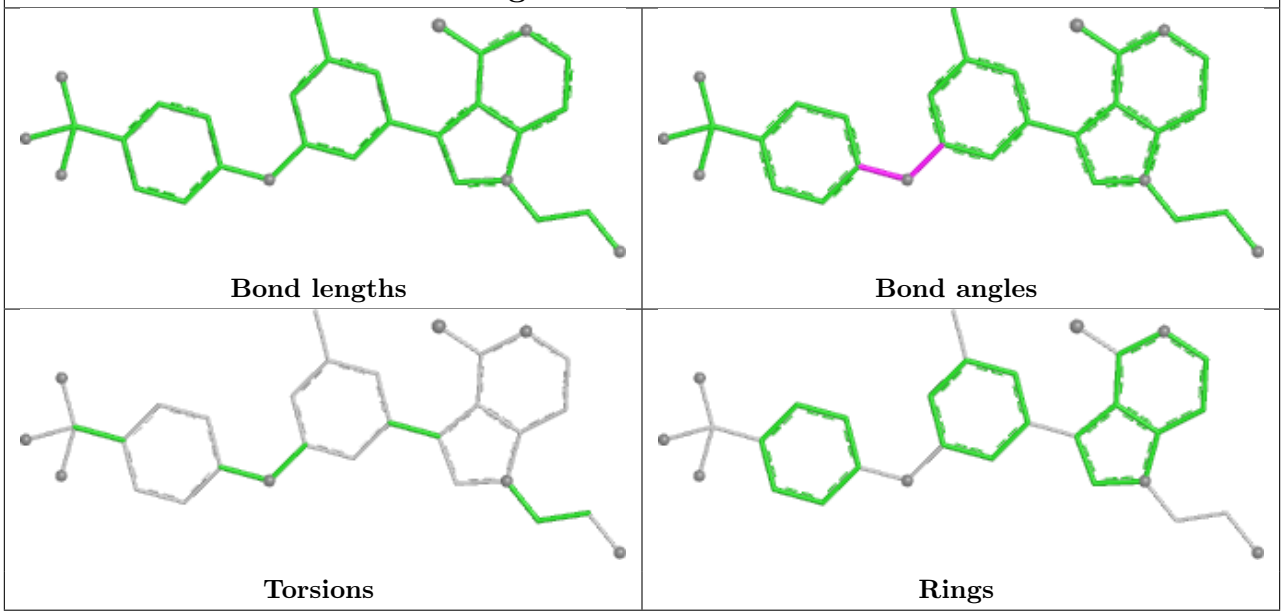
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MYR	1	0
5	C	502	A1JLZ	4	0
5	D	501	A1JLZ	2	0
3	B	502	GOL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1JLZ C 502



Ligand A1JLZ 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	205/220 (93%)	0.44	14 (6%)	23	25	10, 29, 49, 65	11 (5%)
1	B	202/220 (91%)	0.60	19 (9%)	14	14	17, 33, 54, 65	4 (1%)
1	C	203/220 (92%)	0.65	17 (8%)	17	17	11, 37, 58, 70	9 (4%)
1	D	182/220 (82%)	1.26	38 (20%)	2	2	14, 50, 82, 96	6 (3%)
All	All	792/880 (90%)	0.72	88 (11%)	10	10	10, 36, 68, 96	30 (3%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	253	LEU	5.4
1	D	423	LEU	5.0
1	A	414	HIS	4.5
1	D	424	VAL	4.4
1	A	253	LEU	4.3
1	D	298	ILE	4.2
1	D	271	GLY	4.1
1	D	257	VAL	4.0
1	D	259	ILE	4.0
1	D	273	LEU	3.9
1	A	298	ILE	3.9
1	C	228	GLN	3.8
1	C	302	ALA	3.7
1	D	291	TRP	3.7
1	B	247	HIS	3.6
1	D	421	TYR	3.5
1	B	298	ILE	3.5
1	D	277	PHE	3.5
1	D	212	GLY	3.5
1	C	253	LEU	3.5
1	A	413	GLU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	262	ILE	3.3
1	A	232	ASP	3.3
1	D	376	TYR	3.3
1	C	329	PHE	3.3
1	A	426	ASP	3.2
1	B	254	LEU	3.2
1	D	279	LYS	3.1
1	D	263	TYR	3.1
1	D	276	LEU	3.1
1	D	352	ARG	3.0
1	D	359[A]	CYS	3.0
1	B	302	ALA	3.0
1	C	411	ASN	3.0
1	D	303	GLY	2.9
1	D	415	GLY	2.9
1	D	267	PRO	2.8
1	D	425	LYS	2.8
1	D	375	LYS	2.7
1	D	420	ILE	2.7
1	D	422	ARG	2.6
1	A	302	ALA	2.6
1	B	234	TYR	2.5
1	D	304	ALA	2.5
1	B	296	CYS	2.5
1	C	376	TYR	2.5
1	C	414	HIS	2.5
1	B	425	LYS	2.4
1	C	378	MET	2.4
1	D	266	PHE	2.4
1	D	284	ALA	2.4
1	C	268	GLU	2.3
1	B	279	LYS	2.3
1	A	210	SER	2.3
1	D	260	ARG	2.3
1	D	294	LEU	2.3
1	B	271	GLY	2.3
1	B	398	GLU	2.3
1	A	294	LEU	2.3
1	B	369	LEU	2.3
1	A	243	GLY	2.2
1	D	243	GLY	2.2
1	B	371	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	414	HIS	2.2
1	C	269	LYS	2.2
1	A	415	GLY	2.2
1	C	412	SER	2.2
1	B	346[A]	ASN	2.2
1	D	296	CYS	2.2
1	C	330	GLY	2.2
1	A	269	LYS	2.2
1	A	411	ASN	2.1
1	B	211	ILE	2.1
1	D	372	LEU	2.1
1	D	419	HIS	2.1
1	D	219	VAL	2.1
1	C	234	TYR	2.1
1	D	410	SER	2.1
1	B	269	LYS	2.1
1	C	409	VAL	2.1
1	C	298	ILE	2.0
1	B	214	THR	2.0
1	C	419[A]	HIS	2.0
1	C	267	PRO	2.0
1	B	422	ARG	2.0
1	A	425	LYS	2.0
1	D	306	TYR	2.0
1	D	288	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

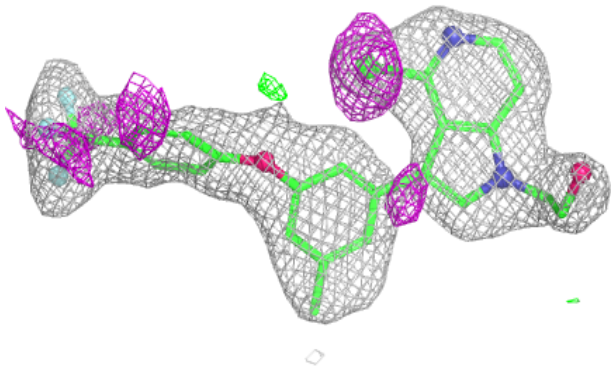
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

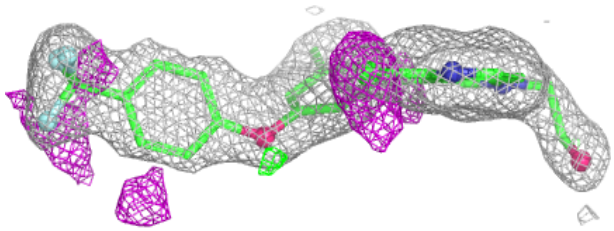
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	A1JLZ	D	501	31/31	0.83	0.12	34,36,44,49	0
2	MYR	B	501	15/16	0.85	0.18	42,43,47,47	0
5	A1JLZ	C	502	31/31	0.86	0.10	29,32,46,52	0
2	MYR	A	501	15/16	0.86	0.15	37,40,44,44	0
4	CL	C	501	1/1	0.90	0.10	59,59,59,59	0
3	GOL	B	502	6/6	0.92	0.09	39,40,41,43	0

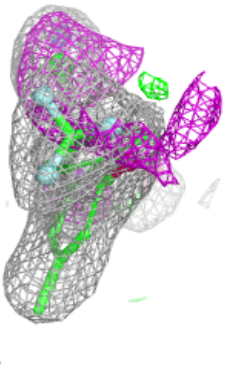
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1JLZ 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)

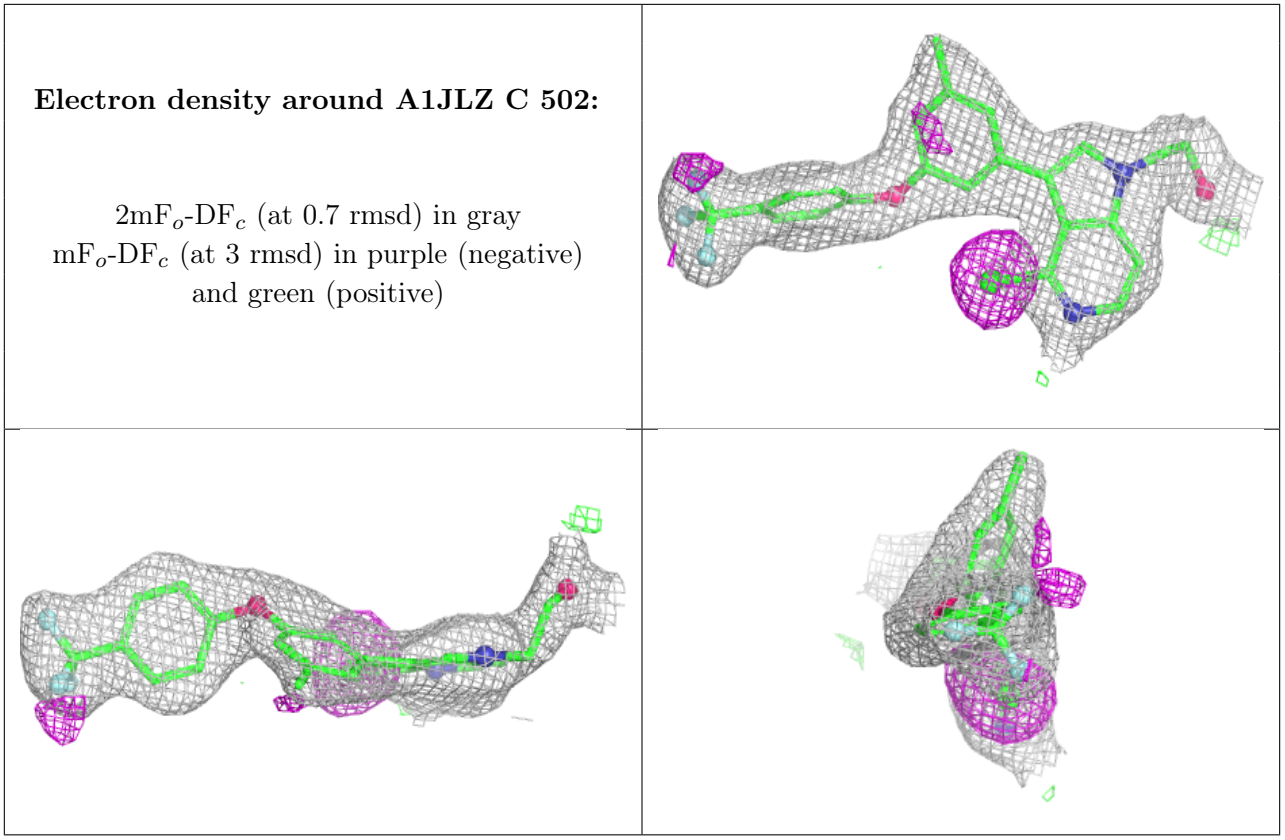






Electron density around A1JLZ C 502:

$2mF_o$-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.