



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:15 PM UTC

PDB ID : 7ZST / pdb_00007zst
Title : Crystal Structure of truncated aspartate transcarbamoylase from Plasmodium falciparum in complex with FLA-01
Authors : Wang, C.; Zhang, B.; Groves, M.R.
Deposited on : 2022-05-08
Resolution : 2.50 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

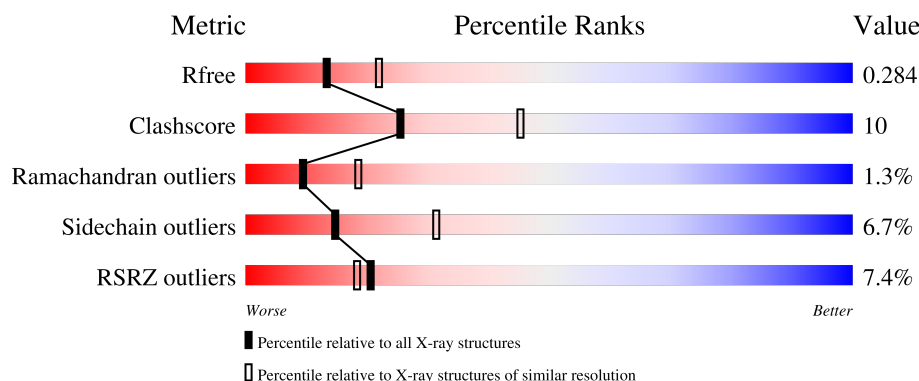
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	349	3% 69% 19% • 9%
1	B	349	2% 70% 21% • 6%
1	C	349	16% 66% 21% • • 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15668 atoms, of which 7833 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 Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	317	Total	C	H	N	O	S	79	0	0
			5125	1629	2571	422	495	8			
1	B	329	Total	C	H	N	O	S	81	0	0
			5315	1690	2662	436	519	8			
1	C	315	Total	C	H	N	O	S	77	0	0
			5110	1626	2568	417	491	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	SER	-	expression tag	UNP A0A5K1K910
A	377	ALA	-	expression tag	UNP A0A5K1K910
A	378	TRP	-	expression tag	UNP A0A5K1K910
A	379	SER	-	expression tag	UNP A0A5K1K910
A	380	HIS	-	expression tag	UNP A0A5K1K910
A	381	PRO	-	expression tag	UNP A0A5K1K910
A	382	GLN	-	expression tag	UNP A0A5K1K910
A	383	PHE	-	expression tag	UNP A0A5K1K910
A	384	GLU	-	expression tag	UNP A0A5K1K910
A	385	LYS	-	expression tag	UNP A0A5K1K910
B	376	SER	-	expression tag	UNP A0A5K1K910
B	377	ALA	-	expression tag	UNP A0A5K1K910
B	378	TRP	-	expression tag	UNP A0A5K1K910
B	379	SER	-	expression tag	UNP A0A5K1K910
B	380	HIS	-	expression tag	UNP A0A5K1K910
B	381	PRO	-	expression tag	UNP A0A5K1K910
B	382	GLN	-	expression tag	UNP A0A5K1K910
B	383	PHE	-	expression tag	UNP A0A5K1K910
B	384	GLU	-	expression tag	UNP A0A5K1K910
B	385	LYS	-	expression tag	UNP A0A5K1K910
C	376	SER	-	expression tag	UNP A0A5K1K910
C	377	ALA	-	expression tag	UNP A0A5K1K910
C	378	TRP	-	expression tag	UNP A0A5K1K910

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Chain	Residue	Modelled	Actual	Comment	Reference
C	379	SER	-	expression tag	UNP A0A5K1K910
C	380	HIS	-	expression tag	UNP A0A5K1K910
C	381	PRO	-	expression tag	UNP A0A5K1K910
C	382	GLN	-	expression tag	UNP A0A5K1K910
C	383	PHE	-	expression tag	UNP A0A5K1K910
C	384	GLU	-	expression tag	UNP A0A5K1K910
C	385	LYS	-	expression tag	UNP A0A5K1K910

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			14	3	8	3		
2	A	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

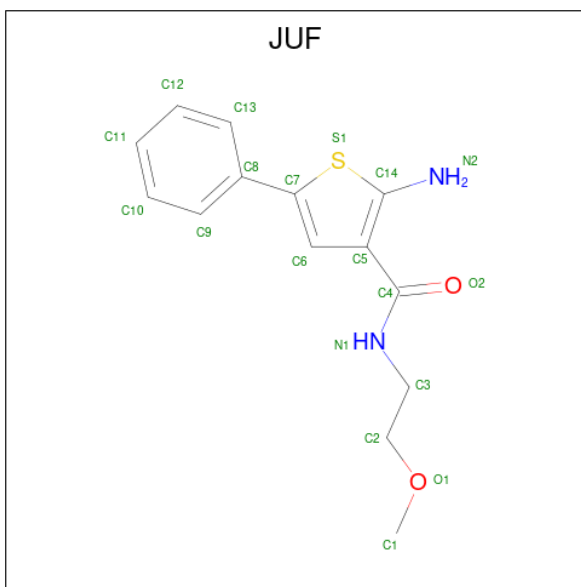


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

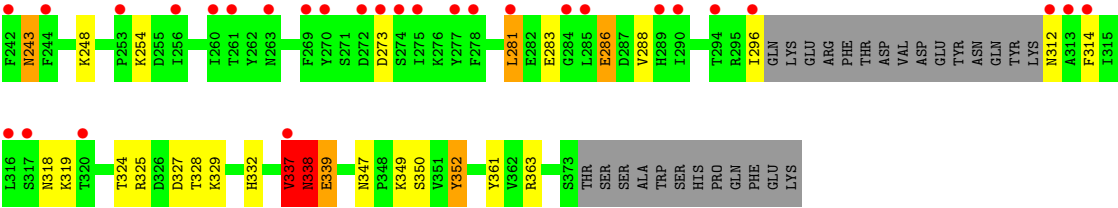
- Molecule 5 is 2-azanyl- {N}-(2-methoxyethyl)-5-phenyl-thiophene-3-carboxamide (CCD ID: JUF) (formula: C₁₄H₁₆N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	S	
			35	14	16	2	2	1	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total	O		
			13	13	0	0
6	B	18	Total	O		
			18	18	0	0
6	C	13	Total	O		
			13	13	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.28Å 89.73Å 137.05Å 90.00° 109.22° 90.00°	Depositor
Resolution (Å)	49.50 – 2.50 49.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.50-2.50) 99.8 (49.50-2.50)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.236 , 0.282 0.238 , 0.284	Depositor DCC
R_{free} test set	2448 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15668	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JUF, GOL, NA, SO4

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	1.09	1/2599 (0.0%)	1.49	2/3510 (0.1%)
1	B	1.12	0/2699	1.53	7/3646 (0.2%)
1	C	1.06	1/2587 (0.0%)	1.48	4/3494 (0.1%)
All	All	1.09	2/7885 (0.0%)	1.50	13/10650 (0.1%)

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	A	0	2
1	B	0	1
1	C	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	GLY	C-O	5.33	1.29	1.24
1	A	188	PRO	C-O	-5.23	1.17	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ASP	CA-CB-CG	6.85	119.45	112.60
1	B	354	THR	CA-CB-OG1	-6.57	99.75	109.60
1	B	312	ASN	CA-C-N	5.71	132.31	122.09
1	B	312	ASN	C-N-CA	5.71	132.31	122.09
1	C	273	ASP	CA-CB-CG	5.71	118.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	THR	CA-CB-OG1	-5.63	101.15	109.60
1	A	68	ASP	CA-CB-CG	5.60	118.20	112.60
1	C	69	GLU	CB-CA-C	-5.47	102.28	110.88
1	A	354	THR	CA-CB-OG1	-5.46	101.42	109.60
1	B	108	THR	CB-CA-C	5.21	119.53	110.68
1	C	337	VAL	CA-C-O	-5.20	115.41	119.46
1	B	247	CYS	CA-C-O	-5.05	115.30	121.36
1	C	126	LEU	CB-CA-C	5.05	117.96	109.48

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ILE	Peptide
1	A	380	HIS	Peptide
1	B	139	GLY	Peptide
1	C	128	ILE	Peptide

5.2 Too-close contacts ⓘ

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	2554	2571	2562	45	2
1	B	2653	2662	2655	54	0
1	C	2542	2568	2561	60	0
2	A	12	16	16	1	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	1	0	0	0	0
5	B	19	16	0	2	0
6	A	13	0	0	1	0
6	B	18	0	0	0	0
6	C	13	0	0	1	0
All	All	7835	7833	7794	150	2

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 10.

All (150) 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:337:VAL:HG23	1:A:338:ASN:H	1.22	1.00
1:A:137:TYR:O	1:A:139:GLY:N	1.96	0.97
1:B:92:LYS:NZ	1:C:96:ASN:OD1	2.11	0.84
1:A:288:VAL:O	1:A:328:THR:HG22	1.79	0.82
1:C:288:VAL:O	1:C:328:THR:HG22	1.79	0.82
1:A:69:GLU:HG2	6:A:512:HOH:O	1.79	0.82
1:B:288:VAL:O	1:B:328:THR:HG22	1.81	0.79
1:A:140:GLU:OE2	1:C:109:ARG:NH1	2.18	0.77
1:A:137:TYR:C	1:A:139:GLY:H	1.94	0.73
1:A:337:VAL:HG23	1:A:338:ASN:N	2.03	0.72
1:A:337:VAL:CG2	1:A:338:ASN:H	2.03	0.71
1:A:185:GLY:HA3	1:A:226:ARG:HD2	1.74	0.70
1:C:332:HIS:NE2	1:C:339:GLU:OE2	2.18	0.68
1:B:49:ASP:OD1	1:B:49:ASP:N	2.22	0.68
1:B:110:THR:OG1	5:B:401:JUF:N2	2.29	0.66
1:B:163:LYS:HB3	1:B:184:THR:HG23	1.79	0.65
1:B:297:GLN:O	1:B:299:GLU:O	2.16	0.64
1:C:296:ILE:HG21	1:C:312:ASN:HB3	1.79	0.64
1:C:286:GLU:O	1:C:288:VAL:N	2.28	0.63
1:C:296:ILE:HD12	1:C:312:ASN:HD22	1.63	0.62
1:C:126:LEU:HD13	1:C:126:LEU:H	1.65	0.62
1:A:350:SER:HB2	1:A:352:TYR:CE1	2.36	0.61
1:C:325:ARG:HB2	1:C:328:THR:HG23	1.82	0.61
1:C:324:THR:OG1	1:C:349:LYS:NZ	2.34	0.60
1:B:325:ARG:HB2	1:B:328:THR:HG23	1.84	0.60
1:A:124:LYS:HD3	1:C:119:LEU:HD22	1.84	0.60
1:B:299:GLU:O	1:B:300:ARG:HB2	2.01	0.59
1:B:193:LEU:C	1:B:193:LEU:HD12	2.28	0.59
1:B:337:VAL:O	1:B:338:ASN:HB2	2.03	0.58
1:A:109:ARG:HE	1:B:148:ILE:HG21	1.69	0.57
1:A:325:ARG:HB2	1:A:328:THR:HG23	1.86	0.57
1:B:334:LEU:HD13	1:C:148:ILE:HD11	1.87	0.57
1:C:185:GLY:HA3	1:C:226:ARG:HB3	1.87	0.57
1:A:193:LEU:HD12	1:A:193:LEU:C	2.30	0.57
1:C:204:PHE:HA	1:C:207:ASP:OD2	2.06	0.56
1:B:149:LEU:HD23	1:B:156:ILE:HD13	1.87	0.56
1:C:163:LYS:HB3	1:C:184:THR:HG23	1.87	0.56
1:C:209:ASN:HB3	1:C:212:LYS:HG3	1.87	0.56
1:B:373:SER:O	1:B:375:SER:N	2.39	0.55
1:C:233:LYS:NZ	6:C:401:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB2	1:B:352:TYR:CE2	2.41	0.55
1:C:193:LEU:C	1:C:193:LEU:HD12	2.31	0.55
1:B:324:THR:OG1	1:B:349:LYS:NZ	2.35	0.55
1:C:327:ASP:O	1:C:329:LYS:NZ	2.36	0.55
1:C:163:LYS:CB	1:C:184:THR:HG23	2.37	0.54
1:B:282:GLU:H	1:B:282:GLU:CD	2.16	0.54
1:C:149:LEU:HD23	1:C:156:ILE:HD13	1.89	0.54
1:B:302:THR:HB	1:B:303:ASP:OD1	2.08	0.54
1:B:337:VAL:O	1:B:337:VAL:HG12	2.08	0.54
1:C:337:VAL:O	1:C:338:ASN:HB2	2.08	0.53
1:B:109:ARG:HH12	1:C:140:GLU:CD	2.16	0.53
1:C:163:LYS:HG2	1:C:164:LYS:N	2.24	0.53
1:C:209:ASN:HB3	1:C:212:LYS:CG	2.39	0.53
1:C:281:LEU:HD13	1:C:314:PHE:CD1	2.44	0.52
1:C:58:LYS:NZ	1:C:65:ASP:O	2.30	0.52
1:C:352:TYR:N	1:C:352:TYR:CD2	2.76	0.51
1:B:312:ASN:OD1	1:B:312:ASN:N	2.42	0.51
1:C:163:LYS:HG2	1:C:164:LYS:H	1.74	0.51
1:B:163:LYS:CB	1:B:184:THR:HG23	2.40	0.51
1:B:163:LYS:HG2	1:B:164:LYS:H	1.76	0.51
1:B:308:ASN:N	1:B:308:ASN:OD1	2.44	0.51
1:B:62:ASN:HB2	1:B:186:GLU:OE1	2.11	0.50
1:B:109:ARG:NE	1:C:148:ILE:HG21	2.25	0.50
1:A:62:ASN:HD22	1:A:186:GLU:HG2	1.76	0.50
1:C:51:ILE:HD12	1:C:51:ILE:N	2.26	0.50
1:A:324:THR:HB	1:A:328:THR:HG21	1.92	0.50
1:C:243:ASN:N	1:C:243:ASN:HD22	2.10	0.49
1:A:133:SER:O	1:A:136:PHE:O	2.30	0.49
1:B:324:THR:HG1	1:B:349:LYS:NZ	2.10	0.49
1:B:221:ASP:OD1	1:B:221:ASP:C	2.55	0.49
1:A:221:ASP:OD1	1:A:221:ASP:C	2.56	0.48
1:B:126:LEU:HD12	1:B:126:LEU:H	1.78	0.48
1:B:179:ASN:ND2	1:B:181:GLY:H	2.10	0.48
1:C:51:ILE:N	1:C:51:ILE:CD1	2.76	0.48
1:B:109:ARG:HB3	5:B:401:JUF:C4	2.43	0.48
1:C:221:ASP:OD1	1:C:221:ASP:C	2.57	0.48
1:A:334:LEU:HD13	1:B:148:ILE:HD11	1.96	0.47
1:C:114:PHE:CE2	1:C:363:ARG:HD3	2.49	0.47
1:C:208:ARG:NH1	1:C:237:ARG:O	2.46	0.47
1:B:282:GLU:CD	1:B:282:GLU:N	2.73	0.47
1:C:62:ASN:HB2	1:C:186:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:SER:O	2:A:401:GOL:H11	2.14	0.47
1:A:137:TYR:C	1:A:139:GLY:N	2.61	0.47
1:B:324:THR:HB	1:B:328:THR:HG21	1.96	0.46
1:C:350:SER:HB2	1:C:352:TYR:CE2	2.51	0.46
1:A:97:LYS:HB2	1:A:123:SER:OG	2.16	0.46
1:B:97:LYS:HB2	1:B:123:SER:OG	2.16	0.46
1:A:71:LEU:HD23	1:A:238:TYR:OH	2.16	0.45
1:C:324:THR:HB	1:C:328:THR:HG21	1.98	0.45
1:C:100:CYS:SG	1:C:126:LEU:CD2	3.04	0.45
1:B:109:ARG:HE	1:C:148:ILE:HG21	1.82	0.45
1:A:62:ASN:ND2	1:A:186:GLU:HG2	2.32	0.45
1:C:48:LEU:H	1:C:51:ILE:HD13	1.81	0.45
1:C:161:PRO:O	1:C:183:GLY:HA3	2.17	0.45
1:C:283:GLU:O	1:C:286:GLU:HG3	2.17	0.45
1:A:62:ASN:HB2	1:A:186:GLU:OE1	2.17	0.45
1:B:214:LEU:O	1:B:240:VAL:HA	2.17	0.44
1:C:45:LYS:O	1:C:46:ILE:HD13	2.18	0.44
1:C:312:ASN:N	1:C:312:ASN:OD1	2.49	0.44
1:A:100:CYS:O	1:A:156:ILE:HA	2.17	0.44
1:A:163:LYS:HG2	1:A:164:LYS:HD2	1.98	0.44
1:B:163:LYS:HG2	1:B:164:LYS:N	2.31	0.44
1:A:94:LEU:HB3	1:A:121:LEU:HB3	1.99	0.44
1:A:160:ASP:O	1:A:182:ASN:HA	2.17	0.44
1:B:161:PRO:O	1:B:183:GLY:N	2.50	0.44
1:A:195:PHE:CZ	1:A:205:ILE:HD12	2.53	0.44
1:C:183:GLY:O	1:C:226:ARG:NH1	2.51	0.44
1:A:111:ARG:HG2	1:A:111:ARG:HH21	1.83	0.43
1:B:133:SER:O	1:B:136:PHE:O	2.36	0.43
1:C:281:LEU:HA	1:C:281:LEU:HD12	1.84	0.43
1:C:100:CYS:SG	1:C:126:LEU:HD22	2.58	0.43
1:C:161:PRO:O	1:C:183:GLY:CA	2.67	0.43
1:A:255:ASP:N	1:A:255:ASP:OD1	2.52	0.42
1:C:161:PRO:O	1:C:183:GLY:N	2.52	0.42
1:C:318:ASN:OD1	1:C:347:ASN:ND2	2.47	0.42
1:B:61:ILE:HG13	1:B:170:VAL:HG21	2.01	0.42
1:C:179:ASN:ND2	1:C:181:GLY:H	2.17	0.42
1:C:217:ALA:HB2	1:C:288:VAL:HG11	2.02	0.42
1:A:118:ILE:HD11	1:A:157:ILE:HD13	2.02	0.42
1:A:161:PRO:O	1:A:183:GLY:N	2.52	0.42
1:B:94:LEU:HB3	1:B:121:LEU:HB3	2.02	0.42
1:C:160:ASP:O	1:C:182:ASN:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:O	1:A:138:LYS:HG2	2.19	0.42
1:B:124:LYS:HG2	3:B:402:SO4:O4	2.19	0.42
1:B:168:ILE:O	1:B:171:SER:OG	2.22	0.42
1:B:161:PRO:O	1:B:183:GLY:HA3	2.20	0.42
1:A:214:LEU:O	1:A:240:VAL:HA	2.20	0.42
1:A:161:PRO:O	1:A:183:GLY:HA3	2.19	0.41
1:A:161:PRO:O	1:A:183:GLY:CA	2.69	0.41
1:A:315:ILE:HG21	1:A:341:LYS:HE3	2.03	0.41
1:B:114:PHE:CE2	1:B:363:ARG:HD3	2.55	0.41
1:A:143:GLU:HA	1:A:172:SER:OG	2.20	0.41
1:A:47:ASP:O	1:A:51:ILE:HG13	2.21	0.41
1:C:71:LEU:HD23	1:C:238:TYR:OH	2.20	0.41
1:A:185:GLY:HA3	1:A:226:ARG:CD	2.49	0.41
1:A:215:ASN:H	1:A:289:HIS:CD2	2.38	0.41
1:B:299:GLU:O	1:B:300:ARG:CB	2.68	0.41
1:C:97:LYS:HB2	1:C:123:SER:OG	2.21	0.41
1:B:100:CYS:O	1:B:156:ILE:HA	2.20	0.41
1:A:281:LEU:HD11	1:A:314:PHE:HA	2.02	0.40
1:B:118:ILE:HD11	1:B:157:ILE:HD13	2.02	0.40
1:A:217:ALA:HB2	1:A:288:VAL:HG11	2.03	0.40
1:B:195:PHE:CZ	1:B:205:ILE:HD12	2.57	0.40
1:B:71:LEU:HD23	1:B:238:TYR:OH	2.21	0.40
1:B:133:SER:O	1:B:137:TYR:HD2	2.03	0.40
1:C:50:LYS:O	1:C:53:THR:HG22	2.21	0.40
1:B:161:PRO:O	1:B:183:GLY:CA	2.70	0.40
1:B:215:ASN:H	1:B:289:HIS:CD2	2.39	0.40
1:C:82:GLU:HG3	1:C:361:TYR:CE2	2.57	0.40
1:C:118:ILE:HD11	1:C:157:ILE:HD13	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:OD2	1:A:379:SER:HG[2_555]	1.19	0.41
1:A:49:ASP:OD2	1:A:379:SER:OG[2_555]	2.17	0.03

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	311/349 (89%)	292 (94%)	16 (5%)	3 (1%)	12	24
1	B	325/349 (93%)	299 (92%)	22 (7%)	4 (1%)	10	20
1	C	311/349 (89%)	286 (92%)	20 (6%)	5 (2%)	7	14
All	All	947/1047 (90%)	877 (93%)	58 (6%)	12 (1%)	9	18

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	LYS
1	A	286	GLU
1	B	374	THR
1	C	248	LYS
1	C	286	GLU
1	C	338	ASN
1	B	286	GLU
1	C	208	ARG
1	B	338	ASN
1	B	302	THR
1	A	337	VAL
1	C	225	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/328 (90%)	279 (94%)	18 (6%)	17	35
1	B	308/328 (94%)	285 (92%)	23 (8%)	12	26
1	C	295/328 (90%)	276 (94%)	19 (6%)	16	33
All	All	900/984 (92%)	840 (93%)	60 (7%)	15	31

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLU
1	A	111	ARG
1	A	113	SER
1	A	126	LEU
1	A	129	THR
1	A	138	LYS
1	A	143	GLU
1	A	147	LYS
1	A	163	LYS
1	A	172	SER
1	A	184	THR
1	A	214	LEU
1	A	248	LYS
1	A	249	SER
1	A	254	LYS
1	A	272	ASP
1	A	319	LYS
1	A	352	TYR
1	B	48	LEU
1	B	49	ASP
1	B	126	LEU
1	B	129	THR
1	B	131	MET
1	B	143	GLU
1	B	163	LYS
1	B	189	THR
1	B	214	LEU
1	B	233	LYS
1	B	248	LYS
1	B	249	SER
1	B	272	ASP

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Mol	Chain	Res	Type
1	B	281	LEU
1	B	299	GLU
1	B	300	ARG
1	B	302	THR
1	B	303	ASP
1	B	306	GLU
1	B	308	ASN
1	B	319	LYS
1	B	339	GLU
1	B	373	SER
1	C	48	LEU
1	C	51	ILE
1	C	52	MET
1	C	53	THR
1	C	126	LEU
1	C	129	THR
1	C	138	LYS
1	C	143	GLU
1	C	163	LYS
1	C	199	HIS
1	C	208	ARG
1	C	243	ASN
1	C	254	LYS
1	C	281	LEU
1	C	319	LYS
1	C	337	VAL
1	C	338	ASN
1	C	339	GLU
1	C	352	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	165	ASN
1	A	179	ASN
1	A	190	GLN
1	A	224	ASN
1	A	243	ASN
1	A	251	ASN
1	A	268	ASN
1	A	280	ASN

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Mol	Chain	Res	Type
1	A	289	HIS
1	A	338	ASN
1	B	62	ASN
1	B	87	ASN
1	B	165	ASN
1	B	179	ASN
1	B	243	ASN
1	B	268	ASN
1	B	280	ASN
1	B	289	HIS
1	B	323	ASN
1	B	358	ASN
1	C	62	ASN
1	C	165	ASN
1	C	179	ASN
1	C	199	HIS
1	C	243	ASN
1	C	268	ASN
1	C	289	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	GOL	A	401	-	5,5,5	0.18	0	5,5,5	0.24	0
5	JUF	B	401	-	20,20,20	0.54	0	26,26,26	1.55	6 (23%)
2	GOL	A	402	-	5,5,5	0.19	0	5,5,5	0.40	0
3	SO4	B	402	-	4,4,4	0.52	0	6,6,6	0.23	0
3	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.10	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	GOL	A	401	-	-	4/4/4/4	-
2	GOL	A	402	-	-	3/4/4/4	-
5	JUF	B	401	-	-	6/13/13/13	0/2/2/2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	JUF	C5-C6-C7	-4.18	105.92	113.50
5	B	401	JUF	C7-S1-C14	-3.08	86.98	90.98
5	B	401	JUF	C6-C5-C4	2.51	131.98	125.97
5	B	401	JUF	C6-C5-C14	-2.49	101.92	109.11
5	B	401	JUF	C6-C7-S1	-2.32	106.94	110.35
5	B	401	JUF	C8-C7-S1	2.06	126.27	121.02

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	C1-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3
5	B	401	JUF	C5-C4-N1-C3
5	B	401	JUF	O2-C4-N1-C3
5	B	401	JUF	S1-C7-C8-C9
5	B	401	JUF	S1-C7-C8-C13

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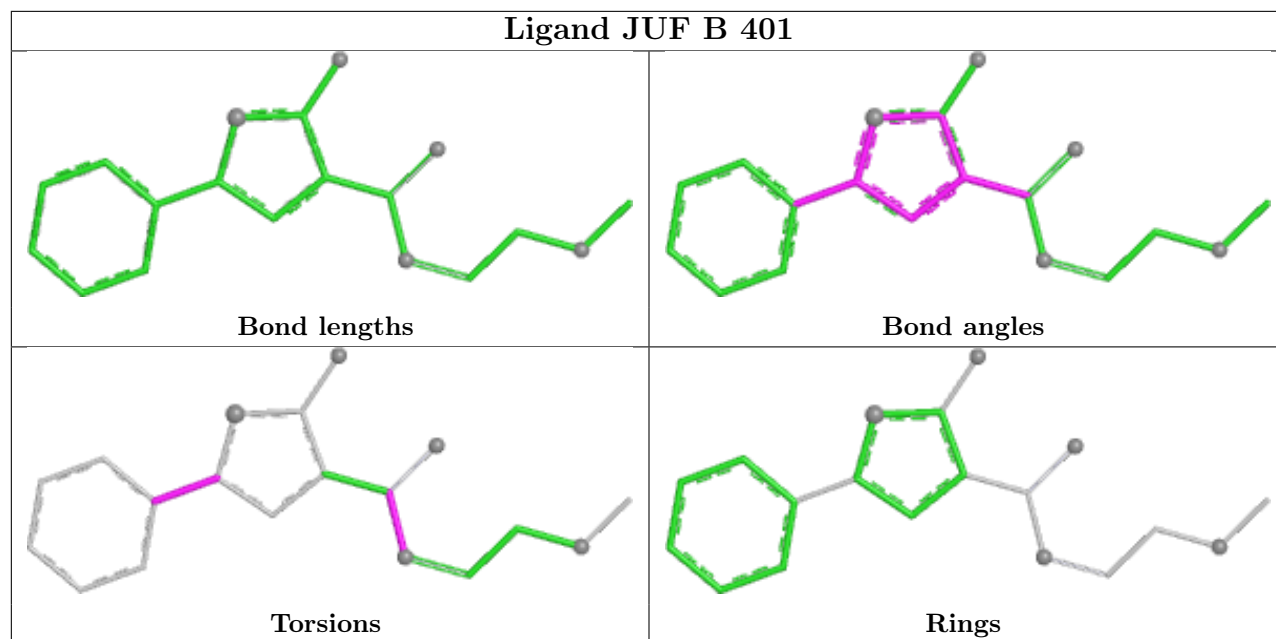
Mol	Chain	Res	Type	Atoms
5	B	401	JUF	C6-C7-C8-C9
5	B	401	JUF	C6-C7-C8-C13
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	C1-C2-C3-O3
2	A	401	GOL	O1-C1-C2-O2
2	A	401	GOL	O2-C2-C3-O3
2	A	402	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	GOL	1	0
5	B	401	JUF	2	0
3	B	402	SO4	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.



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	317/349 (90%)	0.47	9 (2%) 55 50	32, 57, 89, 100	0
1	B	329/349 (94%)	0.25	6 (1%) 67 64	31, 50, 77, 95	0
1	C	315/349 (90%)	1.08	56 (17%) 4 3	35, 72, 105, 127	0
All	All	961/1047 (91%)	0.60	71 (7%) 20 18	31, 58, 95, 127	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	284	GLY	5.2
1	B	46	ILE	4.0
1	C	44	TYR	4.0
1	C	277	TYR	4.0
1	B	377	ALA	3.9
1	C	46	ILE	3.8
1	C	281	LEU	3.7
1	C	45	LYS	3.6
1	C	214	LEU	3.6
1	C	48	LEU	3.6
1	C	296	ILE	3.5
1	C	72	LEU	3.4
1	B	308	ASN	3.3
1	A	183	GLY	3.2
1	C	238	TYR	3.2
1	B	375	SER	3.1
1	C	216	ILE	3.1
1	C	256	ILE	3.1
1	C	231	LEU	3.1
1	C	317	SER	3.0
1	A	297	GLN	2.9
1	A	184	THR	2.9
1	C	227	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	206	LEU	2.8
1	C	275	ILE	2.8
1	C	130	ASP	2.8
1	C	273	ASP	2.8
1	C	274	SER	2.8
1	C	337	VAL	2.8
1	C	285	LEU	2.8
1	C	220	GLY	2.7
1	A	296	ILE	2.7
1	C	294	THR	2.7
1	C	240	VAL	2.6
1	C	270	TYR	2.6
1	C	260	ILE	2.5
1	C	320	THR	2.5
1	B	374	THR	2.4
1	C	316	LEU	2.4
1	C	314	PHE	2.4
1	A	130	ASP	2.4
1	C	215	ASN	2.4
1	C	217	ALA	2.4
1	C	47	ASP	2.4
1	C	244	PHE	2.4
1	C	263	ASN	2.3
1	A	131	MET	2.3
1	C	204	PHE	2.3
1	C	239	ASN	2.2
1	C	261	THR	2.2
1	C	269	PHE	2.2
1	C	253	PRO	2.2
1	C	201	TYR	2.2
1	C	290	ILE	2.2
1	B	312	ASN	2.1
1	C	313	ALA	2.1
1	C	222	LEU	2.1
1	A	133	SER	2.1
1	C	242	PHE	2.1
1	C	163	LYS	2.1
1	C	312	ASN	2.1
1	C	210	ILE	2.1
1	C	278	PHE	2.1
1	C	68	ASP	2.1
1	C	272	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	219	VAL	2.0
1	C	131	MET	2.0
1	C	289	HIS	2.0
1	C	208	ARG	2.0
1	A	48	LEU	2.0
1	A	148	ILE	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](#)

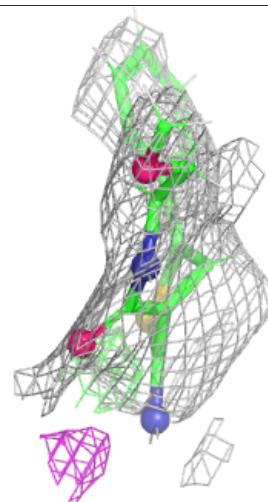
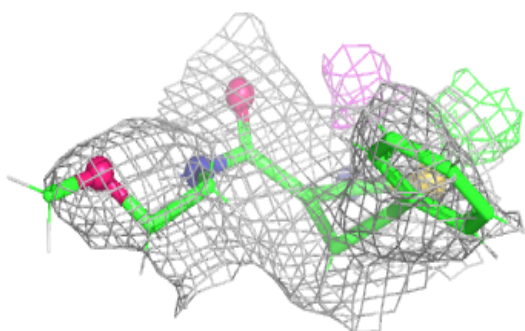
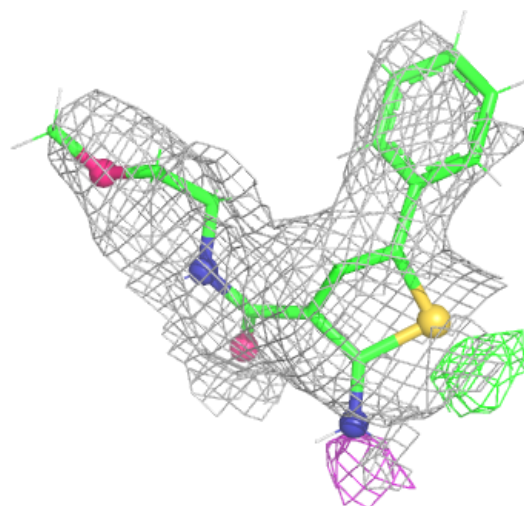
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	JUF	B	401	19/19	0.78	0.21	85,90,94,95	0
2	GOL	A	402	6/6	0.82	0.21	30,82,83,84	2
4	NA	A	404	1/1	0.87	0.07	36,36,36,36	0
2	GOL	A	401	6/6	0.87	0.15	30,74,75,77	2
3	SO4	A	403	5/5	0.88	0.16	67,76,81,82	0
3	SO4	B	402	5/5	0.94	0.13	51,53,54,57	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 JUF B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.