



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 6TZF / pdb_00006tzf
Title : ADC-7 in complex with boronic acid transition state inhibitor S17079
Authors : Fish, E.R.; Powers, R.A.; Wallar, B.J.
Deposited on : 2019-08-12
Resolution : 1.96 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

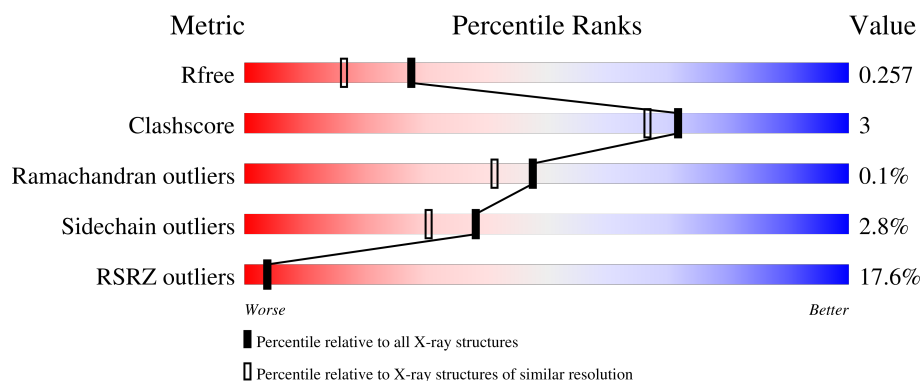
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	361	% 92% 6% ..
1	B	361	32% 90% 6% ..
1	C	361	19% 88% 9% ..
1	D	361	17% 89% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11439 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.

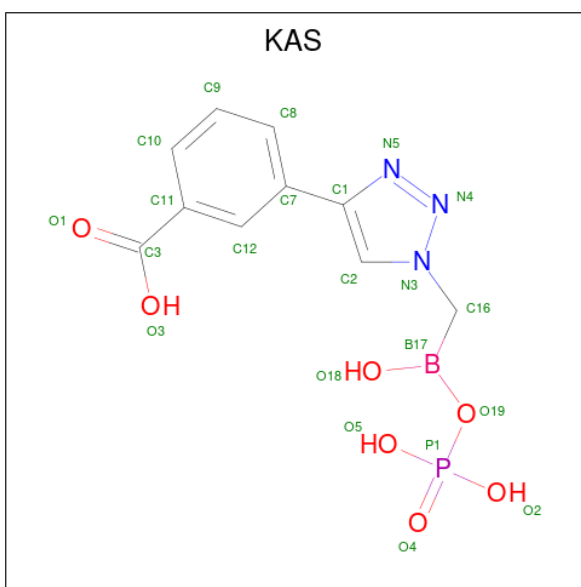
- Molecule 1 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2819	1811	467	532	9			
1	B	356	Total	C	N	O	S	0	0	0
			2690	1733	443	505	9			
1	C	354	Total	C	N	O	S	0	1	0
			2748	1764	452	523	9			
1	D	356	Total	C	N	O	S	0	0	0
			2755	1768	458	520	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP Q6DRA1
B	-1	MET	-	expression tag	UNP Q6DRA1
C	-1	MET	-	expression tag	UNP Q6DRA1
D	-1	MET	-	expression tag	UNP Q6DRA1

- Molecule 2 is 3-(1-{[hydroxy(phosphonooxy)boranyl]methyl}-1H-1,2,3-triazol-4-yl)benzoic acid (CCD ID: KAS) (formula: C₁₀H₁₁BN₃O₇P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 22	B 1	C 10	N 3	O 7	P 1	0	0
2	B	1	Total 22	B 1	C 10	N 3	O 7	P 1	0	0
2	C	1	Total 22	B 1	C 10	N 3	O 7	P 1	0	0
2	D	1	Total 22	B 1	C 10	N 3	O 7	P 1	0	0

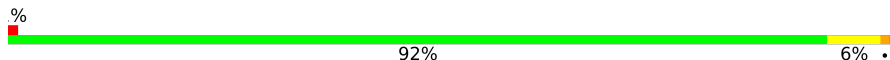
- Molecule 3 is water.

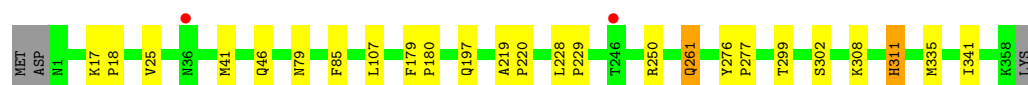
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	3
			164	164		
3	B	28	Total	O	0	1
			29	29		
3	C	78	Total	O	0	2
			81	81		
3	D	64	Total	O	0	1
			65	65		

3 Residue-property plots

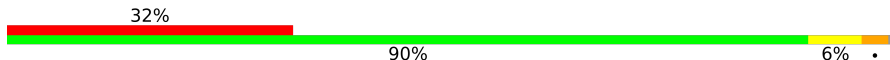
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

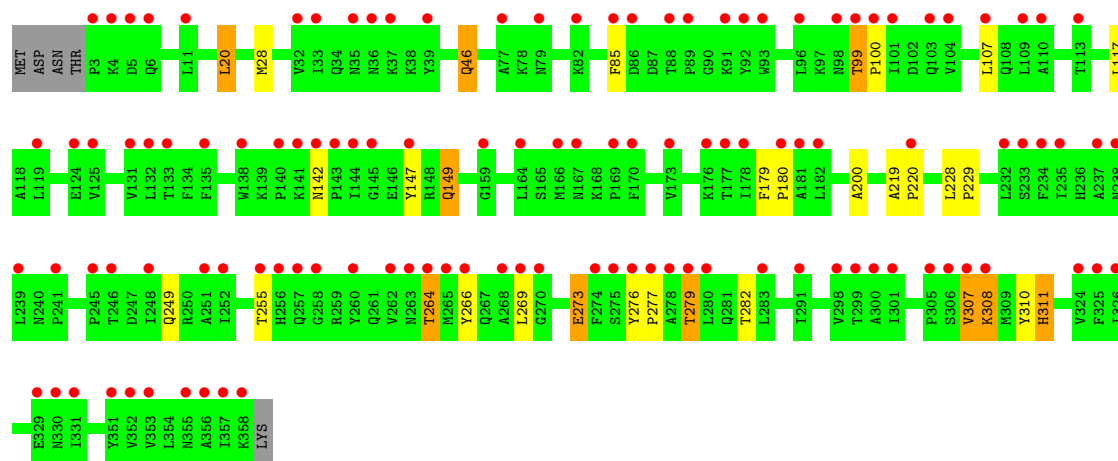
• Molecule 1: Beta-lactamase

Chain A: 



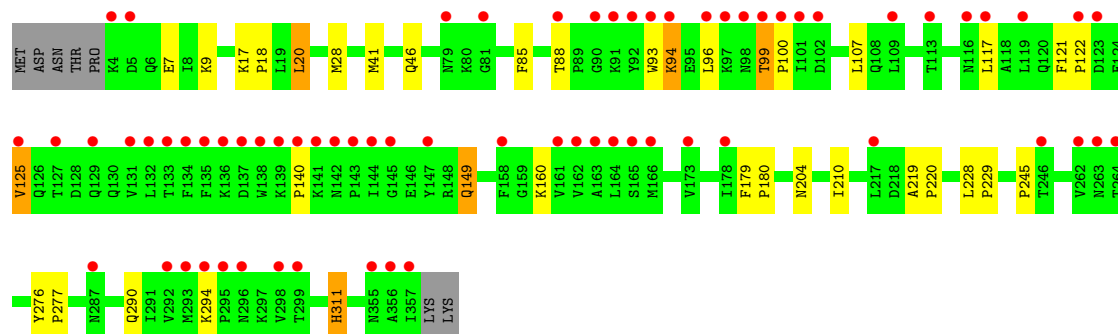
• Molecule 1: Beta-lactamase

Chain B: 

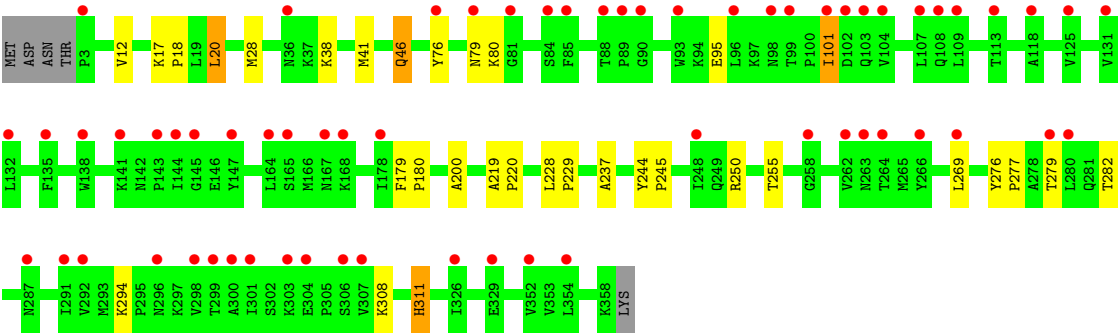
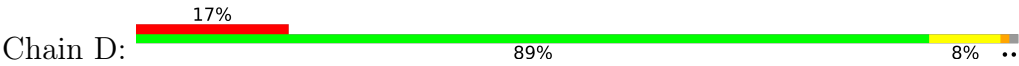


• Molecule 1: Beta-lactamase

Chain C: 



● Molecule 1: Beta-lactamase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.62Å 80.78Å 107.00Å 90.00° 112.47° 90.00°	Depositor
Resolution (Å)	98.88 – 1.96 98.88 – 1.96	Depositor EDS
% Data completeness (in resolution range)	94.5 (98.88-1.96) 94.5 (98.88-1.96)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.219 , 0.251 0.227 , 0.257	Depositor DCC
R_{free} test set	4890 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11439	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 40.29 % 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 2.7952e-04. 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: KAS

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	1.00	1/2887 (0.0%)	1.28	2/3924 (0.1%)
1	B	1.01	0/2758	1.31	0/3772
1	C	1.00	0/2815	1.30	3/3839 (0.1%)
1	D	1.00	0/2823	1.30	0/3845
All	All	1.00	1/11283 (0.0%)	1.30	5/15380 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	VAL	N-CA	5.13	1.50	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	GLU	CA-C-O	-6.27	112.75	119.97
1	C	96	LEU	CA-C-O	-5.43	114.51	120.43
1	A	261	GLN	CB-CA-C	5.19	119.56	109.33
1	C	88	THR	CB-CA-C	5.09	116.70	108.91
1	A	302	SER	N-CA-C	-5.05	107.80	114.31

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	2819	0	2793	10	0
1	B	2690	0	2546	22	0
1	C	2748	0	2650	20	0
1	D	2755	0	2666	22	0
2	A	22	0	0	1	0
2	B	22	0	0	0	0
2	C	22	0	0	0	0
2	D	22	0	0	0	0
3	A	164	0	0	3	0
3	B	29	0	0	0	0
3	C	81	0	0	0	0
3	D	65	0	0	1	0
All	All	11439	0	10655	72	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 3.

All (72) 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:266:TYR:HB2	1:B:273:GLU:HG2	1.50	0.94
1:D:79:ASN:HD21	1:D:250:ARG:NE	1.69	0.89
1:B:20:LEU:HD11	1:B:28:MET:HE2	1.71	0.72
1:D:101:ILE:HD13	1:D:101:ILE:O	1.89	0.72
1:D:20:LEU:HD11	1:D:28:MET:HE2	1.73	0.70
1:C:20:LEU:HD11	1:C:28:MET:HE2	1.74	0.70
2:A:401:KAS:O4	3:A:501[A]:HOH:O	2.10	0.68
1:C:204:ASN:HB3	1:C:210:ILE:HD13	1.80	0.64
1:B:266:TYR:HB2	1:B:273:GLU:CG	2.27	0.62
1:B:264:THR:OG1	1:B:282:THR:HG23	2.00	0.62
1:B:266:TYR:CB	1:B:273:GLU:HG2	2.27	0.61
1:D:255:THR:HA	1:D:269:LEU:HB2	1.82	0.60
1:B:255:THR:HA	1:B:269:LEU:HB2	1.82	0.60
1:B:276:TYR:HB3	1:B:307:VAL:HG22	1.86	0.58
1:D:79:ASN:HD21	1:D:250:ARG:HE	1.50	0.58
1:C:121:PHE:HB3	1:C:125:VAL:HG13	1.85	0.57
1:B:147:TYR:OH	1:D:245:PRO:HA	2.05	0.57
1:A:335:MET:HE1	1:A:341:ILE:HD11	1.85	0.57
1:D:79:ASN:HD21	1:D:250:ARG:CZ	2.19	0.54
1:C:122:PRO:O	1:C:125:VAL:HG13	2.07	0.54
1:A:79:ASN:HB3	1:A:250:ARG:CZ	2.39	0.53
1:C:121:PHE:HB3	1:C:125:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ASN:HB3	1:C:210:ILE:CD1	2.39	0.52
1:B:276:TYR:HB3	1:B:307:VAL:CG2	2.40	0.51
1:C:85:PHE:HB3	1:C:107:LEU:HB2	1.90	0.51
1:A:85:PHE:HB3	1:A:107:LEU:HB2	1.92	0.51
1:D:79:ASN:ND2	1:D:250:ARG:NE	2.50	0.50
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.92	0.50
1:D:76:TYR:CE1	1:D:80:LYS:HD2	2.47	0.50
1:B:99:THR:HG22	1:B:100:PRO:HD2	1.93	0.49
1:B:46:GLN:HG3	1:B:200:ALA:HA	1.95	0.49
1:D:46:GLN:HG3	1:D:200:ALA:HA	1.95	0.48
3:A:588:HOH:O	1:C:245:PRO:HD3	2.13	0.47
1:B:117:LEU:O	1:B:149:GLN:HG2	2.16	0.46
1:D:228:LEU:HB3	1:D:229:PRO:HD3	1.98	0.45
1:D:279:THR:HG23	1:D:282:THR:H	1.81	0.45
1:B:228:LEU:HB3	1:B:229:PRO:HD3	1.98	0.45
1:B:279:THR:HG23	1:B:282:THR:OG1	2.17	0.44
1:C:179:PHE:HB2	1:C:180:PRO:HD3	1.99	0.44
1:C:290:GLN:HA	1:C:294:LYS:HG3	1.98	0.44
1:A:179:PHE:HB2	1:A:180:PRO:HD3	2.00	0.44
1:B:179:PHE:HB2	1:B:180:PRO:HD3	1.99	0.44
1:D:38:LYS:NZ	3:D:505:HOH:O	2.48	0.44
1:A:276:TYR:CD1	1:A:277:PRO:HA	2.53	0.43
1:C:122:PRO:O	1:C:125:VAL:CG1	2.66	0.43
1:C:99:THR:HG22	1:C:100:PRO:HD2	2.00	0.43
1:B:219:ALA:HB3	1:B:220:PRO:HD3	2.01	0.43
1:C:93:TRP:O	1:C:94:LYS:HB2	2.18	0.43
1:D:276:TYR:CD1	1:D:277:PRO:HA	2.53	0.43
1:A:219:ALA:HB3	1:A:220:PRO:HD3	2.01	0.43
1:D:179:PHE:HB2	1:D:180:PRO:HD3	1.99	0.43
1:B:276:TYR:CD1	1:B:277:PRO:HA	2.53	0.42
1:D:12:VAL:HG21	1:D:41:MET:HE3	2.02	0.42
1:C:117:LEU:O	1:C:149:GLN:HG2	2.19	0.42
1:D:237:ALA:HA	1:D:244:TYR:CE1	2.55	0.42
1:D:311:HIS:CD2	1:D:311:HIS:C	2.98	0.42
1:B:308:LYS:HE2	1:B:310:TYR:OH	2.20	0.41
1:C:100:PRO:HB3	1:C:140:PRO:HD3	2.01	0.41
1:C:228:LEU:HB3	1:C:229:PRO:HD3	2.02	0.41
1:B:142:ASN:OD1	1:D:245:PRO:CG	2.68	0.41
1:B:311:HIS:CD2	1:B:311:HIS:C	2.99	0.41
1:A:228:LEU:HB3	1:A:229:PRO:HD3	2.02	0.41
1:C:276:TYR:CD1	1:C:277:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TYR:CZ	1:D:245:PRO:HA	2.55	0.41
1:A:17:LYS:N	1:A:18:PRO:CD	2.84	0.41
1:A:311:HIS:CD2	1:A:311:HIS:C	2.99	0.41
1:C:219:ALA:HB3	1:C:220:PRO:HD3	2.02	0.41
1:C:311:HIS:CD2	1:C:311:HIS:C	2.98	0.41
1:D:219:ALA:HB3	1:D:220:PRO:HD3	2.03	0.41
1:D:17:LYS:N	1:D:18:PRO:CD	2.84	0.41
1:A:299:THR:HG22	3:A:574:HOH:O	2.21	0.40
1:C:17:LYS:N	1:C:18:PRO:CD	2.84	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	356/361 (99%)	349 (98%)	7 (2%)	0	100	100
1	B	354/361 (98%)	347 (98%)	7 (2%)	0	100	100
1	C	353/361 (98%)	342 (97%)	10 (3%)	1 (0%)	36	28
1	D	354/361 (98%)	346 (98%)	8 (2%)	0	100	100
All	All	1417/1444 (98%)	1384 (98%)	32 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	94	LYS

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	308/319 (97%)	302 (98%)	6 (2%)	50	45
1	B	275/319 (86%)	264 (96%)	11 (4%)	28	17
1	C	293/319 (92%)	284 (97%)	9 (3%)	35	26
1	D	292/319 (92%)	285 (98%)	7 (2%)	43	36
All	All	1168/1276 (92%)	1135 (97%)	33 (3%)	38	30

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	MET
1	A	46	GLN
1	A	197	GLN
1	A	261	GLN
1	A	308	LYS
1	A	311	HIS
1	B	20	LEU
1	B	46	GLN
1	B	99	THR
1	B	149	GLN
1	B	249	GLN
1	B	264	THR
1	B	273	GLU
1	B	279	THR
1	B	307	VAL
1	B	308	LYS
1	B	311	HIS
1	C	9	LYS
1	C	20	LEU
1	C	41	MET
1	C	46	GLN
1	C	99	THR
1	C	125	VAL
1	C	149	GLN
1	C	160	LYS
1	C	311	HIS
1	D	20	LEU
1	D	46	GLN

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Mol	Chain	Res	Type
1	D	95	GLU
1	D	101	ILE
1	D	294	LYS
1	D	308	LYS
1	D	311	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	142	ASN
1	A	186	HIS
1	A	195	GLN
1	A	197	GLN
1	A	198	ASN
1	A	205	GLN
1	A	249	GLN
1	A	290	GLN
1	A	343	ASN
1	B	253	ASN
1	B	287	ASN
1	C	14	GLN
1	C	36	ASN
1	C	142	ASN
1	C	290	GLN
1	C	296	ASN
1	C	330	ASN
1	D	79	ASN
1	D	149	GLN
1	D	290	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	KAS	B	401	1	21,23,23	1.99	5 (23%)	26,33,33	1.75	7 (26%)
2	KAS	A	401	1	21,23,23	1.56	3 (14%)	26,33,33	2.01	6 (23%)
2	KAS	C	401	1	21,23,23	1.96	5 (23%)	26,33,33	1.74	6 (23%)
2	KAS	D	401	1	21,23,23	2.08	6 (28%)	26,33,33	1.94	6 (23%)

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	KAS	B	401	1	-	0/8/17/17	0/2/2/2
2	KAS	A	401	1	-	1/8/17/17	0/2/2/2
2	KAS	C	401	1	-	0/8/17/17	0/2/2/2
2	KAS	D	401	1	-	0/8/17/17	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	KAS	P1-O19	5.98	1.61	1.56
2	D	401	KAS	P1-O19	5.77	1.61	1.56
2	C	401	KAS	P1-O19	5.21	1.61	1.56
2	D	401	KAS	N5-N4	5.18	1.40	1.32
2	B	401	KAS	N5-N4	4.49	1.39	1.32
2	C	401	KAS	N5-N4	4.29	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	KAS	N5-N4	4.16	1.38	1.32
2	A	401	KAS	P1-O19	3.29	1.59	1.56
2	C	401	KAS	B17-C16	3.02	1.62	1.57
2	A	401	KAS	C2-C1	2.73	1.41	1.37
2	C	401	KAS	C2-C1	2.68	1.41	1.37
2	B	401	KAS	N3-N4	2.65	1.39	1.34
2	D	401	KAS	N3-N4	2.53	1.38	1.34
2	B	401	KAS	C2-C1	2.35	1.41	1.37
2	C	401	KAS	N3-N4	2.34	1.38	1.34
2	D	401	KAS	B17-C16	2.33	1.61	1.57
2	D	401	KAS	C2-C1	2.17	1.41	1.37
2	B	401	KAS	B17-C16	2.09	1.60	1.57
2	D	401	KAS	C7-C1	2.04	1.50	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	KAS	N3-N4-N5	5.33	111.82	107.02
2	A	401	KAS	C1-N5-N4	-5.02	103.85	109.23
2	B	401	KAS	C1-N5-N4	-4.71	104.18	109.23
2	D	401	KAS	C1-N5-N4	-4.37	104.55	109.23
2	C	401	KAS	C1-N5-N4	-4.34	104.58	109.23
2	C	401	KAS	N3-N4-N5	4.12	110.73	107.02
2	D	401	KAS	C1-C2-N3	4.10	108.58	105.28
2	D	401	KAS	C7-C1-C2	-4.05	123.46	129.65
2	A	401	KAS	C2-N3-N4	-3.97	106.89	110.75
2	B	401	KAS	N3-N4-N5	3.90	110.53	107.02
2	C	401	KAS	C2-N3-N4	-3.38	107.46	110.75
2	D	401	KAS	N3-N4-N5	3.34	110.02	107.02
2	D	401	KAS	C7-C1-N5	3.26	127.29	122.05
2	D	401	KAS	C2-N3-N4	-3.24	107.60	110.75
2	B	401	KAS	C2-N3-N4	-3.10	107.73	110.75
2	A	401	KAS	C1-C2-N3	2.79	107.53	105.28
2	C	401	KAS	C1-C2-N3	2.74	107.48	105.28
2	C	401	KAS	C16-N3-N4	-2.66	116.53	119.86
2	B	401	KAS	C7-C1-C2	-2.63	125.63	129.65
2	B	401	KAS	C2-C1-N5	2.53	110.29	107.85
2	B	401	KAS	C1-C2-N3	2.46	107.27	105.28
2	A	401	KAS	C16-N3-N4	-2.43	116.82	119.86
2	B	401	KAS	C16-N3-N4	-2.28	117.01	119.86
2	A	401	KAS	C2-C1-N5	2.14	109.92	107.85
2	C	401	KAS	C7-C1-C2	-2.03	126.56	129.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

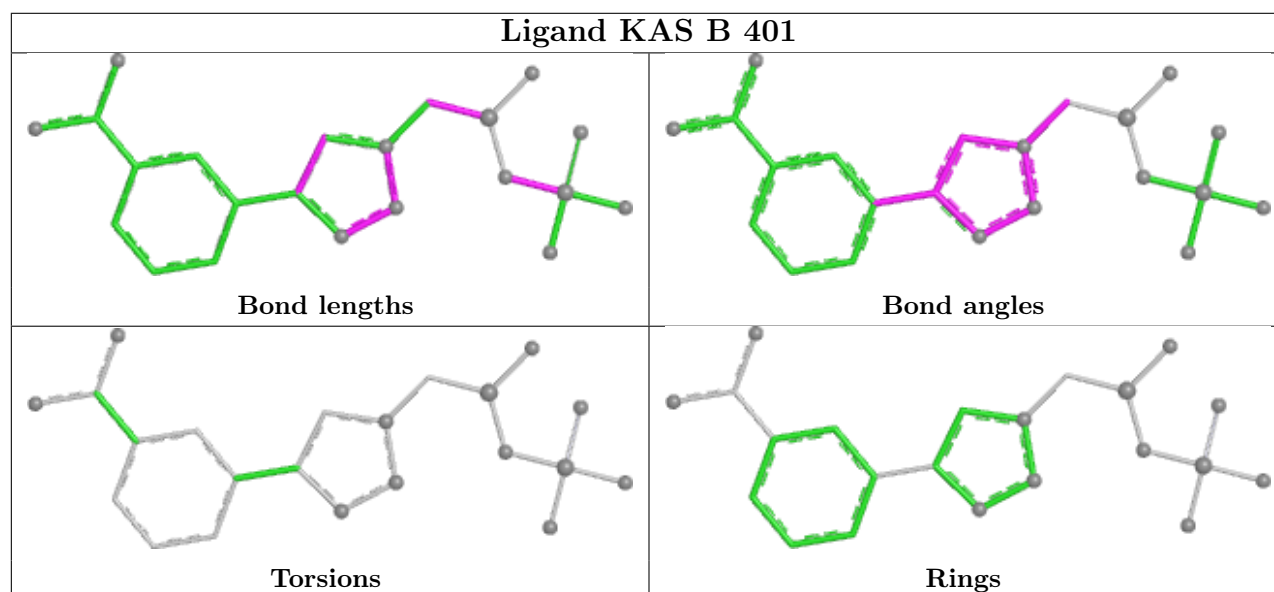
Mol	Chain	Res	Type	Atoms
2	A	401	KAS	C10-C11-C3-O1

There are no ring outliers.

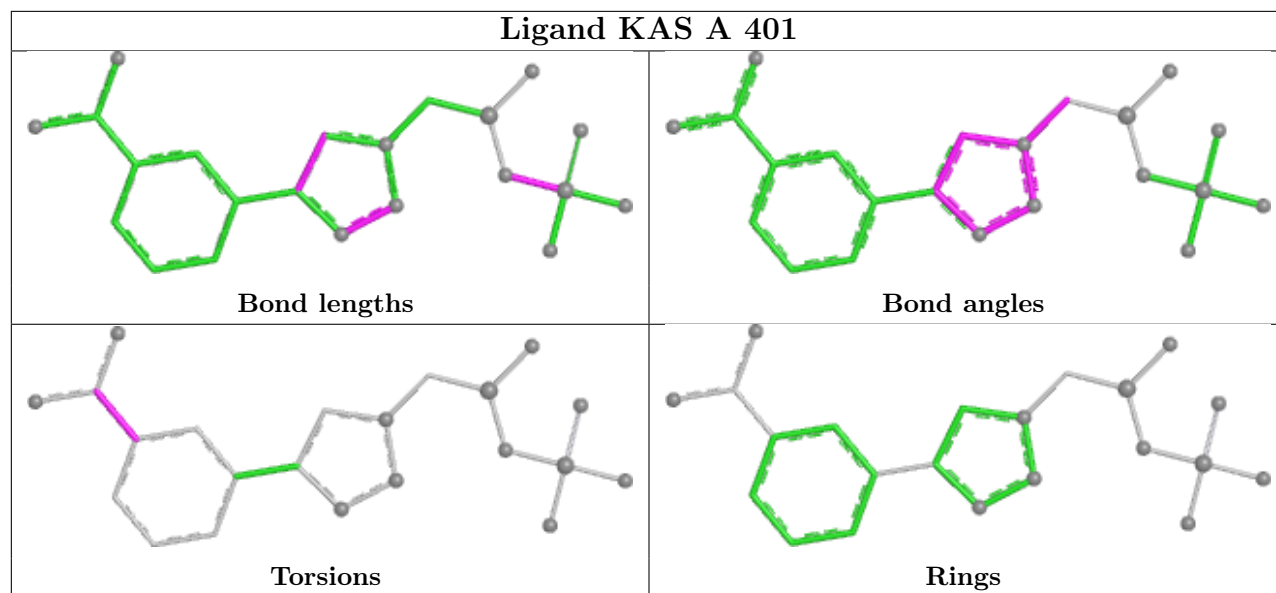
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	KAS	1	0

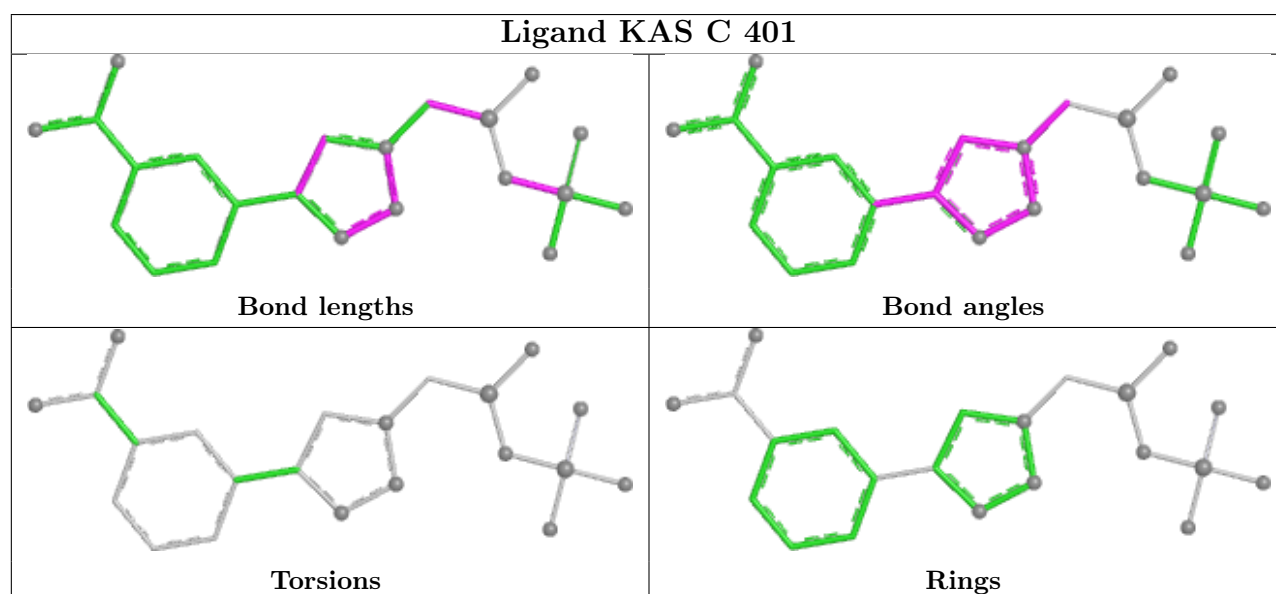
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



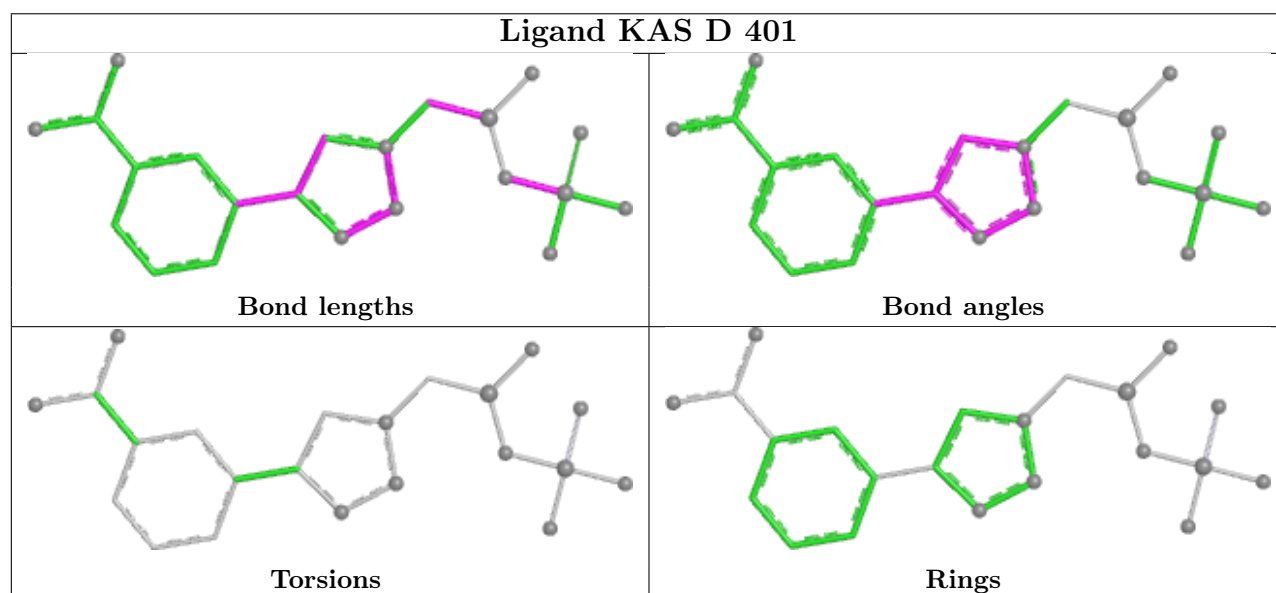
Ligand KAS A 401



Ligand KAS C 401



Ligand KAS D 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	358/361 (99%)	0.22	2 (0%) 85 89	20, 31, 47, 62	0
1	B	356/361 (98%)	1.56	117 (32%) 1 0	25, 54, 80, 93	0
1	C	354/361 (98%)	1.10	68 (19%) 3 3	24, 40, 69, 85	1 (0%)
1	D	356/361 (98%)	1.16	63 (17%) 4 4	24, 48, 74, 90	0
All	All	1424/1444 (98%)	1.01	250 (17%) 4 4	20, 42, 73, 93	1 (0%)

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	PRO	5.9
1	B	107	LEU	4.9
1	C	96	LEU	4.9
1	B	86	ASP	4.8
1	C	131	VAL	4.8
1	B	241	PRO	4.8
1	C	138	TRP	4.7
1	B	5	ASP	4.7
1	C	101	ILE	4.6
1	B	245	PRO	4.6
1	B	101	ILE	4.6
1	D	101	ILE	4.5
1	C	144	ILE	4.4
1	B	264	THR	4.4
1	C	134	PHE	4.4
1	C	135	PHE	4.3
1	C	246	THR	4.3
1	B	99	THR	4.1
1	B	104	VAL	4.1
1	C	122	PRO	4.1
1	C	143	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	107	LEU	3.8
1	B	3	PRO	3.8
1	C	93	TRP	3.8
1	C	125	VAL	3.8
1	C	142	ASN	3.8
1	C	132	LEU	3.8
1	C	263	ASN	3.8
1	D	85	PHE	3.7
1	B	257	GLN	3.7
1	D	3	PRO	3.7
1	D	145	GLY	3.7
1	B	96	LEU	3.6
1	B	300	ALA	3.6
1	B	357	ILE	3.6
1	D	144	ILE	3.6
1	C	99	THR	3.5
1	C	357	ILE	3.5
1	B	238	ASN	3.5
1	B	251	ALA	3.5
1	D	147	TYR	3.5
1	B	93	TRP	3.5
1	D	104	VAL	3.5
1	D	279	THR	3.5
1	B	265	MET	3.5
1	B	11	LEU	3.5
1	D	306	SER	3.4
1	B	252	ILE	3.4
1	B	144	ILE	3.4
1	B	262	VAL	3.4
1	B	237	ALA	3.4
1	D	96	LEU	3.4
1	B	307	VAL	3.3
1	B	306	SER	3.3
1	B	269	LEU	3.3
1	D	138	TRP	3.3
1	B	248	ILE	3.3
1	B	298	VAL	3.3
1	D	98	ASN	3.3
1	C	141	LYS	3.2
1	B	276	TYR	3.2
1	B	180	PRO	3.2
1	C	100	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	326	ILE	3.2
1	D	301	ILE	3.2
1	D	118	ALA	3.1
1	C	295	PRO	3.1
1	D	125	VAL	3.1
1	B	91	LYS	3.1
1	B	301	ILE	3.1
1	C	79	ASN	3.1
1	B	133	THR	3.1
1	C	299	THR	3.1
1	D	262	VAL	3.0
1	B	88	THR	3.0
1	C	127	THR	3.0
1	B	181	ALA	3.0
1	B	278	ALA	3.0
1	C	117	LEU	3.0
1	B	98	ASN	3.0
1	D	79	ASN	3.0
1	B	32	VAL	3.0
1	B	176	LYS	3.0
1	C	133	THR	3.0
1	D	141	LYS	3.0
1	C	116	ASN	3.0
1	C	287	ASN	3.0
1	C	262	VAL	2.9
1	B	39	TYR	2.9
1	D	81	GLY	2.9
1	B	85	PHE	2.9
1	B	331	ILE	2.9
1	C	158	PHE	2.9
1	B	164	LEU	2.9
1	C	139	LYS	2.9
1	B	279	THR	2.8
1	C	97	LYS	2.8
1	B	79	ASN	2.8
1	B	232	LEU	2.8
1	B	4	LYS	2.8
1	B	37	LYS	2.8
1	B	308	LYS	2.8
1	B	143	PRO	2.8
1	C	161	VAL	2.8
1	D	102	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	305	PRO	2.8
1	C	294	LYS	2.7
1	B	145	GLY	2.7
1	B	283	LEU	2.7
1	D	132	LEU	2.7
1	B	275	SER	2.7
1	B	110	ALA	2.7
1	B	141	LYS	2.7
1	B	268	ALA	2.7
1	C	292	VAL	2.7
1	C	5	ASP	2.7
1	C	355	ASN	2.7
1	D	258	GLY	2.6
1	B	246	THR	2.6
1	B	325	PHE	2.6
1	B	140	PRO	2.6
1	D	291	ILE	2.6
1	C	4	LYS	2.6
1	D	299	THR	2.6
1	B	138	TRP	2.6
1	B	256	HIS	2.6
1	B	33	ILE	2.6
1	C	178	ILE	2.6
1	D	84	SER	2.6
1	B	169	PRO	2.6
1	B	260	TYR	2.5
1	C	147	TYR	2.5
1	D	266	TYR	2.5
1	B	135	PHE	2.5
1	C	102	ASP	2.5
1	D	93	TRP	2.5
1	B	159	GLY	2.5
1	C	356	ALA	2.5
1	D	108	GLN	2.5
1	B	266	TYR	2.5
1	D	135	PHE	2.5
1	B	36	ASN	2.5
1	B	124	GLU	2.5
1	B	277	PRO	2.5
1	B	274	PHE	2.5
1	B	125	VAL	2.5
1	C	92	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	98	ASN	2.4
1	C	164	LEU	2.4
1	D	103	GLN	2.4
1	D	329	GLU	2.4
1	B	233	SER	2.4
1	B	356	ALA	2.4
1	C	94	LYS	2.4
1	D	90	GLY	2.4
1	D	88	THR	2.4
1	D	99	THR	2.4
1	C	163	ALA	2.4
1	B	353	VAL	2.4
1	C	173	VAL	2.4
1	D	131	VAL	2.4
1	B	330	ASN	2.4
1	B	355	ASN	2.4
1	B	182	LEU	2.4
1	B	351	TYR	2.4
1	B	291	ILE	2.4
1	B	352	VAL	2.4
1	C	136	LYS	2.4
1	D	352	VAL	2.3
1	D	304	GLU	2.3
1	D	113	THR	2.3
1	D	167	ASN	2.3
1	B	100	PRO	2.3
1	D	143	PRO	2.3
1	D	303	LYS	2.3
1	D	292	VAL	2.3
1	D	164	LEU	2.3
1	B	255	THR	2.3
1	C	166	MET	2.3
1	C	91	LYS	2.3
1	C	123	ASP	2.3
1	B	173	VAL	2.3
1	B	324	VAL	2.3
1	D	287	ASN	2.3
1	B	177	THR	2.3
1	D	354	LEU	2.3
1	B	89	PRO	2.2
1	B	234	PHE	2.2
1	B	270	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	178	ILE	2.2
1	C	129	GLN	2.2
1	C	298	VAL	2.2
1	D	263	ASN	2.2
1	D	296	ASN	2.2
1	C	264	THR	2.2
1	B	239	LEU	2.2
1	C	119	LEU	2.2
1	D	109	LEU	2.2
1	B	147	TYR	2.2
1	B	178	ILE	2.2
1	D	248	ILE	2.2
1	B	166	MET	2.2
1	C	162	VAL	2.2
1	B	119	LEU	2.2
1	B	132	LEU	2.2
1	C	90	GLY	2.2
1	C	137	ASP	2.2
1	C	145	GLY	2.2
1	C	165	SER	2.2
1	C	296	ASN	2.2
1	D	36	ASN	2.2
1	D	298	VAL	2.2
1	D	264	THR	2.2
1	B	258	GLY	2.2
1	B	280	LEU	2.2
1	C	81	GLY	2.2
1	B	167	ASN	2.1
1	C	293	MET	2.1
1	B	170	PHE	2.1
1	A	246	THR	2.1
1	B	131	VAL	2.1
1	B	109	LEU	2.1
1	C	109	LEU	2.1
1	A	36	ASN	2.1
1	B	35	ASN	2.1
1	D	300	ALA	2.1
1	D	165	SER	2.1
1	D	307	VAL	2.1
1	B	82	LYS	2.1
1	B	220	PRO	2.1
1	B	263	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	269	LEU	2.1
1	B	103	GLN	2.1
1	B	235	ILE	2.1
1	D	326	ILE	2.1
1	B	113	THR	2.1
1	B	142	ASN	2.1
1	D	280	LEU	2.1
1	B	77	ALA	2.1
1	D	168	LYS	2.0
1	B	92	TYR	2.0
1	D	76	TYR	2.0
1	C	217	LEU	2.0
1	B	329	GLU	2.0
1	B	358	LYS	2.0
1	B	6	GLN	2.0
1	B	299	THR	2.0
1	C	88	THR	2.0
1	C	113	THR	2.0
1	D	89	PRO	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](#)

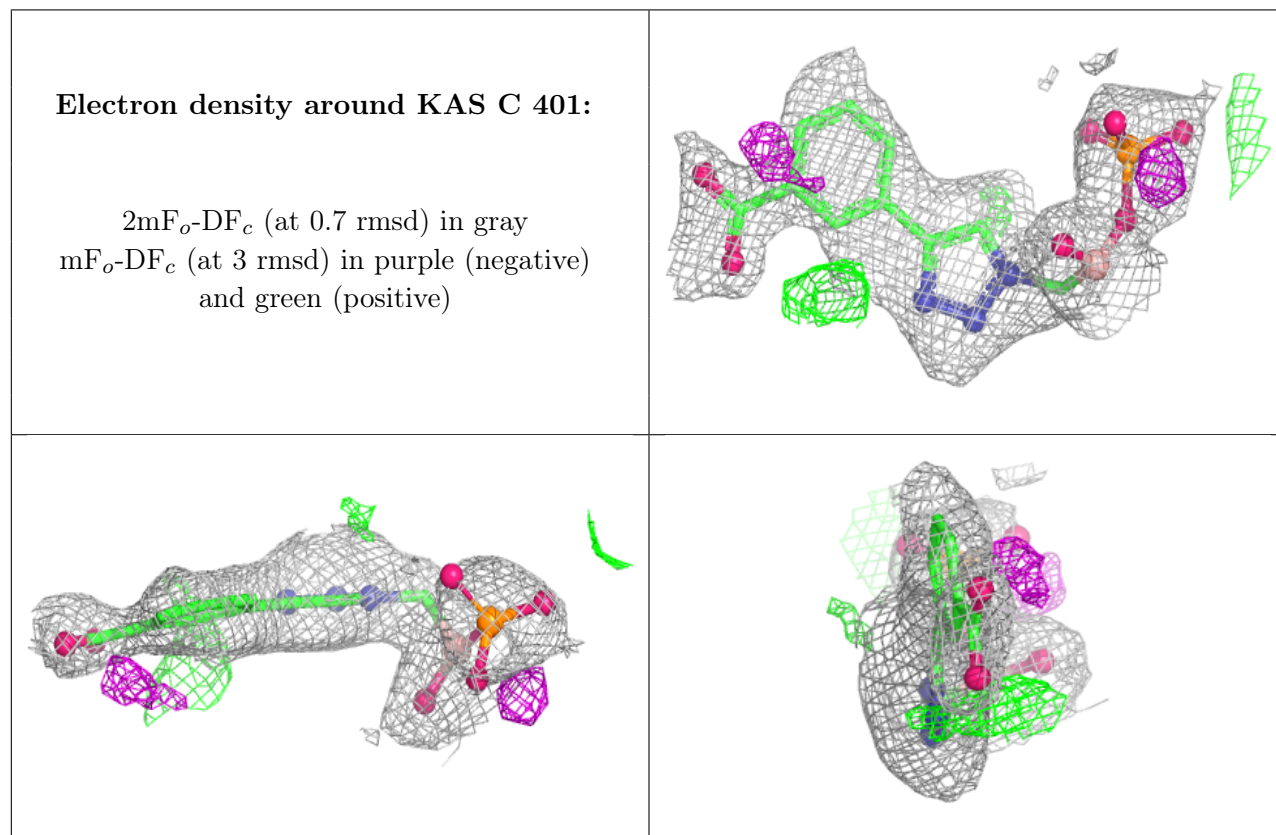
There are no oligosaccharides in this entry.

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.

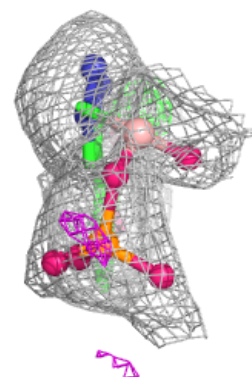
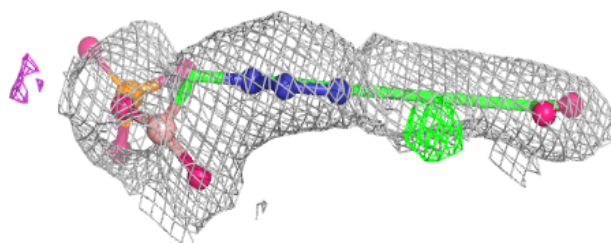
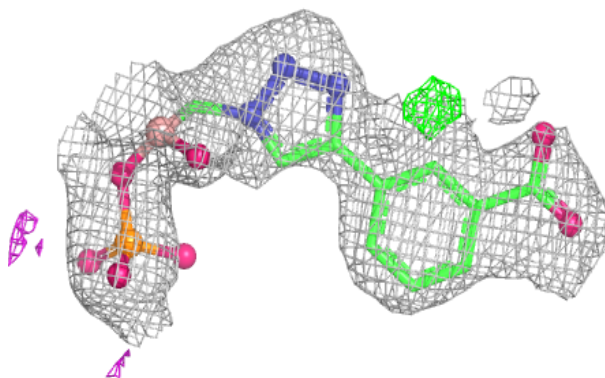
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	KAS	C	401	22/22	0.83	0.16	32,64,91,101	0
2	KAS	D	401	22/22	0.83	0.14	46,64,74,87	0
2	KAS	A	401	22/22	0.89	0.13	27,45,63,86	0
2	KAS	B	401	22/22	0.89	0.12	42,56,63,70	0

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.

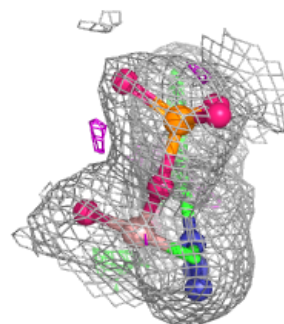
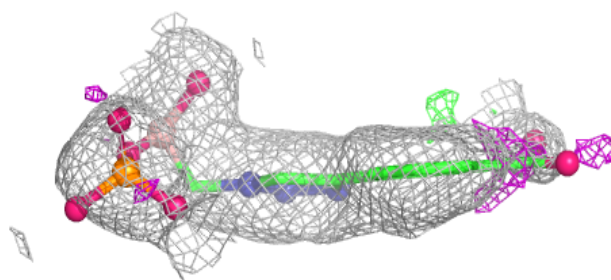
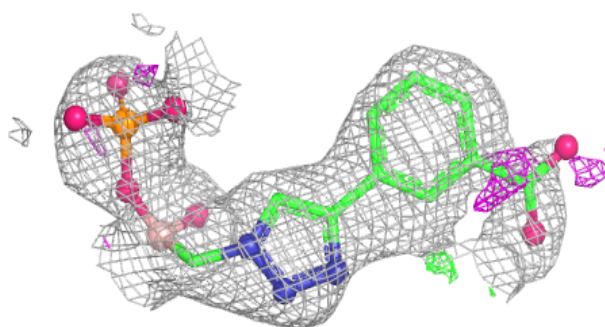


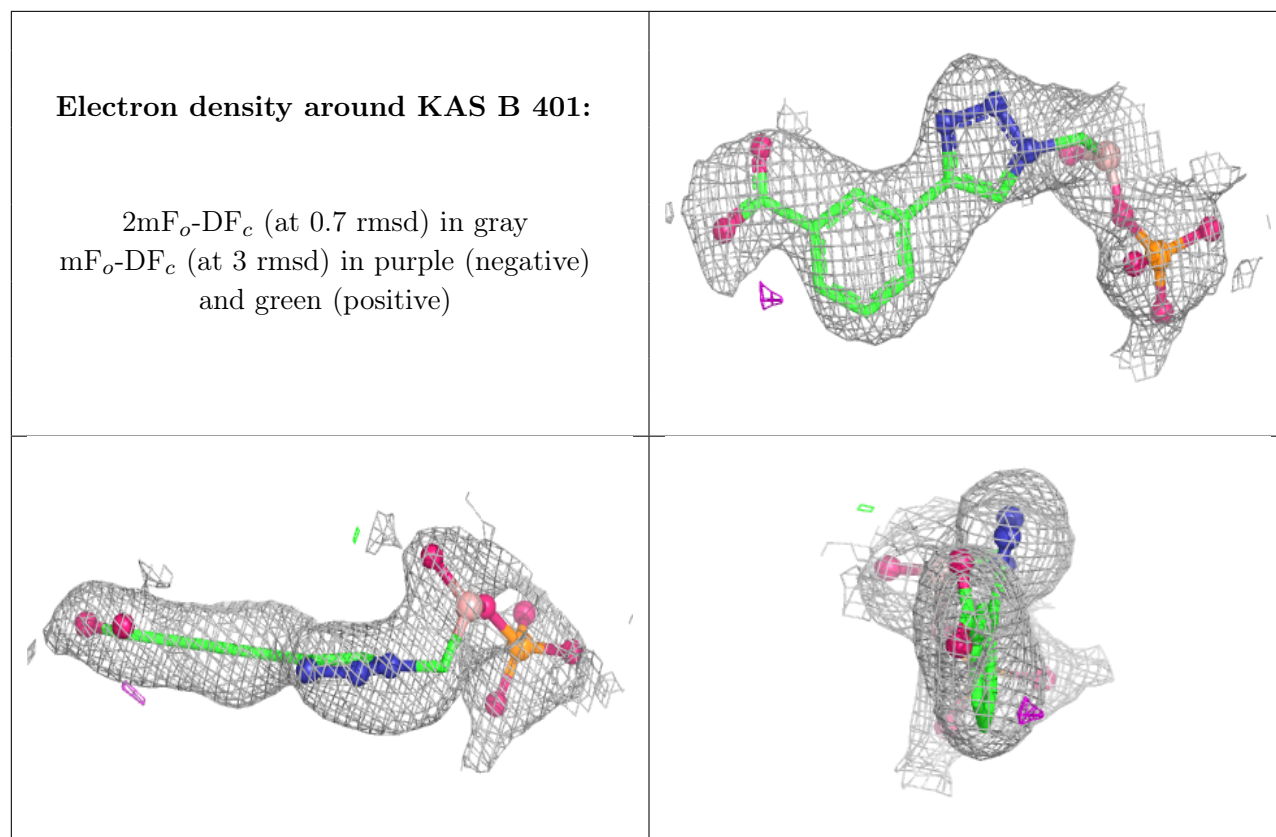
Electron density around KAS D 401:

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

**Electron density around KAS A 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 [i](#)

There are no such residues in this entry.