



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 6N5G / pdb_00006n5g
Title : Crystal structure of an epoxide hydrolase from *Trichoderma reesei* in complex with inhibitor 2
Authors : Oliveira, G.S.; Adriani, P.P.; Ribeiro, J.A.; Morisseau, C.; Hammock, B.D.; Dias, M.V.; Chambergo, F.S.
Deposited on : 2018-11-21
Resolution : 2.60 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

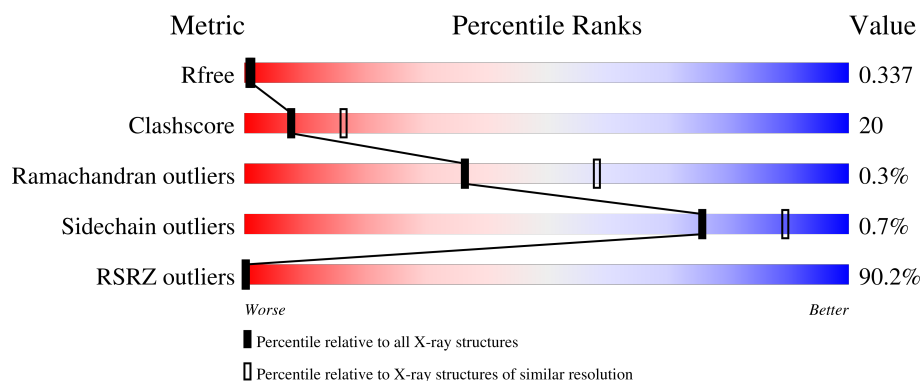
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	336	90% 61%39%

2 Entry composition [i](#)

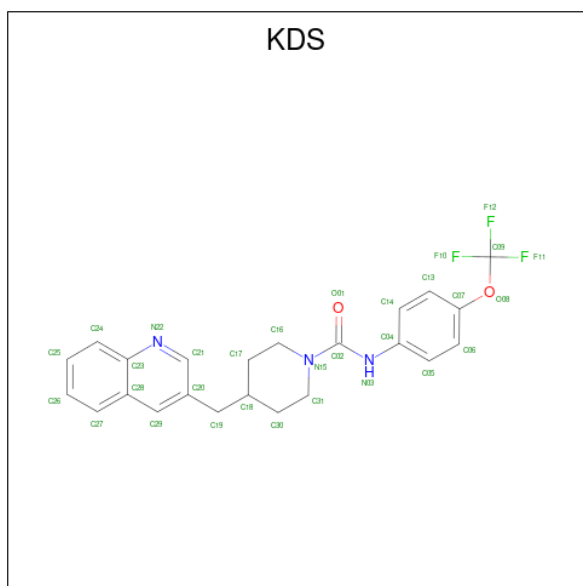
There are 3 unique types of molecules in this entry. The entry contains 2690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Epoxide hydrolase TrEH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2637	1688	454	483	12			

- Molecule 2 is 4-[(quinolin-3-yl)methyl]-N-[4-(trifluoromethoxy)phenyl]piperidine-1-carboxamide (CCD ID: KDS) (formula: $C_{23}H_{22}F_3N_3O_2$).



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

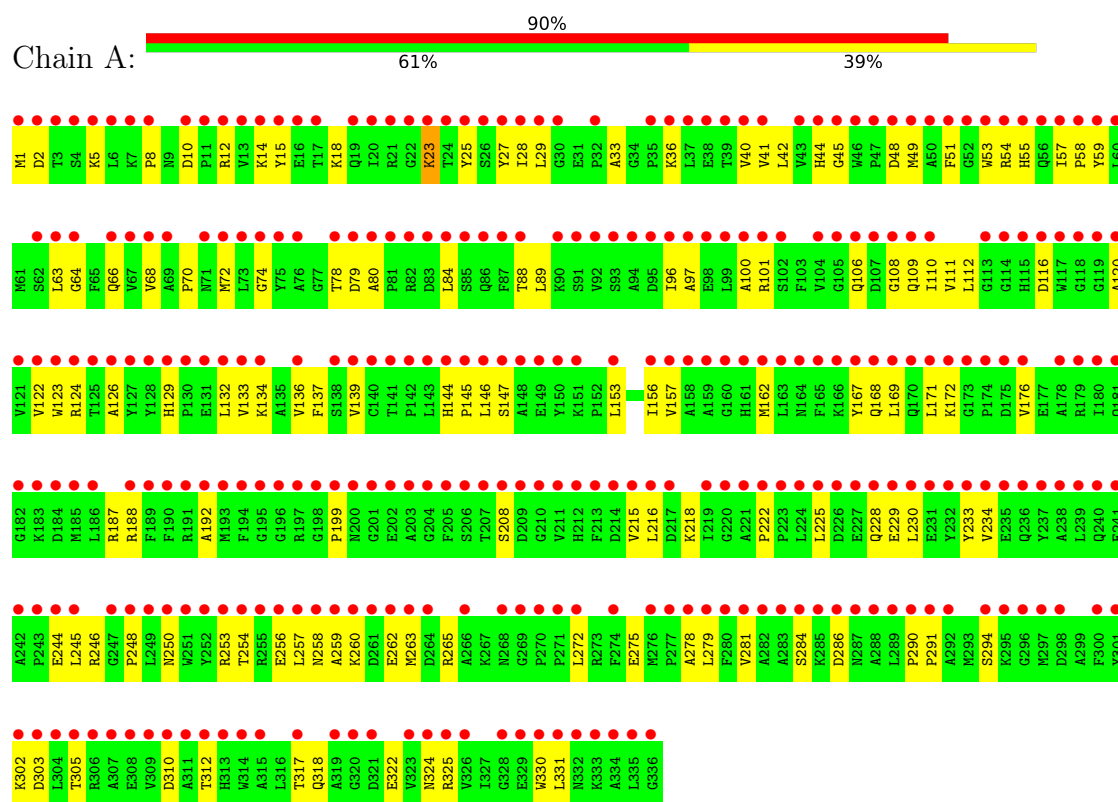
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total 22 O 22	0	0

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: Epoxide hydrolase TrEH



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	50.42Å 77.32Å 86.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.81 – 2.60 37.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.81-2.60) 99.0 (37.81-2.60)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.270 , 0.340 0.277 , 0.337	Depositor DCC
R_{free} test set	517 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	1.703	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2690	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.98% 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: KDS

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	0.19	0/2709	0.43	0/3678

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2637	0	2580	105	0
2	A	31	0	0	2	0
3	A	22	0	0	3	0
All	All	2690	0	2580	105	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 20.

All (105) 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:5:LYS:HD2	1:A:54:ARG:NH1	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:PRO:HG2	1:A:228:GLN:HG2	1.59	0.84
1:A:45:GLY:HA3	1:A:116:ASP:HB3	1.64	0.80
1:A:101:ARG:HG2	1:A:106:GLN:HA	1.69	0.75
1:A:74:GLY:HA2	1:A:80:ALA:HB2	1.71	0.73
1:A:171:LEU:HD23	1:A:176:VAL:HG21	1.72	0.71
1:A:5:LYS:HD2	1:A:54:ARG:HH11	1.56	0.69
1:A:172:LYS:O	1:A:253:ARG:NH1	2.25	0.69
1:A:80:ALA:O	1:A:246:ARG:NH2	2.28	0.67
1:A:291:PRO:O	1:A:294:SER:OG	2.14	0.66
1:A:153:LEU:HA	1:A:156:ILE:HD12	1.79	0.64
1:A:54:ARG:NH2	1:A:317:THR:HB	2.14	0.63
1:A:254:THR:O	1:A:258:ASN:ND2	2.32	0.62
1:A:312:THR:OG1	1:A:318:GLN:OE1	2.17	0.61
1:A:40:VAL:HG22	1:A:111:VAL:HB	1.83	0.60
1:A:169:LEU:HA	1:A:172:LYS:HE3	1.83	0.60
1:A:70:PRO:HG2	1:A:72:MET:HE3	1.84	0.60
1:A:5:LYS:NZ	1:A:54:ARG:HH12	1.99	0.59
1:A:254:THR:OG1	1:A:258:ASN:ND2	2.35	0.59
1:A:18:LYS:HB2	1:A:27:TYR:HE1	1.67	0.58
1:A:111:VAL:HG11	1:A:331:LEU:HD21	1.85	0.58
1:A:124:ARG:NH2	1:A:144:HIS:O	2.34	0.58
1:A:100:ALA:HB1	1:A:110:ILE:HG13	1.87	0.57
1:A:44:HIS:HB2	1:A:48:ASP:HB3	1.87	0.57
1:A:72:MET:HA	1:A:72:MET:HE2	1.85	0.57
1:A:112:LEU:HB3	1:A:136:VAL:HG23	1.87	0.56
1:A:139:VAL:HG22	1:A:281:VAL:HB	1.88	0.56
1:A:23:LYS:HB3	1:A:79:ASP:HB2	1.89	0.55
1:A:116:ASP:OD1	2:A:401:KDS:N03	2.40	0.55
1:A:84:LEU:HD21	1:A:253:ARG:HB2	1.88	0.55
1:A:199:PRO:HD3	1:A:218:LYS:HB3	1.89	0.54
1:A:42:LEU:HB3	1:A:53:TRP:CE2	2.43	0.54
1:A:133:VAL:HG11	1:A:136:VAL:HB	1.89	0.54
1:A:325:ARG:NH2	3:A:507:HOH:O	2.42	0.53
1:A:10:ASP:N	1:A:15:TYR:OH	2.43	0.52
1:A:136:VAL:O	1:A:278:ALA:HA	2.10	0.52
1:A:14:LYS:HB2	1:A:29:LEU:HB3	1.91	0.52
1:A:54:ARG:HH21	1:A:317:THR:HB	1.75	0.52
1:A:41:VAL:HG23	1:A:110:ILE:HG21	1.92	0.51
1:A:145:PRO:HA	1:A:272:LEU:HD12	1.92	0.51
1:A:275:GLU:OE2	1:A:302:LYS:HB2	2.11	0.51
1:A:322:GLU:OE2	3:A:501:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:NH1	1:A:262:GLU:OE1	2.43	0.51
1:A:97:ALA:HB2	1:A:129:HIS:CD2	2.46	0.51
1:A:25:TYR:HA	1:A:78:THR:HG23	1.93	0.51
1:A:147:SER:OG	1:A:259:ALA:HA	2.11	0.50
1:A:72:MET:HE1	1:A:96:ILE:HD11	1.94	0.49
1:A:167:TYR:OH	2:A:401:KDS:O01	2.21	0.49
1:A:84:LEU:HB3	1:A:257:LEU:HD11	1.95	0.49
1:A:146:LEU:HD22	1:A:265:ARG:HB2	1.95	0.49
1:A:55:HIS:O	1:A:324:ASN:ND2	2.30	0.49
1:A:59:TYR:O	1:A:63:LEU:HD13	2.13	0.48
1:A:49:MET:HE3	1:A:51:PHE:HB3	1.94	0.48
1:A:222:PRO:HG3	1:A:230:LEU:HD13	1.95	0.48
1:A:101:ARG:HE	1:A:132:LEU:HD13	1.78	0.48
1:A:88:THR:CG2	1:A:257:LEU:HB3	2.44	0.47
1:A:153:LEU:O	1:A:157:VAL:HG22	2.14	0.47
1:A:187:ARG:HA	1:A:234:VAL:HG21	1.97	0.47
1:A:278:ALA:O	1:A:305:THR:N	2.40	0.47
1:A:156:ILE:HG21	1:A:162:MET:HE2	1.96	0.47
1:A:244:GLU:OE1	1:A:244:GLU:N	2.40	0.47
1:A:18:LYS:HD3	1:A:27:TYR:OH	2.15	0.46
1:A:120:ALA:O	1:A:124:ARG:HG2	2.15	0.46
1:A:51:PHE:HE2	1:A:229:GLU:HB3	1.80	0.46
1:A:28:ILE:HD11	1:A:57:ILE:HD13	1.98	0.46
1:A:215:VAL:HG13	1:A:216:LEU:HD23	1.97	0.46
1:A:101:ARG:HB3	1:A:106:GLN:NE2	2.31	0.45
1:A:41:VAL:HA	1:A:68:VAL:O	2.16	0.45
1:A:1:MET:HE3	1:A:33:ALA:HB2	1.97	0.45
1:A:192:ALA:HB2	1:A:216:LEU:HD21	1.99	0.45
1:A:279:LEU:HB2	1:A:330:TRP:CD2	2.52	0.44
1:A:89:LEU:HB3	1:A:124:ARG:HG3	1.99	0.44
1:A:133:VAL:CG1	1:A:136:VAL:HB	2.47	0.44
1:A:302:LYS:HD3	1:A:303:ASP:HB2	1.99	0.44
1:A:10:ASP:OD2	1:A:12:ARG:HD3	2.17	0.44
1:A:199:PRO:CD	1:A:218:LYS:HB3	2.48	0.43
1:A:29:LEU:HD11	1:A:66:GLN:HE21	1.83	0.43
1:A:101:ARG:NE	1:A:132:LEU:HD13	2.34	0.43
1:A:168:GLN:HA	1:A:171:LEU:HB2	2.00	0.43
1:A:256:GLU:O	1:A:260:LYS:HG2	2.18	0.43
1:A:49:MET:HE1	1:A:233:TYR:HA	2.01	0.43
1:A:259:ALA:O	1:A:263:MET:HG3	2.19	0.42
1:A:108:GLY:O	1:A:132:LEU:HD12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ALA:HA	1:A:133:VAL:HG21	2.02	0.42
1:A:18:LYS:HB2	1:A:27:TYR:CE1	2.49	0.42
1:A:5:LYS:HZ3	1:A:54:ARG:HH12	1.65	0.42
1:A:188:ARG:HD3	1:A:216:LEU:O	2.19	0.42
1:A:1:MET:HG2	1:A:2:ASP:N	2.35	0.42
1:A:27:TYR:HA	1:A:70:PRO:HA	2.02	0.42
1:A:192:ALA:HB2	1:A:216:LEU:CD2	2.49	0.42
1:A:54:ARG:HE	1:A:317:THR:HG21	1.84	0.42
1:A:109:GLN:HB3	1:A:134:LYS:HB2	2.02	0.42
1:A:250:ASN:HA	1:A:253:ARG:HG3	2.02	0.41
1:A:57:ILE:HB	1:A:58:PRO:HD3	2.02	0.41
1:A:84:LEU:HB3	1:A:257:LEU:CD1	2.50	0.41
1:A:284:SER:HB2	1:A:310:ASP:HA	2.03	0.41
1:A:74:GLY:O	1:A:248:PRO:HD3	2.20	0.41
1:A:123:TRP:HB2	3:A:511:HOH:O	2.21	0.41
1:A:137:PHE:HB2	1:A:279:LEU:HB3	2.03	0.41
1:A:5:LYS:CD	1:A:54:ARG:NH1	2.72	0.41
1:A:222:PRO:HG2	1:A:225:LEU:HB2	2.03	0.41
1:A:245:LEU:HA	1:A:248:PRO:HD2	2.03	0.41
1:A:290:PRO:HA	1:A:291:PRO:HD3	1.98	0.41
1:A:112:LEU:HG	1:A:122:VAL:HG12	2.03	0.40
1:A:36:LYS:HA	1:A:64:GLY:O	2.21	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	334/336 (99%)	317 (95%)	16 (5%)	1 (0%)	36 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	271/273 (99%)	269 (99%)	2 (1%)	76 89

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	208	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	144	HIS
1	A	200	ASN

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

1 ligand is 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	KDS	A	401	-	34,34,34	1.77	7 (20%)	48,48,48	1.34	5 (10%)

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	KDS	A	401	-	-	5/17/27/27	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	KDS	C02-N15	5.33	1.45	1.36
2	A	401	KDS	C02-N03	4.90	1.46	1.37
2	A	401	KDS	C28-C23	-3.59	1.36	1.42
2	A	401	KDS	O01-C02	-2.32	1.19	1.23
2	A	401	KDS	C31-N15	2.30	1.51	1.47
2	A	401	KDS	C16-N15	2.25	1.51	1.47
2	A	401	KDS	C04-N03	2.22	1.46	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	KDS	C21-N22-C23	4.20	121.82	116.96
2	A	401	KDS	C29-C20-C21	4.02	120.45	116.88
2	A	401	KDS	C17-C16-N15	2.96	116.46	110.66
2	A	401	KDS	C20-C21-N22	-2.95	119.64	124.01
2	A	401	KDS	C30-C31-N15	2.50	115.57	110.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

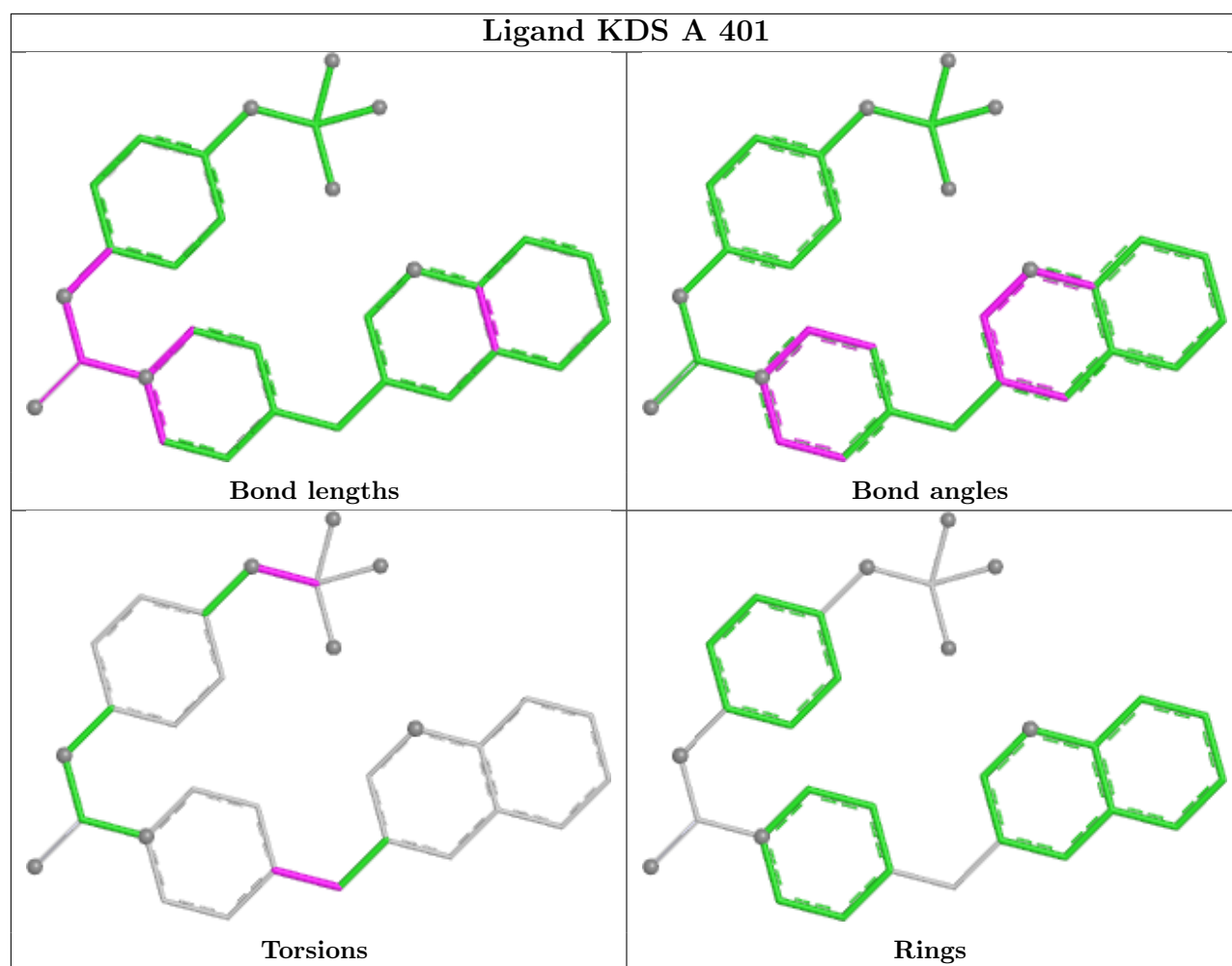
Mol	Chain	Res	Type	Atoms
2	A	401	KDS	F12-C09-O08-C07
2	A	401	KDS	C17-C18-C19-C20
2	A	401	KDS	F11-C09-O08-C07
2	A	401	KDS	C30-C18-C19-C20
2	A	401	KDS	F10-C09-O08-C07

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	KDS	2	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	336/336 (100%)	3.51	303 (90%) 0 0	13, 24, 37, 45	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	ASP	8.8
1	A	215	VAL	8.4
1	A	74	GLY	7.2
1	A	226	ASP	7.0
1	A	287	ASN	6.9
1	A	22	GLY	6.8
1	A	178	ALA	6.8
1	A	212	HIS	6.5
1	A	288	ALA	6.5
1	A	283	ALA	6.4
1	A	266	ALA	6.3
1	A	170	GLN	6.3
1	A	87	PHE	6.2
1	A	32	PRO	6.0
1	A	291	PRO	5.9
1	A	30	GLY	5.8
1	A	214	ASP	5.7
1	A	208	SER	5.5
1	A	85	SER	5.5
1	A	73	LEU	5.4
1	A	238	ALA	5.4
1	A	167	TYR	5.4
1	A	195	GLY	5.4
1	A	203	ALA	5.4
1	A	118	GLY	5.4
1	A	128	TYR	5.4
1	A	196	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	127	TYR	5.3
1	A	206	SER	5.3
1	A	72	MET	5.2
1	A	258	ASN	5.2
1	A	213	PHE	5.1
1	A	119	GLY	5.1
1	A	240	GLN	5.1
1	A	54	ARG	5.0
1	A	290	PRO	5.0
1	A	205	PHE	5.0
1	A	24	THR	4.9
1	A	292	ALA	4.9
1	A	250	ASN	4.9
1	A	114	GLY	4.9
1	A	84	LEU	4.9
1	A	164	ASN	4.9
1	A	263	MET	4.8
1	A	106	GLN	4.8
1	A	194	PHE	4.7
1	A	298	ASP	4.7
1	A	51	PHE	4.7
1	A	184	ASP	4.7
1	A	71	ASN	4.7
1	A	124	ARG	4.6
1	A	259	ALA	4.6
1	A	230	LEU	4.6
1	A	222	PRO	4.6
1	A	285	LYS	4.6
1	A	58	PRO	4.6
1	A	185	MET	4.6
1	A	125	THR	4.5
1	A	102	SER	4.5
1	A	302	LYS	4.5
1	A	269	GLY	4.5
1	A	109	GLN	4.5
1	A	83	ASP	4.5
1	A	309	VAL	4.5
1	A	43	VAL	4.5
1	A	108	GLY	4.4
1	A	63	LEU	4.4
1	A	221	ALA	4.4
1	A	297	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	50	ALA	4.4
1	A	211	VAL	4.4
1	A	247	GLY	4.4
1	A	314	TRP	4.4
1	A	175	ASP	4.3
1	A	192	ALA	4.3
1	A	36	LYS	4.3
1	A	165	PHE	4.3
1	A	332	ASN	4.3
1	A	315	ALA	4.3
1	A	35	PRO	4.3
1	A	204	GLY	4.3
1	A	236	GLN	4.3
1	A	132	LEU	4.3
1	A	216	LEU	4.3
1	A	252	TYR	4.3
1	A	257	LEU	4.3
1	A	179	ARG	4.3
1	A	325	ARG	4.2
1	A	105	GLY	4.2
1	A	3	THR	4.2
1	A	13	VAL	4.2
1	A	29	LEU	4.2
1	A	313	HIS	4.2
1	A	253	ARG	4.2
1	A	145	PRO	4.2
1	A	173	GLY	4.2
1	A	189	PHE	4.2
1	A	126	ALA	4.2
1	A	198	GLY	4.2
1	A	239	LEU	4.2
1	A	81	PRO	4.1
1	A	86	GLN	4.1
1	A	57	ILE	4.1
1	A	66	GLN	4.1
1	A	123	TRP	4.1
1	A	225	LEU	4.1
1	A	20	ILE	4.0
1	A	210	GLY	4.0
1	A	138	SER	4.0
1	A	8	PRO	4.0
1	A	182	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	308	GLU	4.0
1	A	319	ALA	4.0
1	A	75	TYR	4.0
1	A	116	ASP	4.0
1	A	14	LYS	4.0
1	A	17	THR	4.0
1	A	45	GLY	4.0
1	A	303	ASP	4.0
1	A	92	VAL	4.0
1	A	93	SER	3.9
1	A	271	PRO	3.9
1	A	335	LEU	3.9
1	A	281	VAL	3.9
1	A	186	LEU	3.9
1	A	264	ASP	3.9
1	A	305	THR	3.9
1	A	224	LEU	3.9
1	A	254	THR	3.8
1	A	11	PRO	3.8
1	A	262	GLU	3.8
1	A	44	HIS	3.8
1	A	97	ALA	3.8
1	A	161	HIS	3.8
1	A	279	LEU	3.8
1	A	64	GLY	3.8
1	A	149	GLU	3.7
1	A	202	GLU	3.7
1	A	15	TYR	3.7
1	A	223	PRO	3.7
1	A	104	VAL	3.7
1	A	209	ASP	3.6
1	A	295	LYS	3.6
1	A	163	LEU	3.6
1	A	10	ASP	3.6
1	A	78	THR	3.6
1	A	312	THR	3.6
1	A	168	GLN	3.6
1	A	307	ALA	3.5
1	A	59	TYR	3.5
1	A	67	VAL	3.5
1	A	143	LEU	3.5
1	A	55	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	270	PRO	3.5
1	A	16	GLU	3.5
1	A	174	PRO	3.5
1	A	228	GLN	3.5
1	A	62	SER	3.4
1	A	200	ASN	3.4
1	A	129	HIS	3.4
1	A	188	ARG	3.4
1	A	235	GLU	3.4
1	A	6	LEU	3.4
1	A	146	LEU	3.4
1	A	310	ASP	3.4
1	A	232	TYR	3.4
1	A	88	THR	3.4
1	A	289	LEU	3.4
1	A	304	LEU	3.4
1	A	27	TYR	3.3
1	A	171	LEU	3.3
1	A	282	ALA	3.3
1	A	40	VAL	3.3
1	A	68	VAL	3.3
1	A	227	GLU	3.3
1	A	91	SER	3.3
1	A	248	PRO	3.3
1	A	159	ALA	3.3
1	A	280	PHE	3.3
1	A	301	TYR	3.3
1	A	330	TRP	3.2
1	A	199	PRO	3.2
1	A	150	TYR	3.2
1	A	28	ILE	3.2
1	A	201	GLY	3.2
1	A	96	ILE	3.2
1	A	12	ARG	3.2
1	A	47	PRO	3.2
1	A	334	ALA	3.2
1	A	183	LYS	3.1
1	A	193	MET	3.1
1	A	37	LEU	3.1
1	A	333	LYS	3.1
1	A	4	SER	3.1
1	A	284	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	95	ASP	3.1
1	A	139	VAL	3.1
1	A	99	LEU	3.1
1	A	79	ASP	3.1
1	A	107	ASP	3.1
1	A	131	GLU	3.1
1	A	321	ASP	3.1
1	A	323	VAL	3.1
1	A	147	SER	3.1
1	A	244	GLU	3.0
1	A	46	TRP	3.0
1	A	229	GLU	3.0
1	A	142	PRO	3.0
1	A	7	LYS	3.0
1	A	158	ALA	3.0
1	A	261	ASP	3.0
1	A	110	ILE	3.0
1	A	317	THR	3.0
1	A	130	PRO	3.0
1	A	21	ARG	3.0
1	A	274	PHE	3.0
1	A	90	LYS	2.9
1	A	217	ASP	2.9
1	A	180	ILE	2.9
1	A	336	GLY	2.9
1	A	121	VAL	2.9
1	A	176	VAL	2.9
1	A	60	LEU	2.9
1	A	251	TRP	2.9
1	A	56	GLN	2.9
1	A	306	ARG	2.9
1	A	25	TYR	2.9
1	A	120	ALA	2.9
1	A	19	GLN	2.9
1	A	156	ILE	2.9
1	A	320	GLY	2.9
1	A	219	ILE	2.8
1	A	136	VAL	2.8
1	A	157	VAL	2.8
1	A	326	VAL	2.8
1	A	2	ASP	2.8
1	A	278	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASP	2.8
1	A	98	GLU	2.8
1	A	191	ARG	2.8
1	A	277	PRO	2.8
1	A	268	ASN	2.8
1	A	39	THR	2.8
1	A	256	GLU	2.7
1	A	233	TYR	2.7
1	A	166	LYS	2.7
1	A	117	TRP	2.7
1	A	144	HIS	2.7
1	A	82	ARG	2.7
1	A	241	GLU	2.7
1	A	41	VAL	2.7
1	A	122	VAL	2.6
1	A	276	MET	2.6
1	A	169	LEU	2.6
1	A	255	ARG	2.6
1	A	52	GLY	2.6
1	A	113	GLY	2.6
1	A	49	MET	2.6
1	A	162	MET	2.6
1	A	134	LYS	2.6
1	A	38	GLU	2.6
1	A	1	MET	2.5
1	A	5	LYS	2.5
1	A	160	GLY	2.5
1	A	94	ALA	2.5
1	A	181	GLN	2.5
1	A	300	PHE	2.5
1	A	141	THR	2.5
1	A	294	SER	2.5
1	A	172	LYS	2.5
1	A	245	LEU	2.5
1	A	249	LEU	2.5
1	A	296	GLY	2.5
1	A	260	LYS	2.4
1	A	242	ALA	2.4
1	A	272	LEU	2.4
1	A	220	GLY	2.4
1	A	197	ARG	2.4
1	A	207	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	69	ALA	2.4
1	A	23	LYS	2.3
1	A	80	ALA	2.3
1	A	26	SER	2.3
1	A	53	TRP	2.3
1	A	101	ARG	2.3
1	A	311	ALA	2.3
1	A	231	GLU	2.3
1	A	324	ASN	2.3
1	A	153	LEU	2.3
1	A	328	GLY	2.3
1	A	100	ALA	2.2
1	A	76	ALA	2.2
1	A	148	ALA	2.2
1	A	190	PHE	2.2
1	A	329	GLU	2.2
1	A	237	TYR	2.2
1	A	151	LYS	2.1
1	A	133	VAL	2.1
1	A	234	VAL	2.1
1	A	331	LEU	2.1
1	A	115	HIS	2.1
1	A	140	CYS	2.1
1	A	243	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](#)

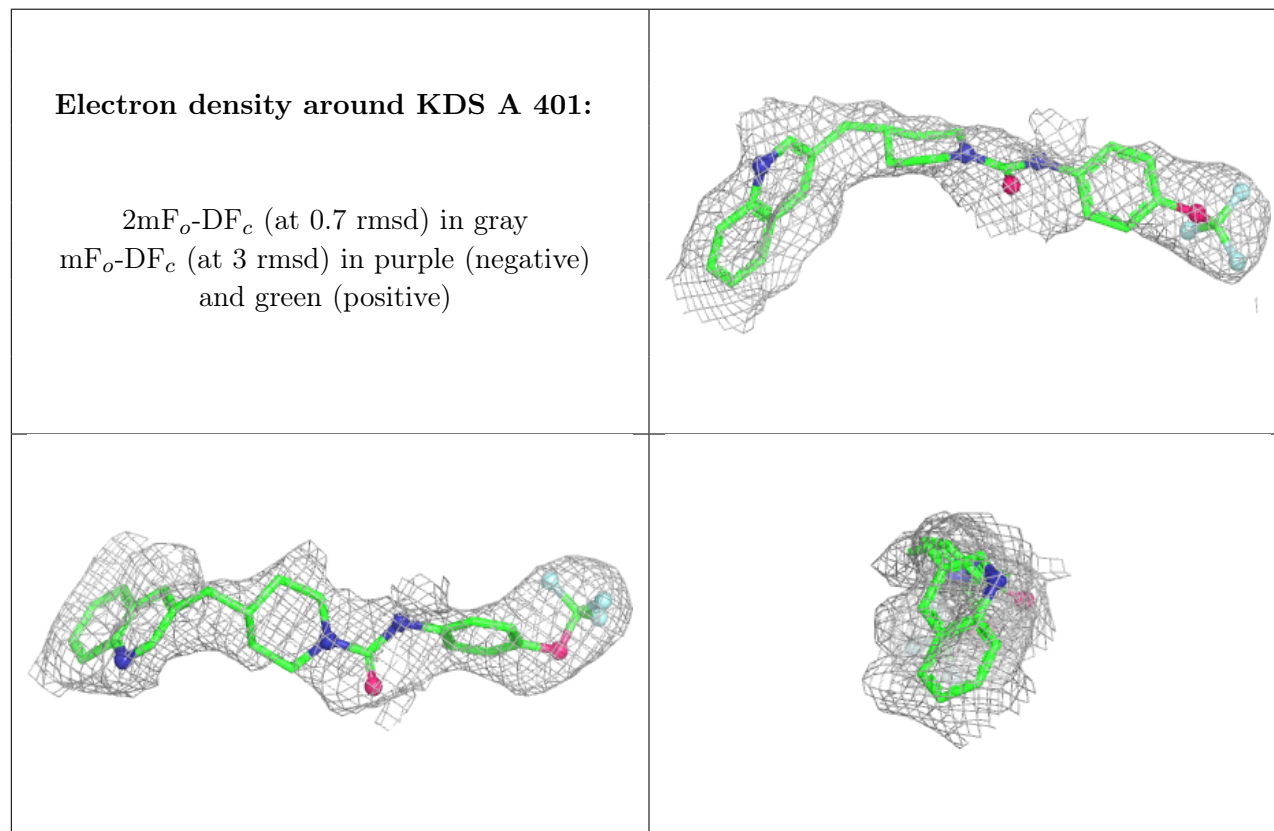
There are no oligosaccharides in this entry.

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	KDS	A	401	31/31	0.72	0.17	22,26,36,40	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.