



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:03 AM BST

PDB ID : 5HES
Title : Human leucine zipper- and sterile alpha motif-containing kinase (ZAK, MLT, HCCS-4, MRK, AZK, MLTK) in complex with vemurafenib
Authors : Mathea, S.; Salah, E.; Abdul Azeez, K.R.; Tallant, C.; Szklarz, M.; Chaikuad, A.; Shrestha, B.; Sorrell, F.J.; Elkins, J.M.; Shrestha, L.; Burgess-Brown, N.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Knapp, S.
Deposited on : 2016-01-06
Resolution : 2.14 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

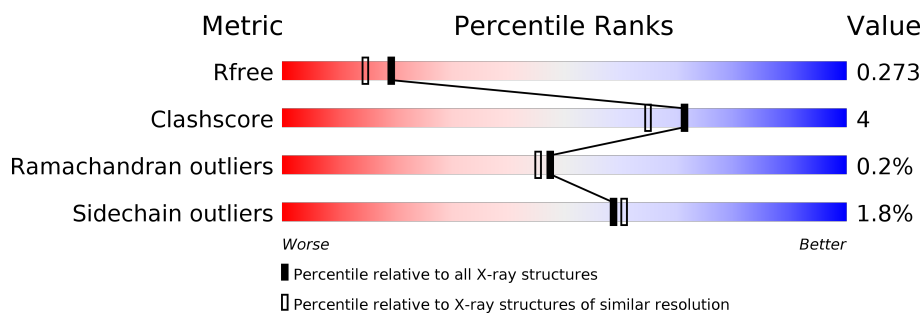
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	307	
1	B	307	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPO	A	161	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4782 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.

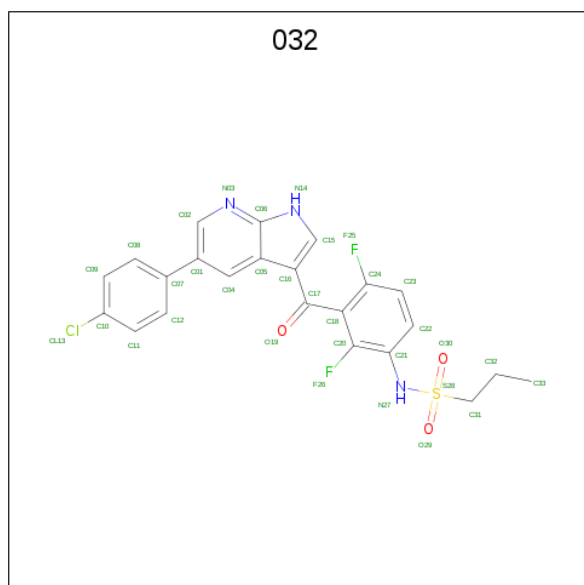
- Molecule 1 is a protein called Mitogen-activated protein kinase kinase kinase MLT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	P	S	0	0	0
			2305	1475	382	432	1	15			
1	B	278	Total	C	N	O	S		0	1	0
			2224	1428	366	415	15				

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	SER	-	expression tag	UNP Q9NYL2
A	4	MET	-	expression tag	UNP Q9NYL2
B	3	SER	-	expression tag	UNP Q9NYL2
B	4	MET	-	expression tag	UNP Q9NYL2

- Molecule 2 is N-(3-{[5-(4-chlorophenyl)-1H-pyrrolo[2,3-b]pyridin-3-yl]carbonyl}-2,4-difluorophenyl)propane-1-sulfonamide (three-letter code: 032) (formula: C₂₃H₁₈ClF₂N₃O₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			33	23	1	2	3	3	1		
2	B	1	Total	C	Cl	F	N	O	S	0	0
			33	23	1	2	3	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

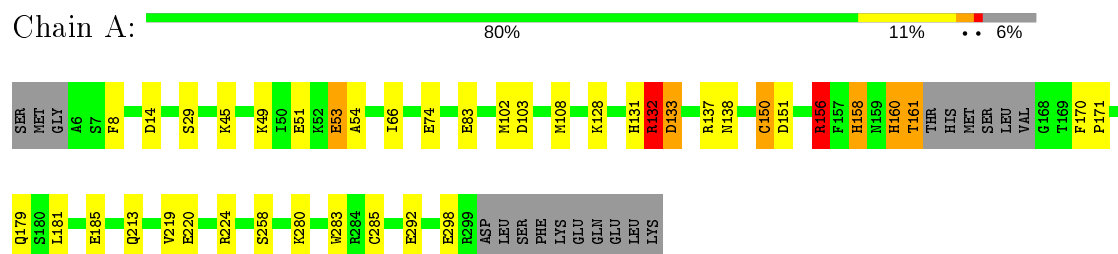
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	86	Total	O	0	0
			86	86		

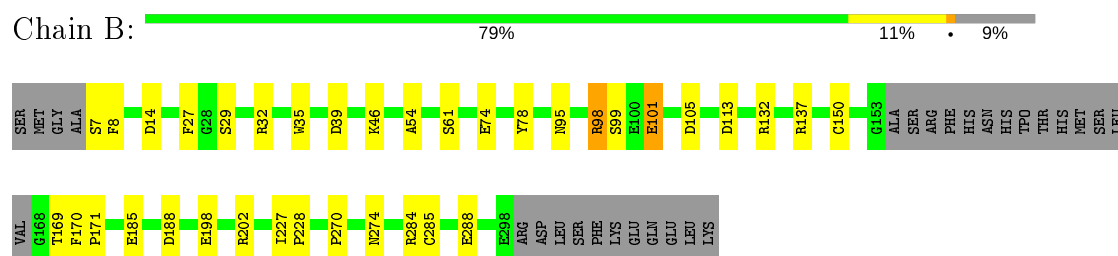
3 Residue-property plots

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. 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. 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: Mitogen-activated protein kinase kinase kinase MLT



- Molecule 1: Mitogen-activated protein kinase kinase kinase MLT



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	78.71Å 78.71Å 133.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.70 – 2.14 29.47 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.6 (78.70-2.14) 99.7 (29.47-2.14)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.7	Depositor
R, R_{free}	0.180 , 0.226 0.228 , 0.273	Depositor DCC
R_{free} test set	2274 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4782	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: TPO, 032, EDO

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	1.35	6/2347 (0.3%)	1.30	15/3173 (0.5%)
1	B	1.37	15/2278 (0.7%)	1.23	9/3082 (0.3%)
All	All	1.36	21/4625 (0.5%)	1.27	24/6255 (0.4%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	GLU	CD-OE2	8.10	1.34	1.25
1	B	78	TYR	CE2-CZ	7.33	1.48	1.38
1	B	198	GLU	CD-OE2	7.07	1.33	1.25
1	B	198	GLU	CD-OE1	6.09	1.32	1.25
1	B	185	GLU	CD-OE1	5.94	1.32	1.25
1	B	113	ASP	CG-OD2	5.91	1.39	1.25
1	A	29	SER	CB-OG	5.71	1.49	1.42
1	A	53	GLU	CD-OE2	5.69	1.31	1.25
1	B	95	ASN	C-O	-5.56	1.12	1.23
1	B	29	SER	CB-OG	5.48	1.49	1.42
1	B	150	CYS	CB-SG	-5.48	1.72	1.81
1	B	35	TRP	CG-CD1	5.46	1.44	1.36
1	A	14	ASP	CB-CG	5.38	1.63	1.51
1	B	27	PHE	CE2-CZ	5.37	1.47	1.37
1	B	98	ARG	CZ-NH1	5.28	1.40	1.33
1	A	292	GLU	CG-CD	5.24	1.59	1.51
1	B	74	GLU	CD-OE2	-5.22	1.20	1.25
1	B	61[A]	SER	C-O	5.12	1.33	1.23
1	B	61[B]	SER	C-O	5.12	1.33	1.23
1	A	53	GLU	CA-CB	5.12	1.65	1.53
1	B	54	ALA	C-O	-5.07	1.13	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH1	12.38	126.49	120.30
1	A	156	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	B	14	ASP	CB-CG-OD1	9.46	126.81	118.30
1	B	137	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	103	ASP	CB-CG-OD1	7.62	125.16	118.30
1	A	224	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	32	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	137	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	B	188	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	137	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	132	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	224	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	B	188	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	74	GLU	OE1-CD-OE2	-5.95	116.16	123.30
1	B	132	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	108	MET	CG-SD-CE	-5.78	90.96	100.20
1	A	133	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	102	MET	CG-SD-CE	-5.52	91.37	100.20
1	A	258	SER	N-CA-CB	-5.42	102.37	110.50
1	A	14	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	292	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	150	CYS	CA-CB-SG	5.27	123.48	114.00
1	B	98	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	132	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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	2305	0	2268	22	0
1	B	2224	0	2195	10	0
2	A	33	0	18	0	0
2	B	33	0	18	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	93	0	0	3	0
4	B	86	0	0	0	0
All	All	4782	0	4511	32	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 4.

All (32) 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:51:GLU:HG3	1:A:161:TPO:O1P	1.41	1.16
1:A:51:GLU:CG	1:A:161:TPO:O1P	2.09	1.00
1:A:158:HIS:NE2	1:A:161:TPO:O2P	2.14	0.81
1:A:128:LYS:HE3	1:A:185:GLU:OE2	1.83	0.78
1:A:51:GLU:CD	1:A:161:TPO:O1P	2.22	0.76
1:A:158:HIS:CD2	1:A:161:TPO:O2P	2.46	0.68
1:A:49:LYS:O	1:A:156:ARG:NH2	2.28	0.66
1:A:45:LYS:NZ	4:A:501:HOH:O	2.35	0.58
1:A:128:LYS:CE	1:A:185:GLU:OE2	2.51	0.58
1:A:160:HIS:O	1:A:161:TPO:OG1	2.23	0.57
1:A:179:GLN:HG3	1:A:181:LEU:HG	1.88	0.54
1:A:219:VAL:HG12	1:A:220:GLU:HG3	1.91	0.53
1:A:51:GLU:N	1:A:53:GLU:OE2	2.36	0.51
1:A:8:PHE:CG	1:A:54:ALA:HB1	2.46	0.50
1:B:270:PRO:O	1:B:274:ASN:ND2	2.43	0.49
1:B:98:ARG:O	1:B:101:GLU:HG2	2.12	0.49
1:A:49:LYS:HE3	1:A:156:ARG:NH1	2.29	0.48
1:A:66:ILE:CG2	1:A:150:CYS:HB3	2.45	0.47
1:A:51:GLU:OE2	1:A:161:TPO:O1P	2.32	0.46
1:A:133:ASP:O	1:A:138:ASN:ND2	2.48	0.46
1:B:227:ILE:O	1:B:228:PRO:C	2.54	0.45
1:B:99:SER:OG	1:B:202:ARG:NE	2.45	0.45
1:A:170:PHE:N	1:A:171:PRO:CD	2.79	0.45
4:A:516:HOH:O	1:B:285:CYS:CB	2.64	0.45
1:B:7:SER:HB3	1:B:8:PHE:CD2	2.51	0.45
4:A:516:HOH:O	1:B:285:CYS:HB3	2.18	0.44
1:A:131:HIS:O	1:A:132:ARG:HB2	2.17	0.44
1:B:169:THR:HG22	1:B:169:THR:O	2.18	0.44
1:B:284:ARG:HD2	1:B:288:GLU:CD	2.39	0.42
1:B:170:PHE:N	1:B:171:PRO:CD	2.83	0.42
1:A:213:GLN:NE2	1:A:298:GLU:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:HA	1:A:283:TRP:CE2	2.56	0.41

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	284/307 (92%)	270 (95%)	13 (5%)	1 (0%)	34	29
1	B	275/307 (90%)	266 (97%)	9 (3%)	0	100	100
All	All	559/614 (91%)	536 (96%)	22 (4%)	1 (0%)	47	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	HIS

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	251/273 (92%)	246 (98%)	5 (2%)	55	57
1	B	244/273 (89%)	240 (98%)	4 (2%)	62	65
All	All	495/546 (91%)	486 (98%)	9 (2%)	59	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ARG
1	A	151	ASP
1	A	156	ARG
1	A	158	HIS
1	A	285	CYS
1	B	39	ASP
1	B	46	LYS
1	B	101	GLU
1	B	105	ASP

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

Mol	Chain	Res	Type
1	A	10	GLN
1	A	278	HIS
1	B	222	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\# Z > 2$
1	TPO	A	161	1	8,10,11	2.45	4 (50%)	10,14,16	1.89	3 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	161	1	-	3/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	TPO	P-O2P	-4.25	1.38	1.54
1	A	161	TPO	P-OG1	2.87	1.64	1.59
1	A	161	TPO	P-O1P	2.76	1.59	1.50
1	A	161	TPO	O-C	2.58	1.30	1.19

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	TPO	CG2-CB-CA	-4.04	105.19	113.16
1	A	161	TPO	O3P-P-O2P	2.40	116.82	107.64
1	A	161	TPO	O3P-P-OG1	2.09	115.38	105.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	161	TPO	CG2-CB-OG1-P
1	A	161	TPO	CB-OG1-P-O3P
1	A	161	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	161	TPO	7	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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$
3	EDO	B	402	-	3,3,3	0.55	0	2,2,2	0.19	0
3	EDO	A	402	-	3,3,3	0.59	0	2,2,2	0.27	0
2	032	A	401	-	35,36,36	1.23	3 (8%)	43,53,53	1.16	6 (13%)
2	032	B	401	-	35,36,36	1.44	2 (5%)	43,53,53	1.06	3 (6%)

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
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
2	032	A	401	-	-	0/17/21/21	0/4/4/4
2	032	B	401	-	-	0/17/21/21	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	032	C16-C17	-6.81	1.42	1.50
2	A	401	032	C16-C17	-4.41	1.45	1.50
2	A	401	032	C16-C05	2.89	1.45	1.42
2	A	401	032	C06-N03	-2.31	1.33	1.37
2	B	401	032	C32-C31	-2.08	1.40	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	032	O29-S28-C31	3.12	112.84	107.86
2	A	401	032	C31-S28-N27	-3.07	102.38	106.77
2	A	401	032	O19-C17-C18	-2.83	114.91	119.74
2	B	401	032	C21-N27-S28	2.72	130.07	123.59
2	A	401	032	C21-N27-S28	2.67	129.97	123.59
2	A	401	032	O29-S28-C31	2.52	111.88	107.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	032	C33-C32-C31	-2.33	105.60	112.45
2	A	401	032	O19-C17-C16	2.25	125.35	120.79
2	A	401	032	C01-C04-C05	-2.00	117.91	122.30

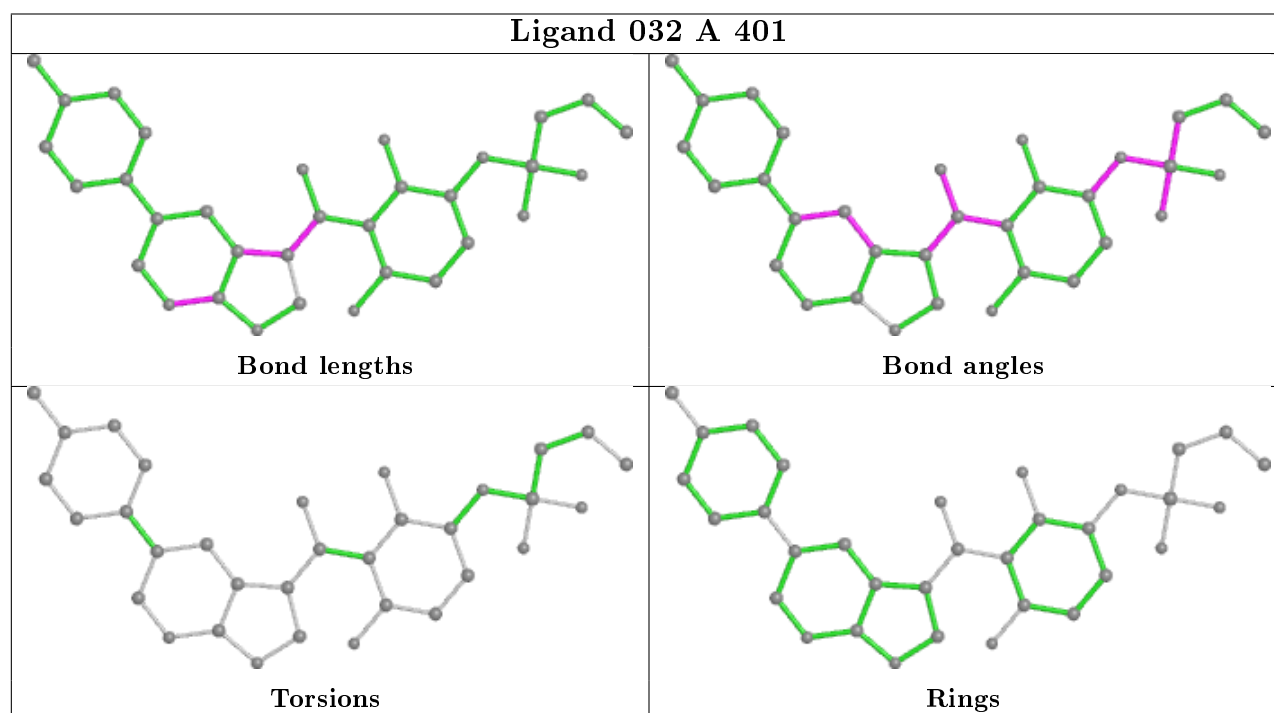
There are no chirality outliers.

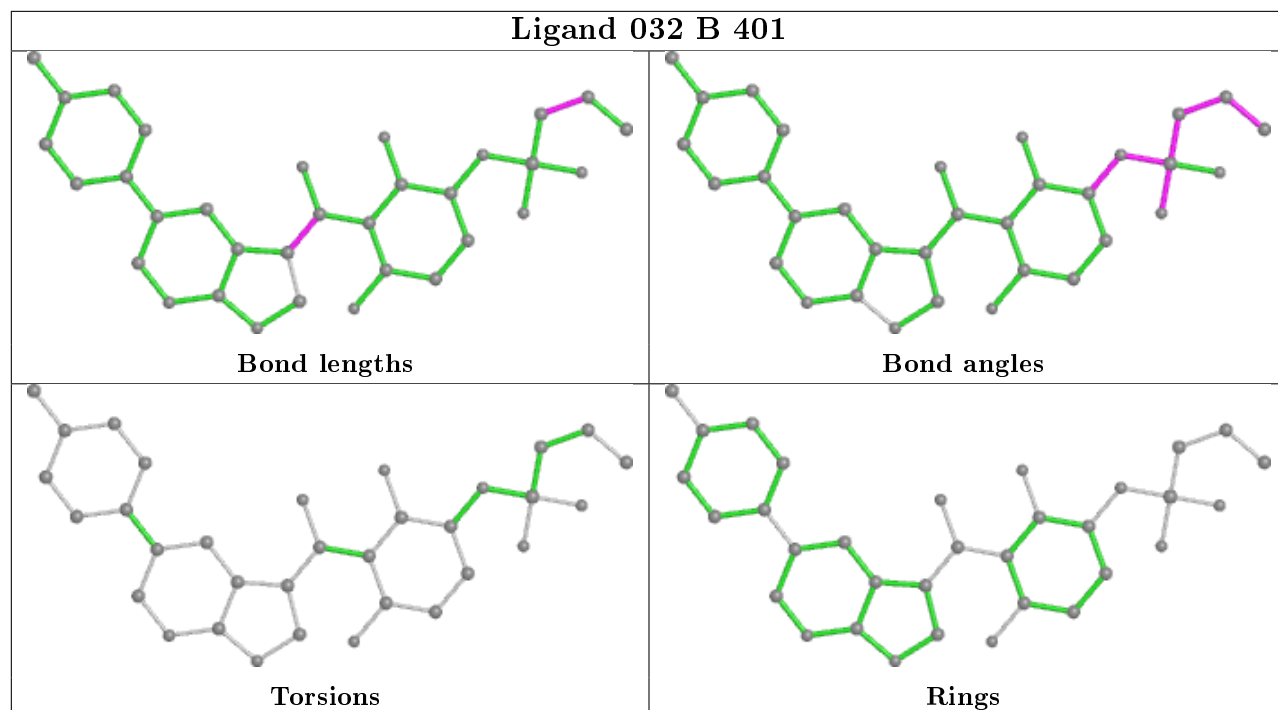
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

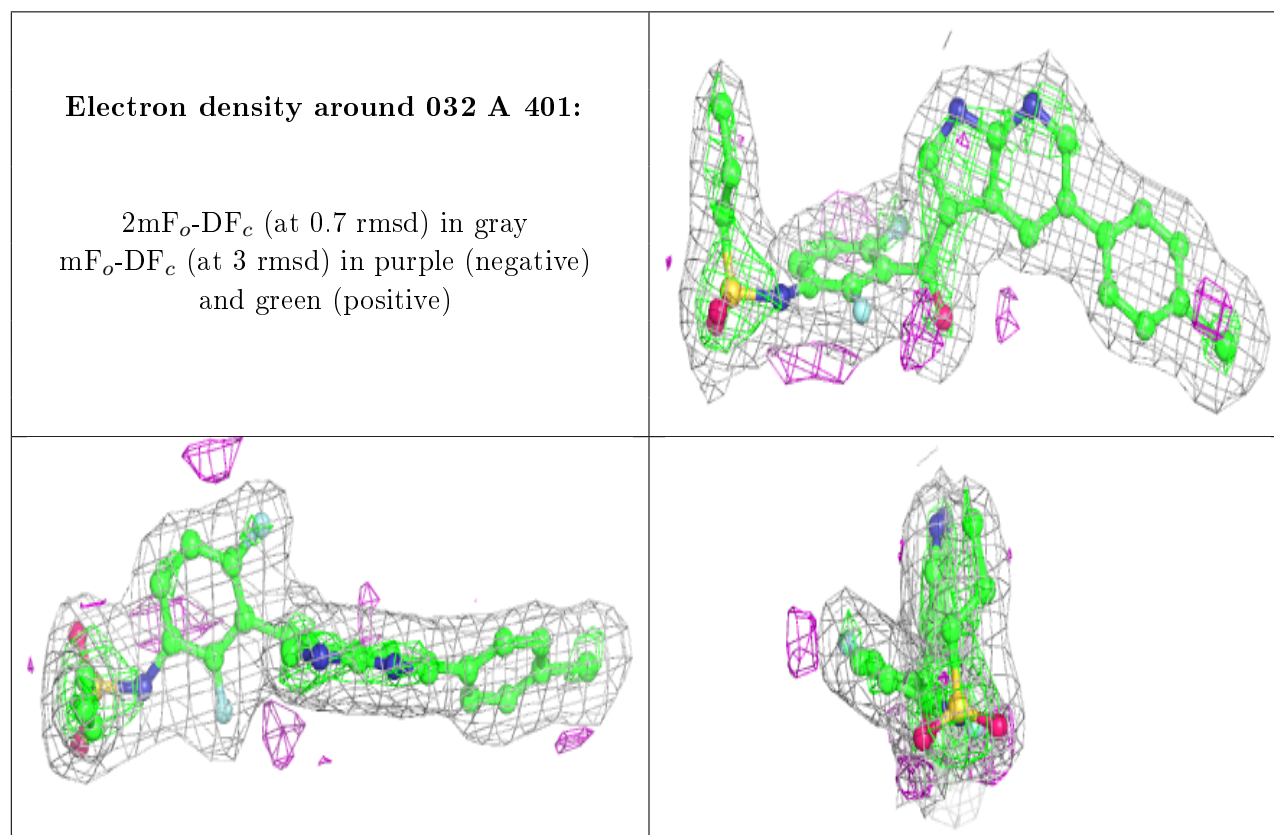
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

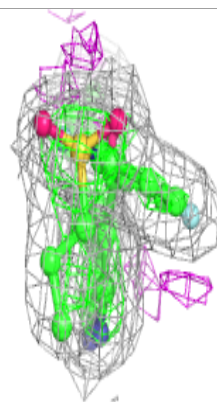
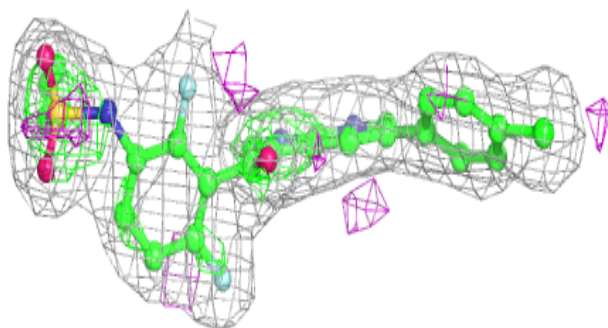
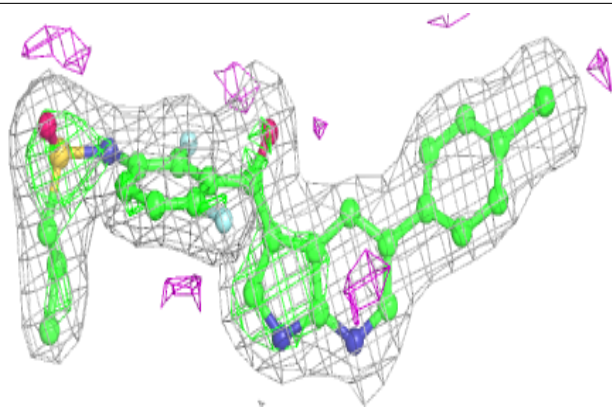
Unable to reproduce the depositors R factor - this section is therefore empty.

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 032 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 [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.