



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 02:26 AM EDT

PDB ID : 8SCV / pdb_00008scv
Title : Crystal structure of IRAK4-HSA complexed with BMS-986126; 6-((5-CYAN O-2-PYRIMIDINYL)AMINO)-N-((2R)-2-FLUORO-3-HYDROXYLBUTYL)-4-(ISOPROPYLAMINO)NICOTINAMIDE
Authors : Muckelbauer, J.K.; Ghosh, K.
Deposited on : 2023-04-05
Resolution : 2.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

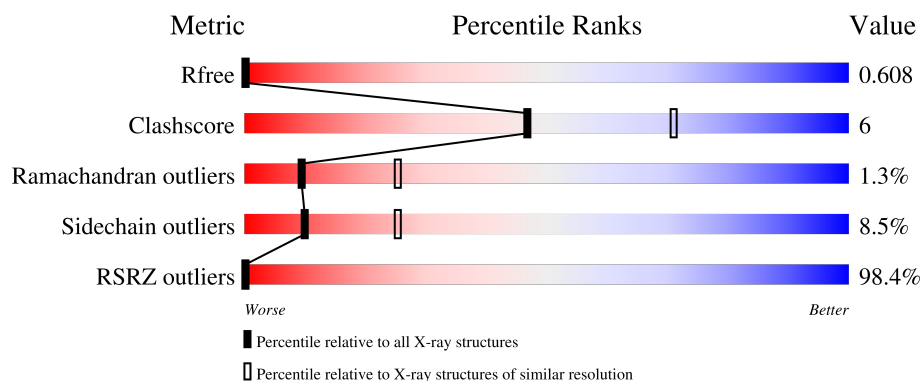
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	305	92% 74% 18% 5%
2	B	305	85% 74% 11% 14%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4214 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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	290	2203	1385	369	431	3	15	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	expression tag	UNP Q9NWZ3
A	157	ALA	-	expression tag	UNP Q9NWZ3
A	158	MET	-	expression tag	UNP Q9NWZ3
A	159	GLY	-	expression tag	UNP Q9NWZ3

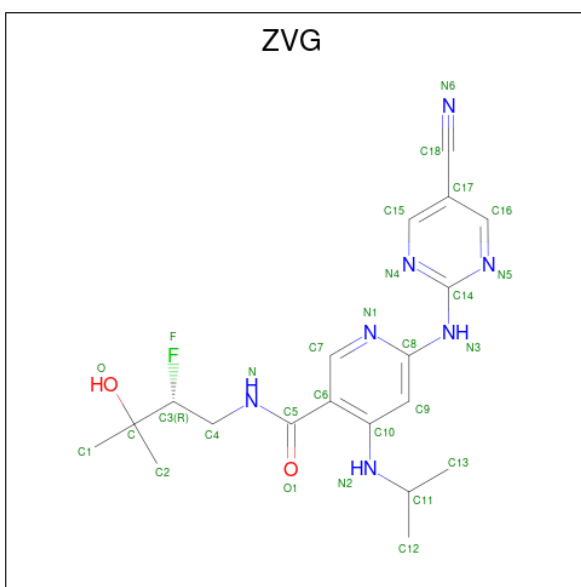
- Molecule 2 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
2	B	263	1879	1180	316	368	2	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 3 is 6-[(5-cyanopyrimidin-2-yl)amino]-N-[(2R)-2-fluoro-3-hydroxy-3-methylbutyl]-4-[(propan-2-yl)amino]pyridine-3-carboxamide (CCD ID: ZVG) (formula: C₁₉H₂₄FN₇O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0
			29	19	1	7	2	
3	B	1	Total	C	F	N	O	0
			29	19	1	7	2	

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total 38	O 38	0	0
5	B	26	Total 26	O 26	0	0

E456	L396	SER	GLU	L397	GLY	L398	GLY	L399	GLY	L400	GLY	L401	GLY	L402	GLY	L403	GLY	L404	GLY	L405	GLY	E406	GLY	E407	GLY	K408	GLY	L409	GLY	L410	GLY	E411	GLY	D412	GLY	L413	GLY	L414	GLY	D415	GLY	K416	GLY	L417	GLY	M418	GLY	M419	GLY	D420	GLY	A421	GLY	D422	GLY	S423	GLY	T424	GLY	S425	GLY	V426	GLY	E427	GLY	A428	GLY	M429	GLY	Y430	GLY	S431	GLY	V432	GLY	A433	GLY	S434	GLY	Q435	GLY	C436	GLY	L437	GLY	H438	GLY	E439	GLY	K440	GLY	K441	GLY	M442	GLY	K443	GLY	R444	GLY	P445	GLY	D446	GLY	L447	GLY	K448	GLY	K449	GLY	V450	GLY	Q451	GLY	Q452	GLY	L453	GLY	L454	GLY	Q455	GLY	L456	GLY	L457	GLY	L458	GLY	L459	GLY	SER	GLY	L342	GLY	V343	GLY	M344	GLY	T345	GLY	S346	GLY	E347	GLY	L348	GLY	T349	GLY	L349	GLY	L350	GLY	T351	GLY	A352	GLY	M353	GLY	A354	GLY	P355	GLY	L356	GLY	E357	GLY	A358	GLY	L359	GLY	L360	GLY	R361	GLY	G362	GLY	E363	GLY	L364	GLY	T365	GLY	P366	GLY	K367	GLY	S368	GLY	D369	GLY	L370	GLY	Y371	GLY	S372	GLY	F373	GLY	G374	GLY	V375	GLY	V376	GLY	L377	GLY	L378	GLY	E379	GLY	L380	GLY	L381	GLY	T382	GLY	G383	GLY	L384	GLY	P385	GLY	A386	GLY	V387	GLY	D388	GLY	E389	GLY	R390	GLY	R391	GLY	E392	GLY	P393	GLY	G394	GLY	L395	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	86.29Å 103.75Å 139.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.69 48.11 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.11-2.69) 99.8 (48.11-2.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.220 , 0.261 0.583 , 0.608	Depositor DCC
R_{free} test set	860 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 218.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.39	EDS
Total number of atoms	4214	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% 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: SO4, TPO, SEP, ZVG

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	0.92	5/2211 (0.2%)	1.41	11/2996 (0.4%)
2	B	0.85	0/1882	1.40	12/2561 (0.5%)
All	All	0.89	5/4093 (0.1%)	1.41	23/5557 (0.4%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLN	CD-OE1	5.78	1.34	1.23
1	A	166	HIS	ND1-CE1	5.60	1.38	1.32
1	A	178	ASN	CG-OD1	5.50	1.34	1.23
1	A	232	GLN	CD-OE1	5.43	1.33	1.23
1	A	207	ASN	CG-OD1	5.17	1.33	1.23

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	HIS	CB-CG-CD2	-7.65	121.26	131.20
1	A	438	HIS	CA-C-N	7.07	130.07	120.38
1	A	438	HIS	C-N-CA	7.07	130.07	120.38
2	B	224	GLU	CA-C-N	5.62	127.81	120.28
2	B	224	GLU	C-N-CA	5.62	127.81	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	345	TPO	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	2203	0	2081	33	0
2	B	1879	0	1695	14	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	38	0	0	2	0
5	B	26	0	0	0	0
All	All	4214	0	3776	45	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 6.

The worst 5 of 45 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:224:GLU:HA	1:A:226:LEU:H	1.17	1.07
1:A:224:GLU:HA	1:A:226:LEU:N	1.96	0.80
1:A:223:THR:O	1:A:224:GLU:CG	2.30	0.80
1:A:224:GLU:CA	1:A:226:LEU:H	1.99	0.74
1:A:345:TPO:HG22	1:A:346:SEP:N	2.09	0.68

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	282/305 (92%)	266 (94%)	11 (4%)	5 (2%)	6	18
2	B	247/305 (81%)	232 (94%)	13 (5%)	2 (1%)	16	37
All	All	529/610 (87%)	498 (94%)	24 (4%)	7 (1%)	9	25

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	GLU
1	A	406	GLU
2	B	406	GLU
1	A	254	ASP
1	A	347	ARG

5.3.2 Protein sidechains

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	225/260 (86%)	203 (90%)	22 (10%)	7	19
2	B	177/261 (68%)	165 (93%)	12 (7%)	14	35
All	All	402/521 (77%)	368 (92%)	34 (8%)	10	25

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	399	ILE

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Mol	Chain	Res	Type
2	B	406	GLU
2	B	439	GLU
1	A	252	SER
1	A	237	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	190	ASN
2	B	305	ASN
2	B	442	ASN
1	A	207	ASN
1	A	286	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	TPO	B	345	2	8,10,11	0.93	0	10,14,16	1.33	1 (10%)
1	TPO	A	345	1	8,10,11	0.85	0	10,14,16	1.32	1 (10%)
1	SEP	A	284	1	8,9,10	2.50	3 (37%)	7,12,14	8.33	4 (57%)
2	SEP	B	346	2	8,9,10	1.05	1 (12%)	7,12,14	3.13	3 (42%)
1	SEP	A	346	1	8,9,10	0.79	0	7,12,14	2.69	1 (14%)

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	TPO	B	345	2	-	3/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	SEP	A	284	1	-	3/6/8/10	-
2	SEP	B	346	2	-	2/6/8/10	-
1	SEP	A	346	1	-	2/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	SEP	P-OG	5.01	1.76	1.60
1	A	284	SEP	CB-CA	3.72	1.62	1.52
1	A	284	SEP	OG-CB	2.48	1.54	1.44
2	B	346	SEP	P-OG	-2.12	1.53	1.60

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	SEP	OG-CB-CA	21.09	128.66	108.14
2	B	346	SEP	OG-CB-CA	6.91	114.87	108.14
1	A	346	SEP	OG-CB-CA	6.65	114.62	108.14
1	A	284	SEP	O2P-P-OG	5.01	119.74	106.67
2	B	346	SEP	O3P-P-O1P	-3.17	98.50	110.83

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	284	SEP	CB-OG-P-O3P
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	CA-CB-OG1-P
1	A	346	SEP	N-CA-CB-OG
1	A	346	SEP	C-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	345	TPO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	346	SEP	3	0

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
3	ZVG	B	501	-	28,30,30	1.94	6 (21%)	37,42,42	1.25	6 (16%)
4	SO4	B	502	-	4,4,4	0.34	0	6,6,6	0.14	0
4	SO4	A	502	-	4,4,4	0.25	0	6,6,6	0.09	0
3	ZVG	A	501	-	28,30,30	1.61	6 (21%)	37,42,42	1.12	3 (8%)

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	ZVG	B	501	-	-	2/22/25/25	0/2/2/2
3	ZVG	A	501	-	-	3/22/25/25	0/2/2/2

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ZVG	C14-N5	5.47	1.42	1.34
3	B	501	ZVG	C14-N4	4.41	1.40	1.34
3	A	501	ZVG	C14-N5	3.90	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	ZVG	C9-C10	3.85	1.45	1.39
3	A	501	ZVG	C5-N	3.38	1.41	1.33

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	ZVG	F-C3-C4	3.28	111.11	108.06
3	A	501	ZVG	C15-C17-C16	2.96	117.59	115.57
3	B	501	ZVG	C10-N2-C11	2.92	128.81	124.66
3	B	501	ZVG	C15-C17-C16	2.53	117.30	115.57
3	A	501	ZVG	N3-C14-N4	2.38	123.04	116.29

There are no chirality outliers.

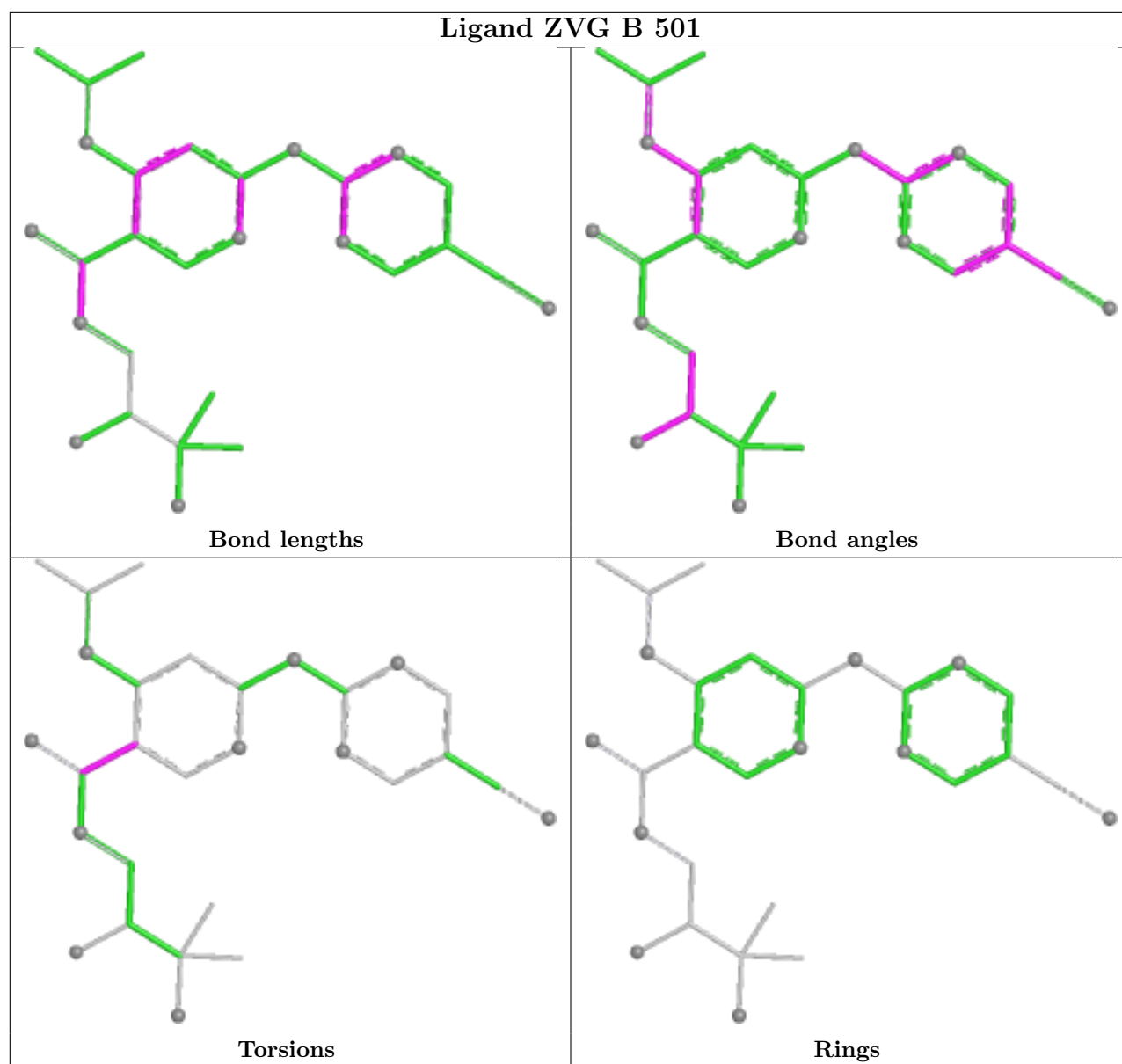
All (5) torsion outliers are listed below:

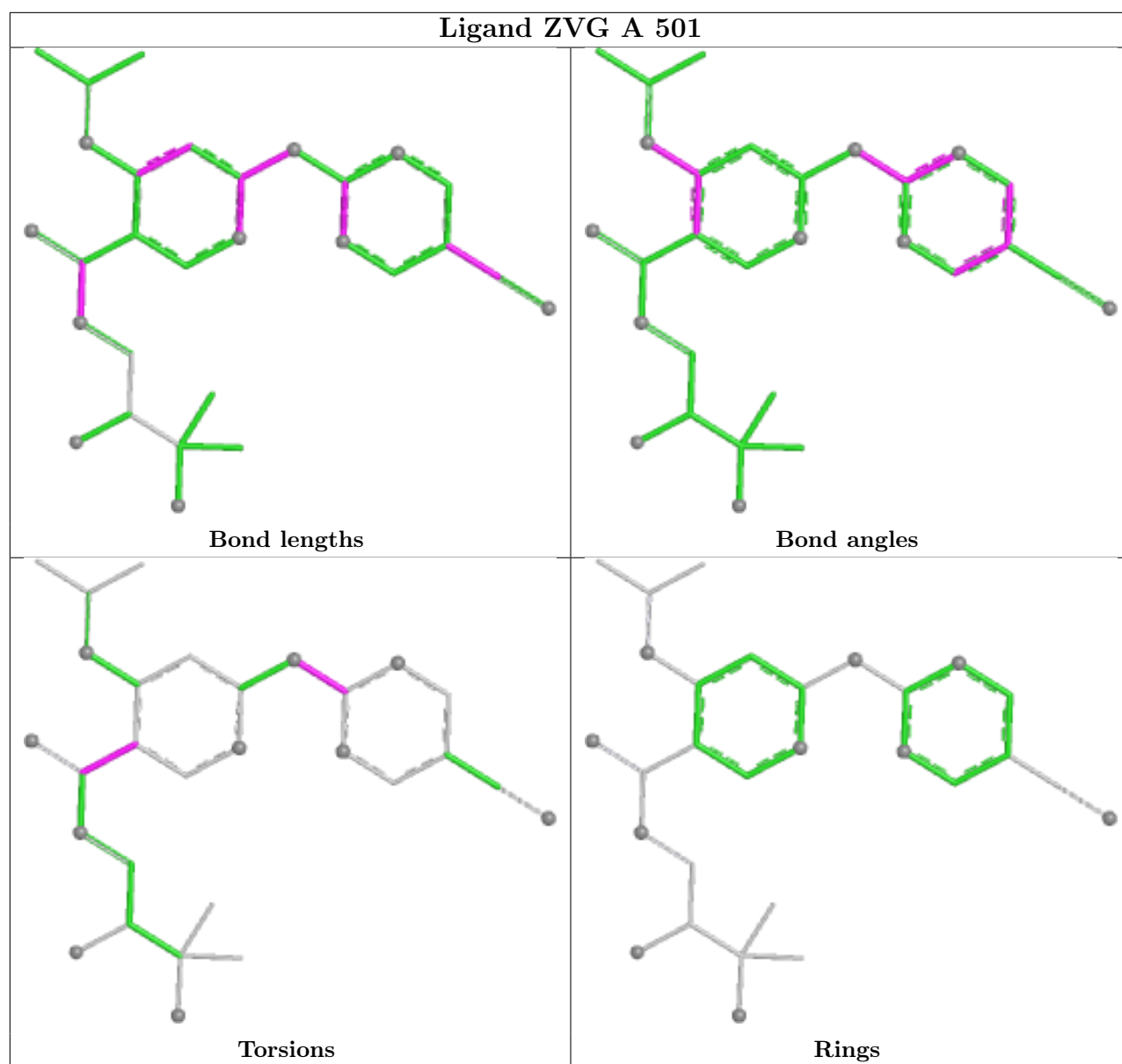
Mol	Chain	Res	Type	Atoms
3	A	501	ZVG	O1-C5-C6-C7
3	B	501	ZVG	O1-C5-C6-C7
3	B	501	ZVG	N-C5-C6-C7
3	A	501	ZVG	N-C5-C6-C7
3	A	501	ZVG	N5-C14-N3-C8

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](#)

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	287/305 (94%)	6.34	281 (97%) 0 0	31, 59, 91, 111	1 (0%)
2	B	261/305 (85%)	6.90	258 (98%) 0 0	44, 78, 142, 159	0
All	All	548/610 (89%)	6.61	539 (98%) 0 0	31, 67, 114, 159	1 (0%)

The worst 5 of 539 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	212	VAL	31.1
2	B	181	ASP	28.6
1	A	436	CYS	26.2
2	B	342	THR	25.7
1	A	450	VAL	25.5

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	284	10/11	0.34	0.30	57,64,71,73	0
2	TPO	B	345	11/12	0.54	0.27	73,75,87,87	0
1	SEP	A	346	10/11	0.66	0.30	95,97,101,102	0
2	SEP	B	346	10/11	0.70	0.19	69,71,74,74	0
1	TPO	A	345	11/12	0.73	0.20	79,93,95,113	0

6.3 Carbohydrates [i](#)

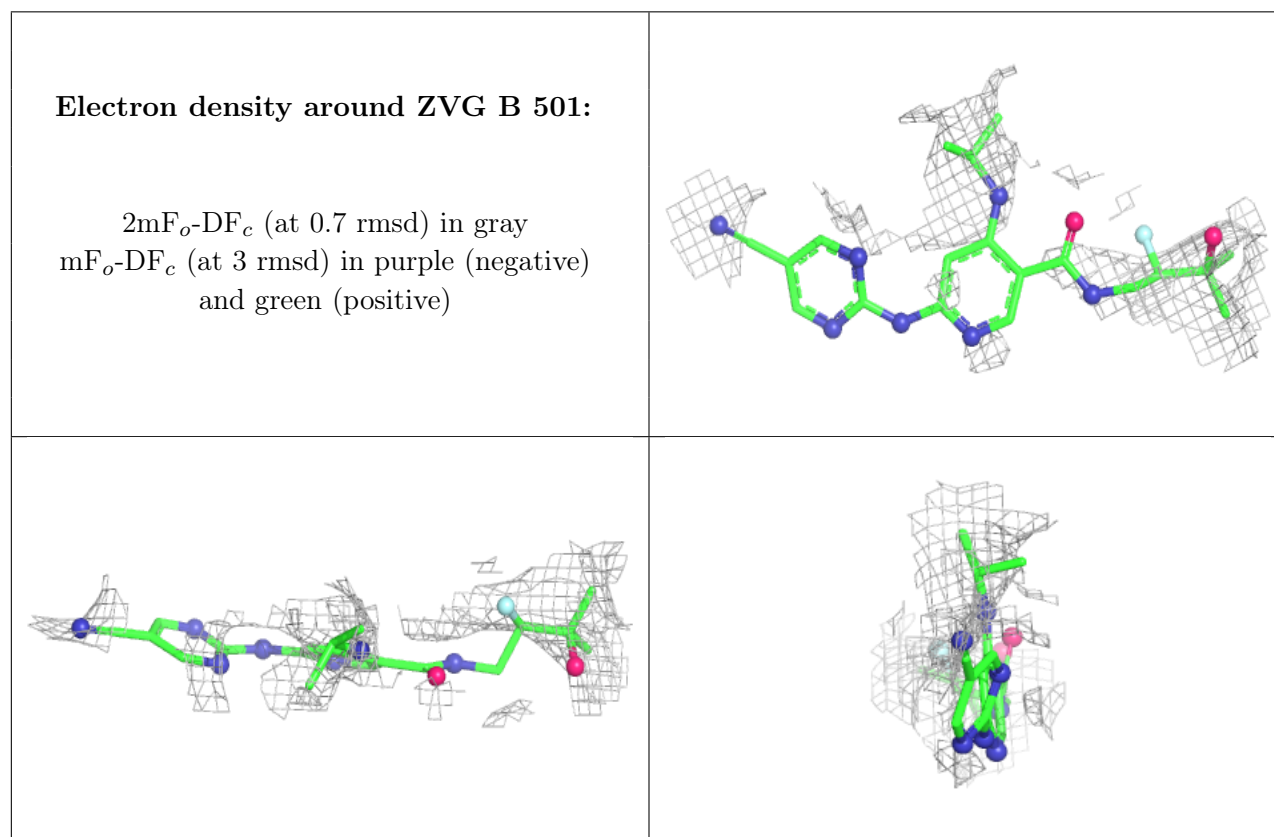
There are no oligosaccharides in this entry.

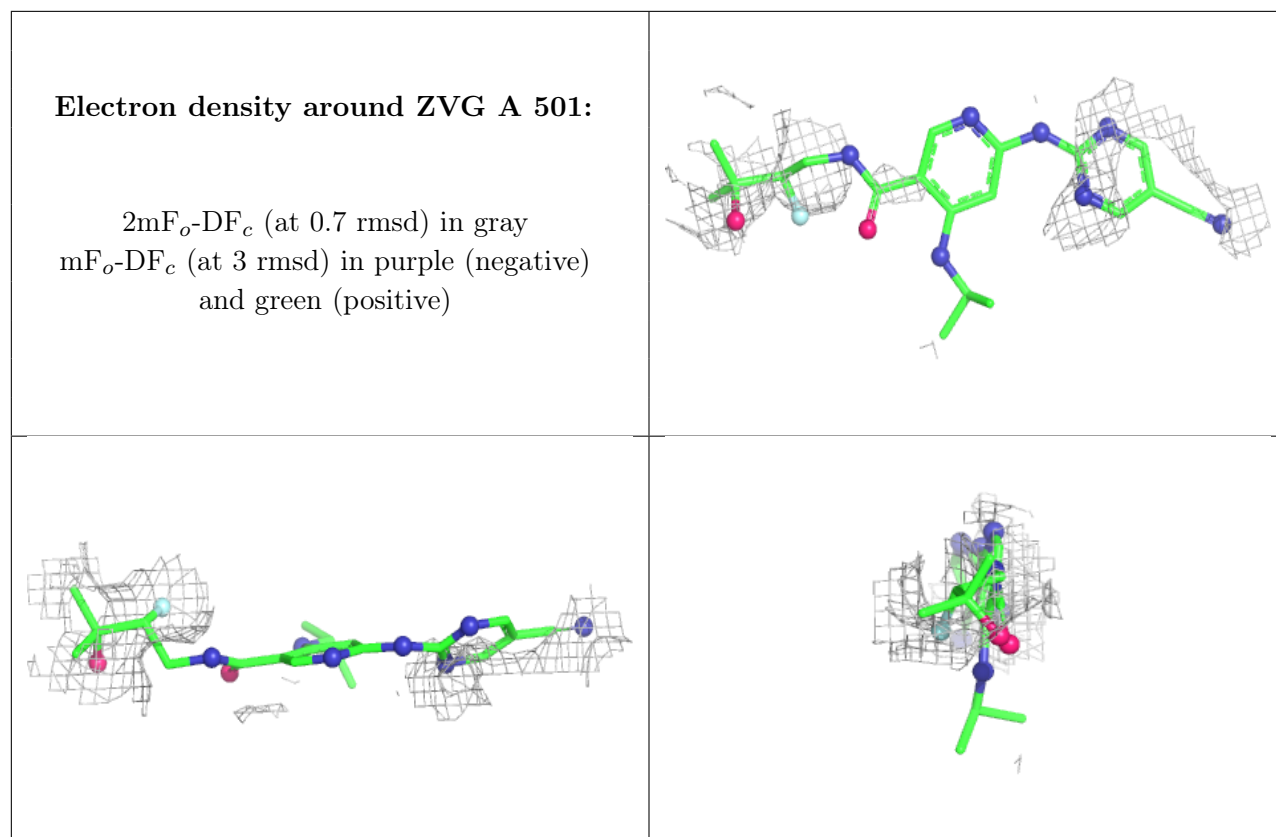
6.4 Ligands [i](#)

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
3	ZVG	B	501	29/29	0.36	0.27	55,68,76,80	0
4	SO4	A	502	5/5	0.39	0.35	144,148,149,150	0
3	ZVG	A	501	29/29	0.53	0.36	24,31,44,55	0
4	SO4	B	502	5/5	0.56	0.30	66,70,71,72	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.