



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:27 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-HYDROXYLBUTY L)-4-(ISOPROPYLAMINO)NICOTINAMIDE
Authors : Muckelbauer, J.K.; Ghosh, K.
Deposited on : 2023-04-05
Resolution : 2.69 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

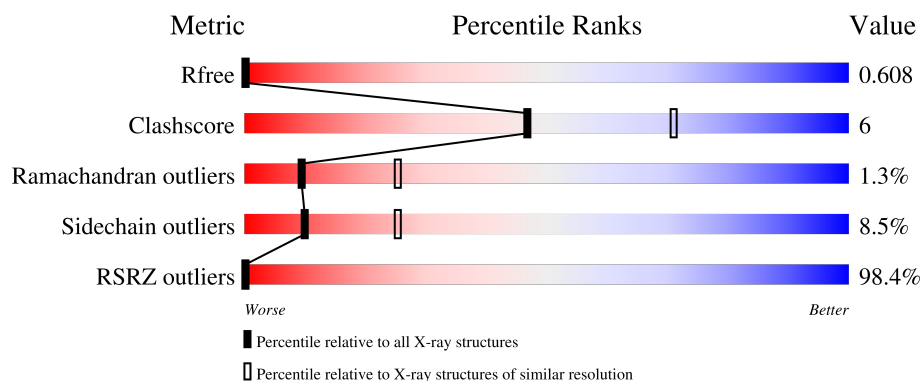
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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

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

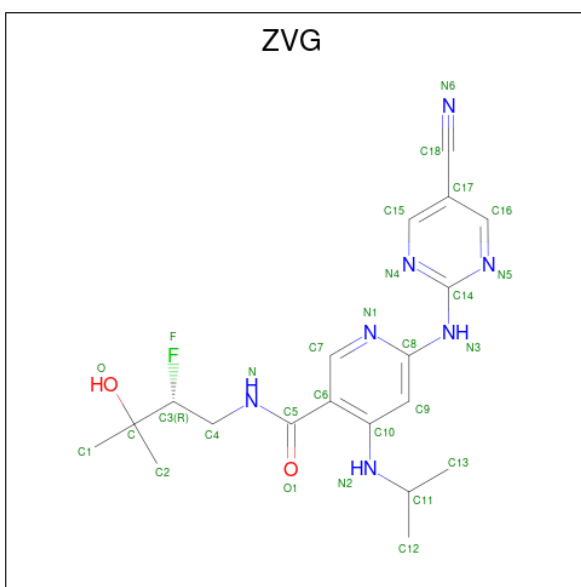
- Molecule 2 is a protein called Interleukin-1 receptor-associated kinase 4.

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	0
			29	19	1	7	2		
3	B	1	Total	C	F	N	O	0	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		

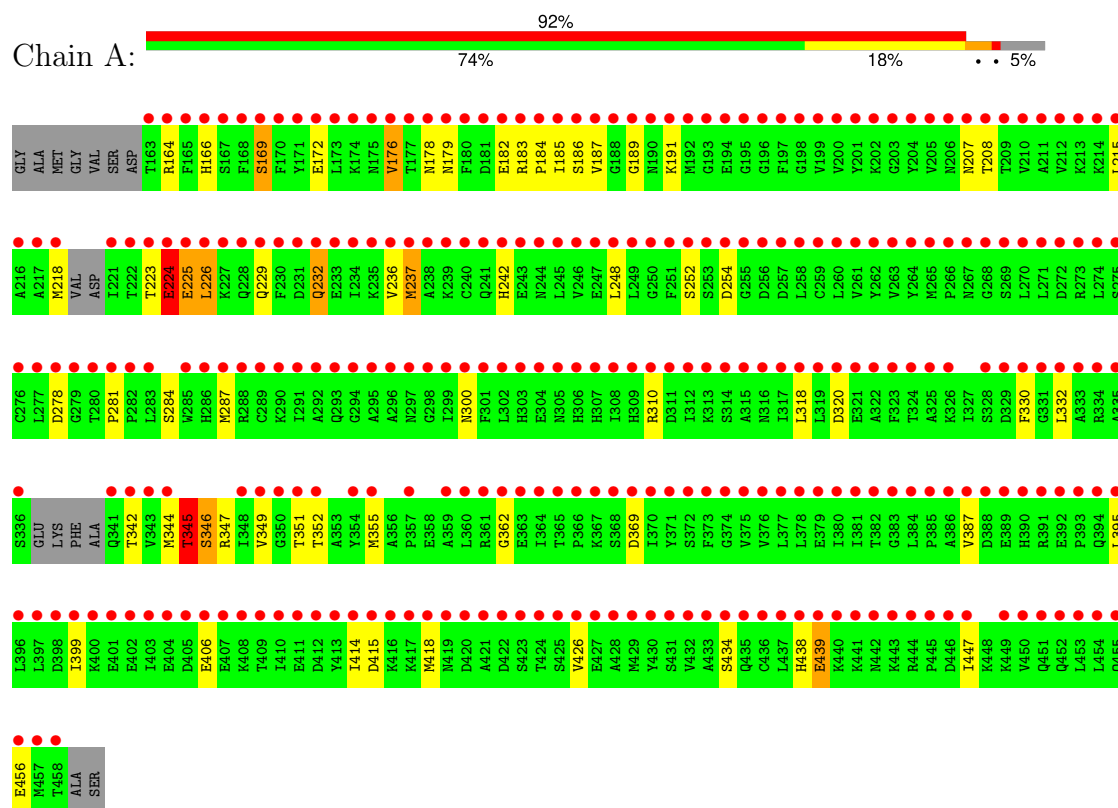
- Molecule 5 is water.

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

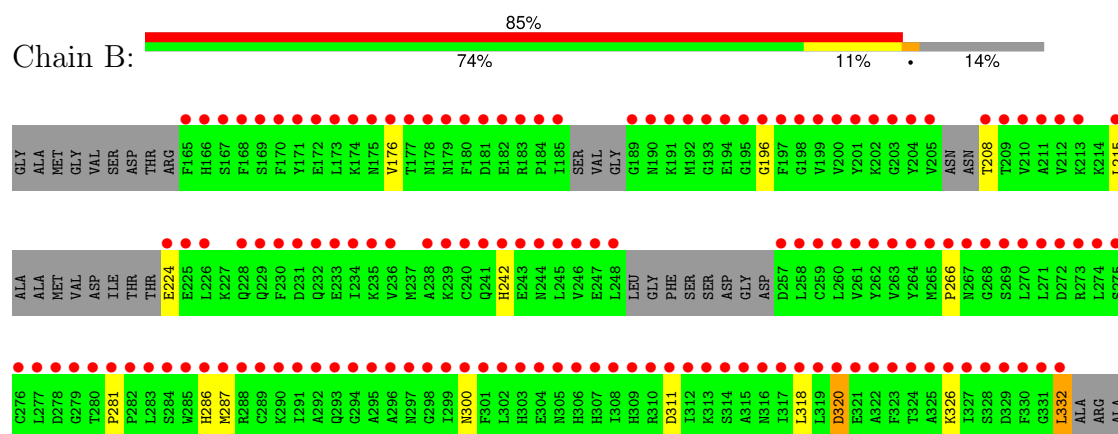
3 Residue-property plots

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: Interleukin-1 receptor-associated kinase 4



- Molecule 2: Interleukin-1 receptor-associated kinase 4



SER	E456	L396	SER
	M457	L397	GLU
	T458	D398	LYS
	A459	I399	PHE
		K400	ALA
		E401	GLN
		E402	T342
		I403	V343
		E404	M344
		D405	T345
	E406	S346	
	E407	E357	
	K408	I348	
	T409	V349	
	I410	GLY	
	E411	THR	
	D412	T352	
	Y413	A353	
	I414	Y354	
	D415	M355	
	K416	A356	
	K417	P357	
	M418	E358	
	M419	A359	
	D420	L360	
	A421	R361	
	D422	G362	
	S423	E363	
	T424	I364	
	S425	T365	
	V426	P366	
	E427	K367	
	A428	S368	
	M429	D369	
	Y430	I370	
	S431	Y371	
	V432	S372	
	A433	F373	
	S434	G374	
	Q435	V375	
	C436	V376	
	L437	L377	
	H438	L378	
	E439	E379	
	K440	I380	
	K441	I381	
	M442	T382	
	K443	G383	
	R444	L384	
	P445	P385	
	D446	A386	
	I447	V387	
	K448	D388	
	K449	E389	
	V450	H390	
	Q451	R391	
	K452	E392	
	L453	P393	
	L454	D394	
	Q455	L395	

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

All (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
1	A	242	HIS	CA-C-N	5.54	128.47	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	HIS	C-N-CA	5.54	128.47	120.38
2	B	369	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	185	ILE	CA-C-N	5.51	128.21	120.28
1	A	185	ILE	C-N-CA	5.51	128.21	120.28
1	A	369	ASP	CA-CB-CG	5.46	118.06	112.60
2	B	242	HIS	CA-C-N	5.43	128.30	120.38
2	B	242	HIS	C-N-CA	5.43	128.30	120.38
2	B	208	THR	CA-C-N	5.42	129.16	121.42
2	B	208	THR	C-N-CA	5.42	129.16	121.42
1	A	342	THR	N-CA-C	5.28	116.52	107.28
1	A	320	ASP	CA-CB-CG	5.28	117.88	112.60
2	B	355	MET	N-CA-C	5.21	117.87	110.10
1	A	439	GLU	CB-CG-CD	5.20	121.43	112.60
2	B	326	LYS	CA-C-N	5.16	127.49	120.63
2	B	326	LYS	C-N-CA	5.16	127.49	120.63
2	B	348	ILE	N-CA-C	-5.13	106.07	110.74
2	B	320	ASP	CA-CB-CG	5.02	117.62	112.60

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 [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	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.

All (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
1:A:345:TPO:O	1:A:346:SEP:HB2	1.96	0.64
1:A:223:THR:O	1:A:224:GLU:CD	2.41	0.64
1:A:223:THR:OG1	1:A:224:GLU:N	2.30	0.62
1:A:345:TPO:O2P	1:A:345:TPO:HA	1.99	0.62
1:A:223:THR:O	1:A:224:GLU:HG3	1.99	0.62
1:A:224:GLU:H	1:A:225:GLU:CB	2.12	0.62
2:B:357:PRO:HG3	2:B:439:GLU:HG3	1.80	0.62
2:B:311:ASP:HB2	2:B:332:LEU:HD21	1.82	0.61
1:A:223:THR:O	1:A:224:GLU:CB	2.48	0.59
1:A:310:ARG:HD3	1:A:332:LEU:O	2.05	0.56
1:A:237:MET:HG2	1:A:248:LEU:HB2	1.88	0.56
2:B:415:ASP:HB3	2:B:418:MET:HE2	1.89	0.55
1:A:179:ASN:HB2	5:A:637:HOH:O	2.06	0.54
1:A:223:THR:HG23	5:A:634:HOH:O	2.06	0.54
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.91	0.53
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.91	0.52
2:B:300:ASN:HA	2:B:447:ILE:HG21	1.92	0.51
2:B:287:MET:HE2	2:B:287:MET:HA	1.94	0.50
1:A:223:THR:O	1:A:224:GLU:OE2	2.30	0.50
2:B:387:VAL:HG23	2:B:395:LEU:HD12	1.93	0.49
1:A:232:GLN:O	1:A:236:VAL:HG23	2.12	0.49
1:A:278:ASP:O	2:B:419:ASN:HB3	2.11	0.49
2:B:440:LYS:H	2:B:440:LYS:CD	2.26	0.48
1:A:184:PRO:HD2	1:A:187:VAL:HG22	1.94	0.48
1:A:387:VAL:HG23	1:A:395:LEU:HD12	1.96	0.48
1:A:351:THR:O	1:A:355:MET:HG3	2.15	0.46
2:B:440:LYS:H	2:B:440:LYS:HD3	1.79	0.46
1:A:345:TPO:CG2	1:A:346:SEP:N	2.79	0.45
1:A:169:SER:H	1:A:172:GLU:CD	2.26	0.44
2:B:353:ALA:HB1	2:B:386:ALA:HB1	2.01	0.42
2:B:286:HIS:CD2	2:B:287:MET:HE3	2.54	0.42
2:B:311:ASP:HB2	2:B:332:LEU:CD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:O	1:A:189:GLY:HA3	2.19	0.42
2:B:266:PRO:HD2	2:B:320:ASP:HA	2.02	0.42
1:A:237:MET:HE1	1:A:330:PHE:CE1	2.55	0.41
1:A:345:TPO:HG23	1:A:362:GLY:O	2.19	0.41
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.02	0.41
1:A:281:PRO:HB3	2:B:281:PRO:HB3	2.04	0.40
1:A:237:MET:HG2	1:A:248:LEU:CB	2.52	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	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

All (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
2	B	196	GLY
1	A	225	GLU

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

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	169	SER
1	A	176	VAL
1	A	182	GLU
1	A	186	SER
1	A	191	LYS
1	A	208	THR
1	A	215	LEU
1	A	218	MET
1	A	224	GLU
1	A	226	LEU
1	A	237	MET
1	A	252	SER
1	A	287	MET
1	A	318	LEU
1	A	344	MET
1	A	349	VAL
1	A	352	THR
1	A	399	ILE
1	A	434	SER
1	A	439	GLU
1	A	456	GLU
2	B	176	VAL
2	B	215	LEU
2	B	318	LEU
2	B	332	LEU
2	B	342	THR

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Mol	Chain	Res	Type
2	B	365	THR
2	B	399	ILE
2	B	406	GLU
2	B	427	GLU
2	B	434	SER
2	B	439	GLU
2	B	440	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	178	ASN
1	A	190	ASN
1	A	207	ASN
1	A	286	HIS
1	A	307	HIS
1	A	390	HIS
2	B	190	ASN
2	B	305	ASN
2	B	442	ASN

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
2	B	345	TPO	P-OG1-CB	-2.87	115.52	123.33
1	A	345	TPO	O-C-CA	-2.76	117.68	124.77
2	B	346	SEP	O3P-P-OG	2.41	112.94	106.67
1	A	284	SEP	O3P-P-O1P	-2.19	102.30	110.83
1	A	284	SEP	OG-P-O1P	2.15	112.26	106.44

There are no chirality outliers.

All (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
2	B	345	TPO	O-C-CA-CB
1	A	284	SEP	CB-OG-P-O1P
2	B	346	SEP	CA-CB-OG-P
2	B	345	TPO	C-CA-CB-CG2
1	A	345	TPO	CG2-CB-OG1-P
2	B	346	SEP	N-CA-CB-OG
1	A	284	SEP	CB-OG-P-O2P
2	B	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O1P

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
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
3	B	501	ZVG	C9-C10	3.85	1.45	1.39
3	A	501	ZVG	C5-N	3.38	1.41	1.33
3	A	501	ZVG	C9-C10	2.99	1.44	1.39
3	B	501	ZVG	C6-C10	2.62	1.45	1.41
3	A	501	ZVG	C17-C18	-2.54	1.39	1.44
3	A	501	ZVG	C8-N3	2.52	1.43	1.38
3	A	501	ZVG	C8-N1	2.47	1.38	1.34
3	B	501	ZVG	C8-N1	2.43	1.38	1.34
3	B	501	ZVG	C5-N	2.31	1.38	1.33

All (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
3	B	501	ZVG	C6-C10-N2	-2.26	119.09	121.08
3	B	501	ZVG	C16-C17-C18	2.14	122.33	120.05
3	B	501	ZVG	N3-C14-N4	2.10	122.23	116.29
3	A	501	ZVG	C6-C10-N2	-2.02	119.30	121.08

There are no chirality outliers.

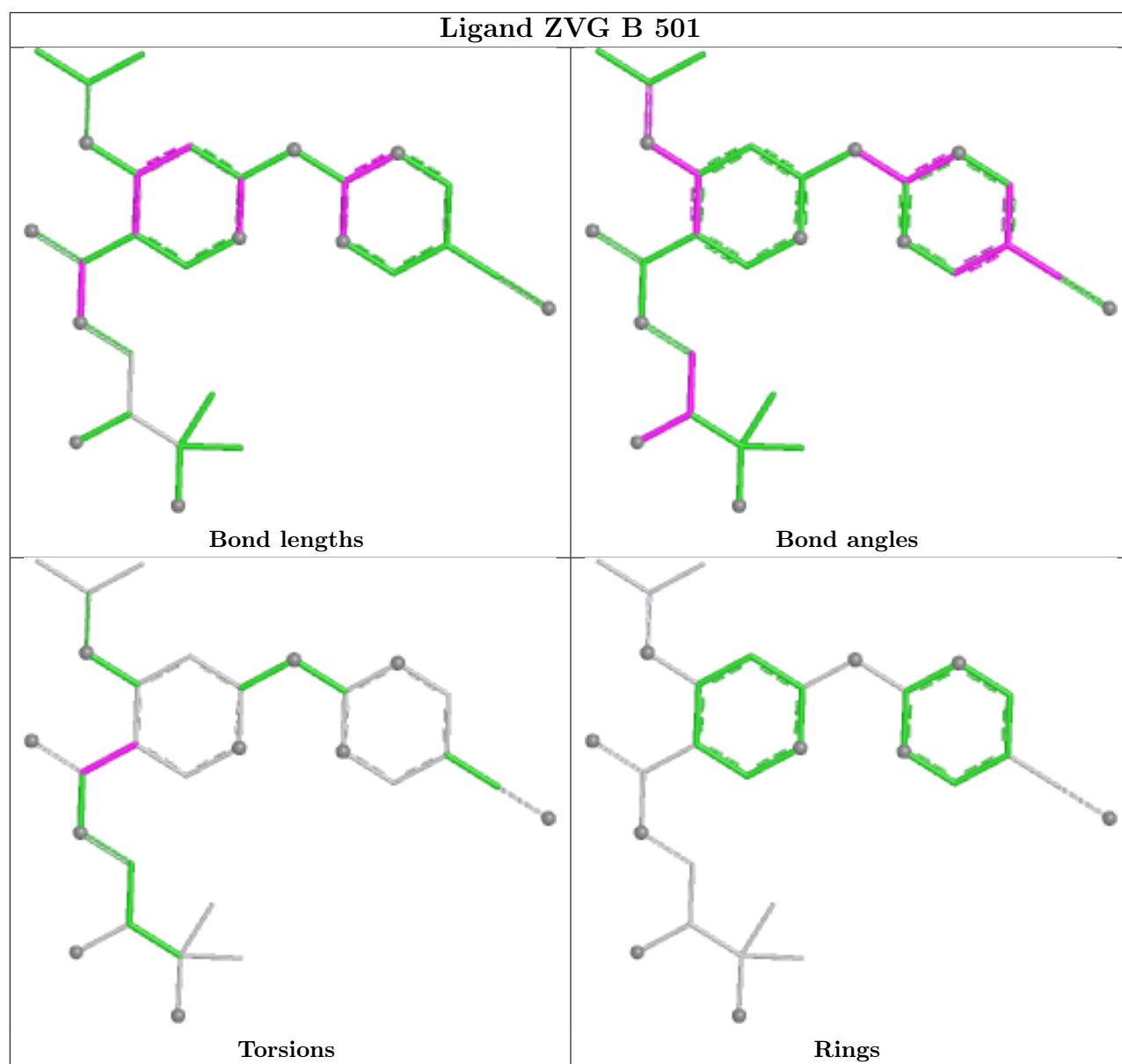
All (5) torsion outliers are listed below:

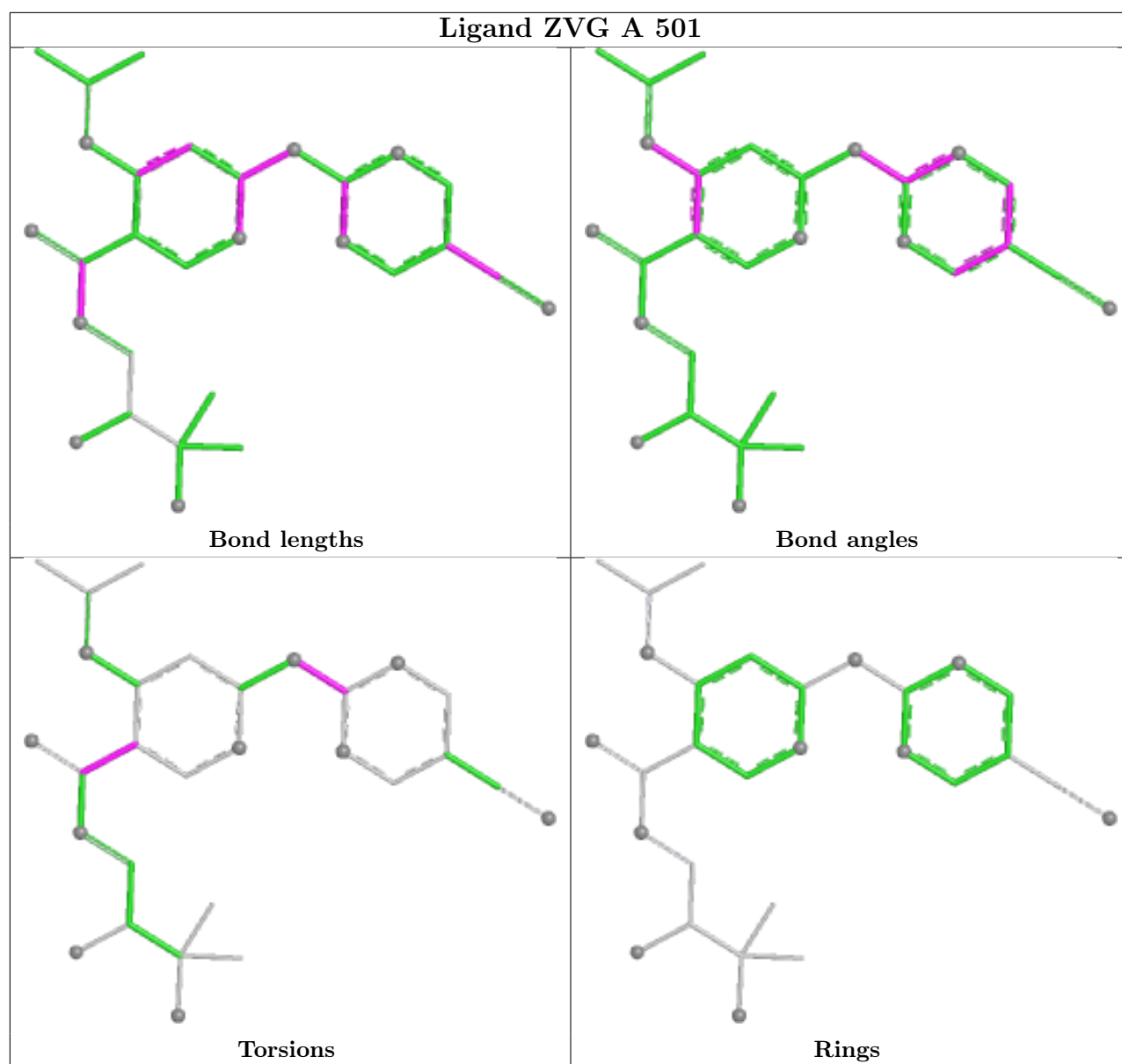
Mol	Chain	Res	Type	Atoms
3	A	501	ZVG	O1-C5-C6-C7
3	B	501	ZVG	O1-C5-C6-C7
3	B	501	ZVG	N-C5-C6-C7
3	A	501	ZVG	N-C5-C6-C7
3	A	501	ZVG	N5-C14-N3-C8

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

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	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%)

All (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
1	A	312	ILE	23.8
1	A	236	VAL	21.9
1	A	366	PRO	21.3
2	B	304	GLU	21.2
2	B	204	TYR	19.9
2	B	260	LEU	19.3
1	A	240	CYS	18.8
2	B	330	PHE	18.3
1	A	454	LEU	18.0
2	B	325	ALA	17.8
1	A	458	THR	17.8
2	B	404	GLU	17.8
1	A	331	GLY	16.9
1	A	388	ASP	16.5
2	B	400	LYS	16.2
1	A	407	GLU	16.2
1	A	424	THR	15.9
2	B	406	GLU	15.8
1	A	437	LEU	15.7

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Mol	Chain	Res	Type	RSRZ
2	B	442	ASN	15.3
2	B	179	ASN	15.2
1	A	439	GLU	15.1
2	B	261	VAL	14.7
2	B	189	GLY	14.5
1	A	303	HIS	14.0
1	A	369	ASP	13.2
2	B	440	LYS	13.1
2	B	435	GLN	12.1
1	A	410	ILE	12.1
2	B	324	THR	12.1
2	B	365	THR	12.0
2	B	360	LEU	12.0
2	B	349	VAL	11.9
2	B	321	GLU	11.8
1	A	218	MET	11.8
1	A	438	HIS	11.7
1	A	178	ASN	11.7
2	B	246	VAL	11.6
2	B	182	GLU	11.6
1	A	389	GLU	11.5
1	A	449	LYS	11.4
2	B	355	MET	11.1
1	A	163	THR	10.9
2	B	401	GLU	10.6
2	B	423	SER	10.4
1	A	355	MET	10.2
2	B	171	TYR	10.2
2	B	313	LYS	10.0
2	B	302	LEU	10.0
2	B	322	ALA	10.0
1	A	320	ASP	9.9
1	A	242	HIS	9.9
1	A	423	SER	9.9
2	B	389	GLU	9.8
2	B	211	ALA	9.8
1	A	429	MET	9.8
1	A	417	LYS	9.8
2	B	343	VAL	9.8
1	A	241	GLN	9.7
1	A	432	VAL	9.7
1	A	253	SER	9.7

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Mol	Chain	Res	Type	RSRZ
2	B	299	ILE	9.6
2	B	279	GLY	9.6
1	A	344	MET	9.5
2	B	178	ASN	9.5
2	B	416	LYS	9.5
2	B	185	ILE	9.5
2	B	363	GLU	9.5
2	B	312	ILE	9.5
1	A	169	SER	9.4
1	A	387	VAL	9.3
1	A	421	ALA	9.3
1	A	330	PHE	9.3
2	B	201	TYR	9.3
2	B	257	ASP	9.3
1	A	426	VAL	9.3
1	A	187	VAL	9.3
1	A	406	GLU	9.2
1	A	304	GLU	9.2
2	B	169	SER	9.0
2	B	318	LEU	9.0
1	A	256	ASP	8.9
2	B	205	VAL	8.9
2	B	432	VAL	8.9
1	A	420	ASP	8.9
1	A	348	ILE	8.9
2	B	364	ILE	8.9
1	A	258	LEU	8.8
2	B	268	GLY	8.8
2	B	245	LEU	8.8
2	B	368	SER	8.8
2	B	443	LYS	8.8
1	A	216	ALA	8.7
2	B	456	GLU	8.6
2	B	278	ASP	8.6
1	A	252	SER	8.6
1	A	397	LEU	8.5
2	B	447	ILE	8.3
2	B	307	HIS	8.3
2	B	230	PHE	8.3
2	B	362	GLY	8.2
1	A	414	ILE	8.2
2	B	453	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
2	B	415	ASP	8.1
1	A	405	ASP	8.1
2	B	446	ASP	8.1
1	A	422	ASP	8.1
2	B	444	ARG	8.1
1	A	335	ALA	8.1
2	B	366	PRO	8.1
2	B	410	ILE	8.0
1	A	333	ALA	8.0
1	A	269	SER	8.0
2	B	357	PRO	8.0
1	A	396	LEU	7.9
1	A	221	ILE	7.9
2	B	441	LYS	7.9
2	B	286	HIS	7.9
2	B	422	ASP	7.8
2	B	175	ASN	7.8
1	A	286	HIS	7.7
2	B	436	CYS	7.7
1	A	305	ASN	7.7
1	A	409	THR	7.6
1	A	223	THR	7.6
2	B	427	GLU	7.6
2	B	449	LYS	7.6
1	A	336	SER	7.6
1	A	291	ILE	7.6
1	A	204[A]	TYR	7.5
1	A	367	LYS	7.5
2	B	193	GLY	7.5
1	A	222	THR	7.5
1	A	404	GLU	7.5
1	A	364	ILE	7.5
2	B	281	PRO	7.5
2	B	315	ALA	7.5
2	B	434	SER	7.4
2	B	236	VAL	7.4
1	A	232	GLN	7.4
1	A	293	GLN	7.4
1	A	164	ARG	7.4
1	A	383	GLY	7.4
2	B	244	ASN	7.4
2	B	454	LEU	7.4

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Mol	Chain	Res	Type	RSRZ
2	B	296	ALA	7.3
1	A	171	TYR	7.3
2	B	395	LEU	7.3
2	B	431	SER	7.3
1	A	229	GLN	7.3
1	A	271	LEU	7.3
2	B	200	VAL	7.2
2	B	300	ASN	7.2
1	A	394	GLN	7.2
1	A	217	ALA	7.2
1	A	297	ASN	7.2
2	B	234	ILE	7.2
2	B	405	ASP	7.1
2	B	370	ILE	7.1
1	A	170	PHE	7.1
2	B	426	VAL	7.1
1	A	165	PHE	7.1
2	B	352	THR	7.1
1	A	376	VAL	7.1
1	A	168	PHE	7.1
1	A	231	ASP	7.1
2	B	430	TYR	7.0
1	A	311	ASP	7.0
1	A	332	LEU	7.0
1	A	287	MET	7.0
1	A	457	MET	7.0
1	A	230	PHE	7.0
1	A	254	ASP	7.0
1	A	390	HIS	7.0
1	A	350	GLY	7.0
1	A	180	PHE	7.0
2	B	354	TYR	7.0
2	B	184	PRO	6.9
1	A	227	LYS	6.9
2	B	277	LEU	6.9
2	B	323	PHE	6.9
1	A	359	ALA	6.9
2	B	266	PRO	6.9
1	A	419	ASN	6.9
1	A	342	THR	6.8
1	A	207	ASN	6.8
1	A	194	GLU	6.8

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Mol	Chain	Res	Type	RSRZ
2	B	314	SER	6.8
1	A	211	ALA	6.8
1	A	290	LYS	6.8
1	A	177	THR	6.8
1	A	412	ASP	6.8
1	A	418	MET	6.7
2	B	297	ASN	6.7
2	B	394	GLN	6.7
1	A	285	TRP	6.7
2	B	353	ALA	6.7
2	B	263	VAL	6.7
1	A	205	VAL	6.6
2	B	403	ILE	6.6
2	B	438	HIS	6.6
2	B	375	VAL	6.6
1	A	275	SER	6.6
2	B	459	ALA	6.6
2	B	388	ASP	6.5
1	A	393	PRO	6.5
1	A	365	THR	6.5
2	B	180	PHE	6.5
2	B	399	ILE	6.5
2	B	208	THR	6.5
2	B	358	GLU	6.5
2	B	374	GLY	6.5
2	B	295	ALA	6.5
1	A	212	VAL	6.5
1	A	191	LYS	6.4
2	B	203	GLY	6.4
2	B	359	ALA	6.4
1	A	292	ALA	6.4
2	B	183	ARG	6.4
2	B	437	LEU	6.3
2	B	292	ALA	6.3
2	B	269	SER	6.3
2	B	451	GLN	6.3
2	B	414	ILE	6.3
2	B	448	LYS	6.2
2	B	445	PRO	6.2
2	B	271	LEU	6.2
2	B	348	ILE	6.2
1	A	384	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
2	B	287	MET	6.2
2	B	242	HIS	6.2
1	A	189	GLY	6.2
2	B	409	THR	6.2
2	B	457	MET	6.2
1	A	262	TYR	6.2
1	A	413	TYR	6.2
1	A	416	LYS	6.2
1	A	181	ASP	6.2
2	B	420	ASP	6.2
2	B	280	THR	6.2
1	A	306	HIS	6.2
2	B	272	ASP	6.1
2	B	290	LYS	6.1
1	A	442	ASN	6.1
2	B	293	GLN	6.1
2	B	439	GLU	6.1
1	A	408	LYS	6.1
1	A	321	GLU	6.1
1	A	398	ASP	6.0
1	A	255	GLY	6.0
2	B	303	HIS	6.0
1	A	206	ASN	6.0
2	B	329	ASP	6.0
2	B	215	LEU	6.0
2	B	170	PHE	6.0
2	B	285	TRP	6.0
2	B	196	GLY	5.9
2	B	267	ASN	5.9
1	A	362	GLY	5.9
1	A	280	THR	5.9
2	B	356	ALA	5.9
1	A	167	SER	5.9
2	B	317	ILE	5.9
2	B	235	LYS	5.9
1	A	411	GLU	5.9
1	A	224	GLU	5.9
1	A	274	LEU	5.8
2	B	385	PRO	5.8
1	A	318	LEU	5.8
1	A	385	PRO	5.8
2	B	455	GLN	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	370	ILE	5.8
2	B	378	LEU	5.8
1	A	197	PHE	5.8
2	B	231	ASP	5.8
2	B	390	HIS	5.7
2	B	413	TYR	5.7
2	B	381	ILE	5.7
1	A	277	LEU	5.7
2	B	411	GLU	5.7
2	B	367	LYS	5.7
1	A	341	GLN	5.7
2	B	309	HIS	5.6
1	A	324	THR	5.6
2	B	428	ALA	5.6
1	A	453	LEU	5.6
2	B	320	ASP	5.6
1	A	391	ARG	5.6
1	A	225	GLU	5.5
1	A	243	GLU	5.5
1	A	430	TYR	5.5
2	B	308	ILE	5.5
1	A	278	ASP	5.5
2	B	274	LEU	5.5
1	A	314	SER	5.5
1	A	185	ILE	5.5
2	B	327	ILE	5.5
2	B	191	LYS	5.5
1	A	188	GLY	5.5
1	A	264	TYR	5.5
2	B	240	CYS	5.4
1	A	234	ILE	5.4
1	A	270	LEU	5.4
2	B	168	PHE	5.4
2	B	419	ASN	5.4
1	A	166	HIS	5.4
1	A	257	ASP	5.4
1	A	226	LEU	5.4
1	A	172	GLU	5.3
2	B	450	VAL	5.3
1	A	182	GLU	5.3
2	B	397	LEU	5.3
2	B	247	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	198	GLY	5.3
2	B	412	ASP	5.3
1	A	300	ASN	5.3
1	A	444	ARG	5.3
2	B	458	THR	5.3
1	A	214	LYS	5.3
1	A	380	ILE	5.3
1	A	399	ILE	5.3
2	B	173	LEU	5.2
1	A	357	PRO	5.2
2	B	418	MET	5.2
1	A	307	HIS	5.2
2	B	384	LEU	5.2
1	A	375	VAL	5.2
2	B	174	LYS	5.1
2	B	270	LEU	5.1
1	A	354	TYR	5.1
2	B	391	ARG	5.1
1	A	381	ILE	5.1
2	B	172	GLU	5.1
2	B	262	TYR	5.1
1	A	237	MET	5.1
2	B	316	ASN	5.1
1	A	299	ILE	5.1
2	B	380	ILE	5.1
1	A	251	PHE	5.1
1	A	174	LYS	5.1
1	A	440	LYS	5.1
1	A	249	LEU	5.0
1	A	360	LEU	5.0
1	A	173	LEU	5.0
2	B	243	GLU	5.0
2	B	373	PHE	5.0
1	A	451	GLN	5.0
2	B	273	ARG	4.9
2	B	306	HIS	4.9
1	A	435	GLN	4.9
1	A	238	ALA	4.9
1	A	176	VAL	4.9
2	B	226	LEU	4.9
2	B	396	LEU	4.9
2	B	398	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	276	CYS	4.9
2	B	344	MET	4.9
1	A	322	ALA	4.8
1	A	279	GLY	4.8
1	A	452	GLN	4.8
1	A	247	GLU	4.8
2	B	371	TYR	4.8
1	A	200	VAL	4.8
2	B	282	PRO	4.8
1	A	215	LEU	4.8
1	A	259	CYS	4.7
2	B	429	MET	4.7
1	A	184	PRO	4.7
2	B	332	LEU	4.7
2	B	202	LYS	4.7
2	B	232	GLN	4.7
1	A	301	PHE	4.7
1	A	260	LEU	4.7
1	A	317	ILE	4.7
1	A	379	GLU	4.7
1	A	368	SER	4.7
1	A	179	ASN	4.7
2	B	213	LYS	4.7
1	A	315	ALA	4.6
2	B	347	ARG	4.6
2	B	361	ARG	4.6
2	B	433	ALA	4.6
2	B	319	LEU	4.6
2	B	425	SER	4.6
1	A	263	VAL	4.6
1	A	392	GLU	4.6
1	A	441	LYS	4.5
2	B	195	GLY	4.5
1	A	228	GLN	4.5
2	B	276	CYS	4.5
1	A	203	GLY	4.5
2	B	387	VAL	4.5
2	B	377	LEU	4.5
2	B	421	ALA	4.5
1	A	382	THR	4.5
2	B	298	GLY	4.4
1	A	208	THR	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	176	VAL	4.4
1	A	186	SER	4.4
1	A	455	GLN	4.4
1	A	289	CYS	4.4
2	B	241	GLN	4.3
2	B	248	LEU	4.3
1	A	372	SER	4.3
1	A	196	GLY	4.3
2	B	209	THR	4.3
1	A	281	PRO	4.3
2	B	452	GLN	4.3
2	B	424	THR	4.3
2	B	264	TYR	4.3
1	A	244	ASN	4.2
1	A	325	ALA	4.2
1	A	294	GLY	4.2
1	A	427	GLU	4.2
2	B	402	GLU	4.2
1	A	209	THR	4.2
2	B	393	PRO	4.2
2	B	165	PHE	4.2
2	B	199	VAL	4.2
1	A	310	ARG	4.2
1	A	175	ASN	4.2
2	B	224	GLU	4.2
2	B	417	LYS	4.2
1	A	446	ASP	4.1
2	B	194	GLU	4.1
1	A	213	LYS	4.1
1	A	443	LYS	4.1
1	A	415	ASP	4.1
1	A	373	PHE	4.1
2	B	284	SER	4.1
2	B	197	PHE	4.1
1	A	456	GLU	4.0
2	B	379	GLU	4.0
2	B	382	THR	3.9
1	A	319	LEU	3.9
1	A	326	LYS	3.9
1	A	395	LEU	3.9
2	B	265	MET	3.9
2	B	392	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	210	VAL	3.9
1	A	349	VAL	3.9
1	A	202	LYS	3.8
1	A	235	LYS	3.8
1	A	361	ARG	3.8
1	A	371	TYR	3.8
2	B	177	THR	3.8
2	B	192	MET	3.7
2	B	288	ARG	3.7
1	A	363	GLU	3.7
1	A	250	GLY	3.7
1	A	334	ARG	3.7
2	B	408	LYS	3.7
1	A	351	THR	3.7
1	A	195	GLY	3.6
2	B	229	GLN	3.6
2	B	310	ARG	3.6
1	A	298	GLY	3.6
2	B	294	GLY	3.6
2	B	386	ALA	3.6
1	A	283	LEU	3.6
1	A	239	LYS	3.6
1	A	428	ALA	3.5
1	A	425	SER	3.5
2	B	291	ILE	3.5
2	B	289	CYS	3.4
1	A	245	LEU	3.4
1	A	403	ILE	3.4
1	A	273	ARG	3.4
2	B	301	PHE	3.4
1	A	400	LYS	3.4
2	B	167	SER	3.4
1	A	288	ARG	3.4
1	A	246	VAL	3.4
1	A	266	PRO	3.3
1	A	296	ALA	3.3
1	A	272	ASP	3.3
1	A	199	VAL	3.3
2	B	275	SER	3.3
2	B	372	SER	3.3
2	B	383	GLY	3.3
1	A	328	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	282	PRO	3.3
1	A	267	ASN	3.3
1	A	323	PHE	3.3
1	A	329	ASP	3.3
2	B	233	GLU	3.3
1	A	308	ILE	3.3
1	A	352	THR	3.2
1	A	433	ALA	3.2
2	B	369	ASP	3.2
2	B	238	ALA	3.2
2	B	190	ASN	3.1
1	A	261	VAL	3.1
2	B	376	VAL	3.1
1	A	192	MET	3.1
2	B	283	LEU	3.1
1	A	447	ILE	3.1
1	A	198	GLY	3.1
1	A	183	ARG	3.1
1	A	316	ASN	3.0
1	A	295	ALA	3.0
2	B	210	VAL	3.0
2	B	259	CYS	3.0
2	B	225	GLU	3.0
1	A	268	GLY	3.0
1	A	248	LEU	3.0
2	B	407	GLU	2.9
1	A	265	MET	2.9
1	A	343	VAL	2.9
1	A	445	PRO	2.8
2	B	328	SER	2.8
2	B	166	HIS	2.8
2	B	258	LEU	2.7
1	A	434	SER	2.7
1	A	233	GLU	2.7
1	A	386	ALA	2.7
2	B	239	LYS	2.7
1	A	201	TYR	2.6
1	A	377	LEU	2.6
2	B	305	ASN	2.6
1	A	309	HIS	2.6
1	A	193	GLY	2.6
1	A	402	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	313	LYS	2.4
2	B	228	GLN	2.4
1	A	431	SER	2.3
2	B	326	LYS	2.3
1	A	401	GLU	2.3
2	B	311	ASP	2.2
1	A	378	LEU	2.2
2	B	331	GLY	2.1
1	A	374	GLY	2.1
1	A	302	LEU	2.0
1	A	190	ASN	2.0

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.

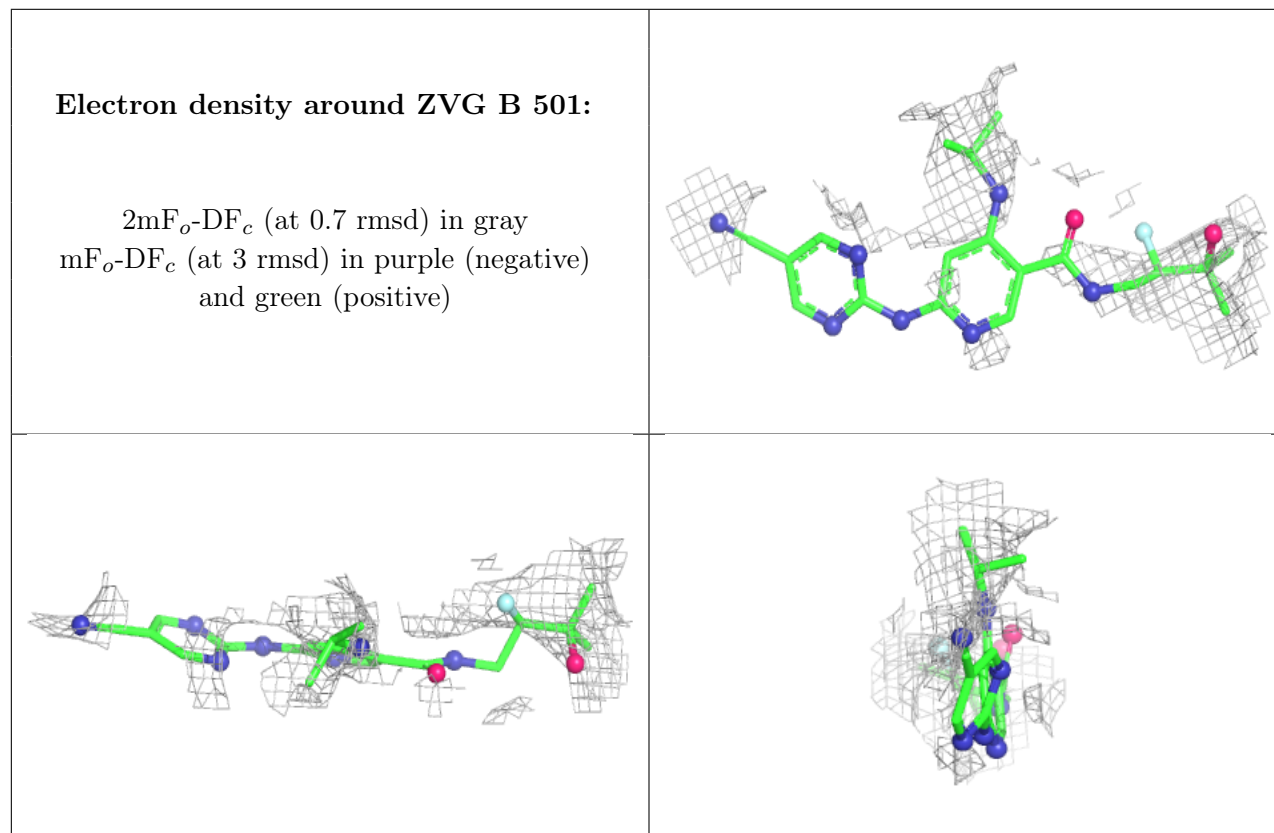
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZVG	B	501	29/29	0.36	0.27	55,68,76,80	0
4	SO4	A	502	5/5	0.39	0.35	144,148,149,150	0

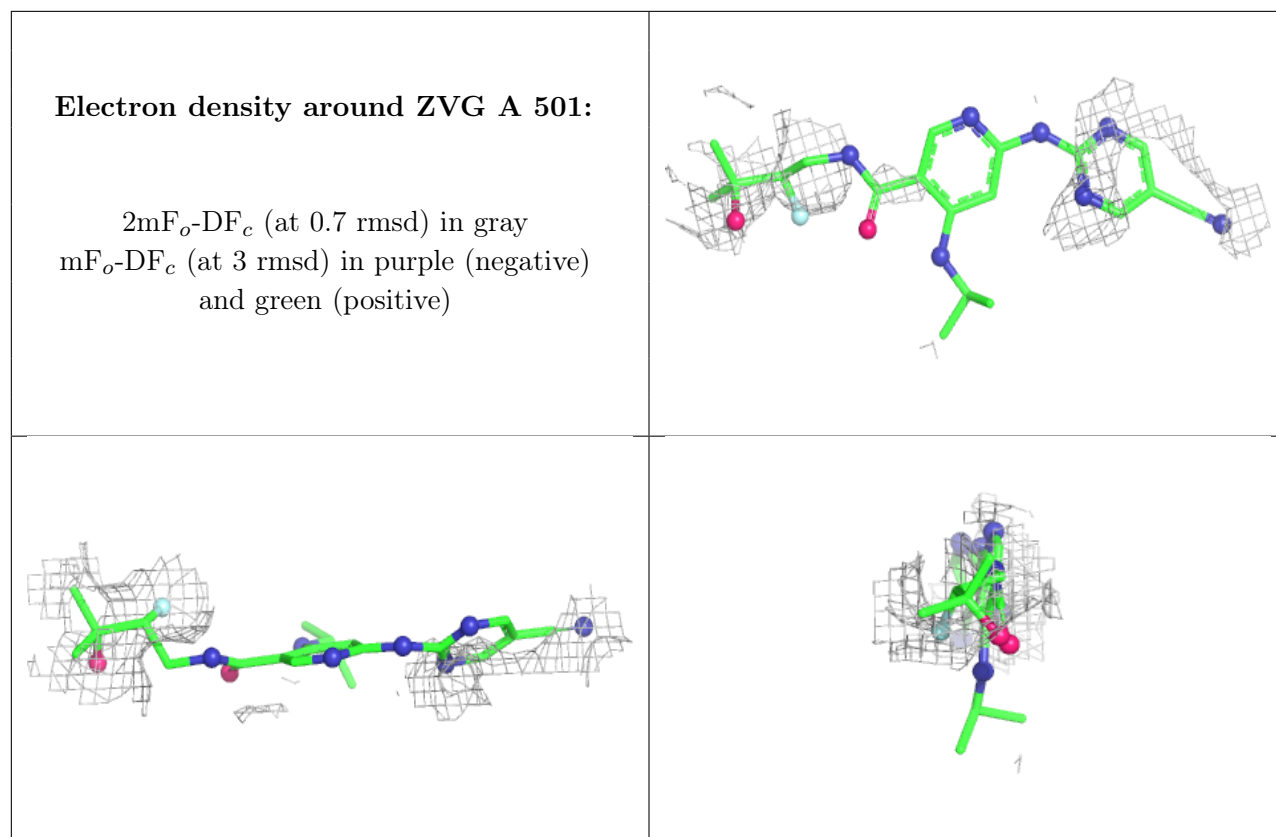
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZVG	A	501	29/29	0.53	0.36	24,31,44,55	0
4	SO4	B	502	5/5	0.56	0.30	66,70,71,72	0

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.