Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2025 – 04:05 PM EST

PDB ID	:	8SCV
Title	:	Crystal structure of IRAK4-HSA complexed with BMS-986126; 6-((5-CYANO-2-PYRIMIDINYL)AMINO)-N-((2R)-2-FLUORO-3-HYDROXHYLBUTYL)-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:

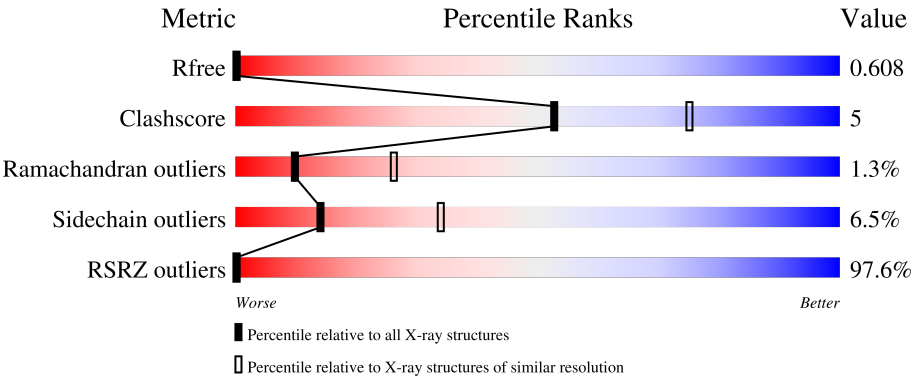
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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 <=5%

Mol	Chain	Length	Quality of chain
1	A	305	91% 80% 13% • 5%
2	B	305	84% 78% 7% • 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
1	A	290	Total	C	N	O	P	S	0	1	0
			2203	1385	369	431	3	15			

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

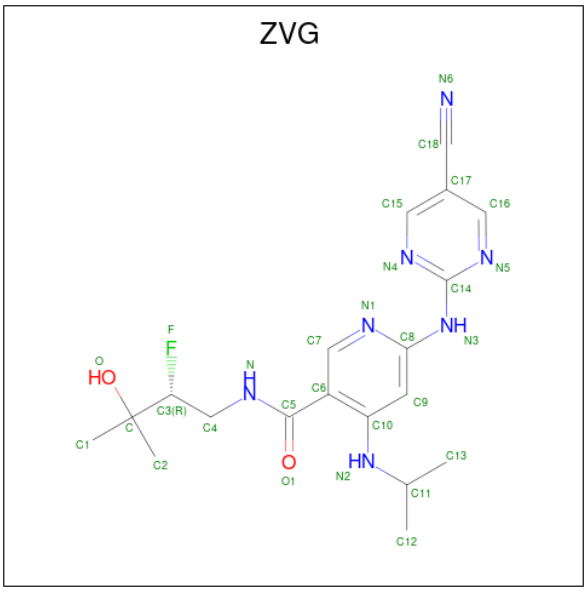
- Molecule 2 is a protein called Interleukin-1 receptor-associated kinase 4.

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

There are 4 discrepancies between the modelled and reference sequences:

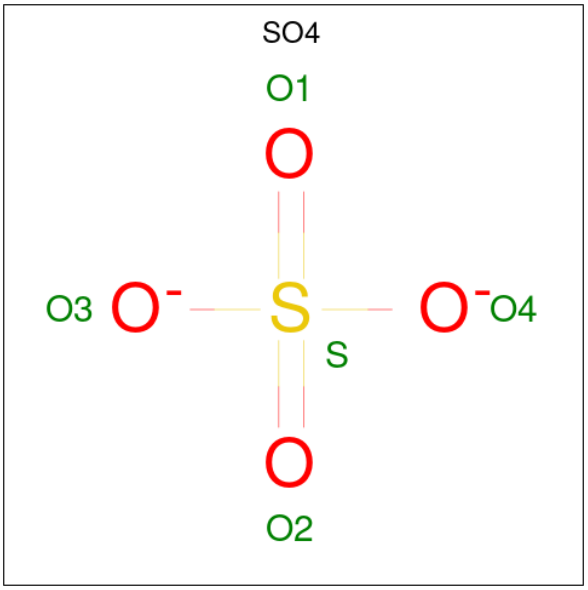
Chain	Residue	Modelled	Actual	Comment	Reference
B	156	GLY	-	expression tag	UNP Q9NWZ3
B	157	ALA	-	expression tag	UNP Q9NWZ3
B	158	MET	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3

- 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 (three-letter code: ZVG) (formula: $C_{19}H_{24}FN_7O_2$) (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 (three-letter code: SO4) (formula: O_4S).



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.

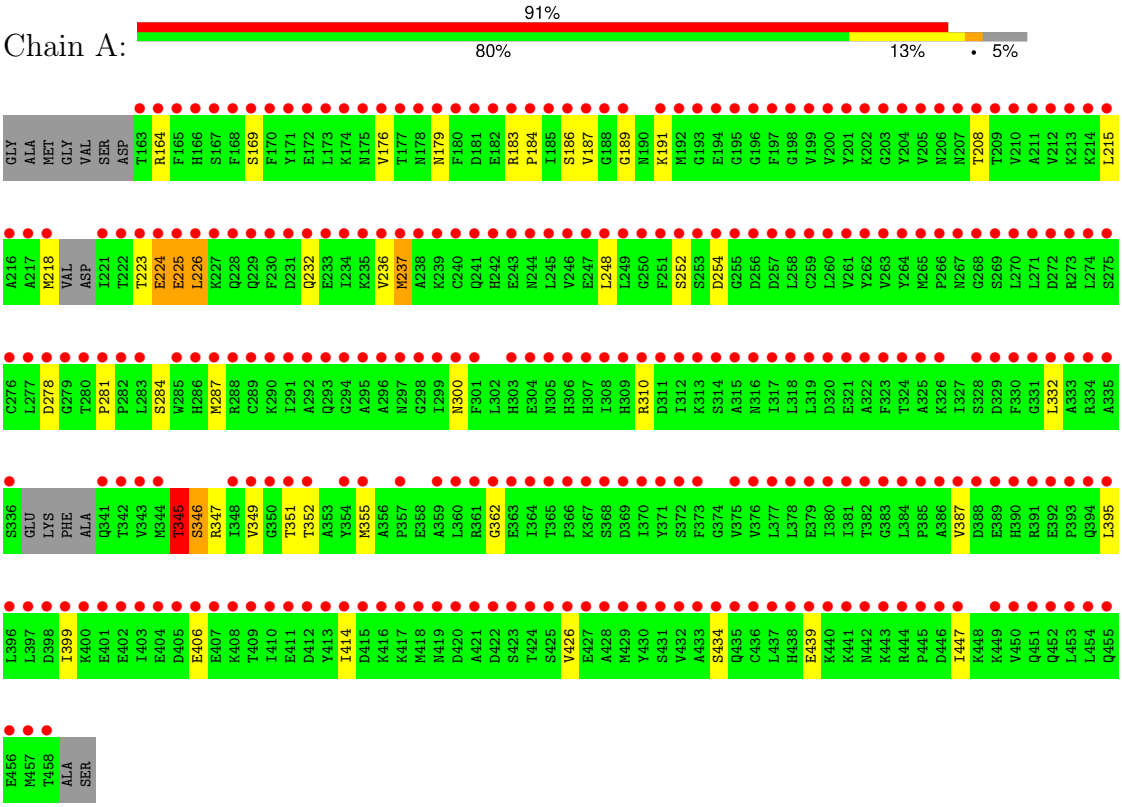
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	B	26	Total O 26 26	0	0

3 Residue-property plots (i)

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.

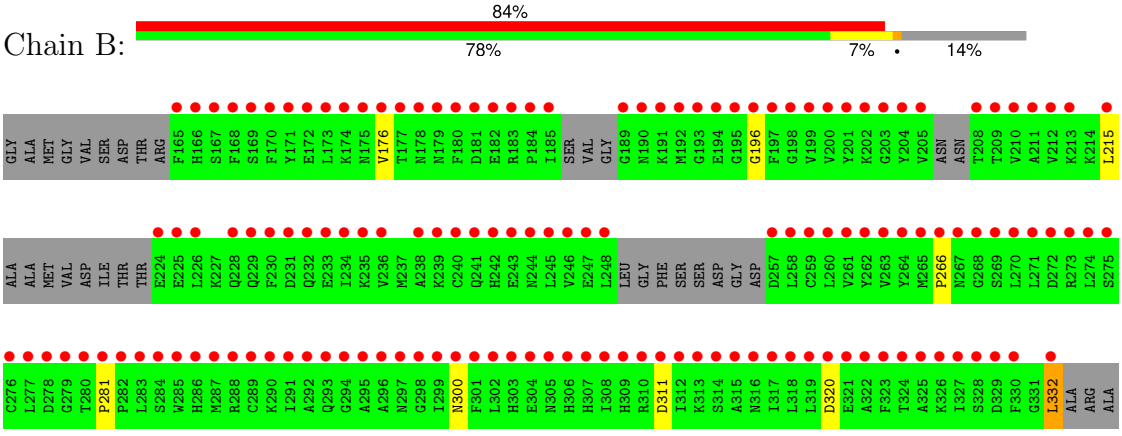
• Molecule 1: Interleukin-1 receptor-associated kinase 4

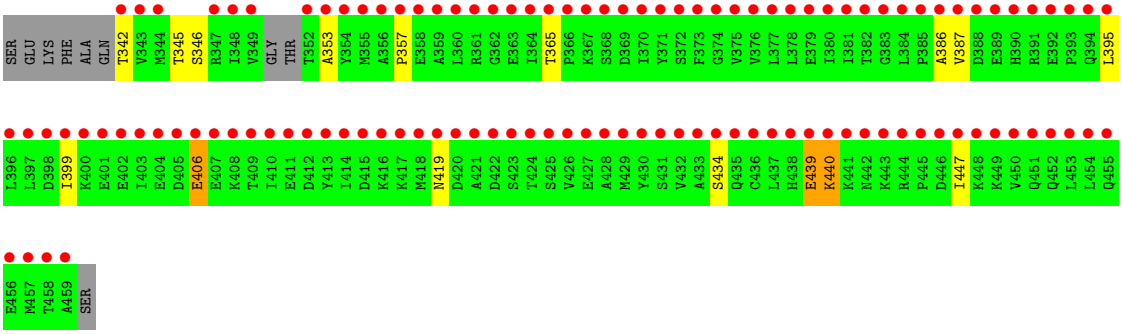
Chain A:



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

Chain B:




SER GLU LYS PHE ALA GLN T342 V343 M344 T345 S346 R347 I348 V349 GLY THR T352 A353 Y354 M355 A356 P357 E358 A359 L360 R361 G362 E363 I364 T365 P366 K367 S368 D369 I370 Y371 S372 P373 G374 V375 V376 L377 L378 E379 I380 I381 T382 G383 L384 P385 A386 V387 D388 E389 H390 R391 E392 P393 Q394 L395
L396 L397 D398 I399 K400 E401 E402 I403 E404 D405 E406 E407 K408 T409 I410 E411 D412 Y413 I414 D415 K416 K417 M418 N419 D420 A421 D422 S423 T424 S425 V426 E427 A428 M429 Y430 S431 V432 A433 S434 Q435 C436 L437 H438 E439 K440 K441 N442 K443 R444 P445 D446 I447 K448 K449 V450 Q451 Q452 L453 L454 Q455
E456 M457 T458 A459 SER

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	870 reflections (4.75%)	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]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SEP, SO4, TPO, 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	0.56	0/2211	0.73	0/2996
2	B	0.48	0/1882	0.69	0/2561
All	All	0.53	0/4093	0.71	0/5557

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

There are no bond length outliers.

There are no bond angle outliers.

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	30	0
2	B	1879	0	1695	11	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	39	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 5.

All (39) 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:OG1	1:A:224:GLU:N	2.30	0.64
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:223:THR:O	1:A:224:GLU:CD	2.41	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:353:ALA:HB1	2:B:386:ALA:HB1	2.01	0.42
2:B:311:ASP:HB2	2:B:332:LEU:CD2	2.50	0.42
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: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%)	7 18
2	B	247/305 (81%)	232 (94%)	13 (5%)	2 (1%)	16 38
All	All	529/610 (87%)	498 (94%)	24 (4%)	7 (1%)	10 26

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

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Mol	Chain	Res	Type
1	A	225	GLU

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	225/260 (86%)	209 (93%)	16 (7%)	12	30
2	B	177/261 (68%)	167 (94%)	10 (6%)	17	41
All	All	402/521 (77%)	376 (94%)	26 (6%)	14	34

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	169	SER
1	A	186	SER
1	A	191	LYS
1	A	208	THR
1	A	215	LEU
1	A	218	MET
1	A	226	LEU
1	A	237	MET
1	A	252	SER
1	A	287	MET
1	A	349	VAL
1	A	352	THR
1	A	399	ILE
1	A	434	SER
1	A	439	GLU
2	B	176	VAL
2	B	215	LEU
2	B	332	LEU
2	B	342	THR
2	B	365	THR
2	B	399	ILE

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Mol	Chain	Res	Type
2	B	406	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. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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%)
2	SEP	B	346	2	8,9,10	1.05	1 (12%)	7,12,14	3.13	3 (42%)
1	SEP	A	284	1	8,9,10	2.50	3 (37%)	7,12,14	8.33	4 (57%)
1	TPO	A	345	1	8,10,11	0.85	0	10,14,16	1.32	1 (10%)
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	-
2	SEP	B	346	2	-	2/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	284	1	-	3/6/8/10	-
1	TPO	A	345	1	-	4/9/11/13	-
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(^{o})	Ideal(^{o})
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

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Mol	Chain	Res	Type	Atoms
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%)
3	ZVG	A	501	-	28,30,30	1.61	6 (21%)	37,42,42	1.12	3 (8%)
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

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(^{o})	Ideal(^{o})
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:

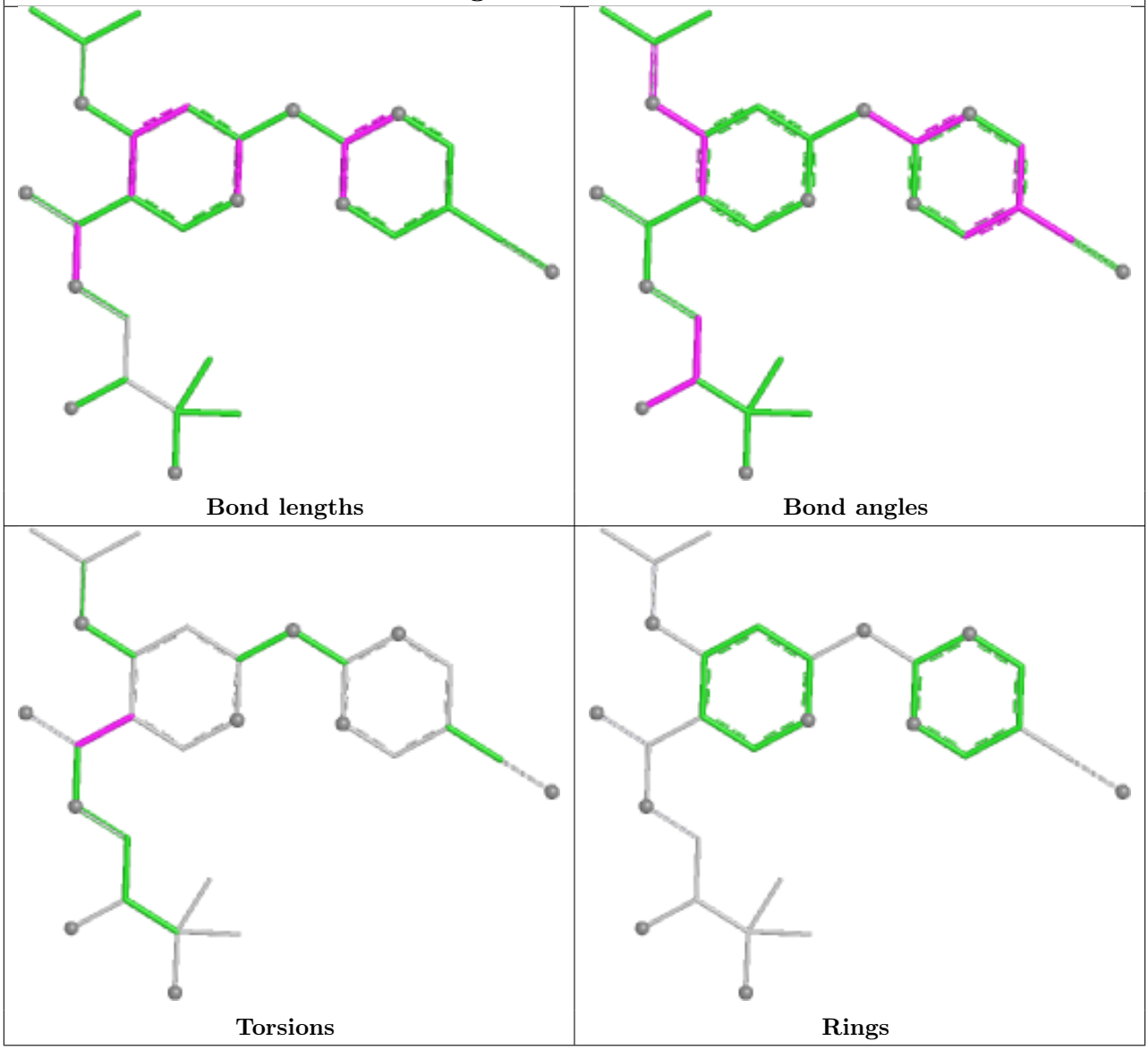
Mol	Chain	Res	Type	Atoms
3	A	501	ZVG	O1-C5-C6-C7
3	B	501	ZVG	O1-C5-C6-C7
3	B	501	ZVG	N-C5-C6-C7
3	A	501	ZVG	N-C5-C6-C7
3	A	501	ZVG	N5-C14-N3-C8

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

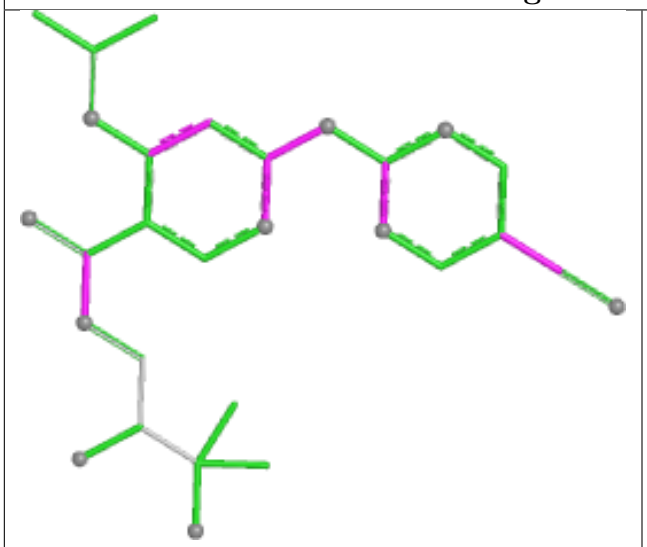
Ligand ZVG B 501



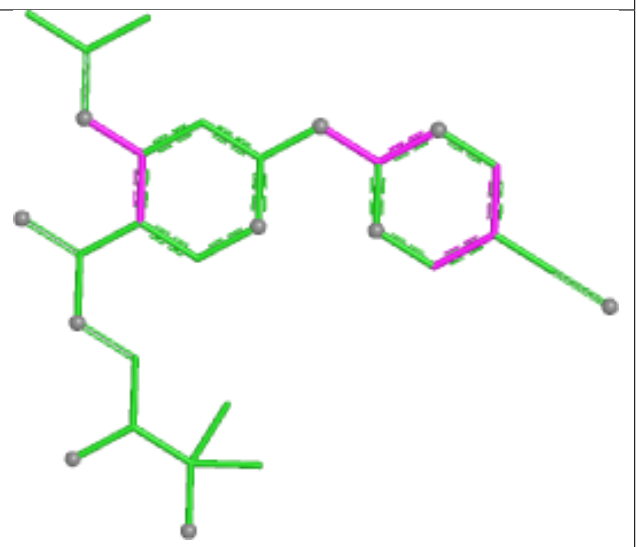
Bond lengths | **Bond angles**

Torsions | **Rings**

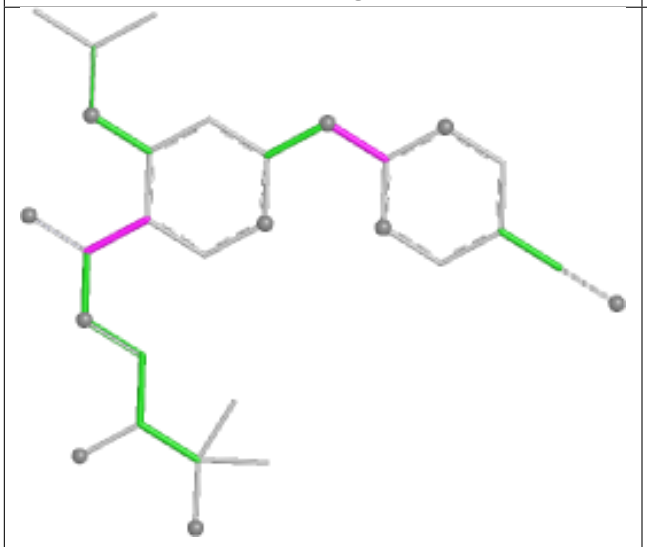
Ligand ZVG A 501



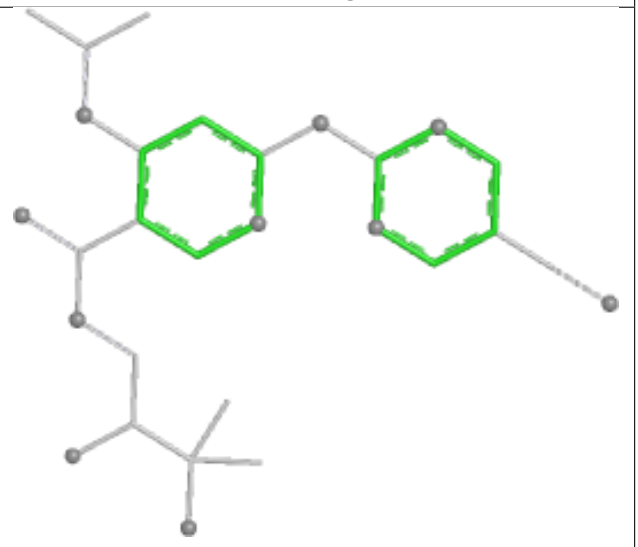
Bond lengths



Bond angles



Torsions



Rings

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

Warning: The R factor obtained from EDS is 0.5938, which does not match the depositor's R factor of 0.22. Please interpret the results in this section carefully.

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, 95^{th} 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%)	6.28	278 (96%)	0	0	31, 59, 91, 111	1 (0%)
2	B	261/305 (85%)	6.85	257 (98%)	0	0	44, 78, 142, 159	0
All	All	548/610 (89%)	6.55	535 (97%)	0	0	31, 67, 114, 159	1 (0%)

All (535) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	212	VAL	31.1
2	B	181	ASP	29.2
1	A	436	CYS	26.2
2	B	342	THR	25.9
1	A	450	VAL	25.5
1	A	312	ILE	23.8
1	A	236	VAL	21.9
2	B	304	GLU	21.7
1	A	366	PRO	21.3
2	B	204	TYR	19.8
2	B	260	LEU	19.2
1	A	240	CYS	18.8
2	B	404	GLU	18.2
2	B	330	PHE	18.1
1	A	458	THR	17.9
1	A	454	LEU	17.9
2	B	325	ALA	17.7
1	A	331	GLY	16.8
1	A	388	ASP	16.8
1	A	407	GLU	16.6
2	B	400	LYS	16.4
2	B	406	GLU	16.1

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Mol	Chain	Res	Type	RSRZ
1	A	424	THR	16.0
1	A	437	LEU	15.5
2	B	442	ASN	15.5
1	A	439	GLU	15.5
2	B	179	ASN	15.4
2	B	261	VAL	14.6
2	B	189	GLY	14.4
1	A	303	HIS	14.0
1	A	369	ASP	13.4
2	B	440	LYS	13.2
2	B	435	GLN	12.2
2	B	324	THR	12.1
2	B	321	GLU	12.1
1	A	410	ILE	12.0
2	B	365	THR	12.0
2	B	182	GLU	11.8
2	B	360	LEU	11.8
2	B	349	VAL	11.8
1	A	389	GLU	11.8
1	A	178	ASN	11.8
1	A	218	MET	11.7
1	A	438	HIS	11.7
2	B	246	VAL	11.5
1	A	449	LYS	11.5
2	B	355	MET	11.0
1	A	163	THR	10.9
2	B	401	GLU	10.8
2	B	423	SER	10.5
1	A	355	MET	10.1
2	B	171	TYR	10.1
2	B	313	LYS	10.0
2	B	389	GLU	10.0
1	A	320	ASP	10.0
1	A	423	SER	10.0
1	A	242	HIS	9.9
1	A	417	LYS	9.9
2	B	322	ALA	9.9
2	B	302	LEU	9.8
1	A	241	GLN	9.8
1	A	253	SER	9.7
2	B	211	ALA	9.7
1	A	429	MET	9.7

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Mol	Chain	Res	Type	RSRZ
2	B	343	VAL	9.7
2	B	363	GLU	9.6
1	A	432	VAL	9.6
2	B	416	LYS	9.6
2	B	178	ASN	9.6
2	B	299	ILE	9.6
1	A	169	SER	9.5
2	B	279	GLY	9.5
1	A	344	MET	9.4
2	B	185	ILE	9.4
2	B	312	ILE	9.4
1	A	406	GLU	9.4
2	B	257	ASP	9.4
1	A	304	GLU	9.3
1	A	387	VAL	9.2
1	A	421	ALA	9.2
2	B	201	TYR	9.2
1	A	426	VAL	9.2
1	A	187	VAL	9.2
1	A	330	PHE	9.1
2	B	169	SER	9.1
1	A	256	ASP	9.0
1	A	420	ASP	8.9
2	B	318	LEU	8.9
2	B	368	SER	8.9
2	B	443	LYS	8.8
2	B	205	VAL	8.8
2	B	432	VAL	8.8
1	A	348	ILE	8.8
2	B	364	ILE	8.8
2	B	456	GLU	8.8
1	A	258	LEU	8.7
2	B	268	GLY	8.7
2	B	245	LEU	8.7
1	A	216	ALA	8.6
2	B	278	ASP	8.6
1	A	252	SER	8.6
1	A	397	LEU	8.4
2	B	307	HIS	8.3
2	B	447	ILE	8.3
2	B	415	ASP	8.2
2	B	444	ARG	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	414	ILE	8.2
1	A	405	ASP	8.2
2	B	446	ASP	8.2
2	B	230	PHE	8.1
2	B	362	GLY	8.1
1	A	422	ASP	8.1
2	B	453	LEU	8.1
1	A	269	SER	8.0
1	A	335	ALA	8.0
2	B	410	ILE	8.0
2	B	366	PRO	8.0
1	A	333	ALA	7.9
2	B	441	LYS	7.9
2	B	422	ASP	7.9
2	B	357	PRO	7.9
2	B	286	HIS	7.8
2	B	175	ASN	7.8
1	A	221	ILE	7.8
1	A	396	LEU	7.8
2	B	427	GLU	7.7
1	A	305	ASN	7.7
1	A	286	HIS	7.7
2	B	449	LYS	7.6
1	A	336	SER	7.6
1	A	409	THR	7.6
2	B	436	CYS	7.6
1	A	404	GLU	7.6
1	A	223	THR	7.6
1	A	367	LYS	7.5
1	A	291	ILE	7.5
1	A	164	ARG	7.5
2	B	434	SER	7.5
1	A	222	THR	7.5
1	A	232	GLN	7.4
1	A	293	GLN	7.4
1	A	204[A]	TYR	7.4
1	A	364	ILE	7.4
2	B	244	ASN	7.4
2	B	193	GLY	7.4
2	B	281	PRO	7.4
2	B	315	ALA	7.4
2	B	236	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
2	B	431	SER	7.3
1	A	229	GLN	7.3
1	A	383	GLY	7.3
2	B	454	LEU	7.2
1	A	394	GLN	7.2
2	B	296	ALA	7.2
2	B	300	ASN	7.2
1	A	171	TYR	7.2
1	A	297	ASN	7.2
2	B	405	ASP	7.2
2	B	395	LEU	7.2
1	A	271	LEU	7.1
2	B	200	VAL	7.1
1	A	217	ALA	7.1
1	A	231	ASP	7.1
2	B	234	ILE	7.1
1	A	311	ASP	7.1
2	B	370	ILE	7.0
2	B	352	THR	7.0
1	A	254	ASP	7.0
2	B	426	VAL	7.0
1	A	376	VAL	7.0
1	A	170	PHE	6.9
1	A	390	HIS	6.9
1	A	227	LYS	6.9
1	A	165	PHE	6.9
2	B	430	TYR	6.9
1	A	287	MET	6.9
1	A	457	MET	6.9
1	A	332	LEU	6.9
1	A	194	GLU	6.9
1	A	168	PHE	6.9
1	A	419	ASN	6.9
1	A	350	GLY	6.9
1	A	230	PHE	6.8
2	B	354	TYR	6.8
1	A	207	ASN	6.8
2	B	314	SER	6.8
2	B	184	PRO	6.8
1	A	290	LYS	6.8
1	A	342	THR	6.8
1	A	359	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
2	B	266	PRO	6.8
1	A	180	PHE	6.8
2	B	277	LEU	6.8
1	A	412	ASP	6.8
1	A	177	THR	6.8
2	B	323	PHE	6.7
2	B	297	ASN	6.7
2	B	394	GLN	6.7
1	A	211	ALA	6.7
1	A	418	MET	6.6
1	A	275	SER	6.6
2	B	358	GLU	6.6
2	B	438	HIS	6.6
2	B	353	ALA	6.5
2	B	388	ASP	6.5
2	B	263	VAL	6.5
1	A	285	TRP	6.5
2	B	403	ILE	6.5
1	A	205	VAL	6.5
1	A	365	THR	6.5
2	B	375	VAL	6.5
1	A	191	LYS	6.4
2	B	459	ALA	6.4
2	B	208	THR	6.4
2	B	183	ARG	6.4
1	A	393	PRO	6.4
2	B	399	ILE	6.4
2	B	295	ALA	6.4
2	B	374	GLY	6.4
2	B	180	PHE	6.3
1	A	212	VAL	6.3
2	B	203	GLY	6.3
2	B	269	SER	6.3
2	B	359	ALA	6.3
1	A	292	ALA	6.3
2	B	451	GLN	6.3
2	B	448	LYS	6.2
2	B	292	ALA	6.2
2	B	437	LEU	6.2
1	A	181	ASP	6.2
2	B	420	ASP	6.2
1	A	416	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
2	B	414	ILE	6.2
2	B	272	ASP	6.1
2	B	242	HIS	6.1
2	B	348	ILE	6.1
2	B	445	PRO	6.1
2	B	409	THR	6.1
2	B	439	GLU	6.1
2	B	290	LYS	6.1
2	B	271	LEU	6.1
2	B	280	THR	6.1
1	A	321	GLU	6.1
2	B	287	MET	6.1
1	A	384	LEU	6.1
1	A	306	HIS	6.1
1	A	442	ASN	6.1
2	B	293	GLN	6.1
2	B	457	MET	6.1
1	A	189	GLY	6.1
1	A	262	TYR	6.1
1	A	413	TYR	6.1
1	A	408	LYS	6.1
1	A	398	ASP	6.0
2	B	329	ASP	6.0
1	A	206	ASN	6.0
2	B	303	HIS	5.9
1	A	411	GLU	5.9
1	A	255	GLY	5.9
1	A	224	GLU	5.9
2	B	267	ASN	5.9
1	A	167	SER	5.9
2	B	235	LYS	5.9
2	B	215	LEU	5.9
1	A	280	THR	5.9
2	B	196	GLY	5.8
2	B	285	TRP	5.8
2	B	170	PHE	5.8
2	B	317	ILE	5.8
1	A	362	GLY	5.8
2	B	356	ALA	5.8
2	B	455	GLN	5.8
2	B	231	ASP	5.7
2	B	411	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
2	B	385	PRO	5.7
1	A	274	LEU	5.7
2	B	390	HIS	5.7
1	A	370	ILE	5.7
1	A	385	PRO	5.7
2	B	367	LYS	5.7
1	A	318	LEU	5.7
1	A	341	GLN	5.7
2	B	378	LEU	5.6
2	B	381	ILE	5.6
2	B	413	TYR	5.6
1	A	197	PHE	5.6
1	A	391	ARG	5.6
1	A	225	GLU	5.6
1	A	243	GLU	5.6
1	A	277	LEU	5.6
2	B	320	ASP	5.6
2	B	309	HIS	5.6
1	A	324	THR	5.5
1	A	278	ASP	5.5
2	B	428	ALA	5.5
1	A	314	SER	5.5
1	A	453	LEU	5.5
2	B	191	LYS	5.5
2	B	308	ILE	5.4
1	A	430	TYR	5.4
1	A	185	ILE	5.4
2	B	327	ILE	5.4
2	B	274	LEU	5.4
1	A	172	GLU	5.4
1	A	182	GLU	5.4
2	B	419	ASN	5.3
1	A	257	ASP	5.3
1	A	188	GLY	5.3
1	A	264	TYR	5.3
2	B	240	CYS	5.3
1	A	234	ILE	5.3
2	B	247	GLU	5.3
1	A	166	HIS	5.3
1	A	270	LEU	5.3
1	A	444	ARG	5.3
2	B	412	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	300	ASN	5.2
1	A	214	LYS	5.2
1	A	226	LEU	5.2
2	B	168	PHE	5.2
2	B	450	VAL	5.2
2	B	458	THR	5.2
2	B	397	LEU	5.2
2	B	198	GLY	5.2
1	A	380	ILE	5.2
1	A	399	ILE	5.2
2	B	391	ARG	5.1
2	B	174	LYS	5.1
2	B	173	LEU	5.1
2	B	172	GLU	5.1
1	A	307	HIS	5.1
1	A	357	PRO	5.1
2	B	418	MET	5.1
1	A	375	VAL	5.0
2	B	384	LEU	5.0
2	B	316	ASN	5.0
2	B	243	GLU	5.0
1	A	174	LYS	5.0
1	A	440	LYS	5.0
2	B	270	LEU	5.0
1	A	354	TYR	5.0
1	A	381	ILE	5.0
1	A	237	MET	5.0
1	A	299	ILE	5.0
2	B	380	ILE	5.0
2	B	262	TYR	5.0
2	B	273	ARG	5.0
1	A	451	GLN	4.9
1	A	249	LEU	4.9
1	A	360	LEU	4.9
1	A	251	PHE	4.9
1	A	173	LEU	4.9
1	A	435	GLN	4.9
2	B	306	HIS	4.8
2	B	398	ASP	4.8
2	B	373	PHE	4.8
1	A	238	ALA	4.8
1	A	247	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	176	VAL	4.8
2	B	226	LEU	4.8
2	B	396	LEU	4.8
1	A	452	GLN	4.8
1	A	276	CYS	4.7
2	B	344	MET	4.7
1	A	322	ALA	4.7
1	A	279	GLY	4.7
2	B	202	LYS	4.7
1	A	379	GLU	4.7
2	B	282	PRO	4.7
1	A	200	VAL	4.7
2	B	371	TYR	4.7
2	B	232	GLN	4.7
2	B	347	ARG	4.6
1	A	259	CYS	4.6
1	A	215	LEU	4.6
2	B	429	MET	4.6
1	A	368	SER	4.6
2	B	361	ARG	4.6
1	A	184	PRO	4.6
2	B	213	LYS	4.6
1	A	179	ASN	4.6
2	B	332	LEU	4.6
1	A	392	GLU	4.6
2	B	425	SER	4.6
1	A	317	ILE	4.6
1	A	260	LEU	4.6
1	A	301	PHE	4.5
1	A	315	ALA	4.5
2	B	433	ALA	4.5
1	A	441	LYS	4.5
1	A	263	VAL	4.5
1	A	228	GLN	4.5
2	B	319	LEU	4.5
2	B	195	GLY	4.4
2	B	276	CYS	4.4
2	B	387	VAL	4.4
1	A	203	GLY	4.4
1	A	382	THR	4.4
2	B	377	LEU	4.4
1	A	208	THR	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	421	ALA	4.4
1	A	186	SER	4.3
2	B	298	GLY	4.3
1	A	455	GLN	4.3
2	B	176	VAL	4.3
2	B	241	GLN	4.3
1	A	289	CYS	4.2
1	A	372	SER	4.2
1	A	427	GLU	4.2
2	B	402	GLU	4.2
2	B	452	GLN	4.2
2	B	209	THR	4.2
1	A	310	ARG	4.2
1	A	244	ASN	4.2
2	B	424	THR	4.2
2	B	248	LEU	4.2
1	A	196	GLY	4.2
1	A	281	PRO	4.2
1	A	209	THR	4.2
2	B	224	GLU	4.2
2	B	264	TYR	4.1
2	B	194	GLU	4.1
1	A	325	ALA	4.1
1	A	294	GLY	4.1
2	B	417	LYS	4.1
2	B	393	PRO	4.1
1	A	175	ASN	4.1
2	B	199	VAL	4.1
1	A	446	ASP	4.1
1	A	213	LYS	4.1
1	A	443	LYS	4.1
1	A	415	ASP	4.1
2	B	165	PHE	4.1
2	B	284	SER	4.0
1	A	456	GLU	4.0
2	B	379	GLU	4.0
1	A	373	PHE	4.0
2	B	197	PHE	3.9
2	B	382	THR	3.9
1	A	326	LYS	3.9
2	B	392	GLU	3.8
1	A	319	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	202	LYS	3.8
1	A	235	LYS	3.8
1	A	361	ARG	3.8
2	B	265	MET	3.8
1	A	395	LEU	3.8
1	A	210	VAL	3.7
1	A	349	VAL	3.7
2	B	177	THR	3.7
2	B	288	ARG	3.7
1	A	363	GLU	3.7
1	A	371	TYR	3.7
1	A	334	ARG	3.7
2	B	192	MET	3.6
2	B	408	LYS	3.6
2	B	310	ARG	3.6
1	A	351	THR	3.6
2	B	229	GLN	3.6
1	A	250	GLY	3.6
1	A	195	GLY	3.5
1	A	239	LYS	3.5
1	A	298	GLY	3.5
2	B	294	GLY	3.5
2	B	386	ALA	3.5
1	A	283	LEU	3.5
1	A	425	SER	3.4
1	A	428	ALA	3.4
2	B	291	ILE	3.4
1	A	273	ARG	3.4
1	A	288	ARG	3.3
2	B	289	CYS	3.3
1	A	400	LYS	3.3
2	B	167	SER	3.3
1	A	403	ILE	3.3
1	A	245	LEU	3.3
1	A	272	ASP	3.3
2	B	275	SER	3.2
2	B	372	SER	3.2
1	A	246	VAL	3.2
2	B	301	PHE	3.2
1	A	266	PRO	3.2
2	B	233	GLU	3.2
1	A	328	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	296	ALA	3.2
1	A	199	VAL	3.2
1	A	329	ASP	3.2
1	A	267	ASN	3.2
2	B	383	GLY	3.2
1	A	282	PRO	3.2
2	B	369	ASP	3.2
1	A	352	THR	3.1
1	A	308	ILE	3.1
1	A	323	PHE	3.1
1	A	433	ALA	3.1
2	B	190	ASN	3.1
2	B	238	ALA	3.0
1	A	183	ARG	3.0
1	A	261	VAL	3.0
1	A	192	MET	3.0
2	B	376	VAL	3.0
2	B	225	GLU	3.0
1	A	447	ILE	3.0
2	B	283	LEU	3.0
1	A	316	ASN	3.0
1	A	198	GLY	2.9
1	A	295	ALA	2.9
2	B	210	VAL	2.9
2	B	259	CYS	2.9
2	B	407	GLU	2.9
1	A	268	GLY	2.9
1	A	248	LEU	2.9
1	A	265	MET	2.8
1	A	343	VAL	2.7
1	A	445	PRO	2.7
2	B	328	SER	2.7
2	B	166	HIS	2.7
1	A	233	GLU	2.6
2	B	258	LEU	2.6
1	A	434	SER	2.6
2	B	239	LYS	2.6
1	A	386	ALA	2.6
1	A	201	TYR	2.5
2	B	305	ASN	2.5
1	A	377	LEU	2.5
1	A	309	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	193	GLY	2.4
1	A	402	GLU	2.4
1	A	313	LYS	2.3
2	B	228	GLN	2.3
1	A	431	SER	2.3
2	B	326	LYS	2.2
1	A	401	GLU	2.2
2	B	311	ASP	2.1
1	A	378	LEU	2.1

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, 95^{th} 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 monosaccharides in this entry.

6.4 Ligands (i)

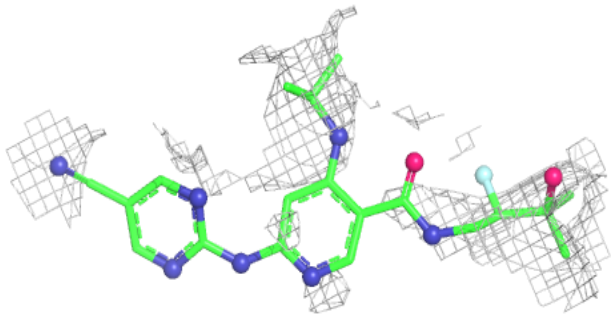
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

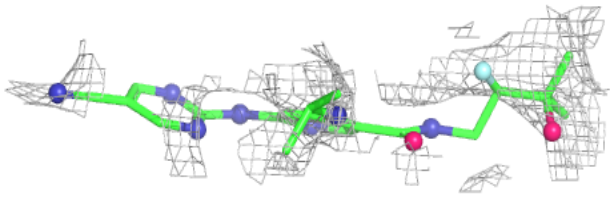
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZVG	B	501	29/29	0.36	0.27	55,68,76,80	0
4	SO4	A	502	5/5	0.39	0.35	144,148,149,150	0
3	ZVG	A	501	29/29	0.53	0.36	24,31,44,55	0
4	SO4	B	502	5/5	0.56	0.30	66,70,71,72	0

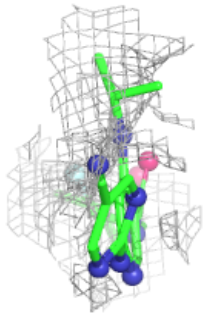
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ZVG B 501:

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

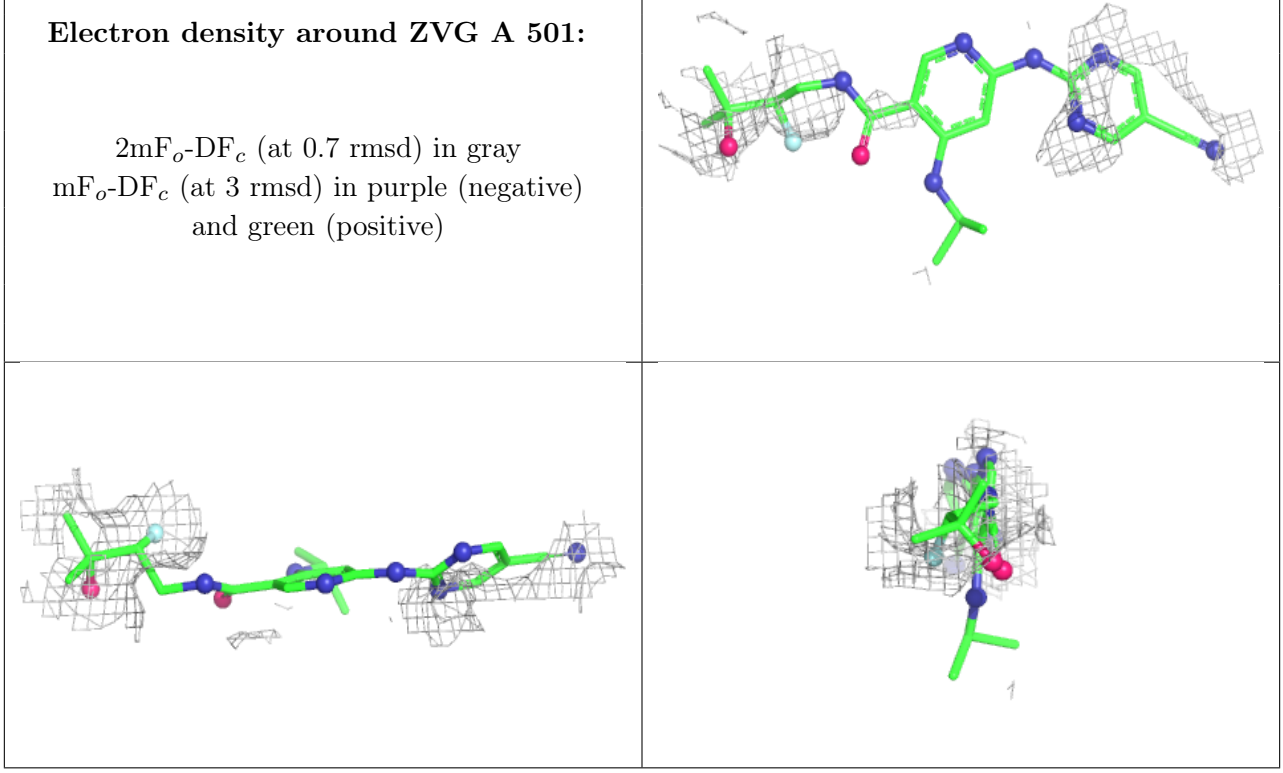






Electron density around ZVG A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.