



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:20 AM UTC

PDB ID : 4AOJ / pdb_00004aoj
Title : Human TrkA in complex with the inhibitor AZ-23
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Ioannidis, S.; Josey, J.A.; Liu, Z.; Lyne, P.D.; MacIntyre, T.; Mohr, P.J.;
Omer, C.A.; Sjogren, T.; Thress, K.; Wang, B.; Wang, H.; Yu, D.; Zhang, H.
Deposited on : 2012-03-28
Resolution : 2.75 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:

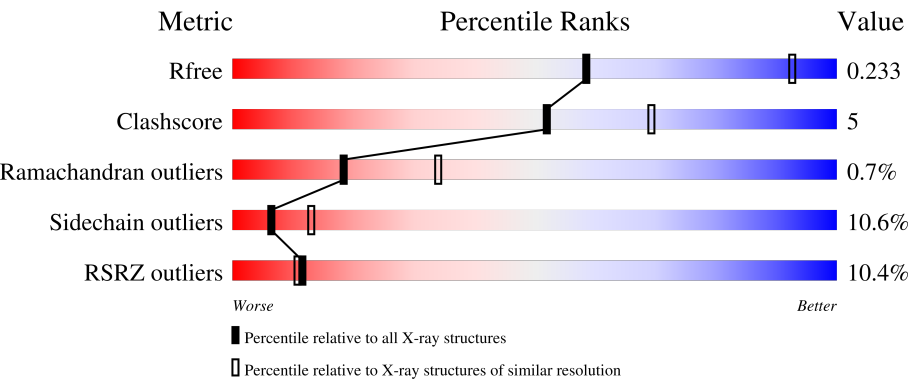
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	329	5% 66% 12% •• 21%
1	B	329	7% 60% 15% • 22%
1	C	329	13% 64% 12% • 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6412 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.

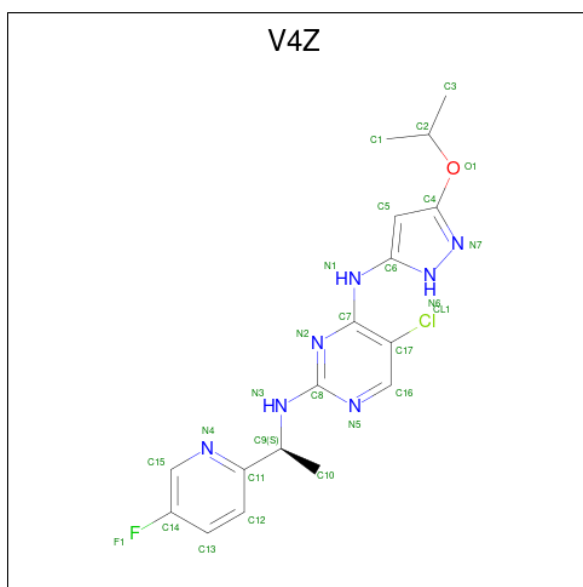
- Molecule 1 is a protein called HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2077	1332	377	353	15			
1	B	258	Total	C	N	O	S	0	1	0
			2077	1338	375	350	14			
1	C	261	Total	C	N	O	S	0	0	0
			2088	1337	379	356	16			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	468	GLY	-	expression tag	UNP P04629
A	469	ALA	-	expression tag	UNP P04629
A	470	MET	-	expression tag	UNP P04629
A	471	GLY	-	expression tag	UNP P04629
A	472	SER	-	expression tag	UNP P04629
B	468	GLY	-	expression tag	UNP P04629
B	469	ALA	-	expression tag	UNP P04629
B	470	MET	-	expression tag	UNP P04629
B	471	GLY	-	expression tag	UNP P04629
B	472	SER	-	expression tag	UNP P04629
C	468	GLY	-	expression tag	UNP P04629
C	469	ALA	-	expression tag	UNP P04629
C	470	MET	-	expression tag	UNP P04629
C	471	GLY	-	expression tag	UNP P04629
C	472	SER	-	expression tag	UNP P04629

- Molecule 2 is 5-chloranyl-N2-[(1S)-1-(5-fluoranylpYridin-2-yl)ethyl]-N4-(3-propan-2-yloxy-1H-pyrazol-5-yl)pyrimidine-2,4-diamine (CCD ID: V4Z) (formula: C₁₇H₁₉ClFN₇O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			27	17	1	1	7	1		
2	B	1	Total	C	Cl	F	N	O	0	0
			27	17	1	1	7	1		
2	C	1	Total	C	Cl	F	N	O	0	0
			27	17	1	1	7	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

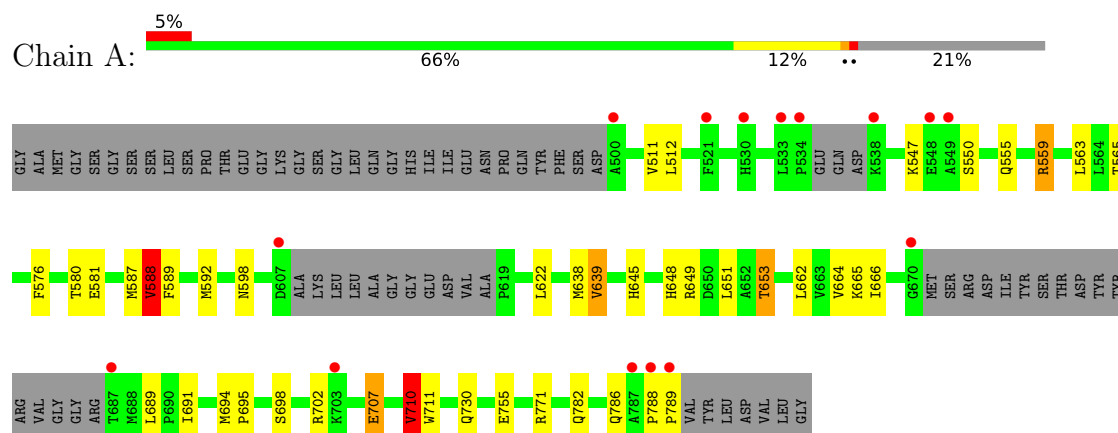
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	31	Total	O	0	0
			31	31		
4	C	11	Total	O	0	0
			11	11		

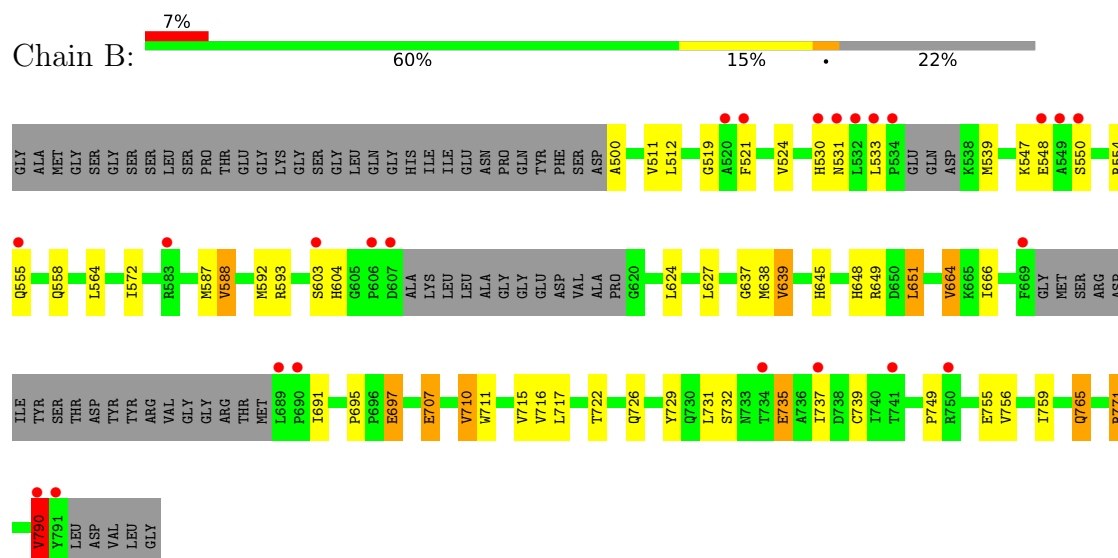
3 Residue-property plots

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.

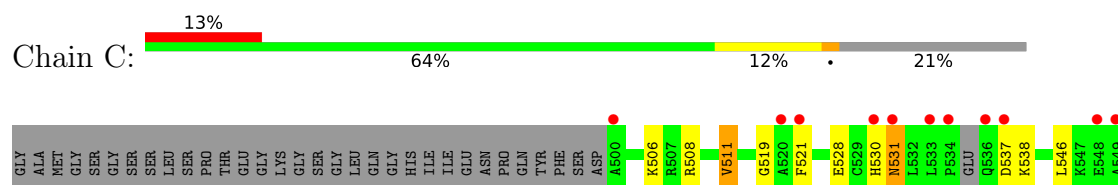
• Molecule 1: HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR

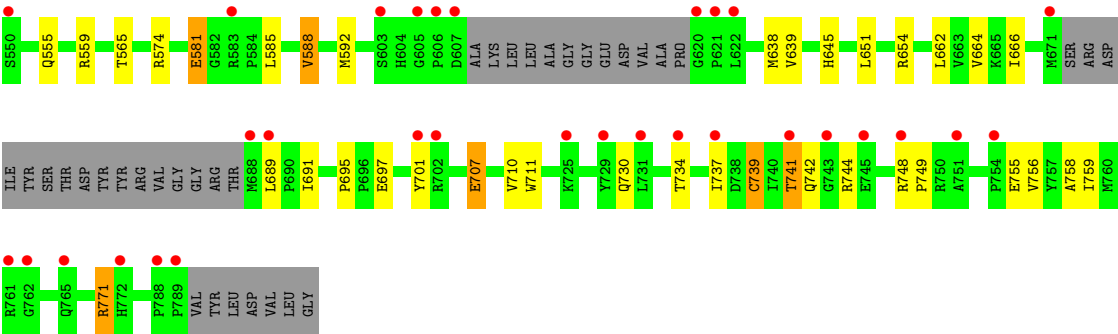


• Molecule 1: HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR



• Molecule 1: HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	130.73Å 158.42Å 152.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.75 40.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.00-2.75) 95.6 (40.00-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.242 0.212 , 0.233	Depositor DCC
R_{free} test set	2085 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6412	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: ZN, V4Z

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	0.93	1/2129 (0.0%)	1.09	2/2878 (0.1%)
1	B	0.90	2/2133 (0.1%)	1.06	6/2884 (0.2%)
1	C	0.83	1/2139 (0.0%)	1.00	1/2890 (0.0%)
All	All	0.89	4/6401 (0.1%)	1.05	9/8652 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	715	VAL	CA-CB	7.24	1.64	1.54
1	B	639	VAL	CA-CB	6.94	1.63	1.54
1	C	639	VAL	CA-CB	6.44	1.62	1.54
1	A	639	VAL	CA-CB	6.00	1.62	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	593	ARG	N-CA-C	6.60	119.30	111.71
1	B	710	VAL	N-CA-CB	6.09	118.83	110.54
1	C	588	VAL	N-CA-C	6.02	116.60	108.17
1	A	588	VAL	N-CA-C	5.97	116.90	108.36
1	B	548	GLU	N-CA-C	5.72	117.97	111.11
1	A	710	VAL	N-CA-CB	5.59	118.14	110.54
1	B	790	VAL	N-CA-C	5.47	120.71	109.34
1	B	588	VAL	N-CA-C	5.20	115.45	108.17
1	B	664	VAL	CB-CA-C	5.18	118.31	110.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2077	0	2078	22	0
1	B	2077	0	2077	21	0
1	C	2088	0	2085	21	0
2	A	27	0	19	1	0
2	B	27	0	19	2	0
2	C	27	0	19	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	41	0	0	0	0
4	B	31	0	0	0	0
4	C	11	0	0	0	0
All	All	6412	0	6297	64	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 (64) 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:C:638:MET:HE3	1:C:651:LEU:HD13	1.38	1.04
1:A:598:ASN:HB2	1:A:653:THR:HG22	1.46	0.97
1:C:592:MET:H	2:C:900:V4Z:H6	1.17	0.93
1:B:592:MET:H	2:B:900:V4Z:H6	1.21	0.85
1:A:592:MET:H	2:A:900:V4Z:H6	1.33	0.73
1:A:638:MET:HE2	1:A:666:ILE:HD13	1.70	0.73
1:A:598:ASN:HB2	1:A:653:THR:CG2	2.21	0.70
1:B:732:SER:H	1:B:735:GLU:HG3	1.56	0.70
1:A:638:MET:HE3	1:A:651:LEU:HD13	1.78	0.65
1:C:695:PRO:HB3	1:C:711:TRP:CD2	2.32	0.64
1:A:782:GLN:O	1:A:786:GLN:HG2	1.98	0.64
1:B:624:LEU:HD23	1:B:790:VAL:HA	1.79	0.62
1:C:638:MET:HE2	1:C:666:ILE:HD13	1.83	0.61
1:C:737:ILE:O	1:C:741:THR:HB	2.03	0.59
1:B:519:GLY:HA3	1:B:521:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:HD13	1:B:716:VAL:HG21	1.88	0.56
1:C:734:THR:O	1:C:737:ILE:HG22	2.07	0.55
1:A:638:MET:HE2	1:A:666:ILE:CD1	2.37	0.54
1:C:697:GLU:OE2	1:C:771:ARG:NH2	2.40	0.53
1:B:638:MET:HE2	1:B:666:ILE:HD13	1.89	0.53
1:B:756:VAL:HA	1:B:759:ILE:HD12	1.91	0.53
1:C:638:MET:HE3	1:C:651:LEU:CD1	2.27	0.52
1:B:695:PRO:HB2	1:B:697:GLU:OE2	2.10	0.51
1:A:695:PRO:HB3	1:A:711:TRP:CD2	2.45	0.51
1:B:637:GLY:HA3	1:B:666:ILE:HD12	1.93	0.50
1:C:581:GLU:O	1:C:581:GLU:HG2	2.12	0.50
1:C:511:VAL:HG13	1:C:528:GLU:HB2	1.95	0.48
1:B:533:LEU:HD12	1:B:539:MET:HE1	1.96	0.48
2:B:900:V4Z:H2	2:B:900:V4Z:H12	1.96	0.47
1:B:564:LEU:HD12	1:B:587:MET:HE2	1.96	0.47
1:C:638:MET:HE2	1:C:666:ILE:CD1	2.44	0.46
1:A:707:GLU:HA	1:A:710:VAL:CG2	2.45	0.46
1:A:555:GLN:HG3	1:A:559:ARG:HH11	1.81	0.46
1:A:598:ASN:CB	1:A:653:THR:CG2	2.93	0.45
1:C:756:VAL:HA	1:C:759:ILE:HD12	1.98	0.45
1:A:689:LEU:HD13	1:A:694:MET:HE1	1.99	0.45
1:C:707:GLU:HA	1:C:710:VAL:HG22	1.99	0.45
1:A:707:GLU:HA	1:A:710:VAL:HG23	1.99	0.44
1:B:722:THR:HG22	1:B:749:PRO:HB3	2.00	0.43
1:A:598:ASN:CB	1:A:653:THR:HG22	2.33	0.43
1:C:530:HIS:ND1	1:C:538:LYS:HG2	2.33	0.43
1:B:717:LEU:HA	1:B:717:LEU:HD23	1.82	0.43
1:C:695:PRO:HB3	1:C:711:TRP:CG	2.54	0.42
1:C:755:GLU:O	1:C:758:ALA:HB3	2.19	0.42
1:B:572:ILE:HD13	1:B:666:ILE:HB	2.01	0.42
1:B:695:PRO:HB3	1:B:711:TRP:CG	2.54	0.42
1:A:587:MET:HE3	1:A:589:PHE:HZ	1.85	0.42
1:B:726:GLN:HE21	1:B:729:TYR:HA	1.83	0.42
1:A:592:MET:HE1	1:A:665:LYS:HG3	2.01	0.42
1:B:603:SER:HB2	1:B:604:HIS:HD2	1.85	0.42
1:A:576:PHE:HB2	1:A:588:VAL:HG22	2.02	0.42
1:A:598:ASN:N	1:A:653:THR:HG23	2.35	0.42
1:C:546:LEU:CD2	1:C:585:LEU:HD12	2.50	0.42
1:B:500:ALA:HB3	1:C:508:ARG:HH22	1.85	0.41
1:A:788:PRO:HA	1:A:789:PRO:HD3	1.90	0.41
1:B:648:HIS:O	1:B:649:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:765:GLN:O	1:B:771:ARG:HD2	2.20	0.41
1:A:648:HIS:O	1:A:649:ARG:HB2	2.19	0.41
1:A:695:PRO:HD2	1:A:698:SER:HB2	2.02	0.41
1:C:739:CYS:SG	1:C:744:ARG:HD3	2.60	0.41
1:A:598:ASN:CA	1:A:653:THR:CG2	2.99	0.40
1:B:707:GLU:HA	1:B:710:VAL:HG22	2.03	0.40
1:C:748:ARG:HA	1:C:749:PRO:HD3	1.90	0.40
1:C:519:GLY:HA3	1:C:521:PHE:CE2	2.56	0.40

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	252/329 (77%)	241 (96%)	10 (4%)	1 (0%)	30	50
1	B	251/329 (76%)	237 (94%)	11 (4%)	3 (1%)	10	20
1	C	253/329 (77%)	239 (94%)	13 (5%)	1 (0%)	30	50
All	All	756/987 (77%)	717 (95%)	34 (4%)	5 (1%)	18	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	550	SER
1	B	790	VAL
1	A	550	SER
1	B	531	ASN
1	C	531	ASN

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	218/272 (80%)	196 (90%)	22 (10%)	7	14
1	B	218/272 (80%)	194 (89%)	24 (11%)	6	11
1	C	219/272 (80%)	196 (90%)	23 (10%)	6	13
All	All	655/816 (80%)	586 (90%)	69 (10%)	6	13

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	VAL
1	A	512	LEU
1	A	547	LYS
1	A	559	ARG
1	A	563	LEU
1	A	565	THR
1	A	580	THR
1	A	581	GLU
1	A	588	VAL
1	A	622	LEU
1	A	639	VAL
1	A	645	HIS
1	A	653	THR
1	A	662	LEU
1	A	664	VAL
1	A	691	ILE
1	A	702	ARG
1	A	707	GLU
1	A	710	VAL
1	A	730	GLN
1	A	755	GLU
1	A	771	ARG
1	B	511	VAL
1	B	512	LEU
1	B	524	VAL
1	B	530	HIS

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Mol	Chain	Res	Type
1	B	547	LYS
1	B	554	ARG
1	B	555	GLN
1	B	558	GLN
1	B	588	VAL
1	B	627	LEU
1	B	639	VAL
1	B	645	HIS
1	B	651	LEU
1	B	664	VAL
1	B	691	ILE
1	B	697	GLU
1	B	707	GLU
1	B	731	LEU
1	B	735	GLU
1	B	737	ILE
1	B	739	CYS
1	B	755	GLU
1	B	765	GLN
1	B	771	ARG
1	C	506	LYS
1	C	511	VAL
1	C	531	ASN
1	C	537	ASP
1	C	555	GLN
1	C	559	ARG
1	C	565	THR
1	C	574	ARG
1	C	581	GLU
1	C	588	VAL
1	C	645	HIS
1	C	654	ARG
1	C	662	LEU
1	C	664	VAL
1	C	689	LEU
1	C	691	ILE
1	C	701	TYR
1	C	707	GLU
1	C	730	GLN
1	C	739	CYS
1	C	741	THR
1	C	742	GLN

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Mol	Chain	Res	Type
1	C	771	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	604	HIS
1	A	645	HIS
1	A	730	GLN
1	A	742	GLN
1	A	765	GLN
1	B	531	ASN
1	B	571	HIS
1	B	604	HIS
1	B	726	GLN
1	B	742	GLN
1	B	772	HIS
1	C	660	GLN
1	C	726	GLN
1	C	733	ASN
1	C	742	GLN
1	C	765	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	V4Z	C	900	-	27,29,29	1.66	5 (18%)	34,40,40	3.50	12 (35%)
2	V4Z	A	900	-	27,29,29	1.71	4 (14%)	34,40,40	4.45	12 (35%)
2	V4Z	B	900	-	27,29,29	1.83	5 (18%)	34,40,40	3.97	11 (32%)

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	V4Z	C	900	-	-	2/16/16/16	0/3/3/3
2	V4Z	A	900	-	-	1/16/16/16	0/3/3/3
2	V4Z	B	900	-	-	1/16/16/16	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	V4Z	C4-N7	5.54	1.37	1.32
2	B	900	V4Z	C8-N3	5.45	1.41	1.34
2	A	900	V4Z	C4-N7	5.25	1.37	1.32
2	B	900	V4Z	C11-C9	-3.99	1.48	1.52
2	C	900	V4Z	C8-N3	3.72	1.39	1.34
2	A	900	V4Z	C8-N3	3.59	1.38	1.34
2	B	900	V4Z	C4-N7	3.58	1.35	1.32
2	B	900	V4Z	C5-C6	3.48	1.43	1.38
2	A	900	V4Z	C5-C6	3.42	1.43	1.38
2	A	900	V4Z	C11-C9	-2.68	1.49	1.52
2	C	900	V4Z	C5-C6	2.63	1.42	1.38
2	C	900	V4Z	C16-C17	-2.39	1.36	1.39
2	B	900	V4Z	C16-C17	-2.22	1.36	1.39
2	C	900	V4Z	C11-C9	-2.19	1.50	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	V4Z	C4-N7-N6	16.10	115.48	102.23
2	B	900	V4Z	C4-N7-N6	14.80	114.41	102.23
2	C	900	V4Z	C4-N7-N6	12.04	112.15	102.23
2	A	900	V4Z	C5-C4-N7	-11.81	104.86	113.69
2	B	900	V4Z	C5-C4-N7	-11.26	105.27	113.69
2	C	900	V4Z	C5-C4-N7	-9.30	106.73	113.69
2	A	900	V4Z	C7-C17-CL1	8.80	126.19	119.76
2	A	900	V4Z	C13-C14-C15	-6.72	118.02	121.55
2	B	900	V4Z	C12-C11-C9	-6.43	116.06	121.89
2	C	900	V4Z	C7-C17-CL1	5.73	123.95	119.76
2	A	900	V4Z	C8-N3-C9	-5.28	113.81	122.67
2	C	900	V4Z	C8-N3-C9	-5.13	114.06	122.67
2	B	900	V4Z	C7-C17-CL1	5.08	123.48	119.76
2	B	900	V4Z	C9-C11-N4	5.02	120.59	116.03
2	B	900	V4Z	C13-C14-C15	-5.00	118.92	121.55
2	A	900	V4Z	C12-C11-C9	-4.98	117.38	121.89
2	C	900	V4Z	C13-C14-C15	-4.90	118.97	121.55
2	C	900	V4Z	C9-C11-N4	4.61	120.21	116.03
2	A	900	V4Z	C9-C11-N4	4.58	120.19	116.03
2	C	900	V4Z	C12-C11-C9	-4.57	117.75	121.89
2	B	900	V4Z	C10-C9-C11	-4.48	105.56	110.98
2	A	900	V4Z	C17-C7-N1	-3.61	117.01	120.23
2	A	900	V4Z	C10-C9-C11	-3.53	106.70	110.98
2	B	900	V4Z	C8-N3-C9	-3.49	116.82	122.67
2	C	900	V4Z	C10-C9-N3	-3.47	102.73	108.91
2	A	900	V4Z	N3-C8-N2	3.39	122.42	117.09
2	A	900	V4Z	C16-C17-C7	-3.08	117.12	119.84
2	C	900	V4Z	C17-C7-N1	-3.03	117.52	120.23
2	C	900	V4Z	C10-C9-C11	-2.96	107.39	110.98
2	A	900	V4Z	N3-C8-N5	-2.95	112.08	116.75
2	B	900	V4Z	C17-C7-N1	-2.77	117.76	120.23
2	C	900	V4Z	N3-C8-N2	2.24	120.60	117.09
2	B	900	V4Z	N3-C8-N2	2.23	120.58	117.09
2	C	900	V4Z	C16-C17-C7	-2.20	117.90	119.84
2	B	900	V4Z	N3-C8-N5	-2.07	113.48	116.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	V4Z	N4-C11-C9-N3
2	C	900	V4Z	N4-C11-C9-N3
2	C	900	V4Z	C12-C11-C9-N3

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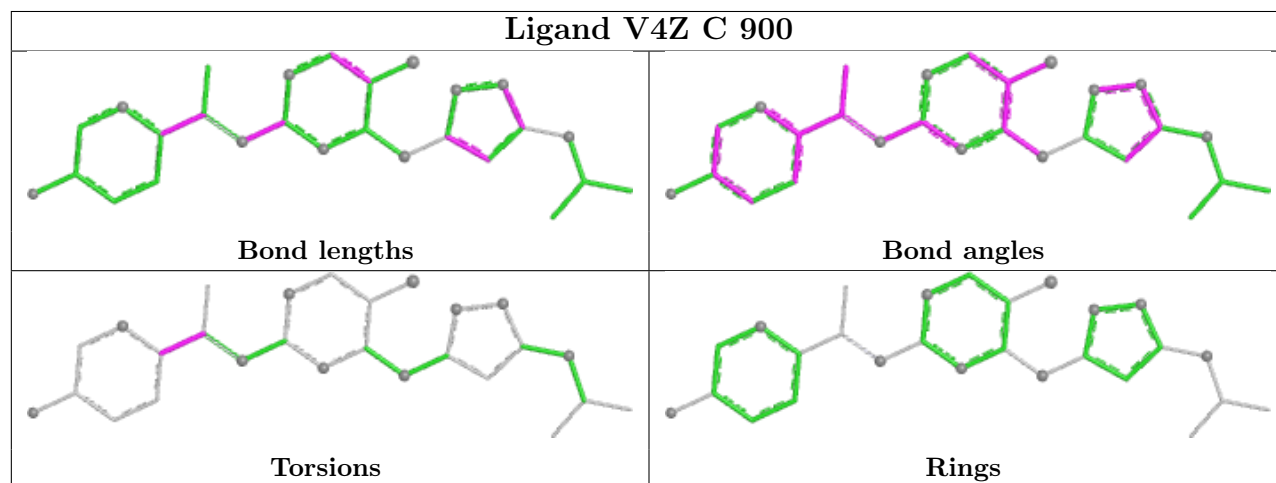
Mol	Chain	Res	Type	Atoms
2	B	900	V4Z	N4-C11-C9-N3

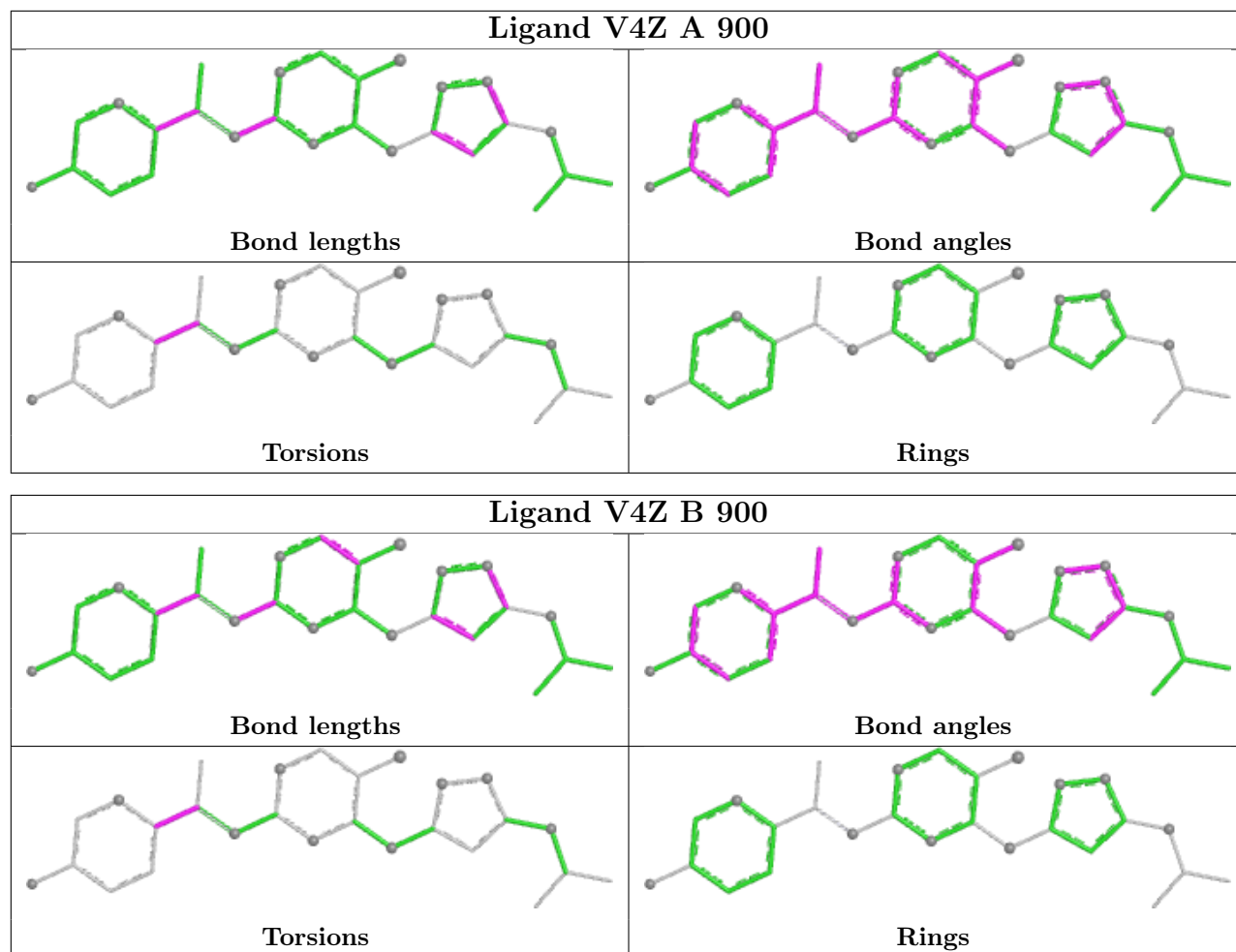
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	V4Z	1	0
2	A	900	V4Z	1	0
2	B	900	V4Z	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	260/329 (79%)	0.28	15 (5%)	29 29	25, 49, 82, 98	0
1	B	258/329 (78%)	0.40	24 (9%)	14 14	23, 49, 87, 97	1 (0%)
1	C	261/329 (79%)	0.77	42 (16%)	4 4	33, 62, 94, 105	0
All	All	779/987 (78%)	0.49	81 (10%)	11 11	23, 53, 88, 105	1 (0%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	791	TYR	7.5
1	A	670	GLY	6.0
1	A	534	PRO	6.0
1	B	790	VAL	5.4
1	A	789	PRO	5.2
1	C	671	MET	5.0
1	B	534	PRO	4.1
1	B	533	LEU	4.1
1	C	789	PRO	4.1
1	B	689	LEU	4.0
1	C	521	PHE	3.8
1	C	534	PRO	3.7
1	A	533	LEU	3.6
1	A	549	ALA	3.6
1	A	521	PHE	3.6
1	A	787	ALA	3.6
1	A	548	GLU	3.3
1	C	689	LEU	3.2
1	B	669	PHE	3.2
1	B	549	ALA	3.1
1	C	520	ALA	3.1
1	C	603	SER	3.0
1	A	500	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	530	HIS	3.0
1	C	533	LEU	2.9
1	B	583	ARG	2.9
1	C	537	ASP	2.9
1	C	548	GLU	2.9
1	B	607	ASP	2.9
1	C	743	GLY	2.9
1	C	606	PRO	2.8
1	C	701	TYR	2.8
1	B	532	LEU	2.8
1	B	750	ARG	2.8
1	C	734	THR	2.8
1	B	606	PRO	2.7
1	A	607	ASP	2.7
1	C	500	ALA	2.7
1	B	603	SER	2.7
1	C	761	ARG	2.6
1	C	621	PRO	2.6
1	C	605	GLY	2.6
1	C	788	PRO	2.6
1	B	520	ALA	2.5
1	B	548	GLU	2.5
1	C	745	GLU	2.5
1	C	729	TYR	2.5
1	B	531	ASN	2.5
1	B	521	PHE	2.4
1	B	734	THR	2.4
1	C	772	HIS	2.4
1	C	536	GLN	2.4
1	B	737	ILE	2.4
1	C	748	ARG	2.3
1	C	549	ALA	2.3
1	C	741	THR	2.3
1	B	690	PRO	2.3
1	B	530	HIS	2.2
1	C	530	HIS	2.2
1	A	687	THR	2.2
1	B	550	SER	2.2
1	C	531	ASN	2.2
1	C	607	ASP	2.2
1	C	737	ILE	2.1
1	A	538	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	555	GLN	2.1
1	C	620	GLY	2.1
1	B	741	THR	2.1
1	C	688	MET	2.1
1	C	731	LEU	2.1
1	C	751	ALA	2.1
1	A	788	PRO	2.1
1	C	725	LYS	2.0
1	C	754	PRO	2.0
1	C	622	LEU	2.0
1	C	762	GLY	2.0
1	C	702	ARG	2.0
1	A	703	LYS	2.0
1	C	550	SER	2.0
1	C	765	GLN	2.0
1	C	583	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	V4Z	C	900	27/27	0.96	0.08	26,33,44,50	0
2	V4Z	B	900	27/27	0.97	0.06	26,30,34,38	0
2	V4Z	A	900	27/27	0.98	0.05	22,29,32,33	0
3	ZN	A	1790	1/1	0.99	0.02	53,53,53,53	0
3	ZN	A	1791	1/1	0.99	0.05	58,58,58,58	0
3	ZN	B	1792	1/1	0.99	0.03	56,56,56,56	0
3	ZN	B	1793	1/1	0.99	0.03	58,58,58,58	0

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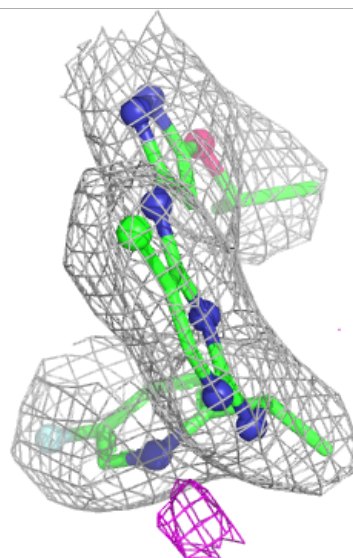
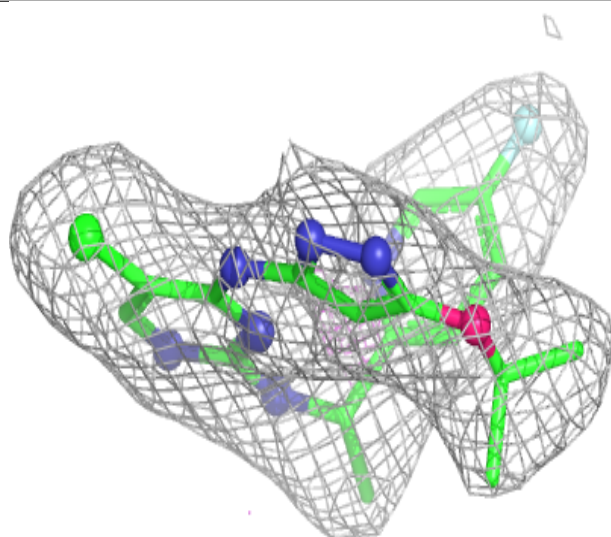
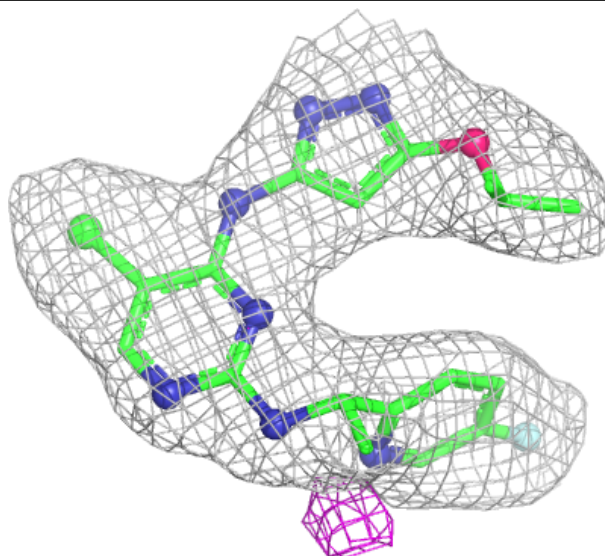
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	1790	1/1	0.99	0.02	52,52,52,52	0
3	ZN	C	1791	1/1	0.99	0.05	64,64,64,64	0

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.

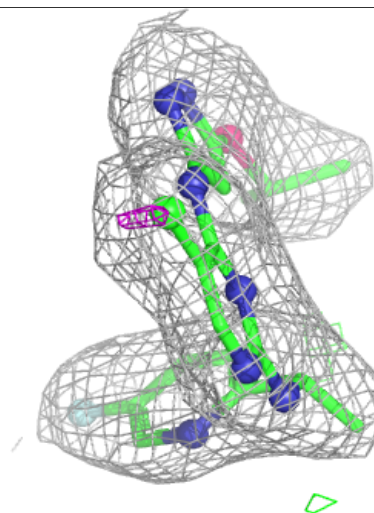
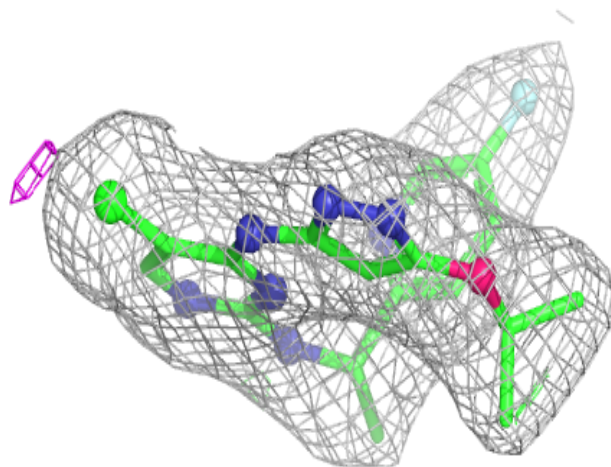
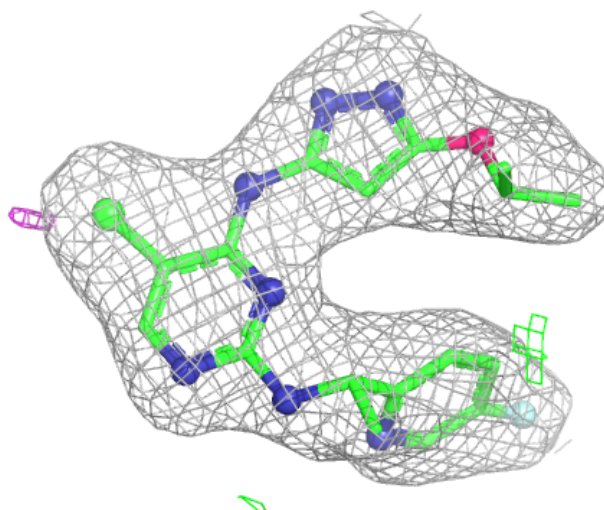
Electron density around V4Z C 900:

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



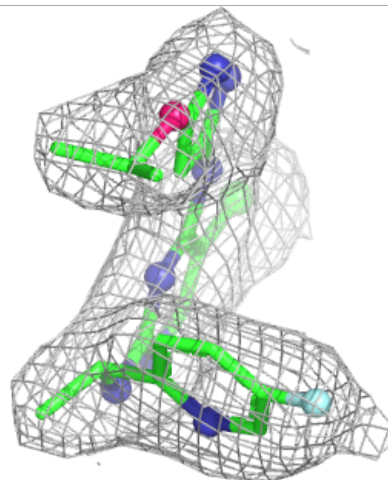
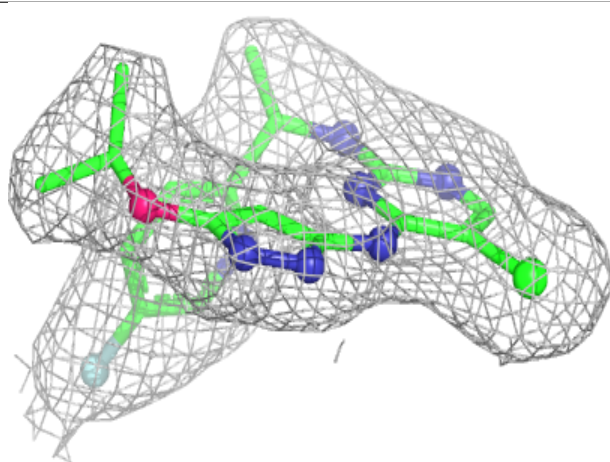
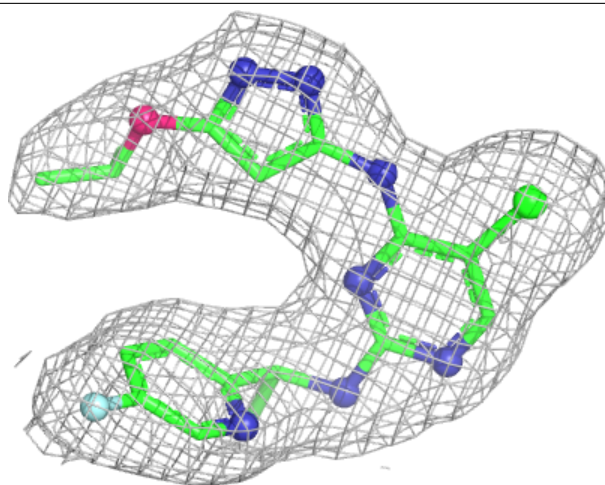
Electron density around V4Z B 900:

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



Electron density around V4Z A 900:

$2mF_o-DF_c$ (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.