Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 03:48 pm GMT

PDB ID	:	4AOJ
Title	:	Human TrkA in complex with the inhibitor AZ-23
Authors	:	Wang, T.; Lamb, M.L.; Block, M.H.; Davies, A.M.; Han, Y.; Hoffmann, E.; 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:

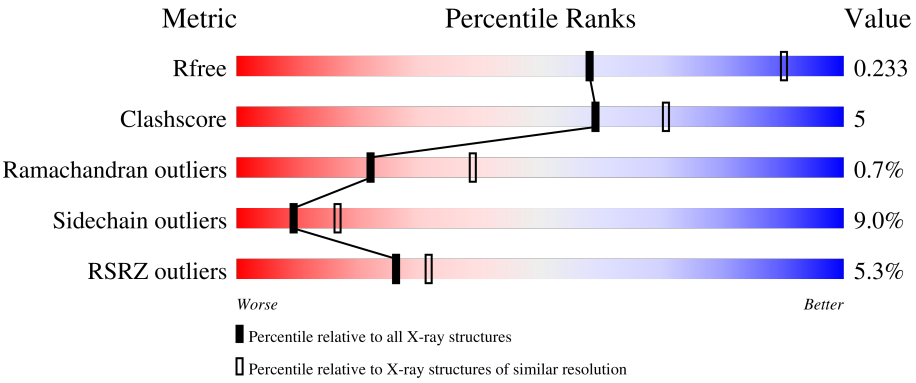
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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% 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	2% 68% 9% • 21%
1	B	329	4% 62% 15% • 22%
1	C	329	6% 66% 12% • 21%

2 Entry composition (i)

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.

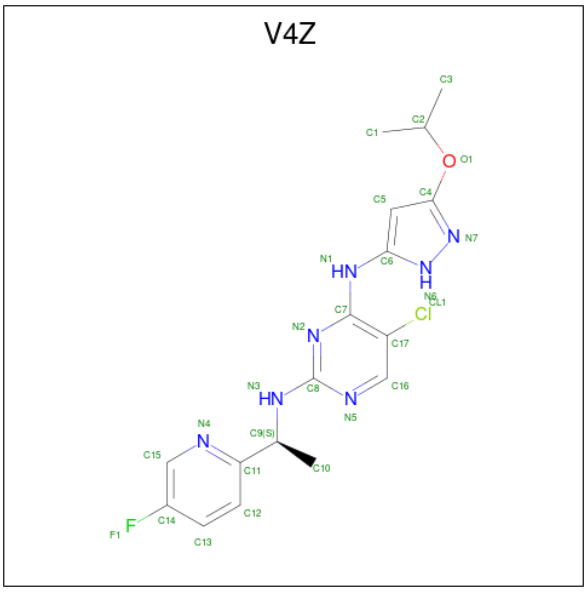
- Molecule 1 is a protein called HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR.

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-1 H-pyrazol-5-yl)pyrimidine-2,4-diamine (three-letter code: V4Z) (formula: $C_{17}H_{19}ClFN_7O$).



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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

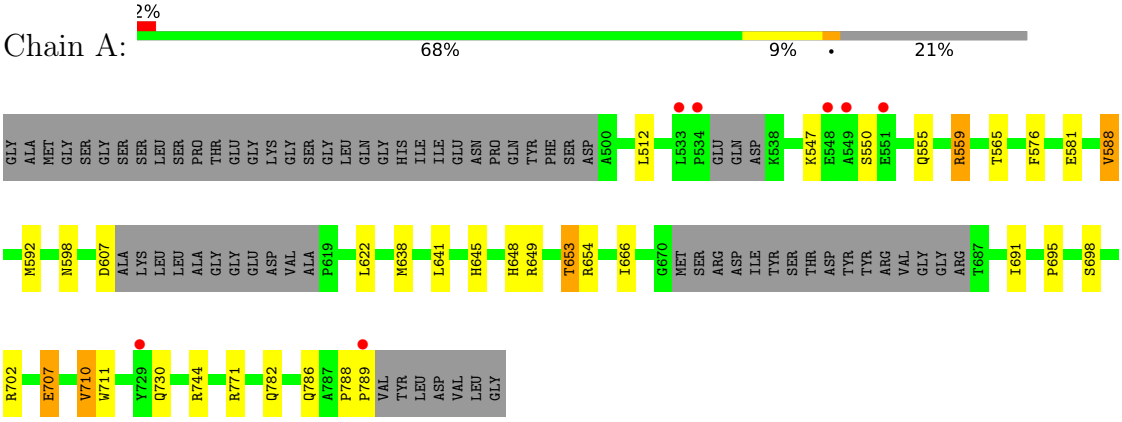
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0
4	B	31	Total O 31 31	0	0
4	C	11	Total O 11 11	0	0

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 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.

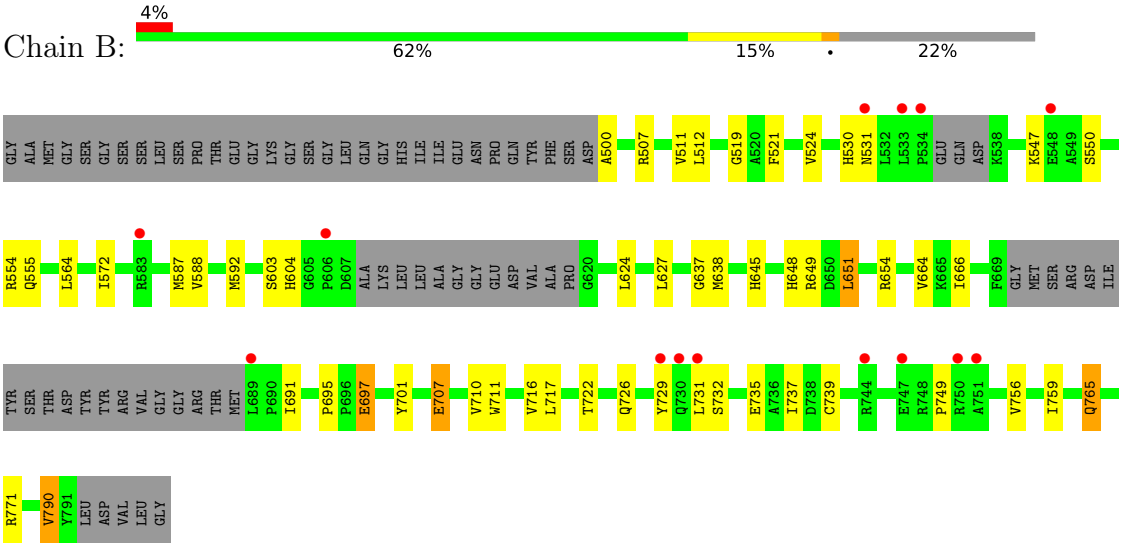
• Molecule 1: HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR

Chain A:



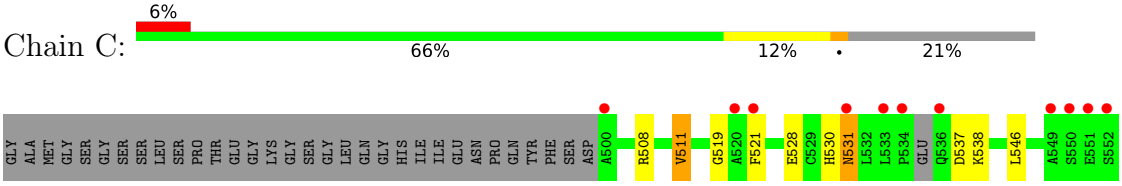
• Molecule 1: HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR

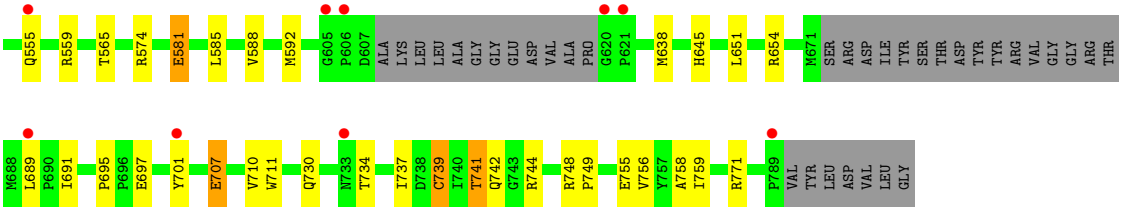
Chain B:



• Molecule 1: HIGH AFFINITY NERVE GROWTH FACTOR RECEPTOR

Chain C:




Q555 R559 T565 R574 E581 L585 V588 M592 G605 P606 D607 ALA LYS LEU LEU ALA GLY GLY GLU ASP VAL ALA PRO G620 P621 M638 H645 L651 R654 M671 SER ARG ASP ILE TYR SER THR ASP TYR TYR ARG VAL GLY GLY ARG THR
M688 L689 P690 I691 P695 P696 E697 Y701 E707 V710 W711 Q730 N733 T734 I737 D738 C739 I740 T741 Q742 G743 R744 R748 P749 E755 V756 Y757 A758 I759 R771 P789 VAL TYR LEU ASP VAL LEU GLY

4 Data and refinement statistics (i)

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 42.06 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.6 (40.00-2.75) 95.6 (42.06-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.36 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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: 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	0.73	0/2129	0.76	0/2878
1	B	0.71	0/2133	0.73	0/2884
1	C	0.66	0/2139	0.68	0/2890
All	All	0.70	0/6401	0.72	0/8652

There are no bond length outliers.

There are no bond angle outliers.

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	19	0
1	B	2077	0	2077	20	0
1	C	2088	0	2085	20	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	0	0	0
4	C	11	0	0	0	0
All	All	6412	0	6297	59	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 (59) 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: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: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: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:C:638:MET:CE	1:C:651:LEU:HD13	2.28	0.63
1:B:624:LEU:HD23	1:B:790:VAL:HA	1.79	0.62
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
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:C:638:MET:HE3	1:C:651:LEU:HD13	1.89	0.54
1:C:697:GLU:OE2	1:C:771:ARG:NH2	2.40	0.53
1:B:756:VAL:HA	1:B:759:ILE:HD12	1.91	0.53
1:C:638:MET:HE2	1:C:651:LEU:HD13	1.91	0.52
1:A:638:MET:HE2	1:A:641:LEU:HD12	1.92	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:564:LEU:HD12	1:B:587:MET:HE2	1.92	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:B:638:MET:HE2	1:B:666:ILE:HD13	1.95	0.49
1:C:511:VAL:HG13	1:C:528:GLU:HB2	1.95	0.48
1:A:638:MET:HE2	1:A:666:ILE:HD13	1.94	0.48
2:B:900:V4Z:H2	2:B:900:V4Z:H12	1.96	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:756:VAL:HA	1:C:759:ILE:HD12	1.98	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:B:726:GLN:HE21	1:B:729:TYR:HA	1.83	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
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:638:MET:CE	1:A:666:ILE:HD13	2.50	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 (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	252/329 (77%)	241 (96%)	10 (4%)	1 (0%)	34	53
1	B	251/329 (76%)	237 (94%)	11 (4%)	3 (1%)	13	23
1	C	253/329 (77%)	239 (94%)	13 (5%)	1 (0%)	34	53
All	All	756/987 (77%)	717 (95%)	34 (4%)	5 (1%)	22	39

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 (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	218/272 (80%)	200 (92%)	18 (8%)	11	20
1	B	218/272 (80%)	196 (90%)	22 (10%)	7	12
1	C	219/272 (80%)	200 (91%)	19 (9%)	10	18
All	All	655/816 (80%)	596 (91%)	59 (9%)	9	16

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	512	LEU
1	A	547	LYS
1	A	559	ARG
1	A	565	THR
1	A	581	GLU
1	A	588	VAL
1	A	607	ASP
1	A	622	LEU

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Mol	Chain	Res	Type
1	A	645	HIS
1	A	653	THR
1	A	654	ARG
1	A	691	ILE
1	A	702	ARG
1	A	707	GLU
1	A	710	VAL
1	A	730	GLN
1	A	744	ARG
1	A	771	ARG
1	B	507	ARG
1	B	511	VAL
1	B	512	LEU
1	B	524	VAL
1	B	530	HIS
1	B	547	LYS
1	B	554	ARG
1	B	555	GLN
1	B	588	VAL
1	B	627	LEU
1	B	645	HIS
1	B	651	LEU
1	B	654	ARG
1	B	664	VAL
1	B	691	ILE
1	B	697	GLU
1	B	701	TYR
1	B	707	GLU
1	B	731	LEU
1	B	737	ILE
1	B	739	CYS
1	B	765	GLN
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

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Mol	Chain	Res	Type
1	C	654	ARG
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	571	HIS
1	A	604	HIS
1	B	555	GLN
1	B	571	HIS
1	B	604	HIS
1	B	726	GLN
1	C	594	HIS
1	C	604	HIS
1	C	660	GLN
1	C	726	GLN
1	C	742	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	B	900	-	27,29,29	1.51	4 (14%)	29,40,40	2.40	8 (27%)
2	V4Z	A	900	-	27,29,29	1.20	4 (14%)	29,40,40	2.54	9 (31%)
2	V4Z	C	900	-	27,29,29	1.25	5 (18%)	29,40,40	2.28	11 (37%)

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	B	900	-	-	0/12/16/16	0/3/3/3
2	V4Z	A	900	-	-	1/12/16/16	0/3/3/3
2	V4Z	C	900	-	-	2/12/16/16	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	V4Z	C8-N3	4.97	1.41	1.34
2	B	900	V4Z	C11-C9	-3.69	1.48	1.52
2	C	900	V4Z	C8-N3	3.41	1.39	1.34
2	A	900	V4Z	C8-N3	3.29	1.38	1.34
2	A	900	V4Z	C11-C9	-2.46	1.49	1.52
2	C	900	V4Z	C16-C17	-2.42	1.36	1.39
2	C	900	V4Z	C7-N1	2.39	1.41	1.36
2	C	900	V4Z	C4-N7	2.30	1.37	1.34
2	B	900	V4Z	C16-C17	-2.26	1.36	1.39
2	B	900	V4Z	C7-N1	2.15	1.40	1.36
2	A	900	V4Z	C4-N7	2.10	1.37	1.34
2	A	900	V4Z	N7-N6	-2.08	1.33	1.37
2	C	900	V4Z	C11-C9	-2.00	1.50	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900	V4Z	C13-C14-C15	-6.71	118.02	121.54
2	B	900	V4Z	C12-C11-C9	-6.35	116.06	121.97
2	B	900	V4Z	C13-C14-C15	-5.00	118.92	121.54
2	A	900	V4Z	C12-C11-C9	-4.94	117.38	121.97
2	C	900	V4Z	C13-C14-C15	-4.89	118.97	121.54
2	B	900	V4Z	C9-C11-N4	4.74	120.59	116.01
2	B	900	V4Z	C10-C9-C11	-4.67	105.56	110.95
2	A	900	V4Z	C5-C4-N7	-4.65	104.86	111.42
2	C	900	V4Z	C12-C11-C9	-4.54	117.75	121.97
2	B	900	V4Z	C5-C4-N7	-4.36	105.27	111.42
2	C	900	V4Z	C9-C11-N4	4.35	120.21	116.01
2	A	900	V4Z	C9-C11-N4	4.32	120.19	116.01
2	C	900	V4Z	C4-O1-C2	-3.87	112.49	118.19
2	A	900	V4Z	C16-C17-C7	-3.86	117.12	120.00
2	A	900	V4Z	C10-C9-C11	-3.68	106.70	110.95
2	A	900	V4Z	N3-C8-N2	3.49	122.42	117.18
2	C	900	V4Z	C5-C4-N7	-3.32	106.73	111.42
2	A	900	V4Z	C14-C15-N4	3.31	123.45	121.46
2	C	900	V4Z	C10-C9-N3	-3.28	102.73	108.95
2	C	900	V4Z	C14-C15-N4	3.24	123.41	121.46
2	C	900	V4Z	C10-C9-C11	-3.08	107.39	110.95
2	C	900	V4Z	C16-C17-C7	-2.82	117.90	120.00
2	A	900	V4Z	N3-C8-N5	-2.68	112.08	116.65
2	C	900	V4Z	N3-C8-N2	2.28	120.60	117.18
2	B	900	V4Z	N3-C8-N2	2.27	120.58	117.18
2	B	900	V4Z	C14-C15-N4	2.18	122.77	121.46
2	B	900	V4Z	F1-C14-C15	2.15	123.89	118.97
2	C	900	V4Z	C4-C5-C6	-2.08	104.39	106.55

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

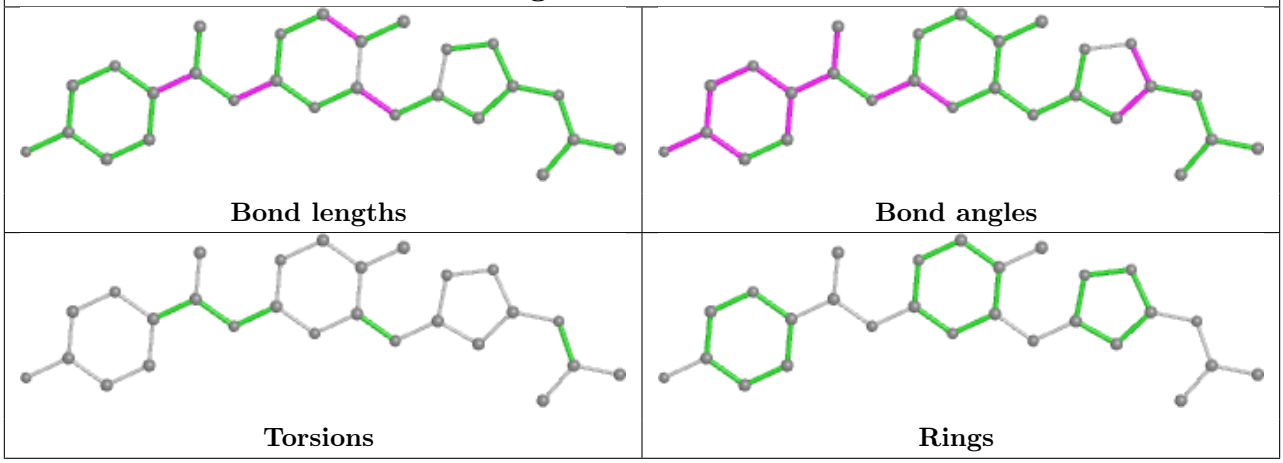
There are no ring outliers.

3 monomers are involved in 4 short contacts:

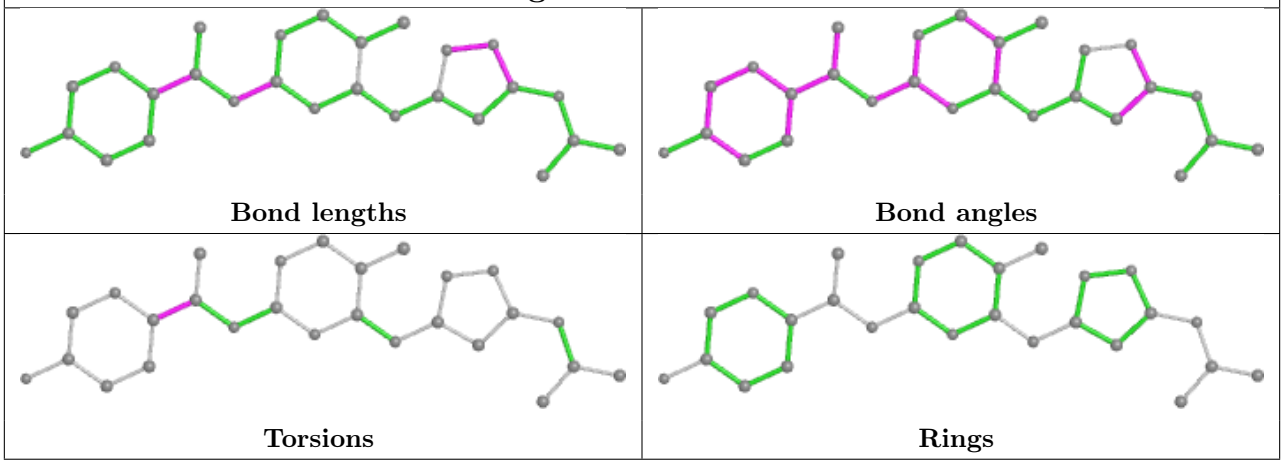
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	V4Z	2	0
2	A	900	V4Z	1	0
2	C	900	V4Z	1	0

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 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.

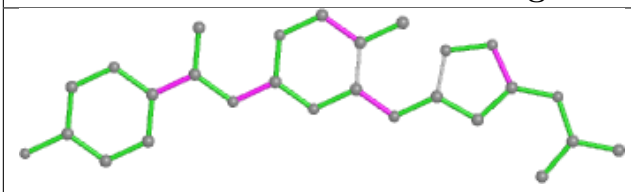
Ligand V4Z B 900



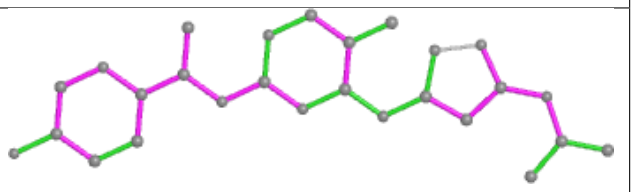
Ligand V4Z A 900



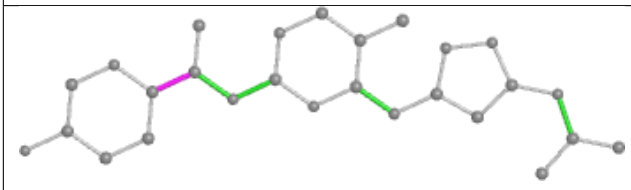
Ligand V4Z C 900



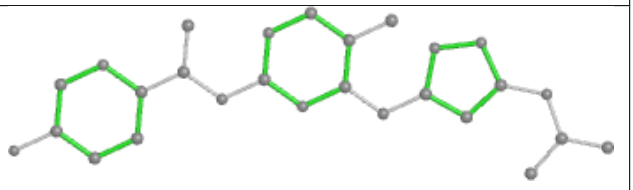
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	260/329 (79%)	0.16	7 (2%)	54	63	25, 49, 82, 98	0
1	B	258/329 (78%)	0.30	14 (5%)	25	31	28, 49, 87, 97	0
1	C	261/329 (79%)	0.46	20 (7%)	13	16	33, 62, 94, 105	0
All	All	779/987 (78%)	0.31	41 (5%)	26	31	25, 53, 88, 105	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	534	PRO	6.5
1	C	534	PRO	5.9
1	B	689	LEU	4.7
1	B	533	LEU	4.5
1	C	533	LEU	4.4
1	A	534	PRO	4.2
1	C	620	GLY	4.1
1	C	689	LEU	3.8
1	C	606	PRO	3.7
1	B	750	ARG	3.7
1	C	551	GLU	3.5
1	C	549	ALA	3.5
1	C	521	PHE	3.3
1	B	730	GLN	3.3
1	A	533	LEU	3.3
1	C	500	ALA	3.2
1	B	731	LEU	3.1
1	B	606	PRO	3.0
1	B	548	GLU	3.0
1	B	583	ARG	3.0
1	C	550	SER	2.8
1	A	789	PRO	2.8
1	B	744	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	531	ASN	2.8
1	C	555	GLN	2.7
1	A	548	GLU	2.7
1	A	549	ALA	2.7
1	C	789	PRO	2.5
1	C	701	TYR	2.5
1	A	551	GLU	2.5
1	A	729	TYR	2.5
1	C	536	GLN	2.3
1	B	747	GLU	2.3
1	C	552	SER	2.3
1	C	605	GLY	2.2
1	C	520	ALA	2.2
1	C	621	PRO	2.2
1	B	729	TYR	2.1
1	C	733	ASN	2.1
1	B	751	ALA	2.0
1	C	531	ASN	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 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
2	V4Z	B	900	27/27	0.98	0.13	26,30,34,38	0
2	V4Z	C	900	27/27	0.98	0.14	26,33,44,50	0
2	V4Z	A	900	27/27	0.99	0.17	22,29,32,33	0
3	ZN	A	1790	1/1	0.99	0.13	53,53,53,53	0
3	ZN	A	1791	1/1	0.99	0.15	58,58,58,58	0

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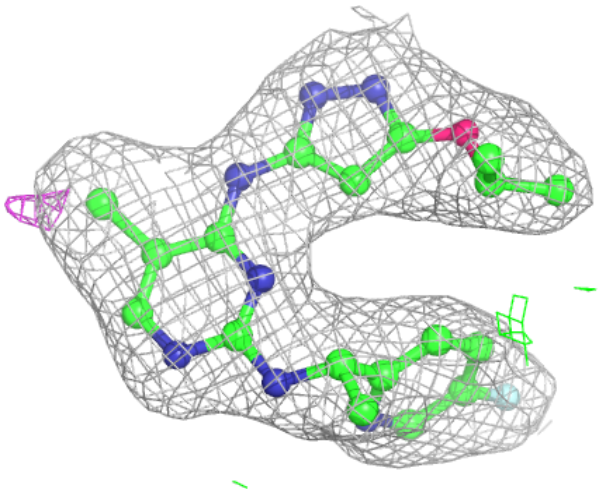
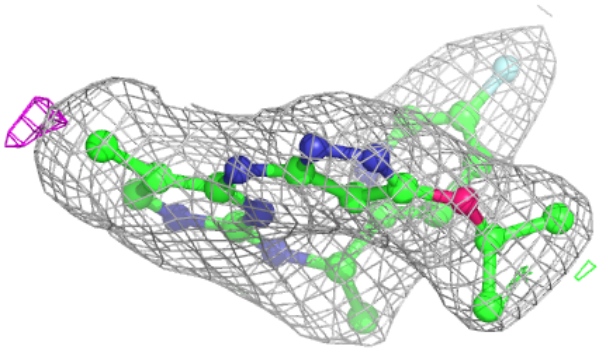
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ZN	B	1792	1/1	0.99	0.14	56,56,56,56	0
3	ZN	B	1793	1/1	0.99	0.11	58,58,58,58	0
3	ZN	C	1790	1/1	0.99	0.14	52,52,52,52	0
3	ZN	C	1791	1/1	0.99	0.13	64,64,64,64	0

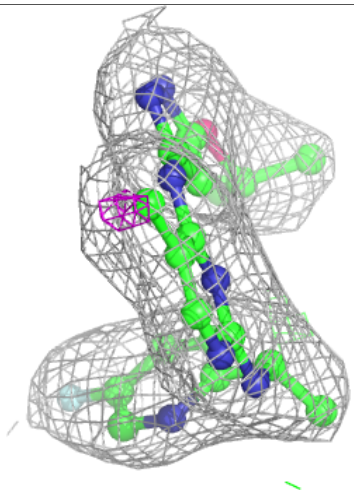
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around V4Z 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)

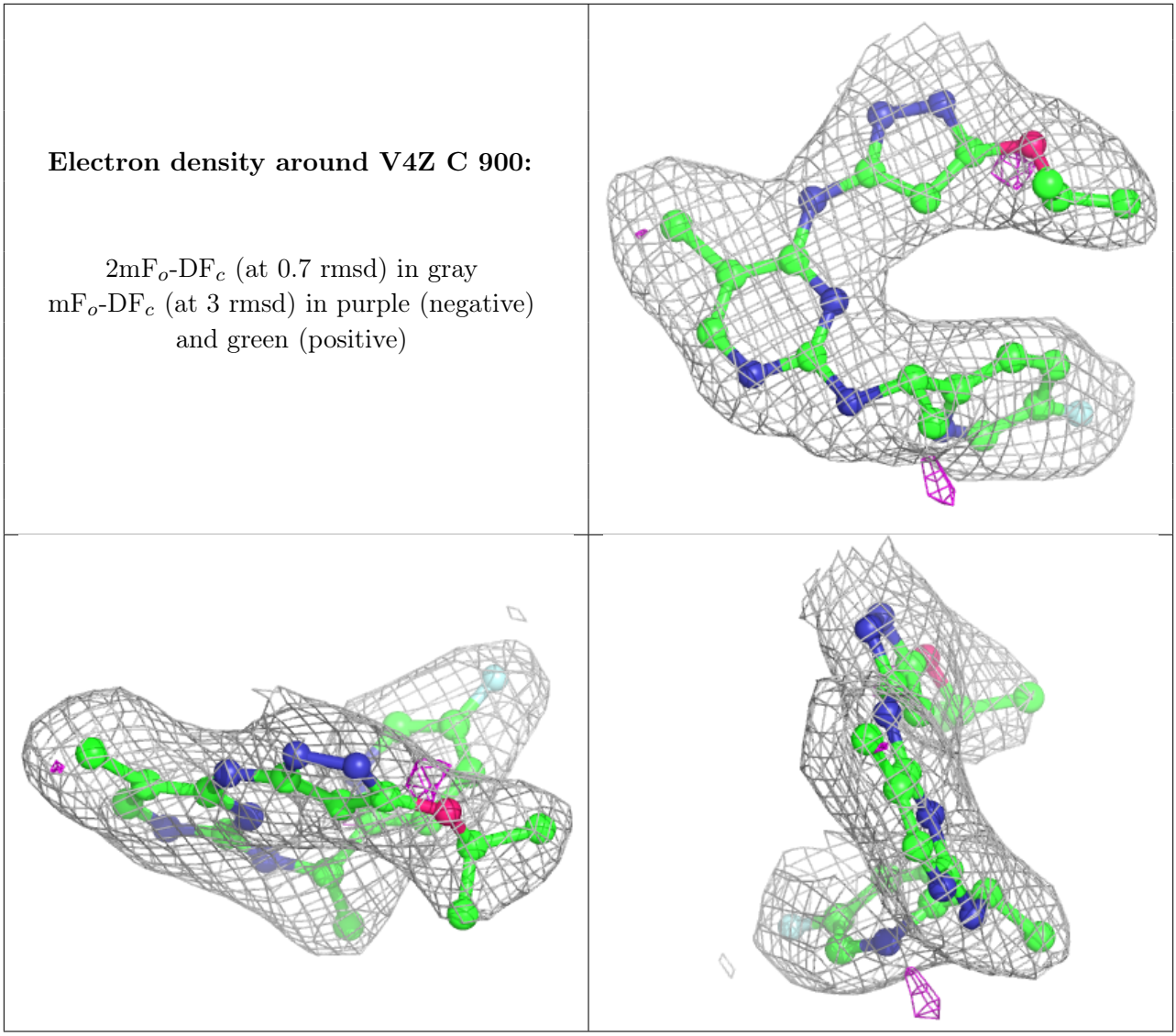






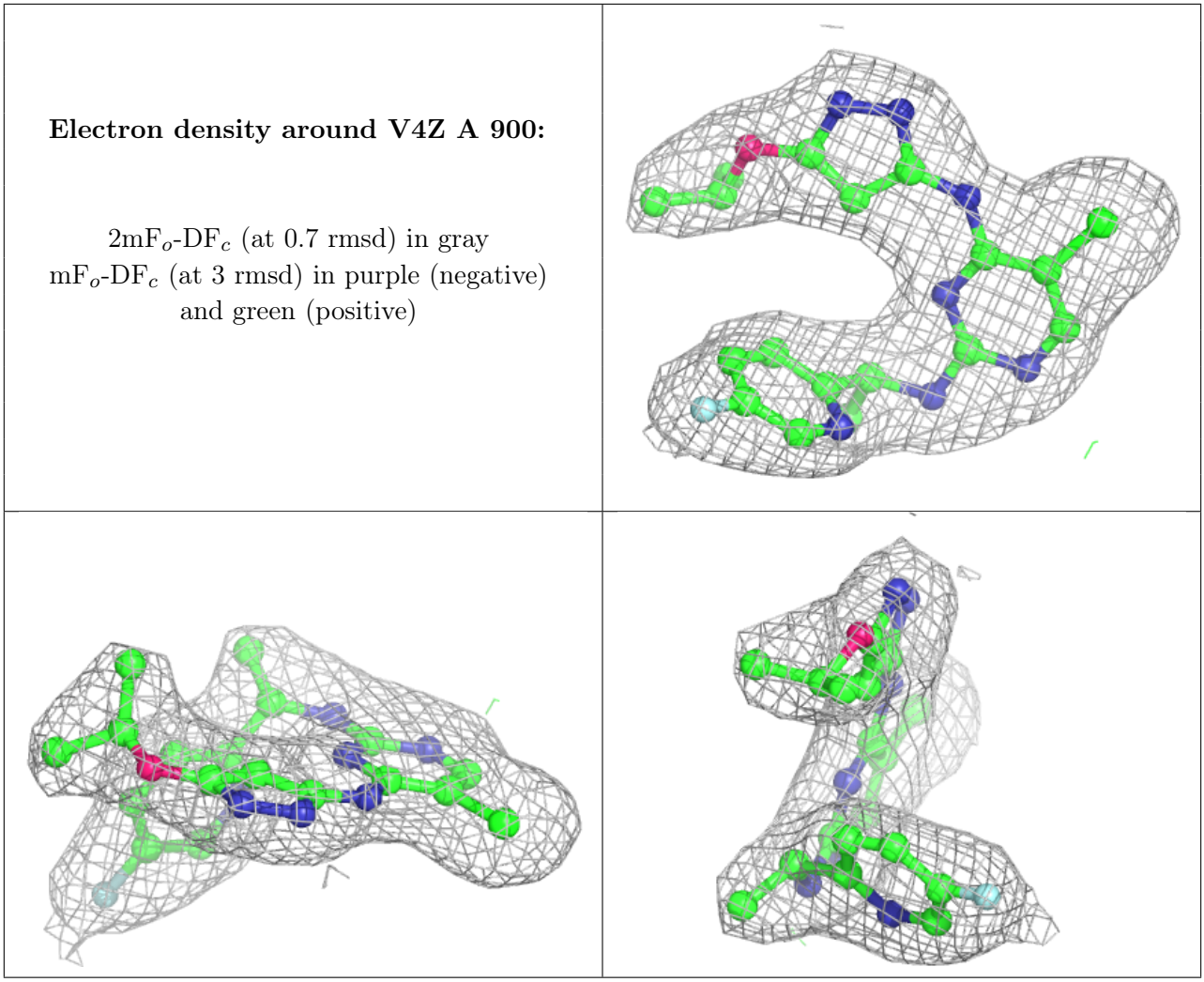
Electron density around V4Z C 900:

$2mF_o$-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 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

There are no such residues in this entry.