

wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 04:04 PM EDT

PDB ID	:	7UN0
Title	:	Structure of MAP kinase phosphatase 5 in complex with 3,3-dimethyl-1-((9
		-chloro-5,6-dihydrobenzo[h]quinazolin-2-yl)thio)butan-2-one, an allosteric
		inhibitor
Authors	:	Gannam, Z.T.K.; Jamali, H.; Lolis, E.; Anderson, K.S.; Ellman, J.A.; Bennett,
		A.M.
Deposited on	:	2022-04-08
Resolution	:	3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467	
Mogul : $1.8.5$ (274361), CSD as541be (2020)	
Xtriage (Phenix) : 1.13	
EDS : 2.35.1	
buster-report : $1.1.7$ (2018)	
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2	019)
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) : 2.35.1	

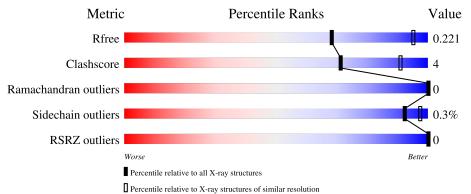


1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	А	152	85%	12%	•
1	В	152	85%	11%	5%
1	С	152	87%	10%	·
1	D	152	87%	10%	•
1	Е	152	88%	9%	•



Mol	Chain	Length	Quality of chain		
1	F	152	90%	7%	·



7UN0

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7266 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	148	Total	С	Ν	0	S	0	0	0
	A	140	1197	767	202	221	7	0	0	0
1	В	145	Total	С	Ν	0	S	0	0	0
	D	140	1176	755	199	215	7	0	0	0
1	С	147	Total	С	Ν	0	S	4	0	0
	U	141	1192	764	201	220	7	4	0	0
1	D	147	Total	С	Ν	0	S	4	0	0
	D	141	1190	763	201	219	7	4	0	0
1	Е	146	Total	С	Ν	0	S	4	0	0
	Ľ	140	1183	758	200	218	7	4	0	0
1	F	147	Total	С	Ν	0	S	1	0	0
	Г	141	1190	763	201	219	7	4		U

• Molecule 1 is a protein called Dual specificity protein phosphatase 10.

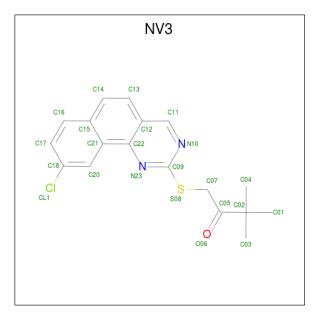
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	316	GLY	-	expression tag	UNP Q9Y6W6
А	317	SER	-	expression tag	UNP Q9Y6W6
А	318	HIS	-	expression tag	UNP Q9Y6W6
А	319	MET	-	expression tag	UNP Q9Y6W6
В	316	GLY	-	expression tag	UNP Q9Y6W6
В	317	SER	-	expression tag	UNP Q9Y6W6
В	318	HIS	-	expression tag	UNP Q9Y6W6
В	319	MET	-	expression tag	UNP Q9Y6W6
С	316	GLY	-	expression tag	UNP Q9Y6W6
С	317	SER	-	expression tag	UNP Q9Y6W6
С	318	HIS	-	expression tag	UNP Q9Y6W6
С	319	MET	-	expression tag	UNP Q9Y6W6
D	316	GLY	-	expression tag	UNP Q9Y6W6
D	317	SER	-	expression tag	UNP Q9Y6W6
D	318	HIS	-	expression tag	UNP Q9Y6W6
D	319	MET	-	expression tag	UNP Q9Y6W6
Е	316	GLY	-	expression tag	UNP Q9Y6W6



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Chain	Residue	Modelled	Actual	Comment	Reference			
E	317	SER	-	expression tag	UNP Q9Y6W6			
Е	318	HIS	-	expression tag	UNP Q9Y6W6			
Е	319	MET	-	expression tag	UNP Q9Y6W6			
F	316	GLY	-	expression tag	UNP Q9Y6W6			
F	317	SER	-	expression tag	UNP Q9Y6W6			
F	318	HIS	-	expression tag	UNP Q9Y6W6			
F	319	MET	-	expression tag	UNP Q9Y6W6			

• Molecule 2 is 1-[(9-chlorobenzo[h]quinazolin-2-yl)sulfanyl]-3,3-dimethylbutan-2-on e (three-letter code: NV3) (formula: C₁₈H₁₇ClN₂OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc AltConf
2	А	1	Total C Cl N O S	0 0
	Л	1	23 18 1 2 1 1	
2	В	1	Total C Cl N O S	0 0
	D	1	23 18 1 2 1 1	0 0
2	С	1	Total C Cl N O S	0 0
2	U	T	23 18 1 2 1 1	0 0
2	D	1	Total C Cl N O S	0 0
2	D	I	23 18 1 2 1 1	0 0
2	Е	1	Total C Cl N O S	0 0
2	Ľ	I	23 18 1 2 1 1	0 0
2	F	1	Total C Cl N O S	0 0
	T	Ĩ	23 18 1 2 1 1	



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: Dual specificity protein phosphatase 10

Chain A:	85%	12% •
CLY SER HITS MET MET E321 E322 E334 0335 0335 0335 0335 0335 0335 1355	L358 K371 K371 E388 E389 E389 E392 F393 1394 L404 C408 C408 C408 C408 C408 C409 C409 C409 C409 C409 C409 C409 C409	
• Molecule 1: Dua	al specificity protein phosphatase 10	
Chain B:	85%	11% 5%
GLY SER MET ALA GLU F330 F330 F330 F330 F330 F359 F359	K371 E389 E389 1394 C408 Q409 Q409 C408 Q409 C408 C408 C408 C408 C408 C408 C408 C408	
• Molecule 1: Dua	al specificity protein phosphatase 10	
Chain C:	87%	10% •
GLY SER HIS MET ALA E321 L322 F330 F330 T348 1348	1355 1355 1355 1355 1357 1 1353 1 1355 1 1355 1 1355 1 1355 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1354 1 1405 1 1467 1 1467 1	
• Molecule 1: Dua	al specificity protein phosphatase 10	
Chain D:	87%	10% •
GLY SER HIS MET A320 E321 L322 L322 E334 C335 C335 C335 C335 C336 C335 C336 C336	K371 E389 1394 1404 1404 1404 0409 0409 0412 1419 1419 1419 1419 1419 1419 1419 1	
• Molecule 1: Dua	al specificity protein phosphatase 10	
Chain E:	88%	9% •
GLY SER HIS MET A320 E334 E334 E389 E389 E389 E389 E389	L404 L406 Q408 Q408 H412 L423 M429 M429 M429 M429 M429 M425 M452 M452 M452 M452 M452 THR	
• Molecule 1: Dua	al specificity protein phosphatase 10	
Chain F:	90%	7% •
	PROTEIN DATA BANK	





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	97.08Å 100.05Å 135.38Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.55 - 3.00	Depositor
Resolution (A)	48.55 - 2.99	EDS
% Data completeness	99.4 (48.55-3.00)	Depositor
(in resolution range)	92.4(48.55-2.99)	EDS
R _{merge}	0.21	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.27 (at 3.01 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
D D	0.174 , 0.214	Depositor
R, R_{free}	0.178 , 0.221	DCC
R_{free} test set	2009 reflections (7.42%)	wwPDB-VP
Wilson B-factor $(Å^2)$	57.2	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29, 28.9	EDS
L-test for twinning ²	$< L > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7266	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: $\rm NV3$

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	
	Unam	$RMSZ \mid \# Z > 5$		RMSZ	# Z > 5
1	А	0.26	0/1223	0.42	0/1653
1	В	0.28	0/1202	0.46	0/1624
1	С	0.24	0/1218	0.41	0/1646
1	D	0.25	0/1216	0.41	0/1643
1	Ε	0.25	0/1209	0.40	0/1633
1	F	0.25	0/1216	0.41	0/1643
All	All	0.25	0/7284	0.42	0/9842

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1197	0	1184	11	0
1	В	1176	0	1166	10	0
1	С	1192	0	1179	10	0
1	D	1190	0	1177	9	0
1	Е	1183	0	1168	8	0
1	F	1190	0	1177	6	0
2	А	23	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	23	0	0	0	0
2	С	23	0	0	0	0
2	D	23	0	0	0	0
2	Е	23	0	0	0	0
2	F	23	0	0	0	0
All	All	7266	0	7051	50	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 4.

The worst 5 of 50 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:388:GLU:O	1:A:392:GLU:HG2	2.03	0.59
1:B:359:PRO:HD3	1:C:359:PRO:HB3	1.84	0.59
1:A:371:LYS:HD3	1:A:389:GLU:HG2	1.86	0.57
1:B:322:LEU:HD21	1:B:330:PHE:HB3	1.87	0.57
1:F:341:ASP:O	1:F:345:ARG:HG2	2.05	0.56

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	А	146/152~(96%)	138 (94%)	8 (6%)	0	100 100
1	В	143/152~(94%)	136~(95%)	7 (5%)	0	100 100
1	С	145/152~(95%)	138 (95%)	7 (5%)	0	100 100
1	D	145/152~(95%)	139 (96%)	6 (4%)	0	100 100
1	Е	144/152~(95%)	137 (95%)	7 (5%)	0	100 100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}			
1	F	145/152~(95%)	138 (95%)	7(5%)	0	100	100			
All	All	868/912~(95%)	826 (95%)	42~(5%)	0	100	100			

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	130/133~(98%)	130 (100%)	0	100 100
1	В	128/133~(96%)	126~(98%)	2(2%)	62 86
1	С	130/133~(98%)	130 (100%)	0	100 100
1	D	129/133~(97%)	129~(100%)	0	100 100
1	Ε	128/133~(96%)	128 (100%)	0	100 100
1	F	129/133~(97%)	129~(100%)	0	100 100
All	All	774/798~(97%)	772 (100%)	2~(0%)	92 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	413	SER
1	В	446	SER

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	Turne	Chain	Res	Link	Bond lengths			Bond angles		
10101	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	NV3	Е	500	-	25,25,25	2.30	8 (32%)	34,37,37	2.46	10 (29%)
2	NV3	F	500	-	25,25,25	2.34	8 (32%)	34,37,37	2.46	9 (26%)
2	NV3	D	500	-	25,25,25	2.33	8 (32%)	34,37,37	2.49	10 (29%)
2	NV3	С	500	-	25,25,25	2.33	8 (32%)	34,37,37	2.51	10 (29%)
2	NV3	В	500	-	25,25,25	1.98	5 (20%)	34,37,37	2.47	9 (26%)
2	NV3	А	500	-	25,25,25	2.33	8 (32%)	34,37,37	2.48	10 (29%)

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	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	NV3	Ε	500	-	-	0/11/11/11	0/3/3/3
2	NV3	F	500	-	-	0/11/11/11	0/3/3/3
2	NV3	D	500	-	-	0/11/11/11	0/3/3/3
2	NV3	С	500	-	-	0/11/11/11	0/3/3/3
2	NV3	В	500	-	-	0/11/11/11	0/3/3/3
2	NV3	A	500	-	-	2/11/11/11	0/3/3/3



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	А	500	NV3	C14-C13	7.60	1.56	1.35
2	С	500	NV3	C14-C13	7.58	1.56	1.35
2	D	500	NV3	C14-C13	7.50	1.56	1.35
2	F	500	NV3	C14-C13	7.50	1.56	1.35
2	Е	500	NV3	C14-C13	7.48	1.56	1.35

The worst 5 of 45 bond length outliers are listed below:

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	500	NV3	C07-S08-C09	10.90	115.68	101.63
2	С	500	NV3	C07-S08-C09	10.85	115.63	101.63
2	D	500	NV3	C07-S08-C09	10.85	115.62	101.63
2	А	500	NV3	C07-S08-C09	10.85	115.62	101.63
2	Е	500	NV3	C07-S08-C09	10.81	115.57	101.63

There are no chirality outliers.

All (2) torsion outliers are listed below:

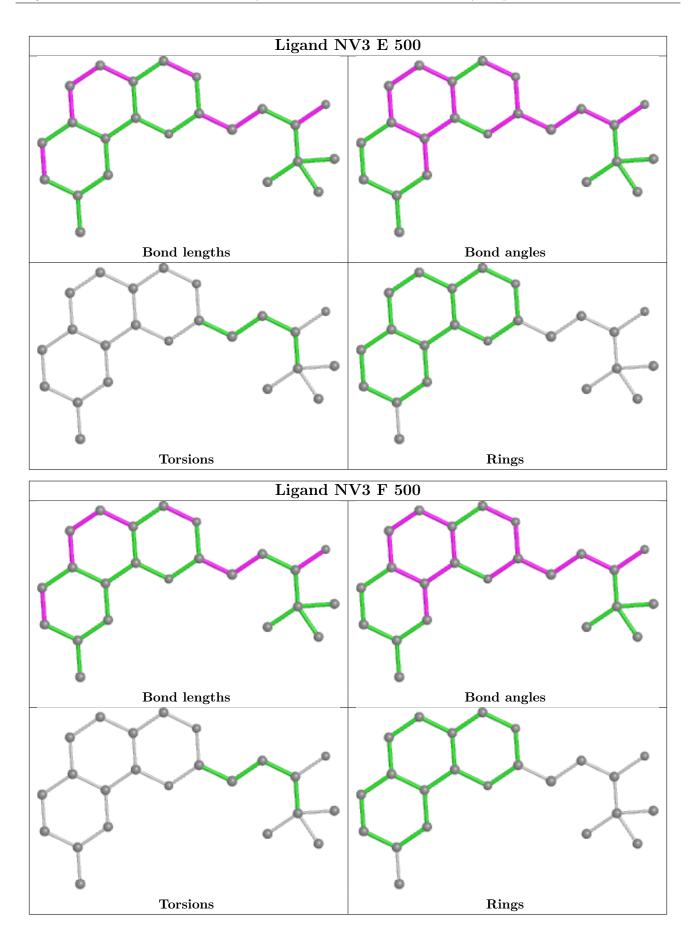
Mol	Chain	Res	Type	Atoms
2	А	500	NV3	C04-C02-C05-C07
2	А	500	NV3	C01-C02-C05-C07

There are no ring outliers.

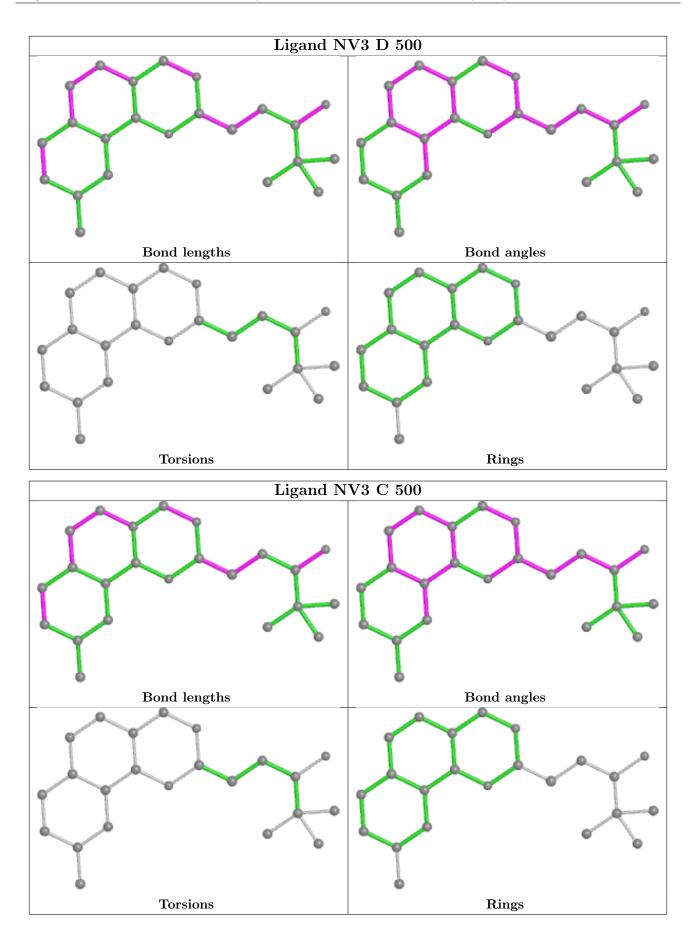
No monomer is involved in short contacts.

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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

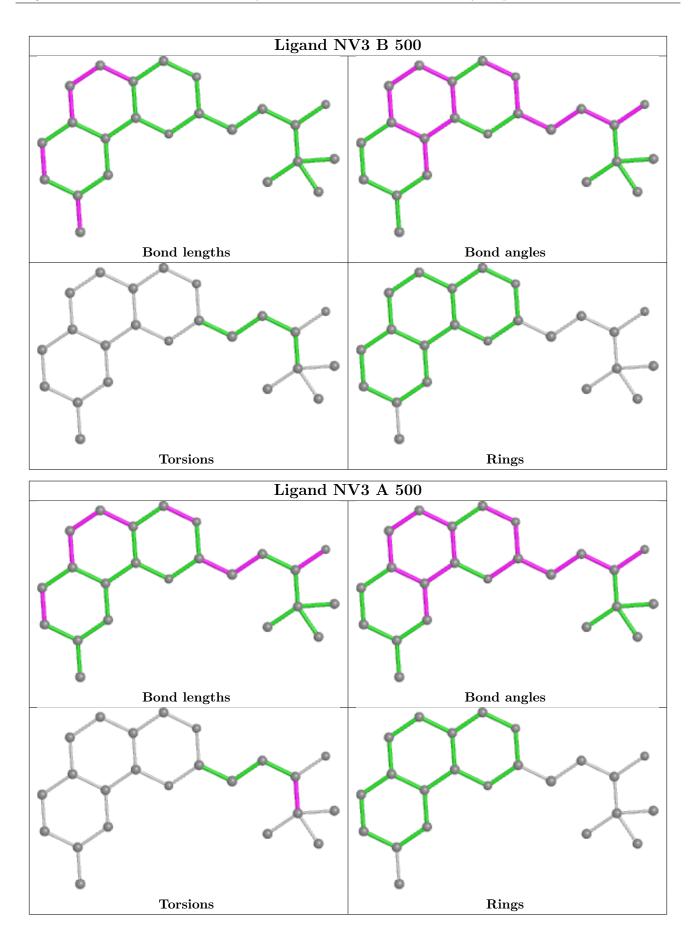














5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	$\langle RSRZ \rangle$	#RSRZ>2		Z>2	$OWAB(Å^2)$	Q<0.9
1	А	148/152~(97%)	-0.50	0	100	100	36, 59, 84, 115	0
1	В	145/152~(95%)	-0.53	0	100	100	35, 56, 89, 108	0
1	С	147/152~(96%)	-0.46	0	100	100	40, 59, 90, 142	1 (0%)
1	D	147/152~(96%)	-0.47	0	100	100	46, 63, 102, 130	1 (0%)
1	Е	146/152~(96%)	-0.41	0	100	100	53, 70, 101, 117	1 (0%)
1	F	147/152~(96%)	-0.54	0	100	100	46, 61, 94, 117	1 (0%)
All	All	880/912~(96%)	-0.48	0	100	100	35, 62, 96, 142	4 (0%)

There are no RSRZ outliers to report.

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.

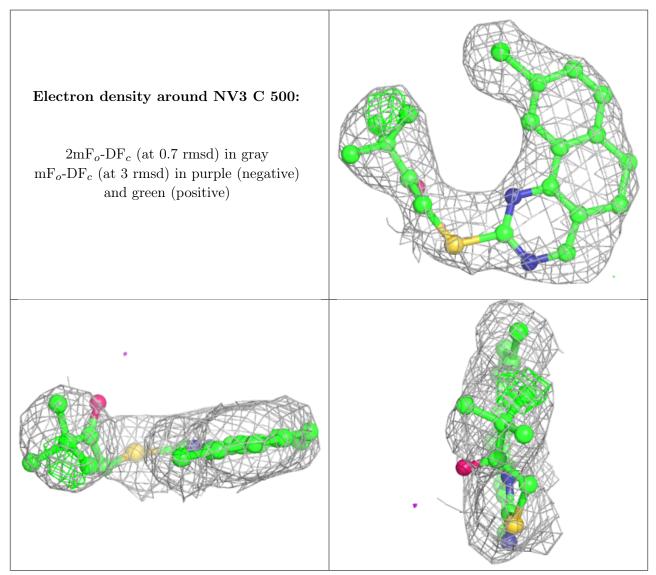
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q < 0.9
2	NV3	С	500	23/23	0.92	0.33	56,76,89,102	0



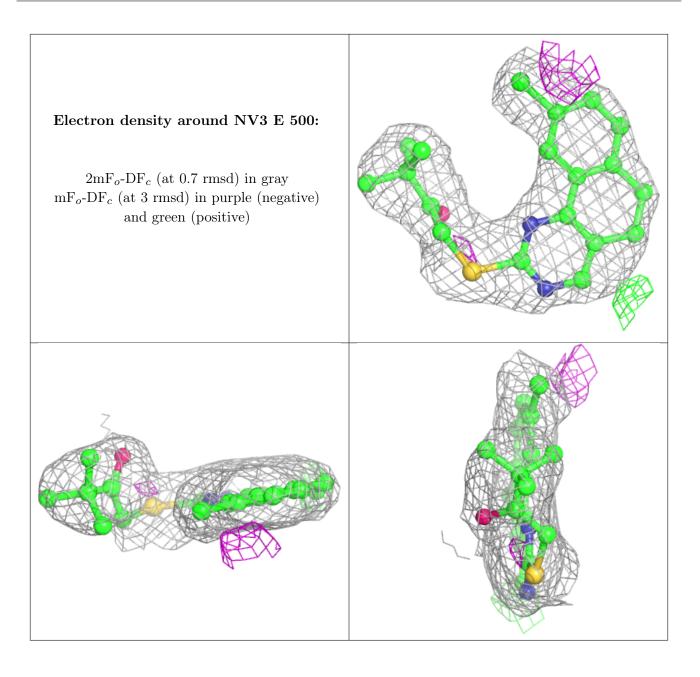
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Mol	Type	Chain	Res	Atoms	RSCC	\mathbf{RSR}	${f B} ext{-factors}({ m \AA}^2)$	Q < 0.9	
2	NV3	Е	500	23/23	0.94	0.24	$53,\!63,\!83,\!86$	0	
2	NV3	F	500	23/23	0.95	0.23	44,62,74,83	0	
2	NV3	D	500	23/23	0.96	0.20	46,60,74,85	0	
2	NV3	В	500	23/23	0.96	0.20	44,71,80,93	0	
2	NV3	А	500	23/23	0.96	0.20	41,74,84,107	0	

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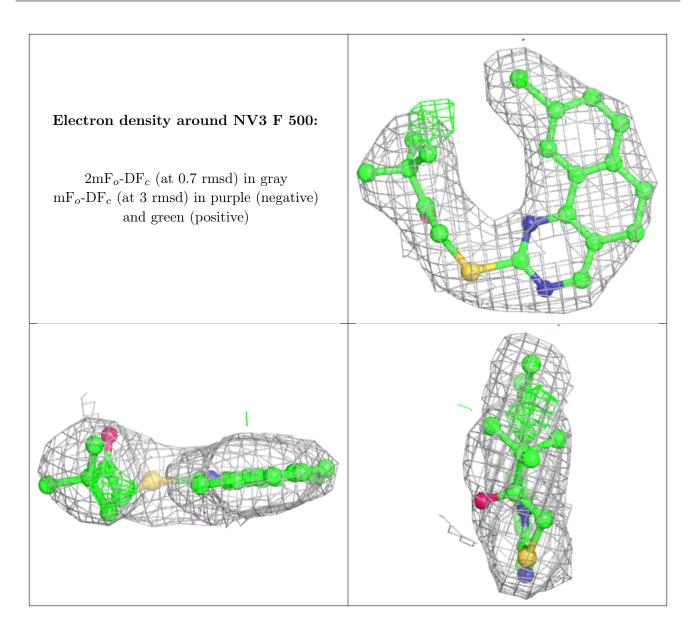
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



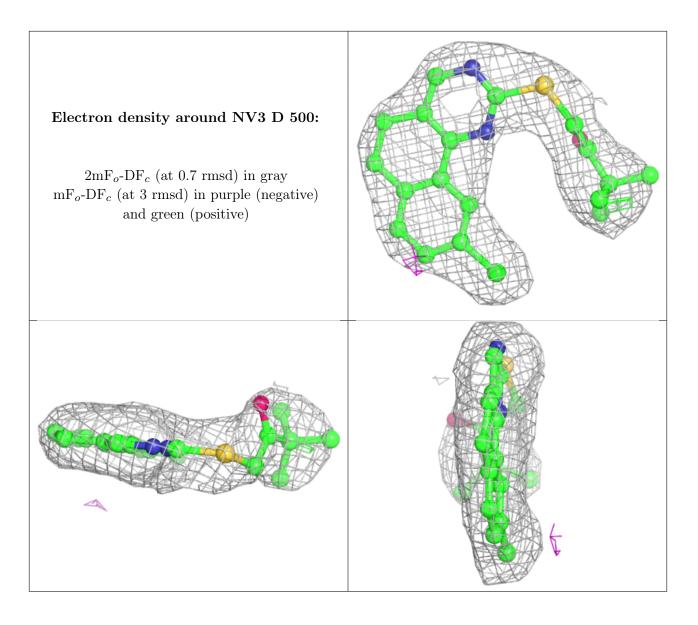




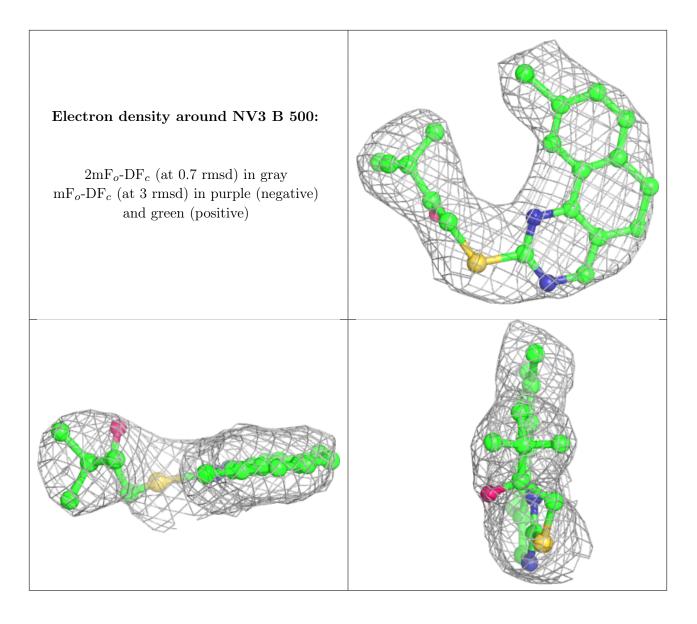




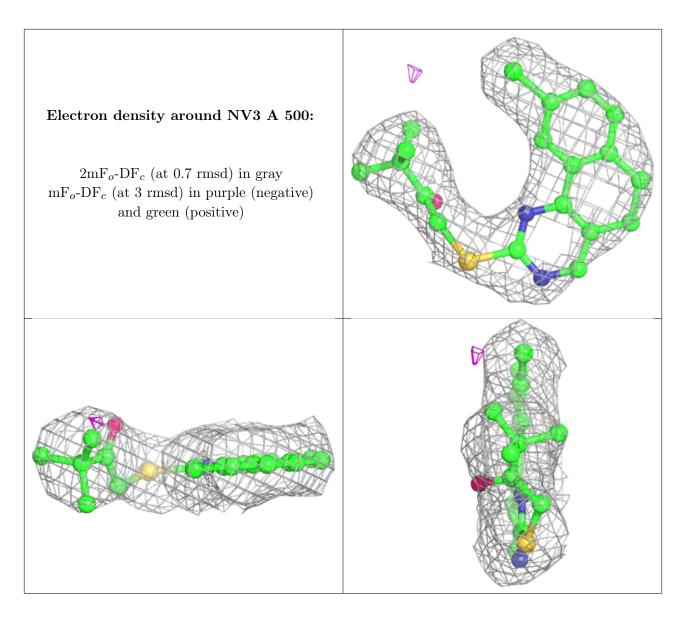












6.5 Other polymers (i)

There are no such residues in this entry.

