



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2023 – 08:19 PM JST

PDB ID : 8HUB
Title : AMP deaminase 2 in complex with an inhibitor
Authors : Adachi, T.; Doi, S.
Deposited on : 2022-12-23
Resolution : 3.25 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.3
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) : 2.31.3

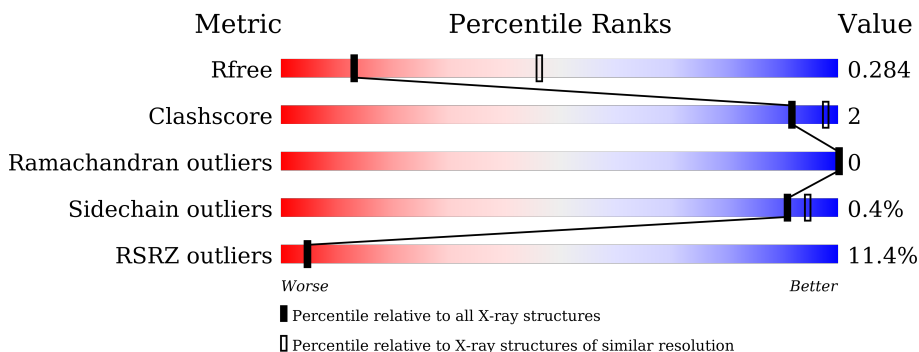
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	678	
1	B	678	
1	C	678	
1	D	678	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 33454 atoms, of which 16575 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 AMP deaminase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	388	6260	2014	3116	542	567	21	0	0	0
1	B	545	8812	2841	4370	769	804	28	0	0	0
1	C	572	9162	2960	4525	809	840	28	0	0	0
1	D	562	9087	2927	4501	802	829	28	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	MET	-	initiating methionine	UNP Q01433
A	203	ASP	-	expression tag	UNP Q01433
A	204	TYR	-	expression tag	UNP Q01433
A	205	LYS	-	expression tag	UNP Q01433
A	206	ASP	-	expression tag	UNP Q01433
A	207	ASP	-	expression tag	UNP Q01433
A	208	ASP	-	expression tag	UNP Q01433
A	209	ASP	-	expression tag	UNP Q01433
A	210	LYS	-	expression tag	UNP Q01433
B	202	MET	-	initiating methionine	UNP Q01433
B	203	ASP	-	expression tag	UNP Q01433
B	204	TYR	-	expression tag	UNP Q01433
B	205	LYS	-	expression tag	UNP Q01433
B	206	ASP	-	expression tag	UNP Q01433
B	207	ASP	-	expression tag	UNP Q01433
B	208	ASP	-	expression tag	UNP Q01433
B	209	ASP	-	expression tag	UNP Q01433
B	210	LYS	-	expression tag	UNP Q01433
C	202	MET	-	initiating methionine	UNP Q01433
C	203	ASP	-	expression tag	UNP Q01433
C	204	TYR	-	expression tag	UNP Q01433

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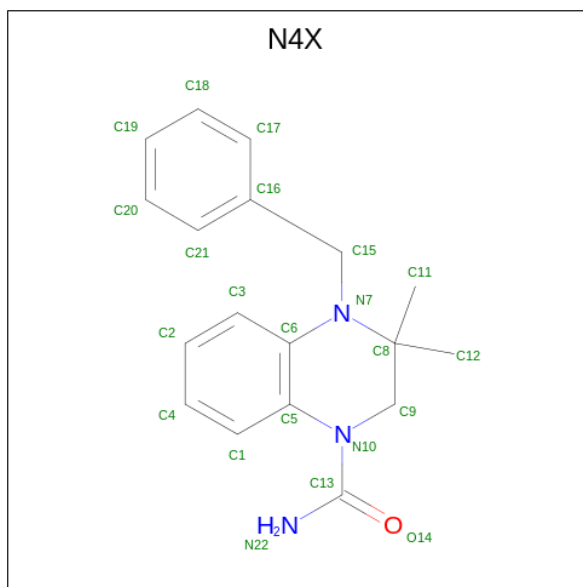
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Chain	Residue	Modelled	Actual	Comment	Reference
C	205	LYS	-	expression tag	UNP Q01433
C	206	ASP	-	expression tag	UNP Q01433
C	207	ASP	-	expression tag	UNP Q01433
C	208	ASP	-	expression tag	UNP Q01433
C	209	ASP	-	expression tag	UNP Q01433
C	210	LYS	-	expression tag	UNP Q01433
D	202	MET	-	initiating methionine	UNP Q01433
D	203	ASP	-	expression tag	UNP Q01433
D	204	TYR	-	expression tag	UNP Q01433
D	205	LYS	-	expression tag	UNP Q01433
D	206	ASP	-	expression tag	UNP Q01433
D	207	ASP	-	expression tag	UNP Q01433
D	208	ASP	-	expression tag	UNP Q01433
D	209	ASP	-	expression tag	UNP Q01433
D	210	LYS	-	expression tag	UNP Q01433

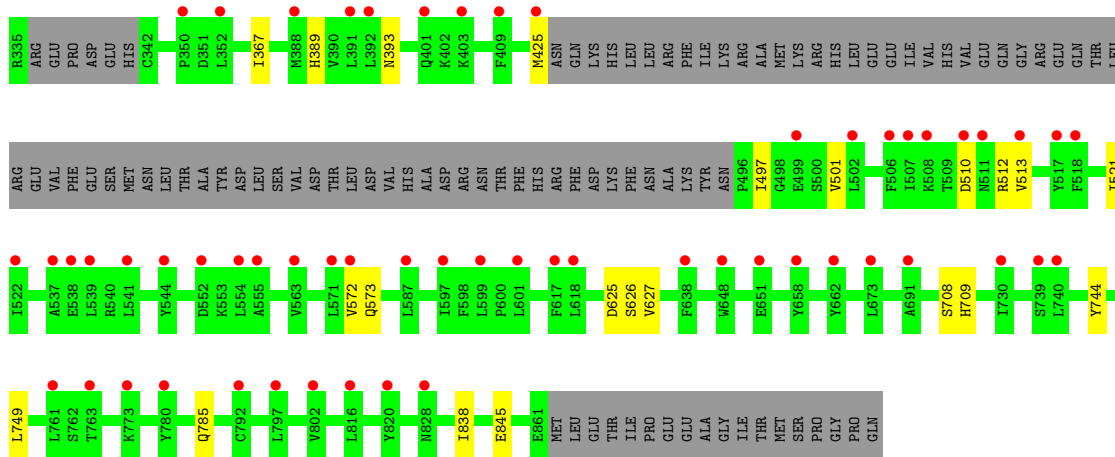
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

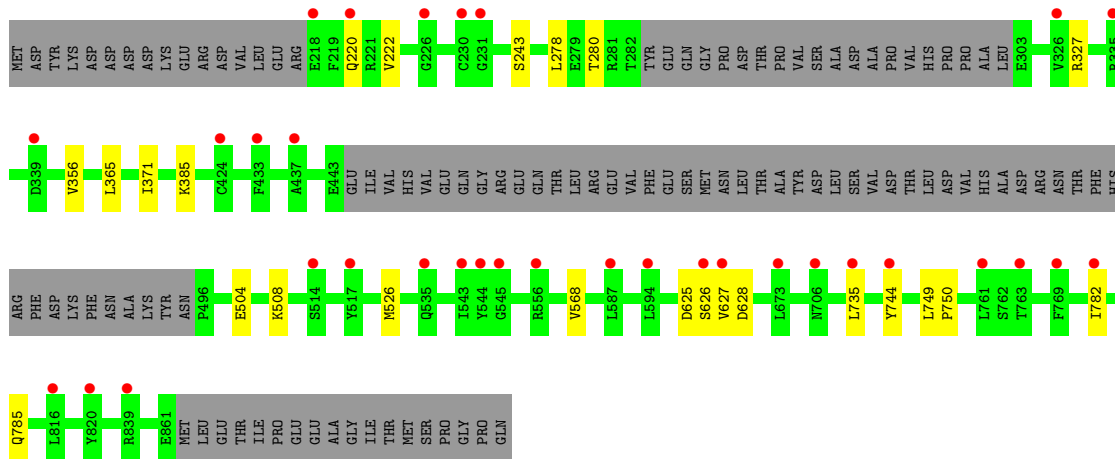
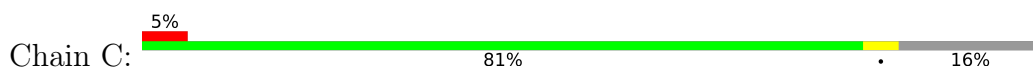
- Molecule 3 is 3,3-dimethyl-4-(phenylmethyl)-2 {H}-quinoxaline-1-carboxamide (three-letter code: N4X) (formula: C₁₈H₂₁N₃O) (labeled as "Ligand of Interest" by depositor).



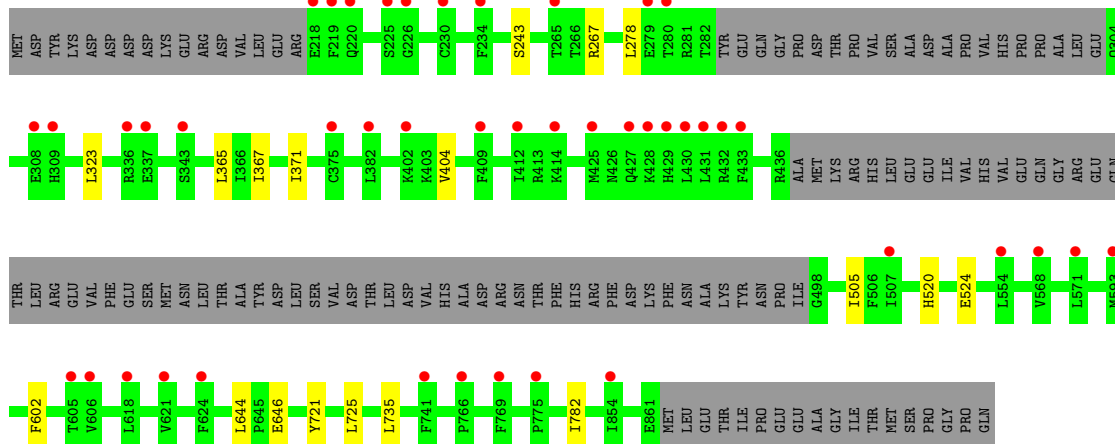
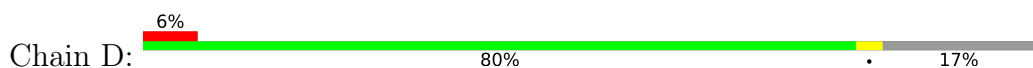
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	B	1	Total	C	H	N	O	0	0
			43	18	21	3	1		
3	C	1	Total	C	H	N	O	0	0
			43	18	21	3	1		
3	D	1	Total	C	H	N	O	0	0
			43	18	21	3	1		



● Molecule 1: AMP deaminase 2



● Molecule 1: AMP deaminase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.52Å 162.53Å 289.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.84 – 3.25 98.84 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (98.84-3.25) 96.5 (98.84-3.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 3.26Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.258 , 0.276 0.261 , 0.284	Depositor DCC
R_{free} test set	2325 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtrriage
Anisotropy	0.443	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	33454	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, N4X

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	0.24	0/3218	0.45	0/4351
1	B	0.24	0/4558	0.45	0/6175
1	C	0.24	0/4758	0.45	0/6449
1	D	0.24	0/4706	0.46	0/6376
All	All	0.24	0/17240	0.45	0/23351

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	A	3144	3116	3116	15	0
1	B	4442	4370	4369	15	0
1	C	4637	4525	4525	13	1
1	D	4586	4501	4499	12	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	22	21	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	22	21	0	0	0
3	D	22	21	0	0	0
All	All	16879	16575	16509	52	1

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 2.

All (52) 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:257:LEU:HD11	1:A:664:PHE:CE2	2.36	0.61
1:A:576:ARG:O	1:A:577:LEU:HD23	2.06	0.56
1:A:577:LEU:HD22	1:A:653:ASN:ND2	2.20	0.56
1:A:660:LEU:HD12	1:A:684:LEU:HD21	1.87	0.56
1:B:219:PHE:CG	1:B:838:ILE:HG23	2.45	0.52
1:B:221:ARG:NH1	1:B:845:GLU:OE2	2.42	0.52
1:A:664:PHE:CG	1:A:703:LEU:HD22	2.45	0.50
1:C:222:VAL:O	1:C:222:VAL:HG13	2.11	0.50
1:A:257:LEU:HD12	1:A:258:SER:N	2.28	0.49
1:D:367:ILE:HG22	1:D:367:ILE:O	2.13	0.48
1:B:625:ASP:OD1	1:B:626:SER:N	2.47	0.48
1:D:505:ILE:HG22	1:D:505:ILE:O	2.13	0.48
1:D:267:ARG:HG3	1:D:278:LEU:HD13	1.96	0.48
1:C:625:ASP:OD1	1:C:626:SER:N	2.46	0.47
1:C:365:LEU:HD11	1:C:371:ILE:HG21	1.96	0.47
1:D:243:SER:HB3	1:D:365:LEU:HD13	1.96	0.47
1:C:785:GLN:HG3	1:D:735:LEU:HD11	1.98	0.46
1:B:708:SER:O	1:B:709:HIS:HB2	2.16	0.46
1:A:365:LEU:HD11	1:A:371:ILE:HG21	1.98	0.45
1:B:497:ILE:HG22	1:B:501:VAL:HG11	1.97	0.45
1:A:257:LEU:HD11	1:A:664:PHE:CZ	2.52	0.44
1:C:735:LEU:HD13	1:C:782:ILE:HD13	1.99	0.44
1:A:749:LEU:C	1:A:749:LEU:HD23	2.37	0.44
1:C:356:VAL:O	1:C:356:VAL:HG12	2.19	0.43
1:A:735:LEU:HD13	1:A:782:ILE:CD1	2.48	0.43
1:B:573:GLN:OE1	1:B:627:VAL:HG21	2.18	0.43
1:C:782:ILE:HG12	1:D:782:ILE:HG12	2.00	0.43
1:B:572:VAL:O	1:B:625:ASP:N	2.51	0.43
1:A:248:LEU:HB2	1:A:270:LEU:HD21	2.01	0.42
1:B:220:GLN:NE2	1:B:393:ASN:OD1	2.52	0.42
1:A:769:PHE:O	1:B:785:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LEU:HD11	1:D:371:ILE:HG21	2.01	0.42
1:B:367:ILE:O	1:B:367:ILE:HG22	2.20	0.42
1:C:627:VAL:O	1:C:628:ASP:HB2	2.20	0.42
1:A:243:SER:HB3	1:A:365:LEU:HD13	2.02	0.42
1:D:404:VAL:O	1:D:404:VAL:HG13	2.20	0.42
1:D:323:LEU:HD13	1:D:602:PHE:HB3	2.02	0.41
1:D:520:HIS:NE2	1:D:524:GLU:OE2	2.53	0.41
1:B:749:LEU:C	1:B:749:LEU:HD23	2.40	0.41
1:D:721:TYR:CE2	1:D:725:LEU:HD11	2.55	0.41
1:C:504:GLU:O	1:C:508:LYS:N	2.53	0.41
1:B:510:ASP:O	1:B:510:ASP:OD1	2.38	0.41
1:C:526:MET:HG2	1:C:568:VAL:HG21	2.02	0.41
1:A:250:ILE:O	1:A:250:ILE:HG22	2.20	0.41
1:B:389:HIS:HE1	1:B:838:ILE:HG22	1.86	0.41
1:B:512:ARG:HG2	1:B:513:VAL:N	2.36	0.41
1:A:571:LEU:HD21	1:A:622:ASP:HB2	2.03	0.40
1:C:749:LEU:N	1:C:750:PRO:HD2	2.36	0.40
1:C:222:VAL:HG11	1:C:385:LYS:HG3	2.03	0.40
1:C:243:SER:HB3	1:C:365:LEU:HD13	2.03	0.40
1:D:644:LEU:N	1:D:644:LEU:HD12	2.37	0.40
1:B:425:MET:HA	1:B:521:ILE:HG21	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:ARG:H	1:D:646:GLU:OE2[5_445]	1.55	0.05

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	374/678 (55%)	365 (98%)	9 (2%)	0	100	100
1	B	537/678 (79%)	517 (96%)	20 (4%)	0	100	100
1	C	566/678 (84%)	540 (95%)	26 (5%)	0	100	100
1	D	556/678 (82%)	537 (97%)	19 (3%)	0	100	100
All	All	2033/2712 (75%)	1959 (96%)	74 (4%)	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 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	350/612 (57%)	348 (99%)	2 (1%)	86	91
1	B	491/612 (80%)	490 (100%)	1 (0%)	93	96
1	C	506/612 (83%)	502 (99%)	4 (1%)	81	89
1	D	505/612 (82%)	505 (100%)	0	100	100
All	All	1852/2448 (76%)	1845 (100%)	7 (0%)	91	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	687	HIS
1	A	744	TYR
1	B	744	TYR
1	C	220	GLN
1	C	278	LEU
1	C	280	THR
1	C	744	TYR

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

Mol	Chain	Res	Type
1	A	360	ASN

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Mol	Chain	Res	Type
1	A	389	HIS
1	A	653	ASN
1	A	770	HIS
1	B	611	HIS
1	B	653	ASN
1	C	271	GLN
1	C	573	GLN
1	C	737	ASN
1	D	737	ASN

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](#)

Of 7 ligands modelled in this entry, 4 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
3	N4X	B	902	-	22,24,24	1.92	5 (22%)	24,35,35	0.99	2 (8%)
3	N4X	C	902	-	22,24,24	1.94	4 (18%)	24,35,35	1.01	2 (8%)
3	N4X	D	902	-	22,24,24	1.94	5 (22%)	24,35,35	0.93	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N4X	B	902	-	-	0/7/27/27	0/2/3/3
3	N4X	C	902	-	-	0/7/27/27	0/2/3/3
3	N4X	D	902	-	-	0/7/27/27	0/2/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	N4X	C13-N22	-5.37	1.26	1.34
3	C	902	N4X	C13-N22	-5.35	1.26	1.34
3	B	902	N4X	C13-N22	-5.31	1.26	1.34
3	C	902	N4X	C5-N10	4.13	1.48	1.41
3	D	902	N4X	C5-N10	4.05	1.48	1.41
3	B	902	N4X	C5-N10	4.01	1.48	1.41
3	D	902	N4X	C6-N7	3.76	1.49	1.39
3	B	902	N4X	C6-N7	3.75	1.49	1.39
3	C	902	N4X	C6-N7	3.71	1.49	1.39
3	B	902	N4X	O14-C13	-2.72	1.19	1.24
3	C	902	N4X	O14-C13	-2.71	1.19	1.24
3	D	902	N4X	O14-C13	-2.70	1.19	1.24
3	B	902	N4X	C9-N10	-2.01	1.41	1.48
3	D	902	N4X	C9-N10	-2.00	1.41	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	N4X	C16-C15-N7	-3.09	110.39	114.16
3	B	902	N4X	C16-C15-N7	-2.97	110.53	114.16
3	D	902	N4X	O14-C13-N22	-2.35	118.25	122.77
3	C	902	N4X	O14-C13-N22	-2.34	118.26	122.77
3	D	902	N4X	C16-C15-N7	-2.32	111.33	114.16
3	B	902	N4X	O14-C13-N22	-2.26	118.42	122.77

There are no chirality outliers.

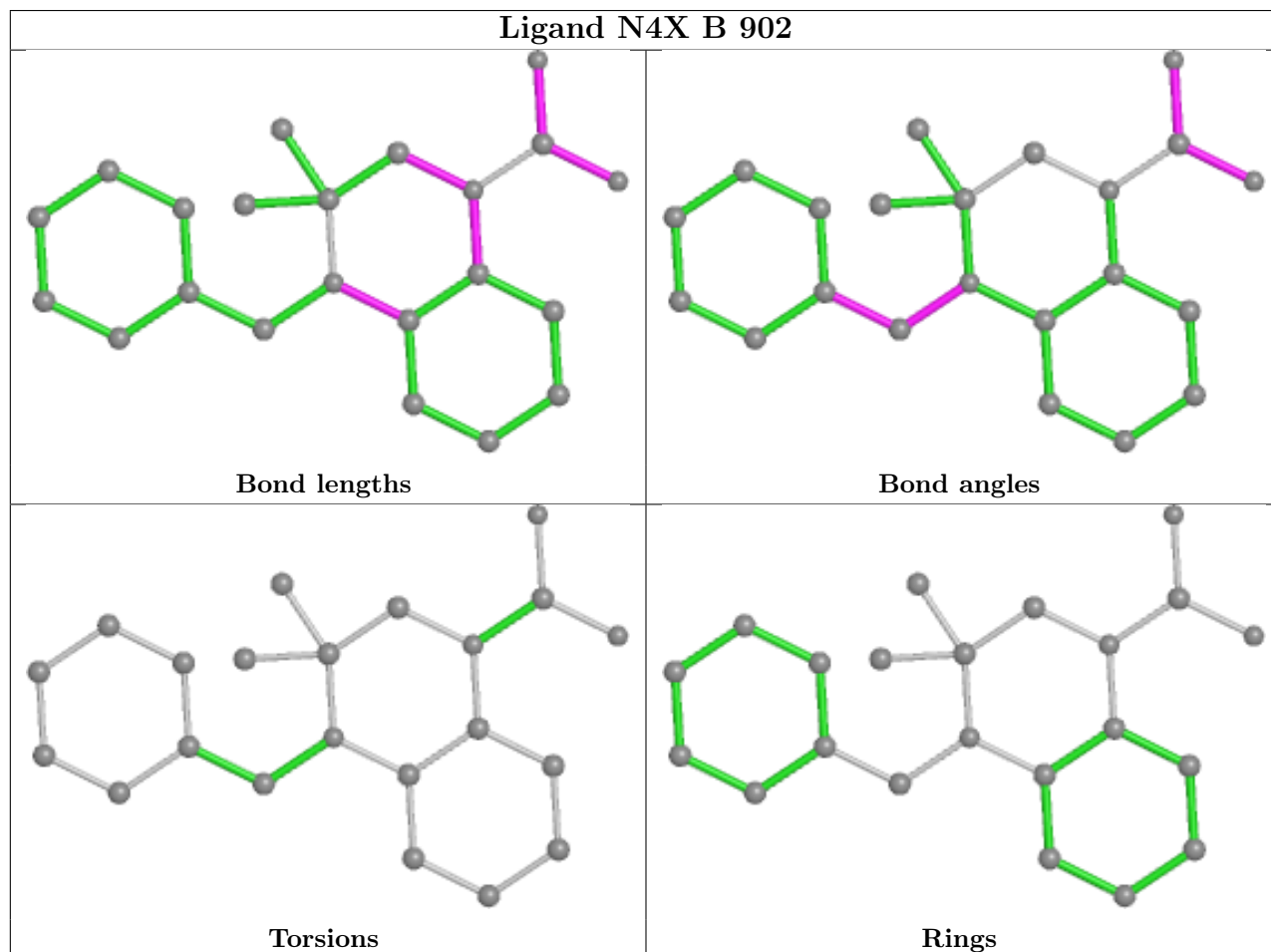
There are no torsion outliers.

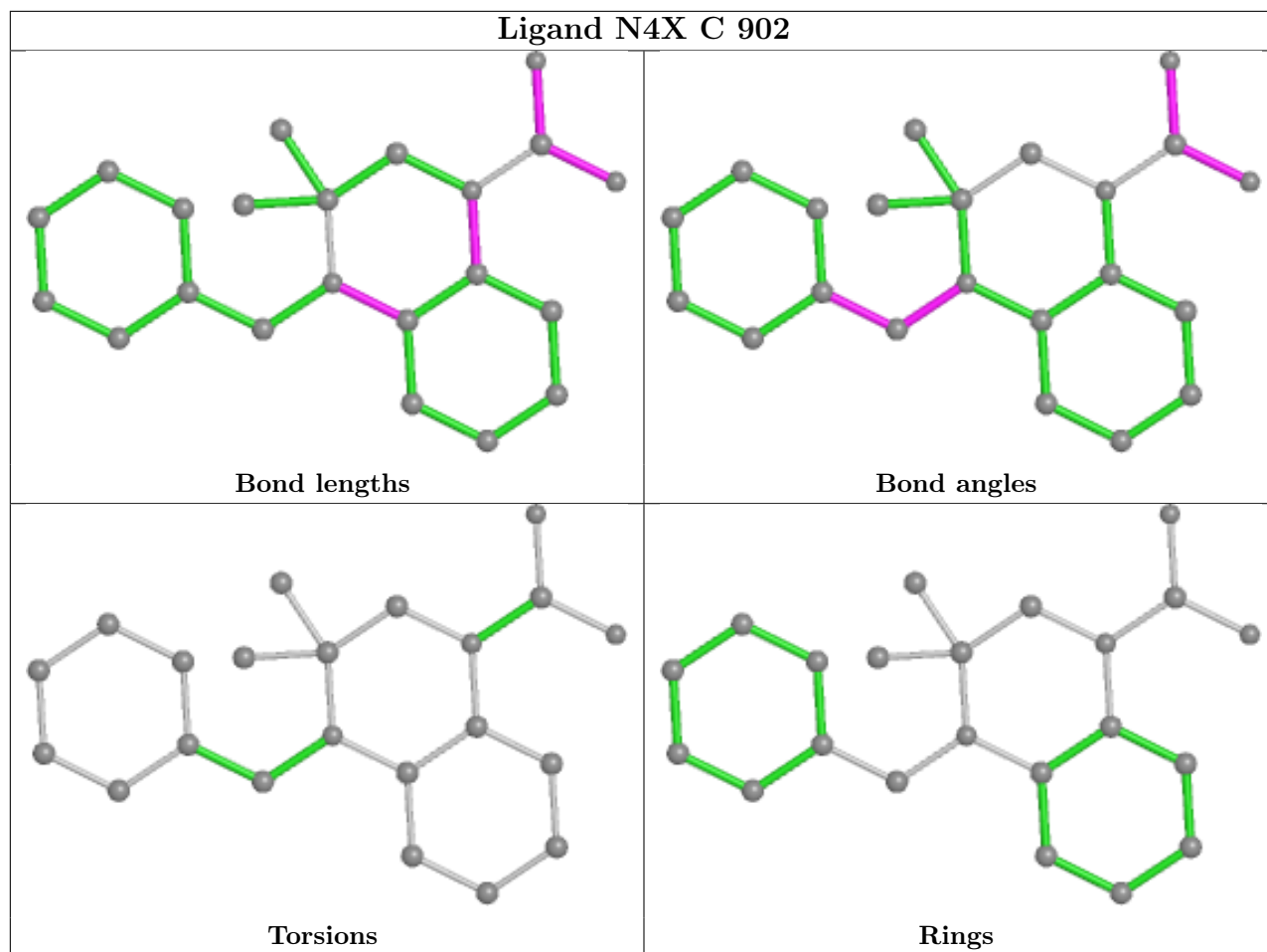
There are no ring outliers.

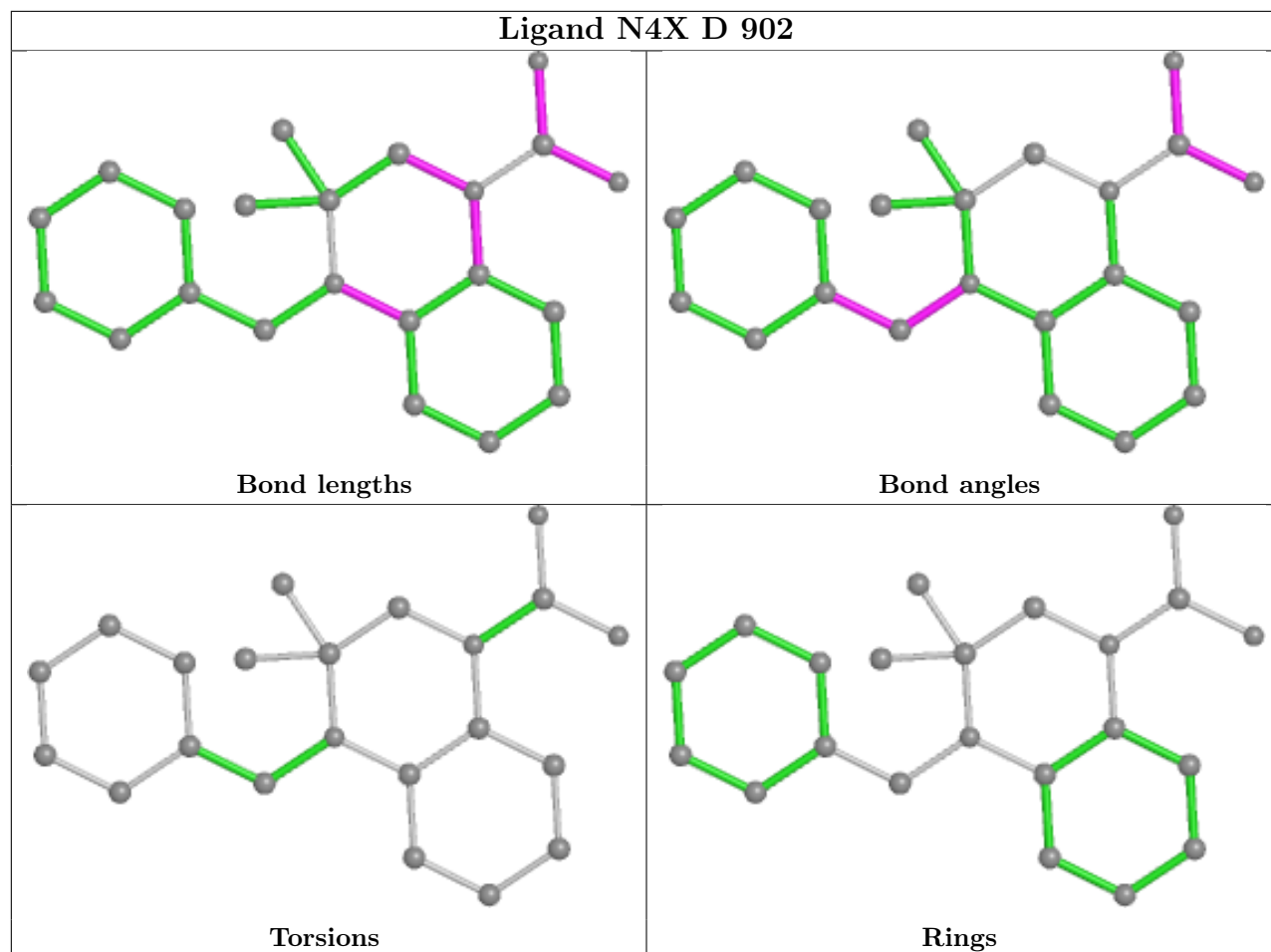
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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







5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	388/678 (57%)	1.34	95 (24%) 0 0	89, 111, 133, 140	0
1	B	545/678 (80%)	0.92	64 (11%) 4 4	79, 98, 123, 139	0
1	C	572/678 (84%)	0.83	33 (5%) 23 22	69, 88, 119, 143	0
1	D	562/678 (82%)	0.90	44 (7%) 13 12	59, 76, 103, 120	0
All	All	2067/2712 (76%)	0.97	236 (11%) 5 5	59, 93, 123, 143	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	511	ASN	8.0
1	A	703	LEU	6.3
1	D	280	THR	6.3
1	A	624	PHE	6.2
1	A	658	TYR	6.0
1	A	521	ILE	5.8
1	A	682	PHE	5.8
1	A	621	VAL	5.7
1	A	769	PHE	5.6
1	A	741	PHE	5.2
1	B	425	MET	5.1
1	A	761	LEU	5.0
1	B	507	ILE	4.6
1	A	535	GLN	4.6
1	A	537	ALA	4.5
1	D	226	GLY	4.4
1	A	230	CYS	4.4
1	A	806	GLY	4.4
1	A	219	PHE	4.4
1	A	702	MET	4.3
1	B	513	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	508	LYS	4.2
1	B	506	PHE	4.2
1	C	339	ASP	4.2
1	D	230	CYS	4.1
1	D	279	GLU	4.1
1	A	425	MET	4.1
1	A	409	PHE	4.1
1	A	273	LEU	4.1
1	B	510	ASP	4.0
1	B	601	LEU	3.9
1	D	430	LEU	3.9
1	A	821	THR	3.8
1	A	362	LEU	3.8
1	B	761	LEU	3.8
1	A	664	PHE	3.7
1	C	220	GLN	3.7
1	A	570	TRP	3.6
1	A	768	GLN	3.6
1	C	218	GLU	3.6
1	A	518	PHE	3.5
1	D	218	GLU	3.5
1	D	428	LYS	3.5
1	A	815	TRP	3.5
1	A	226	GLY	3.5
1	A	258	SER	3.5
1	B	307	TYR	3.5
1	D	593	MET	3.5
1	D	769	PHE	3.3
1	D	427	GLN	3.3
1	A	720	GLN	3.3
1	D	308	GLU	3.3
1	A	568	VAL	3.3
1	A	412	ILE	3.2
1	A	541	LEU	3.2
1	B	502	LEU	3.2
1	D	220	GLN	3.2
1	A	571	LEU	3.2
1	C	437	ALA	3.2
1	A	816	LEU	3.2
1	A	257	LEU	3.1
1	B	518	PHE	3.1
1	A	730	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	701	PHE	3.1
1	A	540	ARG	3.1
1	A	684	LEU	3.1
1	D	741	PHE	3.1
1	A	427	GLN	3.1
1	D	507	ILE	3.0
1	B	409	PHE	3.0
1	A	404	VAL	3.0
1	B	638	PHE	2.9
1	A	364	ALA	2.9
1	B	658	TYR	2.9
1	A	828	ASN	2.9
1	C	326	VAL	2.9
1	D	409	PHE	2.9
1	B	828	ASN	2.9
1	D	425	MET	2.9
1	A	269	TYR	2.8
1	D	605	THR	2.8
1	A	758	MET	2.8
1	A	392	LEU	2.8
1	A	220	GLN	2.8
1	D	265	THR	2.8
1	A	851	LEU	2.8
1	B	539	LEU	2.8
1	C	517	TYR	2.8
1	A	574	VAL	2.8
1	A	805	SER	2.8
1	A	752	TYR	2.8
1	A	800	ASN	2.7
1	A	564	HIS	2.7
1	B	333	TYR	2.7
1	B	618	LEU	2.7
1	A	536	ASN	2.7
1	C	543	ILE	2.7
1	D	618	LEU	2.7
1	C	433	PHE	2.7
1	C	782	ILE	2.7
1	A	713	LEU	2.7
1	B	552	ASP	2.7
1	A	662	TYR	2.6
1	A	740	LEU	2.6
1	A	542	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	544	TYR	2.6
1	C	231	GLY	2.6
1	A	722	LEU	2.6
1	A	635	ASN	2.6
1	B	403	LYS	2.6
1	D	606	VAL	2.6
1	A	576	ARG	2.6
1	D	336	ARG	2.6
1	B	651	GLU	2.5
1	C	226	GLY	2.5
1	A	763	THR	2.5
1	C	424	CYS	2.5
1	B	673	LEU	2.5
1	A	419	ILE	2.5
1	C	761	LEU	2.5
1	A	803	LEU	2.5
1	B	816	LEU	2.5
1	D	429	HIS	2.5
1	C	230	CYS	2.5
1	A	820	TYR	2.5
1	A	729	GLY	2.5
1	A	391	LEU	2.4
1	B	571	LEU	2.4
1	D	554	LEU	2.4
1	B	763	THR	2.4
1	D	234	PHE	2.4
1	A	771	PHE	2.4
1	B	617	PHE	2.4
1	A	260	GLN	2.4
1	A	529	LEU	2.4
1	A	807	PHE	2.4
1	D	337	GLU	2.4
1	C	627	VAL	2.4
1	B	305	HIS	2.4
1	A	406	HIS	2.4
1	A	413	ARG	2.4
1	A	577	LEU	2.4
1	A	259	LEU	2.4
1	B	802	VAL	2.4
1	A	414	LYS	2.4
1	D	375	CYS	2.4
1	B	554	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	388	MET	2.3
1	D	225	SER	2.3
1	D	854	ILE	2.3
1	D	624	PHE	2.3
1	C	735	LEU	2.3
1	B	739	SER	2.3
1	C	769	PHE	2.3
1	C	556	ARG	2.3
1	B	648	TRP	2.3
1	C	816	LEU	2.3
1	B	780	TYR	2.3
1	C	535	GLN	2.3
1	D	621	VAL	2.3
1	A	661	TYR	2.3
1	B	537	ALA	2.3
1	C	335	ARG	2.2
1	B	773	LYS	2.2
1	C	587	LEU	2.2
1	D	775	PRO	2.2
1	B	308	GLU	2.2
1	B	273	LEU	2.2
1	A	244	VAL	2.2
1	D	343	SER	2.2
1	D	766	PRO	2.2
1	A	697	LEU	2.2
1	A	742	LEU	2.2
1	A	794	MET	2.2
1	D	219	PHE	2.2
1	D	432	ARG	2.2
1	D	433	PHE	2.2
1	C	744	TYR	2.2
1	A	681	THR	2.2
1	A	222	VAL	2.2
1	B	517	TYR	2.2
1	B	820	TYR	2.2
1	B	538	GLU	2.2
1	B	350	PRO	2.2
1	D	431	LEU	2.2
1	A	782	ILE	2.2
1	A	855	THR	2.2
1	A	780	TYR	2.2
1	A	859	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	730	ILE	2.2
1	B	587	LEU	2.1
1	C	514	SER	2.1
1	A	633	PRO	2.1
1	B	499	GLU	2.1
1	B	392	LEU	2.1
1	B	691	ALA	2.1
1	A	704	ALA	2.1
1	D	382	LEU	2.1
1	C	673	LEU	2.1
1	D	568	VAL	2.1
1	B	391	LEU	2.1
1	C	544	TYR	2.1
1	B	597	ILE	2.1
1	A	365	LEU	2.1
1	A	797	LEU	2.1
1	B	555	ALA	2.1
1	C	626	SER	2.1
1	D	414	LYS	2.1
1	B	352	LEU	2.1
1	D	309	HIS	2.1
1	D	571	LEU	2.1
1	C	763	THR	2.1
1	B	599	LEU	2.1
1	B	792	CYS	2.1
1	C	706	ASN	2.1
1	C	839	ARG	2.1
1	D	402	LYS	2.1
1	B	563	VAL	2.1
1	A	776	LEU	2.1
1	B	740	LEU	2.1
1	B	797	LEU	2.1
1	A	796	GLU	2.0
1	B	572	VAL	2.0
1	B	541	LEU	2.0
1	D	412	ILE	2.0
1	B	401	GLN	2.0
1	A	744	TYR	2.0
1	C	545	GLY	2.0
1	A	811	VAL	2.0
1	B	662	TYR	2.0
1	B	522	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	266	THR	2.0
1	B	321	LEU	2.0
1	C	594	LEU	2.0
1	C	820	TYR	2.0
1	A	738	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](#)

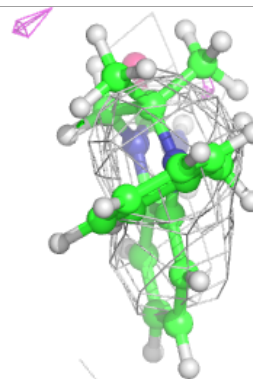
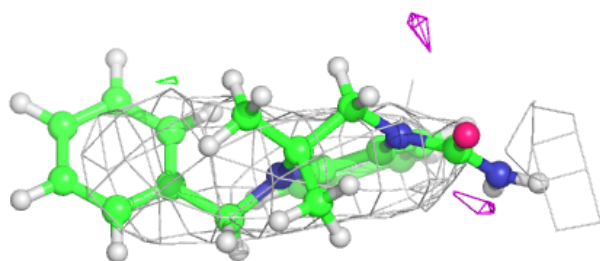
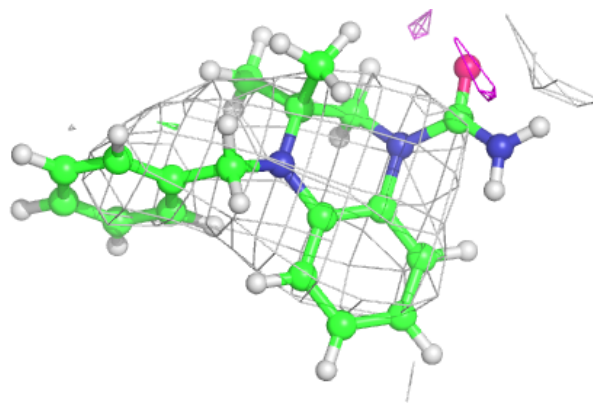
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	N4X	B	902	22/22	0.83	0.63	110,121,145,146	0
3	N4X	D	902	22/22	0.93	0.43	85,95,112,115	0
3	N4X	C	902	22/22	0.95	0.46	88,98,116,119	0
2	ZN	B	901	1/1	0.96	0.23	90,90,90,90	0
2	ZN	D	901	1/1	0.97	0.22	67,67,67,67	0
2	ZN	A	1000	1/1	0.98	0.14	113,113,113,113	0
2	ZN	C	901	1/1	0.98	0.23	77,77,77,77	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.

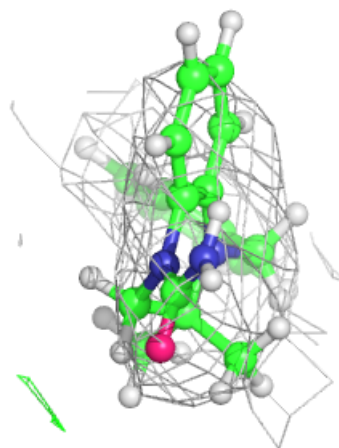
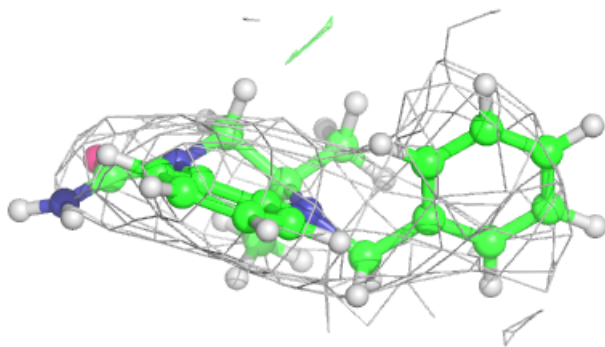
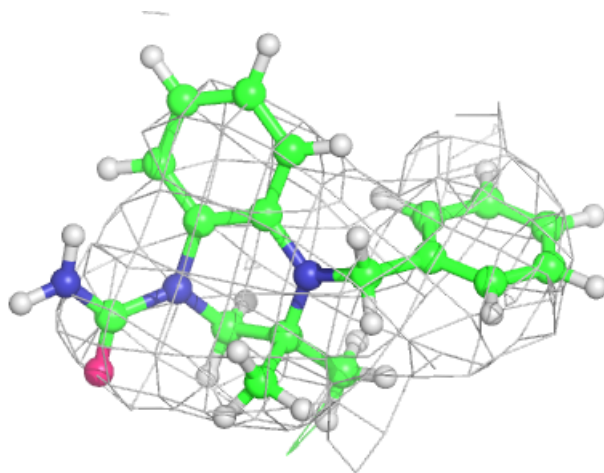
Electron density around N4X B 902:

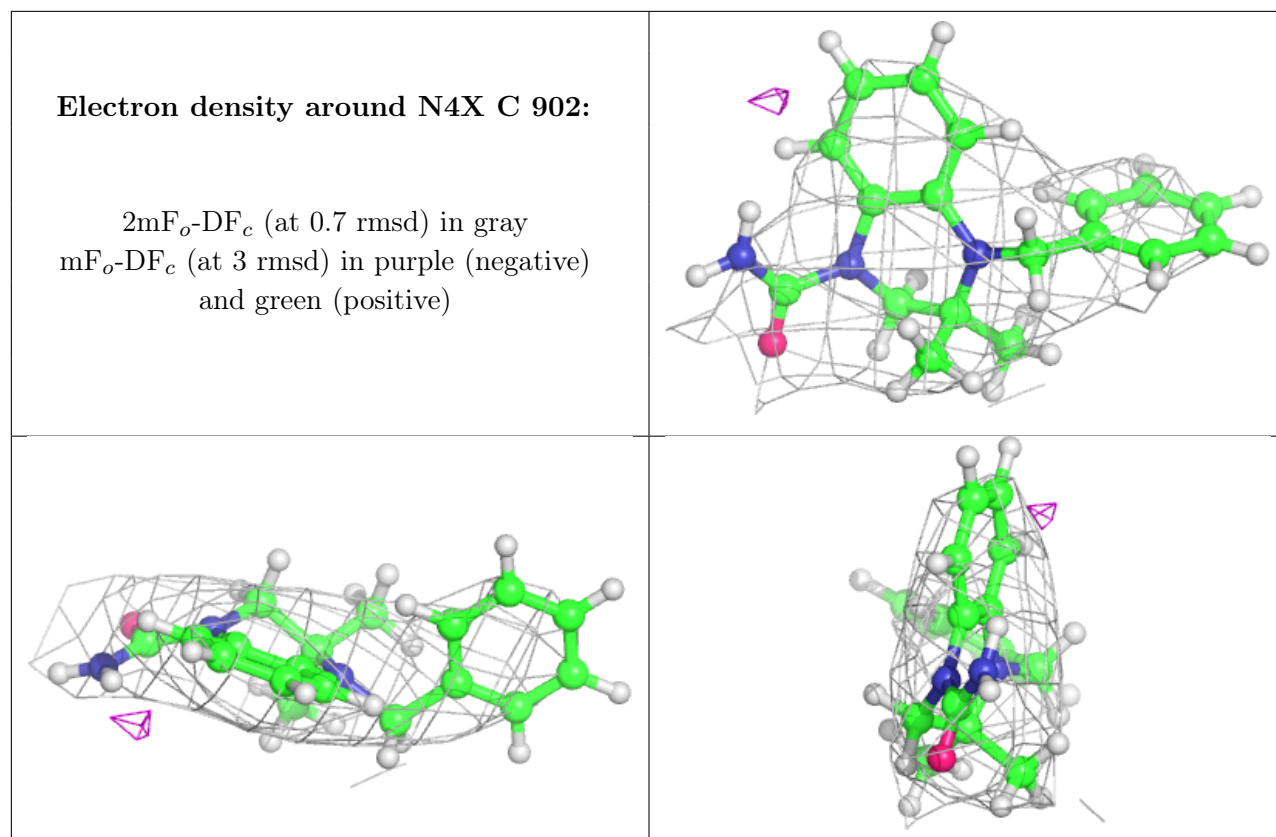
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around N4X D 902:

$2mF_o-DF_c$ (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.