



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:08 PM UTC

PDB ID : 8HUB / pdb_00008hub
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 : 4-5-2 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

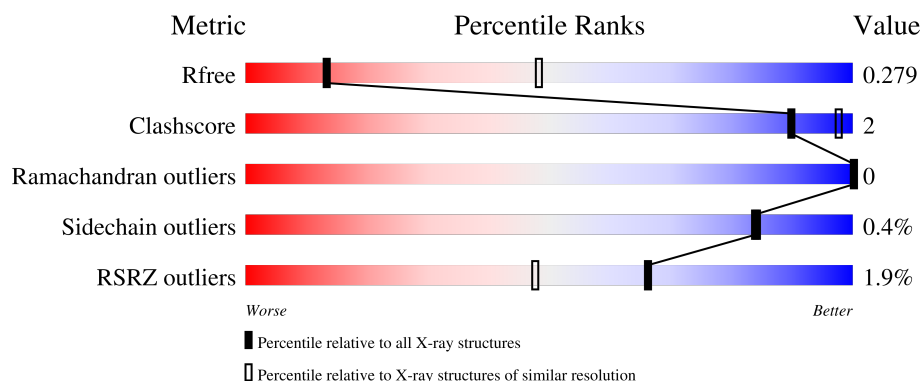
1 Overall quality at a glance

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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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	 3% 53% 1% 43%
1	B	678	 % 76% 5% 20%
1	C	678	 % 81% 1% 16%
1	D	678	 % 79% 1% 17%

2 Entry composition

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

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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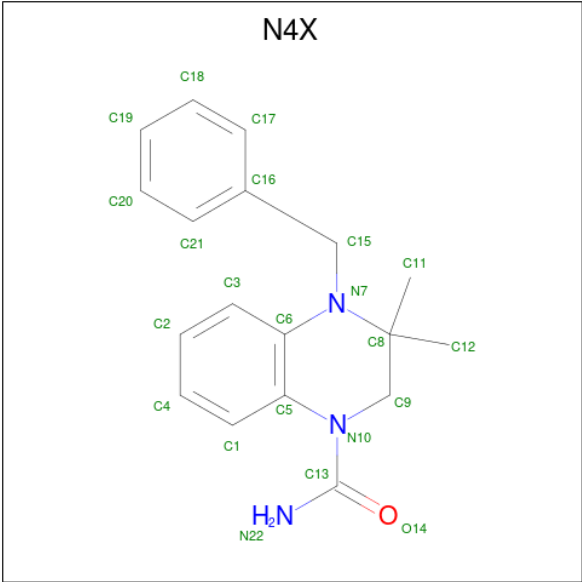
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Chain	Residue	Modelled	Actual	Comment	Reference
C	205	LYS	-	expression tag	UNP Q01433
C	206	ASP	-	expression tag	UNP Q01433
C	207	ASP	-	expression tag	UNP Q01433
C	208	ASP	-	expression tag	UNP Q01433
C	209	ASP	-	expression tag	UNP Q01433
C	210	LYS	-	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

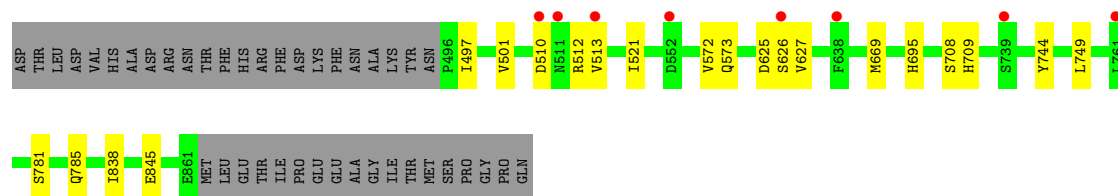
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

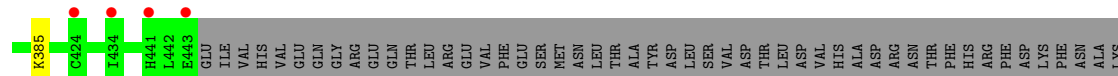
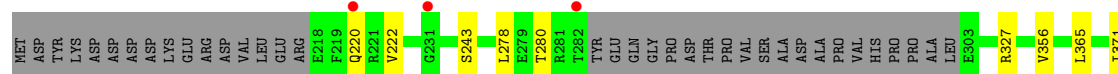
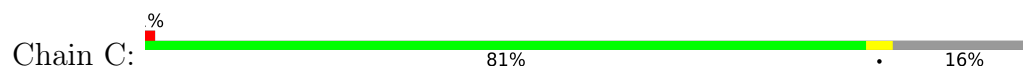
- Molecule 3 is 3,3-dimethyl-4-(phenylmethyl)-2 {H}-quinoxaline-1-carboxamide (CCD ID: N4X) (formula: C₁₈H₂₁N₃O) (labeled as "Ligand of Interest" by depositor).



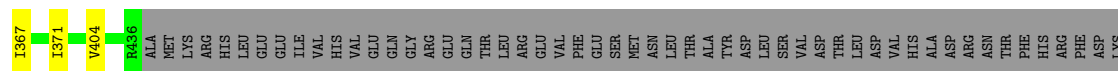
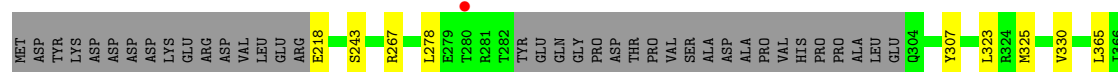
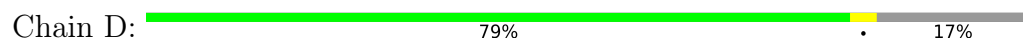
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			43	18	21	3	1		
3	C	1	Total	C	H	N	O	0	0
			43	18	21	3	1		
3	D	1	Total	C	H	N	O	0	0
			43	18	21	3	1		



- 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)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.258 , 0.276 0.258 , 0.279	Depositor DCC
R_{free} test set	2325 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	33454	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage'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	0.07	0/3218	0.22	0/4351
1	B	0.07	0/4558	0.21	0/6175
1	C	0.07	0/4758	0.22	0/6449
1	D	0.07	0/4706	0.23	0/6376
All	All	0.07	0/17240	0.22	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	18	0
1	B	4442	4370	4369	19	0
1	C	4637	4525	4525	13	1
1	D	4586	4501	4499	14	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	60	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 (60) 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:A:749:LEU:C	1:A:749:LEU:HD23	2.37	0.48
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:B:749:LEU:C	1:B:749:LEU:HD23	2.40	0.46
1:C:785:GLN:HG3	1:D:735:LEU:HD11	1.98	0.46
1:B:363:MET:HE1	1:B:695:HIS:HB3	1.97	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:B:350:PRO:HD3	1:B:669:MET:HE3	2.00	0.44
1:B:253:LYS:NZ	1:B:354:GLU:OE2	2.49	0.44
1:D:307:TYR:OH	1:D:620:HIS:ND1	2.49	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:ILE:HG12	1:D:782:ILE:HG12	2.00	0.43
1:D:325:MET:HE2	1:D:330:VAL:HG23	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
1:D:365:LEU:HD11	1:D:371:ILE:HG21	2.01	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:A:666:ASN:O	1:A:667:MET:C	2.63	0.41
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: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:A:778:GLU:OE2	1:B:781:SER:OG	2.26	0.41
1:B:367:ILE:O	1:B:367: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:627:VAL:O	1:C:628:ASP:HB2	2.20	0.40
1:C:749:LEU:N	1:C:750:PRO:HD2	2.36	0.40
1:A:257:LEU:HD12	1:A:257:LEU:C	2.47	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

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	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

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%)	78	81
1	B	491/612 (80%)	490 (100%)	1 (0%)	87	87
1	C	506/612 (83%)	503 (99%)	3 (1%)	78	81
1	D	505/612 (82%)	504 (100%)	1 (0%)	87	87
All	All	1852/2448 (76%)	1845 (100%)	7 (0%)	84	84

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

Mol	Chain	Res	Type
1	A	687	HIS
1	A	744	TYR

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Mol	Chain	Res	Type
1	B	744	TYR
1	C	220	GLN
1	C	278	LEU
1	C	280	THR
1	D	218	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	389	HIS
1	A	653	ASN
1	A	770	HIS
1	B	331	HIS
1	B	520	HIS
1	B	727	GLN
1	B	737	ASN
1	C	271	GLN
1	C	561	HIS
1	C	680	HIS
1	C	706	ASN
1	C	727	GLN
1	C	737	ASN
1	C	814	HIS

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 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	C	902	-	22,24,24	1.92	5 (22%)	23,35,35	1.02	2 (8%)
3	N4X	B	902	-	22,24,24	1.90	5 (22%)	23,35,35	1.01	2 (8%)
3	N4X	D	902	-	22,24,24	1.92	5 (22%)	23,35,35	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	C	902	-	-	0/7/27/27	0/2/3/3
3	N4X	B	902	-	-	0/7/27/27	0/2/3/3
3	N4X	D	902	-	-	0/7/27/27	0/2/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	902	N4X	C13-N22	-5.13	1.26	1.34
3	C	902	N4X	C13-N22	-5.12	1.26	1.34
3	B	902	N4X	C13-N22	-5.07	1.26	1.34
3	C	902	N4X	C5-N10	4.18	1.48	1.41
3	D	902	N4X	C5-N10	4.11	1.48	1.41
3	B	902	N4X	C5-N10	4.06	1.48	1.41
3	D	902	N4X	C6-N7	3.51	1.49	1.39
3	B	902	N4X	C6-N7	3.50	1.49	1.39
3	C	902	N4X	C6-N7	3.46	1.49	1.39
3	B	902	N4X	O14-C13	-2.69	1.19	1.24
3	C	902	N4X	O14-C13	-2.68	1.19	1.24
3	D	902	N4X	O14-C13	-2.67	1.19	1.24
3	B	902	N4X	C9-N10	-2.17	1.41	1.47
3	D	902	N4X	C9-N10	-2.15	1.41	1.47
3	C	902	N4X	C9-N10	-2.14	1.41	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	N4X	C16-C15-N7	-2.93	110.39	114.11
3	B	902	N4X	C16-C15-N7	-2.81	110.53	114.11
3	D	902	N4X	O14-C13-N22	-2.25	118.25	122.63
3	C	902	N4X	O14-C13-N22	-2.25	118.26	122.63
3	D	902	N4X	C16-C15-N7	-2.18	111.33	114.11
3	B	902	N4X	O14-C13-N22	-2.16	118.42	122.63

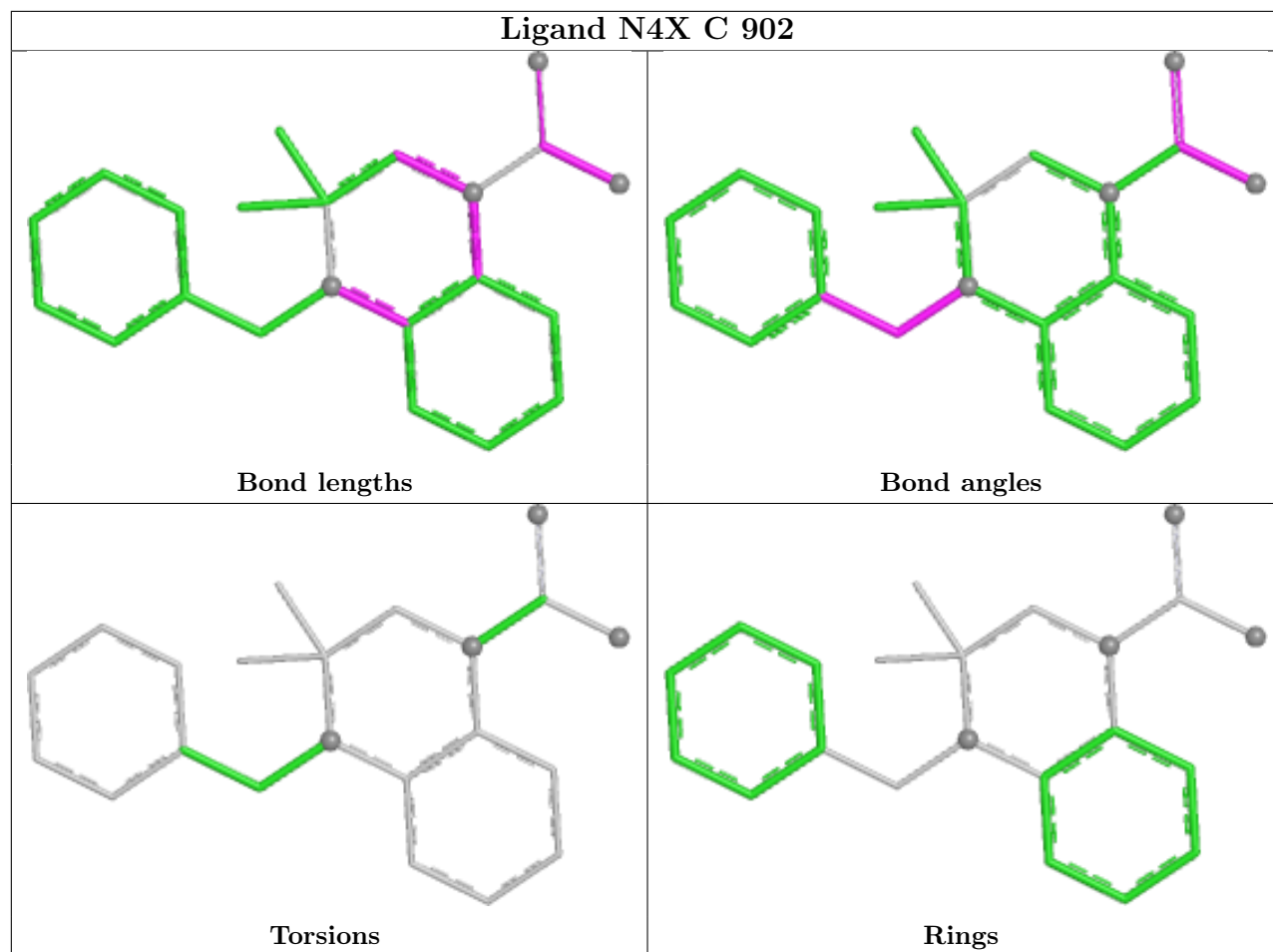
There are no chirality outliers.

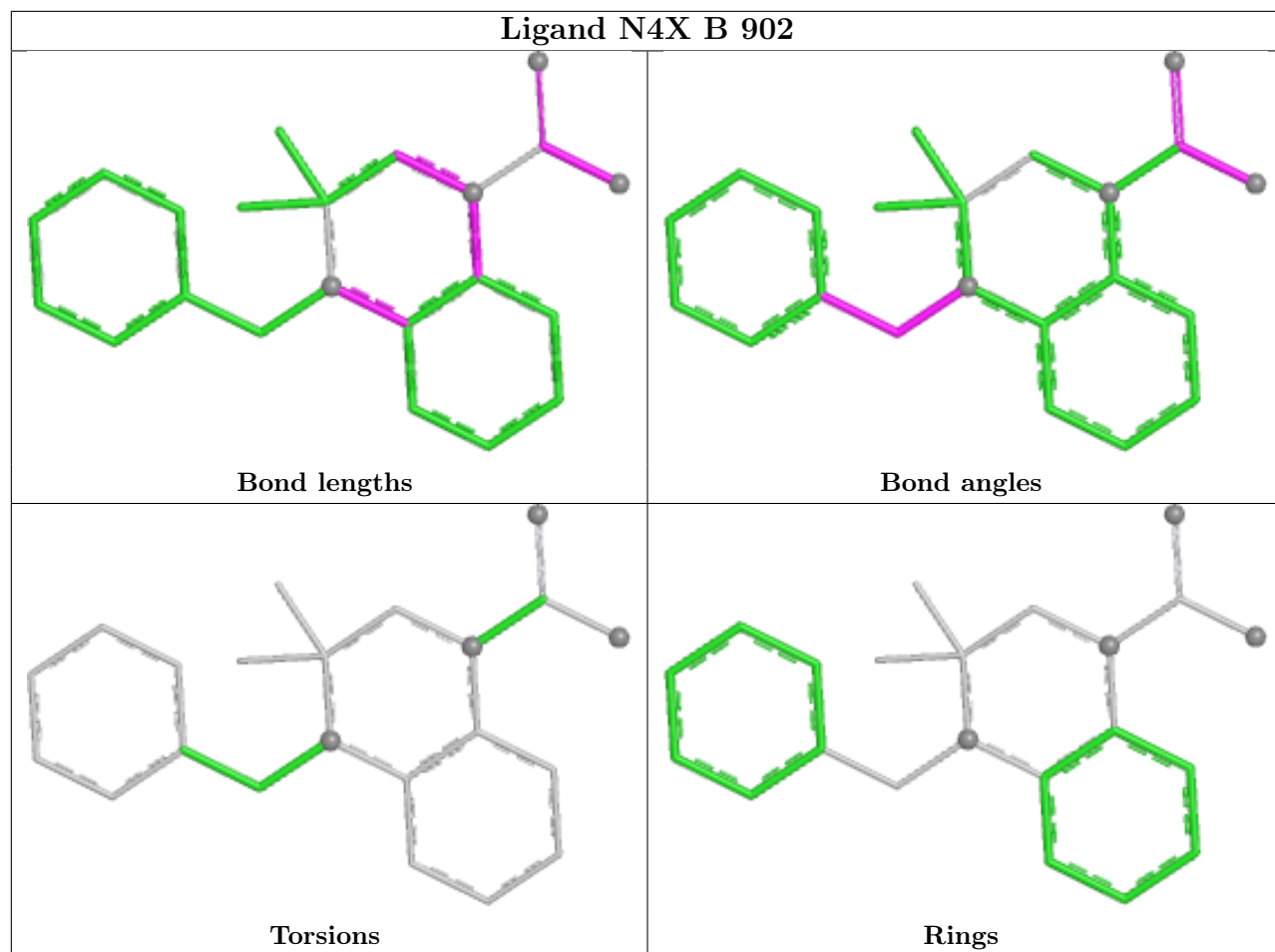
There are no torsion outliers.

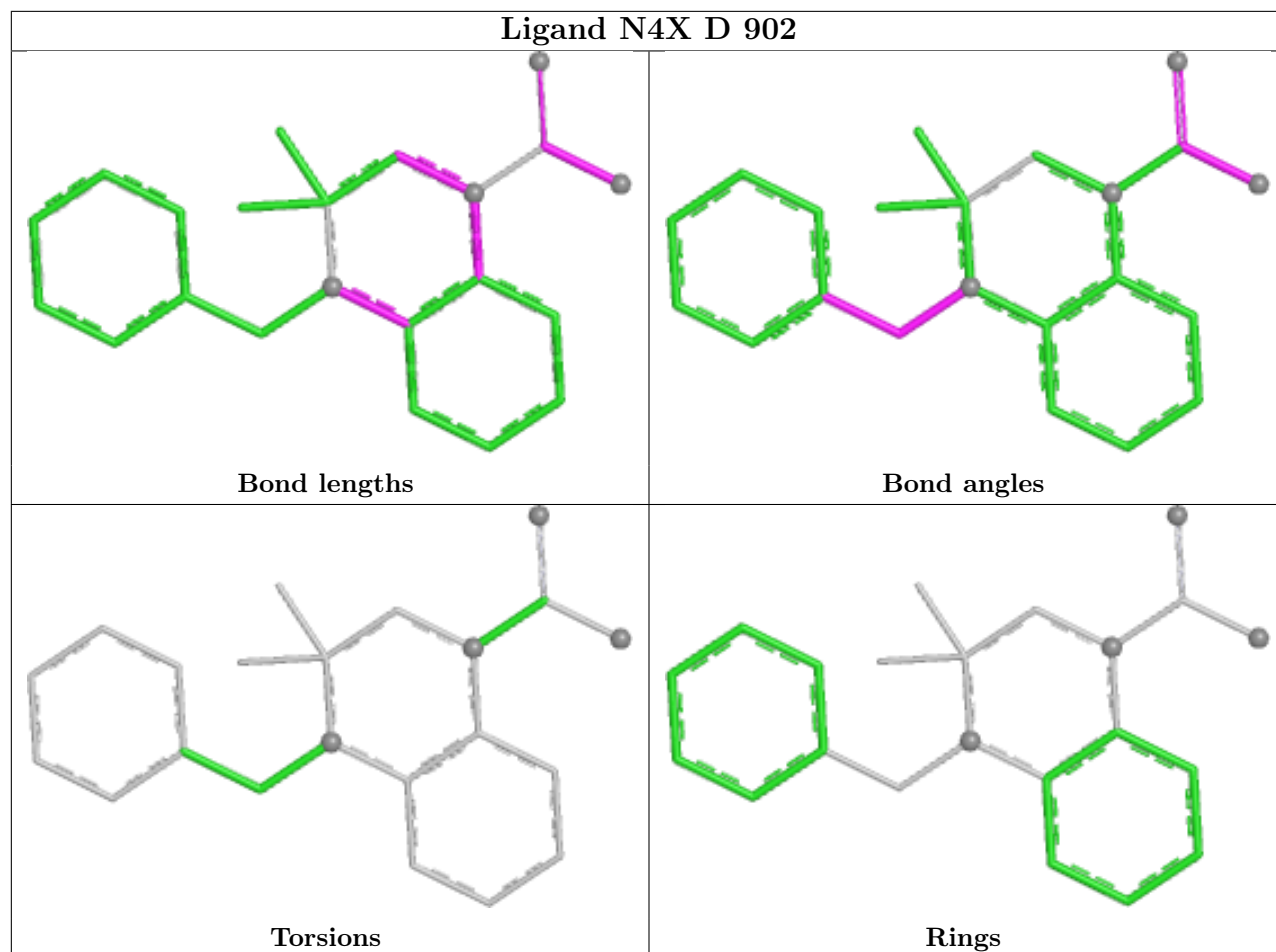
There are no ring outliers.

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%)	0.62	20 (5%) 33 22	97, 121, 144, 157	0
1	B	545/678 (80%)	0.30	10 (1%) 67 48	87, 108, 136, 150	0
1	C	572/678 (84%)	0.23	8 (1%) 73 54	75, 97, 130, 151	0
1	D	562/678 (82%)	0.14	1 (0%) 91 85	64, 84, 114, 130	0
All	All	2067/2712 (76%)	0.30	39 (1%) 66 48	64, 102, 135, 157	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	682	PHE	4.3
1	A	626	SER	4.2
1	C	443	GLU	4.1
1	B	511	ASN	4.1
1	A	624	PHE	3.6
1	A	621	VAL	3.4
1	D	280	THR	3.2
1	B	425	MET	3.1
1	C	424	CYS	3.1
1	A	741	PHE	2.9
1	A	656	TYR	2.9
1	A	658	TYR	2.9
1	C	441	HIS	2.8
1	C	231	GLY	2.7
1	C	282	THR	2.7
1	A	657	ALA	2.7
1	A	806	GLY	2.7
1	A	761	LEU	2.6
1	B	739	SER	2.6
1	A	638	PHE	2.6
1	A	769	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	552	ASP	2.6
1	B	510	ASP	2.5
1	A	620	HIS	2.4
1	B	626	SER	2.4
1	A	230	CYS	2.4
1	C	626	SER	2.3
1	B	761	LEU	2.3
1	B	513	VAL	2.3
1	A	425	MET	2.2
1	C	220	GLN	2.2
1	A	518	PHE	2.2
1	A	257	LEU	2.1
1	A	273	LEU	2.1
1	A	426	ASN	2.1
1	B	638	PHE	2.1
1	C	434	ILE	2.1
1	A	767	LEU	2.0
1	B	352	LEU	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
3	N4X	B	902	22/22	0.83	0.18	110,121,145,146	0
3	N4X	D	902	22/22	0.93	0.14	85,95,112,115	0
3	N4X	C	902	22/22	0.95	0.14	88,98,116,119	0
2	ZN	A	1000	1/1	0.97	0.05	113,113,113,113	0
2	ZN	C	901	1/1	0.98	0.03	77,77,77,77	0

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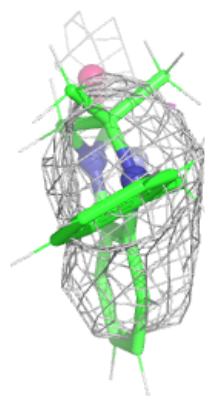
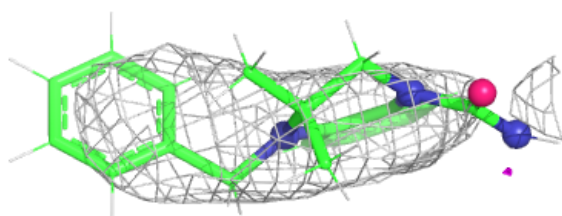
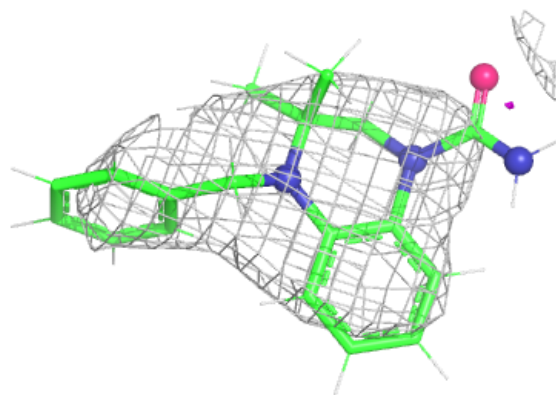
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	901	1/1	0.98	0.07	90,90,90,90	0
2	ZN	D	901	1/1	0.99	0.04	67,67,67,67	0

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.

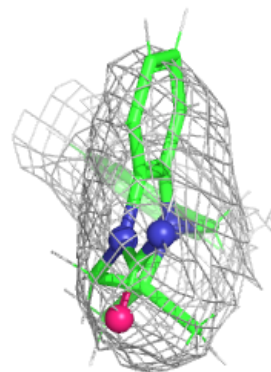
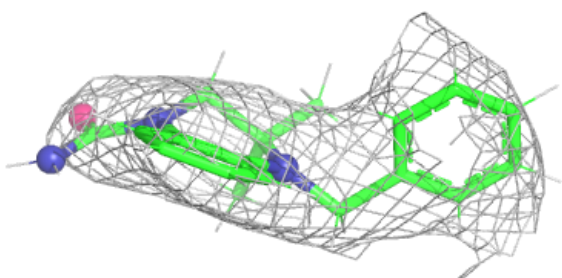
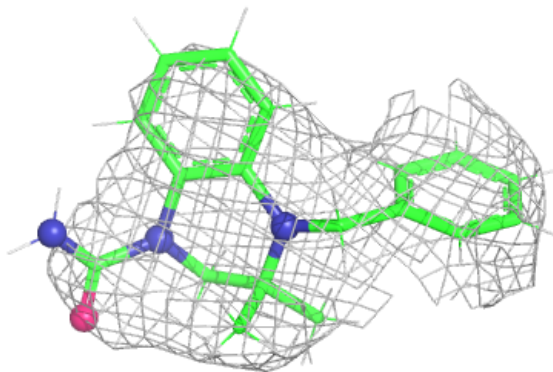
Electron density around N4X B 902:

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

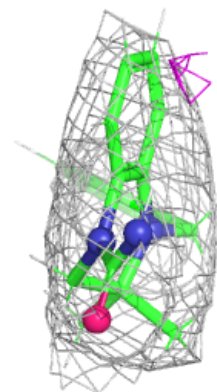
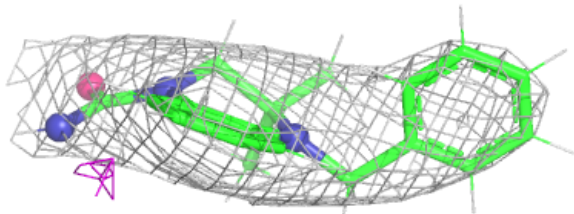
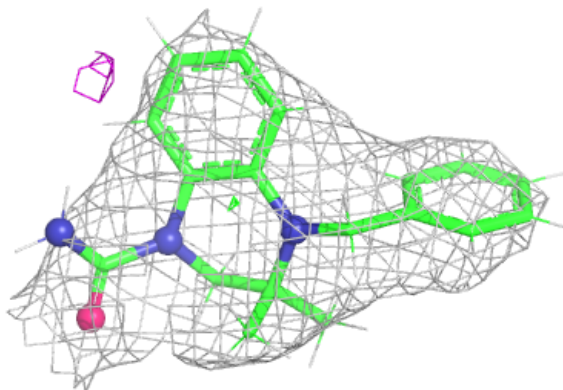


Electron density around N4X D 902:

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

**Electron density around N4X C 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.