



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:20 PM UTC

PDB ID : 7GTG / pdb_00007gtg
Title : PanDDA Analysis group deposition – Crystal structure of PTP1B in complex with FMOOA000684a
Authors : Mehlman, T.; Ginn, H.M.; Keedy, D.A.
Deposited on : 2024-01-03
Resolution : 1.69 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

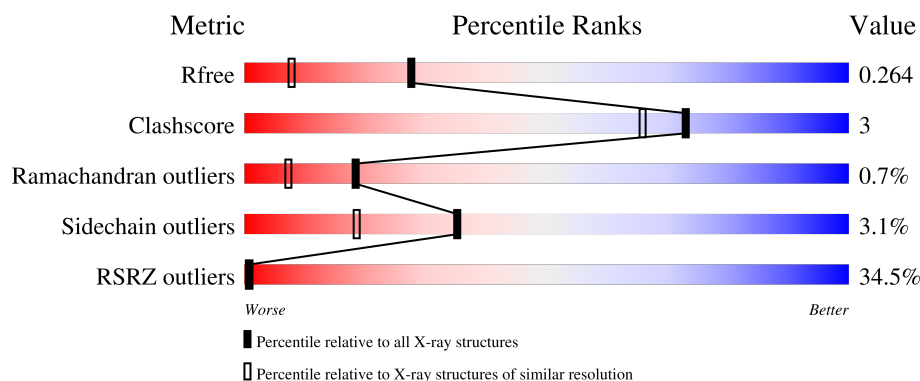
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	321	31% 78% 10% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	A1ABN	A	402	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4926 atoms, of which 2341 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 Tyrosine-protein phosphatase non-receptor type 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	284	4621	1471	2304	399	432	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	SER	CYS	engineered mutation	UNP P18031
A	92	VAL	CYS	engineered mutation	UNP P18031

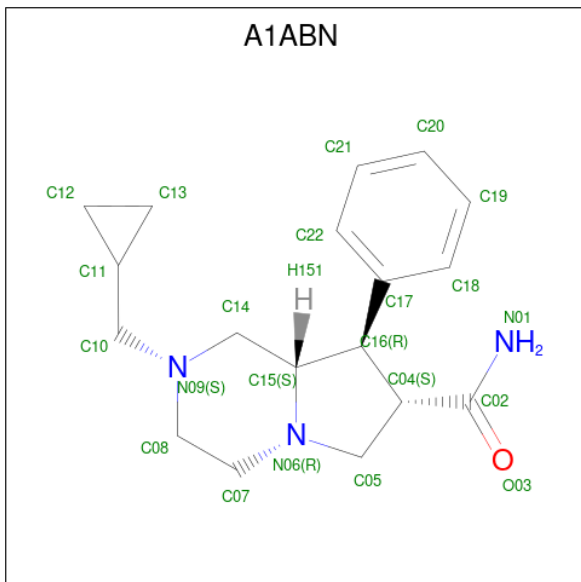
- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	20	4	12	1	3	0	0

- Molecule 3 is (5R,7S,8R,8aS)-2-(cyclopropylmethyl)-8-phenyloctahydropyrrolo[1,2-a]pyrazin

e-7-carboxamide (CCD ID: A1ABN) (formula: $C_{18}H_{25}N_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			47	18	25	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	234	Total	O	0	6
			238	238		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.20Å 90.20Å 106.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.04 – 1.69 63.04 – 1.69	Depositor EDS
% Data completeness (in resolution range)	100.0 (63.04-1.69) 100.0 (63.04-1.69)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.233 0.241 , 0.264	Depositor DCC
R_{free} test set	2220 reflections (3.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4926	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1ABN, TRS

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	1.31	8/2369 (0.3%)	1.31	3/3192 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	VAL	C-O	7.14	1.31	1.24
1	A	212	VAL	C-O	6.95	1.31	1.24
1	A	153	TYR	C-O	5.22	1.30	1.23
1	A	173	HIS	CE1-NE2	5.20	1.37	1.32
1	A	233	LEU	C-O	5.17	1.30	1.24
1	A	208	HIS	CE1-NE2	5.10	1.37	1.32
1	A	227	LEU	C-O	5.09	1.29	1.24
1	A	70	SER	C-O	5.00	1.30	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ARG	CA-C-N	5.70	125.53	121.65
1	A	105	ARG	C-N-CA	5.70	125.53	121.65
1	A	72	ILE	CA-CB-CG1	5.49	119.73	110.40

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	2317	2304	2296	14	2
2	A	8	12	12	0	2
3	A	22	25	0	1	0
4	A	238	0	0	8	0
All	All	2585	2341	2308	15	2

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 3.

All (15) 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:90:ASN:OD1	4:A:501[B]:HOH:O	1.68	1.12
1:A:128:LYS:NZ	4:A:502:HOH:O	2.24	0.70
1:A:73:LYS:CE	4:A:513:HOH:O	2.47	0.62
3:A:402:A1ABN:C13	4:A:700:HOH:O	2.49	0.60
1:A:58:LYS:HE2	4:A:701:HOH:O	2.04	0.57
1:A:60:HIS:HE1	4:A:607:HOH:O	1.87	0.56
1:A:136:GLU:HB2	4:A:622:HOH:O	2.05	0.56
1:A:92:VAL:HG12	1:A:135:PHE:CE1	2.43	0.52
1:A:2:GLU:HG3	1:A:5:LYS:HG2	1.94	0.49
1:A:56:ARG:NH2	1:A:58:LYS:HE3	2.30	0.47
1:A:133:MET:HE2	1:A:135:PHE:CZ	2.52	0.45
1:A:92:VAL:CG1	1:A:135:PHE:CE1	3.00	0.44
1:A:105:ARG:HH11	1:A:105:ARG:HG2	1.83	0.43
1:A:73:LYS:NZ	4:A:513:HOH:O	2.51	0.43
1:A:28:SER:HB3	1:A:30:PHE:CE2	2.56	0.40

All (2) 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:A:130:GLU:OE2	2:A:401:TRS:O2[4_565]	1.85	0.35
1:A:130:GLU:OE2	2:A:401:TRS:HO2[4_565]	1.53	0.07

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	282/321 (88%)	272 (96%)	8 (3%)	2 (1%)	18 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	261	ILE

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	257/294 (87%)	249 (97%)	8 (3%)	35 18

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	62	GLU
1	A	72	ILE
1	A	121	CYS
1	A	140	LEU
1	A	162	ASN
1	A	279	LYS
1	A	282	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	A1ABN	A	402	-	25,25,25	1.79	5 (20%)	33,36,36	2.12	9 (27%)
2	TRS	A	401	-	7,7,7	1.05	0	9,9,9	1.24	0

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	A1ABN	A	402	-	-	6/12/39/39	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	401	-	-	7/9/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	A1ABN	C15-N06	5.52	1.54	1.47
3	A	402	A1ABN	C02-N01	3.91	1.42	1.32
3	A	402	A1ABN	C05-N06	2.72	1.51	1.47
3	A	402	A1ABN	C22-C17	2.45	1.43	1.39
3	A	402	A1ABN	C18-C17	2.17	1.42	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	A1ABN	C07-N06-C15	5.11	116.77	112.06
3	A	402	A1ABN	C10-N09-C14	-4.96	102.04	111.33
3	A	402	A1ABN	C15-C14-N09	-4.80	103.07	111.39
3	A	402	A1ABN	C11-C10-N09	-4.38	107.11	114.06
3	A	402	A1ABN	C07-C08-N09	-3.37	103.85	110.65
3	A	402	A1ABN	C08-N09-C10	-2.74	103.77	111.35
3	A	402	A1ABN	C18-C17-C22	-2.14	115.65	118.30
3	A	402	A1ABN	C04-C05-N06	2.02	106.26	103.44
3	A	402	A1ABN	O03-C02-C04	2.01	123.16	121.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

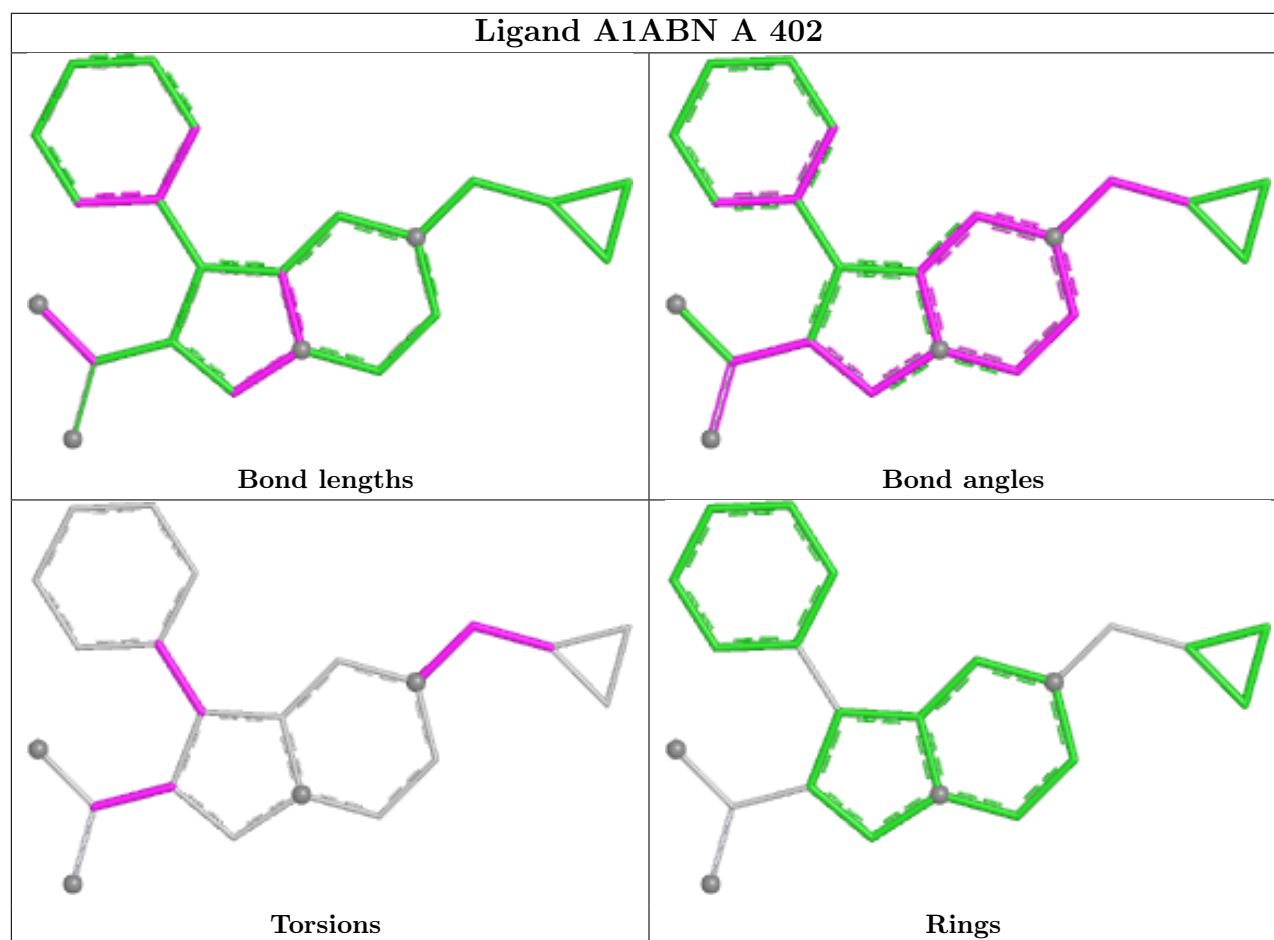
Mol	Chain	Res	Type	Atoms
2	A	401	TRS	C2-C-C1-O1
2	A	401	TRS	C3-C-C1-O1
2	A	401	TRS	N-C-C2-O2
3	A	402	A1ABN	O03-C02-C04-C05
3	A	402	A1ABN	N09-C10-C11-C12
2	A	401	TRS	N-C-C1-O1
3	A	402	A1ABN	C15-C16-C17-C22
2	A	401	TRS	C1-C-C2-O2
3	A	402	A1ABN	C11-C10-N09-C08
3	A	402	A1ABN	C15-C16-C17-C18
2	A	401	TRS	C1-C-C3-O3
3	A	402	A1ABN	C11-C10-N09-C14
2	A	401	TRS	N-C-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	A1ABN	1	0
2	A	401	TRS	0	2

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	284/321 (88%)	3.07	98 (34%) 1 1	12, 33, 66, 129	51 (17%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	TRP	19.7
1	A	165	THR	19.0
1	A	164	THR	17.3
1	A	140	LEU	17.0
1	A	168	THR	16.8
1	A	96	TRP	16.7
1	A	163	LEU	16.6
1	A	135	PHE	16.2
1	A	99	VAL	16.2
1	A	160	LEU	16.0
1	A	59	LEU	14.7
1	A	162	ASN	14.6
1	A	174	PHE	14.0
1	A	283	GLY	14.0
1	A	152	TYR	13.8
1	A	138	THR	13.7
1	A	153	TYR	13.6
1	A	93	GLY	13.5
1	A	60	HIS	13.5
1	A	61	GLN	12.9
1	A	169	ARG	12.9
1	A	103	LYS	12.8
1	A	281	ILE	12.7
1	A	139	ASN	12.1
1	A	166	GLN	12.0
1	A	284	ASP	12.0
1	A	137	ASP	11.8

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Mol	Chain	Res	Type	RSRZ
1	A	98	MET	11.6
1	A	167	GLU	11.6
1	A	62	GLU	11.4
1	A	58	LYS	11.4
1	A	101	GLU	11.3
1	A	102	GLN	11.1
1	A	136	GLU	10.9
1	A	161	GLU	10.4
1	A	63	ASP	10.4
1	A	94	HIS	10.3
1	A	280	PHE	10.3
1	A	282	MET	9.6
1	A	97	GLU	9.3
1	A	237	LYS	7.9
1	A	236	ASP	7.4
1	A	277	GLY	7.4
1	A	278	ALA	7.3
1	A	241	PRO	7.2
1	A	279	LYS	7.2
1	A	239	LYS	7.0
1	A	243	SER	6.6
1	A	10	ILE	6.0
1	A	242	SER	5.8
1	A	3	MET	5.6
1	A	240	ASP	5.5
1	A	238	ARG	5.3
1	A	1	MET	5.1
1	A	5	LYS	5.0
1	A	7	PHE	5.0
1	A	276	GLU	4.4
1	A	9	GLN	4.1
1	A	2	GLU	4.0
1	A	92	VAL	4.0
1	A	271	TYR	3.6
1	A	275	ILE	3.6
1	A	155	VAL	3.5
1	A	272	LEU	3.5
1	A	188	PRO	3.5
1	A	193	ASN	3.4
1	A	12	LYS	3.3
1	A	134	ILE	3.3
1	A	21	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	25	HIS	3.2
1	A	207	GLU	2.9
1	A	131	LYS	2.9
1	A	24	ARG	2.9
1	A	150	LYS	2.7
1	A	90	ASN	2.6
1	A	184	VAL	2.6
1	A	206	PRO	2.6
1	A	233	LEU	2.5
1	A	47	ARG	2.5
1	A	119	LEU	2.5
1	A	181	ASP	2.4
1	A	182	PHE	2.4
1	A	196	PHE	2.4
1	A	195	LEU	2.4
1	A	46	TYR	2.4
1	A	145	ILE	2.3
1	A	186	GLU	2.3
1	A	121	CYS	2.3
1	A	246	ILE	2.3
1	A	36	LYS	2.3
1	A	226	CYS	2.2
1	A	189	ALA	2.1
1	A	248	LYS	2.1
1	A	32	SER	2.1
1	A	148	ASP	2.1
1	A	14	GLY	2.0
1	A	16	TRP	2.0
1	A	269	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

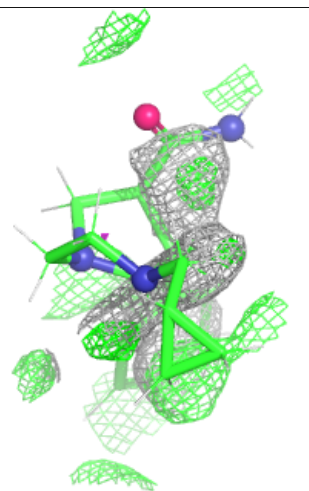
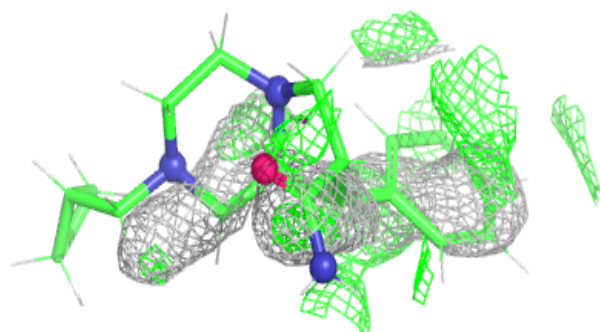
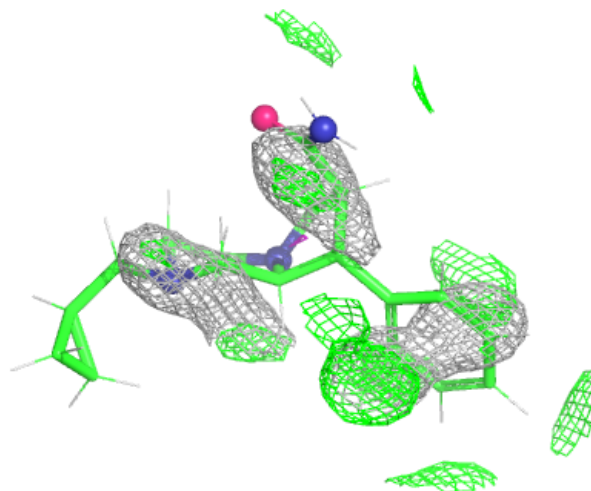
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1ABN	A	402	22/22	0.57	0.57	45,56,61,61	47
2	TRS	A	401	8/8	0.78	0.19	31,48,63,70	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 A1ABN A 402:

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.