



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 01:05 AM UTC

PDB ID : 9GL7 / pdb_00009gl7
Title : EGFR Exon20 insertion mutant NPG bound with (S)-3-((3-chloro-2-methoxyphenyl)amino)-2-(3-((tetrahydrofuran-2-yl)methoxy)pyridin-4-yl)-1,5,6,7-tetrahydro-4H-pyrrolo[3,2-c]pyridin-4-one
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Deposited on : 2024-08-27
Resolution : 1.88 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

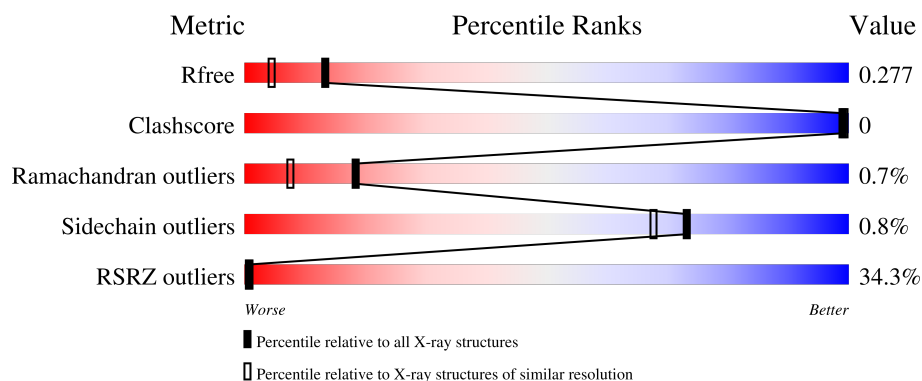
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	338	30% 86% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5054 atoms, of which 2483 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.

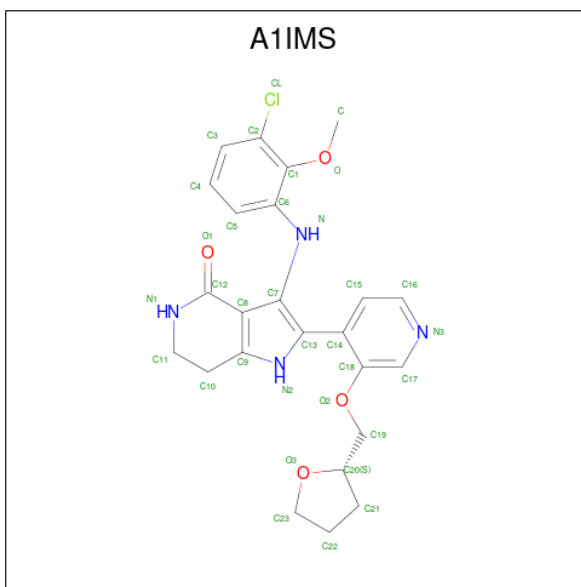
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	H	N	O	S	2483	4	0
			4914	1567	2483	415	433	16			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	694	MET	-	initiating methionine	UNP P00533
A	770A	ASN	-	insertion	UNP P00533
A	770B	PRO	-	insertion	UNP P00533
A	770C	GLY	-	insertion	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
A	1023	HIS	-	expression tag	UNP P00533
A	1024	HIS	-	expression tag	UNP P00533
A	1025	HIS	-	expression tag	UNP P00533
A	1026	HIS	-	expression tag	UNP P00533
A	1027	HIS	-	expression tag	UNP P00533
A	1028	HIS	-	expression tag	UNP P00533

- Molecule 2 is 3-[(3-chloranyl-2-methoxy-phenyl)amino]-2-[3-[[[(2S)-oxolan-2-yl]methoxy]pyridin-4-yl]-1,5,6,7-tetrahydropyrrolo[3,2-c]pyridin-4-one (CCD ID: A1IMS) (formula: C₂₄H₂₅ClN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 33	C 24	Cl 1	N 4	O 4	0	0

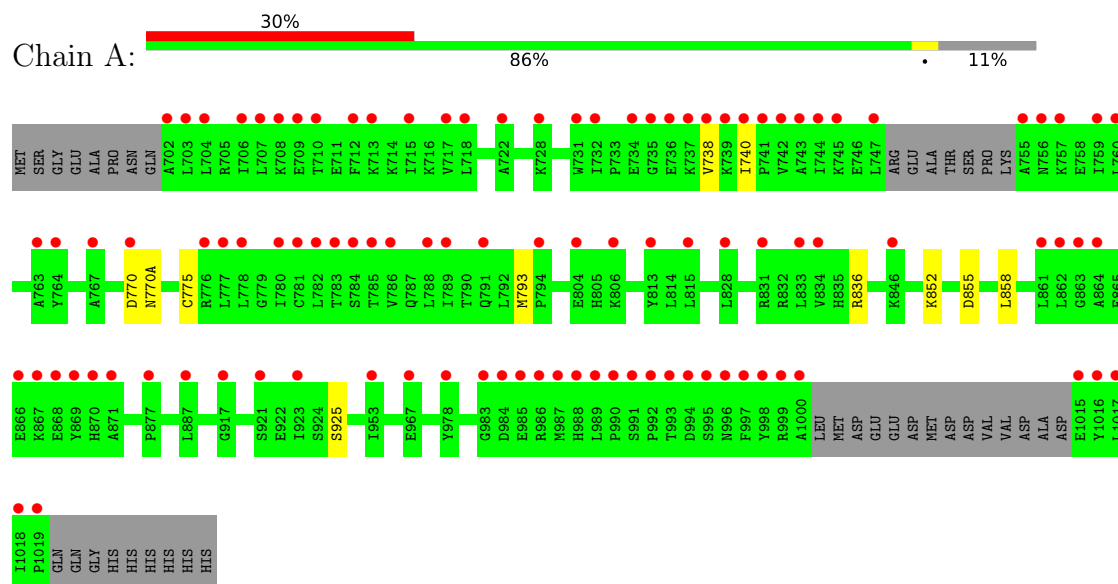
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	106	Total O 107 107	0	2

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: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	39.74Å 105.78Å 174.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.22 – 1.88 34.22 – 1.88	Depositor EDS
% Data completeness (in resolution range)	53.9 (34.22-1.88) 53.9 (34.22-1.88)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.88Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.268 , 0.287 0.256 , 0.277	Depositor DCC
R_{free} test set	794 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.4	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	0.89	EDS
Total number of atoms	5054	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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: A1IMS

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	0.79	0/2503	1.01	3/3382 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	770(A)	ASN	CA-CB-CG	-7.38	105.22	112.60
1	A	740	ILE	N-CA-C	5.65	113.46	107.76
1	A	770	ASP	CA-CB-CG	-5.29	107.31	112.60

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	2431	2483	2464	2	0
2	A	33	0	0	0	0
3	A	107	0	0	0	0
All	All	2571	2483	2464	2	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 0.

All (2) 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:793:MET:SD	1:A:852:LYS:HD2	2.58	0.43
1:A:836:ARG:HD3	1:A:858:LEU:O	2.18	0.43

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	298/338 (88%)	288 (97%)	8 (3%)	2 (1%)	18 7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	855	ASP
1	A	738	VAL

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	268/297 (90%)	266 (99%)	2 (1%)	76 69

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

Mol	Chain	Res	Type
1	A	775	CYS
1	A	925	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	791	GLN
1	A	842	ASN
1	A	870	HIS
1	A	988	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](#)

1 ligand is 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	$\# Z > 2$
2	A1IMS	A	2001	-	37,37,37	1.57	4 (10%)	43,52,52	1.18	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1IMS	A	2001	-	-	2/15/32/32	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	A1IMS	C7-C13	5.69	1.44	1.38
2	A	2001	A1IMS	C12-N1	5.56	1.40	1.34
2	A	2001	A1IMS	C7-N	2.31	1.41	1.35
2	A	2001	A1IMS	C17-C18	2.01	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	A1IMS	O2-C18-C17	-4.91	118.68	124.43
2	A	2001	A1IMS	O1-C12-N1	-2.48	118.95	123.24
2	A	2001	A1IMS	C19-O2-C18	-2.38	112.94	118.21
2	A	2001	A1IMS	O2-C18-C14	2.36	122.17	116.97
2	A	2001	A1IMS	C10-C9-C8	-2.21	123.80	125.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

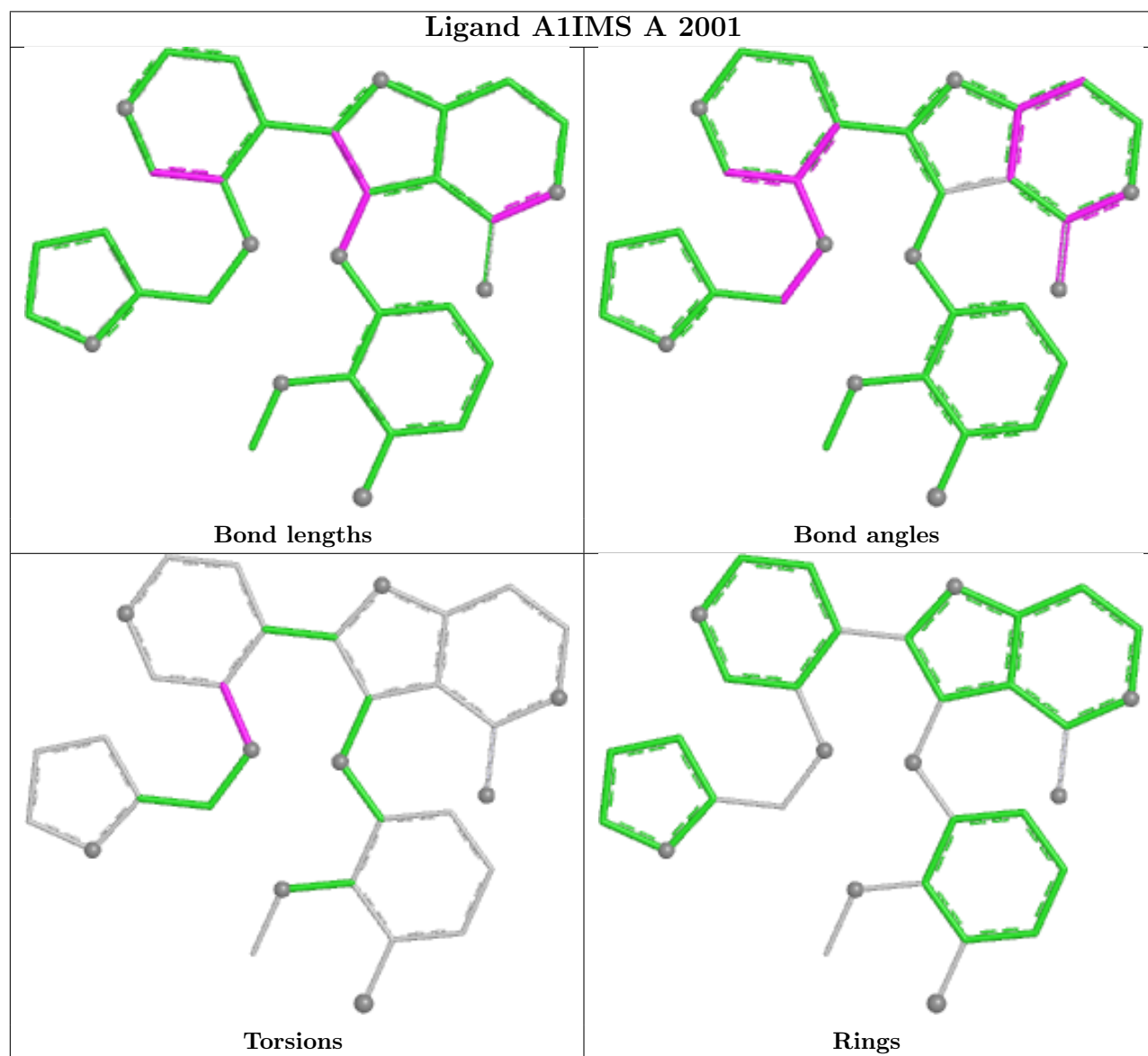
Mol	Chain	Res	Type	Atoms
2	A	2001	A1IMS	C17-C18-O2-C19
2	A	2001	A1IMS	C14-C18-O2-C19

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	300/338 (88%)	1.70	103 (34%) 1 1	6, 21, 39, 48	2 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1000	ALA	7.1
1	A	737	LYS	6.0
1	A	997	PHE	5.8
1	A	806[A]	LYS	5.5
1	A	993	THR	5.2
1	A	992	PRO	4.9
1	A	755	ALA	4.8
1	A	738	VAL	4.8
1	A	759	ILE	4.7
1	A	785	THR	4.6
1	A	703	LEU	4.4
1	A	747	LEU	4.4
1	A	996	ASN	4.4
1	A	989	LEU	4.3
1	A	778	LEU	4.3
1	A	861	LEU	4.3
1	A	998	TYR	4.2
1	A	788	LEU	4.2
1	A	991	SER	4.0
1	A	1018	ILE	3.9
1	A	988	HIS	3.8
1	A	734	GLU	3.8
1	A	741	PRO	3.8
1	A	756	ASN	3.7
1	A	740	ILE	3.7
1	A	999	ARG	3.7
1	A	718	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	869	TYR	3.6
1	A	777	LEU	3.6
1	A	739	LYS	3.5
1	A	702	ALA	3.5
1	A	1019	PRO	3.5
1	A	722	ALA	3.5
1	A	710	THR	3.4
1	A	1016	TYR	3.4
1	A	707	LEU	3.4
1	A	706	ILE	3.4
1	A	917	GLY	3.4
1	A	780	ILE	3.3
1	A	986	ARG	3.3
1	A	871	ALA	3.2
1	A	783	THR	3.2
1	A	704	LEU	3.2
1	A	862	LEU	3.2
1	A	735	GLY	3.2
1	A	708	LYS	3.2
1	A	1017	LEU	3.1
1	A	994	ASP	3.1
1	A	923	ILE	3.0
1	A	985	GLU	2.9
1	A	870	HIS	2.9
1	A	867	LYS	2.9
1	A	743	ALA	2.9
1	A	995	SER	2.9
1	A	717	VAL	2.8
1	A	794	PRO	2.8
1	A	786	VAL	2.7
1	A	731	TRP	2.7
1	A	983	GLY	2.7
1	A	732	ILE	2.7
1	A	866	GLU	2.7
1	A	782	LEU	2.6
1	A	828	LEU	2.6
1	A	757	LYS	2.6
1	A	791	GLN	2.6
1	A	744	ILE	2.6
1	A	864	ALA	2.5
1	A	987	MET	2.5
1	A	978	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	877	PRO	2.4
1	A	715	ILE	2.4
1	A	713	LYS	2.4
1	A	990	PRO	2.4
1	A	921	SER	2.3
1	A	804	GLU	2.3
1	A	712	PHE	2.3
1	A	887	LEU	2.3
1	A	813	TYR	2.3
1	A	846	LYS	2.3
1	A	833	LEU	2.3
1	A	763	ALA	2.2
1	A	728	LYS	2.2
1	A	776	ARG	2.2
1	A	736	GLU	2.2
1	A	984	ASP	2.2
1	A	709	GLU	2.2
1	A	781	CYS	2.2
1	A	815	LEU	2.2
1	A	767	ALA	2.2
1	A	764	TYR	2.1
1	A	868	GLU	2.1
1	A	742	VAL	2.1
1	A	834	VAL	2.1
1	A	863	GLY	2.1
1	A	770	ASP	2.1
1	A	789	ILE	2.1
1	A	953	ILE	2.1
1	A	784	SER	2.1
1	A	831	ARG	2.1
1	A	967	GLU	2.1
1	A	1015	GLU	2.1
1	A	760	LEU	2.0
1	A	745	LYS	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

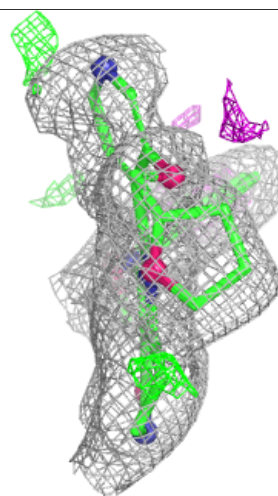
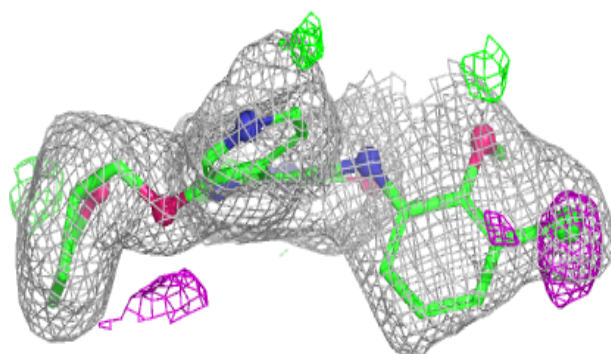
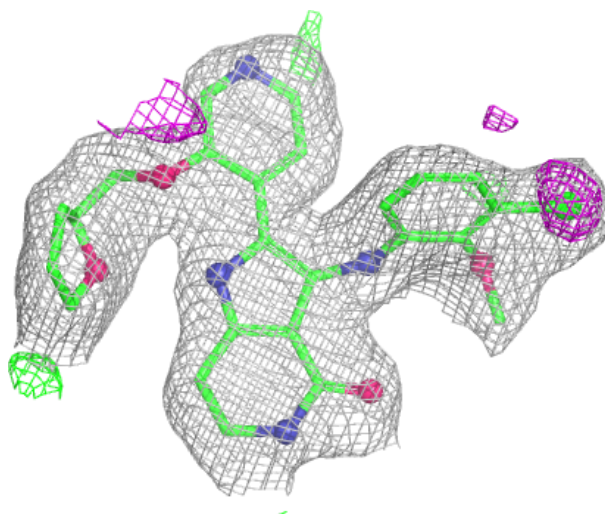
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	A1IMS	A	2001	33/33	0.84	0.13	36,39,41,42	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 A1IMS A 2001:

$2mF_o-DF_c$ (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.