



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:48 PM UTC

PDB ID : 9QD4 / pdb_00009qd4
Title : Crystal structure of the neurotensin receptor 1 in complex with the small-molecule full agonist cp30a
Authors : Deluigi, M.; Hilge, M.; Plueckthun, A.
Deposited on : 2025-03-06
Resolution : 3.11 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

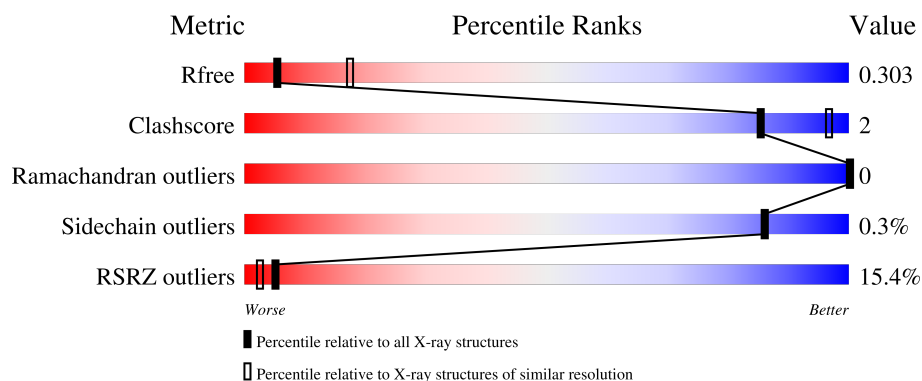
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	500	14% 87% 5% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6661 atoms, of which 3322 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 Neurotensin receptor type 1, DARPin fusion.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	460	6600	2151	3296	553	588	12	155	0	0

There are 30 discrepancies between the modelled and reference sequences:

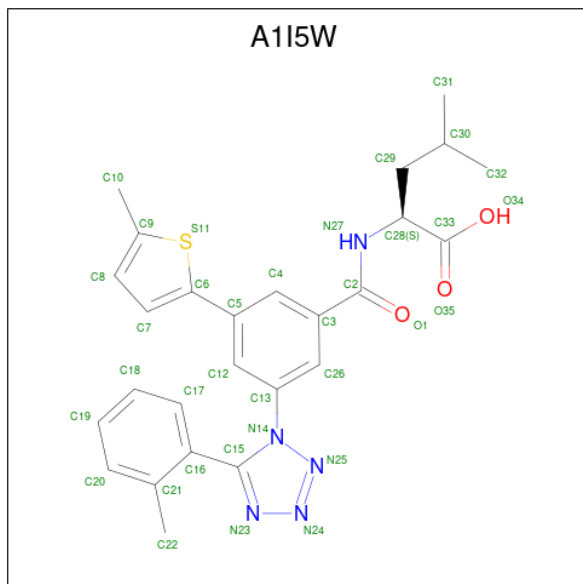
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLY	-	expression tag	UNP P20789
A	47	PRO	-	expression tag	UNP P20789
A	48	GLY	-	expression tag	UNP P20789
A	49	SER	-	expression tag	UNP P20789
A	83	GLY	SER	engineered mutation	UNP P20789
A	86	LEU	ALA	engineered mutation	UNP P20789
A	101	ARG	THR	engineered mutation	UNP P20789
A	103	ASP	HIS	engineered mutation	UNP P20789
A	105	TYR	HIS	engineered mutation	UNP P20789
A	119	PHE	LEU	engineered mutation	UNP P20789
A	121	LEU	MET	engineered mutation	UNP P20789
A	124	ASP	GLU	engineered mutation	UNP P20789
A	143	LYS	ARG	engineered mutation	UNP P20789
A	150	GLU	ASP	engineered mutation	UNP P20789
A	161	VAL	ALA	engineered mutation	UNP P20789
A	167	LEU	ARG	engineered mutation	UNP P20789
A	213	LEU	ARG	engineered mutation	UNP P20789
A	234	LEU	VAL	engineered mutation	UNP P20789
A	235	ARG	LYS	engineered mutation	UNP P20789
A	240	LEU	VAL	engineered mutation	UNP P20789
A	253	ALA	ILE	engineered mutation	UNP P20789
A	260	ALA	ILE	engineered mutation	UNP P20789
A	262	ARG	ASN	engineered mutation	UNP P20789
A	263	ARG	LYS	engineered mutation	UNP P20789
A	305	ARG	HIS	engineered mutation	UNP P20789
A	332	VAL	CYS	engineered mutation	UNP P20789
A	342	ALA	PHE	engineered mutation	UNP P20789

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Chain	Residue	Modelled	Actual	Comment	Reference
A	354	SER	THR	engineered mutation	UNP P20789
A	358	VAL	PHE	engineered mutation	UNP P20789
A	362	ALA	SER	engineered mutation	UNP P20789

- Molecule 2 is (2 {S})-4-methyl-2-[[3-[5-(2-methylphenyl)-1,2,3,4-tetrazol-1-yl]-5-(5-methylthiophen-2-yl)phenyl]carbonylamino]pentanoic acid (CCD ID: A1I5W) (formula: C₂₆H₂₇N₅O₃S) (labeled as "Ligand of Interest" by depositor).

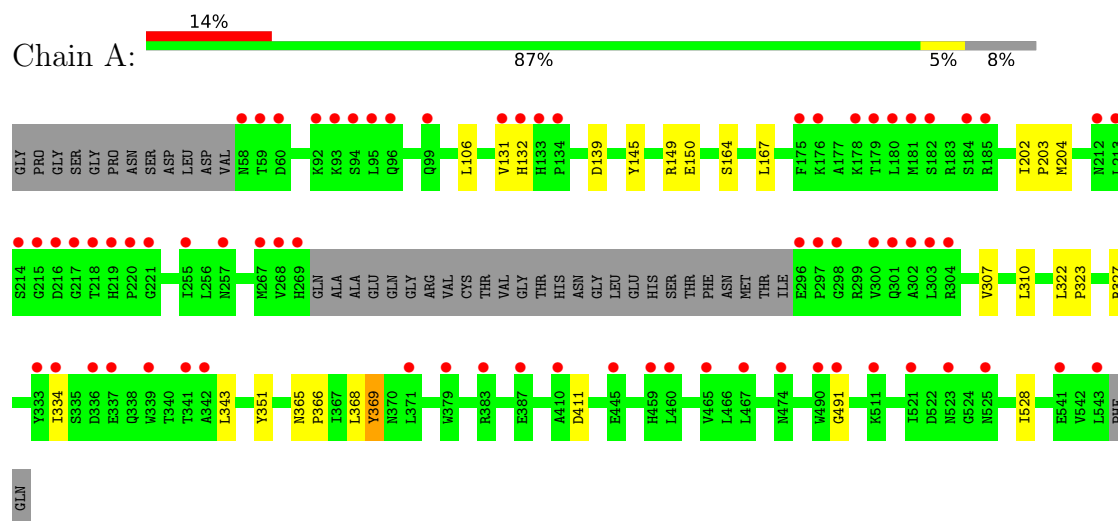


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			61	26	26	5	3	1		

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: Neurotensin receptor type 1, DARPin fusion



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.89Å 216.06Å 96.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.60 – 3.11 71.60 – 3.11	Depositor EDS
% Data completeness (in resolution range)	79.6 (71.60-3.11) 79.6 (71.60-3.11)	Depositor EDS
R_{merge}	1.00	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.312 , 0.325 0.301 , 0.303	Depositor DCC
R_{free} test set	571 reflections (3.85%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.6	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	0.81	EDS
Total number of atoms	6661	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% 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: A1I5W

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	0.52	0/3374	0.97	2/4638 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	CA-CB-CG	6.12	118.72	112.60
1	A	411	ASP	CA-CB-CG	5.22	117.82	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	3304	3296	3145	14	0
2	A	35	26	0	0	0
All	All	3339	3322	3145	14	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 2.

All (14) 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:365:ASN:OD1	1:A:366:PRO:HD3	1.67	0.94
1:A:131:VAL:O	1:A:132:HIS:C	2.56	0.48
1:A:491:GLY:HA2	1:A:528:ILE:HD12	1.96	0.48
1:A:365:ASN:O	1:A:368:LEU:N	2.48	0.47
1:A:322:LEU:HB3	1:A:323:PRO:HD3	1.97	0.46
1:A:202:ILE:N	1:A:203:PRO:CD	2.79	0.45
1:A:106:LEU:HD13	1:A:369:TYR:HD1	1.81	0.45
1:A:145:TYR:CZ	1:A:149:ARG:HD2	2.52	0.44
1:A:150:GLU:HG3	1:A:204:MET:HG3	1.99	0.44
1:A:167:LEU:HD21	1:A:307:VAL:HG22	1.99	0.44
1:A:164:SER:HA	1:A:310:LEU:HD21	2.01	0.43
1:A:327:ARG:CD	1:A:351:TYR:HA	2.50	0.42
1:A:334:ILE:HD13	1:A:343:LEU:HD21	2.02	0.42
1:A:365:ASN:O	1:A:366:PRO:C	2.63	0.40

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	456/500 (91%)	448 (98%)	8 (2%)	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	307/412 (74%)	306 (100%)	1 (0%)	86 86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	369	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	159	ASN
1	A	443	ASN
1	A	448	HIS
1	A	492	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A1I5W	A	1000	-	38,38,38	0.45	0	54,54,54	0.44	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
2	A1I5W	A	1000	-	-	1/28/28/28	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

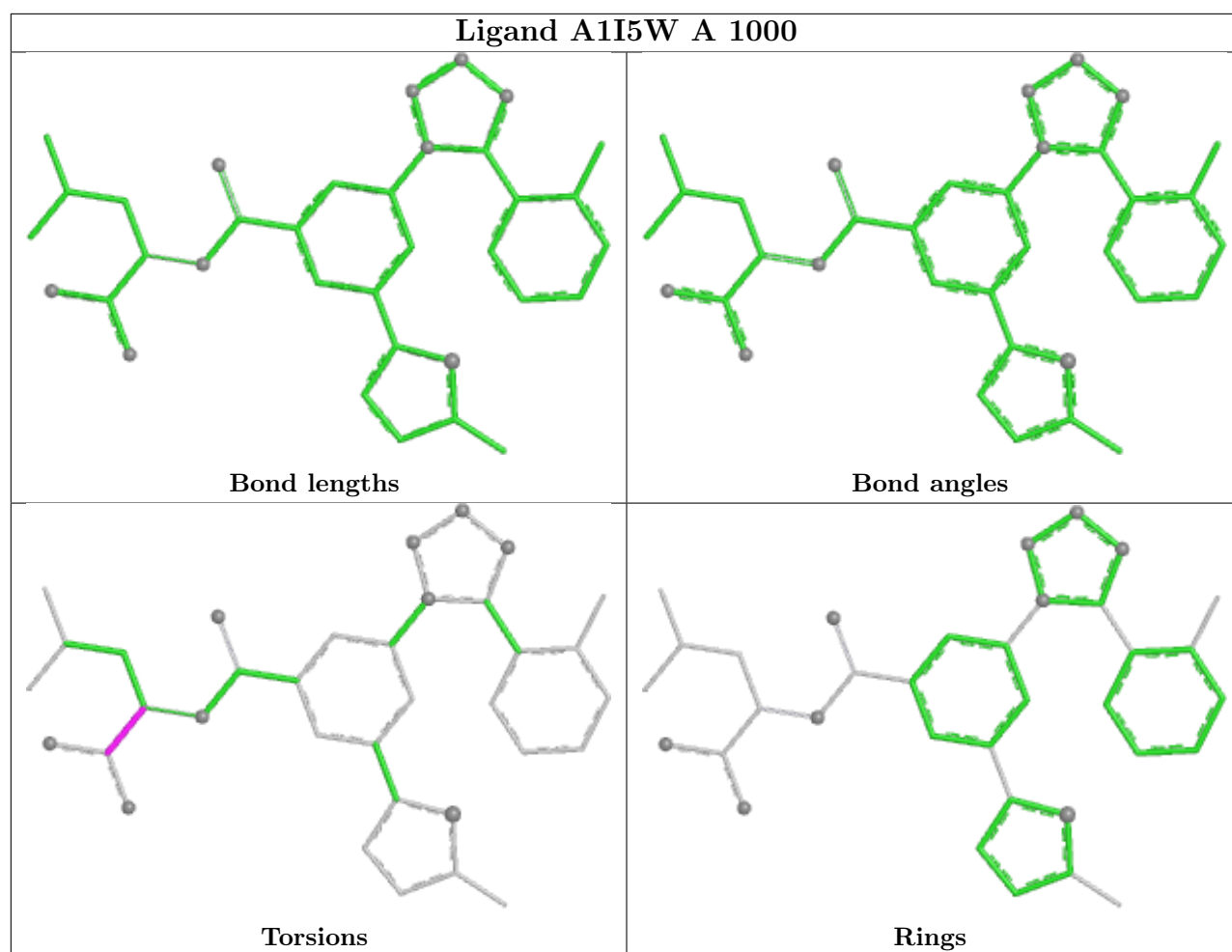
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1000	A1I5W	N27-C28-C33-O34

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	460/500 (92%)	1.09	71 (15%) 5 2	9, 25, 74, 100	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	PRO	7.2
1	A	298	GLY	7.2
1	A	296	GLU	7.1
1	A	267	MET	6.8
1	A	95	LEU	6.6
1	A	219	HIS	5.6
1	A	269	HIS	5.2
1	A	218	THR	5.1
1	A	94	SER	4.9
1	A	268	VAL	4.9
1	A	523	ASN	4.6
1	A	217	GLY	4.6
1	A	220	PRO	4.5
1	A	221	GLY	4.5
1	A	336	ASP	4.0
1	A	132	HIS	4.0
1	A	175	PHE	3.9
1	A	182	SER	3.8
1	A	179	THR	3.8
1	A	337	GLU	3.7
1	A	59	THR	3.6
1	A	543	LEU	3.6
1	A	379	TRP	3.6
1	A	134	PRO	3.5
1	A	180	LEU	3.5
1	A	490	TRP	3.5
1	A	96	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLY	3.1
1	A	181	MET	3.1
1	A	58	ASN	3.1
1	A	341	THR	3.0
1	A	459	HIS	3.0
1	A	445	GLU	2.9
1	A	525	ASN	2.9
1	A	131	VAL	2.9
1	A	333	TYR	2.8
1	A	301	GLN	2.8
1	A	216	ASP	2.7
1	A	184	SER	2.7
1	A	371	LEU	2.7
1	A	176	LYS	2.7
1	A	303	LEU	2.7
1	A	339	TRP	2.6
1	A	255	ILE	2.5
1	A	214	SER	2.5
1	A	99	GLN	2.5
1	A	300	VAL	2.5
1	A	334	ILE	2.5
1	A	304	ARG	2.5
1	A	491	GLY	2.4
1	A	212	ASN	2.4
1	A	387	GLU	2.4
1	A	93	LYS	2.3
1	A	474	ASN	2.3
1	A	521	ILE	2.3
1	A	511	LYS	2.3
1	A	465	VAL	2.3
1	A	460	LEU	2.2
1	A	342	ALA	2.2
1	A	467	LEU	2.2
1	A	213	LEU	2.1
1	A	92	LYS	2.1
1	A	383	ARG	2.1
1	A	410	ALA	2.1
1	A	541	GLU	2.1
1	A	60	ASP	2.1
1	A	257	ASN	2.1
1	A	302	ALA	2.1
1	A	185	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	178	LYS	2.0
1	A	133	HIS	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](#)

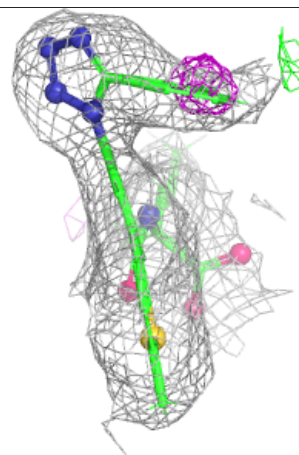
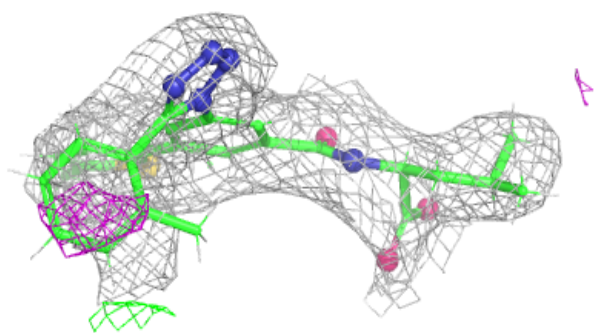
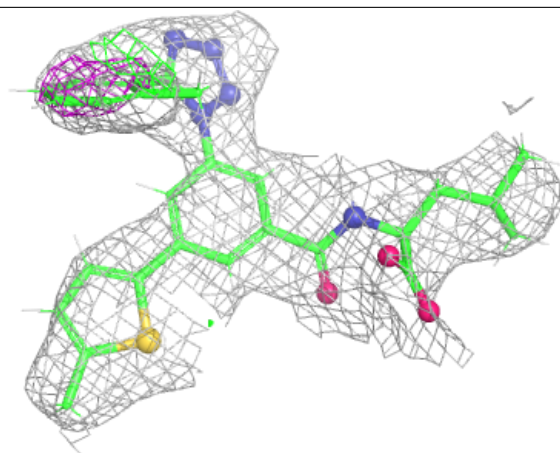
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	A1I5W	A	1000	35/35	0.88	0.14	13,15,17,18	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 A1I5W A 1000:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.