



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2021 – 06:07 PM GMT

PDB ID : 6Z4S
Title : Crystal structure of the neurotensin receptor 1 (NTSR1-H4bmx) in complex with the small molecule inverse agonist SR48692
Authors : Deluigi, M.; Klipp, A.; Hilge, M.; Merklinger, L.; Klenk, C.; Plueckthun, A.
Deposited on : 2020-05-25
Resolution : 2.71 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 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 : 2.16
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) : 2.16

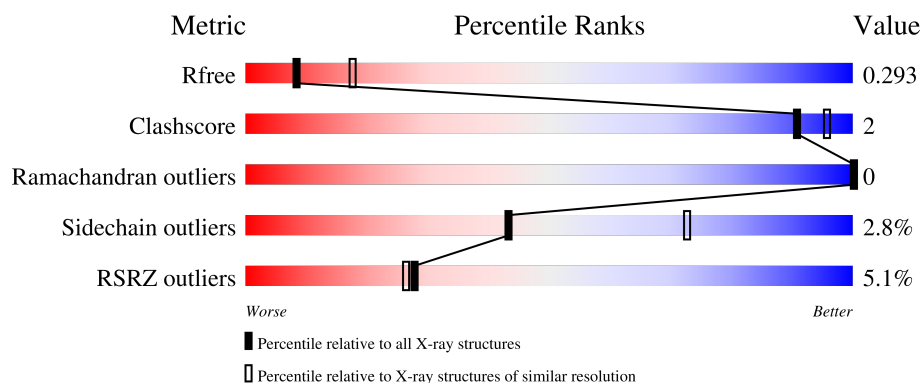
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	AAA	482	<div> <div>5%</div> <div>88%</div> <div>5%</div> <div>7%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6617 atoms, of which 3287 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,HRV 3C protease recognition sequence.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	448	Total	C	H	N	O	S	193	0	0
			6544	2140	3256	542	594	12			

There are 53 discrepancies between the modelled and reference sequences:

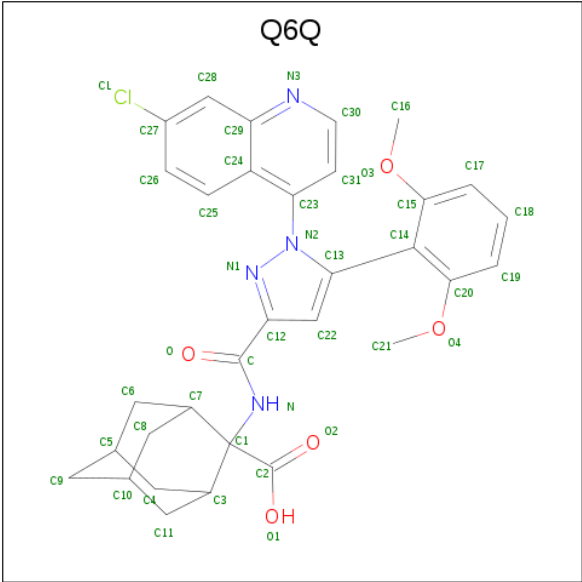
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	46	GLY	-	expression tag	UNP P20789
AAA	47	PRO	-	expression tag	UNP P20789
AAA	48	GLY	-	expression tag	UNP P20789
AAA	49	SER	-	expression tag	UNP P20789
AAA	83	GLY	SER	engineered mutation	UNP P20789
AAA	86	LEU	ALA	engineered mutation	UNP P20789
AAA	101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

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	?	-	VAL	deletion	UNP P20789
AAA	?	-	CYS	deletion	UNP P20789
AAA	?	-	THR	deletion	UNP P20789
AAA	?	-	VAL	deletion	UNP P20789
AAA	?	-	GLY	deletion	UNP P20789
AAA	?	-	THR	deletion	UNP P20789
AAA	?	-	HIS	deletion	UNP P20789
AAA	?	-	ASN	deletion	UNP P20789
AAA	?	-	GLY	deletion	UNP P20789
AAA	?	-	LEU	deletion	UNP P20789
AAA	?	-	GLU	deletion	UNP P20789
AAA	?	-	HIS	deletion	UNP P20789
AAA	?	-	SER	deletion	UNP P20789
AAA	?	-	THR	deletion	UNP P20789
AAA	305	ARG	HIS	engineered mutation	UNP P20789
AAA	332	VAL	CYS	engineered mutation	UNP P20789
AAA	342	ALA	PHE	engineered mutation	UNP P20789
AAA	354	SER	THR	engineered mutation	UNP P20789
AAA	372	ALA	-	linker	UNP P20789
AAA	373	GLU	-	linker	UNP P20789
AAA	374	ASP	-	linker	UNP P20789
AAA	375	LEU	-	linker	UNP P20789
AAA	376	VAL	-	linker	UNP P20789
AAA	377	GLU	-	linker	UNP P20789
AAA	378	ASP	-	linker	UNP P20789
AAA	379	TRP	-	linker	UNP P20789
AAA	380	GLU	-	linker	UNP P20789

- Molecule 2 is 2-[[1-(7-chloranylquinolin-4-yl)-5-(2,6-dimethoxyphenyl)pyrazol-3-yl]carbonylamino]adamantane-2-carboxylic acid (three-letter code: Q6Q) (formula: C₃₂H₃₁ClN₄O₅) (labeled as "Ligand of Interest" by depositor).

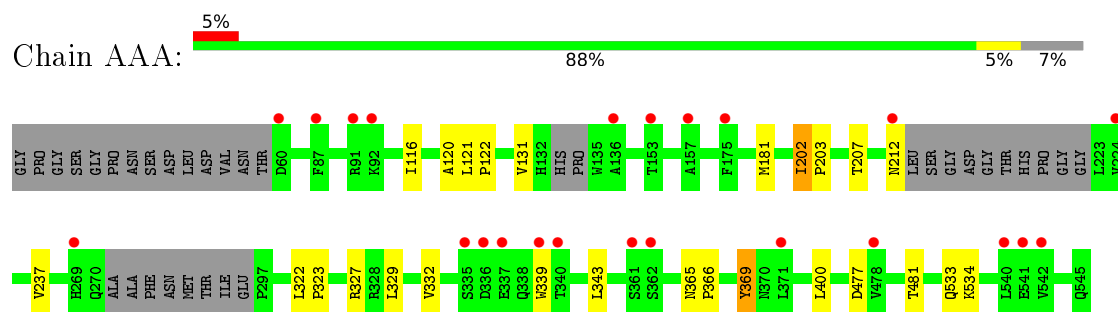


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	H	N	O		
2	AAA	1	73	32	1	31	4	5	1	0

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,HRV 3C protease recognition sequence



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.52Å 77.73Å 158.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 2.71 29.34 – 2.71	Depositor EDS
% Data completeness (in resolution range)	68.4 (29.35-2.71) 68.5 (29.34-2.71)	Depositor EDS
R_{merge}	0.53	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.273 , 0.289 0.276 , 0.293	Depositor DCC
R_{free} test set	552 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 15.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	6617	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: Q6Q

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	AAA	0.68	0/3357	0.70	0/4603

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	AAA	3288	3256	3136	11	0
2	AAA	42	31	0	1	0
All	All	3330	3287	3136	11	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 (11) 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:AAA:366:PRO:HA	1:AAA:369:TYR:CE1	2.46	0.50
1:AAA:322:LEU:HB3	1:AAA:323:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:202:ILE:N	1:AAA:203:PRO:CD	2.79	0.46
1:AAA:116:ILE:O	1:AAA:120:ALA:HB3	2.15	0.46
1:AAA:207:THR:HG21	1:AAA:237:VAL:HG21	2.00	0.44
1:AAA:365:ASN:HB3	1:AAA:366:PRO:HD3	2.00	0.44
1:AAA:121:LEU:HB3	1:AAA:122:PRO:HD3	2.00	0.43
1:AAA:327:ARG:NH2	2:AAA:4000:Q6Q:O1	2.35	0.42
1:AAA:477:ASP:OD1	1:AAA:481:THR:N	2.51	0.41
1:AAA:212:ASN:N	1:AAA:212:ASN:OD1	2.54	0.41
1:AAA:329:LEU:HA	1:AAA:332:VAL:HG12	2.03	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	AAA	440/482 (91%)	423 (96%)	17 (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	AAA	316/398 (79%)	307 (97%)	9 (3%)	43	73

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	131	VAL
1	AAA	181	MET
1	AAA	202	ILE
1	AAA	339	TRP
1	AAA	343	LEU
1	AAA	369	TYR
1	AAA	400	LEU
1	AAA	533	GLN
1	AAA	534	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	Q6Q	AAA	4000	-	43,48,48	0.31	0	56,73,73	0.41	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	Q6Q	AAA	4000	-	-	1/18/59/59	0/8/7/7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

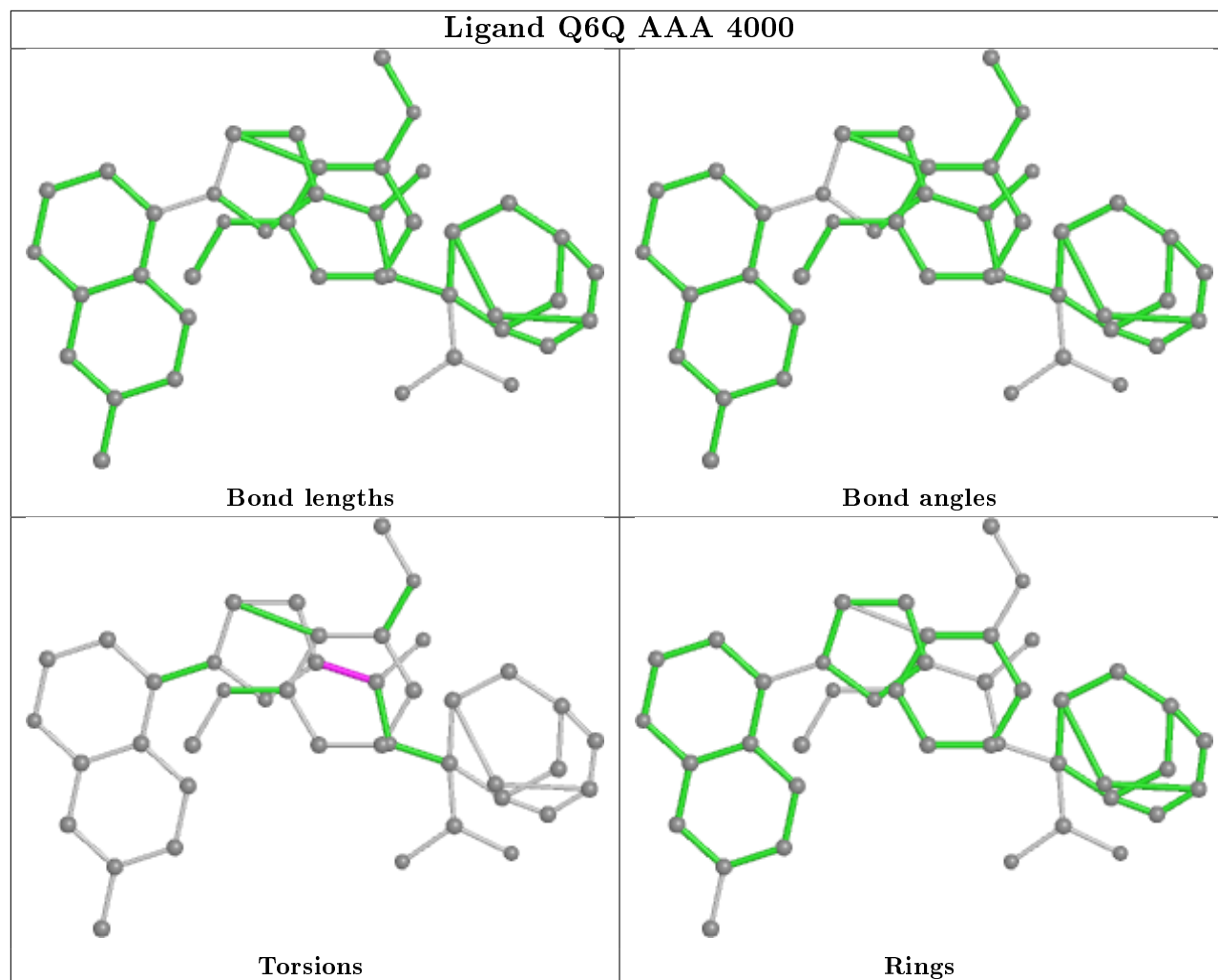
Mol	Chain	Res	Type	Atoms
2	AAA	4000	Q6Q	O-C-C12-C22

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	4000	Q6Q	1	0

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	AAA	448/482 (92%)	0.44	23 (5%)	28 26	32, 41, 63, 80	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	339	TRP	4.4
1	AAA	224	VAL	4.1
1	AAA	212	ASN	4.0
1	AAA	87	PHE	3.9
1	AAA	542	VAL	2.9
1	AAA	337	GLU	2.9
1	AAA	478	VAL	2.9
1	AAA	541	GLU	2.8
1	AAA	153	THR	2.7
1	AAA	335	SER	2.7
1	AAA	175	PHE	2.7
1	AAA	361	SER	2.6
1	AAA	91	ARG	2.6
1	AAA	362	SER	2.6
1	AAA	336	ASP	2.5
1	AAA	371	LEU	2.5
1	AAA	92	LYS	2.3
1	AAA	60	ASP	2.3
1	AAA	136	ALA	2.1
1	AAA	540	LEU	2.1
1	AAA	157	ALA	2.1
1	AAA	269	HIS	2.1
1	AAA	340	THR	2.1

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](#)

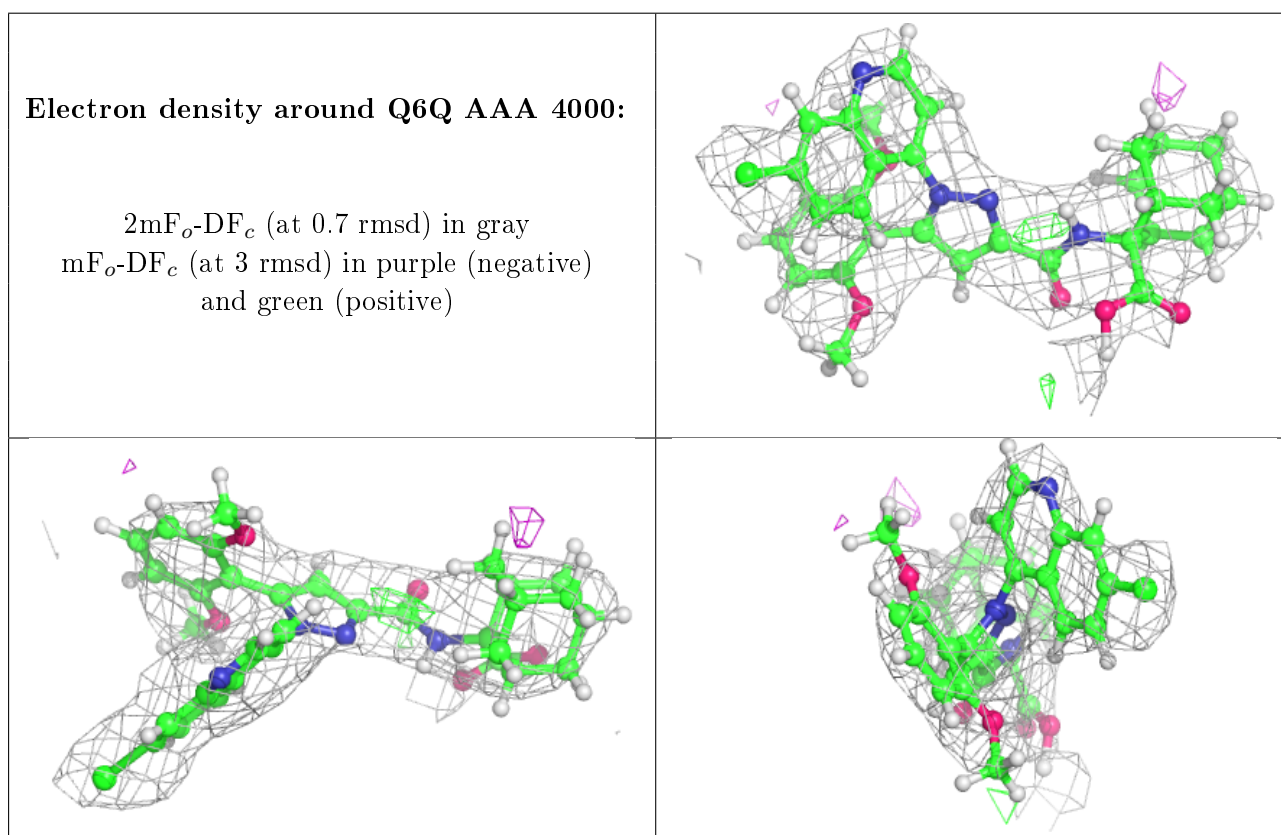
There are no monosaccharides in this entry.

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
2	Q6Q	AAA	4000	42/42	0.89	0.23	54,55,57,75	1

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.



6.5 Other polymers

There are no such residues in this entry.