



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2026 – 04:32 pm BST

PDB ID : 9HZ3 / pdb_00009hz3
Title : PCSK9 AZD0780 complex
Authors : Johansson, P.
Deposited on : 2025-01-13
Resolution : 1.43 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 : 1.8.4, CSD as541be (2020)
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

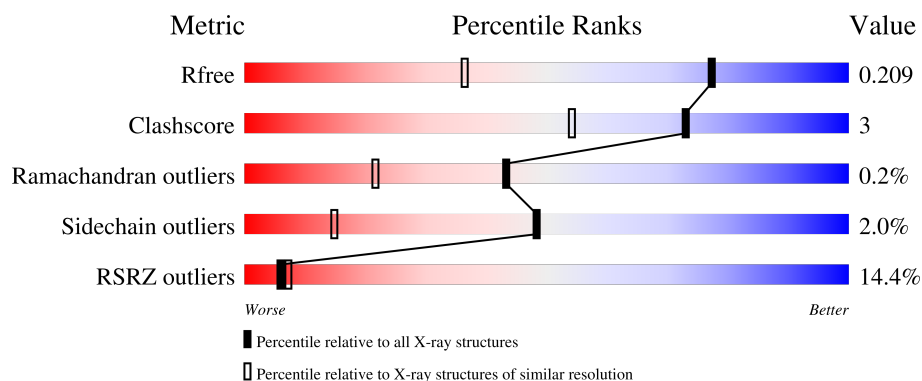
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.43 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	3234 (1.46-1.42)
Clashscore	190562	3289 (1.46-1.42)
Ramachandran outliers	187476	3248 (1.46-1.42)
Sidechain outliers	187428	3248 (1.46-1.42)
RSRZ outliers	180081	3234 (1.46-1.42)

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	152	<div> <div>7%</div> <div>58%</div> <div>39%</div> </div>
2	B	553	<div> <div>13%</div> <div>78%</div> <div>7%</div> <div>15%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4719 atoms, of which 0 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			740	474	133	131	2			

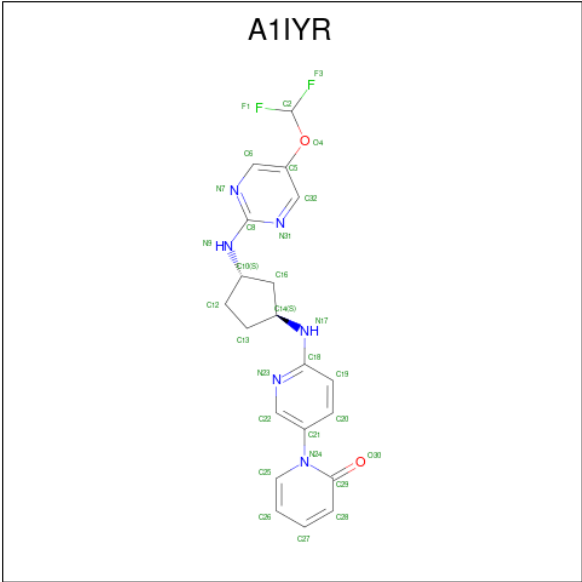
- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	472	Total	C	N	O	S	0	0	0
			3506	2167	645	663	31			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	474	ILE	VAL	variant	UNP Q8NBP7
B	670	GLU	GLY	variant	UNP Q8NBP7
B	693	GLU	-	expression tag	UNP Q8NBP7
B	694	ASN	-	expression tag	UNP Q8NBP7
B	695	LEU	-	expression tag	UNP Q8NBP7
B	696	TYR	-	expression tag	UNP Q8NBP7
B	697	PHE	-	expression tag	UNP Q8NBP7
B	698	GLN	-	expression tag	UNP Q8NBP7
B	699	GLY	-	expression tag	UNP Q8NBP7
B	700	HIS	-	expression tag	UNP Q8NBP7
B	701	HIS	-	expression tag	UNP Q8NBP7
B	702	HIS	-	expression tag	UNP Q8NBP7
B	703	HIS	-	expression tag	UNP Q8NBP7
B	704	HIS	-	expression tag	UNP Q8NBP7
B	705	HIS	-	expression tag	UNP Q8NBP7

- Molecule 3 is 1-[6-[(1 {S},3 {S})-3-[[5-[bis(fluoranyl)methoxy]pyrimidin-2-yl]amino]cyclopentyl]amino]pyridin-3-yl]pyridin-2-one (CCD ID: A1IYR) (formula: C₂₀H₂₀F₂N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			30	20	2	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	B	343	Total	O	0	0
			343	343		

- Molecule 1: Proprotein convertase subtilisin/kexin type 9



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.97Å 70.72Å 149.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.89 – 1.43 74.89 – 1.43	Depositor EDS
% Data completeness (in resolution range)	79.3 (74.89-1.43) 79.3 (74.89-1.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.43Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.193 , 0.213 0.187 , 0.209	Depositor DCC
R_{free} test set	4835 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4719	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: A1IYR

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	0.82	0/757	1.00	2/1023 (0.2%)
2	B	0.90	2/3567 (0.1%)	1.02	5/4839 (0.1%)
All	All	0.89	2/4324 (0.0%)	1.02	7/5862 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	330	ALA	CA-C	7.05	1.61	1.52
2	B	201	MET	SD-CE	-6.33	1.63	1.79

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	186	ASP	CA-CB-CG	9.70	122.30	112.60
2	B	224	ASP	CA-CB-CG	7.64	120.24	112.60
2	B	320	ASP	CA-CB-CG	5.66	118.25	112.60
1	A	132	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	118	LEU	N-CA-C	-5.08	105.32	112.12
2	B	644	VAL	N-CA-C	5.06	115.62	109.30
2	B	330	ALA	O-C-N	-5.04	116.67	121.20

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	740	0	750	1	0
2	B	3506	0	3433	24	0
3	B	30	0	0	0	0
4	A	100	0	0	1	0
4	B	343	0	0	3	0
All	All	4719	0	4183	25	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 3.

All (25) 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:120:PRO:HD2	4:A:246:HOH:O	1.72	0.90
2:B:476:ARG:HH21	2:B:503:GLN:HE22	1.22	0.82
2:B:186:ASP:OD2	2:B:230:LEU:HD12	1.84	0.78
2:B:223:CYS:HG	2:B:255:CYS:HG	0.81	0.71
2:B:201:MET:HE3	2:B:248:ARG:HH21	1.57	0.70
2:B:398:MET:HE3	2:B:444:LEU:HD21	1.79	0.64
2:B:185:LEU:HD11	2:B:271:ILE:HD11	1.84	0.60
2:B:273:LYS:HG3	4:B:1119:HOH:O	2.02	0.58
2:B:548:THR:HG22	2:B:596:ILE:HG22	1.83	0.58
2:B:557:HIS:CE1	2:B:602:HIS:HB2	2.39	0.57
2:B:201:MET:CE	2:B:248:ARG:HH21	2.17	0.57
2:B:499:ARG:HG2	2:B:512:HIS:HE1	1.69	0.56
2:B:189:ILE:CD1	2:B:200:VAL:HG11	2.37	0.55
2:B:476:ARG:NH2	2:B:503:GLN:HE22	1.98	0.53
2:B:201:MET:HE3	2:B:248:ARG:HD3	1.91	0.52
2:B:423:VAL:HG22	4:B:1097:HOH:O	2.10	0.51
2:B:549:ARG:HG2	2:B:589:VAL:HG22	1.94	0.49
2:B:548:THR:HG22	2:B:596:ILE:CG2	2.44	0.47
2:B:273:LYS:NZ	4:B:903:HOH:O	2.48	0.46
2:B:398:MET:HE3	2:B:444:LEU:CD2	2.45	0.46
2:B:367:ASP:HA	2:B:381:SER:OG	2.16	0.46
2:B:476:ARG:HH21	2:B:503:GLN:NE2	2.03	0.43
2:B:206:GLU:HG2	2:B:251:ARG:HB3	1.99	0.43
2:B:566:TRP:CD2	2:B:571:LEU:HD11	2.54	0.43
2:B:201:MET:CE	2:B:248:ARG:HD3	2.50	0.42

There are no symmetry-related clashes.

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	90/152 (59%)	88 (98%)	2 (2%)	0	100	100
2	B	454/553 (82%)	444 (98%)	9 (2%)	1 (0%)	43	22
All	All	544/705 (77%)	532 (98%)	11 (2%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	280	VAL

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	79/127 (62%)	78 (99%)	1 (1%)	61	29
2	B	378/443 (85%)	370 (98%)	8 (2%)	47	13
All	All	457/570 (80%)	448 (98%)	9 (2%)	48	15

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

Mol	Chain	Res	Type
1	A	96	ARG
2	B	167	ARG
2	B	178	SER
2	B	375	CYS
2	B	499	ARG

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Mol	Chain	Res	Type
2	B	567	GLU
2	B	606	LEU
2	B	619	GLN
2	B	645	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
2	B	302	GLN
2	B	382	GLN
2	B	387	GLN
2	B	503	GLN
2	B	512	HIS
2	B	553	HIS
2	B	621	GLN

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
3	A1IYR	B	801	-	33,33,33	1.27	3 (9%)	42,45,45	1.92	13 (30%)

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	A1IYR	B	801	-	-	0/16/25/25	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	A1IYR	C8-N9	5.14	1.41	1.34
3	B	801	A1IYR	C28-C29	2.96	1.51	1.43
3	B	801	A1IYR	C18-N17	2.14	1.41	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	A1IYR	O30-C29-N24	4.59	124.47	119.94
3	B	801	A1IYR	N9-C8-N31	4.09	123.62	116.65
3	B	801	A1IYR	N31-C8-N7	-3.76	122.47	126.43
3	B	801	A1IYR	N17-C18-N23	3.71	122.97	116.84
3	B	801	A1IYR	C19-C18-N17	-3.30	114.97	120.89
3	B	801	A1IYR	C8-N9-C10	-3.04	119.18	124.31
3	B	801	A1IYR	C6-N7-C8	2.89	120.25	115.88
3	B	801	A1IYR	C16-C10-N9	-2.56	105.87	112.44
3	B	801	A1IYR	C28-C29-N24	2.44	115.87	114.46
3	B	801	A1IYR	C5-O4-C2	-2.41	109.92	119.05
3	B	801	A1IYR	C12-C10-N9	2.40	116.87	111.76
3	B	801	A1IYR	C20-C21-N24	2.18	122.45	119.63
3	B	801	A1IYR	C25-N24-C29	-2.13	121.73	122.74

There are no chirality outliers.

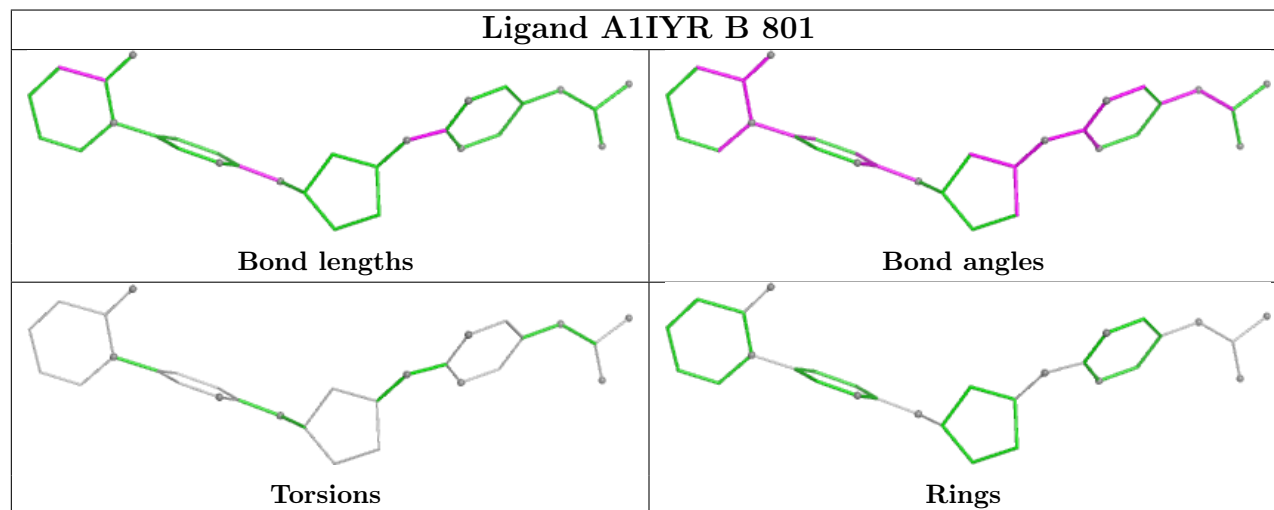
There are no torsion outliers.

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	92/152 (60%)	0.32	10 (10%)	10 12	13, 19, 34, 44	0
2	B	472/553 (85%)	0.61	71 (15%)	5 7	11, 20, 44, 64	0
All	All	564/705 (80%)	0.56	81 (14%)	6 7	11, 20, 42, 64	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	515	PHE	8.4
2	B	615	ILE	7.4
2	B	505	GLY	5.8
2	B	571	LEU	5.7
2	B	585	PRO	5.4
2	B	331	PRO	5.2
2	B	469	ARG	5.0
2	B	220	ALA	4.6
2	B	471	ALA	4.5
2	B	672	VAL	4.4
2	B	671	ALA	4.3
2	B	556	GLY	4.2
2	B	534	CYS	4.1
2	B	167	ARG	4.0
2	B	554	GLN	4.0
2	B	530	PRO	4.0
1	A	117	GLY	3.9
2	B	553	HIS	3.9
2	B	533	ASN	3.8
1	A	61	THR	3.8
2	B	619	GLN	3.7
2	B	153	SER	3.6
2	B	569	GLU	3.5
1	A	85	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	658	SER	3.5
1	A	108	LEU	3.4
2	B	502	ALA	3.3
2	B	470	MET	3.3
2	B	516	GLY	3.3
2	B	602	HIS	3.3
2	B	643	HIS	3.2
2	B	620	GLU	3.2
2	B	178	SER	3.2
2	B	453	TRP	3.2
2	B	568	VAL	3.2
2	B	166	TYR	3.2
2	B	517	GLY	3.2
2	B	555	GLN	3.1
2	B	223	CYS	3.0
2	B	504	GLY	2.9
2	B	503	GLN	2.9
1	A	118	LEU	2.9
2	B	303	ARG	2.8
2	B	570	ASP	2.8
2	B	645	LEU	2.8
1	A	104	ARG	2.8
1	A	119	LEU	2.7
2	B	542	ALA	2.7
2	B	194	ARG	2.6
2	B	491	ARG	2.6
2	B	374	ASP	2.6
1	A	116	HIS	2.6
2	B	472	THR	2.5
2	B	222	LYS	2.5
2	B	682	ARG	2.5
2	B	640	GLY	2.5
2	B	501	GLU	2.5
2	B	567	GLU	2.5
2	B	221	SER	2.5
2	B	641	THR	2.5
2	B	507	LEU	2.4
2	B	514	ALA	2.4
2	B	557	HIS	2.4
2	B	605	GLY	2.4
2	B	211	GLU	2.4
1	A	96	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	468	THR	2.3
2	B	548	THR	2.3
2	B	245	ALA	2.2
2	B	549	ARG	2.2
2	B	198	GLY	2.2
2	B	592	ARG	2.2
1	A	84	GLU	2.2
2	B	601	CYS	2.2
2	B	369	ILE	2.1
2	B	535	SER	2.1
2	B	189	ILE	2.1
2	B	547	GLY	2.1
2	B	499	ARG	2.0
2	B	494	LYS	2.0
2	B	375	CYS	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](#)

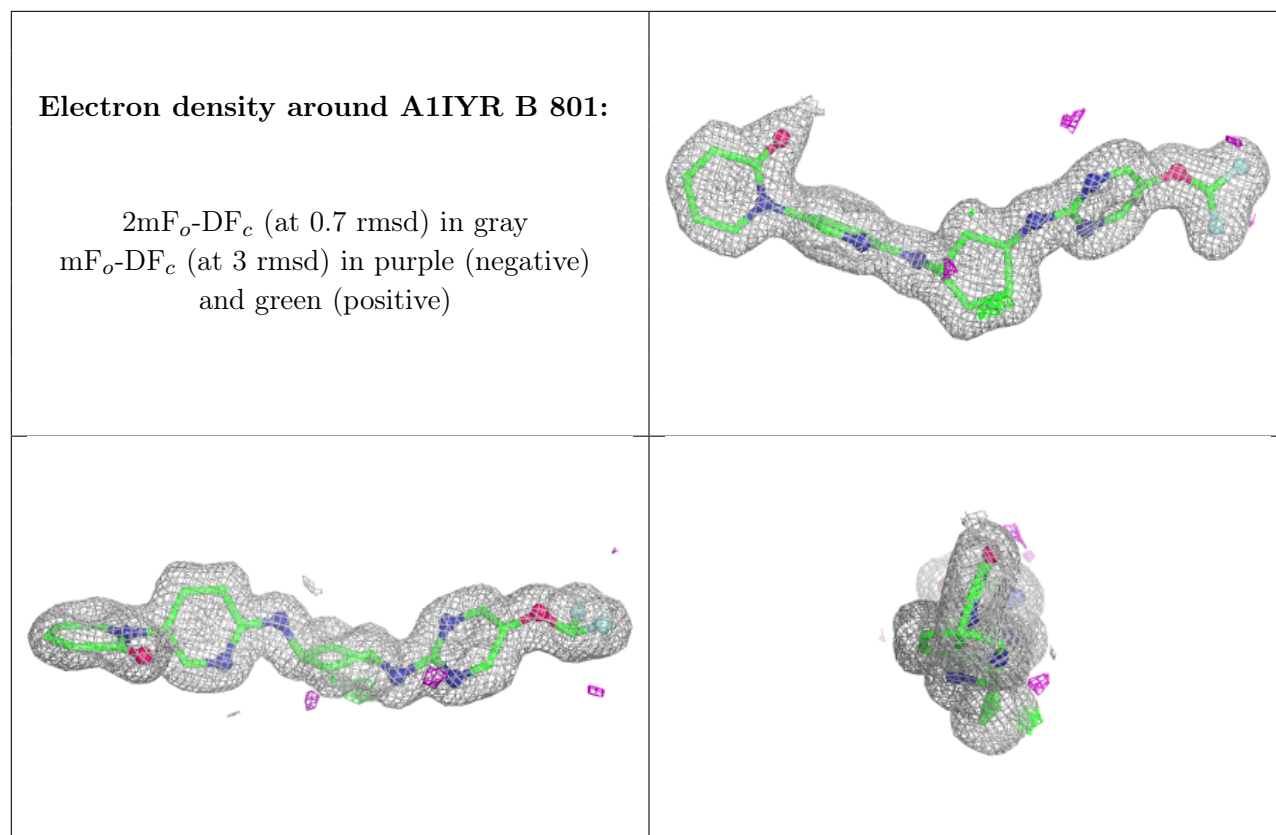
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
3	A1IYR	B	801	30/30	0.96	0.08	19,24,29,29	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.