



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2026 – 04:27 pm BST

PDB ID : 9SZY / pdb_00009szy
Title : PCSK9 CTD fragment structure
Authors : Johansson, P.
Deposited on : 2025-10-16
Resolution : 1.76 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

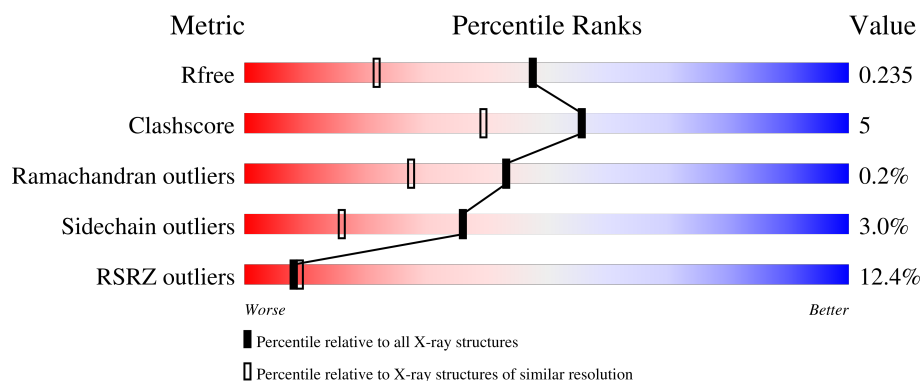
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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>3%</div> <div>59%</div> <div>39%</div> </div>
2	B	692	<div> <div>10%</div> <div>61%</div> <div>9%</div> <div>30%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4692 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			

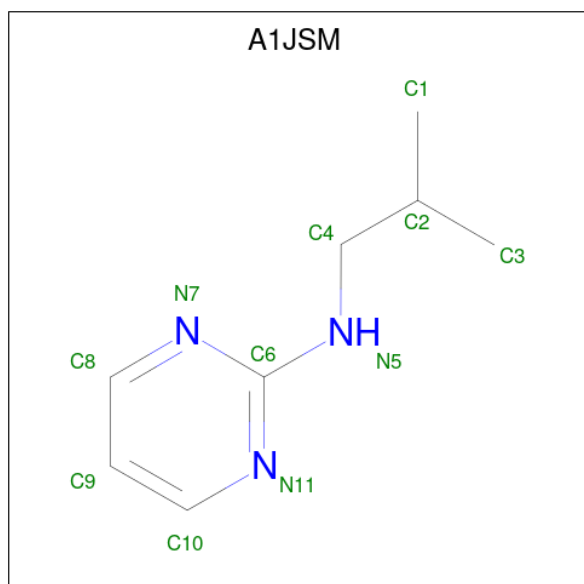
- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	487	Total	C	N	O	S	0	1	0
			3616	2229	667	688	32			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	474	ILE	VAL	variant	UNP Q8NBP7

- Molecule 3 is {N}-(2-methylpropyl)pyrimidin-2-amine (CCD ID: A1JSM) (formula: C₈H₁₃N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			11	8	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	254	Total	O	0	0
			254	254		

- 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	62.60Å 70.12Å 148.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.02 – 1.76 74.02 – 1.76	Depositor EDS
% Data completeness (in resolution range)	59.6 (74.02-1.76) 59.6 (74.02-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.76Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.198 , 0.236 0.192 , 0.235	Depositor DCC
R_{free} test set	1986 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4692	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: A1JSM

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	0.67	0/757	0.98	0/1023
2	B	0.73	0/3681	1.01	2/4996 (0.0%)
All	All	0.72	0/4438	1.01	2/6019 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	418	PHE	CA-CB-CG	-5.10	108.70	113.80
2	B	336	VAL	N-CA-C	5.09	115.18	107.75

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	3616	0	3543	34	0
3	B	11	0	0	1	0
4	A	71	0	0	0	0
4	B	254	0	0	1	0
All	All	4692	0	4293	35	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 5.

All (35) 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)
2:B:626:CYS:HG	2:B:678:CYS:HG	0.99	0.98
2:B:641:THR:HB	2:B:643:HIS:CE1	2.03	0.94
2:B:503:GLN:NE2	2:B:510:ARG:HH12	1.74	0.84
2:B:499:ARG:HD3	2:B:512:HIS:HE1	1.47	0.79
2:B:562:CYS:HG	2:B:588:CYS:HG	0.83	0.77
2:B:638:LEU:HB2	2:B:673:THR:HB	1.77	0.67
2:B:186:ASP:OD2	2:B:230:LEU:HD12	1.96	0.65
2:B:185:LEU:HD11	2:B:271:ILE:HD11	1.83	0.60
2:B:608:CYS:HG	2:B:679:CYS:HG	0.86	0.60
2:B:200:VAL:HG22	2:B:247:MET:HB2	1.83	0.59
2:B:499:ARG:HD3	2:B:512:HIS:CE1	2.36	0.57
2:B:201:MET:HE3	2:B:248:ARG:HD3	1.87	0.57
2:B:177:GLY:HA2	2:B:401:SER:HB2	1.87	0.56
2:B:612:GLU:HG2	2:B:675:VAL:HG22	1.89	0.55
2:B:503:GLN:NE2	2:B:510:ARG:NH1	2.52	0.54
2:B:643:HIS:HD2	2:B:658:SER:HB2	1.74	0.53
2:B:638:LEU:HD13	2:B:675:VAL:HG21	1.90	0.53
2:B:179:LEU:HD22	2:B:401:SER:HA	1.90	0.52
2:B:206:GLU:HG2	2:B:251:ARG:HB3	1.95	0.48
2:B:221:SER:O	2:B:373:SER:OG	2.31	0.48
2:B:423:VAL:HG22	4:B:900:HOH:O	2.14	0.47
2:B:477:CYS:HG	2:B:526:CYS:CB	2.27	0.47
2:B:503:GLN:HE21	2:B:510:ARG:HH12	1.60	0.46
2:B:563:SER:HB2	2:B:597:HIS:HB2	1.97	0.45
2:B:186:ASP:OD1	2:B:226:HIS:ND1	2.43	0.44
2:B:548:THR:HG22	2:B:596:ILE:HG22	2.00	0.44
2:B:465:SER:HB3	2:B:473:ALA:HB2	2.01	0.43
2:B:399:MET:HE2	2:B:445:PRO:HG3	2.00	0.43
2:B:435:VAL:HG12	2:B:461:TRP:CH2	2.54	0.43
1:A:98:LEU:HB2	1:A:137:LEU:HD11	2.00	0.43
2:B:185:LEU:O	2:B:288:PRO:HD2	2.19	0.42
2:B:503:GLN:HE21	2:B:510:ARG:NH1	2.17	0.42
2:B:453:TRP:CZ2	2:B:530:PRO:HD2	2.54	0.41
2:B:562:CYS:SG	3:B:701:A1JSM:C8	3.09	0.41
2:B:608:CYS:HG	2:B:679:CYS:CB	2.29	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	90/152 (59%)	87 (97%)	3 (3%)	0	100	100
2	B	474/692 (68%)	466 (98%)	7 (2%)	1 (0%)	43	27
All	All	564/844 (67%)	553 (98%)	10 (2%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	280	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	79/127 (62%)	78 (99%)	1 (1%)	61	46
2	B	389/557 (70%)	376 (97%)	13 (3%)	33	13
All	All	468/684 (68%)	454 (97%)	14 (3%)	36	16

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
2	B	179	LEU
2	B	277	VAL
2	B	333	VAL
2	B	375	CYS

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Mol	Chain	Res	Type
2	B	398	MET
2	B	421	LYS
2	B	449	HIS
2	B	491	ARG
2	B	499	ARG
2	B	546	MET
2	B	619	GLN
2	B	623	THR
2	B	638	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
2	B	342	GLN
2	B	382	GLN
2	B	387	GLN
2	B	503	GLN
2	B	512	HIS
2	B	513	ASN
2	B	613	HIS
2	B	619	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	A1JSM	B	701	-	11,11,11	1.55	1 (9%)	13,13,13	2.59	5 (38%)

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	A1JSM	B	701	-	-	0/5/5/5	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	701	A1JSM	C6-N5	4.95	1.42	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	A1JSM	C4-N5-C6	-6.53	114.06	123.53
3	B	701	A1JSM	N11-C6-N7	-3.79	122.43	126.43
3	B	701	A1JSM	N5-C6-N7	3.32	122.20	117.22
3	B	701	A1JSM	C10-N11-C6	2.75	117.89	115.45
3	B	701	A1JSM	C8-N7-C6	2.06	117.28	115.45

There are no chirality outliers.

There are no torsion outliers.

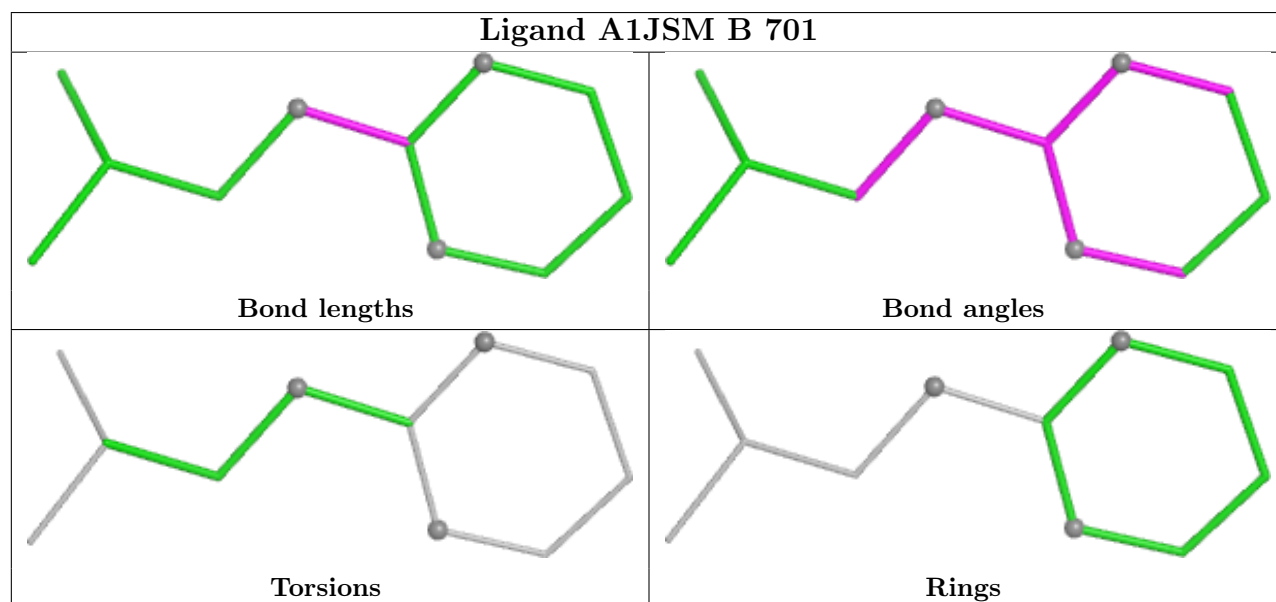
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	A1JSM	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	A	92/152 (60%)	0.30	5 (5%) 31 35	25, 33, 48, 57	0
2	B	487/692 (70%)	0.75	67 (13%) 6 7	13, 37, 65, 84	1 (0%)
All	All	579/844 (68%)	0.68	72 (12%) 8 9	13, 36, 62, 84	1 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	571	LEU	5.8
2	B	671	ALA	5.7
2	B	641	THR	5.2
2	B	220	ALA	4.8
2	B	585	PRO	4.7
2	B	616	PRO	4.5
2	B	505	GLY	4.5
2	B	544	ALA	4.5
2	B	531	GLN	4.4
2	B	672	VAL	4.2
2	B	546	MET	4.1
2	B	448	THR	4.0
2	B	449	HIS	3.9
2	B	515	PHE	3.9
2	B	223	CYS	3.8
2	B	471	ALA	3.8
2	B	177	GLY	3.7
2	B	568	VAL	3.7
2	B	642	SER	3.7
2	B	553	HIS	3.6
2	B	178	SER	3.5
2	B	615	ILE	3.4
2	B	569	GLU	3.4
2	B	435	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	453	TRP	3.4
2	B	176	GLY	3.3
2	B	640	GLY	3.3
2	B	179	LEU	3.2
2	B	554	GLN	3.1
2	B	447	SER	3.1
2	B	547	GLY	3.0
2	B	620	GLU	3.0
2	B	245	ALA	3.0
2	B	375	CYS	3.0
2	B	644	VAL	3.0
2	B	619	GLN	3.0
2	B	530	PRO	2.9
2	B	470	MET	2.9
2	B	422	ASP	2.8
2	B	331	PRO	2.8
2	B	469	ARG	2.7
2	B	643	HIS	2.6
1	A	61	THR	2.5
2	B	496	ARG	2.5
2	B	153	SER	2.5
1	A	117	GLY	2.5
2	B	468	THR	2.5
2	B	659	ARG	2.5
2	B	614	GLY	2.4
2	B	426	GLU	2.4
2	B	167	ARG	2.4
2	B	221	SER	2.4
2	B	477	CYS	2.4
2	B	545	SER	2.4
1	A	132	GLU	2.3
2	B	474	ILE	2.3
2	B	428	TRP	2.3
2	B	473	ALA	2.3
2	B	502	ALA	2.3
2	B	189	ILE	2.3
2	B	504	GLY	2.3
2	B	604	PRO	2.2
1	A	119	LEU	2.2
2	B	194	ARG	2.2
2	B	562	CYS	2.2
2	B	452	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	212	ASP	2.1
2	B	656	VAL	2.1
2	B	501	GLU	2.0
2	B	333	VAL	2.0
1	A	108	LEU	2.0
2	B	542	ALA	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](#)

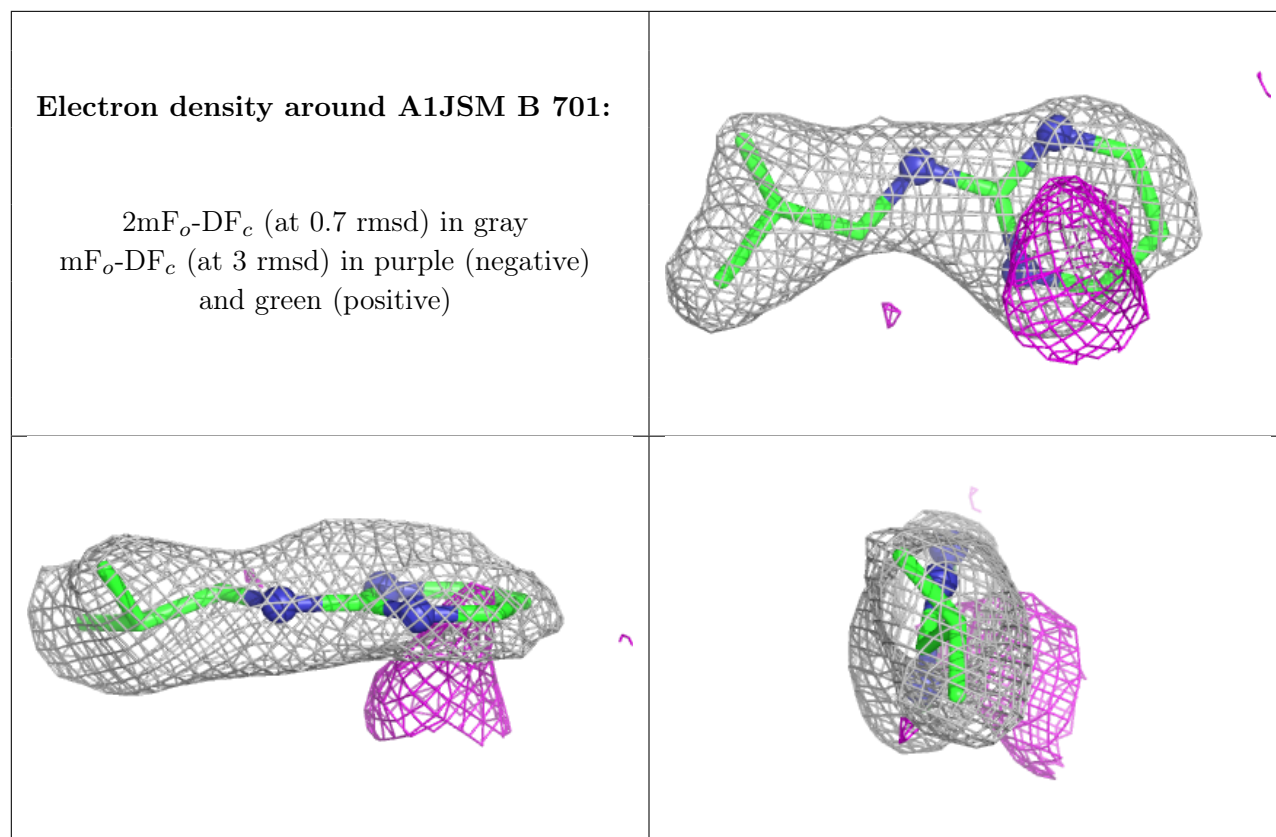
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
3	A1JSM	B	701	11/11	0.80	0.18	47,48,48,48	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.