



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:15 pm BST

PDB ID : 4P1N
Title : Crystal structure of Atg1-Atg13 complex
Authors : Fujioka, Y.; Noda, N.N.
Deposited on : 2014-02-27
Resolution : 2.20 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

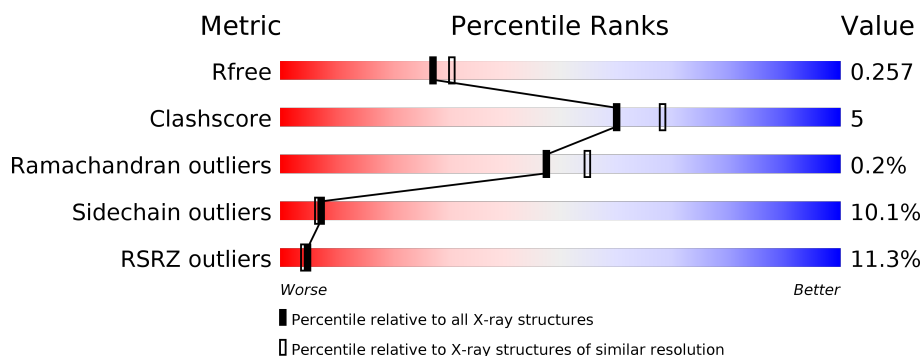
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	275	<div> <div>13%</div> <div>56%</div> <div>11%</div> <div>•</div> <div>31%</div> </div>
1	B	275	<div> <div>5%</div> <div>61%</div> <div>13%</div> <div>•</div> <div>25%</div> </div>
2	C	61	<div> <div>10%</div> <div>69%</div> <div>8%</div> <div>23%</div> </div>
2	D	61	<div> <div>3%</div> <div>69%</div> <div>16%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3900 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 Atg1 tMIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1473	943	242	277	11			
1	B	207	Total	C	N	O	S	0	0	0
			1636	1050	261	313	12			

- Molecule 2 is a protein called Atg13 MIM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	47	Total	C	N	O	S	0	0	0
			356	221	55	76	4			
2	D	53	Total	C	N	O	S	0	0	0
			409	256	64	86	3			

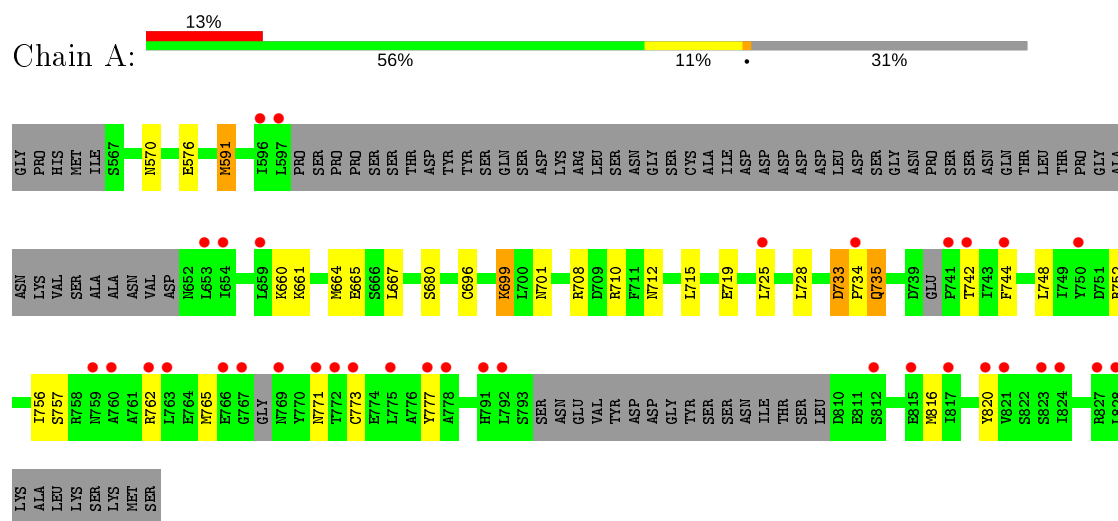
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	14	Total	O	0	0
			14	14		
3	C	5	Total	O	0	0
			5	5		

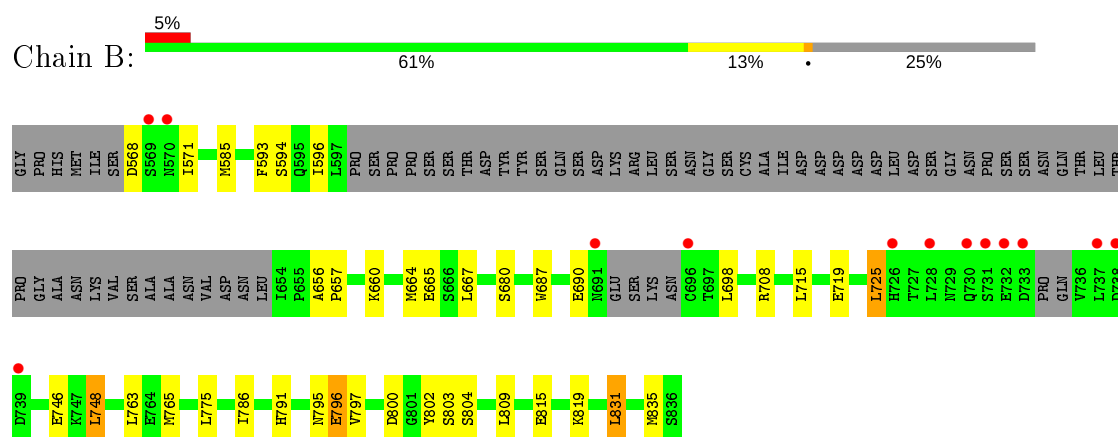
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

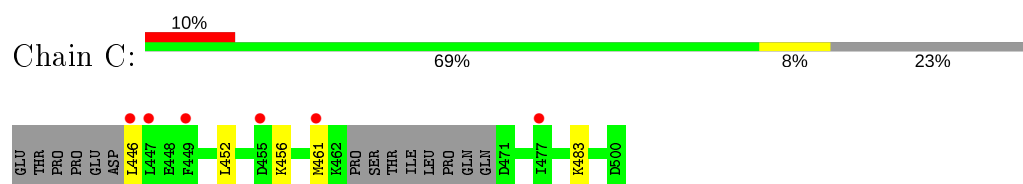
• Molecule 1: Atg1 tMIT



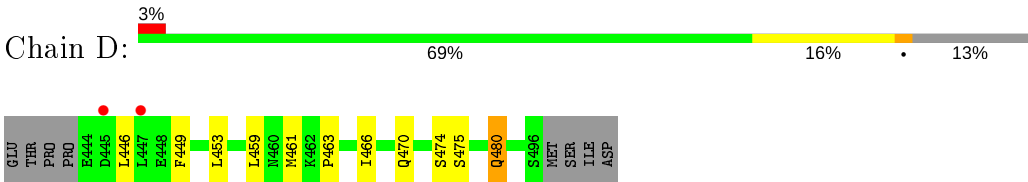
• Molecule 1: Atg1 tMIT



• Molecule 2: Atg13 MIM



● Molecule 2: Atg13 MIM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.99Å 96.62Å 63.33Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	45.77 – 2.20 45.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (45.77-2.20) 99.5 (45.73-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.209 , 0.255 0.213 , 0.257	Depositor DCC
R_{free} test set	3140 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3900	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% 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](#)

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	0.55	0/1496	0.68	1/2020 (0.0%)
1	B	0.62	0/1662	0.74	3/2241 (0.1%)
2	C	0.50	0/357	0.60	0/476
2	D	0.46	0/413	0.59	0/557
All	All	0.57	0/3928	0.69	4/5294 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	796	GLU	CA-CB-CG	7.61	130.15	113.40
1	A	708	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	708	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	B	708	ARG	NE-CZ-NH1	5.99	123.30	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	733	ASP	Peptide

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	1473	0	1421	12	0
1	B	1636	0	1616	18	0
2	C	356	0	340	1	0
2	D	409	0	404	10	0
3	A	7	0	0	0	0
3	B	14	0	0	0	0
3	C	5	0	0	0	0
All	All	3900	0	3781	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)
1:A:661:LYS:NZ	1:A:665:GLU:OE2	2.15	0.79
1:B:809:LEU:HD23	2:D:461:MET:CE	2.28	0.63
1:A:735:GLN:H	1:A:735:GLN:CD	2.03	0.62
1:A:576:GLU:OE2	1:A:699:LYS:NZ	2.35	0.60
1:B:585:MET:HE3	1:B:786:ILE:HD13	1.83	0.60
1:B:831:LEU:HD13	1:B:835:MET:CE	2.35	0.56
1:A:712:ASN:OD1	2:C:483:LYS:HD2	2.07	0.55
1:B:809:LEU:HD23	2:D:461:MET:HE1	1.88	0.55
1:A:752:ARG:HD2	1:A:756:ILE:HD11	1.91	0.53
2:D:449:PHE:CZ	2:D:453:LEU:HD11	2.44	0.53
1:B:800:ASP:HB3	1:B:802:TYR:H	1.75	0.51
1:B:665:GLU:HG2	1:B:748:LEU:HD21	1.93	0.51
1:A:733:ASP:C	1:A:733:ASP:OD1	2.51	0.48
1:B:800:ASP:HB2	1:B:804:SER:O	2.14	0.47
1:B:656:ALA:N	1:B:657:PRO:HD2	2.29	0.47
1:B:568:ASP:HA	1:B:687:TRP:HE1	1.81	0.46
1:A:742:THR:HG21	1:A:744:PHE:CE1	2.51	0.46
1:B:765:MET:HB3	2:D:446:LEU:HD13	1.98	0.45
1:B:795:ASN:OD1	1:B:797:VAL:HG22	2.16	0.45
1:B:815:GLU:O	1:B:819:LYS:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:MET:SD	1:A:752:ARG:NH2	2.90	0.45
1:B:719:GLU:OE2	2:D:480:GLN:NE2	2.50	0.45
2:D:459:LEU:HB3	2:D:461:MET:HE2	1.98	0.44
1:B:802:TYR:O	1:B:803:SER:HB3	2.18	0.44
1:B:809:LEU:HD23	2:D:461:MET:HE3	1.97	0.44
2:D:459:LEU:HD13	2:D:461:MET:HE3	2.00	0.43
1:B:593:PHE:O	1:B:596:ILE:HB	2.19	0.43
2:D:459:LEU:HB3	2:D:461:MET:CE	2.49	0.42
1:B:725:LEU:HA	1:B:725:LEU:HD12	1.94	0.42
1:B:800:ASP:N	1:B:804:SER:O	2.48	0.42
2:D:463:PRO:HD2	2:D:466:ILE:HD11	2.02	0.42
1:A:735:GLN:N	1:A:735:GLN:CD	2.72	0.42
1:A:773:CYS:O	1:A:777:TYR:CD2	2.73	0.42
1:A:696:CYS:SG	1:A:701:ASN:ND2	2.93	0.41
1:A:715:LEU:O	1:A:719:GLU:HG2	2.20	0.40

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	180/275 (66%)	177 (98%)	2 (1%)	1 (1%)	25	26
1	B	199/275 (72%)	197 (99%)	2 (1%)	0	100	100
2	C	43/61 (70%)	43 (100%)	0	0	100	100
2	D	51/61 (84%)	50 (98%)	1 (2%)	0	100	100
All	All	473/672 (70%)	467 (99%)	5 (1%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	734	PRO

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	155/251 (62%)	137 (88%)	18 (12%)	5	5
1	B	179/251 (71%)	162 (90%)	17 (10%)	8	8
2	C	42/61 (69%)	38 (90%)	4 (10%)	8	8
2	D	50/61 (82%)	46 (92%)	4 (8%)	12	12
All	All	426/624 (68%)	383 (90%)	43 (10%)	7	7

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	ASN
1	A	591	MET
1	A	660	LYS
1	A	664	MET
1	A	667	LEU
1	A	680	SER
1	A	699	LYS
1	A	710	ARG
1	A	725	LEU
1	A	728	LEU
1	A	735	GLN
1	A	748	LEU
1	A	757	SER
1	A	762	ARG
1	A	765	MET
1	A	771	ASN
1	A	816	MET
1	A	820	TYR
1	B	571	ILE
1	B	594	SER
1	B	660	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	664	MET
1	B	667	LEU
1	B	680	SER
1	B	690	GLU
1	B	698	LEU
1	B	715	LEU
1	B	725	LEU
1	B	746	GLU
1	B	748	LEU
1	B	763	LEU
1	B	775	LEU
1	B	791	HIS
1	B	796	GLU
1	B	831	LEU
2	C	446	LEU
2	C	452	LEU
2	C	456	LYS
2	C	461	MET
2	D	470	GLN
2	D	474	SER
2	D	475	SER
2	D	480	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	ASN
1	A	701	ASN
1	A	729	ASN
1	B	759	ASN
1	B	771	ASN
2	C	486	ASN
2	C	492	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	190/275 (69%)	0.90	35 (18%) 1 1	31, 68, 120, 134	0
1	B	207/275 (75%)	0.42	13 (6%) 20 19	26, 55, 100, 118	0
2	C	47/61 (77%)	0.83	6 (12%) 3 3	42, 73, 114, 134	0
2	D	53/61 (86%)	0.25	2 (3%) 40 38	41, 75, 107, 116	0
All	All	497/672 (73%)	0.62	56 (11%) 5 4	26, 63, 115, 134	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	828	LEU	8.1
1	A	824	ILE	7.2
1	A	653	LEU	6.4
1	B	737	LEU	6.3
1	B	738	ASP	6.0
1	A	773	CYS	5.8
2	C	455	ASP	5.7
2	C	446	LEU	5.2
1	B	731	SER	4.9
1	B	732	GLU	4.6
2	C	449	PHE	4.3
1	A	741	PRO	4.2
1	B	739	ASP	4.0
2	C	461	MET	3.9
1	A	742	THR	3.8
1	A	654	ILE	3.7
1	B	730	GLN	3.7
1	A	817	ILE	3.7
1	B	733	ASP	3.6
1	A	777	TYR	3.4
1	A	812	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	827	ARG	3.1
1	B	696	CYS	3.0
1	A	778	ALA	3.0
1	A	597	LEU	2.9
1	A	772	THR	2.9
1	A	750	TYR	2.9
1	B	569	SER	2.8
1	A	791	HIS	2.8
1	A	744	PHE	2.8
1	A	771	ASN	2.7
1	B	570	ASN	2.7
2	C	477	ILE	2.7
2	D	447	LEU	2.7
1	A	815	GLU	2.6
1	B	726	HIS	2.6
1	A	820	TYR	2.6
1	A	821	VAL	2.5
1	A	734	PRO	2.4
1	A	767	GLY	2.4
1	A	775	LEU	2.4
1	A	766	GLU	2.4
1	A	659	LEU	2.3
1	A	763	LEU	2.3
1	A	596	ILE	2.3
1	A	760	ALA	2.3
1	A	792	LEU	2.2
1	B	691	ASN	2.2
1	B	728	LEU	2.2
1	A	759	ASN	2.1
1	A	762	ARG	2.1
1	A	769	ASN	2.1
2	C	447	LEU	2.1
1	A	823	SER	2.1
1	A	725	LEU	2.1
2	D	445	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.