



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:01 PM GMT

PDB ID : 3SE6  
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2  
Authors : Birtley, J.R.; Saridakis, E.; Stratikos, E; Mavridis, I.M.  
Deposited on : 2011-06-10  
Resolution : 3.08 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

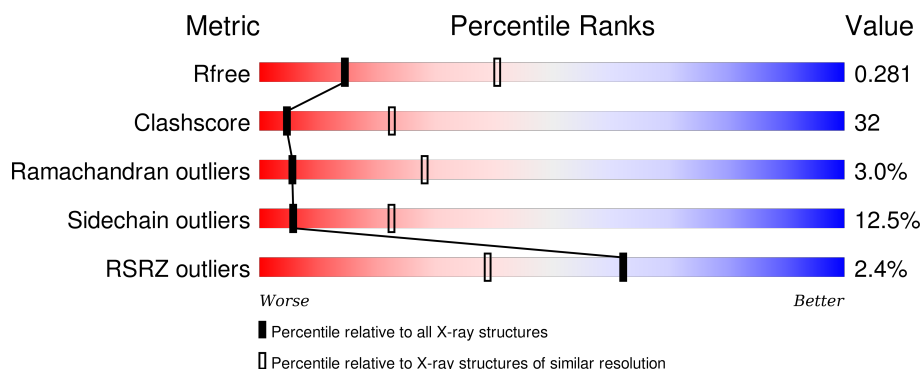
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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))
$R_{free}$	91344	1119 (3.12-3.04)
Clashscore	102246	1098 (3.10-3.06)
Ramachandran outliers	100387	1057 (3.10-3.06)
Sidechain outliers	100360	1057 (3.10-3.06)
RSRZ outliers	91569	1001 (3.10-3.06)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	967	<div> <div></div> <div>43%</div> <div>39%</div> <div>8%</div> <div>10%</div> </div>
1	B	967	<div> <div>3%</div> <div>39%</div> <div>41%</div> <div>8%</div> <div>11%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1073	-	-	-	X
5	NAG	A	1075	-	-	-	X
5	NAG	B	1081	-	-	-	X
7	MAN	B	1079	X	-	-	-
7	MAN	B	1080	X	-	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14348 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 Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	2	2	0
			7050	4548	1173	1302	27			
1	B	859	Total	C	N	O	S	0	0	0
			6978	4504	1160	1287	27			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	ENGINEERED MUTATION	UNP Q6P179
A	392	ASN	LYS	SEE REMARK 999	UNP Q6P179
A	961	ARG	-	EXPRESSION TAG	UNP Q6P179
A	962	HIS	-	EXPRESSION TAG	UNP Q6P179
A	963	HIS	-	EXPRESSION TAG	UNP Q6P179
A	964	HIS	-	EXPRESSION TAG	UNP Q6P179
A	965	HIS	-	EXPRESSION TAG	UNP Q6P179
A	966	HIS	-	EXPRESSION TAG	UNP Q6P179
A	967	HIS	-	EXPRESSION TAG	UNP Q6P179
B	2	VAL	PHE	ENGINEERED MUTATION	UNP Q6P179
B	392	ASN	LYS	SEE REMARK 999	UNP Q6P179
B	961	ARG	-	EXPRESSION TAG	UNP Q6P179
B	962	HIS	-	EXPRESSION TAG	UNP Q6P179
B	963	HIS	-	EXPRESSION TAG	UNP Q6P179
B	964	HIS	-	EXPRESSION TAG	UNP Q6P179
B	965	HIS	-	EXPRESSION TAG	UNP Q6P179
B	966	HIS	-	EXPRESSION TAG	UNP Q6P179
B	967	HIS	-	EXPRESSION TAG	UNP Q6P179

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

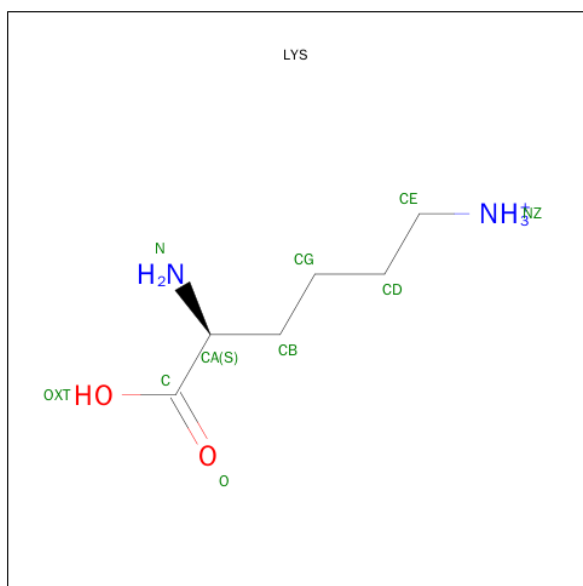
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			10	6	2	2		
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

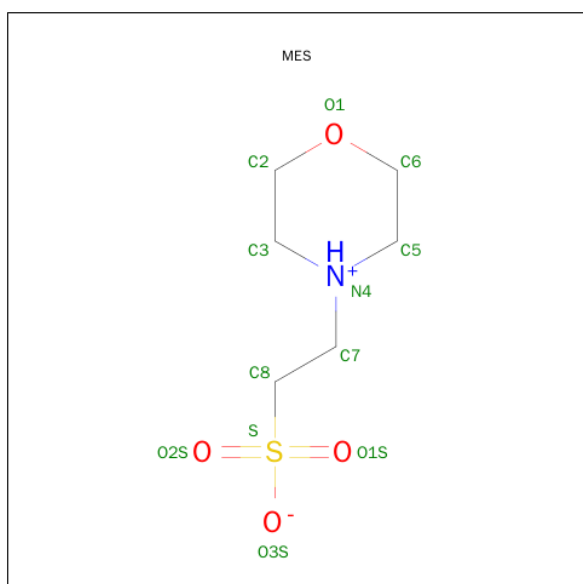
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	4	Total	C	N	O	0	0
			50	28	2	20		

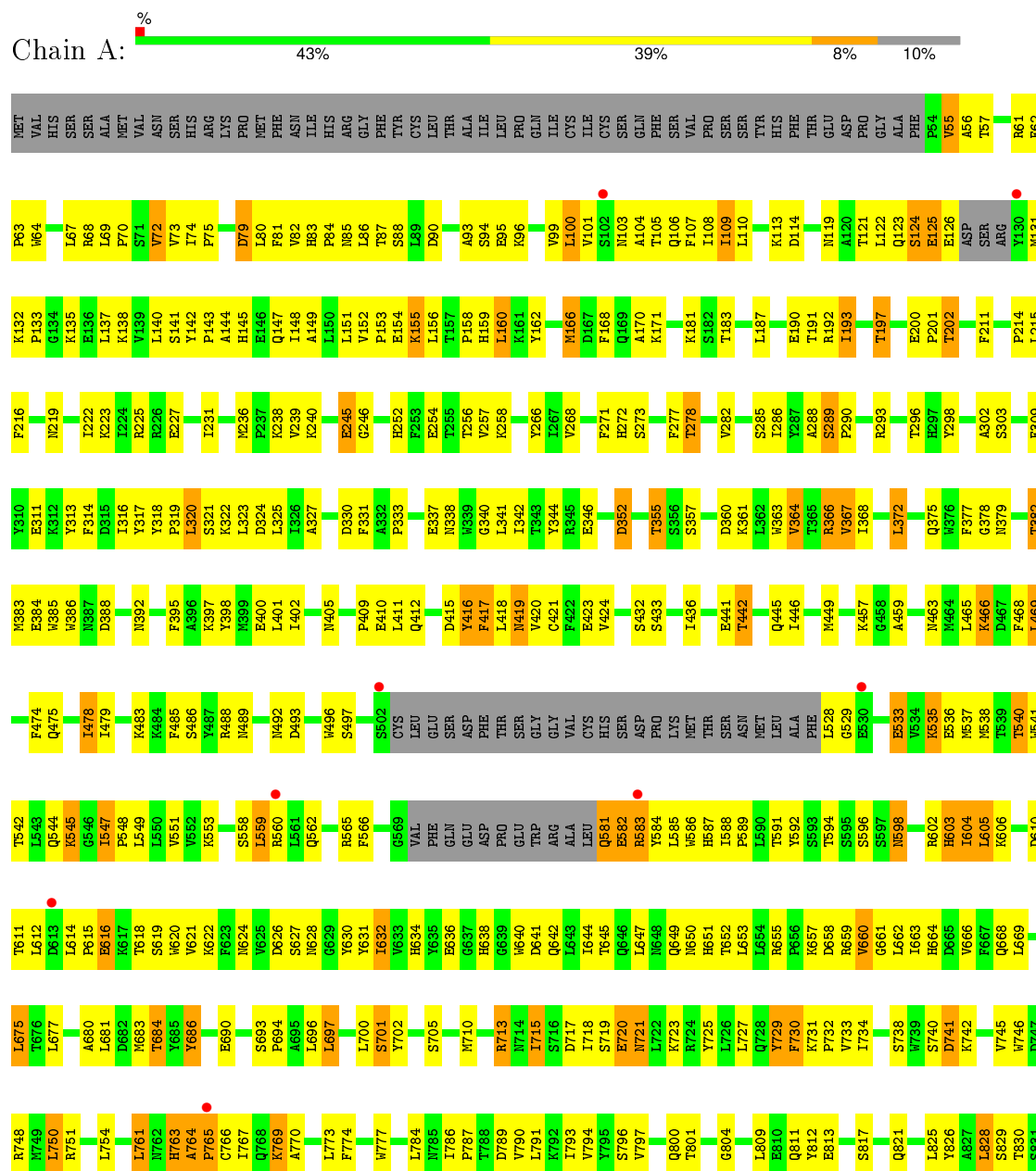
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	73	Total	O	0	0
			73	73		
8	B	53	Total	O	0	0
			53	53		

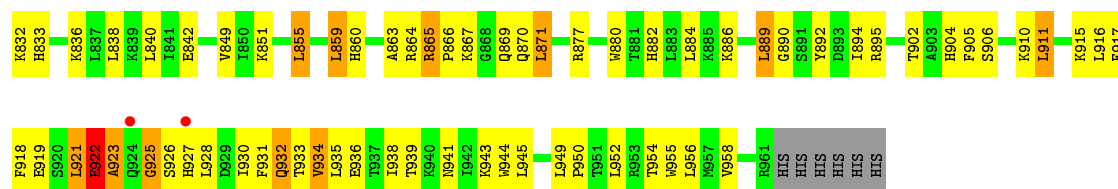
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

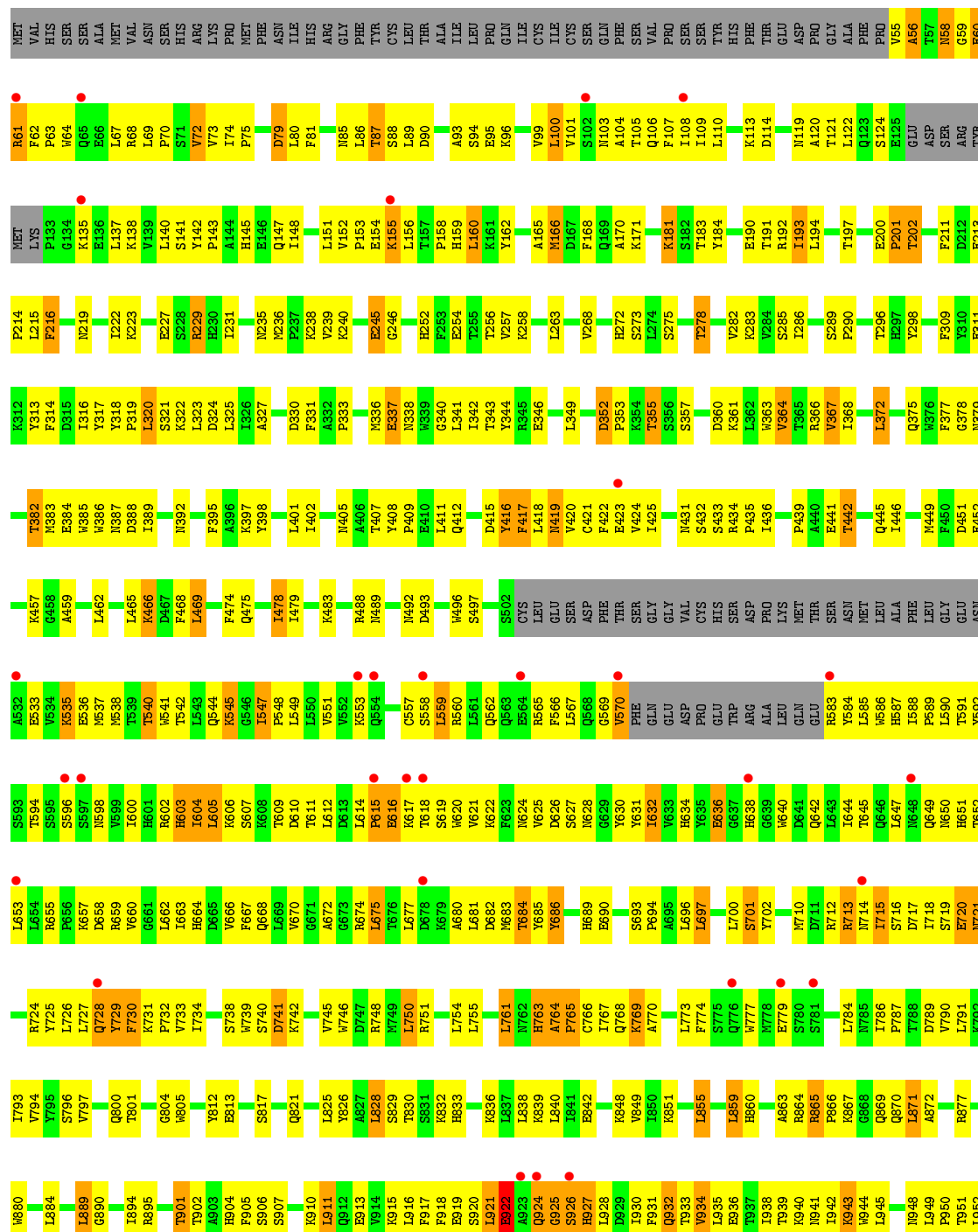
#### • Molecule 1: Endoplasmic reticulum aminopeptidase 2







# • Molecule 1: Endoplasmic reticulum aminopeptidase 2



1955	1956
R961	HIS
	HIS
	HIS
	HIS
	HIS
	HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.58Å 134.36Å 128.01Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	11.00 – 3.08 20.03 – 3.08	Depositor EDS
% Data completeness (in resolution range)	94.3 (11.00-3.08) 93.3 (20.03-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 3.09Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.212 , 0.277 0.214 , 0.281	Depositor DCC
$R_{free}$ test set	2194 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.6	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 70.6	EDS
Estimated twinning fraction	0.018 for -h,-l,-k 0.005 for -h,l,k 0.034 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46141 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	14348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, NAG, MES, MAN

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	0.40	0/7227	0.58	1/9794 (0.0%)
1	B	0.41	0/7148	0.58	0/9686
All	All	0.41	0/14375	0.58	1/19480 (0.0%)

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
7	B	2	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	923	ALA	N-CA-C	-5.60	95.88	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1079	MAN	C1
7	B	1080	MAN	C1

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	7050	0	6987	431	0
1	B	6978	0	6946	474	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	12	1	0
3	B	10	0	12	2	0
4	A	56	0	50	5	0
5	A	28	0	26	0	0
5	B	14	0	13	3	0
6	A	12	0	12	2	0
6	B	12	0	12	4	0
7	B	50	0	43	1	0
8	A	73	0	0	4	0
8	B	53	0	0	12	0
All	All	14348	0	14113	904	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 32.

The worst 5 of 904 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:B:56:ALA:HB1	1:B:61:ARG:HA	1.23	1.09
1:A:56:ALA:HB1	1:A:57:THR:HA	1.34	1.06
1:B:245:GLU:HG2	1:B:246:GLY:H	1.27	0.98
1:A:245:GLU:HG2	1:A:246:GLY:H	1.23	0.98
1:A:544:GLN:HE21	1:A:584:TYR:HD1	1.16	0.93

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	863/967 (89%)	746 (86%)	95 (11%)	22 (2%)	7	33
1	B	851/967 (88%)	732 (86%)	89 (10%)	30 (4%)	4	25
All	All	1714/1934 (89%)	1478 (86%)	184 (11%)	52 (3%)	5	28

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	245	GLU
1	A	417	PHE
1	A	596	SER
1	A	616	GLU

### 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	773/870 (89%)	677 (88%)	96 (12%)	6	23
1	B	770/870 (88%)	672 (87%)	98 (13%)	5	22
All	All	1543/1740 (89%)	1349 (87%)	194 (13%)	6	22

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	871	LEU

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Mol	Chain	Res	Type
1	B	181	LYS
1	B	855	LEU
1	A	911	LEU
1	B	72	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	870	GLN
1	B	58	ASN
1	B	870	GLN
1	A	882	HIS
1	A	927	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 ⓘ

8 carbohydrates are 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	$\# Z  > 2$
4	NAG	A	1071	1,4	14,14,15	0.65	0	15,19,21	1.11	1 (6%)
4	NAG	A	1072	4	14,14,15	0.47	0	15,19,21	1.62	2 (13%)
4	NAG	A	1073	1,4	14,14,15	0.59	0	15,19,21	1.89	2 (13%)
4	NAG	A	1074	4	14,14,15	0.51	0	15,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	1077	1,7	14,14,15	0.45	0	15,19,21	1.59	3 (20%)
7	NAG	B	1078	7	14,14,15	0.56	0	15,19,21	1.42	2 (13%)
7	MAN	B	1079	7	11,11,12	0.69	0	14,15,17	1.03	0
7	MAN	B	1080	7	11,11,12	0.57	0	14,15,17	0.69	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
4	NAG	A	1071	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1072	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1073	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1074	4	-	0/6/23/26	0/1/1/1
7	NAG	B	1077	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1078	7	-	0/6/23/26	0/1/1/1
7	MAN	B	1079	7	1/1/4/5	0/2/19/22	0/1/1/1
7	MAN	B	1080	7	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1071	NAG	C2-N2-C7	-3.07	119.10	123.04
7	B	1077	NAG	C4-C3-C2	-2.90	106.72	111.23
4	A	1072	NAG	C2-N2-C7	-2.89	119.33	123.04
4	A	1073	NAG	C2-N2-C7	-2.10	120.35	123.04
7	B	1078	NAG	C6-C5-C4	-2.04	107.98	113.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	B	1080	MAN	C1
7	B	1079	MAN	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1071	NAG	3	0
4	A	1072	NAG	1	0
4	A	1073	NAG	2	0
4	A	1074	NAG	1	0
7	B	1079	MAN	1	0

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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$
5	NAG	A	1075	1	14,14,15	0.49	0	15,19,21	1.11	1 (6%)
5	NAG	A	1076	1	14,14,15	0.69	0	15,19,21	1.86	4 (26%)
6	MES	A	1083	-	11,12,12	0.83	0	14,16,16	2.54	6 (42%)
3	LYS	A	968	2	6,9,9	0.29	0	4,10,10	0.36	0
5	NAG	B	1081	1	14,14,15	0.68	0	15,19,21	0.85	0
6	MES	B	1084	-	11,12,12	0.70	0	14,16,16	2.72	8 (57%)
3	LYS	B	968	2	6,9,9	0.41	0	4,10,10	0.31	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
5	NAG	A	1075	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1076	1	-	0/6/23/26	0/1/1/1
6	MES	A	1083	-	-	0/6/14/14	0/1/1/1
3	LYS	A	968	2	-	0/5/9/9	0/0/0/0
5	NAG	B	1081	1	-	0/6/23/26	0/1/1/1
6	MES	B	1084	-	-	0/6/14/14	0/1/1/1
3	LYS	B	968	2	-	0/5/9/9	0/0/0/0

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1084	MES	C6-C5-N4	-4.44	103.39	110.12
5	A	1076	NAG	C2-N2-C7	-4.04	117.85	123.04
6	A	1083	MES	C6-C5-N4	-3.76	104.43	110.12
6	A	1083	MES	C2-C3-N4	-3.47	104.87	110.12
6	B	1084	MES	C2-C3-N4	-3.33	105.07	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1083	MES	2	0
3	A	968	LYS	1	0
5	B	1081	NAG	3	0
6	B	1084	MES	4	0
3	B	968	LYS	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	869/967 (89%)	-0.25	10 (1%) 81 63	26, 61, 108, 138	2 (0%)
1	B	859/967 (88%)	-0.11	31 (3%) 46 23	27, 63, 111, 139	0
All	All	1728/1934 (89%)	-0.18	41 (2%) 62 39	26, 62, 109, 139	2 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	VAL	4.1
1	B	617	LYS	4.1
1	B	596	SER	3.6
1	A	102	SER	3.6
1	B	102	SER	3.3

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	A	1073	14/15	0.89	0.33	4.01	44,63,69,71	0
7	NAG	B	1077	14/15	0.93	0.21	1.06	45,65,74,75	0
4	NAG	A	1071	14/15	0.94	0.20	0.64	43,58,70,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1072	14/15	0.91	0.22	0.13	62,77,82,90	0
7	NAG	B	1078	14/15	0.89	0.23	-	57,74,91,95	0
7	MAN	B	1080	11/12	0.86	0.35	-	98,112,120,124	0
7	MAN	B	1079	11/12	0.82	0.33	-	94,102,111,115	0
4	NAG	A	1074	14/15	0.63	0.63	-	78,88,106,128	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	1081	14/15	0.88	0.37	5.71	53,72,97,99	0
5	NAG	A	1075	14/15	0.91	0.30	2.97	58,81,86,93	0
3	LYS	B	968	10/10	0.95	0.20	1.58	36,51,71,71	0
6	MES	B	1084	12/12	0.88	0.27	1.52	53,71,88,100	0
6	MES	A	1083	12/12	0.91	0.22	1.19	46,68,81,96	0
3	LYS	A	968	10/10	0.99	0.12	-1.41	32,39,51,51	0
2	ZN	A	5000	1/1	1.00	0.09	-2.87	31,31,31,31	0
2	ZN	B	6000	1/1	0.99	0.07	-4.66	36,36,36,36	0
5	NAG	A	1076	14/15	0.84	0.31	-	59,91,103,108	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.