



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 12:51 AM GMT

PDB ID : 4E36
Title : Crystal structure of the human Endoplasmic Reticulum Aminopeptidase 2 variant N392K
Authors : Birtley, J.R.; Saridakis, E.; Pegias, P.; Stratikos, E.; Mavridis, I.M.
Deposited on : 2012-03-09
Resolution : 3.22 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

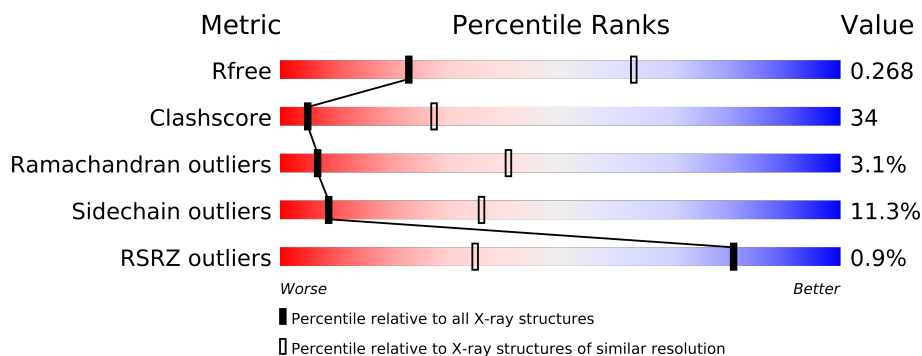
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.22 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}	66092	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	967	
1	B	967	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	LYS	B	1005	-	X
5	MES	A	1009	-	X
5	MES	B	1010	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14341 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

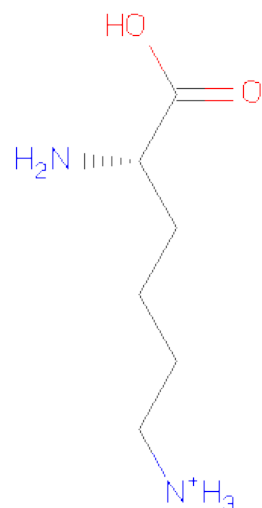
- Molecule 1 is a protein called Endoplasmic reticulum aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	869	Total	C	N	O	S	2	2	0
			7030	4537	1167	1299	27			
1	B	859	Total	C	N	O	S	0	0	0
			6969	4501	1157	1284	27			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	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	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 LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

There are 24 discrepancies between the modelled and reference sequences:

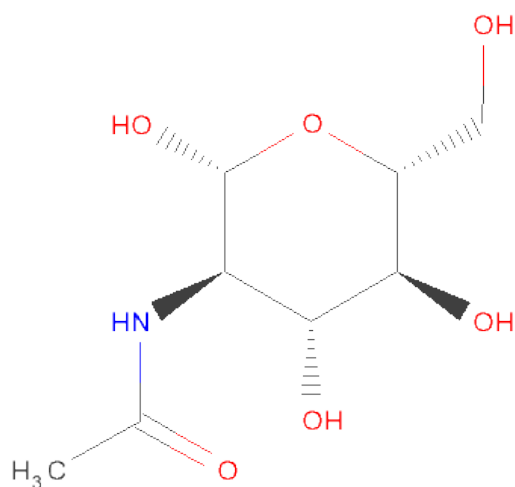
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	PHE	SEE REMARK 999	UNP Q6P179
A	961	ARG	-	EXPRESSION TAG	UNP Q6P179
A	962	HIS	-	EXPRESSION TAG	UNP Q6P179
A	963	HIS	-	EXPRESSION TAG	UNP Q6P179
A	964	HIS	-	EXPRESSION TAG	UNP Q6P179
A	965	HIS	-	EXPRESSION TAG	UNP Q6P179
A	966	HIS	-	EXPRESSION TAG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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	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 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



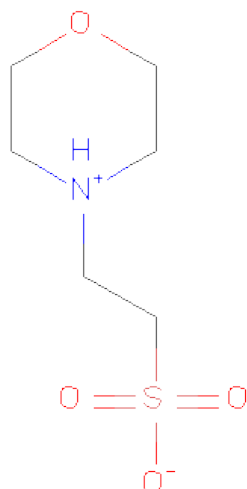
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	A	1	Total	Zn	0	0
			1	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		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	VAL	PHE	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 8 is water.

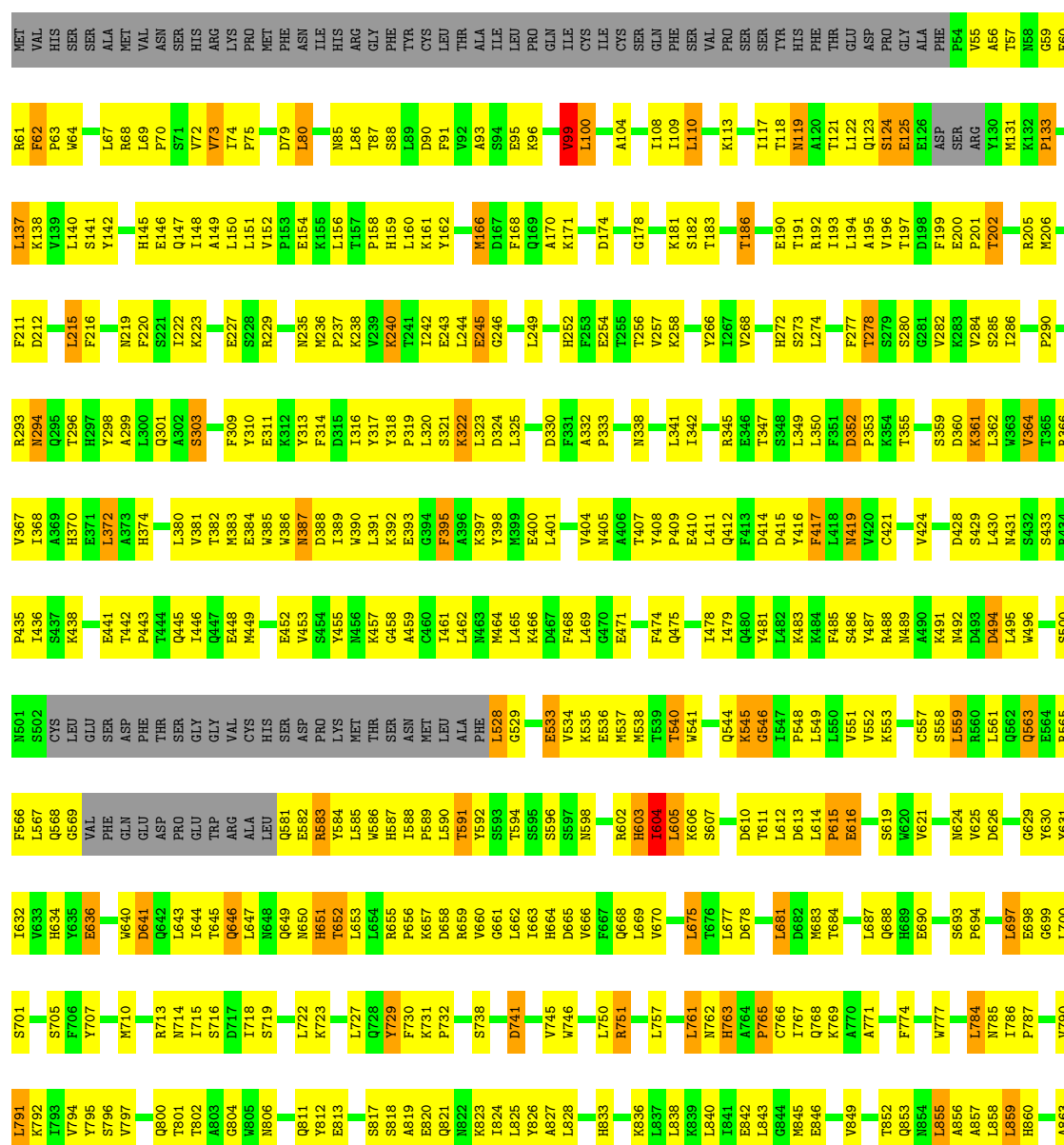
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	66	Total O 66 66	0	0
8	B	40	Total O 40 40	0	0

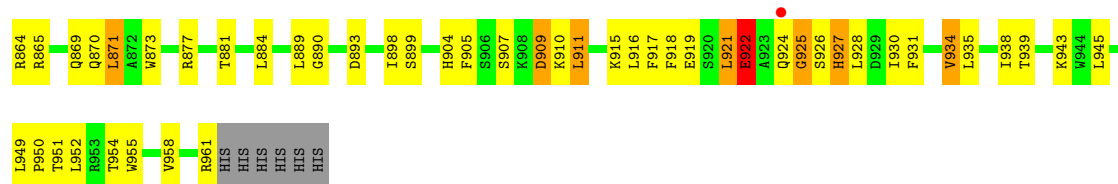
3 Residue-property plots

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 ($RSRZ > 2$). 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

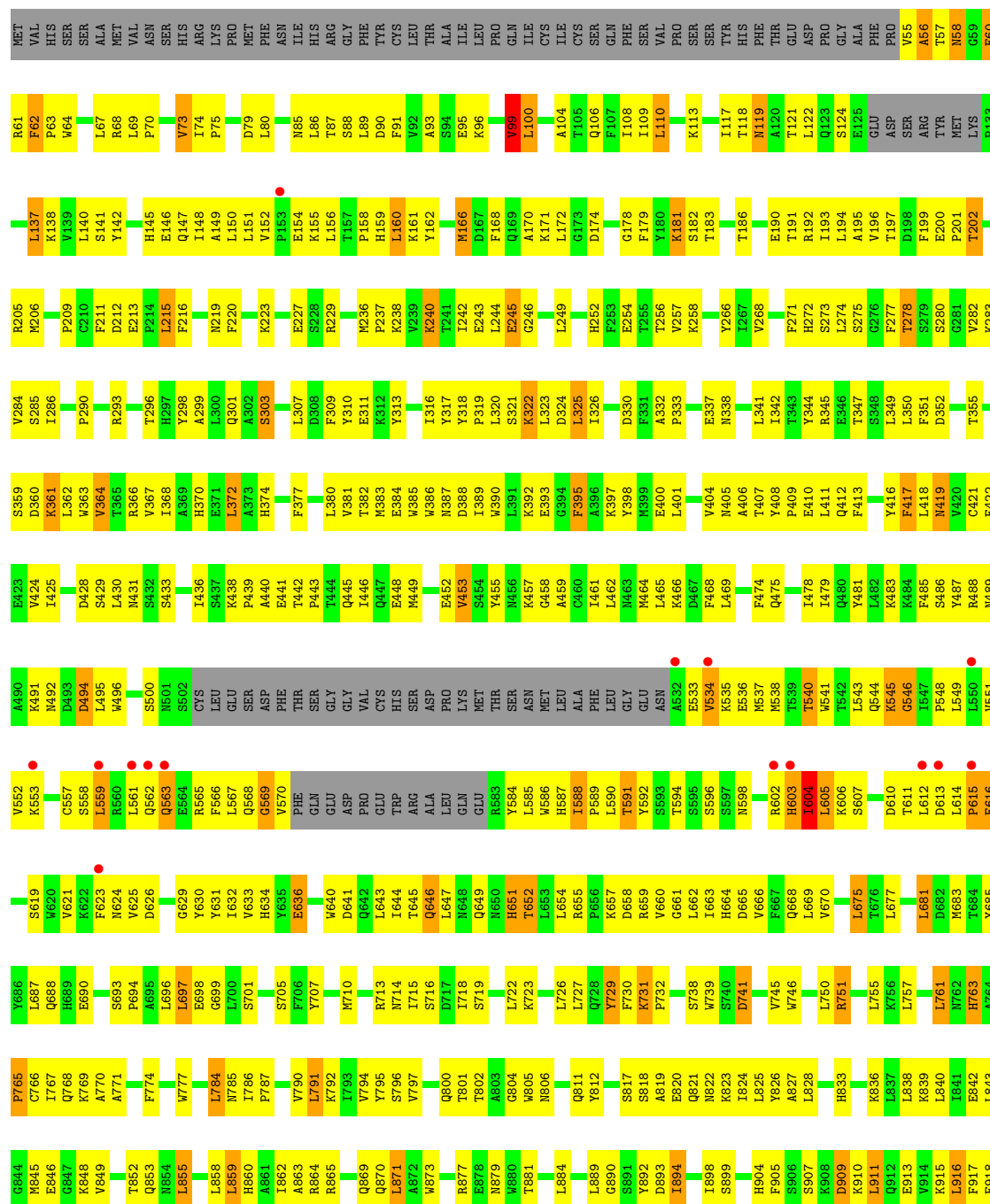
Chain A: 





• Molecule 1: Endoplasmic reticulum aminopeptidase 2

Chain B:



E919	S920	L921	E922	A923	Q924	Q925	S926	H927	L928	D929	I930	F931		Y934	L935		I938	T939		R943	W944	L945		L949	P950	T951	L952	R953	T954	W955		Y958		R961	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.34Å 134.45Å 127.37Å 90.00° 90.85° 90.00°	Depositor
Resolution (Å)	11.00 – 3.22 59.45 – 3.22	Depositor EDS
% Data completeness (in resolution range)	89.4 (11.00-3.22) 99.1 (59.45-3.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.209 , 0.261 0.216 , 0.268	Depositor DCC
R_{free} test set	2013 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.7	EDS
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 40288 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14341	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.37	0/7207	0.54	0/9769
1	B	0.39	0/7139	0.54	0/9674
All	All	0.38	0/14346	0.54	0/19443

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	922	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7030	0	6950	459	1
1	B	6969	0	6937	495	1
2	A	10	0	12	0	0
2	B	10	0	12	4	0
3	A	56	0	50	7	0
3	B	28	0	25	2	0
4	A	42	0	39	2	0
4	B	14	0	13	0	0
5	A	12	0	12	1	0
5	B	12	0	12	4	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	50	0	43	6	0
8	A	66	0	0	5	0
8	B	40	0	0	8	0
All	All	14341	0	14105	961	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

The worst 5 of 961 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:227:GLU:HG3	3:A:1002:NAG:H82	1.27	1.07
1:A:227:GLU:HG3	3:A:1002:NAG:C8	1.84	1.07
1:A:56:ALA:HB1	1:A:57:THR:HA	1.40	1.02
1:B:488:ARG:HG2	1:B:489:ASN:H	1.24	1.00
1:B:741:ASP:OD2	1:B:787:PRO:HB3	1.61	0.99

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:SER:O	1:A:961:ARG:NH2[2_655]	2.11	0.09
1:B:320:LEU:O	1:B:961:ARG:NH1[2_556]	2.19	0.01

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%)	729 (84%)	108 (12%)	26 (3%)	7	42
1	B	851/967 (88%)	710 (83%)	114 (13%)	27 (3%)	6	39
All	All	1714/1934 (89%)	1439 (84%)	222 (13%)	53 (3%)	7	41

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	119	ASN
1	A	583	ARG
1	A	596	SER
1	A	603	HIS

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	768/870 (88%)	679 (88%)	89 (12%)	8	35
1	B	768/870 (88%)	684 (89%)	84 (11%)	9	37
All	All	1536/1740 (88%)	1363 (89%)	173 (11%)	9	36

5 of 173 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	871	LEU
1	B	117	ILE
1	B	855	LEU
1	A	893	ASP
1	A	934	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	GLN

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Mol	Chain	Res	Type
1	B	145	HIS
1	B	879	ASN
1	A	959	ASN
1	B	147	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

10 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	$\# Z > 2$
3	NAG	A	1002	1,3	12,14,15	0.91	1 (8%)	15,19,21	2.94	6 (40%)
3	NAG	A	1003	3	12,14,15	0.56	0	15,19,21	1.21	2 (13%)
3	NAG	A	1004	1,3	12,14,15	0.89	1 (8%)	15,19,21	1.44	3 (20%)
3	NAG	A	1005	3	12,14,15	0.78	1 (8%)	15,19,21	1.05	1 (6%)
7	MAN	B	1001	7	10,11,12	0.86	1 (10%)	11,15,17	1.03	1 (9%)
7	MAN	B	1002	7	10,11,12	0.79	0	11,15,17	1.06	1 (9%)
7	NAG	B	1003	1,7	12,14,15	0.53	0	15,19,21	1.17	2 (13%)
7	NAG	B	1004	7	12,14,15	0.70	0	15,19,21	0.80	0
3	NAG	B	1007	1,3	12,14,15	0.69	1 (8%)	15,19,21	0.87	1 (6%)
3	NAG	B	1008	3	12,14,15	0.56	0	15,19,21	1.05	1 (6%)

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	NAG	A	1002	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1003	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1004	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1005	3	-	0/6/23/26	0/1/1/1
7	MAN	B	1001	7	-	0/2/19/22	0/1/1/1
7	MAN	B	1002	7	-	0/2/19/22	0/1/1/1
7	NAG	B	1003	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	1004	7	-	0/6/23/26	0/1/1/1
3	NAG	B	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1008	3	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	NAG	O5-C5	-2.46	1.40	1.45
3	A	1005	NAG	O5-C5	-2.30	1.41	1.45
3	B	1007	NAG	O5-C5	-2.19	1.41	1.45
7	B	1001	MAN	O5-C5	-2.15	1.41	1.45
3	A	1002	NAG	O5-C5	-2.12	1.41	1.45

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	NAG	O5-C5-C6	7.34	114.68	106.98
3	A	1002	NAG	O5-C5-C4	-5.22	104.03	110.65
3	A	1002	NAG	C3-C4-C5	-4.19	102.73	110.20
7	B	1002	MAN	O5-C5-C6	3.28	110.42	106.98
3	A	1002	NAG	O4-C4-C3	3.09	117.28	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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$
2	LYS	A	1001	6	9,9,9	0.74	1 (11%)	10,10,10	0.74	0
4	NAG	A	1006	1	12,14,15	0.61	0	15,19,21	1.06	0
4	NAG	A	1007	1	12,14,15	0.68	0	15,19,21	2.34	5 (33%)
4	NAG	A	1008	1	12,14,15	0.59	0	15,19,21	0.90	0
5	MES	A	1009	-	12,12,12	2.10	1 (8%)	16,16,16	2.67	6 (37%)
2	LYS	B	1005	6	9,9,9	0.77	1 (11%)	10,10,10	1.09	1 (10%)
4	NAG	B	1009	1	12,14,15	0.53	0	15,19,21	0.92	0
5	MES	B	1010	-	12,12,12	2.13	1 (8%)	16,16,16	2.70	7 (43%)

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	LYS	A	1001	6	-	0/9/9/9	0/0/0/0
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
5	MES	A	1009	-	-	0/6/14/14	1/1/1/1
2	LYS	B	1005	6	-	0/9/9/9	0/0/0/0
4	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
5	MES	B	1010	-	-	0/6/14/14	1/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1010	MES	C8-S	-6.32	1.67	1.78
5	A	1009	MES	C8-S	-6.30	1.67	1.78
2	B	1005	LYS	OXT-C	-2.13	1.22	1.30
2	A	1001	LYS	OXT-C	-2.00	1.23	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	NAG	O5-C5-C6	5.39	112.64	106.98
5	B	1010	MES	C6-C5-N4	-5.11	103.41	109.96
5	B	1010	MES	C5-N4-C3	4.89	119.45	109.75
5	A	1009	MES	C5-N4-C3	4.89	119.44	109.75
5	A	1009	MES	C8-C7-N4	-4.46	104.81	112.44

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1010	MES	C2-C3-C5-C6-N4-O1
5	A	1009	MES	C2-C3-C5-C6-N4-O1

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	869/967 (89%)	-0.13	1 (0%) 93 75	33, 67, 111, 147	2 (0%)
1	B	859/967 (88%)	-0.00	15 (1%) 67 20	34, 70, 116, 146	0
All	All	1728/1934 (89%)	-0.07	16 (0%) 81 35	33, 68, 114, 147	2 (0%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	561	LEU	3.5
1	B	612	LEU	3.0
1	B	563	GLN	2.9
1	B	550	LEU	2.8
1	B	559	LEU	2.7

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 ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	1002	14/15	0.24	0.76	64,79,83,87	0
3	NAG	B	1007	14/15	0.22	-0.23	68,91,111,112	0
7	NAG	B	1003	14/15	0.18	-0.31	56,73,85,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1003	14/15	0.15	-0.57	65,82,87,91	0
7	NAG	B	1004	14/15	0.16	-0.71	50,77,92,102	0
3	NAG	A	1004	14/15	0.13	-3.20	46,53,69,70	0
7	MAN	B	1001	11/12	0.15	-	72,97,108,112	0
7	MAN	B	1002	11/12	0.27	-	96,113,135,142	0
3	NAG	B	1008	14/15	0.29	-	84,113,127,133	0
3	NAG	A	1005	14/15	0.20	-	60,81,88,99	0

6.4 Ligands

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MES	A	1009	12/12	0.35	4.09	57,72,86,95	12
5	MES	B	1010	12/12	0.34	3.26	57,65,73,84	12
2	LYS	B	1005	10/10	0.32	2.99	46,59,65,69	0
4	NAG	A	1007	14/15	0.26	1.93	88,104,121,130	0
4	NAG	B	1009	14/15	0.24	1.92	76,101,110,112	0
2	LYS	A	1001	10/10	0.31	1.30	34,45,52,53	0
6	ZN	B	1006	1/1	0.20	0.10	46,46,46,46	0
4	NAG	A	1006	14/15	0.17	-1.89	62,85,87,88	0
6	ZN	A	1010	1/1	0.26	-2.70	32,32,32,32	0
4	NAG	A	1008	14/15	0.12	-	96,107,114,117	0

6.5 Other polymers

There are no such residues in this entry.