



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:33 AM GMT

PDB ID : 3MDJ
Title : ER Aminopeptidase, ERAP1, Bound to the Zinc Aminopeptidase Inhibitor, Bestatin
Authors : Nguyen, T.T.; Stern, L.J.
Deposited on : 2010-03-30
Resolution : 2.95 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
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

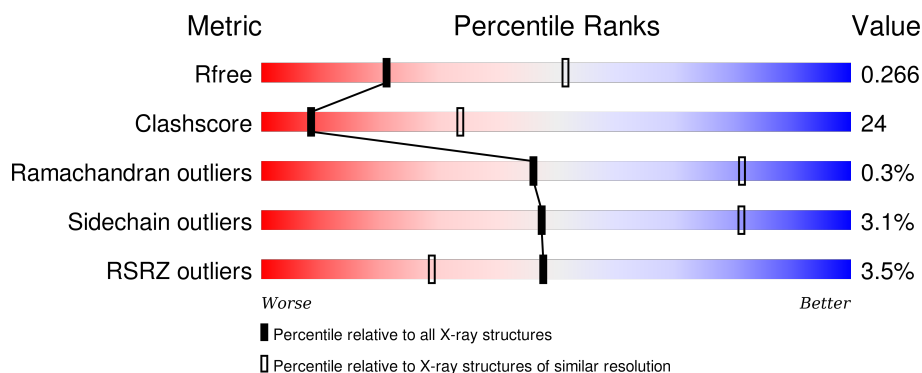
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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. 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	921	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>36%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	921	<div> <div>4%</div> <div> <div></div> <div>54%</div> <div>33%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	921	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>38%</div> <div>•</div> <div>11%</div> </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
3	BES	A	1001	-	-	-	X
3	BES	B	1001	-	-	X	X
3	BES	C	1001	-	-	-	X
4	NAG	C	5001	X	-	-	-
5	NAG	A	6001	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20163 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	818	Total	C	N	O	S	55	0	0
			6625	4271	1096	1227	31			
1	B	821	Total	C	N	O	S	50	0	0
			6643	4281	1099	1232	31			
1	C	819	Total	C	N	O	S	68	0	0
			6634	4276	1097	1230	31			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08
A	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
A	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
A	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
A	940	HIS	-	EXPRESSION TAG	UNP Q9NZ08
A	941	ASP	-	EXPRESSION TAG	UNP Q9NZ08
A	942	PRO	-	EXPRESSION TAG	UNP Q9NZ08
A	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
A	944	ALA	-	EXPRESSION TAG	UNP Q9NZ08
A	945	ASP	-	EXPRESSION TAG	UNP Q9NZ08
A	946	ALA	-	EXPRESSION TAG	UNP Q9NZ08
A	947	THR	-	EXPRESSION TAG	UNP Q9NZ08
A	948	GLY	-	EXPRESSION TAG	UNP Q9NZ08
A	949	LEU	-	EXPRESSION TAG	UNP Q9NZ08
A	950	GLU	-	EXPRESSION TAG	UNP Q9NZ08
A	951	ARG	-	EXPRESSION TAG	UNP Q9NZ08
A	952	MET	-	EXPRESSION TAG	UNP Q9NZ08
A	953	LEU	-	EXPRESSION TAG	UNP Q9NZ08
A	954	GLU	-	EXPRESSION TAG	UNP Q9NZ08
A	955	SER	-	EXPRESSION TAG	UNP Q9NZ08
A	956	ARG	-	EXPRESSION TAG	UNP Q9NZ08
A	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08
B	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08

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Chain	Residue	Modelled	Actual	Comment	Reference
B	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
B	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
B	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
B	940	HIS	-	EXPRESSION TAG	UNP Q9NZ08
B	941	ASP	-	EXPRESSION TAG	UNP Q9NZ08
B	942	PRO	-	EXPRESSION TAG	UNP Q9NZ08
B	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
B	944	ALA	-	EXPRESSION TAG	UNP Q9NZ08
B	945	ASP	-	EXPRESSION TAG	UNP Q9NZ08
B	946	ALA	-	EXPRESSION TAG	UNP Q9NZ08
B	947	THR	-	EXPRESSION TAG	UNP Q9NZ08
B	948	GLY	-	EXPRESSION TAG	UNP Q9NZ08
B	949	LEU	-	EXPRESSION TAG	UNP Q9NZ08
B	950	GLU	-	EXPRESSION TAG	UNP Q9NZ08
B	951	ARG	-	EXPRESSION TAG	UNP Q9NZ08
B	952	MET	-	EXPRESSION TAG	UNP Q9NZ08
B	953	LEU	-	EXPRESSION TAG	UNP Q9NZ08
B	954	GLU	-	EXPRESSION TAG	UNP Q9NZ08
B	955	SER	-	EXPRESSION TAG	UNP Q9NZ08
B	956	ARG	-	EXPRESSION TAG	UNP Q9NZ08
B	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08
C	346	ASP	GLY	SEE REMARK 999	UNP Q9NZ08
C	514	ARG	GLY	SEE REMARK 999	UNP Q9NZ08
C	528	ARG	LYS	SEE REMARK 999	UNP Q9NZ08
C	730	GLU	GLN	SEE REMARK 999	UNP Q9NZ08
C	940	HIS	-	EXPRESSION TAG	UNP Q9NZ08
C	941	ASP	-	EXPRESSION TAG	UNP Q9NZ08
C	942	PRO	-	EXPRESSION TAG	UNP Q9NZ08
C	943	GLU	-	EXPRESSION TAG	UNP Q9NZ08
C	944	ALA	-	EXPRESSION TAG	UNP Q9NZ08
C	945	ASP	-	EXPRESSION TAG	UNP Q9NZ08
C	946	ALA	-	EXPRESSION TAG	UNP Q9NZ08
C	947	THR	-	EXPRESSION TAG	UNP Q9NZ08
C	948	GLY	-	EXPRESSION TAG	UNP Q9NZ08
C	949	LEU	-	EXPRESSION TAG	UNP Q9NZ08
C	950	GLU	-	EXPRESSION TAG	UNP Q9NZ08
C	951	ARG	-	EXPRESSION TAG	UNP Q9NZ08
C	952	MET	-	EXPRESSION TAG	UNP Q9NZ08
C	953	LEU	-	EXPRESSION TAG	UNP Q9NZ08
C	954	GLU	-	EXPRESSION TAG	UNP Q9NZ08
C	955	SER	-	EXPRESSION TAG	UNP Q9NZ08
C	956	ARG	-	EXPRESSION TAG	UNP Q9NZ08

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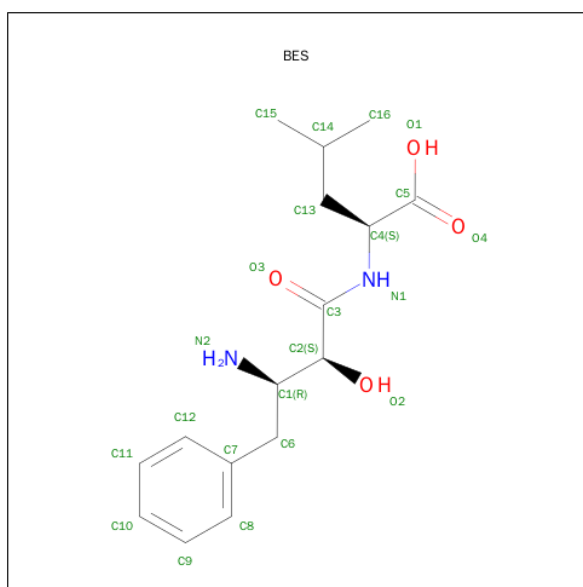
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Chain	Residue	Modelled	Actual	Comment	Reference
C	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08

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

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

- Molecule 3 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: C₁₆H₂₄N₂O₄).

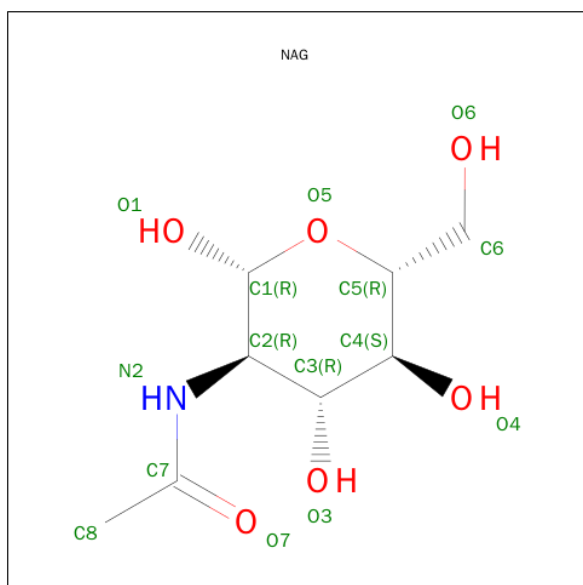


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 22 16 2 4	0	0
3	B	1	Total C N O 22 16 2 4	0	0
3	C	1	Total C N O 22 16 2 4	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		
4	C	5	Total	C	N	O	0	0
			61	34	2	25		

- 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		

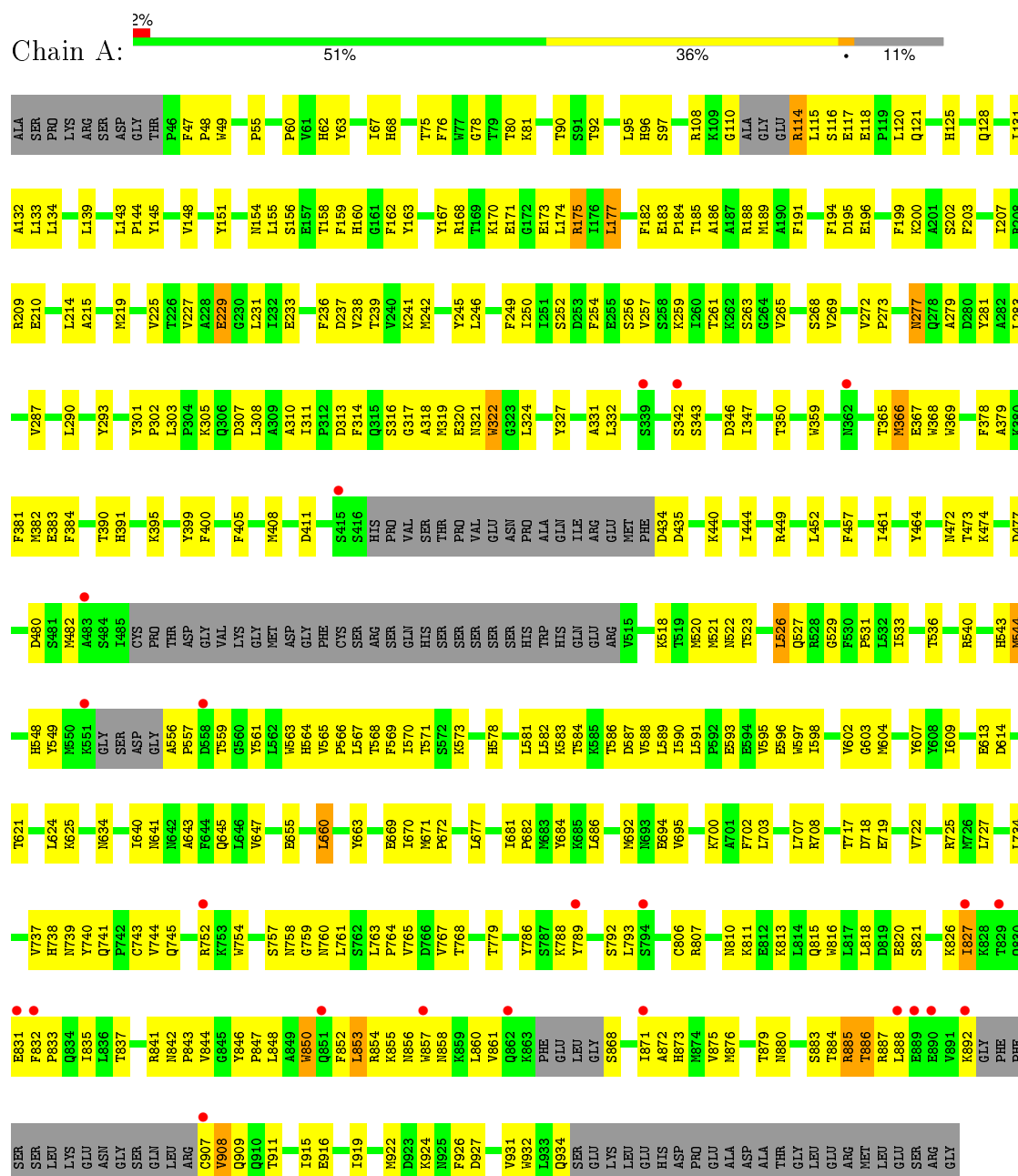
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

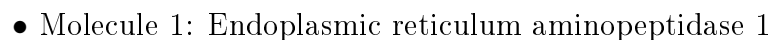
3 Residue-property plots

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 1



Chain B:



Chain C:



LYS	S869	S795	L707	D614	K545	W479	V396	W322	T236
LEU	S870	T796	L710	D615	Q546	D480	V399	G323	V227
HIS	A871	E547	L711	G616	E548	S481	F400	L324	A228
ASP	H873	I801	T717	D618	E549	N482	F405	T325	E229
PRO	M874	E802	D718	S619	K550	L485	M408	T326	G230
GLU	N875	F803	E719	L620	K551	CYS	A331	Y327	L231
ALA	M876	A804		T621	GLY	PRO	A331	R328	T232
ASP	T879	L805		L624	SER	THR	A331	R328	E233
THR	N880	C806		K625	ASP	GLY	A331	A331	E233
GLY		R807		L624	GLY	GLY	D411	L332	D237
LEU				G625	VAL	LYS	A412	L333	V238
GLU	S883	N810		H628	P557	GLY	L413	F334	T239
ARG	T884	K811	L731		E556	MET	M414		V240
MET	R885	B812	L732	L639	T559	ASP	S415	E337	K241
LEU	T886	K813	L733	I640	E560	ASP	HIS	R338	
GLU	R887	L734	A735	A643	Y561	GLY	PRO	K338	
GLU	L888		C736		H564	PHE	VAL	S343	S252
ARG	K892	E820	H737	V647	V565	CYS	SER	K344	D263
GLY			N739	S648	P566	ARG	THR	L345	F254
			I649	L567	L567	SER	PRO	D346	
						GLN	VAL	I347	K259
						HIS	GLU	T348	I260
						SER	ASN	K349	T261
						SER	PRO	K349	K262
						SER	ALA	T350	S263
						SER	GLN	L355	G264
						SER	ILE	A356	V265
						SER	ARG	H357	
						HIS	GLU	V269	
						TRP	MET	N362	
						HIS	PHE	L363	N277
						GLN	D434	V364	Q278
						GLU	D435	T365	A279
						ARG	V436	N366	D280
						V515	S437	E367	Y281
						K518	Y438	K368	K286
						T519	D439	K369	V287
						N520	K440	D371	
						N521	I444	L372	L290
						N524	R449	W373	E291
						T525	L452	L374	F292
						L526		N375	Y293
							F457	F378	L303
							F457	K380	F304
							I461	F381	K305
							Y464	N382	A310
							Y470	E383	D313
							T473	F384	F314
							K474	V385	Q315
							M475	S386	S316
							E476	V387	G317
							H541	T390	A318
							V542	H391	K319
							H543	E320	E320
							L478	D477	E321
								K395	N321

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.03 Å 234.63 Å 95.86 Å 90.00° 103.59° 90.00°	Depositor
Resolution (Å)	38.11 – 2.95 38.11 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.11-2.95) 99.8 (38.11-2.95)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.95 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.199 , 0.264 0.200 , 0.266	Depositor DCC
R_{free} test set	3208 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 63770 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20163	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BES, ZN, BMA, NAG, 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	0.27	0/6785	0.45	0/9195
1	B	0.28	0/6804	0.46	0/9222
1	C	0.27	0/6794	0.45	0/9207
All	All	0.27	0/20383	0.45	0/27624

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
4	C	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	5001	NAG	C1

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6625	0	6567	327	0
1	B	6643	0	6582	315	0
1	C	6634	0	6574	322	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	22	0	22	2	0
3	B	22	0	22	10	0
3	C	22	0	23	6	0
4	A	61	0	52	4	0
4	C	61	0	52	1	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
6	B	28	0	25	1	0
All	All	20163	0	19958	955	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 24.

The worst 5 of 955 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:C:640:ILE:HD11	1:C:663:TYR:HE2	1.13	1.12
1:B:113:GLU:O	1:B:117:GLU:HG3	1.49	1.12
1:A:210:GLU:HG3	4:A:5001:NAG:H83	1.37	1.07
1:A:875:VAL:HG11	1:A:908:VAL:CG2	1.86	1.04
1:C:319:MET:HE1	3:C:1001:BES:HN21	1.23	1.03

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	804/921 (87%)	750 (93%)	50 (6%)	4 (0%)	34	74
1	B	809/921 (88%)	755 (93%)	52 (6%)	2 (0%)	52	86
1	C	805/921 (87%)	753 (94%)	51 (6%)	1 (0%)	56	89
All	All	2418/2763 (88%)	2258 (93%)	153 (6%)	7 (0%)	46	81

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	908	VAL
1	A	229	GLU
1	A	908	VAL
1	B	908	VAL
1	A	855	LYS

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	733/819 (90%)	710 (97%)	23 (3%)	47	81
1	B	734/819 (90%)	711 (97%)	23 (3%)	47	81
1	C	734/819 (90%)	711 (97%)	23 (3%)	47	81
All	All	2201/2457 (90%)	2132 (97%)	69 (3%)	47	81

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	322	TRP
1	B	660	LEU
1	C	743	CYS
1	B	366	MET
1	B	575	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	GLN
1	B	634	ASN
1	C	698	GLN
1	B	277	ASN
1	B	391	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 ⓘ

12 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	5001	1,4	14,14,15	0.83	0	15,19,21	2.12	5 (33%)
4	NAG	A	5002	4	14,14,15	0.62	0	15,19,21	2.12	3 (20%)
4	BMA	A	5003	4	11,11,12	0.41	0	14,15,17	0.71	0
4	MAN	A	5004	4	11,11,12	0.57	0	14,15,17	0.90	0
4	MAN	A	5005	4	11,11,12	0.89	0	14,15,17	1.71	3 (21%)
6	NAG	B	5001	1,6	14,14,15	0.74	0	15,19,21	1.21	1 (6%)
6	NAG	B	5002	6	14,14,15	0.63	0	15,19,21	2.18	3 (20%)
4	NAG	C	5001	1,4	14,14,15	1.03	2 (14%)	15,19,21	2.15	5 (33%)
4	NAG	C	5002	4	14,14,15	0.72	0	15,19,21	2.53	4 (26%)
4	BMA	C	5003	4	11,11,12	0.38	0	14,15,17	0.68	0
4	MAN	C	5004	4	11,11,12	0.44	0	14,15,17	0.80	0
4	MAN	C	5005	4	11,11,12	0.74	0	14,15,17	1.21	2 (14%)

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	5001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	5002	4	-	0/6/23/26	0/1/1/1
4	BMA	A	5003	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5004	4	-	0/2/19/22	0/1/1/1
4	MAN	A	5005	4	-	0/2/19/22	0/1/1/1
6	NAG	B	5001	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	5002	6	-	0/6/23/26	0/1/1/1
4	NAG	C	5001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	5002	4	-	0/6/23/26	0/1/1/1
4	BMA	C	5003	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5004	4	-	0/2/19/22	0/1/1/1
4	MAN	C	5005	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5001	NAG	C4-C3	-2.07	1.47	1.52
4	C	5001	NAG	O4-C4	-2.02	1.38	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5002	NAG	O5-C5-C6	-6.76	92.71	107.35
4	A	5002	NAG	O5-C5-C6	-5.98	94.40	107.35
6	B	5002	NAG	O5-C5-C6	-5.91	94.55	107.35
4	C	5001	NAG	C3-C2-N2	-4.34	100.17	110.56
4	C	5001	NAG	O4-C4-C3	-4.26	100.75	110.34

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	5001	NAG	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	5001	NAG	3	0
4	A	5004	MAN	1	0
6	B	5001	NAG	1	0
4	C	5002	NAG	1	0
4	C	5005	MAN	1	0

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z > 2$
3	BES	A	1001	2	19,22,22	0.50	0	19,29,29	0.82	1 (5%)
5	NAG	A	6000	1	14,14,15	0.89	1 (7%)	15,19,21	1.37	1 (6%)
5	NAG	A	6001	1	14,14,15	1.26	2 (14%)	15,19,21	1.38	3 (20%)
3	BES	B	1001	2	19,22,22	0.52	0	19,29,29	0.88	1 (5%)
5	NAG	B	6000	1	14,14,15	0.63	0	15,19,21	1.03	1 (6%)
3	BES	C	1001	2	19,22,22	0.44	0	19,29,29	0.96	1 (5%)

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	BES	A	1001	2	-	0/20/24/24	0/1/1/1
5	NAG	A	6000	1	-	0/6/23/26	0/1/1/1
5	NAG	A	6001	1	1/1/5/7	0/6/23/26	0/1/1/1
3	BES	B	1001	2	-	0/20/24/24	0/1/1/1
5	NAG	B	6000	1	-	0/6/23/26	0/1/1/1
3	BES	C	1001	2	-	0/20/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	6000	NAG	O5-C1	2.22	1.47	1.43
5	A	6001	NAG	O5-C1	2.61	1.48	1.43
5	A	6001	NAG	C1-C2	3.20	1.56	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	BES	C4-N1-C3	-2.92	118.88	123.43
5	A	6001	NAG	C6-C5-C4	-2.74	106.26	113.02
3	B	1001	BES	C4-N1-C3	-2.41	119.67	123.43
3	A	1001	BES	C7-C6-C1	-2.07	109.17	113.53
5	A	6001	NAG	C4-C3-C2	-2.03	108.08	111.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	6001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	BES	2	0
5	A	6001	NAG	1	0
3	B	1001	BES	10	0
3	C	1001	BES	6	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, 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	818/921 (88%)	-0.22	23 (2%)	56 36	26, 57, 133, 238	11 (1%)
1	B	821/921 (89%)	-0.14	36 (4%)	38 22	24, 57, 130, 223	11 (1%)
1	C	818/921 (88%)	-0.24	28 (3%)	49 30	28, 57, 130, 223	12 (1%)
All	All	2457/2763 (88%)	-0.20	87 (3%)	48 29	24, 57, 131, 238	34 (1%)

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	SER	9.9
1	B	558	ASP	9.0
1	B	557	PRO	8.6
1	B	794	SER	8.6
1	B	825	ASP	7.6

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, 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	LLDF	B-factors(Å ²)	Q<0.9
4	MAN	C	5004	11/12	0.84	0.24	1.54	75,95,103,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	C	5001	14/15	0.90	0.19	1.43	20,79,110,127	0
4	NAG	A	5001	14/15	0.89	0.21	1.11	49,90,110,161	0
6	NAG	B	5001	14/15	0.91	0.21	1.00	50,93,110,139	0
6	NAG	B	5002	14/15	0.75	0.25	-	118,161,189,212	0
4	BMA	C	5003	11/12	0.85	0.26	-	43,135,191,223	0
4	MAN	A	5004	11/12	0.56	0.34	-	111,168,187,189	0
4	NAG	C	5002	14/15	0.86	0.34	-	47,135,257,284	0
4	NAG	A	5002	14/15	0.88	0.18	-	60,85,108,108	0
4	BMA	A	5003	11/12	0.89	0.17	-	51,86,129,131	0
4	MAN	A	5005	11/12	0.83	0.30	-	33,95,172,209	0
4	MAN	C	5005	11/12	0.81	0.35	-	86,142,212,223	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	BES	A	1001	22/22	0.79	0.45	5.06	86,184,208,217	0
3	BES	C	1001	22/22	0.82	0.37	3.86	79,178,213,218	0
3	BES	B	1001	22/22	0.88	0.38	3.50	121,167,185,218	0
2	ZN	B	1000	1/1	0.99	0.11	-0.88	38,38,38,38	0
2	ZN	C	1000	1/1	0.99	0.12	-0.93	38,38,38,38	0
2	ZN	A	1000	1/1	0.99	0.13	-1.25	40,40,40,40	0
5	NAG	A	6000	14/15	0.82	0.19	-	76,119,141,145	0
5	NAG	A	6001	14/15	0.74	0.17	-	72,140,150,153	0
5	NAG	B	6000	14/15	0.74	0.28	-	59,128,146,153	0

6.5 Other polymers [i](#)

There are no such residues in this entry.