



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 30, 2017 – 06:14 PM EDT

PDB ID : 3MDJ
Title : ER Aminopeptidase, ERAP1, Bound to the Zinc Aminopeptidase Inhibitor, Bestatin
Authors : Nguyen, T.T.; Stern, L.J.
Deposited on : unknown
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

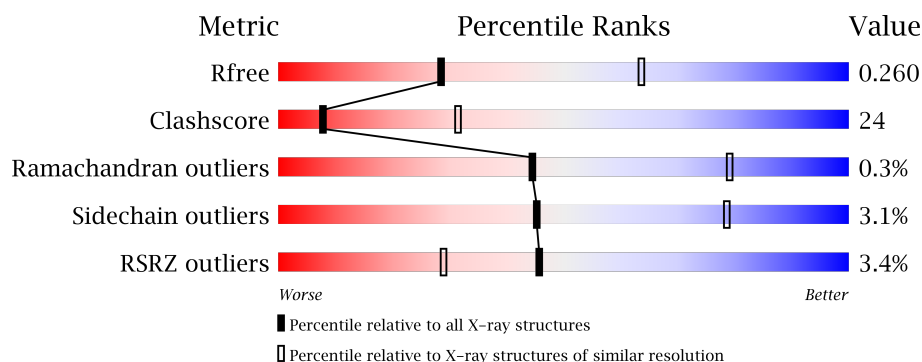
1 Overall quality at a glance ⓘ

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}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (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>51% 36% 11%</div> </div>
1	B	921	<div> <div>4%</div> <div>54% 33% 11%</div> </div>
1	C	921	<div> <div>3%</div> <div>50% 38% 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
3	BES	A	1001	-	-	-	X
3	BES	B	1001	-	-	X	X
3	BES	C	1001	-	-	-	X
4	NAG	A	6001	X	-	-	-
4	NAG	C	5001	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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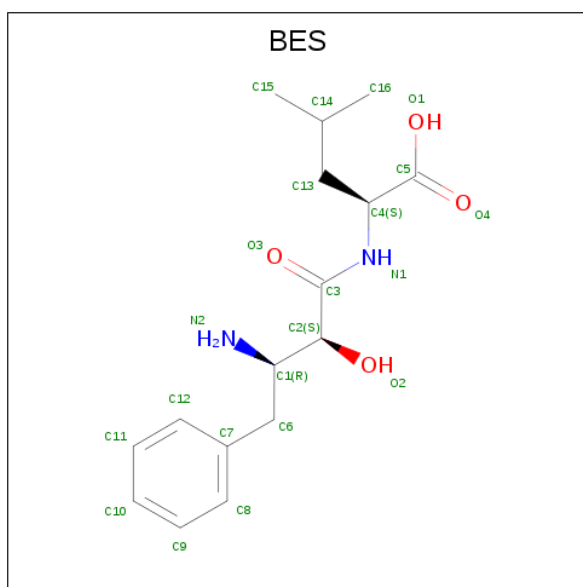
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Chain	Residue	Modelled	Actual	Comment	Reference
C	957	GLY	-	EXPRESSION TAG	UNP Q9NZ08

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

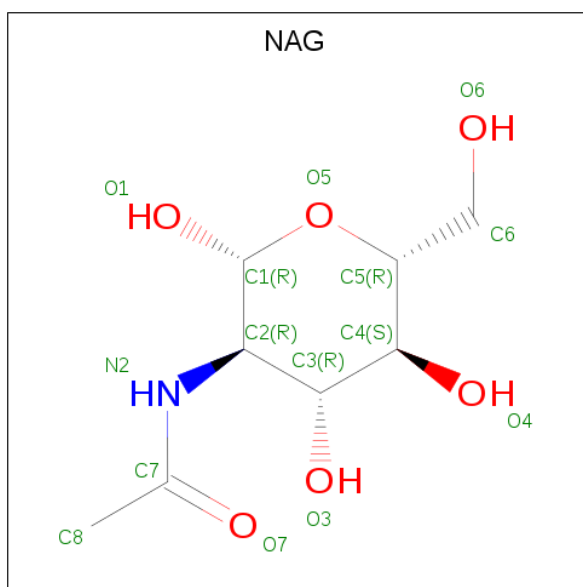
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

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



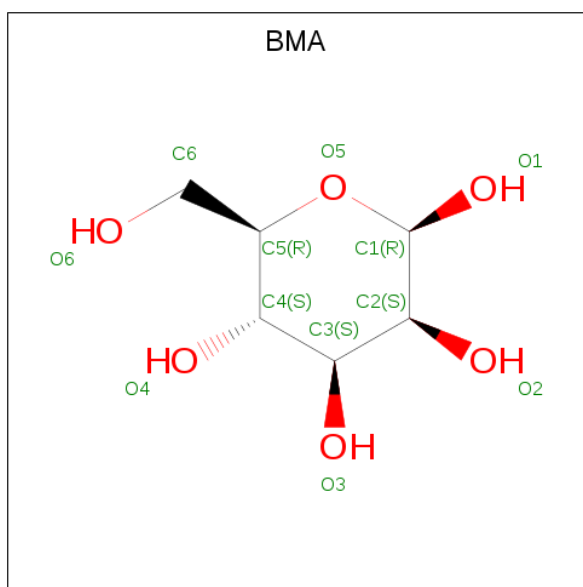
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 22 16 2 4	0	0
3	B	1	Total C N O 22 16 2 4	0	0
3	C	1	Total C N O 22 16 2 4	0	0

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



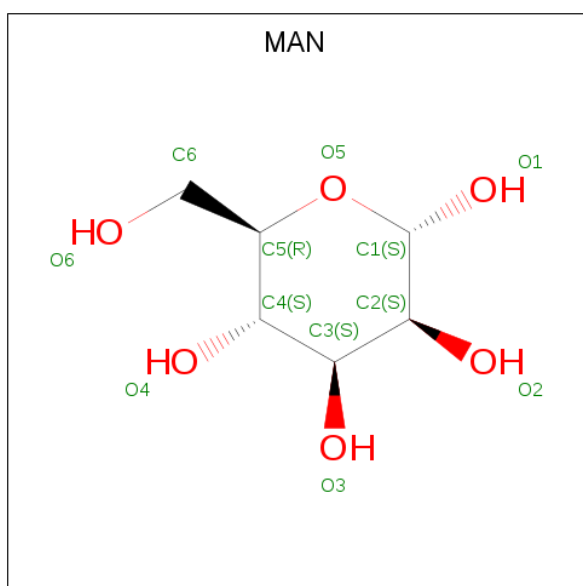
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1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

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

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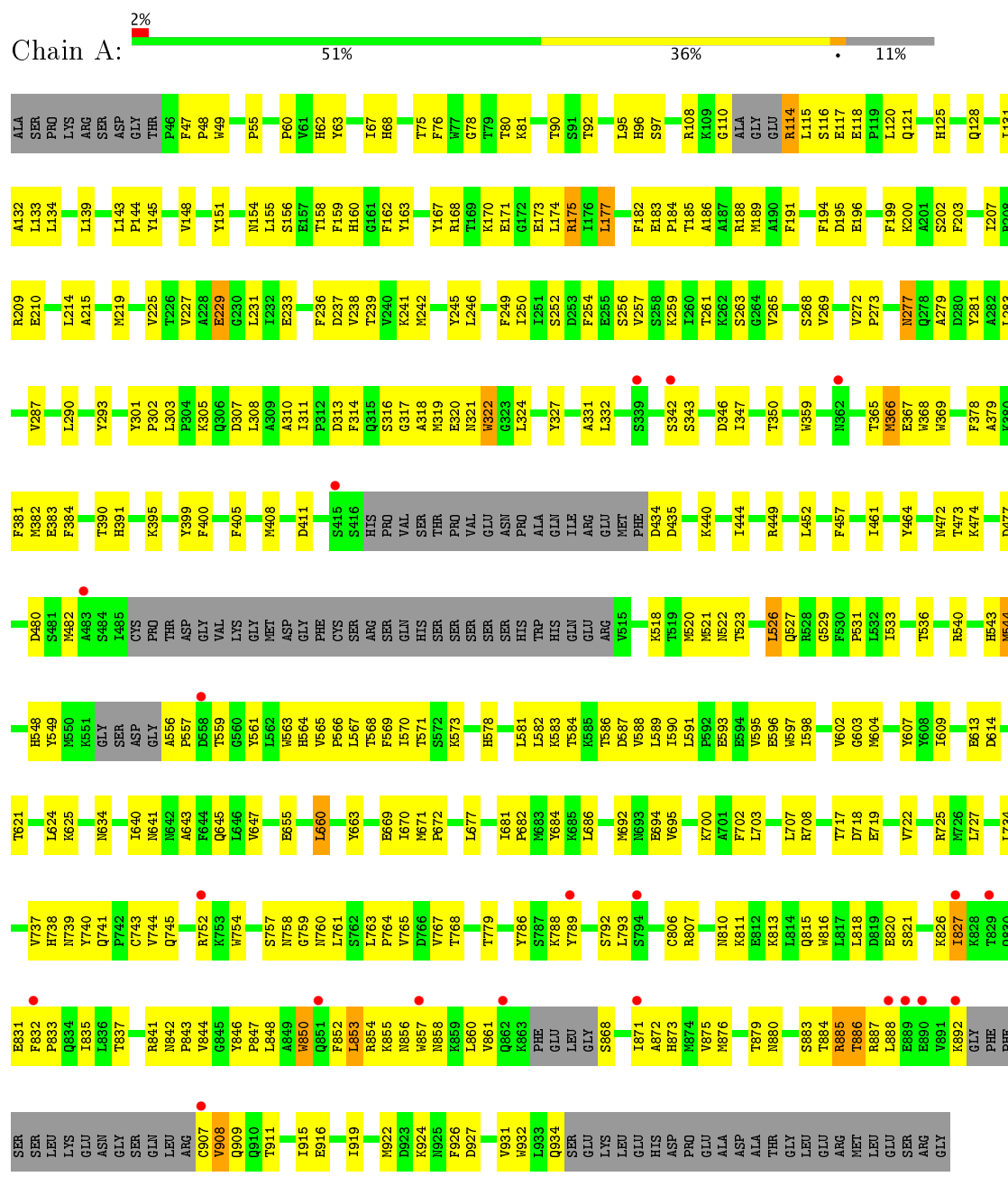
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		

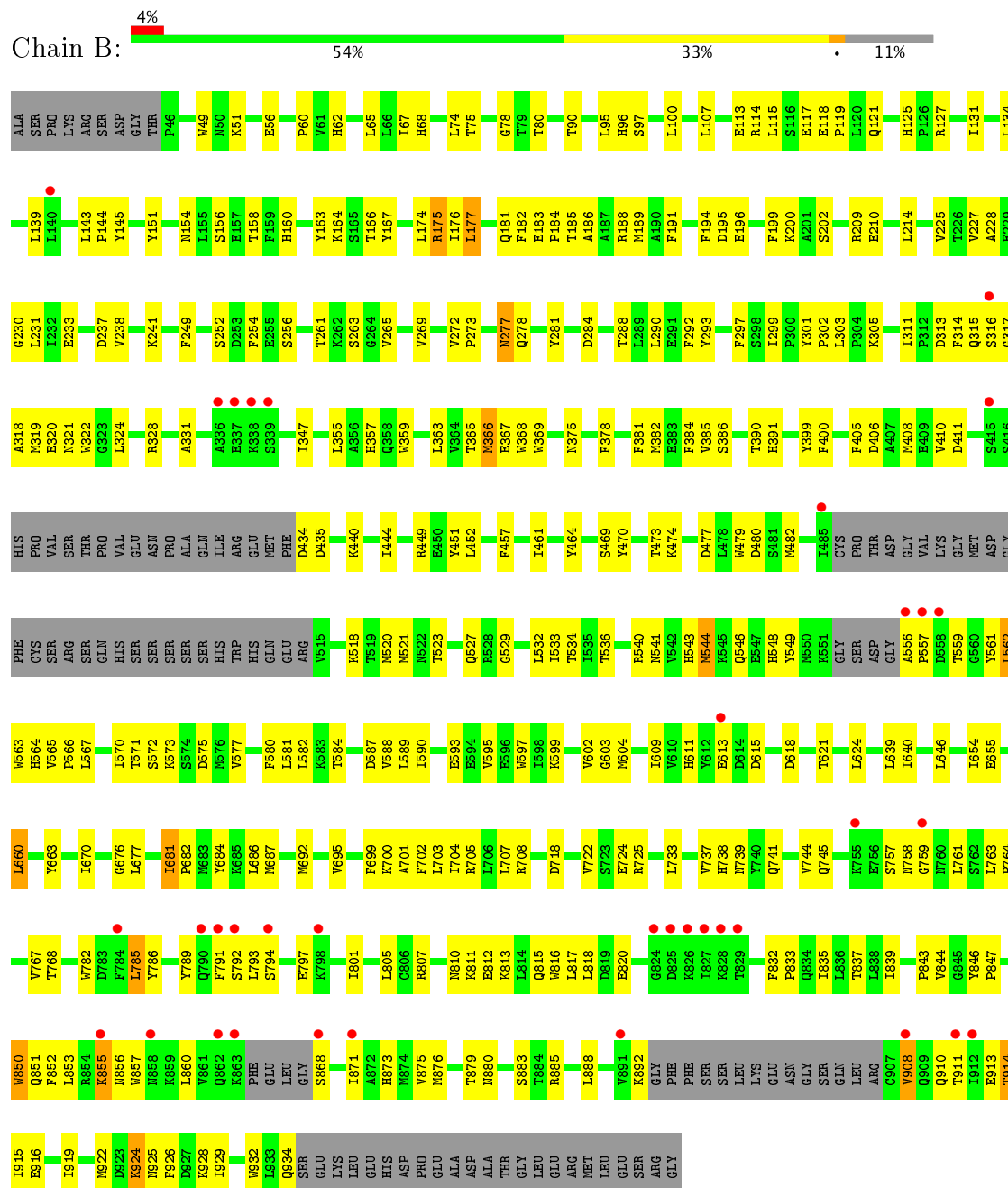
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

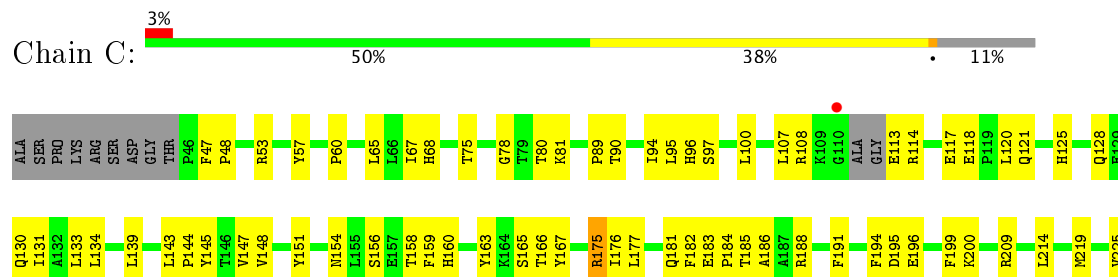
- Molecule 1: Endoplasmic reticulum aminopeptidase 1



• Molecule 1: Endoplasmic reticulum aminopeptidase 1



• Molecule 1: Endoplasmic reticulum aminopeptidase 1



LYS	S869	S795	L707	D614	K545	M479	V396	K322	T236
LEU	S870	T796	L710	D615	Q546	D480	V399	G323	V227
HIS	A871	E547	L711	G616	E548	S481	F400	T324	A228
ASP	H873	I801	T717	D618	E549	M482	F405	T325	E229
PRO	M874	E802	D718	S619	K550	L485	M408	T326	G230
GLU	V875	F803	E719	L620	K551	CYS	F405	Y327	L231
ALA	M876	A804		T621	GLY	PRO		R328	T232
ASP	T879	L805		L624	ASP	THR		A331	E233
ALA	R806	R807		K625	ASP	THR		A331	D237
THR	R807			L624	GLY	GLY		L332	V238
GLY				G628	VAL	VAL		F334	T239
LEU	S883	N810		L628	P557	LYS		E337	V240
GLU	T884	K811		L630	E558	GLY		R338	K241
ARG	R885	B812		L639	T559	MET		S339	F249
MET	T886	K813		I640	G560	ASP		HIS	
LEU	R887	L734		I649	Y561	GLY		S343	S252
GLU	L888	A735		A643	Y561	THR		K344	D263
ARG	K892			V647	E564	CYS		L345	F254
GLY		E820		S648	P566	ARG		D346	
		G824		I649	L567	SER		T347	K259
		D825		L652	I570	HIS		T348	I260
		K826		E655	T571	SER		K349	T261
		I827		L660	S572	SER		K262	K262
		K828		L660	S573	SER		G264	S263
		T829		L660	S574	SER		A356	V265
		K830		L660	D575	SER		R357	
		B831		L663	M576	HIS		V269	
		F832		V663	V577	TRP		N362	
		P833		E667	F580	HIS		L363	N277
		K834		I670	L581	GLN		V364	Q278
		I835		M671	L582	GLU		T365	A279
		L836		P672	K583	ARG		N366	D280
		T837		L677	T584	V515		E367	Y281
		V844			K585	K518		K368	K286
		G845			T586	T519		K369	V287
		Y846			D587	M520		D371	
		P847			V588	M521		L372	L290
					L589			W373	E291
		W850			I590	M524		L374	F292
		Q851			L591	T525		N375	Y293
		P852			L686	L526		F378	L303
		L853			M687			A379	P304
		K854			V596	E529		K380	K305
		N855			W597	F530		F381	
		W857			F600			N382	A310
		N858			M601			E383	
		K859			T602			F384	D313
		L860			V602			V385	F314
		V861			G603			S386	Q315
		Q862			M604			V387	S316
		K863			A701			T473	G317
		P864			F702			K474	G317
		GLU			L703			M475	A318
		LEU			I704			E476	R319
		GLY			V612			D477	E320
		S868			B613			L478	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 1.5_2	Depositor
R, R_{free}	0.199 , 0.264 0.193 , 0.260	Depositor DCC
R_{free} test set	3206 reflections (5.03%)	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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	56	0	50	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	42	0	38	1	0
4	C	28	0	24	1	0
5	A	11	0	8	0	0
5	C	11	0	8	0	0
6	A	22	0	20	1	0
6	C	22	0	20	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 ⓘ

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	804/921 (87%)	750 (93%)	50 (6%)	4 (0%)	32	71
1	B	809/921 (88%)	755 (93%)	52 (6%)	2 (0%)	51	84
1	C	805/921 (87%)	753 (94%)	51 (6%)	1 (0%)	55	87
All	All	2418/2763 (88%)	2258 (93%)	153 (6%)	7 (0%)	44	79

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%)	45	78
1	B	734/819 (90%)	711 (97%)	23 (3%)	45	78
1	C	734/819 (90%)	711 (97%)	23 (3%)	45	78
All	All	2201/2457 (90%)	2132 (97%)	69 (3%)	45	78

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 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	0.46	0	19,29,29	0.77	1 (5%)
4	NAG	A	5001	1,4	14,14,15	0.85	0	15,19,21	2.07	5 (33%)
4	NAG	A	5002	5,4	14,14,15	0.61	0	15,19,21	1.49	2 (13%)
5	BMA	A	5003	4,6	11,11,12	0.42	0	13,15,17	0.60	0
6	MAN	A	5004	5	11,11,12	0.59	0	13,15,17	0.86	0
6	MAN	A	5005	5	11,11,12	0.91	0	13,15,17	1.55	2 (15%)
4	NAG	A	6000	1	14,14,15	0.91	1 (7%)	15,19,21	1.41	2 (13%)
4	NAG	A	6001	1	14,14,15	1.27	2 (14%)	15,19,21	1.57	4 (26%)
3	BES	B	1001	2	19,22,22	0.48	0	19,29,29	0.84	1 (5%)
4	NAG	B	5001	1,4	14,14,15	0.74	0	15,19,21	1.18	1 (6%)
4	NAG	B	5002	4	14,14,15	0.63	0	15,19,21	1.59	2 (13%)
4	NAG	B	6000	1	14,14,15	0.64	0	15,19,21	0.99	1 (6%)
3	BES	C	1001	2	19,22,22	0.43	0	19,29,29	0.88	1 (5%)
4	NAG	C	5001	1,4	14,14,15	1.06	3 (21%)	15,19,21	1.96	6 (40%)
4	NAG	C	5002	5,4	14,14,15	0.71	0	15,19,21	1.84	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BMA	C	5003	4,6	11,11,12	0.39	0	13,15,17	0.50	0
6	MAN	C	5004	5	11,11,12	0.45	0	13,15,17	0.80	0
6	MAN	C	5005	5	11,11,12	0.77	0	13,15,17	1.01	1 (7%)

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
4	NAG	A	5001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	5002	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	5003	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	5004	5	-	0/2/19/22	0/1/1/1
6	MAN	A	5005	5	-	0/2/19/22	0/1/1/1
4	NAG	A	6000	1	-	0/6/23/26	0/1/1/1
4	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
4	NAG	B	5001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	5002	4	-	0/6/23/26	0/1/1/1
4	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
4	NAG	C	5001	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	C	5002	5,4	-	0/6/23/26	0/1/1/1
5	BMA	C	5003	4,6	-	0/2/19/22	0/1/1/1
6	MAN	C	5004	5	-	0/2/19/22	0/1/1/1
6	MAN	C	5005	5	-	0/2/19/22	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5001	NAG	C4-C3	-2.12	1.47	1.52
4	C	5001	NAG	O4-C4	-2.10	1.38	1.43
4	C	5001	NAG	O5-C1	2.02	1.47	1.43
4	A	6000	NAG	O5-C1	2.27	1.47	1.43
4	A	6001	NAG	O5-C1	2.67	1.48	1.43

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5001	NAG	O4-C4-C3	-4.42	100.75	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	6001	NAG	O5-C1-C2	-3.60	106.46	111.47
4	A	5001	NAG	O3-C3-C4	-3.57	102.59	110.36
4	B	5002	NAG	C4-C3-C2	-3.54	105.84	111.02
4	C	5002	NAG	C4-C3-C2	-3.51	105.88	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	6001	NAG	C1
4	C	5001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	BES	2	0
4	A	5001	NAG	3	0
6	A	5004	MAN	1	0
4	A	6001	NAG	1	0
3	B	1001	BES	10	0
4	B	5001	NAG	1	0
3	C	1001	BES	6	0
4	C	5002	NAG	1	0
6	C	5005	MAN	1	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%)	-0.23	21 (2%) 56 37	26, 57, 133, 238	11 (1%)
1	B	821/921 (89%)	-0.15	36 (4%) 35 21	24, 57, 130, 223	11 (1%)
1	C	818/921 (88%)	-0.25	27 (3%) 47 30	28, 57, 130, 223	12 (1%)
All	All	2457/2763 (88%)	-0.21	84 (3%) 46 29	24, 57, 131, 238	34 (1%)

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	SER	9.7
1	B	558	ASP	8.8
1	B	794	SER	8.4
1	B	557	PRO	8.3
1	B	827	ILE	7.4

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 carbohydrates 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. 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
6	MAN	C	5004	11/12	0.84	0.24	1.54	75,95,103,110	0
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
4	NAG	B	5001	14/15	0.91	0.21	1.00	50,93,110,139	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
4	NAG	B	6000	14/15	0.74	0.28	-	59,128,146,153	0
4	NAG	A	6000	14/15	0.82	0.19	-	76,119,141,145	0
4	NAG	C	5002	14/15	0.86	0.34	-	47,135,257,284	0
5	BMA	A	5003	11/12	0.89	0.17	-	51,86,129,131	0
4	NAG	A	5002	14/15	0.88	0.18	-	60,85,108,108	0
4	NAG	B	5002	14/15	0.75	0.25	-	118,161,189,212	0
6	MAN	C	5005	11/12	0.81	0.35	-	86,142,212,223	0
4	NAG	A	6001	14/15	0.74	0.17	-	72,140,150,153	0
6	MAN	A	5004	11/12	0.56	0.34	-	111,168,187,189	0
5	BMA	C	5003	11/12	0.85	0.26	-	43,135,191,223	0
6	MAN	A	5005	11/12	0.83	0.30	-	33,95,172,209	0

6.5 Other polymers [i](#)

There are no such residues in this entry.