wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1BJR
Title	:	COMPLEX FORMED BETWEEN PROTEOLYTICALLY GENERATED LACTOFERRIN FRAGMENT AND PROTEINASE K
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Deposited on	:	1998-06-27
Resolution	:	2.44 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 (i) symbol.

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

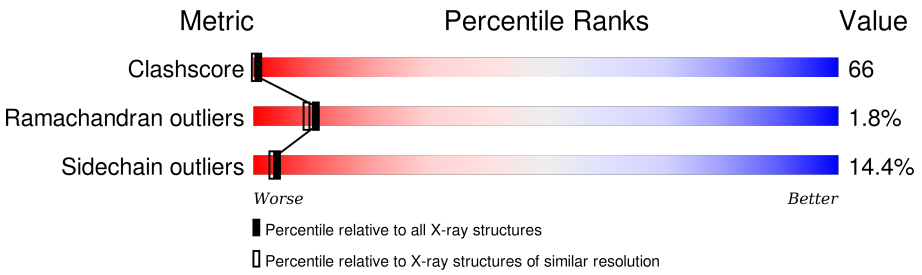
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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))
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	279	55% 36% 6% •
2	I	10	60% 30% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2289 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 PROTEINASE K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	279	2030	1247	357	416	10	0	0	0

- Molecule 2 is a protein called LACTOFERRIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	I	10	56	34	11	11	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	E	2	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	200	200	200	0	0
4	I	1	1	1	0	0

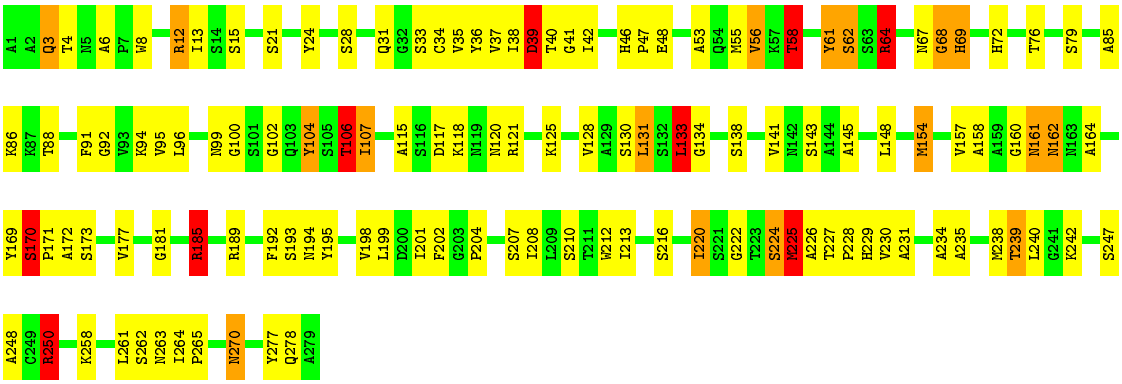
3 Residue-property plots (i)

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

Note EDS was not executed.

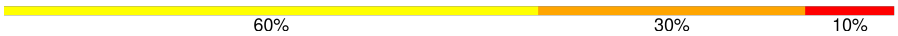
- Molecule 1: PROTEINASE K

Chain E:



- Molecule 2: LACTOFERRIN

Chain I:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.60Å 38.58Å 79.22Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	12.00 – 2.44	Depositor
% Data completeness (in resolution range)	92.2 (12.00-2.44)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CCP4	Depositor
R, R_{free}	0.160 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2289	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

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: CA

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	E	0.77	9/2069 (0.4%)	1.12	16/2810 (0.6%)
2	I	1.49	0/55	1.92	1/73 (1.4%)
All	All	0.80	9/2124 (0.4%)	1.15	17/2883 (0.6%)

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	E	0	2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	225	MET	C-N	15.35	1.69	1.34
1	E	162	ASN	N-CA	10.47	1.67	1.46
1	E	225	MET	N-CA	7.65	1.61	1.46
1	E	68	GLY	C-N	-7.09	1.17	1.34
1	E	106	THR	C-N	-7.04	1.17	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	69	HIS	O-C-N	-10.05	106.12	123.20
1	E	250	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	E	68	GLY	O-C-N	8.28	135.95	122.70
1	E	69	HIS	CA-C-N	7.78	131.76	116.20
2	I	282	GLN	N-CA-CB	7.59	124.25	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	106	THR	Mainchain
1	E	107	ILE	Mainchain

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	E	2030	0	1931	257	10
2	I	56	0	56	110	9
3	E	2	0	0	0	0
4	E	200	0	0	60	1
4	I	1	0	0	0	0
All	All	2289	0	1987	268	10

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 66.

The worst 5 of 268 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:E:225:MET:C	1:E:226:ALA:N	1.69	1.46
1:E:224:SER:OG	2:I:286:ALA:CA	1.80	1.29
1:E:100:GLY:O	2:I:281:ALA:HB3	1.36	1.21
1:E:224:SER:OG	2:I:286:ALA:HA	1.08	1.20
1:E:100:GLY:C	2:I:281:ALA:HB3	1.61	1.19

The worst 5 of 10 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	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ARG:NE	2:I:282:GLN:NE2[1_565]	1.04	1.16
1:E:250:ARG:NH1	2:I:282:GLN:OE1[1_565]	1.76	0.44
1:E:250:ARG:NE	2:I:282:GLN:CD[1_565]	1.81	0.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ARG:CD	2:I:282:GLN:NE2[1_565]	1.82	0.38
1:E:250:ARG:NH1	4:E:346:HOH:O[1_565]	1.88	0.32

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	E	277/279 (99%)	266 (96%)	9 (3%)	2 (1%)	26 32
2	I	8/10 (80%)	2 (25%)	3 (38%)	3 (38%)	0 0
All	All	285/289 (99%)	268 (94%)	12 (4%)	5 (2%)	11 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	170	SER
2	I	282	GLN
2	I	283	GLY
2	I	285	ALA
1	E	39	ASP

5.3.2 Protein sidechains (i)

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	E	213/213 (100%)	184 (86%)	29 (14%)	5 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	3/3 (100%)	1 (33%)	2 (67%)	0 0
All	All	216/216 (100%)	185 (86%)	31 (14%)	4 3

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	131	LEU
1	E	154	MET
1	E	270	ASN
1	E	133	LEU
1	E	170	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	162	ASN
1	E	270	ASN
1	E	229	HIS
1	E	119	ASN
1	E	194	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.