

Full wwPDB X-ray Structure Validation Report (i)

Dec 4, 2023 - 05:08 pm GMT

PDB ID : 2JE6

Title: Structure of a 9-subunit archaeal exosome

Authors : Lorentzen, E.; Conti, E.

Deposited on : 2007-01-15

Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS : NOT EXECUTED

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

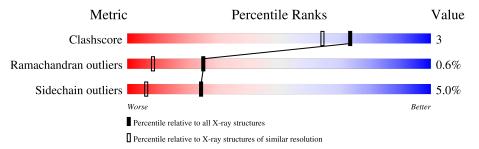
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.60 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain	
1	A	277	89%	9%
2	В	250	85%	8% 6%
3	I	251	72% 9%	• 18%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5849 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 EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	274	Total 2119	C 1357	N 341	O 414	S 7	0	10	0

• Molecule 2 is a protein called EXOSOME COMPLEX EXONUCLEASE 1.

Mo	l Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	234	Total 1813	C 1155	N 309	O 338	S 11	0	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
В	182	ALA	ASP	engineered mutation	UNP Q9UXC2	

• Molecule 3 is a protein called EXOSOME COMPLEX RNA-BINDING PROTEIN 1.

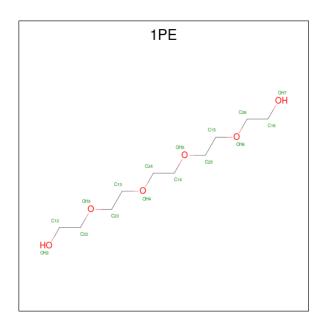
Mo	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	I	207	Total 1495	C 973	N 240	O 280	S 2	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	8	GLU	LYS	$\operatorname{conflict}$	UNP Q9UXC4

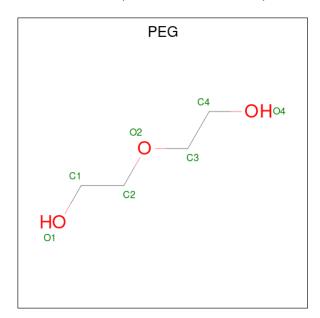
• Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).





Mol	Chain	Residues	\mathbf{At}	$\overline{\mathrm{oms}}$		ZeroOcc	AltConf
4	A	1	Total 16	C 10	O 6	0	0

 $\bullet \ \ Molecule \ 5 \ is \ DI(HYDROXYETHYL)ETHER \ (three-letter \ code: \ PEG) \ (formula: \ C_4H_{10}O_3).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0

 \bullet Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Cl 1 1	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	211	Total O 211 211	0	0
7	В	151	Total O 151 151	0	0
7	I	36	Total O 36 36	0	0

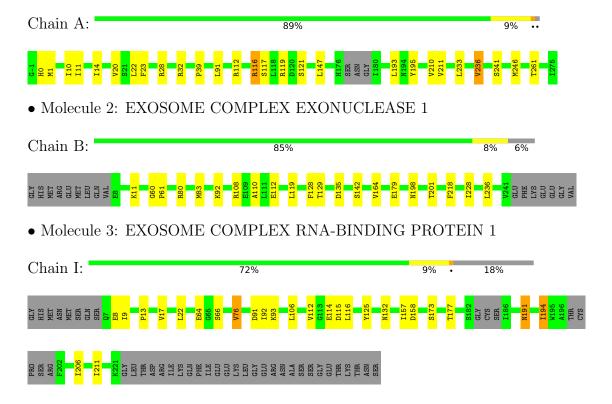


3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: EXOSOME COMPLEX EXONUCLEASE 2





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 3	Depositor	
Cell constants	135.49Å 135.49Å 135.49Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	45.18 - 1.60	Depositor	
% Data completeness	100.0 (45.18-1.60)	Depositor	
(in resolution range)	100.0 (49.10 1.00)		
R_{merge}	0.10	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	REFMAC 5.2.0005	Depositor	
R, R_{free}	0.215 , 0.249	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	5849	wwPDB-VP	
Average B, all atoms (Å ²)	40.0	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: 1PE, CL, PEG

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).

Mal	Clasia	Bond lengths		Bond angles	
Mol Chain		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.72	1/2178 (0.0%)	0.95	8/2961 (0.3%)
2	В	0.68	0/1865	0.84	0/2524
3	I	0.43	0/1526	0.60	0/2091
All	All	0.64	$1/5569 \ (0.0\%)$	0.83	8/7576 (0.1%)

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 maintain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	2

All (1) bond length outliers are listed below:

I	Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(ext{\AA})$
	1	A	116	ARG	CD-NE	-5.07	1.37	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	116	ARG	NE-CZ-NH2	-17.94	111.33	120.30
1	A	116	ARG	NE-CZ-NH1	15.95	128.27	120.30
1	A	236	VAL	CG1-CB-CG2	7.42	122.77	110.90
1	A	112	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	236	VAL	N-CA-CB	-5.44	99.52	111.50
1	A	32	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	116	ARG	CD-NE-CZ	5.39	131.15	123.60
1	A	116	ARG	CG-CD-NE	-5.21	100.86	111.80



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	60	GLY	Peptide, 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	A	2119	0	2172	16	0
2	В	1813	0	1866	12	0
3	I	1495	0	1395	11	1
4	A	16	0	22	0	0
5	A	7	0	10	1	0
6	В	1	0	0	0	0
7	A	211	0	0	1	1
7	В	151	0	0	3	1
7	I	36	0	0	0	0
All	All	5849	0	5465	36	2

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 3.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:116:ARG:HD2	7:B:2120:HOH:O	1.85	0.75
2:B:129:THR:HG21	2:B:142:SER:OG	1.90	0.70
1:A:0:HIS:ND1	7:A:2001:HOH:O	2.25	0.67
3:I:93:LYS:NZ	3:I:158:ASP:HB3	2.12	0.65
2:B:135:ASP:OD1	2:B:179:GLU:HB2	1.99	0.62
1:A:28:ARG:CZ	1:A:210[B]:VAL:CG2	2.79	0.61
1:A:20:VAL:O	1:A:20:VAL:HG12	2.01	0.60
3:I:206:ILE:O	3:I:206:ILE:HG23	2.02	0.60
3:I:93:LYS:HZ3	3:I:158:ASP:HB3	1.67	0.59
2:B:80:ARG:HD3	7:B:2080:HOH:O	2.02	0.58
1:A:14:ILE:HD12	1:A:14:ILE:H	1.69	0.58

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Atom 1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
1:A:91:LEU:HD12	1:A:147:LEU:HD23	1.84	0.58
1:A:20:VAL:HG13	1:A:23:PHE:CD2	2.40	0.57
1:A:28:ARG:NH1	1:A:210[A]:VAL:HG13	2.19	0.57
1:A:1[B]:MET:HG2	2:B:80:ARG:HB2	1.87	0.57
3:I:76:VAL:HG22	3:I:191:ASN:CG	2.28	0.53
3:I:92:ILE:O	3:I:191:ASN:ND2	2.42	0.52
2:B:108:ARG:O	2:B:112:GLU:HG2	2.10	0.51
1:A:39:PRO:HB2	5:A:1277:PEG:H32	1.93	0.50
1:A:28:ARG:CZ	1:A:210[B]:VAL:HG22	2.42	0.49
3:I:194:ILE:HD13	3:I:211:ILE:HD13	1.95	0.48
2:B:80:ARG:O	2:B:129:THR:HG22	2.14	0.48
1:A:1[B]:MET:SD	2:B:128:PHE:HE2	2.36	0.48
1:A:14:ILE:HD13	3:I:125:TYR:CD1	2.49	0.47
1:A:28:ARG:NH1	1:A:210[B]:VAL:HG22	2.31	0.46
3:I:194:ILE:HD13	3:I:211:ILE:CD1	2.46	0.46
1:A:117:SER:O	1:A:121:SER:HB3	2.16	0.46
1:A:211:VAL:HG11	1:A:261:THR:HG21	1.98	0.45
2:B:164[A]:VAL:HG13	2:B:228:ILE:CD1	2.45	0.45
3:I:157:ILE:HD12	3:I:194:ILE:HD11	2.00	0.43
3:I:173:SER:O	3:I:177:THR:HG22	2.19	0.43
2:B:110:ALA:HA	2:B:201[A]:THR:OG1	2.19	0.42
2:B:198:ASN:HB2	7:B:2118:HOH:O	2.19	0.42
2:B:198:ASN:O	2:B:198:ASN:CG	2.59	0.41
3:I:191:ASN:HD22	3:I:191:ASN:HA	1.62	0.41
2:B:164[A]:VAL:CG1	2:B:228:ILE:CD1	3.00	0.40

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	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
3:I:112:VAL:O	3:I:132:ASN:OD1[10_545]	2.06	0.14
7:A:2125:HOH:O	7:B:2041:HOH:O[7_555]	2.12	0.08

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	Perce	\mathbf{ntiles}
1	A	280/277 (101%)	272 (97%)	8 (3%)	0	100	100
2	В	240/250 (96%)	235 (98%)	4 (2%)	1 (0%)	34	15
3	I	202/251 (80%)	185 (92%)	14 (7%)	3 (2%)	10	2
All	All	722/778 (93%)	692 (96%)	26 (4%)	4 (1%)	25	8

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	13	PRO
2	В	61	PRO
3	I	116	LEU
3	I	115	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	A	238/243 (98%)	227 (95%)	11 (5%)	27 8
2	В	194/208 (93%)	186 (96%)	8 (4%)	30 9
3	I	144/223 (65%)	132 (92%)	12 (8%)	11 2
All	All	576/674 (86%)	545 (95%)	31 (5%)	24 5

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	ILE
1	A	22	LEU
1	A	119	ARG
1	A	193	LEU
1	A	195	TYR

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Mol	Chain	Res	Type
1	A	233	LEU
1	A	236	VAL
1	A	241	SER
1	A	246[A]	MET
1	A	246[B]	MET
2	В	11	LYS
2	В	83[A]	MET
2	В	83[B]	MET
2 2	В	92	LYS
	В	119	LEU
2	В	218[A]	PHE
2	В	218[B]	PHE
2	В	236	LEU
3	I	8	GLU
3	I	9	ILE
3	I	17	VAL
3	I	22	LEU
3	I	64	GLU
3	I	66	SER
3	I	76	VAL
3	I	91	ASP
3	I	106	LEU
3	I	114	GLU
3	I	191	ASN
3	I	194	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	\mathbf{Type}	
1	A	272	HIS	
2	В	198	ASN	
3	I	57	GLN	
3	I	190	ASN	
3	I	191	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	Bo	ond leng	ths	В	ond ang	les
IVIOI	туре	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PEG	A	1277	-	6,6,6	0.48	0	5,5,5	0.20	0
4	1PE	A	1276	-	15,15,15	0.49	0	14,14,14	0.20	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	PEG	A	1277	-	-	3/4/4/4	-
4	1PE	A	1276	-	-	4/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1276	1PE	OH4-C13-C23-OH3
5	A	1277	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	1277	PEG	O2-C3-C4-O4
5	A	1277	PEG	C4-C3-O2-C2
4	A	1276	1PE	C16-C26-OH6-C15
4	A	1276	1PE	C12-C22-OH3-C23
4	A	1276	1PE	C24-C14-OH5-C25

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1277	PEG	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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

