



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:54 AM UTC

PDB ID : 1SSB / pdb_00001ssb
Title : A STRUCTURAL INVESTIGATION OF CATALYTICALLY MODIFIED
F12OL AND F12OY SEMISYNTHETIC RIBONUCLEASES
Authors : Demel, V.S.J.; Doscher, M.S.; Glinn, M.A.; Martin, P.D.; Ram, M.L.; Ed-
wards, B.F.P.
Deposited on : 1993-08-03
Resolution : 2.00 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

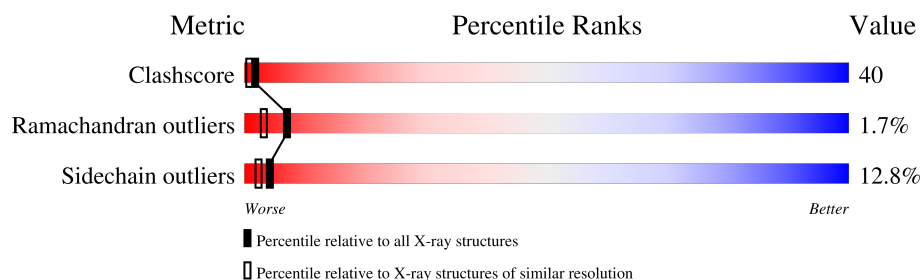
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

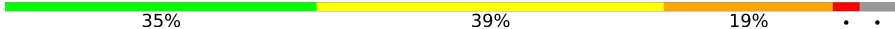
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	118	 35% 39% 19% . .
2	B	14	 29% 21% 21% 7% 21%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1052 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 RIBONUCLEASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	113	863	516	158	177	12	0	0	0

- Molecule 2 is a protein called RIBONUCLEASE A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	11	89	59	13	17	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	113	SER	ASN	conflict	UNP P61823

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	14	Total	O	0	0
			14	14		

Note EDS was not executed.

Chain A: 35% 39% 19% . .



Chain B:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	68.15Å 68.15Å 65.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.184 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1052	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	1.73	8/874 (0.9%)	2.49	63/1175 (5.4%)
2	B	1.70	2/93 (2.2%)	2.87	8/127 (6.3%)
All	All	1.73	10/967 (1.0%)	2.53	71/1302 (5.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	VAL	N-CA	7.42	1.54	1.46
1	A	46	PHE	N-CA	6.24	1.53	1.46
1	A	55	GLN	N-CA	6.03	1.53	1.46
2	B	123	SER	C-N	-5.63	1.25	1.33
1	A	12	HIS	CG-CD2	5.39	1.41	1.35
1	A	87	THR	CB-OG1	5.29	1.52	1.43
1	A	85	ARG	N-CA	5.15	1.52	1.46
1	A	85	ARG	CD-NE	-5.14	1.39	1.46
1	A	75	SER	N-CA	5.10	1.52	1.46
2	B	123	SER	CA-C	5.05	1.58	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122	ALA	CA-C-N	11.46	139.55	122.93
2	B	122	ALA	C-N-CA	11.46	139.55	122.93
2	B	123	SER	CA-C-N	11.12	141.71	121.70
2	B	123	SER	C-N-CA	11.12	141.71	121.70
1	A	108	VAL	N-CA-CB	-10.82	91.92	111.93
1	A	98	LYS	N-CA-CB	10.34	126.98	110.23
1	A	63	VAL	N-CA-CB	-10.11	93.67	112.36
1	A	108	VAL	CB-CA-C	9.28	125.54	110.69
2	B	118	VAL	N-CA-CB	-9.07	96.26	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ASN	CA-C-O	-8.79	110.89	120.30
1	A	60	GLN	OE1-CD-NE2	-8.43	114.17	122.60
1	A	98	LYS	CB-CA-C	-8.15	96.08	109.53
1	A	113	ASN	CA-C-O	-8.12	107.00	120.80
1	A	103	ASN	CA-CB-CG	-7.83	104.77	112.60
1	A	54	VAL	N-CA-C	-7.33	103.64	110.53
1	A	113	ASN	OD1-CG-ND2	7.22	129.82	122.60
1	A	33	ARG	NE-CZ-NH2	-7.09	112.82	119.20
1	A	65	CYS	N-CA-C	-7.09	100.31	110.59
1	A	107	ILE	O-C-N	7.02	130.78	123.20
1	A	105	HIS	CA-C-O	-7.00	113.08	121.05
1	A	41	LYS	N-CA-C	-6.99	99.41	109.48
1	A	53	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	22	SER	CA-C-N	6.67	130.46	120.31
1	A	22	SER	C-N-CA	6.67	130.46	120.31
1	A	76	TYR	CA-C-O	6.62	127.59	119.97
1	A	40	CYS	CA-C-O	-6.44	113.89	120.84
2	B	118	VAL	CB-CA-C	6.36	121.72	111.29
1	A	47	VAL	O-C-N	6.28	130.00	123.03
1	A	109	ALA	CA-C-O	-6.28	113.70	120.92
1	A	98	LYS	N-CA-C	-6.27	99.43	109.96
1	A	33	ARG	NE-CZ-NH1	6.21	127.71	121.50
1	A	99	THR	OG1-CB-CG2	6.21	121.71	109.30
1	A	33	ARG	CD-NE-CZ	6.04	132.86	124.40
1	A	79	MET	CA-C-O	-5.96	114.49	121.46
1	A	74	GLN	OE1-CD-NE2	5.89	128.49	122.60
1	A	37	LYS	CA-C-O	-5.85	114.22	120.42
1	A	86	GLU	CB-CG-CD	5.85	122.54	112.60
1	A	49	GLU	N-CA-CB	5.81	121.03	111.62
1	A	113	ASN	N-CA-CB	5.75	120.27	110.50
1	A	82	THR	N-CA-CB	5.75	119.79	110.77
2	B	123	SER	CB-CA-C	-5.74	99.05	109.38
1	A	5	ALA	CA-C-N	5.71	128.41	120.29
1	A	5	ALA	C-N-CA	5.71	128.41	120.29
1	A	47	VAL	CA-C-O	-5.70	114.47	120.57
1	A	87	THR	CA-C-N	5.62	126.22	119.98
1	A	87	THR	C-N-CA	5.62	126.22	119.98
1	A	19	ALA	CA-C-N	5.62	129.34	121.02
1	A	19	ALA	C-N-CA	5.62	129.34	121.02
1	A	85	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	A	74	GLN	CB-CG-CD	-5.57	103.13	112.60
1	A	61	LYS	CA-CB-CG	5.55	125.21	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ILE	CA-C-O	-5.55	116.20	121.64
1	A	39	ARG	N-CA-CB	-5.54	102.51	110.87
1	A	29	MET	CA-C-O	-5.43	114.79	120.55
1	A	10	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	A	80	SER	CA-C-O	-5.33	114.61	120.69
1	A	37	LYS	N-CA-C	5.29	117.13	111.36
1	A	62	ASN	CB-CA-C	5.27	118.43	109.84
1	A	24	ASN	CA-C-O	-5.26	112.91	119.28
1	A	12	HIS	N-CA-CB	-5.26	102.96	110.80
1	A	30	MET	N-CA-C	-5.21	105.68	111.36
1	A	82	THR	CA-CB-CG2	5.20	119.34	110.50
1	A	106	ILE	O-C-N	5.15	128.54	122.36
2	B	115	TYR	CA-CB-CG	5.15	123.17	113.90
1	A	54	VAL	CB-CA-C	5.10	118.70	112.02
1	A	32	SER	CB-CA-C	-5.09	102.02	110.68
1	A	69	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	11	GLN	N-CA-C	5.04	117.89	111.69
1	A	106	ILE	CA-C-O	-5.03	116.30	121.93
1	A	101	GLN	CA-CB-CG	5.02	124.15	114.10
1	A	43	VAL	CA-C-O	-5.00	115.25	120.76

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	863	0	825	71	0
2	B	89	0	80	7	0
3	B	5	0	0	0	0
4	A	81	0	0	15	0
4	B	14	0	0	2	0
All	All	1052	0	905	75	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 40.

All (75) 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:A:61:LYS:HZ2	1:A:74:GLN:NE2	1.32	1.26
1:A:91:LYS:HD2	1:A:92:TYR:N	1.56	1.17
1:A:85:ARG:O	4:A:187:HOH:O	1.66	1.12
1:A:61:LYS:NZ	1:A:74:GLN:NE2	1.97	1.10
1:A:61:LYS:NZ	1:A:74:GLN:HE22	1.49	1.06
1:A:91:LYS:HD2	1:A:92:TYR:H	0.90	1.05
1:A:1:LYS:O	1:A:1:LYS:HG3	1.53	1.02
1:A:32:SER:HB3	4:A:198:HOH:O	1.59	1.02
1:A:7:LYS:HG2	4:A:141:HOH:O	1.58	1.01
1:A:87:THR:HG22	1:A:98:LYS:CD	1.90	1.01
1:A:87:THR:HG22	1:A:98:LYS:CE	1.97	0.94
1:A:87:THR:HG22	1:A:98:LYS:HE3	1.51	0.88
1:A:34:ASN:HA	1:A:37:LYS:NZ	1.91	0.86
1:A:7:LYS:CG	4:A:141:HOH:O	2.21	0.84
1:A:34:ASN:HA	1:A:37:LYS:HZ2	1.43	0.83
1:A:91:LYS:CD	1:A:92:TYR:H	1.85	0.83
1:A:87:THR:HG22	1:A:98:LYS:HD2	1.61	0.82
1:A:88:GLY:HA2	4:A:213:HOH:O	1.81	0.80
1:A:61:LYS:HZ2	1:A:74:GLN:HE22	0.81	0.79
1:A:37:LYS:N	1:A:37:LYS:HE3	2.00	0.76
1:A:112:GLY:HA2	2:B:114:PRO:O	1.85	0.76
1:A:61:LYS:HD3	4:A:221:HOH:O	1.86	0.75
1:A:98:LYS:HD3	4:A:187:HOH:O	1.85	0.75
1:A:1:LYS:O	1:A:1:LYS:CG	2.33	0.72
1:A:26:CYS:HB2	1:A:99:THR:HG22	1.70	0.72
1:A:34:ASN:CA	1:A:37:LYS:HZ2	2.03	0.71
1:A:87:THR:CG2	1:A:98:LYS:HE3	2.22	0.69
1:A:27:ASN:HD21	1:A:97:TYR:H	1.38	0.69
1:A:26:CYS:SG	1:A:99:THR:HB	2.32	0.68
1:A:36:THR:C	1:A:37:LYS:HE3	2.19	0.67
1:A:86:GLU:OE2	1:A:90:SER:OG	2.07	0.66
1:A:26:CYS:H	1:A:99:THR:HG21	1.62	0.65
1:A:66:LYS:HE3	2:B:121:ASP:O	1.97	0.64
1:A:98:LYS:HD3	1:A:98:LYS:N	2.14	0.63
1:A:104:LYS:HD2	2:B:123:SER:HB3	1.80	0.62
2:B:124:VAL:C	4:B:225:HOH:O	2.42	0.62
1:A:71:ASN:H	1:A:71:ASN:HD22	1.48	0.62
1:A:34:ASN:C	1:A:37:LYS:HZ2	2.08	0.62
1:A:11:GLN:HG2	1:A:35:LEU:HD21	1.83	0.61
1:A:98:LYS:HD3	1:A:98:LYS:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HG3	4:A:141:HOH:O	2.01	0.60
1:A:98:LYS:N	4:A:187:HOH:O	1.64	0.60
1:A:61:LYS:HZ1	1:A:74:GLN:NE2	1.95	0.60
1:A:24:ASN:OD1	1:A:28:GLN:NE2	2.29	0.59
1:A:67:ASN:HD21	1:A:69:GLN:CD	2.11	0.58
1:A:43:VAL:HG13	4:A:211:HOH:O	2.04	0.58
1:A:87:THR:CB	1:A:98:LYS:HE3	2.35	0.57
2:B:114:PRO:HG2	2:B:115:TYR:H	1.70	0.56
1:A:1:LYS:O	1:A:1:LYS:NZ	2.33	0.55
1:A:28:GLN:HG3	4:A:181:HOH:O	2.06	0.55
1:A:91:LYS:CD	1:A:92:TYR:N	2.50	0.55
1:A:87:THR:O	4:A:207:HOH:O	2.18	0.54
1:A:55:GLN:NE2	4:A:158:HOH:O	2.22	0.53
1:A:87:THR:HA	1:A:98:LYS:HE3	1.92	0.51
1:A:98:LYS:CD	1:A:98:LYS:N	2.72	0.51
1:A:7:LYS:HG3	4:A:183:HOH:O	2.11	0.50
1:A:24:ASN:ND2	1:A:27:ASN:HB2	2.27	0.50
1:A:34:ASN:HA	1:A:37:LYS:HZ3	1.72	0.49
2:B:114:PRO:HD3	4:B:176:HOH:O	2.12	0.49
1:A:14:ASP:O	1:A:48:HIS:HA	2.12	0.48
1:A:26:CYS:H	1:A:99:THR:CG2	2.26	0.48
1:A:17:THR:O	1:A:48:HIS:HB3	2.14	0.48
1:A:14:ASP:OD2	1:A:17:THR:OG1	2.31	0.47
1:A:113:ASN:N	1:A:113:ASN:OD1	2.48	0.47
1:A:27:ASN:HD21	1:A:97:TYR:N	2.11	0.46
2:B:124:VAL:HG22	2:B:124:VAL:O	2.18	0.44
1:A:87:THR:CG2	1:A:98:LYS:HD2	2.40	0.43
1:A:61:LYS:HE3	1:A:61:LYS:HB2	1.58	0.43
1:A:62:ASN:HB2	1:A:73:TYR:CE2	2.54	0.43
1:A:91:LYS:HD3	1:A:91:LYS:HA	1.80	0.42
1:A:106:ILE:HG21	1:A:106:ILE:HD13	1.81	0.42
1:A:26:CYS:CB	1:A:99:THR:HG22	2.43	0.42
1:A:30:MET:HE3	1:A:30:MET:HB3	1.90	0.42
1:A:87:THR:HA	1:A:98:LYS:CE	2.50	0.41
1:A:2:GLU:HA	4:A:142:HOH:O	2.18	0.41

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	111/118 (94%)	105 (95%)	5 (4%)	1 (1%)	14	9
2	B	9/14 (64%)	7 (78%)	1 (11%)	1 (11%)	0	0
All	All	120/132 (91%)	112 (93%)	6 (5%)	2 (2%)	7	3

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
2	B	122	ALA

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	99/104 (95%)	87 (88%)	12 (12%)	5	3
2	B	10/12 (83%)	8 (80%)	2 (20%)	1	0
All	All	109/116 (94%)	95 (87%)	14 (13%)	4	2

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	28	GLN
1	A	32	SER
1	A	37	LYS

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Mol	Chain	Res	Type
1	A	39	ARG
1	A	63	VAL
1	A	71	ASN
1	A	91	LYS
1	A	93	PRO
1	A	98	LYS
1	A	99	THR
1	A	108	VAL
2	B	115	TYR
2	B	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	74	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	SO4	B	125	-	4,4,4	0.94	0	6,6,6	0.70	0

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.