WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 18, 2023 – 09:38 AM EST

PDB ID	:	1VI5
Title	:	Crystal structure of ribosomal protein S2P
Authors	:	Structural GenomiX
Deposited on	:	2003-12-01
Resolution	:	2.65 Å(reported)

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

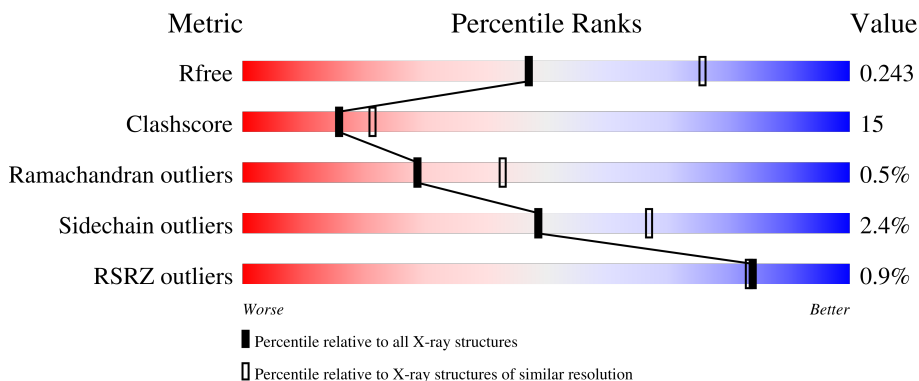|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.65 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		15
Ramachandran outliers		0.5%
Sidechain outliers		2.4%
RSRZ outliers		0.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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% 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	208	74% 19% • 5%
1	B	208	74% 19% • 6%
1	C	208	67% 25% • 7%
1	D	208	2% 59% 31% • 8%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6456 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 30S ribosomal protein S2P.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	Se	0	0	0
			1564	1003	265	292	1	3			
1	B	195	Total	C	N	O	S	Se	0	0	0
			1549	996	261	288	1	3			
1	C	193	Total	C	N	O	S	Se	0	0	0
			1531	985	258	284	1	3			
1	D	192	Total	C	N	O	S	Se	0	0	0
			1510	973	256	277	1	3			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MSE	-	cloning artifact	UNP O29132
A	1	SER	-	cloning artifact	UNP O29132
A	2	LEU	-	cloning artifact	UNP O29132
A	31	MSE	MET	modified residue	UNP O29132
A	85	MSE	MET	modified residue	UNP O29132
A	108	MSE	MET	modified residue	UNP O29132
A	198	GLU	-	cloning artifact	UNP O29132
A	199	GLY	-	cloning artifact	UNP O29132
A	200	GLY	-	cloning artifact	UNP O29132
A	201	SER	-	cloning artifact	UNP O29132
A	202	HIS	-	cloning artifact	UNP O29132
A	203	HIS	-	cloning artifact	UNP O29132
A	204	HIS	-	cloning artifact	UNP O29132
A	205	HIS	-	cloning artifact	UNP O29132
A	206	HIS	-	cloning artifact	UNP O29132
A	207	HIS	-	cloning artifact	UNP O29132
B	0	MSE	-	cloning artifact	UNP O29132
B	1	SER	-	cloning artifact	UNP O29132
B	2	LEU	-	cloning artifact	UNP O29132
B	31	MSE	MET	modified residue	UNP O29132
B	85	MSE	MET	modified residue	UNP O29132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	MSE	MET	modified residue	UNP O29132
B	198	GLU	-	cloning artifact	UNP O29132
B	199	GLY	-	cloning artifact	UNP O29132
B	200	GLY	-	cloning artifact	UNP O29132
B	201	SER	-	cloning artifact	UNP O29132
B	202	HIS	-	cloning artifact	UNP O29132
B	203	HIS	-	cloning artifact	UNP O29132
B	204	HIS	-	cloning artifact	UNP O29132
B	205	HIS	-	cloning artifact	UNP O29132
B	206	HIS	-	cloning artifact	UNP O29132
B	207	HIS	-	cloning artifact	UNP O29132
C	0	MSE	-	cloning artifact	UNP O29132
C	1	SER	-	cloning artifact	UNP O29132
C	2	LEU	-	cloning artifact	UNP O29132
C	31	MSE	MET	modified residue	UNP O29132
C	85	MSE	MET	modified residue	UNP O29132
C	108	MSE	MET	modified residue	UNP O29132
C	198	GLU	-	cloning artifact	UNP O29132
C	199	GLY	-	cloning artifact	UNP O29132
C	200	GLY	-	cloning artifact	UNP O29132
C	201	SER	-	cloning artifact	UNP O29132
C	202	HIS	-	cloning artifact	UNP O29132
C	203	HIS	-	cloning artifact	UNP O29132
C	204	HIS	-	cloning artifact	UNP O29132
C	205	HIS	-	cloning artifact	UNP O29132
C	206	HIS	-	cloning artifact	UNP O29132
C	207	HIS	-	cloning artifact	UNP O29132
D	0	MSE	-	cloning artifact	UNP O29132
D	1	SER	-	cloning artifact	UNP O29132
D	2	LEU	-	cloning artifact	UNP O29132
D	31	MSE	MET	modified residue	UNP O29132
D	85	MSE	MET	modified residue	UNP O29132
D	108	MSE	MET	modified residue	UNP O29132
D	198	GLU	-	cloning artifact	UNP O29132
D	199	GLY	-	cloning artifact	UNP O29132
D	200	GLY	-	cloning artifact	UNP O29132
D	201	SER	-	cloning artifact	UNP O29132
D	202	HIS	-	cloning artifact	UNP O29132
D	203	HIS	-	cloning artifact	UNP O29132
D	204	HIS	-	cloning artifact	UNP O29132
D	205	HIS	-	cloning artifact	UNP O29132
D	206	HIS	-	cloning artifact	UNP O29132

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Chain	Residue	Modelled	Actual	Comment	Reference
D	207	HIS	-	cloning artifact	UNP O29132

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	83	Total 83	O 83	0	0
2	B	91	Total 91	O 91	0	0
2	C	82	Total 82	O 82	0	0
2	D	46	Total 46	O 46	0	0

3   Residue-property plots ⓘ

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 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.
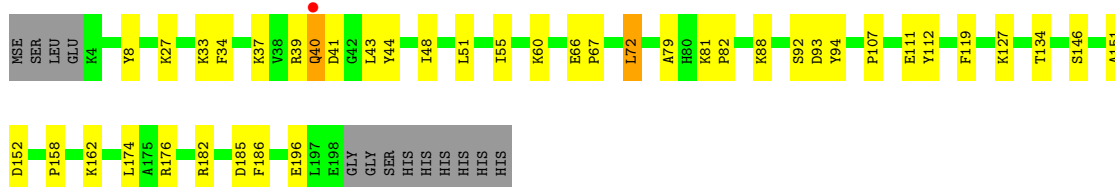
• Molecule 1: 30S ribosomal protein S2P

Chain A:
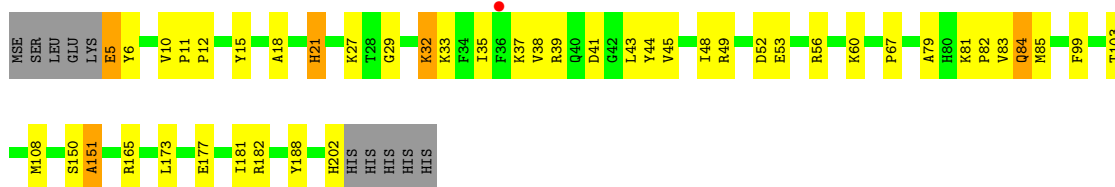
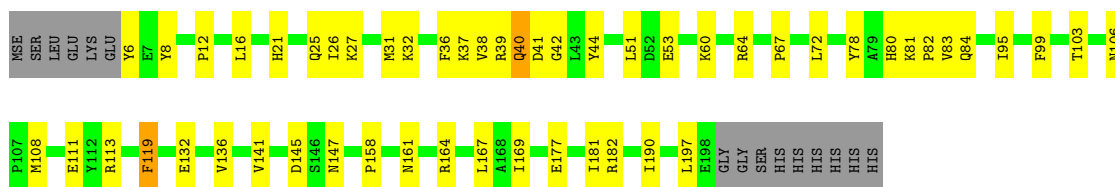• Molecule 1: 30S ribosomal protein S2P

Chain B:

• Molecule 1: 30S ribosomal protein S2P
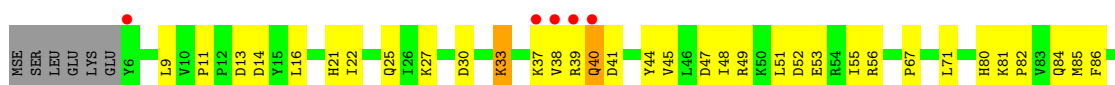
Chain C:

• Molecule 1: 30S ribosomal protein S2P

Chain D:

V90 I95 R98 F99 I100 T103 L104 T105 N106 P107 M108 E111 Y112 R113 E114 P115 E116 V117 V118 K127 Q128 V136 G337 I138 P139 S150 L155 P158 R165 I169 V170 L173 L174 A175 R176 E177 I181 R182 F186 E191 D192 F193 E194 L197

GLU GLY GLY SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.02Å 96.21Å 160.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.70 – 2.65 54.70 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (54.70-2.65) 99.9 (54.70-2.65)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.65Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.246 , 0.288 0.204 , 0.243	Depositor DCC
R_{free} test set	1707 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.7	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6456	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	0.36	0/1593	0.62	0/2155
1	B	0.39	0/1577	0.65	0/2133
1	C	0.37	0/1559	0.62	0/2110
1	D	0.34	0/1538	0.58	0/2083
All	All	0.37	0/6267	0.62	0/8481

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 ⓘ

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	1564	0	1575	47	0
1	B	1549	0	1570	29	0
1	C	1531	0	1551	48	0
1	D	1510	0	1523	66	0
2	A	83	0	0	0	0
2	B	91	0	0	2	0
2	C	82	0	0	0	0
2	D	46	0	0	1	0
All	All	6456	0	6219	181	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 15.

The worst 5 of 181 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:D:37:LYS:HG3	1:D:38:VAL:H	1.38	0.89
1:A:27:LYS:HG3	1:A:35:ILE:HD12	1.56	0.87
1:D:39:ARG:HB2	1:D:45:VAL:HG22	1.58	0.84
1:B:134:THR:HG21	1:B:152:ASP:HB3	1.60	0.82
1:D:39:ARG:HB2	1:D:45:VAL:CG2	2.11	0.80

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	196/208 (94%)	186 (95%)	8 (4%)	2 (1%)	15	23
1	B	193/208 (93%)	187 (97%)	5 (3%)	1 (0%)	29	43
1	C	191/208 (92%)	184 (96%)	7 (4%)	0	100	100
1	D	190/208 (91%)	173 (91%)	16 (8%)	1 (0%)	29	43
All	All	770/832 (92%)	730 (95%)	36 (5%)	4 (0%)	29	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	ALA
1	B	151	ALA
1	D	40	GLN
1	A	67	PRO

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	168/174 (97%)	164 (98%)	4 (2%)	49	67
1	B	167/174 (96%)	163 (98%)	4 (2%)	49	67
1	C	165/174 (95%)	163 (99%)	2 (1%)	71	84
1	D	160/174 (92%)	154 (96%)	6 (4%)	33	49
All	All	660/696 (95%)	644 (98%)	16 (2%)	49	67

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	155	LEU
1	D	127	LYS
1	C	40	GLN
1	D	113	ARG
1	B	185	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	84	GLN
1	C	147	ASN
1	D	184	GLN
1	D	77	GLN
1	D	84	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	195/208 (93%)	-0.14	1 (0%)	91	91	22, 35, 54, 83	0
1	B	192/208 (92%)	-0.10	1 (0%)	91	91	23, 34, 49, 71	0
1	C	190/208 (91%)	-0.20	0	100	100	20, 36, 55, 71	0
1	D	189/208 (90%)	0.24	5 (2%)	56	52	28, 51, 77, 97	0
All	All	766/832 (92%)	-0.05	7 (0%)	84	83	20, 37, 66, 97	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	VAL	4.5
1	D	39	ARG	4.1
1	A	36	PHE	3.2
1	D	40	GLN	2.8
1	D	6	TYR	2.7

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.