



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 12:24 PM EDT

PDB ID : 6HUA
Title : the competence regulator ComR from *Streptococcus vestibularis* in complex with its cognate signaling peptide XIP
Authors : Nessler, S.; Thuillier, J.; Ledesma, L.; Hols, P.
Deposited on : 2018-10-05
Resolution : 3.39 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

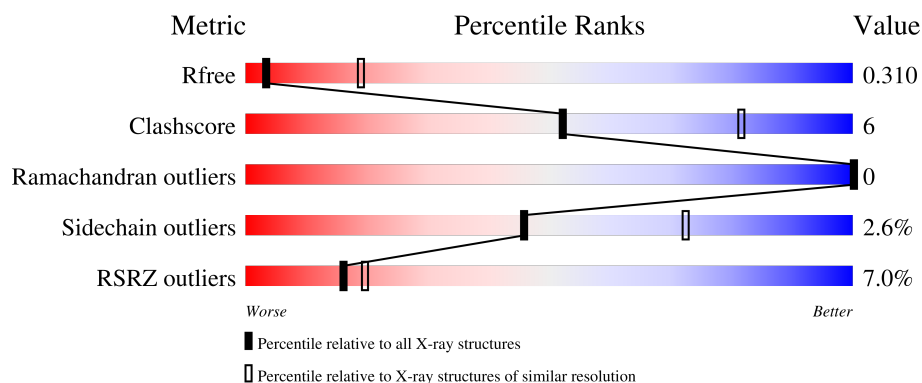
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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}	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 $\leq 5\%$. 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	310	<div> <div>11%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>5%</div> </div> </div>
1	B	310	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>15%</div> <div>26%</div> </div> </div>
2	C	8	<div> <div></div> <div> <div>62%</div> <div>38%</div> </div> </div>
2	D	8	<div> <div></div> <div>100%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4509 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2442	1572	398	465	7			
1	B	229	Total	C	N	O	S	0	0	0
			1913	1244	302	364	3			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	GLY	-	expression tag	UNP E3CNF6
A	301	ALA	-	expression tag	UNP E3CNF6
A	302	GLY	-	expression tag	UNP E3CNF6
A	303	TRP	-	expression tag	UNP E3CNF6
A	304	SER	-	expression tag	UNP E3CNF6
A	305	HIS	-	expression tag	UNP E3CNF6
A	306	PRO	-	expression tag	UNP E3CNF6
A	307	GLN	-	expression tag	UNP E3CNF6
A	308	PHE	-	expression tag	UNP E3CNF6
A	309	GLU	-	expression tag	UNP E3CNF6
A	310	LYS	-	expression tag	UNP E3CNF6
B	300	GLY	-	expression tag	UNP E3CNF6
B	301	ALA	-	expression tag	UNP E3CNF6
B	302	GLY	-	expression tag	UNP E3CNF6
B	303	TRP	-	expression tag	UNP E3CNF6
B	304	SER	-	expression tag	UNP E3CNF6
B	305	HIS	-	expression tag	UNP E3CNF6
B	306	PRO	-	expression tag	UNP E3CNF6
B	307	GLN	-	expression tag	UNP E3CNF6
B	308	PHE	-	expression tag	UNP E3CNF6
B	309	GLU	-	expression tag	UNP E3CNF6
B	310	LYS	-	expression tag	UNP E3CNF6

- Molecule 2 is a protein called XIP signaling peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	0	0
			77	57	8	11	1			
2	D	8	Total	C	N	O	S	0	0	0
			77	57	8	11	1			

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.19Å 84.03Å 152.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.87 – 3.39 38.87 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.87-3.39) 99.8 (38.87-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.245 , 0.301 0.260 , 0.310	Depositor DCC
R_{free} test set	564 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	121.6	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 88.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4509	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.37 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2135e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

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	0.21	0/2482	0.35	0/3335
1	B	0.22	0/1951	0.36	0/2628
2	C	0.24	0/81	0.33	0/108
2	D	0.25	0/81	0.32	0/108
All	All	0.21	0/4595	0.36	0/6179

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	2442	0	2484	28	0
1	B	1913	0	1922	23	0
2	C	77	0	71	2	0
2	D	77	0	71	0	0
All	All	4509	0	4548	50	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 6.

All (50) 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:B:152:VAL:O	1:B:190:ARG:NH2	2.29	0.66
1:A:20:MET:SD	1:A:58:ARG:NH1	2.70	0.64
1:B:203:ASN:HD22	1:B:240:SER:HB3	1.66	0.61
1:A:10:ARG:HH21	1:A:66:LEU:HD23	1.66	0.60
1:A:241:GLN:HG3	1:B:87:LYS:HB3	1.84	0.59
1:A:204:ILE:O	1:A:208:ASN:ND2	2.33	0.59
1:A:124:ASP:O	1:A:128:ASN:ND2	2.36	0.58
1:B:75:PRO:HG2	1:B:111:PHE:HE2	1.70	0.56
1:B:139:PRO:HG2	1:B:144:ILE:HD11	1.87	0.55
1:A:90:THR:HA	1:A:96:ARG:HE	1.72	0.55
1:A:230:ILE:HA	1:A:233:LEU:HD12	1.88	0.55
1:A:293:GLU:HG3	2:C:19:PHE:HE1	1.73	0.54
1:B:85:LEU:HD21	1:B:104:ILE:HG12	1.91	0.52
1:A:174:TYR:CZ	2:C:18:PRO:HD3	2.46	0.50
1:B:152:VAL:HG13	1:B:158:PHE:HE1	1.76	0.50
1:A:21:SER:HB3	1:A:24:VAL:HG23	1.94	0.50
1:A:203:ASN:HD22	1:A:240:SER:HB3	1.76	0.50
1:B:133:THR:OG1	1:B:134:SER:N	2.43	0.49
1:A:141:VAL:HG11	1:A:169:TYR:HD1	1.78	0.49
1:A:93:ASP:HB3	1:A:96:ARG:HB2	1.95	0.48
1:B:162:ASP:O	1:B:166:ILE:HG13	2.14	0.48
1:A:294:LYS:HG2	1:A:299:LEU:HB2	1.96	0.47
1:B:213:ILE:O	1:B:217:LYS:HG2	2.14	0.47
1:A:192:LEU:HD22	1:A:232:LYS:HG3	1.97	0.47
1:A:158:PHE:HB3	1:A:162:ASP:HB2	1.97	0.46
1:B:145:TYR:HB3	1:B:148:LEU:HB3	1.97	0.46
1:B:230:ILE:HA	1:B:233:LEU:HD12	1.96	0.46
1:A:7:ILE:HG13	1:A:10:ARG:HH11	1.81	0.46
1:A:89:PRO:O	1:A:96:ARG:NH2	2.38	0.46
1:A:12:LYS:O	1:A:16:GLU:HG2	2.15	0.45
1:B:84:ARG:NH2	1:B:99:GLN:OE1	2.50	0.45
1:A:75:PRO:HB2	1:A:77:THR:HG22	1.98	0.45
1:B:182:LYS:O	1:B:186:ARG:HB2	2.17	0.44
1:A:140:LYS:HG2	1:A:172:HIS:NE2	2.33	0.43
1:A:185:ASP:HA	1:A:188:VAL:HG22	2.00	0.43
1:A:38:ILE:HG22	1:A:42:LYS:HE3	1.99	0.43
1:A:247:PRO:HG3	1:A:277:PHE:HB3	2.00	0.43
1:B:100:LYS:O	1:B:104:ILE:HG13	2.18	0.43
1:B:135:TRP:O	1:B:172:HIS:HE1	2.02	0.43
1:B:257:GLU:O	1:B:263:ASN:N	2.52	0.42
1:B:287:GLU:OE1	1:B:291:ARG:NH1	2.52	0.42
1:B:118:GLU:OE1	1:B:118:GLU:N	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:CZ	1:B:245:TYR:HB3	2.54	0.42
1:B:113:ASP:OD1	1:B:113:ASP:N	2.46	0.41
1:A:177:LYS:HE2	1:A:177:LYS:HB3	1.95	0.41
1:A:28:ASP:OD1	1:A:28:ASP:N	2.53	0.41
1:B:115:LEU:HA	1:B:116:PRO:HD3	1.89	0.41
1:A:135:TRP:CD2	1:A:136:GLU:HG3	2.56	0.40
1:A:189:ASP:O	1:A:193:LYS:HG2	2.22	0.40
1:B:140:LYS:HA	1:B:172:HIS:CD2	2.57	0.40

There are no symmetry-related clashes.

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	A	292/310 (94%)	282 (97%)	10 (3%)	0	100	100
1	B	227/310 (73%)	219 (96%)	8 (4%)	0	100	100
2	C	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
All	All	531/636 (84%)	511 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	270/282 (96%)	265 (98%)	5 (2%)	57	78
1	B	210/282 (74%)	203 (97%)	7 (3%)	38	67
2	C	8/8 (100%)	7 (88%)	1 (12%)	4	18
2	D	8/8 (100%)	8 (100%)	0	100	100
All	All	496/580 (86%)	483 (97%)	13 (3%)	46	72

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	33	THR
1	A	59	LEU
1	A	115	LEU
1	A	277	PHE
1	B	105	GLU
1	B	108	TYR
1	B	190	ARG
1	B	194	GLN
1	B	208	ASN
1	B	220	LEU
1	B	232	LYS
2	C	24	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	296/310 (95%)	0.57	33 (11%) 5 7	80, 127, 210, 286	0
1	B	229/310 (73%)	0.21	5 (2%) 62 66	83, 113, 167, 220	0
2	C	8/8 (100%)	0.30	0 100 100	98, 109, 123, 129	0
2	D	8/8 (100%)	0.53	0 100 100	98, 106, 120, 123	0
All	All	541/636 (85%)	0.42	38 (7%) 16 20	80, 118, 195, 286	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	SER	6.7
1	A	55	ILE	4.8
1	A	45	SER	4.5
1	A	5	ASP	4.3
1	A	52	LEU	4.3
1	A	51	LYS	3.9
1	A	68	ASP	3.5
1	A	50	ASP	3.5
1	A	27	LEU	3.4
1	B	111	PHE	3.4
1	A	65	ASP	3.4
1	B	112	PHE	3.3
1	A	44	GLU	3.2
1	A	4	LYS	3.2
1	A	31	GLU	3.1
1	A	26	CYS	3.1
1	A	49	LEU	3.1
1	A	23	GLU	3.1
1	A	114	ILE	3.0
1	A	64	ALA	2.9
1	A	54	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	2.8
1	A	33	THR	2.8
1	A	35	ARG	2.8
1	A	39	ARG	2.8
1	A	58	ARG	2.8
1	A	57	LYS	2.7
1	A	134	SER	2.7
1	A	46	LEU	2.7
1	A	36	GLN	2.5
1	A	53	SER	2.3
1	A	24	VAL	2.2
1	A	262	GLY	2.1
1	A	11	ILE	2.1
1	B	74	ILE	2.0
1	A	10	ARG	2.0
1	B	107	VAL	2.0
1	B	113	ASP	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.