



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:36 pm BST

PDB ID : 3UR1
Title : The structure of a ternary complex between CheA domains P4 and P5 with CheW and with a truncated fragment of TM14, a chemoreceptor analog from *Thermotoga maritima*.
Authors : Li, X.; Crane, B.R.; Bilwes, A.M.
Deposited on : 2011-11-21
Resolution : 4.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

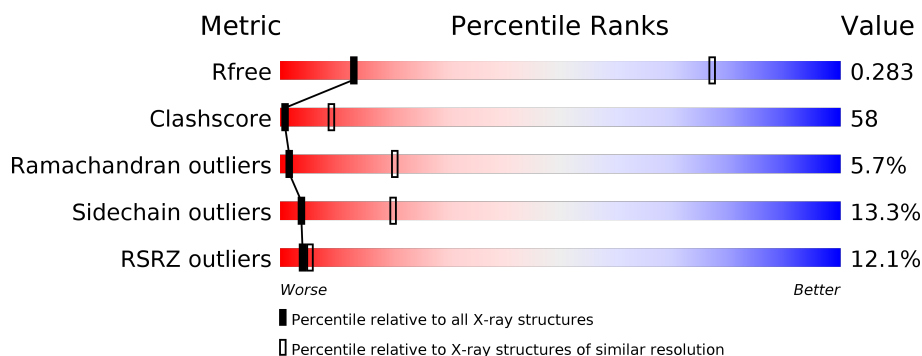
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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 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	320	<div> <div>21%</div> <div>23% 50% 9% 18%</div> </div>
2	B	139	<div> <div>39% 48% 13%</div> </div>
3	C	85	<div> <div>29% 59% 12%</div> </div>
3	D	85	<div> <div>4% 13% 76% 9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4488 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 Chemotaxis protein CheA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2063	1312	354	392	5			

There are 3 discrepancies between the modelled and reference sequences:

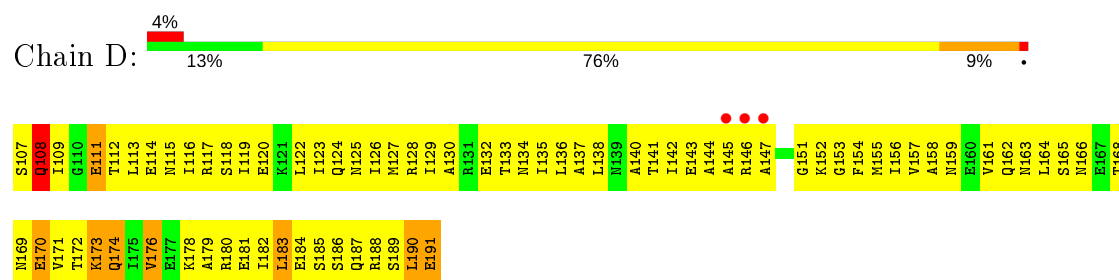
Chain	Residue	Modelled	Actual	Comment	Reference
A	352	GLY	-	EXPRESSION TAG	UNP Q56310
A	353	SER	-	EXPRESSION TAG	UNP Q56310
A	354	HIS	-	EXPRESSION TAG	UNP Q56310

- Molecule 2 is a protein called Chemotaxis protein CheW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1105	710	183	210	2			

- Molecule 3 is a protein called Methyl-accepting chemotaxis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	85	Total	C	N	O	S	0	0	0
			660	402	120	136	2			
3	D	85	Total	C	N	O	S	0	0	0
			660	402	120	136	2			



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	213.99Å 213.99Å 208.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 4.50 49.90 – 4.49	Depositor EDS
% Data completeness (in resolution range)	86.0 (29.75-4.50) 86.0 (49.90-4.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 4.45Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.266 , 0.291 0.240 , 0.283	Depositor DCC
R_{free} test set	1119 reflections (10.24%)	wwPDB-VP
Wilson B-factor (Å ²)	177.6	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 220.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4488	wwPDB-VP
Average B, all atoms (Å ²)	245.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

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	0.42	0/2087	0.63	1/2818 (0.0%)
2	B	0.44	0/1116	0.59	0/1501
3	C	0.55	0/660	0.66	0/884
3	D	0.51	0/660	0.61	0/884
All	All	0.46	0/4523	0.62	1/6087 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	ALA	N-CA-C	10.20	138.54	111.00

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	2063	0	2147	272	0
2	B	1105	0	1166	91	0
3	C	660	0	678	105	0
3	D	660	0	678	122	1
All	All	4488	0	4669	534	1

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 58.

The worst 5 of 534 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:402:PRO:HB3	1:A:514:VAL:HG22	1.43	1.00
1:A:443:VAL:CG2	1:A:539:LEU:HB3	1.92	0.99
3:C:115:ASN:HD21	3:D:178:LYS:HD2	1.25	0.97
1:A:653:ALA:HB2	1:A:663:LEU:HD23	1.46	0.96
1:A:365:PHE:H	1:A:366:PRO:HD2	1.34	0.93

All (1) 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)
3:D:188:ARG:NH1	3:D:188:ARG:NH1[12_555]	2.14	0.06

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	259/320 (81%)	177 (68%)	65 (25%)	17 (7%)	1	18
2	B	137/139 (99%)	93 (68%)	33 (24%)	11 (8%)	1	14
3	C	83/85 (98%)	63 (76%)	18 (22%)	2 (2%)	6	36
3	D	83/85 (98%)	57 (69%)	24 (29%)	2 (2%)	6	36
All	All	562/629 (89%)	390 (69%)	140 (25%)	32 (6%)	1	20

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL
1	A	579	ASP
1	A	605	GLU
1	A	608	GLU

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Mol	Chain	Res	Type
3	C	147	ALA

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	233/280 (83%)	205 (88%)	28 (12%)	5	22
2	B	127/127 (100%)	109 (86%)	18 (14%)	3	18
3	C	72/72 (100%)	63 (88%)	9 (12%)	4	21
3	D	72/72 (100%)	60 (83%)	12 (17%)	2	14
All	All	504/551 (92%)	437 (87%)	67 (13%)	4	20

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	26	ASP
2	B	98	VAL
3	D	173	LYS
2	B	29	ASN
2	B	80	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
2	B	64	ASN
3	D	115	ASN
1	A	603	HIS
1	A	632	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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](#)

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	263/320 (82%)	1.05	66 (25%) 0 1	125, 296, 446, 623	0
2	B	139/139 (100%)	-0.08	0 100 100	137, 195, 260, 313	0
3	C	85/85 (100%)	-0.10	0 100 100	93, 202, 269, 332	0
3	D	85/85 (100%)	0.01	3 (3%) 44 35	152, 215, 295, 365	0
All	All	572/629 (90%)	0.45	69 (12%) 4 5	93, 212, 418, 623	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	435	SER	6.4
3	D	146	ARG	5.5
1	A	375	LYS	5.1
1	A	409	ASN	5.0
1	A	385	ARG	4.9

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 carbohydrates 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.