



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:20 PM UTC

PDB ID : 5J1M / pdb_00005j1m
Title : Crystal structure of Csd1-Csd2 dimer II
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Deposited on : 2016-03-29
Resolution : 2.35 Å(reported)

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

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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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

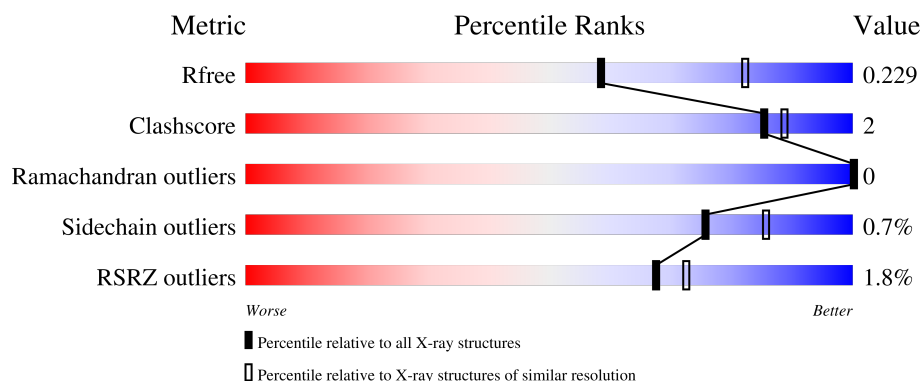
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	216	 2% 73% 23%
1	C	216	 3% 69% 5% 26%
2	B	189	 % 87% 6% 7%
2	D	189	 % 86% 7% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5560 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 ToxR-activated gene (TagE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1328	860	231	232	5			
1	C	159	Total	C	N	O	S	0	0	0
			1271	822	220	224	5			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	MET	-	initiating methionine	UNP O26068
A	106	GLY	-	expression tag	UNP O26068
A	107	SER	-	expression tag	UNP O26068
A	108	SER	-	expression tag	UNP O26068
A	109	HIS	-	expression tag	UNP O26068
A	110	HIS	-	expression tag	UNP O26068
A	111	HIS	-	expression tag	UNP O26068
A	112	HIS	-	expression tag	UNP O26068
A	113	HIS	-	expression tag	UNP O26068
A	114	HIS	-	expression tag	UNP O26068
A	115	SER	-	expression tag	UNP O26068
A	116	SER	-	expression tag	UNP O26068
A	117	GLY	-	expression tag	UNP O26068
A	118	LEU	-	expression tag	UNP O26068
A	119	VAL	-	expression tag	UNP O26068
A	120	PRO	-	expression tag	UNP O26068
A	121	ARG	-	expression tag	UNP O26068
A	122	GLY	-	expression tag	UNP O26068
A	123	SER	-	expression tag	UNP O26068
A	124	HIS	-	expression tag	UNP O26068
A	313	LEU	-	expression tag	UNP O26068
A	314	GLU	-	expression tag	UNP O26068
A	315	HIS	-	expression tag	UNP O26068
A	316	HIS	-	expression tag	UNP O26068
A	317	HIS	-	expression tag	UNP O26068

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Chain	Residue	Modelled	Actual	Comment	Reference
A	318	HIS	-	expression tag	UNP O26068
A	319	HIS	-	expression tag	UNP O26068
A	320	HIS	-	expression tag	UNP O26068
C	105	MET	-	initiating methionine	UNP O26068
C	106	GLY	-	expression tag	UNP O26068
C	107	SER	-	expression tag	UNP O26068
C	108	SER	-	expression tag	UNP O26068
C	109	HIS	-	expression tag	UNP O26068
C	110	HIS	-	expression tag	UNP O26068
C	111	HIS	-	expression tag	UNP O26068
C	112	HIS	-	expression tag	UNP O26068
C	113	HIS	-	expression tag	UNP O26068
C	114	HIS	-	expression tag	UNP O26068
C	115	SER	-	expression tag	UNP O26068
C	116	SER	-	expression tag	UNP O26068
C	117	GLY	-	expression tag	UNP O26068
C	118	LEU	-	expression tag	UNP O26068
C	119	VAL	-	expression tag	UNP O26068
C	120	PRO	-	expression tag	UNP O26068
C	121	ARG	-	expression tag	UNP O26068
C	122	GLY	-	expression tag	UNP O26068
C	123	SER	-	expression tag	UNP O26068
C	124	HIS	-	expression tag	UNP O26068
C	313	LEU	-	expression tag	UNP O26068
C	314	GLU	-	expression tag	UNP O26068
C	315	HIS	-	expression tag	UNP O26068
C	316	HIS	-	expression tag	UNP O26068
C	317	HIS	-	expression tag	UNP O26068
C	318	HIS	-	expression tag	UNP O26068
C	319	HIS	-	expression tag	UNP O26068
C	320	HIS	-	expression tag	UNP O26068

- Molecule 2 is a protein called ToxR-activated gene (TagE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	176	Total	C	N	O	S	0	0	0
			1405	911	238	254	2			
2	D	177	Total	C	N	O	S	0	0	0
			1414	916	239	257	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	MET	-	initiating methionine	UNP O26069
D	120	MET	-	initiating methionine	UNP O26069

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

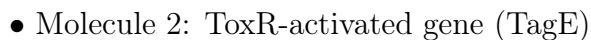
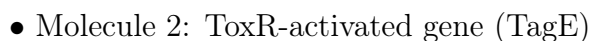
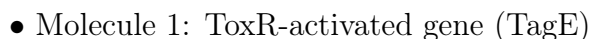
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	47	Total O 47 47	0	0
4	C	22	Total O 22 22	0	0
4	D	46	Total O 46 46	0	0

i

- Molecule 1: ToxR-activated gene (TagE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.15Å 80.01Å 74.59Å 90.00° 104.43° 90.00°	Depositor
Resolution (Å)	50.01 – 2.35 50.01 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.01-2.35) 99.7 (50.01-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.168 , 0.233 0.171 , 0.229	Depositor DCC
R_{free} test set	1246 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5560	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% 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](#)

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

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	0.71	0/1364	0.84	1/1844 (0.1%)
1	C	0.67	0/1304	0.89	0/1760
2	B	0.71	0/1440	0.85	0/1947
2	D	0.76	0/1449	0.86	0/1959
All	All	0.71	0/5557	0.86	1/7510 (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	151	VAL	N-CA-C	5.47	116.11	110.36

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	1328	0	1330	4	0
1	C	1271	0	1273	7	0
2	B	1405	0	1406	7	0
2	D	1414	0	1412	8	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	25	0	0	0	0
4	B	47	0	0	1	0
4	C	22	0	0	0	1
4	D	46	0	0	0	1
All	All	5560	0	5421	24	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 2.

All (24) 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)
2:B:156:HIS:HB3	2:B:159:LYS:O	2.03	0.59
2:D:197:TYR:O	2:D:214:THR:HG23	2.06	0.54
2:B:212:ILE:HG22	2:B:250:GLU:HB2	1.90	0.54
2:D:292:ASP:O	2:D:295:GLN:HG2	2.08	0.54
1:A:216:TYR:HB2	1:A:254:GLU:HB2	1.92	0.52
2:B:174:LEU:HD12	2:B:237:GLY:HA2	1.92	0.52
1:C:216:TYR:HB2	1:C:254:GLU:HB2	1.92	0.51
1:A:146:GLU:HA	1:A:149:ARG:HD2	1.91	0.51
1:C:128:THR:HB	1:C:131:GLN:HB3	1.94	0.49
1:C:137:ARG:HH11	2:D:296:LEU:HD21	1.78	0.48
2:D:295:GLN:HG3	2:D:296:LEU:N	2.30	0.46
2:D:127:ALA:HB3	2:D:294:VAL:HG11	1.98	0.46
1:A:232:LYS:HE3	2:B:288:TRP:CZ2	2.51	0.46
2:B:136:ILE:HD11	2:B:286:LEU:HD21	1.98	0.46
2:B:197:TYR:O	2:B:214:THR:HG23	2.15	0.45
1:A:169:HIS:CE1	1:A:261:PRO:HA	2.52	0.44
1:C:132:LYS:HB2	1:C:272:MET:HE1	2.00	0.44
2:D:168:ILE:CD1	2:D:264:LEU:HD11	2.49	0.43
2:B:159:LYS:O	2:B:161:ILE:N	2.53	0.42
4:B:402:HOH:O	1:C:286:ARG:NH1	2.44	0.42
1:C:197:TRP:CZ3	1:C:244:GLY:HA2	2.55	0.41
2:D:126:LEU:HD21	2:D:130:HIS:CE1	2.55	0.41
2:D:174:LEU:HD12	2:D:237:GLY:HA2	2.02	0.41
1:C:131:GLN:HA	1:C:298:MET:SD	2.61	0.40

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)
4:C:511:HOH:O	4:D:441:HOH:O[2_656]	1.65	0.55

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	162/216 (75%)	152 (94%)	10 (6%)	0	100	100
1	C	155/216 (72%)	145 (94%)	10 (6%)	0	100	100
2	B	174/189 (92%)	169 (97%)	5 (3%)	0	100	100
2	D	175/189 (93%)	167 (95%)	8 (5%)	0	100	100
All	All	666/810 (82%)	633 (95%)	33 (5%)	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	144/188 (77%)	143 (99%)	1 (1%)	76	86
1	C	137/188 (73%)	137 (100%)	0	100	100
2	B	152/164 (93%)	151 (99%)	1 (1%)	76	86
2	D	153/164 (93%)	151 (99%)	2 (1%)	61	76
All	All	586/704 (83%)	582 (99%)	4 (1%)	76	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
2	B	214	THR
2	D	214	THR
2	D	284	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	HIS
2	B	155	ASN
2	B	285	ASN
2	D	123	ASN
2	D	128	GLN
2	D	130	HIS
2	D	285	ASN
2	D	295	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 [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	166/216 (76%)	-0.00	5 (3%) 52 59	28, 41, 83, 118	0
1	C	159/216 (73%)	0.06	6 (3%) 44 50	29, 45, 90, 123	0
2	B	176/189 (93%)	-0.28	1 (0%) 85 89	25, 38, 65, 100	0
2	D	177/189 (93%)	-0.30	0 100 100	25, 37, 59, 99	0
All	All	678/810 (83%)	-0.14	12 (1%) 67 72	25, 39, 79, 123	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	TYR	3.7
1	C	147	SER	3.5
1	C	151	VAL	3.1
1	C	154	ALA	2.7
2	B	160	LYS	2.6
1	A	153	ALA	2.5
1	C	153	ALA	2.5
1	A	154	ALA	2.3
1	A	279	PHE	2.2
1	A	167	HIS	2.1
1	C	170	THR	2.1
1	A	298	MET	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	401	1/1	0.98	0.04	74,74,74,74	0
3	ZN	A	401	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.