



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 7PTB / pdb_00007ptb
Title : Crystal structure of the SPD-2 domain of human CEP192
Authors : Rosa e Silva, I.; van Breugel, M.
Deposited on : 2021-09-26
Resolution : 2.08 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) : 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

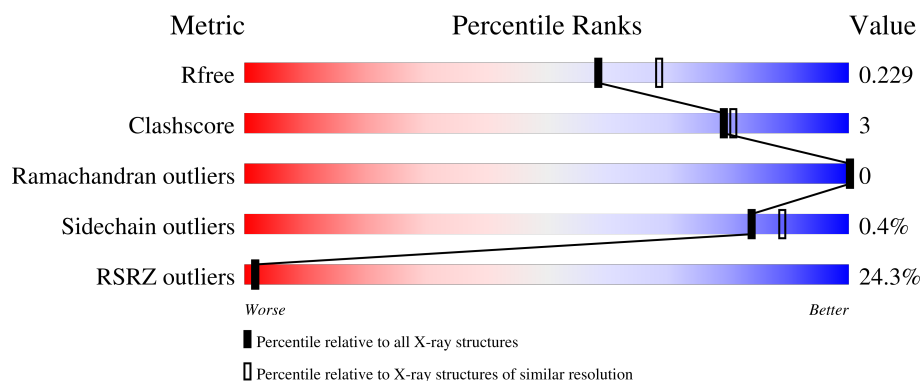
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	352	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2735 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.

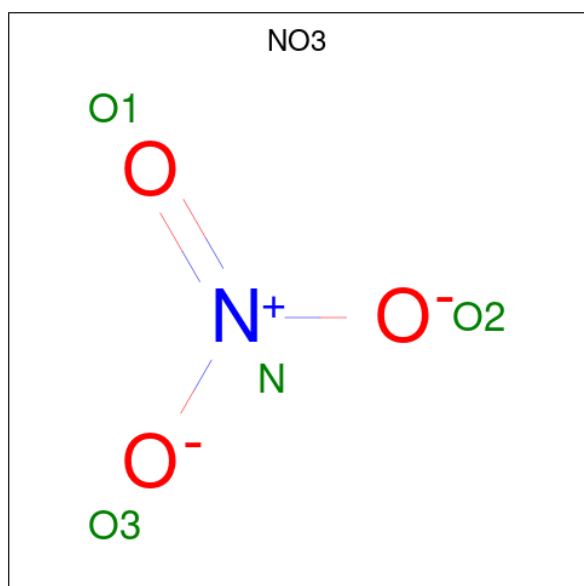
- Molecule 1 is a protein called Centrosomal protein of 192 kDa.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	317	2563	1634	451	468	5	5	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1741	GLY	-	expression tag	UNP Q8TEP8
A	1742	PRO	-	expression tag	UNP Q8TEP8

- Molecule 2 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
2	A	1	4	1	3	0	0
2	A	1	4	1	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	N	O	0	0
			4	1	3		

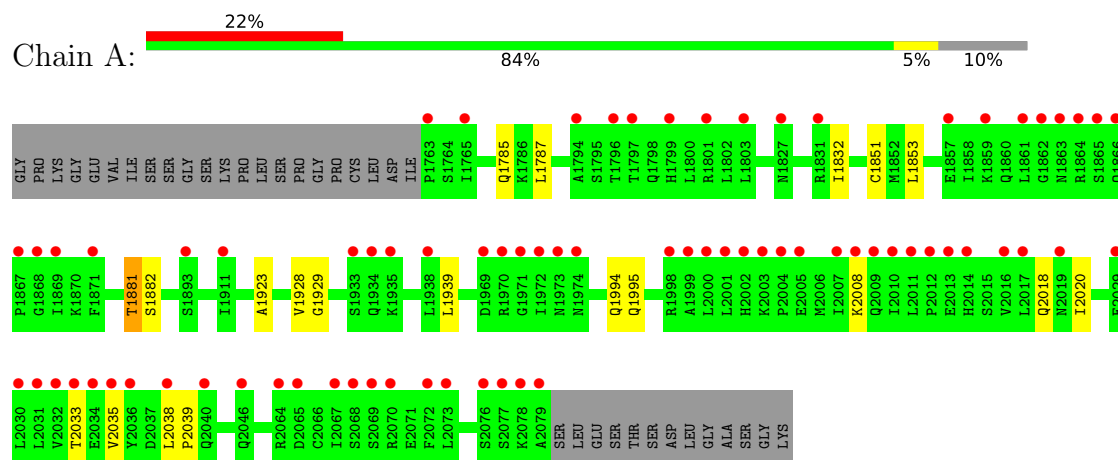
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		

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: Centrosomal protein of 192 kDa



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	104.59Å 104.59Å 90.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	90.58 – 2.08 90.58 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.58-2.08) 100.0 (90.58-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267, PHENIX 1.18	Depositor
R, R_{free}	0.212 , 0.224 0.216 , 0.229	Depositor DCC
R_{free} test set	1629 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2735	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: NO3

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	1.01	0/2631	1.30	0/3541

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	2563	0	2665	14	0
2	A	12	0	0	0	0
3	A	160	0	0	1	0
All	All	2735	0	2665	14	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 3.

All (14) 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:1881[A]:THR:HG22	1:A:1882:SER:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1853:LEU:HD21	1:A:2039:PRO:HD3	1.90	0.54
1:A:1994:GLN:HG3	1:A:2033:THR:HG21	1.91	0.51
1:A:2033:THR:HG23	1:A:2035:VAL:HG12	1.92	0.51
1:A:1787:LEU:HD12	1:A:1787:LEU:C	2.36	0.50
1:A:1929:GLY:HA3	1:A:1939:LEU:HD12	1.93	0.49
1:A:1882:SER:HB2	1:A:1923:ALA:HB2	1.96	0.47
1:A:1785:GLN:NE2	3:A:2201:HOH:O	2.38	0.46
1:A:1995[B]:GLN:NE2	1:A:2038:LEU:HD13	2.33	0.44
1:A:1928[B]:VAL:HG11	1:A:2020:ILE:HD12	2.00	0.43
1:A:2008:LYS:HA	1:A:2018:GLN:HE22	1.83	0.42
1:A:1851:CYS:SG	1:A:2038:LEU:HG	2.60	0.42
1:A:1832:ILE:O	1:A:1832:ILE:HG23	2.20	0.41
1:A:1928[A]:VAL:HG21	1:A:2020:ILE:HD12	2.02	0.41

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	324/352 (92%)	317 (98%)	7 (2%)	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	294/309 (95%)	292 (99%)	2 (1%)	76	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1881[A]	THR
1	A	1881[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1783	GLN
1	A	1809	GLN
1	A	1815	GLN
1	A	1901	ASN
1	A	2018	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are 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	$\# Z > 2$
2	NO3	A	2103	-	1,3,3	0.27	0	0,3,3	-	-
2	NO3	A	2102	-	1,3,3	0.25	0	0,3,3	-	-
2	NO3	A	2101	-	1,3,3	0.23	0	0,3,3	-	-

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 ⓘ

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	313/352 (88%)	1.15	76 (24%) 2 2	19, 42, 84, 112	8 (2%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2031	LEU	9.9
1	A	2014[A]	HIS	8.3
1	A	2007	ILE	7.1
1	A	2068	SER	6.8
1	A	2079	ALA	5.4
1	A	1763	PRO	5.3
1	A	2004	PRO	5.3
1	A	1867	PRO	5.0
1	A	2010	ILE	5.0
1	A	1974	ASN	5.0
1	A	2032	VAL	4.9
1	A	2003	LYS	4.7
1	A	2033	THR	4.4
1	A	1972	ILE	4.3
1	A	2002	HIS	4.1
1	A	1861	LEU	4.1
1	A	2069	SER	4.0
1	A	2001	LEU	3.8
1	A	1864	ARG	3.5
1	A	2013	GLU	3.5
1	A	2012	PRO	3.4
1	A	2011	LEU	3.4
1	A	2036	TYR	3.3
1	A	2078	LYS	3.3
1	A	2065	ASP	3.3
1	A	2008	LYS	3.3
1	A	1865	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2067	ILE	3.2
1	A	1971	GLY	3.1
1	A	2030	LEU	3.1
1	A	1796	THR	3.1
1	A	1863	ASN	3.1
1	A	2009	GLN	3.0
1	A	1831	ARG	3.0
1	A	2076	SER	3.0
1	A	1933	SER	2.9
1	A	1973	ASN	2.9
1	A	2016	VAL	2.9
1	A	2070	ARG	2.9
1	A	2046	GLN	2.8
1	A	2072	PHE	2.8
1	A	1868	GLY	2.7
1	A	1866	GLN	2.6
1	A	2005	GLU	2.6
1	A	1998	ARG	2.6
1	A	2034	GLU	2.6
1	A	1969	ASP	2.6
1	A	1799	HIS	2.5
1	A	1794	ALA	2.5
1	A	1801	ARG	2.5
1	A	1869	ILE	2.4
1	A	2077	SER	2.4
1	A	2064	ARG	2.4
1	A	1893	SER	2.3
1	A	1999	ALA	2.3
1	A	1935	LYS	2.2
1	A	2038	LEU	2.2
1	A	1803	LEU	2.2
1	A	1934	GLN	2.2
1	A	2019	ASN	2.2
1	A	1765	ILE	2.2
1	A	1911	ILE	2.2
1	A	1862	GLY	2.2
1	A	2040	GLN	2.2
1	A	2029	GLU	2.1
1	A	2035	VAL	2.1
1	A	1970	ARG	2.1
1	A	1859	LYS	2.1
1	A	2000	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	2073	LEU	2.1
1	A	1938	LEU	2.1
1	A	1857	GLU	2.1
1	A	1797	THR	2.1
1	A	1827	ASN	2.0
1	A	1871	PHE	2.0
1	A	2017	LEU	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
2	NO3	A	2102	4/4	0.84	0.11	67,68,68,68	0
2	NO3	A	2103	4/4	0.91	0.26	49,52,52,53	0
2	NO3	A	2101	4/4	0.96	0.13	44,44,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.