



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:35 PM UTC

PDB ID : 2OEN / pdb_00002oen
Title : Structural mechanism for the fine-tuning of CcpA function by the small molecule effectors glucose-6-phosphate and fructose-1,6-bisphosphate
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Deposited on : 2006-12-30
Resolution : 3.17 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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

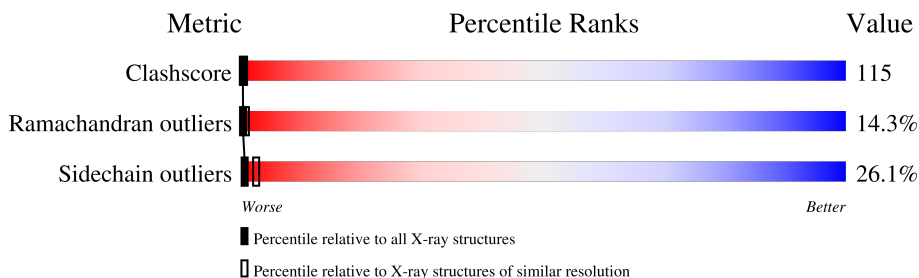
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.17 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))
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	G	280	7% 55% 30% 7% .
2	L	88	11% 47% 33% 8% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2773 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 Catabolite control protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	G	275	2141	1349	356	428	8	0	0	0

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P				S
2	L	87	632	386	104	138	1	3	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	46	SEP	SER	modified residue	UNP O69250

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.33Å 69.33Å 229.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.37 – 3.17	Depositor
% Data completeness (in resolution range)	98.9 (66.37-3.17)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.278 , 0.318	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2773	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

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: SEP

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	G	0.96	1/2174 (0.0%)	1.58	47/2945 (1.6%)
2	L	1.05	1/625 (0.2%)	1.42	8/839 (1.0%)
All	All	0.98	2/2799 (0.1%)	1.54	55/3784 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	241	THR	CA-CB	5.88	1.63	1.53
2	L	5	THR	CA-CB	5.36	1.62	1.53

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	71	SER	N-CA-C	-13.68	96.73	113.41
1	G	197	VAL	N-CA-C	-11.15	101.08	111.45
1	G	128	THR	N-CA-C	10.90	125.17	110.35
1	G	151	THR	N-CA-C	10.51	125.37	112.54
1	G	138	SER	CA-C-N	10.26	132.67	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	29	PHE	Sidechain

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	G	2141	0	2147	477	1
2	L	632	0	624	167	0
All	All	2773	0	2771	635	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 115.

The worst 5 of 635 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:G:293:PRO:HB2	1:G:296:ASP:HB2	1.25	1.14
1:G:288:THR:HG23	1:G:327:PHE:HA	1.24	1.10
1:G:304:LEU:HD13	2:L:48:MET:HE1	1.28	1.09
2:L:8:VAL:HG13	2:L:58:GLY:H	1.17	1.09
1:G:58:LYS:HE3	1:G:58:LYS:HA	1.34	1.07

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)
1:G:94:ILE:CD1	1:G:94:ILE:CD1[8_665]	1.71	0.49

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	G	273/280 (98%)	164 (60%)	77 (28%)	32 (12%)	0	1
2	L	84/88 (96%)	47 (56%)	18 (21%)	19 (23%)	0	0
All	All	357/368 (97%)	211 (59%)	95 (27%)	51 (14%)	0	1

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	100	GLN
1	G	108	LEU
1	G	109	LEU
1	G	110	ASN
1	G	131	HIS

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	G	241/244 (99%)	181 (75%)	60 (25%)	0	3
2	L	66/67 (98%)	46 (70%)	20 (30%)	0	1
All	All	307/311 (99%)	227 (74%)	80 (26%)	0	2

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	328	ARG
2	L	55	ILE
1	G	332	LYS
2	L	23	VAL
2	L	63	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	276	ASN
1	G	292	GLN
2	L	56	GLN
1	G	310	ASN
1	G	153	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](#)

1 non-standard protein/DNA/RNA residue is 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	SEP	L	46	2	8,9,10	1.11	0	7,12,14	2.68	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	L	46	2	-	5/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	46	SEP	OG-CB-CA	6.26	114.23	108.14
2	L	46	SEP	O3P-P-O1P	2.43	120.29	110.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	46	SEP	C-CA-CB-OG
2	L	46	SEP	CB-OG-P-O2P
2	L	46	SEP	CB-OG-P-O3P
2	L	46	SEP	CA-CB-OG-P
2	L	46	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	46	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.