



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 1, 2023 – 03:38 AM EDT

PDB ID : 3L8R  
Title : The crystal structure of PtcA from *S. mutans*  
Authors : Lei, J.; Liu, X.; Li, L.  
Deposited on : 2010-01-03  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

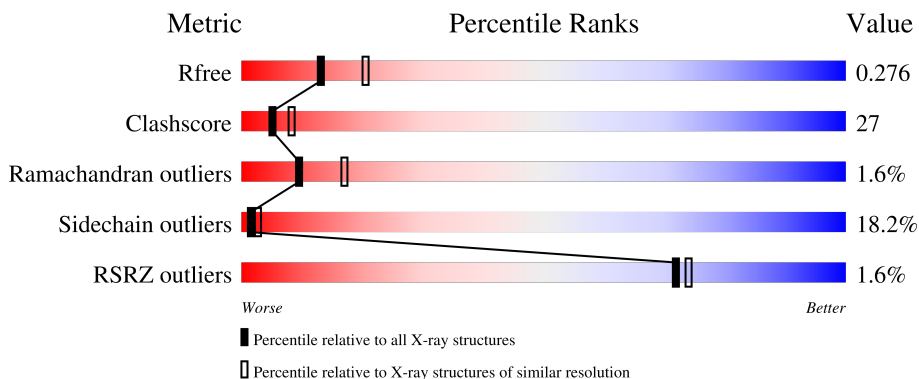
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	120	
1	B	120	
1	C	120	
1	D	120	
1	E	120	

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Mol	Chain	Length	Quality of chain
1	F	120	 50% 24% 11% 15%
1	G	120	 3% 46% 31% 8% 15%
1	H	120	 2% 48% 33% 15%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6823 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 Putative PTS system, cellobiose-specific IIA component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	102	818	513	137	162	6	0	0	0
1	B	102	818	513	137	162	6	0	0	0
1	C	102	818	513	137	162	6	0	0	0
1	D	102	818	513	137	162	6	0	0	0
1	E	102	818	513	137	162	6	0	0	0
1	F	102	818	513	137	162	6	0	0	0
1	G	102	823	516	138	163	6	0	1	0
1	H	102	818	513	137	162	6	0	0	0

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLY	-	expression tag	UNP Q8DT03
A	-15	SER	-	expression tag	UNP Q8DT03
A	-14	HIS	-	expression tag	UNP Q8DT03
A	-13	MET	-	expression tag	UNP Q8DT03
A	-12	ALA	-	expression tag	UNP Q8DT03
A	-11	SER	-	expression tag	UNP Q8DT03
A	-10	MET	-	expression tag	UNP Q8DT03
A	-9	THR	-	expression tag	UNP Q8DT03
A	-8	GLY	-	expression tag	UNP Q8DT03
A	-7	GLY	-	expression tag	UNP Q8DT03
A	-6	GLN	-	expression tag	UNP Q8DT03
A	-5	GLN	-	expression tag	UNP Q8DT03
A	-4	MET	-	expression tag	UNP Q8DT03

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q8DT03
A	-2	ARG	-	expression tag	UNP Q8DT03
A	-1	GLY	-	expression tag	UNP Q8DT03
A	0	SER	-	expression tag	UNP Q8DT03
B	-16	GLY	-	expression tag	UNP Q8DT03
B	-15	SER	-	expression tag	UNP Q8DT03
B	-14	HIS	-	expression tag	UNP Q8DT03
B	-13	MET	-	expression tag	UNP Q8DT03
B	-12	ALA	-	expression tag	UNP Q8DT03
B	-11	SER	-	expression tag	UNP Q8DT03
B	-10	MET	-	expression tag	UNP Q8DT03
B	-9	THR	-	expression tag	UNP Q8DT03
B	-8	GLY	-	expression tag	UNP Q8DT03
B	-7	GLY	-	expression tag	UNP Q8DT03
B	-6	GLN	-	expression tag	UNP Q8DT03
B	-5	GLN	-	expression tag	UNP Q8DT03
B	-4	MET	-	expression tag	UNP Q8DT03
B	-3	GLY	-	expression tag	UNP Q8DT03
B	-2	ARG	-	expression tag	UNP Q8DT03
B	-1	GLY	-	expression tag	UNP Q8DT03
B	0	SER	-	expression tag	UNP Q8DT03
C	-16	GLY	-	expression tag	UNP Q8DT03
C	-15	SER	-	expression tag	UNP Q8DT03
C	-14	HIS	-	expression tag	UNP Q8DT03
C	-13	MET	-	expression tag	UNP Q8DT03
C	-12	ALA	-	expression tag	UNP Q8DT03
C	-11	SER	-	expression tag	UNP Q8DT03
C	-10	MET	-	expression tag	UNP Q8DT03
C	-9	THR	-	expression tag	UNP Q8DT03
C	-8	GLY	-	expression tag	UNP Q8DT03
C	-7	GLY	-	expression tag	UNP Q8DT03
C	-6	GLN	-	expression tag	UNP Q8DT03
C	-5	GLN	-	expression tag	UNP Q8DT03
C	-4	MET	-	expression tag	UNP Q8DT03
C	-3	GLY	-	expression tag	UNP Q8DT03
C	-2	ARG	-	expression tag	UNP Q8DT03
C	-1	GLY	-	expression tag	UNP Q8DT03
C	0	SER	-	expression tag	UNP Q8DT03
D	-16	GLY	-	expression tag	UNP Q8DT03
D	-15	SER	-	expression tag	UNP Q8DT03
D	-14	HIS	-	expression tag	UNP Q8DT03
D	-13	MET	-	expression tag	UNP Q8DT03

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	ALA	-	expression tag	UNP Q8DT03
D	-11	SER	-	expression tag	UNP Q8DT03
D	-10	MET	-	expression tag	UNP Q8DT03
D	-9	THR	-	expression tag	UNP Q8DT03
D	-8	GLY	-	expression tag	UNP Q8DT03
D	-7	GLY	-	expression tag	UNP Q8DT03
D	-6	GLN	-	expression tag	UNP Q8DT03
D	-5	GLN	-	expression tag	UNP Q8DT03
D	-4	MET	-	expression tag	UNP Q8DT03
D	-3	GLY	-	expression tag	UNP Q8DT03
D	-2	ARG	-	expression tag	UNP Q8DT03
D	-1	GLY	-	expression tag	UNP Q8DT03
D	0	SER	-	expression tag	UNP Q8DT03
E	-16	GLY	-	expression tag	UNP Q8DT03
E	-15	SER	-	expression tag	UNP Q8DT03
E	-14	HIS	-	expression tag	UNP Q8DT03
E	-13	MET	-	expression tag	UNP Q8DT03
E	-12	ALA	-	expression tag	UNP Q8DT03
E	-11	SER	-	expression tag	UNP Q8DT03
E	-10	MET	-	expression tag	UNP Q8DT03
E	-9	THR	-	expression tag	UNP Q8DT03
E	-8	GLY	-	expression tag	UNP Q8DT03
E	-7	GLY	-	expression tag	UNP Q8DT03
E	-6	GLN	-	expression tag	UNP Q8DT03
E	-5	GLN	-	expression tag	UNP Q8DT03
E	-4	MET	-	expression tag	UNP Q8DT03
E	-3	GLY	-	expression tag	UNP Q8DT03
E	-2	ARG	-	expression tag	UNP Q8DT03
E	-1	GLY	-	expression tag	UNP Q8DT03
E	0	SER	-	expression tag	UNP Q8DT03
F	-16	GLY	-	expression tag	UNP Q8DT03
F	-15	SER	-	expression tag	UNP Q8DT03
F	-14	HIS	-	expression tag	UNP Q8DT03
F	-13	MET	-	expression tag	UNP Q8DT03
F	-12	ALA	-	expression tag	UNP Q8DT03
F	-11	SER	-	expression tag	UNP Q8DT03
F	-10	MET	-	expression tag	UNP Q8DT03
F	-9	THR	-	expression tag	UNP Q8DT03
F	-8	GLY	-	expression tag	UNP Q8DT03
F	-7	GLY	-	expression tag	UNP Q8DT03
F	-6	GLN	-	expression tag	UNP Q8DT03
F	-5	GLN	-	expression tag	UNP Q8DT03

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	MET	-	expression tag	UNP Q8DT03
F	-3	GLY	-	expression tag	UNP Q8DT03
F	-2	ARG	-	expression tag	UNP Q8DT03
F	-1	GLY	-	expression tag	UNP Q8DT03
F	0	SER	-	expression tag	UNP Q8DT03
G	-16	GLY	-	expression tag	UNP Q8DT03
G	-15	SER	-	expression tag	UNP Q8DT03
G	-14	HIS	-	expression tag	UNP Q8DT03
G	-13	MET	-	expression tag	UNP Q8DT03
G	-12	ALA	-	expression tag	UNP Q8DT03
G	-11	SER	-	expression tag	UNP Q8DT03
G	-10	MET	-	expression tag	UNP Q8DT03
G	-9	THR	-	expression tag	UNP Q8DT03
G	-8	GLY	-	expression tag	UNP Q8DT03
G	-7	GLY	-	expression tag	UNP Q8DT03
G	-6	GLN	-	expression tag	UNP Q8DT03
G	-5	GLN	-	expression tag	UNP Q8DT03
G	-4	MET	-	expression tag	UNP Q8DT03
G	-3	GLY	-	expression tag	UNP Q8DT03
G	-2	ARG	-	expression tag	UNP Q8DT03
G	-1	GLY	-	expression tag	UNP Q8DT03
G	0	SER	-	expression tag	UNP Q8DT03
H	-16	GLY	-	expression tag	UNP Q8DT03
H	-15	SER	-	expression tag	UNP Q8DT03
H	-14	HIS	-	expression tag	UNP Q8DT03
H	-13	MET	-	expression tag	UNP Q8DT03
H	-12	ALA	-	expression tag	UNP Q8DT03
H	-11	SER	-	expression tag	UNP Q8DT03
H	-10	MET	-	expression tag	UNP Q8DT03
H	-9	THR	-	expression tag	UNP Q8DT03
H	-8	GLY	-	expression tag	UNP Q8DT03
H	-7	GLY	-	expression tag	UNP Q8DT03
H	-6	GLN	-	expression tag	UNP Q8DT03
H	-5	GLN	-	expression tag	UNP Q8DT03
H	-4	MET	-	expression tag	UNP Q8DT03
H	-3	GLY	-	expression tag	UNP Q8DT03
H	-2	ARG	-	expression tag	UNP Q8DT03
H	-1	GLY	-	expression tag	UNP Q8DT03
H	0	SER	-	expression tag	UNP Q8DT03

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	39	Total O 39 39	0	0
2	C	40	Total O 40 40	0	0
2	D	35	Total O 35 35	0	0
2	E	37	Total O 37 37	0	0
2	F	37	Total O 37 37	0	0
2	G	28	Total O 28 28	0	0
2	H	29	Total O 29 29	0	0







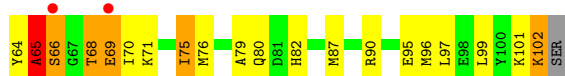
- Molecule 1: Putative PTS system, cellobiose-specific IIA component



- Molecule 1: Putative PTS system, cellobiose-specific IIA component



- Molecule 1: Putative PTS system, cellobiose-specific IIA component



- Molecule 1: Putative PTS system, cellobiose-specific IIA component



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.40Å 127.40Å 190.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.40 – 2.50 19.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.40-2.50) 100.0 (19.40-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.28 (at 2.49Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.208 , 0.280 0.207 , 0.276	Depositor DCC
$R_{free}$ test set	2027 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.3	Xtrriage
Anisotropy	0.353	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 15.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.306 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.53 % 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 4.5766e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.80	0/826	0.94	2/1111 (0.2%)
1	B	0.88	0/826	0.89	0/1111
1	C	0.90	1/826 (0.1%)	0.92	1/1111 (0.1%)
1	D	0.80	0/826	0.89	2/1111 (0.2%)
1	E	0.92	0/826	0.92	0/1111
1	F	0.91	0/826	0.90	1/1111 (0.1%)
1	G	0.84	0/834	0.86	1/1122 (0.1%)
1	H	0.84	0/826	0.87	1/1111 (0.1%)
All	All	0.86	1/6616 (0.0%)	0.90	8/8899 (0.1%)

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
1	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLU	CG-CD	6.16	1.61	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	81	ASP	CB-CG-OD1	9.48	126.83	118.30
1	D	81	ASP	CB-CG-OD2	-9.22	110.00	118.30
1	H	99	LEU	CA-CB-CG	7.28	132.05	115.30
1	C	81	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	81	ASP	CB-CG-OD1	5.68	123.42	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	65	ALA	Peptide

## 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	818	0	822	54	0
1	B	818	0	822	61	0
1	C	818	0	822	74	0
1	D	818	0	822	41	0
1	E	818	0	822	51	0
1	F	818	0	822	44	0
1	G	823	0	828	37	0
1	H	818	0	822	35	0
2	A	29	0	0	8	0
2	B	39	0	0	12	0
2	C	40	0	0	13	0
2	D	35	0	0	7	0
2	E	37	0	0	12	0
2	F	37	0	0	8	0
2	G	28	0	0	8	0
2	H	29	0	0	9	0
All	All	6823	0	6582	353	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 27.

The worst 5 of 353 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:C:37:ILE:HG22	2:C:119:HOH:O	1.18	1.26
1:A:1:MET:N	1:A:2:ASN:HB3	1.63	1.11
1:H:57:GLN:HG3	2:H:104:HOH:O	1.50	1.10
1:C:21:ARG:HH12	1:C:85:THR:CG2	1.67	1.08
1:B:72:ILE:O	1:B:73:GLU:CB	2.03	1.06

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	100/120 (83%)	95 (95%)	3 (3%)	2 (2%)	7	12
1	B	100/120 (83%)	90 (90%)	7 (7%)	3 (3%)	4	6
1	C	100/120 (83%)	91 (91%)	8 (8%)	1 (1%)	15	28
1	D	100/120 (83%)	100 (100%)	0	0	100	100
1	E	100/120 (83%)	94 (94%)	4 (4%)	2 (2%)	7	12
1	F	100/120 (83%)	97 (97%)	3 (3%)	0	100	100
1	G	101/120 (84%)	94 (93%)	4 (4%)	3 (3%)	4	6
1	H	100/120 (83%)	93 (93%)	5 (5%)	2 (2%)	7	12
All	All	801/960 (83%)	754 (94%)	34 (4%)	13 (2%)	9	17

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	ALA
1	B	72	ILE
1	G	66	SER
1	A	2	ASN
1	B	66	SER

### 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	88/100 (88%)	69 (78%)	19 (22%)	1	1
1	B	88/100 (88%)	70 (80%)	18 (20%)	1	2
1	C	88/100 (88%)	70 (80%)	18 (20%)	1	2
1	D	88/100 (88%)	76 (86%)	12 (14%)	3	7
1	E	88/100 (88%)	71 (81%)	17 (19%)	1	2
1	F	88/100 (88%)	68 (77%)	20 (23%)	1	1
1	G	89/100 (89%)	77 (86%)	12 (14%)	4	7
1	H	88/100 (88%)	76 (86%)	12 (14%)	3	7
All	All	705/800 (88%)	577 (82%)	128 (18%)	1	3

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	102	LYS
1	H	15	LEU
1	C	61	LEU
1	C	58	THR
1	H	57	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	80	GLN
1	G	82	HIS
1	H	57	GLN
1	C	47	ASN
1	C	44	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	102/120 (85%)	-0.02	1 (0%) 82 84	9, 26, 40, 48	0
1	B	102/120 (85%)	-0.00	1 (0%) 82 84	11, 30, 44, 56	0
1	C	102/120 (85%)	0.04	1 (0%) 82 84	9, 30, 43, 48	0
1	D	102/120 (85%)	-0.04	0 100 100	10, 26, 40, 49	0
1	E	102/120 (85%)	0.07	3 (2%) 51 55	8, 28, 43, 60	0
1	F	102/120 (85%)	-0.03	0 100 100	9, 30, 41, 47	0
1	G	102/120 (85%)	0.15	4 (3%) 39 42	11, 29, 49, 56	0
1	H	102/120 (85%)	0.06	3 (2%) 51 55	12, 30, 46, 50	0
All	All	816/960 (85%)	0.03	13 (1%) 72 74	8, 28, 45, 60	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	65	ALA	6.1
1	G	66	SER	3.3
1	B	1	MET	2.9
1	G	1	MET	2.7
1	E	2	ASN	2.6

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.