



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 07:56 pm BST

PDB ID : 3K4D
Title : Crystal structure of E. coli beta-glucuronidase with the glucaro-d-lactam inhibitor bound
Authors : Wallace, B.D.; Redinbo, M.R.
Deposited on : 2009-10-05
Resolution : 2.39 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

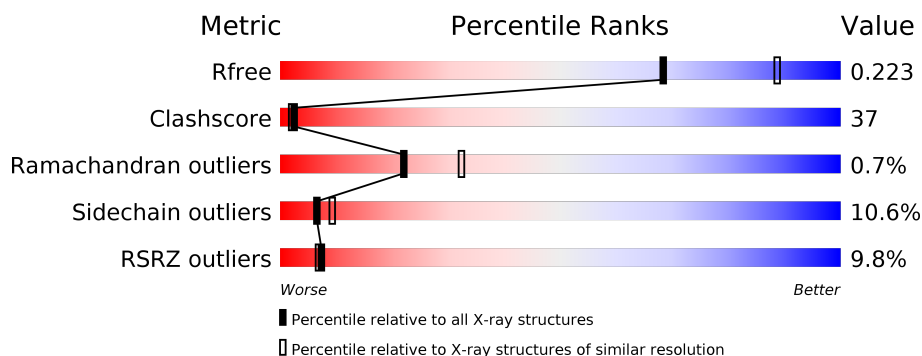
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	605	<div> <div>6%</div> <div>59%</div> <div>31%</div> <div>6%</div> <div>..</div> </div>
1	B	605	<div> <div>13%</div> <div>46%</div> <div>43%</div> <div>8%</div> <div>..</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9933 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.

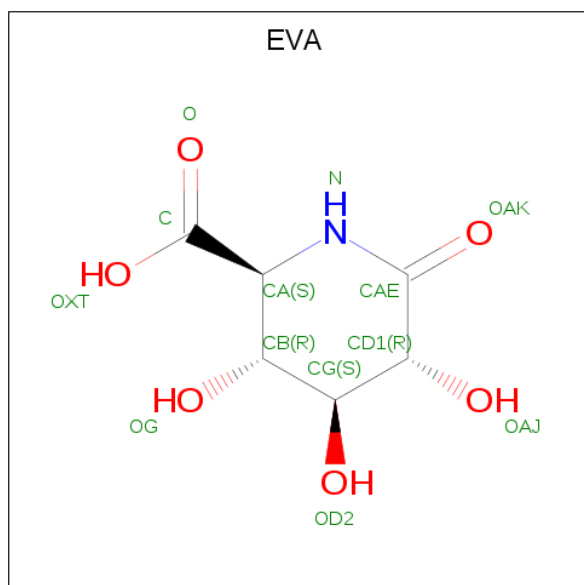
- Molecule 1 is a protein called Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4776	3032	825	897	22			
1	B	596	Total	C	N	O	S	0	0	0
			4776	3032	825	897	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P05804
A	0	HIS	-	EXPRESSION TAG	UNP P05804
B	-1	SER	-	EXPRESSION TAG	UNP P05804
B	0	HIS	-	EXPRESSION TAG	UNP P05804

- Molecule 2 is (2S,3R,4S,5R)-3,4,5-trihydroxy-6-oxopiperidine-2-carboxylic acid (three-letter code: EVA) (formula: C₆H₉NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 13	C 6	N 1	O 6	0	0
2	B	1	Total 13	C 6	N 1	O 6	0	0

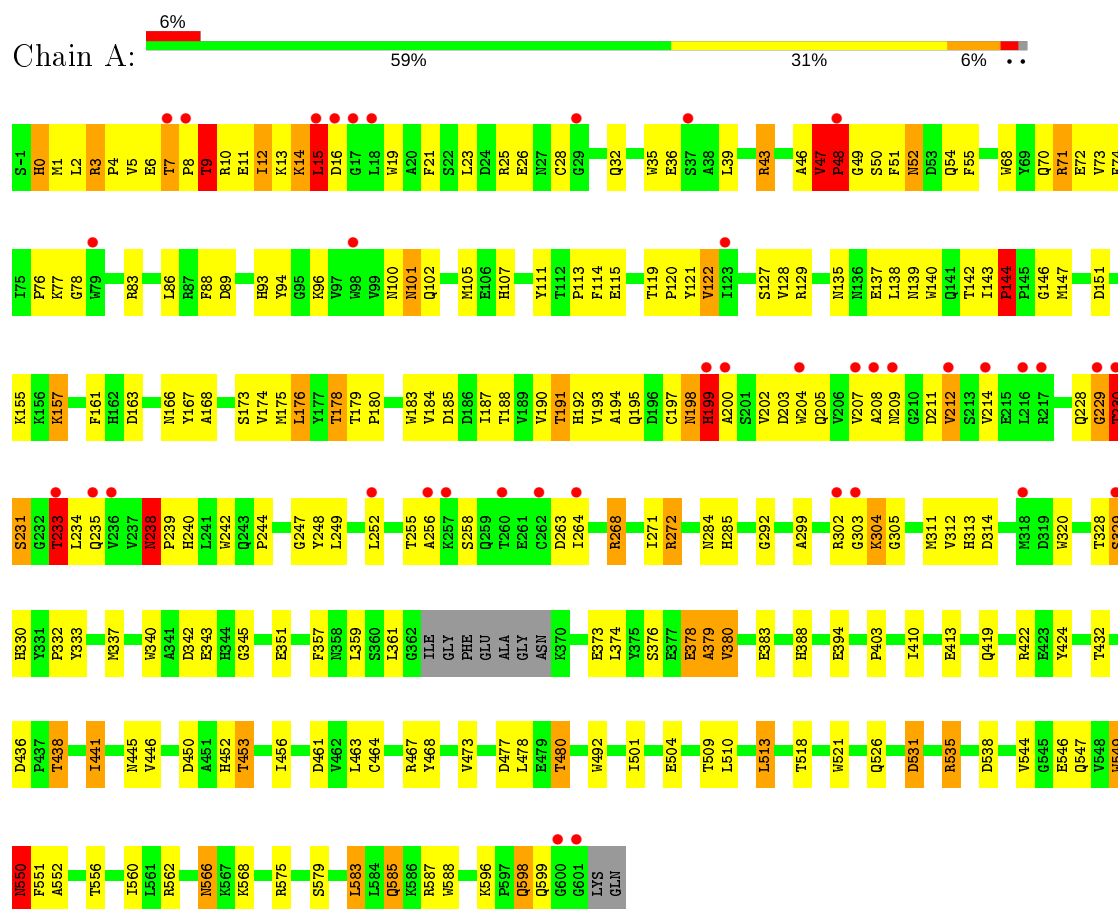
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total 244	O 244	0	0
3	B	111	Total 111	O 111	0	0

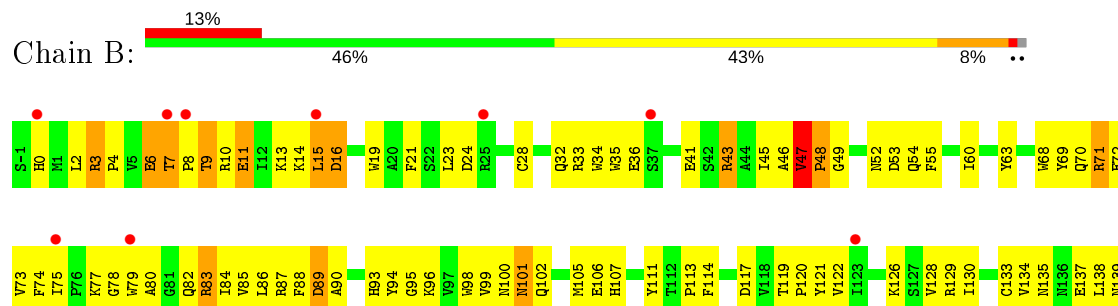
3 Residue-property plots

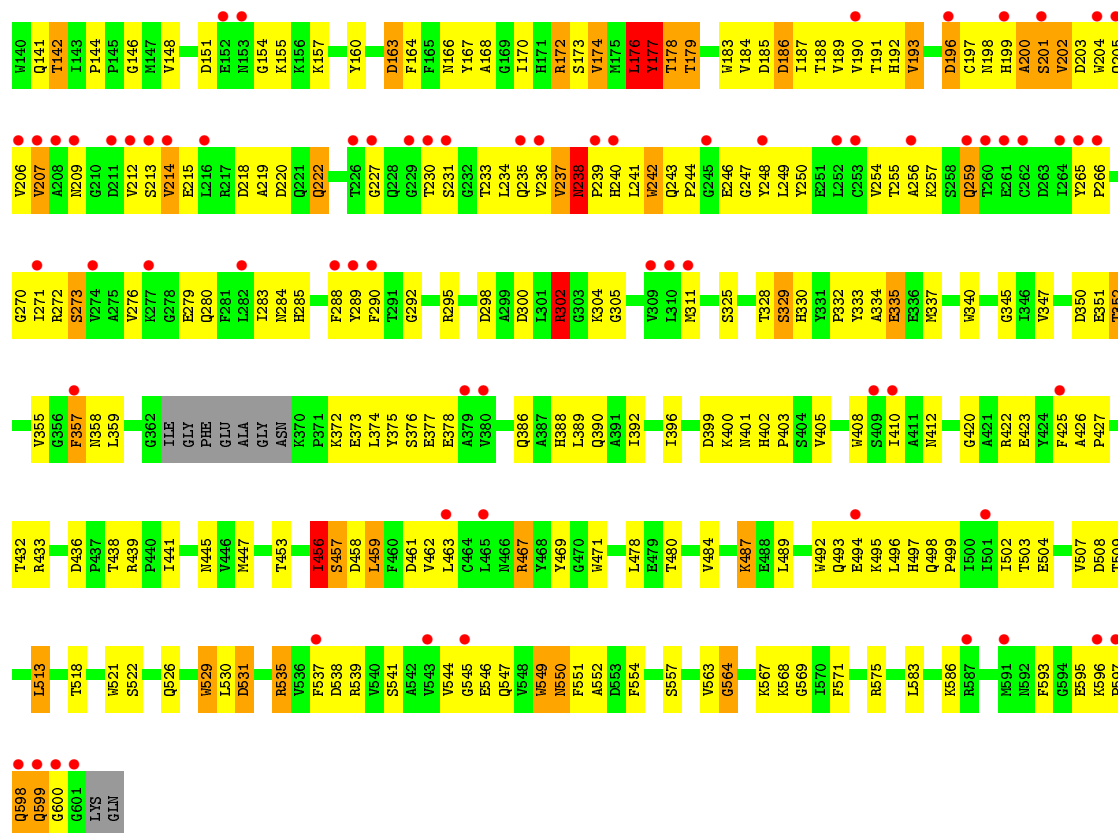
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Beta-glucuronidase



• Molecule 1: Beta-glucuronidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.65Å 76.97Å 125.47Å 90.00° 124.98° 90.00°	Depositor
Resolution (Å)	29.57 – 2.39 47.79 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.57-2.39) 98.2 (47.79-2.39)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102, PHENIX	Depositor
R, R_{free}	0.205 , 0.237 0.208 , 0.223	Depositor DCC
R_{free} test set	2602 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9933	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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	0.65	3/4904 (0.1%)	0.91	26/6673 (0.4%)
1	B	0.49	0/4904	0.85	22/6673 (0.3%)
All	All	0.57	3/9808 (0.0%)	0.88	48/13346 (0.4%)

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	A	0	7
1	B	0	6
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	TYR	CD2-CE2	-6.67	1.29	1.39
1	A	468	TYR	CD1-CE1	-5.42	1.31	1.39
1	A	468	TYR	CE1-CZ	-5.22	1.31	1.38

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	SER	N-CA-CB	-14.31	89.04	110.50
1	B	80	ALA	CB-CA-C	-11.67	92.59	110.10
1	B	599	GLN	N-CA-CB	-10.65	91.43	110.60
1	B	358	ASN	N-CA-CB	-10.25	92.15	110.60
1	A	229	GLY	N-CA-C	-9.35	89.72	113.10

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	ILE	Mainchain,Peptide
1	A	198	ASN	Peptide
1	A	238	ASN	Peptide
1	A	47	VAL	Peptide
1	A	549	TRP	Mainchain

5.2 Too-close contacts ⓘ

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	4776	0	4557	309	0
1	B	4776	0	4558	408	0
2	A	13	0	8	2	0
2	B	13	0	8	3	0
3	A	244	0	0	15	0
3	B	111	0	0	19	0
All	All	9933	0	9131	696	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 37.

The worst 5 of 696 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:7:THR:CG2	1:A:8:PRO:HD3	1.44	1.47
1:B:7:THR:HB	1:B:8:PRO:CD	1.29	1.43
1:A:183:TRP:CZ3	1:A:185:ASP:HB3	1.63	1.34
1:B:7:THR:CB	1:B:8:PRO:CD	2.00	1.23
1:B:456:ILE:O	1:B:456:ILE:CG2	1.86	1.21

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	592/605 (98%)	568 (96%)	19 (3%)	5 (1%)	19	29
1	B	592/605 (98%)	566 (96%)	23 (4%)	3 (0%)	29	41
All	All	1184/1210 (98%)	1134 (96%)	42 (4%)	8 (1%)	22	32

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	B	7	THR
1	B	48	PRO
1	A	304	LYS
1	A	48	PRO

5.3.2 Protein sidechains

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	506/513 (99%)	459 (91%)	47 (9%)	9	13
1	B	506/513 (99%)	446 (88%)	60 (12%)	5	6
All	All	1012/1026 (99%)	905 (89%)	107 (11%)	6	9

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	THR

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	487	LYS
1	B	11	GLU
1	B	71	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	599	GLN
1	B	101	ASN
1	B	498	GLN
1	B	0	HIS
1	B	54	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](#)

2 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	EVA	A	604	-	10,13,13	0.61	0	11,19,19	1.52	1 (9%)
2	EVA	B	604	-	10,13,13	2.29	2 (20%)	11,19,19	1.91	4 (36%)

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	EVA	A	604	-	-	0/0/24/24	0/1/1/1
2	EVA	B	604	-	-	0/0/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	EVA	CAE-N	6.13	1.43	1.33
2	B	604	EVA	CA-N	2.88	1.48	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	604	EVA	OAK-CAE-N	-3.85	117.51	122.69
2	A	604	EVA	OAK-CAE-N	-3.52	117.96	122.69
2	B	604	EVA	OD2-CG-CD1	-2.45	105.01	109.68
2	B	604	EVA	CD1-CAE-N	2.34	123.53	117.93
2	B	604	EVA	OAJ-CD1-CG	-2.12	106.15	110.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	EVA	2	0
2	B	604	EVA	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	596/605 (98%)	0.32	39 (6%) 18 17	19, 46, 107, 127	0
1	B	596/605 (98%)	0.83	78 (13%) 3 3	26, 87, 178, 207	0
All	All	1192/1210 (98%)	0.58	117 (9%) 7 7	19, 67, 152, 207	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	VAL	10.5
1	A	207	VAL	8.7
1	A	303	GLY	8.5
1	B	601	GLY	7.9
1	B	230	THR	7.5

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](#)

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(\AA^2)	Q<0.9
2	EVA	B	604	13/13	0.89	0.16	22,23,29,30	0
2	EVA	A	604	13/13	0.95	0.15	20,21,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.