



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 24, 2017 – 09:59 PM EDT

PDB ID : 3HUM
Title : Crystal structure of Penicillin binding protein 4 from Staphylococcus aureus COL in complex with Cefotaxime
Authors : Navratna, V.; Gopal, B.
Deposited on : unknown
Resolution : 2.30 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

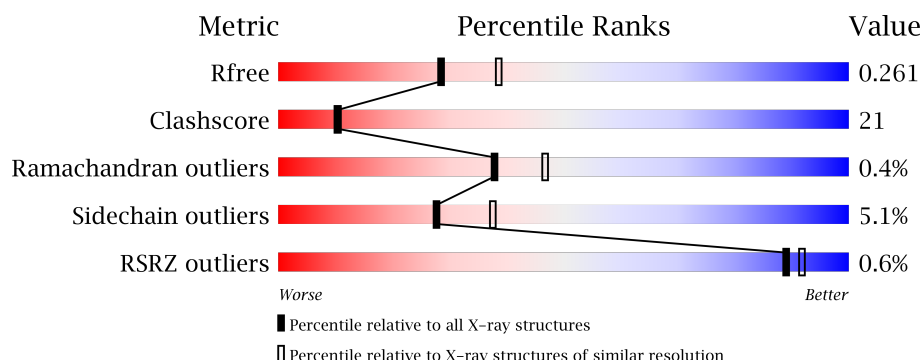
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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. 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	453	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; bottom: 0; width: 57%; background-color: green;"></div> <div style="position: absolute; left: 57%; top: 0; bottom: 0; width: 21%; background-color: yellow;"></div> <div style="position: absolute; left: 78%; top: 0; bottom: 0; width: 21%; background-color: grey;"></div> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 10px; background-color: red;"></div> </div> <div>57% 21% 21%</div> </div>
1	B	453	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; bottom: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; left: 0; top: 0; bottom: 0; width: 57%; background-color: green;"></div> <div style="position: absolute; left: 57%; top: 0; bottom: 0; width: 19%; background-color: yellow;"></div> <div style="position: absolute; left: 76%; top: 0; bottom: 0; width: 21%; background-color: grey;"></div> </div> <div>57% 19% 21%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CEW	A	501	X	-	X	X
2	CEW	B	501	X	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5856 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 Penicillin-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2817	1779	474	552	12			
1	B	358	Total	C	N	O	S	0	0	0
			2817	1779	474	552	12			

There are 46 discrepancies between the modelled and reference sequences:

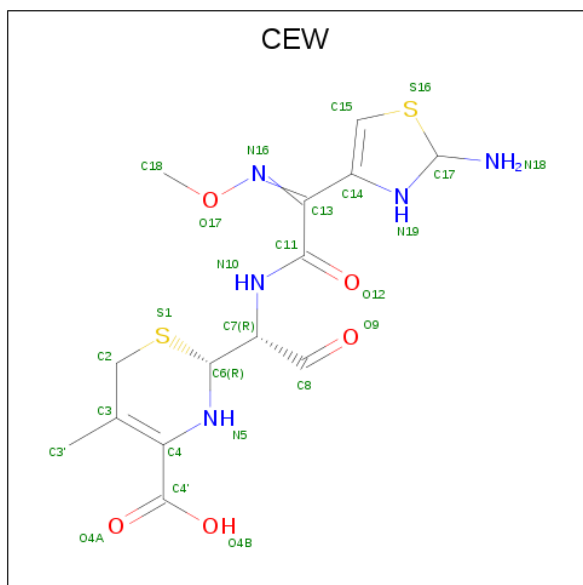
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP Q5HI26
A	-20	GLY	-	EXPRESSION TAG	UNP Q5HI26
A	-19	SER	-	EXPRESSION TAG	UNP Q5HI26
A	-18	SER	-	EXPRESSION TAG	UNP Q5HI26
A	-17	HIS	-	EXPRESSION TAG	UNP Q5HI26
A	-16	HIS	-	EXPRESSION TAG	UNP Q5HI26
A	-15	HIS	-	EXPRESSION TAG	UNP Q5HI26
A	-14	HIS	-	EXPRESSION TAG	UNP Q5HI26
A	-13	HIS	-	EXPRESSION TAG	UNP Q5HI26
A	-12	HIS	-	EXPRESSION TAG	UNP Q5HI26
A	-11	SER	-	EXPRESSION TAG	UNP Q5HI26
A	-10	SER	-	EXPRESSION TAG	UNP Q5HI26
A	-9	GLY	-	EXPRESSION TAG	UNP Q5HI26
A	-8	LEU	-	EXPRESSION TAG	UNP Q5HI26
A	-7	VAL	-	EXPRESSION TAG	UNP Q5HI26
A	-6	PRO	-	EXPRESSION TAG	UNP Q5HI26
A	-5	ARG	-	EXPRESSION TAG	UNP Q5HI26
A	-4	GLY	-	EXPRESSION TAG	UNP Q5HI26
A	-3	SER	-	EXPRESSION TAG	UNP Q5HI26
A	-2	HIS	-	EXPRESSION TAG	UNP Q5HI26
A	-1	MET	-	EXPRESSION TAG	UNP Q5HI26
A	0	ALA	-	EXPRESSION TAG	UNP Q5HI26
A	189	SER	THR	ENGINEERED	UNP Q5HI26
B	-21	MET	-	EXPRESSION TAG	UNP Q5HI26
B	-20	GLY	-	EXPRESSION TAG	UNP Q5HI26

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	EXPRESSION TAG	UNP Q5HI26
B	-18	SER	-	EXPRESSION TAG	UNP Q5HI26
B	-17	HIS	-	EXPRESSION TAG	UNP Q5HI26
B	-16	HIS	-	EXPRESSION TAG	UNP Q5HI26
B	-15	HIS	-	EXPRESSION TAG	UNP Q5HI26
B	-14	HIS	-	EXPRESSION TAG	UNP Q5HI26
B	-13	HIS	-	EXPRESSION TAG	UNP Q5HI26
B	-12	HIS	-	EXPRESSION TAG	UNP Q5HI26
B	-11	SER	-	EXPRESSION TAG	UNP Q5HI26
B	-10	SER	-	EXPRESSION TAG	UNP Q5HI26
B	-9	GLY	-	EXPRESSION TAG	UNP Q5HI26
B	-8	LEU	-	EXPRESSION TAG	UNP Q5HI26
B	-7	VAL	-	EXPRESSION TAG	UNP Q5HI26
B	-6	PRO	-	EXPRESSION TAG	UNP Q5HI26
B	-5	ARG	-	EXPRESSION TAG	UNP Q5HI26
B	-4	GLY	-	EXPRESSION TAG	UNP Q5HI26
B	-3	SER	-	EXPRESSION TAG	UNP Q5HI26
B	-2	HIS	-	EXPRESSION TAG	UNP Q5HI26
B	-1	MET	-	EXPRESSION TAG	UNP Q5HI26
B	0	ALA	-	EXPRESSION TAG	UNP Q5HI26
B	189	SER	THR	ENGINEERED	UNP Q5HI26

- Molecule 2 is (2R)-2-[(1R)-1-({[(2R)-2-amino-2,3-dihydro-1,3-thiazol-4-yl](methoxyimino)acetyl]amino)-2-oxoethyl]-5-methyl-3,6-dihydro-2H-1,3-thiazine-4-carboxylic acid (three-letter code: CEW) (formula: C₁₄H₁₉N₅O₅S₂).




Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	5	5	2		
2	B	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total	O	0	0
			88	88		
3	B	82	Total	O	0	0
			82	82		

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 
- Sequence logo for Chain A, showing amino acid conservation across 100 positions. The y-axis represents the amino acid, and the x-axis represents the position. The logo is color-coded by conservation: green for highly conserved, yellow for moderately conserved, and grey for non-conserved. The sequence is: MET, GLY, SER, SER, HIS, HIS, HIS, HIS, HIS, HIS, SER, SER, GLY, VAL, PRO, ARG, ARG, GLY, SER, HIS, MET, MET, MET, LYS, ASN, LEU, ILE, ILE, ILE, LEU, CYS, LEU, THR, LEU, LEU, SER, THR, PRO, TYR, ALA, GLN, ALA, T25, D28, V29, T30, P31, V32, Q33, A34, A35, N36, D37, Y40.

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows positions 1 to 100. A color scale at the top indicates the percentage of positions with a given amino acid: 57% (green), 19% (yellow), and 21% (grey).
- Key amino acids and their approximate information content (bits) at specific positions:
- Position 1: MET (0.8 bits)
 - Position 2: GLY (0.4 bits)
 - Position 3: SER (0.4 bits)
 - Position 4: SER (0.4 bits)
 - Position 5: HIS (0.4 bits)
 - Position 6: HIS (0.4 bits)
 - Position 7: HIS (0.4 bits)
 - Position 8: HIS (0.4 bits)
 - Position 9: HIS (0.4 bits)
 - Position 10: HIS (0.4 bits)
 - Position 11: HIS (0.4 bits)
 - Position 12: HIS (0.4 bits)
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 - Position 86: HIS (0.4 bits)
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 - Position 88: HIS (0.4 bits)
 - Position 89: HIS (0.4 bits)
 - Position 90: HIS (0.4 bits)
 - Position 91: HIS (0.4 bits)
 - Position 92: HIS (0.4 bits)
 - Position 93: HIS (0.4 bits)
 - Position 94: HIS (0.4 bits)
 - Position 95: HIS (0.4 bits)
 - Position 96: HIS (0.4 bits)
 - Position 97: HIS (0.4 bits)
 - Position 98: HIS (0.4 bits)
 - Position 99: HIS (0.4 bits)
 - Position 100: HIS (0.4 bits)

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.15Å 97.97Å 98.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.30 37.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.34-2.30) 99.7 (37.49-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.202 , 0.265 0.208 , 0.261	Depositor DCC
R_{free} test set	1946 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.468 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5856	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 3.10% 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: CEW

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	0.89	0/2872	0.88	1/3891 (0.0%)
1	B	0.89	0/2872	0.90	3/3891 (0.1%)
All	All	0.89	0/5744	0.89	4/7782 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	LEU	CA-CB-CG	5.84	128.74	115.30
1	B	343	LEU	CA-CB-CG	5.57	128.12	115.30
1	B	97	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	B	100	VAL	N-CA-C	-5.15	97.10	111.00

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	2817	0	2802	97	0
1	B	2817	0	2802	124	0
2	A	26	0	17	17	0
2	B	26	0	17	39	0
3	A	88	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	82	0	0	3	0
All	All	5856	0	5638	234	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 21.

The worst 5 of 234 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:336:GLU:HG3	1:A:380:GLU:CB	1.71	1.20
2:B:501:CEW:H3'	2:B:501:CEW:O4B	1.40	1.19
1:B:262:SER:N	2:B:501:CEW:H2	1.57	1.18
1:A:336:GLU:CG	1:A:380:GLU:HB2	1.73	1.17
1:B:337:ASN:HB3	3:B:482:HOH:O	1.46	1.16

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	356/453 (79%)	339 (95%)	17 (5%)	0	100	100
1	B	356/453 (79%)	336 (94%)	17 (5%)	3 (1%)	22	26
All	All	712/906 (79%)	675 (95%)	34 (5%)	3 (0%)	38	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	LYS
1	B	381	VAL
1	B	330	GLY

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	311/393 (79%)	297 (96%)	14 (4%)	32	44
1	B	311/393 (79%)	293 (94%)	18 (6%)	23	31
All	All	622/786 (79%)	590 (95%)	32 (5%)	28	37

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	SER
1	B	128	ILE
1	B	350	LYS
1	B	119	LYS
1	B	155	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	ASN
1	B	37	GLN
1	B	269	ASN
1	A	382	HIS
1	B	26	ASN

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 [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	CEW	A	501	-	18,27,27	3.89	9 (50%)	17,37,37	3.10	9 (52%)
2	CEW	B	501	-	18,27,27	3.64	8 (44%)	17,37,37	3.46	11 (64%)

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	CEW	A	501	-	1/1/9/14	1/15/47/47	0/1/2/2
2	CEW	B	501	-	1/1/9/14	2/15/47/47	0/1/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	CEW	C2-C3	-10.77	1.37	1.51
2	B	501	CEW	C2-C3	-9.64	1.39	1.51
2	B	501	CEW	C3'-C3	-7.15	1.38	1.51
2	A	501	CEW	C3'-C3	-7.12	1.38	1.51
2	A	501	CEW	C2-S1	-5.92	1.68	1.82

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	CEW	C3'-C3-C4	-5.68	116.46	123.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	CEW	C14-C15-S16	-4.70	106.80	111.62
2	B	501	CEW	O17-N16-C13	-3.68	103.75	111.49
2	B	501	CEW	C14-C15-S16	-3.37	108.17	111.62
2	B	501	CEW	O12-C11-C13	-2.85	116.86	121.57

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	CEW	C17
2	B	501	CEW	C17

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CEW	C18-O17-N16-C13
2	B	501	CEW	C13-C11-N10-C7
2	B	501	CEW	O12-C11-N10-C7

There are no ring outliers.

2 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	CEW	17	0
2	B	501	CEW	39	0

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	358/453 (79%)	-0.22	3 (0%) 86 89	33, 46, 69, 83	14 (3%)
1	B	358/453 (79%)	-0.21	1 (0%) 93 96	33, 46, 71, 82	8 (2%)
All	All	716/906 (79%)	-0.22	4 (0%) 89 92	33, 46, 69, 83	22 (3%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	3.4
1	A	329	ASN	2.4
1	B	381	VAL	2.2
1	A	325	GLU	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	CEW	A	501	26/26	0.67	0.39	9.19	47,54,60,60	26
2	CEW	B	501	26/26	0.75	0.35	8.44	33,46,56,57	26

6.5 Other polymers [i](#)

There are no such residues in this entry.