



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:06 AM EDT

PDB ID : 1W54 / pdb_00001w54
Title : Stepwise introduction of a zinc binding site into Porphobilinogen synthase from *Pseudomonas aeruginosa* (mutation D139C)
Authors : Frere, F.; Reents, H.; Schubert, W.-D.; Heinz, D.W.; Jahn, D.
Deposited on : 2004-08-05
Resolution : 2.20 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

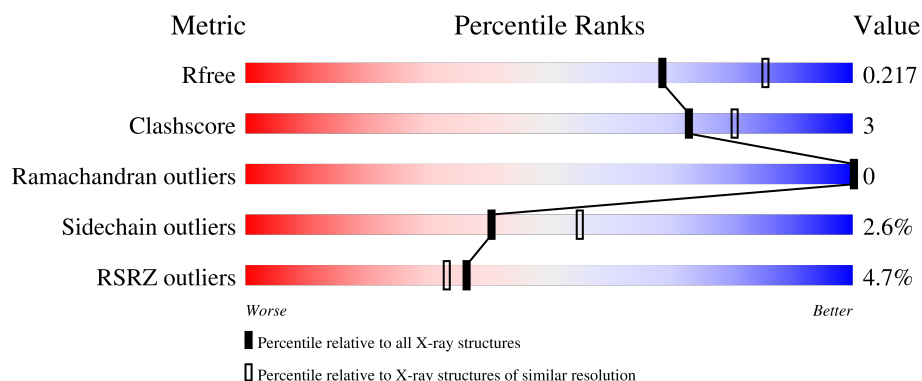
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	337	
1	B	337	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5297 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.

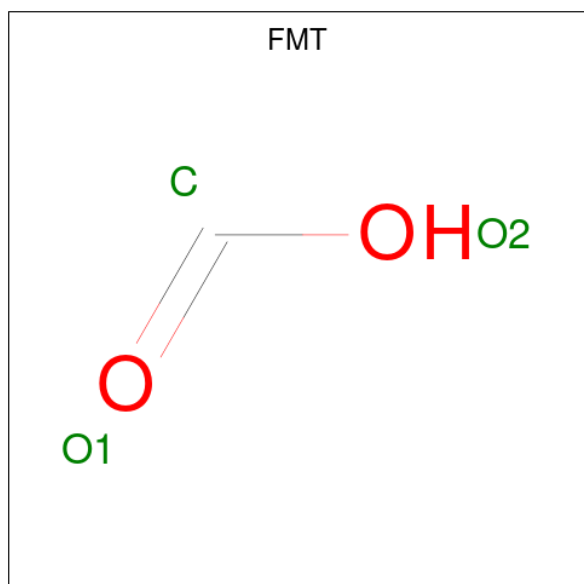
- Molecule 1 is a protein called DELTA-AMINOLEVULINIC ACID DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	4	1
			2452	1538	438	464	12			
1	B	322	Total	C	N	O	S	0	4	1
			2529	1587	452	478	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	CYS	ASP	engineered mutation	UNP Q59643
B	139	CYS	ASP	engineered mutation	UNP Q59643
A	199	VAL	ILE	engineered mutation	UNP Q59643
B	199	VAL	ILE	engineered mutation	UNP Q59643

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 3 1 2	0	0
2	B	1	Total C O 3 1 2	0	0

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0
3	B	1	Total K 1 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0

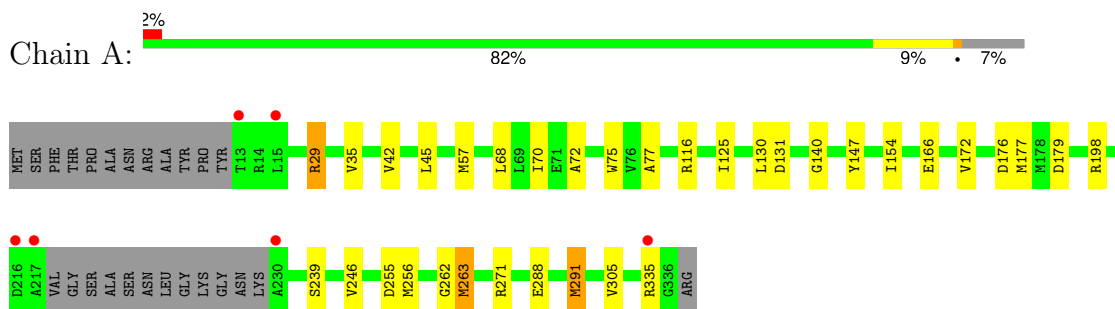
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	178	Total O 178 178	0	0
6	B	126	Total O 126 126	0	0

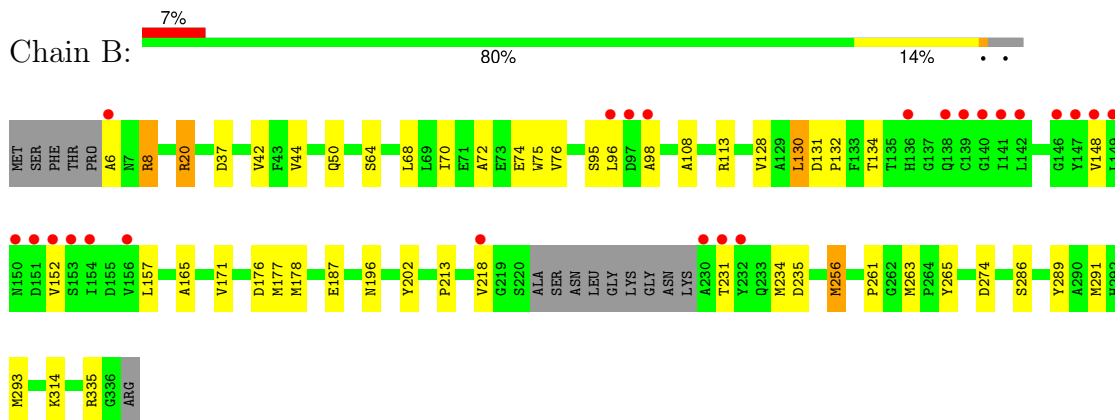
3 Residue-property plots

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: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



• Molecule 1: DELTA-AMINOLEVULINIC ACID DEHYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.23Å 125.23Å 86.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.71 – 2.20 87.71 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (87.71-2.20) 99.7 (87.71-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.86 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.154 , 0.217 0.164 , 0.217	Depositor DCC
R_{free} test set	1811 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5297	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ZN, FMT

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	1.47	14/2495 (0.6%)	1.20	3/3383 (0.1%)
1	B	1.47	20/2575 (0.8%)	1.20	7/3493 (0.2%)
All	All	1.47	34/5070 (0.7%)	1.20	10/6876 (0.1%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	MET	SD-CE	-11.38	1.51	1.79
1	A	291	MET	SD-CE	-9.66	1.55	1.79
1	B	256	MET	SD-CE	-9.43	1.55	1.79
1	B	291	MET	SD-CE	-8.21	1.59	1.79
1	A	70	ILE	CA-CB	7.42	1.63	1.54
1	A	131	ASP	C-O	-6.65	1.18	1.24
1	B	196	ASN	CG-OD1	6.61	1.36	1.23
1	B	234	MET	SD-CE	-6.53	1.63	1.79
1	B	177	MET	SD-CE	6.05	1.94	1.79
1	A	166	GLU	C-O	-5.96	1.16	1.24
1	B	218	VAL	CA-CB	5.93	1.62	1.54
1	A	57	MET	SD-CE	5.92	1.94	1.79
1	A	29	ARG	CD-NE	-5.85	1.38	1.46
1	B	108	ALA	CA-C	-5.79	1.45	1.52
1	B	8	ARG	CD-NE	-5.68	1.38	1.46
1	B	113	ARG	N-CA	5.67	1.53	1.46
1	B	289	TYR	C-O	-5.60	1.17	1.24
1	A	45	LEU	CA-C	-5.53	1.45	1.52
1	A	246	VAL	C-O	-5.48	1.17	1.24
1	A	239	SER	CA-C	-5.48	1.48	1.52
1	A	77	ALA	CA-CB	5.43	1.61	1.53
1	A	172	VAL	C-O	5.37	1.29	1.24
1	B	231	THR	CA-CB	5.33	1.63	1.53
1	B	70	ILE	CA-CB	5.29	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	VAL	CA-C	-5.23	1.46	1.52
1	B	202	TYR	C-O	-5.19	1.16	1.23
1	B	165	ALA	CA-CB	5.17	1.61	1.53
1	B	152	VAL	CA-CB	5.14	1.60	1.54
1	B	171	VAL	CA-CB	5.13	1.61	1.54
1	A	271	ARG	C-O	-5.10	1.18	1.24
1	B	274	ASP	C-O	-5.08	1.18	1.24
1	A	125	ILE	CA-CB	5.08	1.60	1.53
1	B	148	VAL	CA-CB	5.02	1.59	1.53
1	A	35	VAL	C-O	-5.01	1.17	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	GLY	N-CA-C	8.36	117.82	110.21
1	B	178	MET	N-CA-C	-6.56	101.69	110.55
1	B	176	ASP	N-CA-C	6.53	119.21	111.71
1	A	177	MET	N-CA-C	6.31	120.23	111.90
1	B	234	MET	N-CA-C	5.72	118.57	110.50
1	A	176	ASP	N-CA-C	5.67	119.46	112.54
1	B	98	ALA	N-CA-C	5.51	119.03	111.54
1	B	64	SER	N-CA-C	-5.40	103.40	110.53
1	B	8	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	B	291	MET	CG-SD-CE	-5.07	89.75	100.90

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	2452	0	2428	18	0
1	B	2529	0	2500	24	0
2	A	3	0	1	0	0
2	B	3	0	1	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	178	0	0	1	0
6	B	126	0	0	1	0
All	All	5297	0	4930	32	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 (32) 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:263[B]:MET:CE	1:B:263[B]:MET:HE2	1.98	0.92
1:A:263[B]:MET:CE	1:B:263[B]:MET:CE	2.51	0.89
1:A:263[B]:MET:HE3	1:B:263[B]:MET:HE2	1.66	0.78
1:A:263[B]:MET:HE2	1:B:263[B]:MET:CE	2.13	0.76
1:A:263[B]:MET:HE2	1:B:263[B]:MET:HE3	1.72	0.70
1:A:263[B]:MET:HE3	1:B:263[B]:MET:CE	2.24	0.66
1:A:29:ARG:HD3	1:B:235:ASP:OD2	1.99	0.62
1:A:263[B]:MET:CE	1:B:263[B]:MET:HE3	2.28	0.62
1:A:42:VAL:HG11	1:A:68:LEU:CD1	2.31	0.61
1:B:128:VAL:HG12	1:B:157:LEU:HD22	1.84	0.60
1:A:42:VAL:HG11	1:A:68:LEU:HD13	1.85	0.59
1:B:6:ALA:HB1	1:B:8:ARG:HG3	1.85	0.58
1:B:213:PRO:HB2	1:B:286:SER:HB2	1.85	0.58
1:B:130:LEU:N	1:B:130:LEU:HD23	2.24	0.53
1:A:130:LEU:HD12	1:A:140:GLY:HA2	1.91	0.53
1:B:42:VAL:HG11	1:B:68:LEU:HD13	1.91	0.52
1:A:263[A]:MET:HG2	1:B:263[A]:MET:HG2	1.94	0.49
1:B:20[B]:ARG:NH2	6:B:2017:HOH:O	2.49	0.46
1:B:95:SER:O	1:B:134:THR:HA	2.18	0.44
1:A:72:ALA:HA	1:A:75:TRP:CE3	2.53	0.44
1:B:6:ALA:HB1	1:B:8:ARG:CG	2.47	0.43
1:A:154:ILE:HD11	1:A:179:ASP:O	2.18	0.43
1:B:261:PRO:HD2	1:B:265:TYR:CE2	2.54	0.43
1:A:198:ARG:HA	1:A:255:ASP:OD2	2.20	0.42
1:B:72:ALA:HA	1:B:75:TRP:CE3	2.54	0.42
1:B:72:ALA:O	1:B:76:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:N	1:B:132:PRO:HD3	2.35	0.42
1:B:131:ASP:N	1:B:132:PRO:CD	2.83	0.41
1:A:288:GLU:HA	1:A:291:MET:HE2	2.03	0.41
1:A:147:TYR:CE1	1:B:20[B]:ARG:HD3	2.56	0.41
1:A:116:ARG:HA	6:A:2075:HOH:O	2.21	0.41
1:B:37:ASP:CG	1:B:314:LYS:HD3	2.46	0.40

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	312/337 (93%)	306 (98%)	6 (2%)	0	100	100
1	B	322/337 (96%)	315 (98%)	7 (2%)	0	100	100
All	All	634/674 (94%)	621 (98%)	13 (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	254/269 (94%)	249 (98%)	5 (2%)	48	64
1	B	261/269 (97%)	251 (96%)	10 (4%)	29	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	515/538 (96%)	500 (97%)	15 (3%)	40	51

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	256	MET
1	A	263[A]	MET
1	A	263[B]	MET
1	A	305	VAL
1	A	335	ARG
1	B	20[A]	ARG
1	B	20[B]	ARG
1	B	44	VAL
1	B	50	GLN
1	B	74	GLU
1	B	96	LEU
1	B	130	LEU
1	B	187	GLU
1	B	256	MET
1	B	335	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	244	HIS
1	A	298	ASN
1	A	332	GLN
1	B	7	ASN
1	B	297	GLN
1	B	298	ASN
1	B	332	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	FMT	B	1337	-	2,2,2	0.31	0	1,1,1	0.73	0
2	FMT	A	1337	-	2,2,2	0.75	0	1,1,1	0.45	0

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	312/337 (92%)	-0.42	6 (1%) 66 63	11, 25, 46, 85	4 (1%)
1	B	322/337 (95%)	0.11	24 (7%) 20 17	10, 31, 80, 103	4 (1%)
All	All	634/674 (94%)	-0.15	30 (4%) 36 33	10, 28, 73, 103	8 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	ILE	6.9
1	B	149	LEU	5.4
1	B	154	ILE	5.0
1	A	13	THR	4.7
1	B	142	LEU	4.6
1	B	151	ASP	4.5
1	B	153	SER	4.2
1	B	152	VAL	4.0
1	B	146	GLY	4.0
1	B	96	LEU	3.9
1	B	148	VAL	3.4
1	B	147	TYR	3.4
1	B	150	ASN	3.4
1	B	156	VAL	3.4
1	A	217	ALA	3.2
1	B	98	ALA	3.1
1	B	230	ALA	2.8
1	B	139	CYS	2.8
1	B	232	TYR	2.8
1	A	230	ALA	2.7
1	A	335	ARG	2.7
1	A	15	LEU	2.5
1	B	97	ASP	2.5
1	B	231	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLY	2.2
1	B	136	HIS	2.2
1	B	218	VAL	2.1
1	B	138	GLN	2.1
1	A	216	ASP	2.1
1	B	6	ALA	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(Å ²)	Q<0.9
4	MG	B	1339	1/1	0.82	0.18	48,48,48,48	0
5	ZN	B	1340	1/1	0.89	0.13	73,73,73,73	1
2	FMT	B	1337	3/3	0.95	0.08	27,27,33,39	0
2	FMT	A	1337	3/3	0.96	0.08	32,32,36,38	0
3	K	B	1338	1/1	0.96	0.07	42,42,42,42	1
5	ZN	A	1340	1/1	0.97	0.04	38,38,38,38	1
3	K	A	1338	1/1	0.98	0.04	50,50,50,50	0
4	MG	A	1339	1/1	0.99	0.02	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.