



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:06 AM UTC

PDB ID : 6CMK / pdb_00006cmk
Title : Crystal structure of Citrobacter koseri AztD
Authors : Yukl, E.T.
Deposited on : 2018-03-05
Resolution : 1.73 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

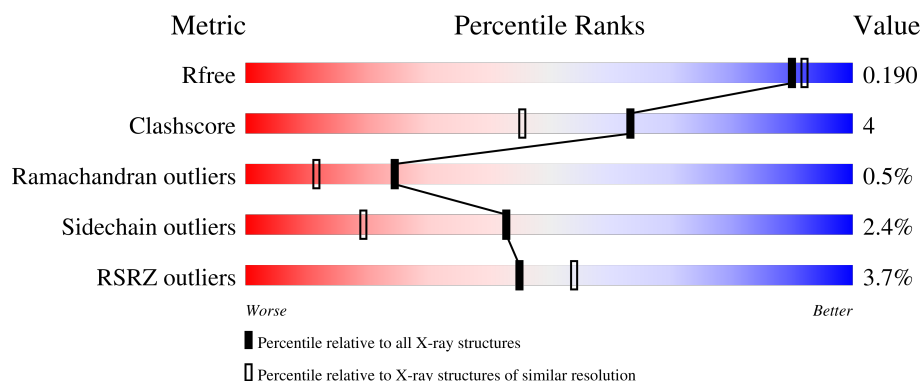
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

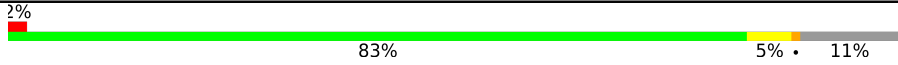
The reported resolution of this entry is 1.73 Å.

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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	421	
1	B	421	

2 Entry composition [i](#)

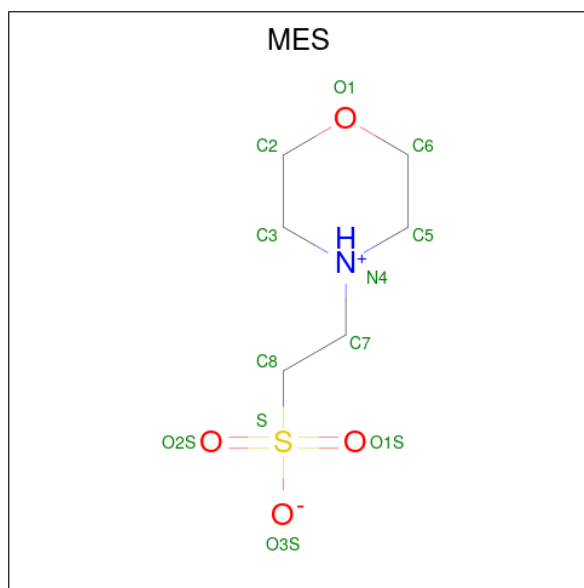
There are 7 unique types of molecules in this entry. The entry contains 12143 atoms, of which 5663 are hydrogens and 0 are deuteriums.

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 AztD protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	373	Total	C	H	N	O	S	0	5	0
			5660	1819	2797	499	541	4			
1	A	375	Total	C	H	N	O	S	0	5	0
			5675	1827	2792	507	545	4			

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).

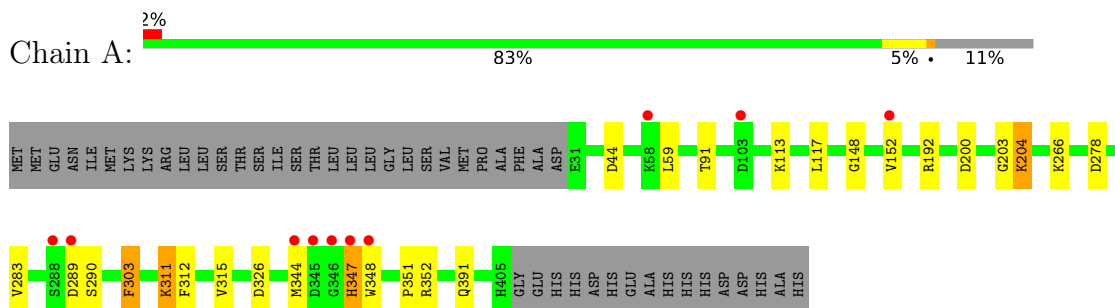
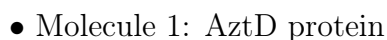


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	299	Total 299	O 299	0	0
7	A	371	Total 374	O 374	0	3

- Molecule 1: AztD protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.23Å 128.79Å 56.85Å 90.00° 105.20° 90.00°	Depositor
Resolution (Å)	64.39 – 1.73 64.39 – 1.73	Depositor EDS
% Data completeness (in resolution range)	99.1 (64.39-1.73) 99.1 (64.39-1.73)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 1.73Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.153 , 0.188 0.154 , 0.190	Depositor DCC
R_{free} test set	1998 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12143	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: ZN, PEG, MES, EDO, PGE

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	0.23	0/2946	0.56	4/4006 (0.1%)
1	B	0.25	0/2926	0.53	2/3980 (0.1%)
All	All	0.24	0/5872	0.54	6/7986 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	GLY	CA-C-N	7.47	131.41	120.95
1	A	203	GLY	C-N-CA	7.47	131.41	120.95
1	B	387	SER	CA-C-N	6.89	133.24	122.70
1	B	387	SER	C-N-CA	6.89	133.24	122.70
1	A	351	PRO	CA-C-N	6.04	133.93	123.11
1	A	351	PRO	C-N-CA	6.04	133.93	123.11

There are no chirality outliers.

There are no planarity outliers.

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	2883	2792	2882	18	0
1	B	2863	2797	2869	27	0
2	A	12	13	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	13	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	8	12	12	0	0
4	B	8	12	12	1	0
5	A	10	14	14	0	0
6	A	7	10	10	0	0
7	A	374	0	0	5	2
7	B	299	0	0	6	2
All	All	6480	5663	5825	46	2

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 4.

All (46) 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:B:326:ASP:OD1	7:B:601:HOH:O	1.91	0.88
1:B:324:GLN:NE2	7:B:603:HOH:O	2.08	0.86
1:A:303:PHE:HB3	1:A:315[A]:VAL:HG12	1.60	0.83
1:B:149:GLU:OE1	7:B:602:HOH:O	2.00	0.79
1:A:347:HIS:O	1:A:352:ARG:NH2	2.23	0.71
1:B:310:ALA:O	7:B:604:HOH:O	2.09	0.69
1:B:365:THR:HG22	1:B:372:ILE:HD12	1.73	0.69
1:A:117:LEU:HD22	1:A:152:VAL:HG22	1.77	0.67
1:B:278:ASP:OD1	7:B:605:HOH:O	2.14	0.64
1:A:44:ASP:OD2	1:A:391:GLN:NE2	2.31	0.63
1:A:278:ASP:OD1	7:A:601:HOH:O	2.16	0.62
4:B:505:EDO:O1	7:B:606:HOH:O	2.16	0.61
1:B:74:GLU:N	1:B:129:GLU:OE1	2.28	0.60
1:A:326:ASP:OD1	7:A:602:HOH:O	2.16	0.60
1:A:303:PHE:CB	1:A:315[A]:VAL:HG12	2.31	0.58
1:A:192[B]:ARG:NH1	7:A:604:HOH:O	2.23	0.58
1:A:148:GLY:O	1:A:152:VAL:HG23	2.03	0.57
1:A:91:THR:HG21	1:A:117:LEU:HD23	1.86	0.56
1:A:311:LYS:NZ	7:A:606:HOH:O	2.35	0.54
1:B:103:ASP:OD1	1:B:104[B]:HIS:N	2.41	0.53
1:B:405:HIS:ND1	1:B:405:HIS:O	2.41	0.53
1:B:355[B]:ILE:HD12	1:B:364:VAL:HG22	1.91	0.53
1:B:192:ARG:NH2	1:B:230:GLU:OE2	2.42	0.52
1:B:103:ASP:O	1:B:104[A]:HIS:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:NZ	7:A:608:HOH:O	2.43	0.50
1:B:104[B]:HIS:O	1:B:105:ALA:HB2	2.12	0.49
1:A:348:TRP:HA	1:A:352:ARG:HH22	1.77	0.49
1:B:65:LYS:NZ	1:B:118:GLU:OE2	2.47	0.48
1:B:99:HIS:CE1	1:B:106:ASP:HB2	2.50	0.46
1:A:348:TRP:CD1	1:A:348:TRP:H	2.35	0.45
1:B:371:LYS:HE3	1:B:373:ILE:HD11	1.99	0.44
1:A:117:LEU:HD22	1:A:152:VAL:CG2	2.47	0.44
1:B:101:HIS:N	1:B:104[A]:HIS:O	2.49	0.44
1:B:91:THR:OG1	1:B:115:LEU:HB2	2.17	0.44
1:B:99:HIS:C	1:B:99:HIS:HD1	2.25	0.44
1:B:355[A]:ILE:HG22	1:B:356:ALA:N	2.33	0.44
1:A:200:ASP:OD2	1:A:204:LYS:NZ	2.42	0.43
1:B:101:HIS:HB2	1:B:104[A]:HIS:HB3	2.00	0.42
1:A:311:LYS:HG3	1:A:312:PHE:CD2	2.55	0.42
1:B:404:VAL:O	1:B:405:HIS:ND1	2.53	0.41
1:B:372:ILE:HD11	1:B:392:PRO:HB2	2.02	0.41
1:A:283:VAL:HA	1:A:290:SER:O	2.21	0.41
1:B:65:LYS:HD2	1:B:88:VAL:HG11	2.03	0.41
1:B:129:GLU:HG3	1:B:134:ILE:CG1	2.51	0.40
1:B:134:ILE:O	1:B:146:ILE:HA	2.21	0.40
1:B:188:ASP:OD1	1:B:191:LYS:HD2	2.21	0.40

All (2) 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)
7:B:792:HOH:O	7:A:959:HOH:O[1_556]	1.94	0.26
7:B:878:HOH:O	7:A:614:HOH:O[2_545]	2.14	0.06

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	378/421 (90%)	364 (96%)	14 (4%)	0	100	100
1	B	376/421 (89%)	357 (95%)	14 (4%)	5 (1%)	9	1
All	All	754/842 (90%)	721 (96%)	28 (4%)	5 (1%)	24	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	104[A]	HIS
1	B	104[B]	HIS
1	B	103	ASP
1	B	187	ASP
1	B	105	ALA

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	312/348 (90%)	304 (97%)	8 (3%)	40	17
1	B	311/348 (89%)	304 (98%)	7 (2%)	44	20
All	All	623/696 (90%)	608 (98%)	15 (2%)	43	19

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

Mol	Chain	Res	Type
1	B	99	HIS
1	B	119	LEU
1	B	154	LYS
1	B	157	LYS
1	B	187	ASP
1	B	303	PHE
1	B	389	GLU
1	A	59	LEU
1	A	204	LYS
1	A	266	LYS
1	A	289	ASP

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Mol	Chain	Res	Type
1	A	303	PHE
1	A	311	LYS
1	A	344	MET
1	A	347	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	156	GLN
1	B	391	GLN
1	A	69	ASN
1	A	240	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\# Z > 2$
5	PGE	A	506	-	9,9,9	0.35	0	8,8,8	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	B	501	-	12,12,12	2.02	1 (8%)	15,16,16	1.48	4 (26%)
2	MES	A	501	-	12,12,12	1.86	1 (8%)	15,16,16	1.20	1 (6%)
4	EDO	A	505	-	3,3,3	0.42	0	2,2,2	0.35	0
4	EDO	A	504	-	3,3,3	0.42	0	2,2,2	0.39	0
6	PEG	A	507	-	6,6,6	0.49	0	5,5,5	0.31	0
4	EDO	B	504	-	3,3,3	0.42	0	2,2,2	0.31	0
4	EDO	B	505	-	3,3,3	0.42	0	2,2,2	0.26	0

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
5	PGE	A	506	-	-	0/7/7/7	-
2	MES	B	501	-	-	1/6/14/14	0/1/1/1
2	MES	A	501	-	-	0/6/14/14	0/1/1/1
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
6	PEG	A	507	-	-	3/4/4/4	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	MES	C8-S	-6.74	1.68	1.77
2	A	501	MES	C8-S	-6.10	1.69	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MES	O1S-S-C8	3.28	111.68	106.73
2	B	501	MES	C6-C5-N4	-2.81	105.85	110.12
2	B	501	MES	O1S-S-C8	2.68	110.78	106.73
2	B	501	MES	C5-N4-C3	2.36	113.92	108.84
2	B	501	MES	O2S-S-C8	2.16	109.99	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	507	PEG	O2-C3-C4-O4
2	B	501	MES	N4-C7-C8-S
4	A	504	EDO	O1-C1-C2-O2
6	A	507	PEG	O1-C1-C2-O2
6	A	507	PEG	C1-C2-O2-C3
4	B	504	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	EDO	1	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	375/421 (89%)	-0.20	10 (2%) 56 64	9, 25, 53, 84	5 (1%)
1	B	373/421 (88%)	0.09	18 (4%) 35 43	8, 27, 68, 120	5 (1%)
All	All	748/842 (88%)	-0.05	28 (3%) 45 54	8, 26, 62, 120	10 (1%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	152	VAL	6.5
1	B	104[A]	HIS	6.3
1	A	348	TRP	5.9
1	B	102	GLY	5.2
1	A	152	VAL	4.6
1	B	103	ASP	4.1
1	A	347	HIS	4.0
1	B	405	HIS	3.9
1	B	101	HIS	3.7
1	B	240	ASN	3.6
1	B	99	HIS	3.5
1	B	105	ALA	3.2
1	A	346	GLY	3.1
1	B	151	ALA	3.0
1	B	100	ASP	2.9
1	B	187	ASP	2.9
1	B	132	GLY	2.8
1	B	54	LEU	2.6
1	A	344	MET	2.4
1	A	289	ASP	2.4
1	A	103	ASP	2.4
1	A	345	ASP	2.4
1	B	360	ASN	2.3
1	A	288	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	58	LYS	2.1
1	B	131	GLN	2.1
1	B	156	GLN	2.1
1	B	404	VAL	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	EDO	A	504	4/4	0.74	0.20	61,74,81,86	0
6	PEG	A	507	7/7	0.82	0.20	46,66,91,91	0
4	EDO	B	505	4/4	0.83	0.12	46,55,63,63	0
5	PGE	A	506	10/10	0.88	0.11	28,44,58,58	0
4	EDO	A	505	4/4	0.89	0.12	46,56,67,67	0
4	EDO	B	504	4/4	0.90	0.14	51,61,67,68	0
3	ZN	B	502	1/1	0.94	0.08	64,64,64,64	0
3	ZN	A	502	1/1	0.95	0.07	37,37,37,37	1
2	MES	B	501	12/12	0.96	0.15	17,71,90,94	0
2	MES	A	501	12/12	0.98	0.06	18,24,29,30	0
3	ZN	A	503	1/1	0.98	0.05	36,36,36,36	1
3	ZN	B	503	1/1	0.99	0.02	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.