



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:42 AM UTC

PDB ID : 1VZY / pdb_00001vzy
Title : Crystal structure of the Bacillus subtilis HSP33
Authors : Janda, I.K.; Devedjiev, Y.; Derewenda, U.; Dauter, Z.; Bielnicki, J.; Cooper, D.R.; Joachimiak, A.; Derewenda, Z.S.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-05-29
Resolution : 1.97 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

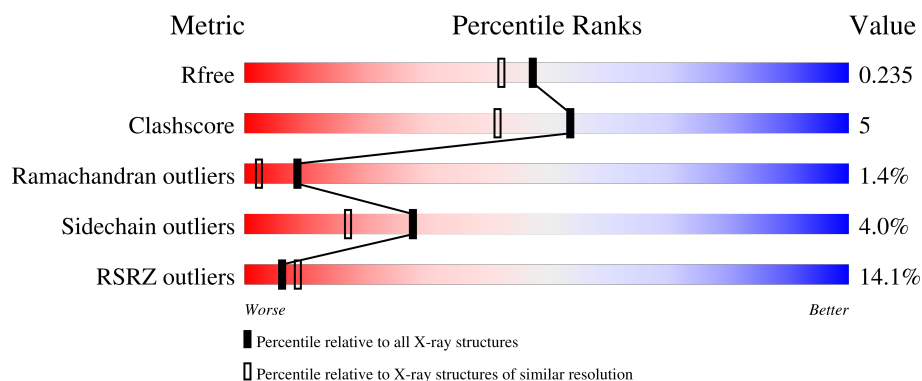
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	291	10% 83% 14% .
1	B	291	18% 86% 10% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4685 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 33 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2209	1386	374	437	12			
1	B	286	Total	C	N	O	S	0	0	0
			2173	1367	366	428	12			

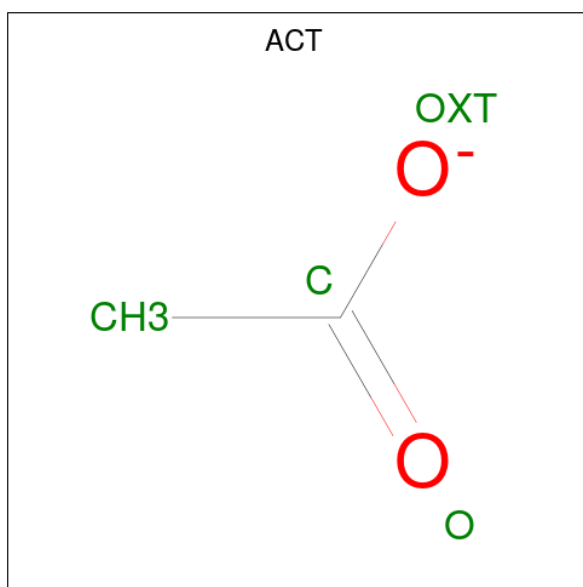
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ALA	GLU	engineered mutation	UNP P37565
A	101	ALA	GLN	engineered mutation	UNP P37565
B	100	ALA	GLU	engineered mutation	UNP P37565
B	101	ALA	GLN	engineered mutation	UNP P37565

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

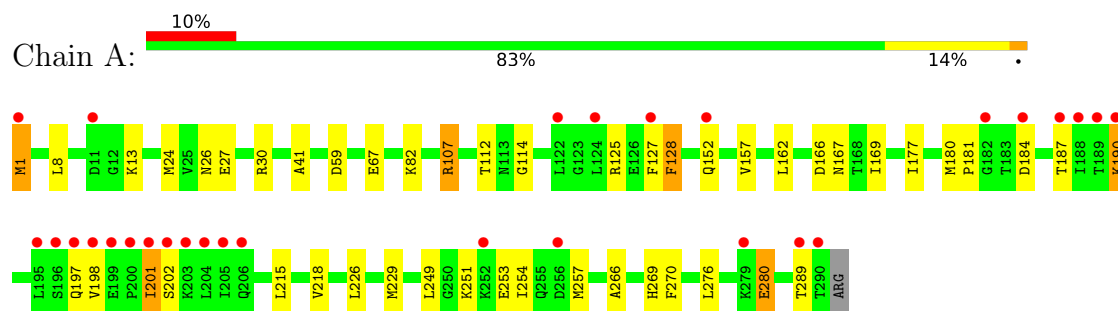
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	146	Total O 146 146	0	0
4	B	131	Total O 131 131	0	0

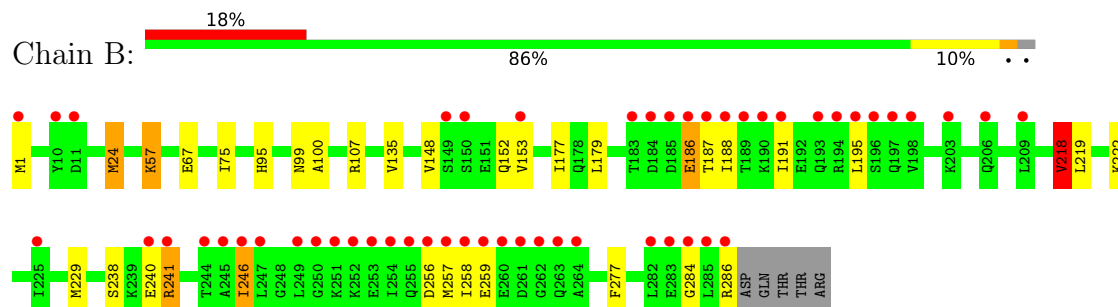
3 Residue-property plots

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: 33 KDA CHAPERONIN



• Molecule 1: 33 KDA CHAPERONIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.29Å 115.29Å 106.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.97 20.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-1.97) 99.5 (20.00-1.97)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.197 , 0.225 0.210 , 0.235	Depositor DCC
R_{free} test set	1103 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4685	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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: ZN, ACT

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	1.40	9/2241 (0.4%)	1.19	4/3028 (0.1%)
1	B	1.38	6/2205 (0.3%)	1.08	1/2980 (0.0%)
All	All	1.39	15/4446 (0.3%)	1.14	5/6008 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	MET	SD-CE	-12.47	1.48	1.79
1	B	24	MET	CG-SD	8.44	2.01	1.80
1	A	229	MET	SD-CE	-8.05	1.59	1.79
1	A	1	MET	CG-SD	6.49	1.97	1.80
1	B	135	VAL	CA-CB	-6.44	1.46	1.54
1	A	24	MET	SD-CE	-6.32	1.63	1.79
1	A	30	ARG	CA-C	-6.19	1.44	1.52
1	A	215	LEU	C-O	-6.19	1.16	1.24
1	A	24	MET	CG-SD	5.94	1.95	1.80
1	A	41	ALA	CA-CB	-5.73	1.44	1.53
1	B	99	ASN	CA-CB	5.67	1.61	1.53
1	B	75	ILE	CA-CB	-5.44	1.48	1.54
1	A	266	ALA	CA-CB	-5.29	1.44	1.53
1	B	218	VAL	CA-C	5.26	1.59	1.52
1	A	201	ILE	CA-CB	5.19	1.61	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	MET	CG-SD-CE	-5.98	87.75	100.90
1	B	153	VAL	CA-C-O	-5.46	117.10	119.94
1	A	157	VAL	CA-C-N	-5.19	118.54	122.33
1	A	157	VAL	C-N-CA	-5.19	118.54	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	VAL	N-CA-C	5.13	116.99	108.99

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	2209	0	2210	24	0
1	B	2173	0	2175	18	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	12	0	0
3	B	8	0	6	1	0
4	A	146	0	0	5	1
4	B	131	0	0	2	0
All	All	4685	0	4403	41	1

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 5.

All (41) 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:24:MET:CG	1:B:24:MET:SD	2.01	1.46
1:A:190:LYS:HD3	4:A:2006:HOH:O	1.79	0.83
1:B:95:HIS:HD2	4:B:2053:HOH:O	1.67	0.77
1:A:162:LEU:HG	1:A:202:SER:HB2	1.69	0.74
1:A:27:GLU:CD	4:A:2020:HOH:O	2.30	0.74
1:B:24:MET:CG	1:B:24:MET:CE	2.66	0.73
1:A:27:GLU:HG3	4:A:2020:HOH:O	1.89	0.73
1:A:59:ASP:OD1	1:A:82:LYS:NZ	2.22	0.72
1:A:27:GLU:CG	4:A:2020:HOH:O	2.36	0.72
1:A:269:HIS:HD2	4:A:2135:HOH:O	1.73	0.72
1:A:125:ARG:HA	1:A:127:PHE:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:MET:SD	1:B:24:MET:CB	2.81	0.68
1:B:240:GLU:O	1:B:241:ARG:CB	2.48	0.61
1:B:177:ILE:HD13	1:B:219:LEU:HD21	1.84	0.60
1:A:26:ASN:ND2	1:A:169:ILE:H	2.03	0.56
1:A:166:ASP:O	1:A:167:ASN:HB2	2.07	0.54
1:B:100:ALA:H	3:B:1289:ACT:H2	1.72	0.53
1:B:95:HIS:HE1	4:B:2056:HOH:O	1.93	0.52
1:A:8:LEU:HG	1:A:226:LEU:HD11	1.92	0.51
1:A:184:ASP:OD1	1:A:187:THR:HG23	2.11	0.51
1:B:195:LEU:CD2	1:B:218:VAL:HG13	2.41	0.51
1:A:26:ASN:HD22	1:A:169:ILE:H	1.59	0.49
1:B:240:GLU:O	1:B:241:ARG:HB2	2.14	0.48
1:A:249:LEU:HD12	1:A:257:MET:HE1	1.96	0.47
1:A:177:ILE:CD1	1:A:218:VAL:HG11	2.45	0.46
1:B:179:LEU:HD13	1:B:188:ILE:HG12	1.98	0.45
1:B:177:ILE:HD13	1:B:219:LEU:CD2	2.45	0.45
1:A:280:GLU:H	1:A:280:GLU:CD	2.24	0.45
1:A:254:ILE:HA	1:A:257:MET:HE3	1.98	0.44
1:A:67:GLU:O	1:A:114:GLY:HA3	2.18	0.44
1:A:249:LEU:HD22	1:A:253:GLU:OE1	2.18	0.44
1:B:246:ILE:CD1	1:B:277:PHE:CE2	3.00	0.44
1:A:251:LYS:HE2	1:A:289:THR:O	2.17	0.43
1:A:152:GLN:OE1	1:B:57:LYS:HG2	2.19	0.42
1:A:180:MET:HB3	1:A:181:PRO:HD2	2.01	0.42
1:A:128:PHE:CD2	1:A:128:PHE:C	2.97	0.42
1:B:148:VAL:O	1:B:152:GLN:HA	2.20	0.42
1:A:107:ARG:CZ	1:A:112:THR:HG21	2.51	0.41
1:B:24:MET:CE	1:B:24:MET:CB	2.99	0.40
1:B:238:SER:O	1:B:241:ARG:HB3	2.21	0.40
1:B:191:ILE:O	1:B:195:LEU:HG	2.21	0.40

All (1) 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)
4:A:2084:HOH:O	4:A:2084:HOH:O[4_555]	0.99	1.21

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	288/291 (99%)	278 (96%)	9 (3%)	1 (0%)	36	27
1	B	284/291 (98%)	269 (95%)	8 (3%)	7 (2%)	4	0
All	All	572/582 (98%)	547 (96%)	17 (3%)	8 (1%)	9	2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	B	186	GLU
1	B	241	ARG
1	B	257	MET
1	B	259	GLU
1	B	256	ASP
1	B	284	GLY
1	B	258	ILE

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	238/239 (100%)	229 (96%)	9 (4%)	29	19
1	B	233/239 (98%)	223 (96%)	10 (4%)	26	14
All	All	471/478 (98%)	452 (96%)	19 (4%)	28	17

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	13	LYS
1	A	107	ARG
1	A	128	PHE
1	A	190	LYS
1	A	201	ILE
1	A	270	PHE
1	A	276	LEU
1	A	280	GLU
1	B	1	MET
1	B	57	LYS
1	B	67	GLU
1	B	107	ARG
1	B	186	GLU
1	B	187	THR
1	B	218	VAL
1	B	222	LYS
1	B	246	ILE
1	B	286	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	131	GLN
1	A	234	HIS
1	A	269	HIS
1	B	95	HIS
1	B	164	ASN
1	B	234	HIS

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, 2 are monoatomic - leaving 6 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	$\# Z > 2$
3	ACT	B	1288	-	3,3,3	0.91	0	3,3,3	1.80	2 (66%)
3	ACT	A	1293	-	3,3,3	0.60	0	3,3,3	2.08	2 (66%)
3	ACT	B	1289	-	3,3,3	0.67	0	3,3,3	1.77	1 (33%)
3	ACT	A	1294	-	3,3,3	0.65	0	3,3,3	2.72	2 (66%)
3	ACT	A	1295	-	3,3,3	1.35	0	3,3,3	1.32	0
3	ACT	A	1292	-	3,3,3	2.00	1 (33%)	3,3,3	1.70	1 (33%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1292	ACT	O-C	3.03	1.35	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1294	ACT	OXT-C-CH3	3.52	129.82	115.05
3	A	1294	ACT	OXT-C-O	-3.04	110.75	122.03
3	A	1293	ACT	OXT-C-CH3	2.67	126.25	115.05
3	B	1289	ACT	OXT-C-O	-2.40	113.12	122.03
3	A	1293	ACT	OXT-C-O	-2.38	113.19	122.03
3	A	1292	ACT	O-C-CH3	2.28	131.88	122.53
3	B	1288	ACT	OXT-C-O	-2.24	113.73	122.03
3	B	1288	ACT	OXT-C-CH3	2.18	124.18	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1289	ACT	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	290/291 (99%)	0.38	29 (10%)	12 18	19, 29, 58, 69	10 (3%)
1	B	286/291 (98%)	1.84	52 (18%)	3 4	1, 33, 66, 96	27 (9%)
All	All	576/582 (98%)	1.10	81 (14%)	6 9	1, 31, 63, 96	37 (6%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	GLY	35.1
1	B	261	ASP	29.7
1	B	258	ILE	28.3
1	B	250	GLY	26.5
1	B	254	ILE	25.7
1	B	251	LYS	24.5
1	B	253	GLU	22.8
1	B	257	MET	22.0
1	B	259	GLU	20.2
1	B	260	GLU	20.1
1	B	252	LYS	19.2
1	B	255	GLN	17.9
1	B	256	ASP	17.8
1	B	286	ARG	14.8
1	A	198	VAL	9.7
1	A	197	GLN	9.6
1	B	185	ASP	8.4
1	B	240	GLU	8.3
1	B	285	LEU	7.9
1	A	199	GLU	7.5
1	B	190	LYS	7.0
1	A	279	LYS	5.8
1	B	153	VAL	5.7
1	B	187	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	184	ASP	5.2
1	B	263	GLN	4.5
1	B	188	ILE	4.5
1	B	189	THR	4.4
1	A	127	PHE	4.3
1	A	201	ILE	4.3
1	B	197	GLN	4.2
1	B	249	LEU	4.1
1	A	205	ILE	4.0
1	B	283	GLU	3.9
1	A	182	GLY	3.8
1	B	284	GLY	3.8
1	B	203	LYS	3.7
1	A	196	SER	3.6
1	A	187	THR	3.6
1	B	198	VAL	3.4
1	A	289	THR	3.4
1	B	183	THR	3.4
1	B	150	SER	3.3
1	B	193	GLN	3.3
1	A	200	PRO	3.3
1	A	195	LEU	3.2
1	B	191	ILE	3.2
1	A	189	THR	3.1
1	B	10	TYR	3.1
1	A	190	LYS	3.0
1	A	203	LYS	3.0
1	B	282	LEU	3.0
1	B	195	LEU	2.9
1	A	252	LYS	2.9
1	B	194	ARG	2.9
1	B	245	ALA	2.8
1	A	124	LEU	2.8
1	B	241	ARG	2.8
1	B	1	MET	2.8
1	B	149	SER	2.6
1	A	204	LEU	2.6
1	A	184	ASP	2.6
1	B	196	SER	2.6
1	A	152	GLN	2.5
1	B	186	GLU	2.4
1	B	209	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	256	ASP	2.3
1	A	1	MET	2.3
1	A	290	THR	2.3
1	B	247	LEU	2.3
1	A	206	GLN	2.2
1	A	11	ASP	2.2
1	A	202	SER	2.2
1	B	264	ALA	2.2
1	A	188	ILE	2.2
1	A	122	LEU	2.2
1	B	11	ASP	2.2
1	B	206	GLN	2.1
1	B	244	THR	2.1
1	B	246	ILE	2.1
1	B	225	ILE	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($\text{\AA}^2$)	Q<0.9
3	ACT	A	1293	4/4	0.51	0.28	61,61,61,62	0
3	ACT	B	1289	4/4	0.66	0.20	54,54,54,55	0
3	ACT	A	1295	4/4	0.75	0.23	58,58,59,59	0
3	ACT	A	1294	4/4	0.76	0.21	59,59,59,61	0
3	ACT	A	1292	4/4	0.77	0.21	34,36,36,39	0
3	ACT	B	1288	4/4	0.78	0.20	55,56,56,56	0
2	ZN	B	1287	1/1	0.98	0.03	33,33,33,33	0
2	ZN	A	1291	1/1	0.99	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.