



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 02:58 AM UTC

PDB ID : 6GZB / pdb_00006gzb
Title : Tandem GerMN domains of the sporulation protein GerM from *Bacillus subtilis*
Authors : Trouve, J.; Mohamed, A.; Leisico, F.; Contreras-Martel, C.; Liu, B.; Mas, C.; Rudner, D.Z.; Rodrigues, C.D.A.; Morlot, C.
Deposited on : 2018-07-03
Resolution : 2.10 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

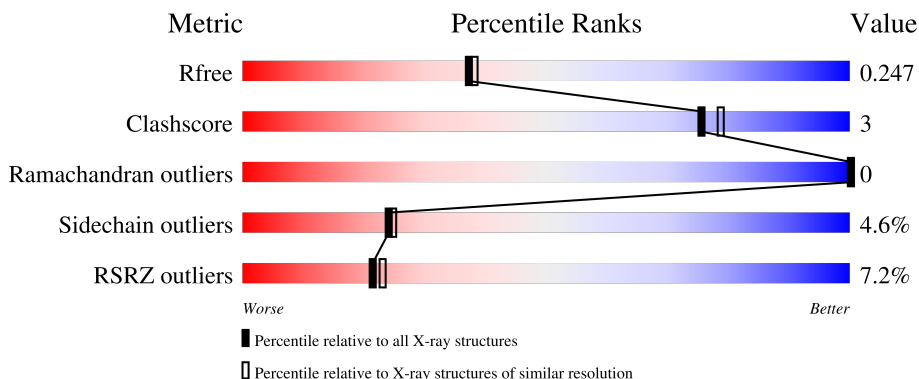
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	341	0% 76% 8% 16%
1	B	341	4% 75% 7% 17%
1	C	341	10% 71% 11% 17%
1	D	341	9% 75% 7% 17%

2 Entry composition [i](#)

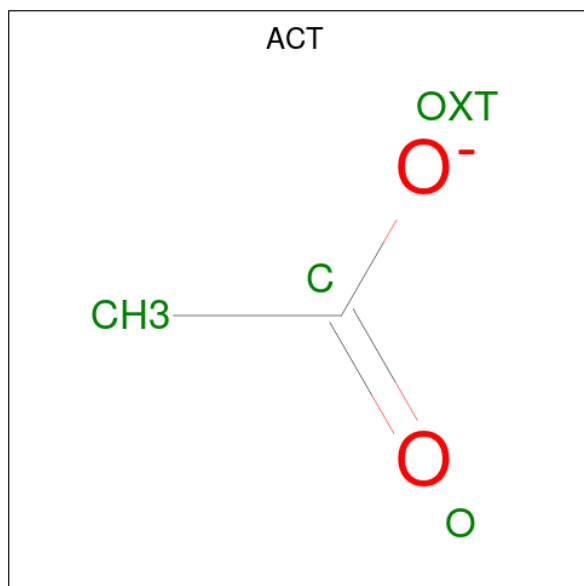
There are 4 unique types of molecules in this entry. The entry contains 9144 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Spore germination protein GerM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2218	1396	365	454	3			
1	B	282	Total	C	N	O	S	0	0	0
			2185	1376	360	446	3			
1	C	284	Total	C	N	O	S	0	0	0
			2199	1386	362	448	3			
1	D	282	Total	C	N	O	S	0	0	0
			2174	1366	359	446	3			

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

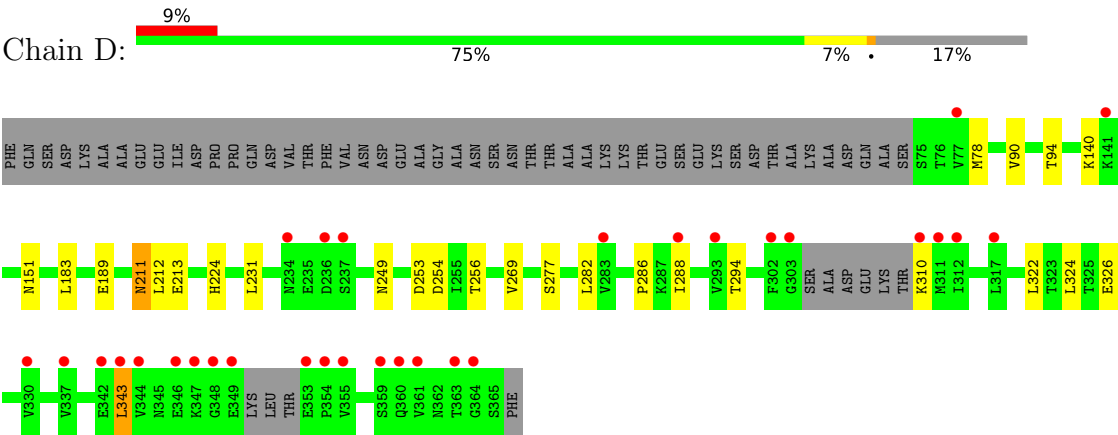
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total 124	O 124	0	0
4	B	61	Total 61	O 61	0	0
4	C	33	Total 33	O 33	0	0
4	D	86	Total 86	O 86	0	0

- Molecule 1: Spore germination protein GerM



● Molecule 1: Spore germination protein GerM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.36Å 103.94Å 162.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.46 – 2.10 46.46 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.46-2.10) 99.8 (46.46-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.204 , 0.236 0.215 , 0.247	Depositor DCC
R_{free} test set	3583 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9144	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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: EDO, 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	0.58	2/2250 (0.1%)	0.68	0/3049
1	B	0.85	2/2216 (0.1%)	0.72	0/3004
1	C	0.87	2/2231 (0.1%)	0.85	8/3023 (0.3%)
1	D	0.78	3/2204 (0.1%)	0.73	1/2985 (0.0%)
All	All	0.78	9/8901 (0.1%)	0.75	9/12061 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	GLU	C-N	-8.77	1.20	1.33
1	D	211	ASN	C-N	8.02	1.44	1.33
1	A	175	PHE	C-N	-7.84	1.23	1.34
1	A	176	SER	C-N	6.83	1.44	1.33
1	C	116	PRO	C-N	5.94	1.41	1.34
1	C	109	GLU	C-N	5.77	1.41	1.33
1	D	213	GLU	C-O	-5.44	1.17	1.24
1	B	243	VAL	C-O	-5.41	1.18	1.24
1	B	344	VAL	C-O	-5.28	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	VAL	N-CA-C	8.28	119.30	107.88
1	C	237	SER	N-CA-C	6.65	118.31	108.60
1	C	115	GLY	CA-C-N	6.59	126.84	119.32
1	C	115	GLY	C-N-CA	6.59	126.84	119.32
1	C	340	LYS	N-CA-C	5.74	118.13	109.41
1	C	111	LEU	N-CA-C	-5.73	105.01	113.61
1	C	236	ASP	N-CA-C	5.54	119.73	112.92
1	D	343	LEU	N-CA-C	5.17	118.02	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	343	LEU	N-CA-C	5.15	118.33	110.20

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	2218	0	2245	10	0
1	B	2185	0	2218	17	0
1	C	2199	0	2228	27	0
1	D	2174	0	2195	8	0
2	A	12	0	9	0	0
2	B	12	0	9	0	0
2	C	4	0	3	0	0
2	D	12	0	9	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	124	0	0	0	0
4	B	61	0	0	0	0
4	C	33	0	0	0	0
4	D	86	0	0	0	0
All	All	9144	0	8952	53	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 (53) 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:246:ARG:HH12	1:C:269:VAL:CG1	1.72	1.02
1:B:246:ARG:HH12	1:C:269:VAL:HG12	1.34	0.92
1:B:246:ARG:NH1	1:C:269:VAL:CG1	2.32	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:NH1	1:C:269:VAL:HG11	1.85	0.91
1:B:90:VAL:H	1:B:211:ASN:HD21	1.21	0.88
1:C:90:VAL:H	1:C:211:ASN:HD21	1.21	0.87
1:A:90:VAL:H	1:A:211:ASN:HD21	1.21	0.84
1:C:269:VAL:HG12	1:C:269:VAL:O	1.78	0.83
1:D:90:VAL:H	1:D:211:ASN:HD21	1.28	0.82
1:D:78:MET:HE3	1:D:94:THR:HG22	1.66	0.77
1:B:246:ARG:NH1	1:C:269:VAL:HG12	2.02	0.70
1:A:221:THR:HG22	1:B:89:TYR:CE1	2.34	0.62
1:B:246:ARG:HH12	1:C:269:VAL:HG11	1.48	0.62
1:B:78:MET:HE3	1:B:94:THR:HG22	1.83	0.60
1:A:224:HIS:HE1	1:A:254:ASP:OD1	1.85	0.59
1:C:224:HIS:HE1	1:C:254:ASP:OD1	1.85	0.59
1:D:224:HIS:HE1	1:D:254:ASP:OD1	1.84	0.59
1:C:269:VAL:CG1	1:C:269:VAL:O	2.52	0.58
1:C:219:ASP:OD1	1:C:221:THR:HG22	2.04	0.57
1:C:224:HIS:HD2	1:C:249:ASN:OD1	1.88	0.57
1:A:224:HIS:HD2	1:A:249:ASN:OD1	1.91	0.55
1:B:224:HIS:HD2	1:B:249:ASN:OD1	1.90	0.54
1:C:78:MET:HG3	1:C:360:GLN:HE22	1.72	0.54
1:B:224:HIS:HE1	1:B:254:ASP:OD1	1.90	0.54
1:C:302:PHE:CZ	1:C:310:LYS:HG2	2.43	0.54
1:C:302:PHE:CE2	1:C:310:LYS:HD3	2.45	0.52
1:D:224:HIS:HD2	1:D:249:ASN:OD1	1.93	0.52
1:C:311:MET:HE2	1:C:345:ASN:O	2.10	0.52
1:B:246:ARG:HH11	1:C:269:VAL:HG11	1.73	0.51
1:A:253:ASP:OD2	1:A:256:THR:OG1	2.29	0.50
1:C:253:ASP:OD2	1:C:256:THR:OG1	2.30	0.49
1:D:253:ASP:OD2	1:D:256:THR:OG1	2.29	0.49
1:C:302:PHE:C	1:C:302:PHE:CD1	2.91	0.48
1:C:77:VAL:HG12	1:C:78:MET:N	2.29	0.48
1:B:302:PHE:C	1:B:302:PHE:CD1	2.93	0.46
1:A:221:THR:HG22	1:B:89:TYR:CD1	2.52	0.44
1:C:237:SER:OG	1:C:238:GLU:N	2.47	0.44
1:B:268:LYS:C	1:B:269:VAL:HG23	2.44	0.42
1:C:302:PHE:CE2	1:C:310:LYS:CD	3.02	0.42
1:A:110:TYR:CZ	1:A:116:PRO:HB2	2.54	0.42
1:C:193:MET:HA	1:C:194:PRO:HD3	1.88	0.42
1:B:322:LEU:O	1:B:326:GLU:HG2	2.20	0.42
1:D:282:LEU:HD13	1:D:286:PRO:HG3	2.02	0.41
1:D:322:LEU:O	1:D:326:GLU:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:PHE:CE2	1:C:310:LYS:HG2	2.55	0.41
1:A:302:PHE:CD1	1:A:302:PHE:C	2.98	0.41
1:C:135:VAL:HG22	1:C:136:ASN:N	2.36	0.41
1:A:272:LEU:C	1:A:273:LEU:HD23	2.45	0.41
1:C:224:HIS:CD2	1:C:249:ASN:OD1	2.72	0.41
1:B:78:MET:HE1	1:B:96:PRO:HD3	2.03	0.40
1:D:310:LYS:N	1:D:310:LYS:HD3	2.36	0.40
1:C:324:LEU:HA	1:C:324:LEU:HD12	1.75	0.40
1:A:322:LEU:O	1:A:326:GLU:HG2	2.21	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	283/341 (83%)	279 (99%)	4 (1%)	0	100	100
1	B	278/341 (82%)	274 (99%)	4 (1%)	0	100	100
1	C	280/341 (82%)	271 (97%)	9 (3%)	0	100	100
1	D	276/341 (81%)	267 (97%)	9 (3%)	0	100	100
All	All	1117/1364 (82%)	1091 (98%)	26 (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	258/300 (86%)	245 (95%)	13 (5%)	22	22
1	B	254/300 (85%)	244 (96%)	10 (4%)	28	31
1	C	255/300 (85%)	242 (95%)	13 (5%)	21	21
1	D	252/300 (84%)	241 (96%)	11 (4%)	25	26
All	All	1019/1200 (85%)	972 (95%)	47 (5%)	24	25

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LYS
1	A	140	LYS
1	A	183	LEU
1	A	204	LEU
1	A	252	LYS
1	A	268	LYS
1	A	269	VAL
1	A	273	LEU
1	A	285	LYS
1	A	290	ASP
1	A	309	THR
1	A	324	LEU
1	A	359	SER
1	B	183	LEU
1	B	186	ASN
1	B	231	LEU
1	B	237	SER
1	B	252	LYS
1	B	269	VAL
1	B	324	LEU
1	B	350	LYS
1	B	359	SER
1	B	363	THR
1	C	79	ARG
1	C	86	LYS
1	C	189	GLU
1	C	204	LEU
1	C	231	LEU
1	C	238	GLU
1	C	245	LYS
1	C	290	ASP
1	C	299	GLN
1	C	324	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	337	VAL
1	C	341	SER
1	C	344	VAL
1	D	140	LYS
1	D	151	ASN
1	D	183	LEU
1	D	212	LEU
1	D	231	LEU
1	D	269	VAL
1	D	277	SER
1	D	288	ILE
1	D	294	THR
1	D	324	LEU
1	D	343	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	151	ASN
1	A	186	ASN
1	A	211	ASN
1	A	224	HIS
1	B	87	ASN
1	B	136	ASN
1	B	211	ASN
1	B	224	HIS
1	C	87	ASN
1	C	186	ASN
1	C	211	ASN
1	C	224	HIS
1	C	249	ASN
1	C	360	GLN
1	D	87	ASN
1	D	123	ASN
1	D	136	ASN
1	D	211	ASN
1	D	224	HIS

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](#)

16 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	$\# Z > 2$
3	EDO	C	402	-	3,3,3	0.24	0	2,2,2	0.51	0
2	ACT	A	401	-	3,3,3	0.77	0	3,3,3	0.82	0
2	ACT	D	401	-	3,3,3	0.84	0	3,3,3	0.72	0
3	EDO	D	404	-	3,3,3	0.47	0	2,2,2	0.33	0
2	ACT	B	403	-	3,3,3	0.81	0	3,3,3	0.76	0
3	EDO	B	405	-	3,3,3	0.41	0	2,2,2	0.39	0
2	ACT	B	402	-	3,3,3	0.85	0	3,3,3	0.70	0
2	ACT	A	403	-	3,3,3	1.03	0	3,3,3	0.81	0
2	ACT	C	401	-	3,3,3	0.87	0	3,3,3	0.85	0
2	ACT	D	403	-	3,3,3	1.04	0	3,3,3	0.83	0
2	ACT	D	402	-	3,3,3	0.80	0	3,3,3	0.76	0
2	ACT	B	401	-	3,3,3	0.87	0	3,3,3	0.69	0
3	EDO	A	405	-	3,3,3	0.44	0	2,2,2	0.30	0
3	EDO	B	404	-	3,3,3	0.45	0	2,2,2	0.32	0
2	ACT	A	402	-	3,3,3	0.88	0	3,3,3	0.53	0
3	EDO	A	404	-	3,3,3	0.46	0	2,2,2	0.23	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
3	EDO	C	402	-	-	0/1/1/1	-
3	EDO	D	404	-	-	0/1/1/1	-
3	EDO	B	405	-	-	1/1/1/1	-
3	EDO	A	405	-	-	0/1/1/1	-
3	EDO	B	404	-	-	1/1/1/1	-
3	EDO	A	404	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	EDO	O1-C1-C2-O2
3	B	404	EDO	O1-C1-C2-O2
3	B	405	EDO	O1-C1-C2-O2

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	287/341 (84%)	0.01	5 (1%) 69 71	24, 37, 62, 91	0
1	B	282/341 (82%)	0.37	12 (4%) 40 41	27, 43, 77, 121	0
1	C	284/341 (83%)	1.00	34 (11%) 9 9	31, 62, 93, 112	0
1	D	282/341 (82%)	0.62	31 (10%) 10 11	28, 46, 90, 128	0
All	All	1135/1364 (83%)	0.50	82 (7%) 21 23	24, 46, 87, 128	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	77	VAL	5.2
1	D	353	GLU	4.7
1	A	309	THR	4.2
1	D	302	PHE	4.1
1	D	354	PRO	4.1
1	C	188	HIS	4.0
1	D	355	VAL	3.8
1	C	217	VAL	3.8
1	D	342	GLU	3.6
1	D	343	LEU	3.5
1	D	361	VAL	3.5
1	C	366	PHE	3.4
1	C	310	LYS	3.4
1	B	200	ILE	3.4
1	C	236	ASP	3.4
1	C	343	LEU	3.3
1	D	310	LYS	3.2
1	C	348	GLY	3.2
1	B	201	SER	3.1
1	B	185	ILE	3.1
1	D	348	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	363	THR	3.0
1	A	273	LEU	3.0
1	B	309	THR	3.0
1	C	329	ASP	2.8
1	C	344	VAL	2.8
1	C	302	PHE	2.8
1	C	110	TYR	2.7
1	A	74	SER	2.7
1	D	236	ASP	2.7
1	C	269	VAL	2.7
1	D	344	VAL	2.7
1	C	309	THR	2.6
1	D	312	ILE	2.6
1	D	346	GLU	2.6
1	D	283	VAL	2.6
1	D	288	ILE	2.6
1	A	274	THR	2.6
1	C	103	THR	2.5
1	D	359	SER	2.5
1	C	114	GLY	2.5
1	B	140	LYS	2.5
1	D	317	LEU	2.5
1	B	203	ASP	2.4
1	B	361	VAL	2.4
1	C	237	SER	2.4
1	C	350	LYS	2.4
1	B	236	ASP	2.4
1	C	186	ASN	2.3
1	C	99	LYS	2.3
1	C	117	VAL	2.3
1	D	330	VAL	2.3
1	D	337	VAL	2.3
1	D	237	SER	2.3
1	A	235	GLU	2.3
1	C	112	VAL	2.3
1	B	191	LYS	2.3
1	D	347	LYS	2.3
1	D	141	LYS	2.3
1	D	311	MET	2.2
1	C	113	GLN	2.2
1	C	97	LEU	2.2
1	C	132	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	185	ILE	2.2
1	D	349	GLU	2.2
1	D	360	GLN	2.2
1	C	273	LEU	2.2
1	B	202	ASP	2.2
1	B	329	ASP	2.2
1	D	293	VAL	2.1
1	D	303	GLY	2.1
1	D	364	GLY	2.1
1	D	234	ASN	2.1
1	C	135	VAL	2.1
1	C	356	SER	2.1
1	D	363	THR	2.1
1	C	187	GLY	2.1
1	C	178	ILE	2.1
1	D	77	VAL	2.1
1	C	235	GLU	2.0
1	C	194	PRO	2.0
1	C	351	LEU	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
2	ACT	C	401	4/4	0.68	0.18	68,70,73,74	0
2	ACT	B	403	4/4	0.71	0.16	57,64,77,81	0
2	ACT	A	403	4/4	0.80	0.15	56,56,59,71	0
2	ACT	B	402	4/4	0.81	0.17	36,51,53,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	D	402	4/4	0.82	0.13	49,54,71,71	0
3	EDO	A	405	4/4	0.85	0.14	47,53,55,59	0
3	EDO	B	405	4/4	0.85	0.15	57,58,64,66	0
2	ACT	A	401	4/4	0.86	0.12	52,56,59,62	0
3	EDO	C	402	4/4	0.86	0.11	47,53,55,59	0
3	EDO	B	404	4/4	0.87	0.14	57,60,64,64	0
2	ACT	D	403	4/4	0.87	0.12	52,56,59,62	0
2	ACT	A	402	4/4	0.87	0.18	45,47,56,57	0
2	ACT	B	401	4/4	0.89	0.20	41,59,64,66	0
3	EDO	D	404	4/4	0.89	0.12	54,55,60,62	0
2	ACT	D	401	4/4	0.90	0.09	69,70,70,74	0
3	EDO	A	404	4/4	0.94	0.15	46,47,48,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.