



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 AM UTC

PDB ID : 4G9O / pdb_00004g9o
Title : Crystal Structure of H234A Mutant of Stationary Phase Survival Protein (SurE) from Salmonella typhimurium
Authors : Mathiharan, Y.K.; Murthy, M.R.N.
Deposited on : 2012-07-24
Resolution : 2.12 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

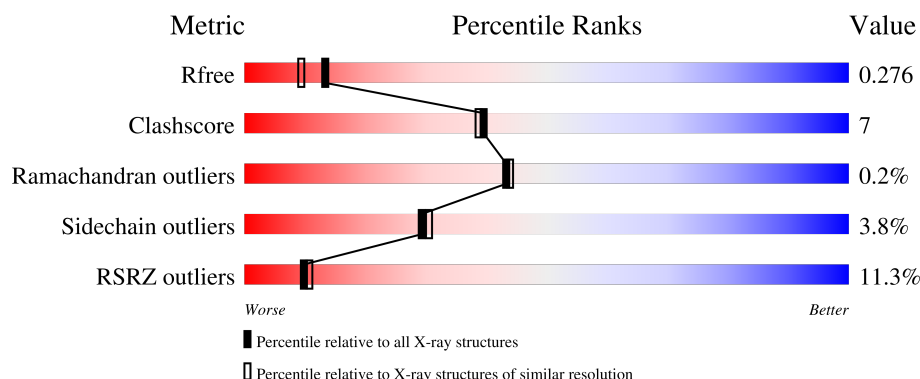
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	267	
1	B	267	

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	EDO	A	301	-	-	X	-
2	EDO	B	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3886 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 5'/3'-nucleotidase SurE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	0	4	0
			1795	1121	319	347	8			
1	B	252	Total	C	N	O	S	0	1	0
			1813	1136	311	359	7			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP P66881
A	-12	ARG	-	expression tag	UNP P66881
A	-11	GLY	-	expression tag	UNP P66881
A	-10	SER	-	expression tag	UNP P66881
A	-9	HIS	-	expression tag	UNP P66881
A	-8	HIS	-	expression tag	UNP P66881
A	-7	HIS	-	expression tag	UNP P66881
A	-6	HIS	-	expression tag	UNP P66881
A	-5	HIS	-	expression tag	UNP P66881
A	-4	HIS	-	expression tag	UNP P66881
A	-3	GLY	-	expression tag	UNP P66881
A	-2	MET	-	expression tag	UNP P66881
A	-1	ALA	-	expression tag	UNP P66881
A	0	SER	-	expression tag	UNP P66881
A	234	ALA	HIS	engineered mutation	UNP P66881
B	-13	MET	-	expression tag	UNP P66881
B	-12	ARG	-	expression tag	UNP P66881
B	-11	GLY	-	expression tag	UNP P66881
B	-10	SER	-	expression tag	UNP P66881
B	-9	HIS	-	expression tag	UNP P66881
B	-8	HIS	-	expression tag	UNP P66881
B	-7	HIS	-	expression tag	UNP P66881
B	-6	HIS	-	expression tag	UNP P66881
B	-5	HIS	-	expression tag	UNP P66881
B	-4	HIS	-	expression tag	UNP P66881

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P66881
B	-2	MET	-	expression tag	UNP P66881
B	-1	ALA	-	expression tag	UNP P66881
B	0	SER	-	expression tag	UNP P66881
B	234	ALA	HIS	engineered mutation	UNP P66881

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



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		
2	A	1	Total	C	O	0	0
			4	2	2		
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		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total 137	O 137	0	0
4	B	111	Total 111	O 111	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.04Å 98.14Å 127.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.12 35.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	100.0 (35.00-2.12) 99.9 (35.00-2.12)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.219 , 0.273 0.221 , 0.276	Depositor DCC
R_{free} test set	1482 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3886	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: MG, EDO

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	0.59	0/1850	0.81	0/2529
1	B	0.59	0/1856	0.82	2/2550 (0.1%)
All	All	0.59	0/3706	0.81	2/5079 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	GLY	CA-C-N	5.63	125.74	119.32
1	B	209	GLY	C-N-CA	5.63	125.74	119.32

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	1795	0	1751	26	0
1	B	1813	0	1719	22	0
2	A	16	0	24	11	0
2	B	12	0	18	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	137	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	111	0	0	1	0
All	All	3886	0	3512	48	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 7.

All (48) 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:68:PRO:HD3	2:A:301:EDO:H11	1.43	1.01
1:A:68:PRO:CD	2:A:301:EDO:H11	1.98	0.93
1:A:52:ARG:HH11	1:A:52:ARG:HG3	1.37	0.89
1:B:8:ASP:OD2	2:B:302:EDO:H12	1.82	0.80
1:A:52:ARG:HG3	1:A:52:ARG:NH1	1.98	0.74
1:B:180:HIS:HD2	1:B:182:ALA:H	1.37	0.72
1:A:22:ALA:HB2	2:A:303:EDO:H22	1.77	0.66
1:B:39:SER:O	2:B:302:EDO:H21	1.95	0.66
2:A:303:EDO:H21	4:A:511:HOH:O	1.96	0.64
1:A:38:ARG:HB3	2:A:301:EDO:H22	1.81	0.63
1:A:184:LYS:HD3	1:A:185:VAL:H	1.68	0.59
1:B:4:LEU:HD11	1:B:32:VAL:HG12	1.85	0.58
1:A:41:ALA:O	2:A:301:EDO:H21	2.04	0.57
1:A:68:PRO:HD2	2:A:301:EDO:H11	1.85	0.57
1:A:120:ALA:HB3	1:A:155:ILE:HG22	1.87	0.56
1:B:236:ALA:O	1:B:239:VAL:HG12	2.07	0.55
1:A:249:VAL:HG13	1:A:250:GLY:H	1.72	0.55
1:A:38:ARG:NH1	1:A:65:MET:HE2	2.23	0.53
1:B:143:ARG:HD3	2:B:303:EDO:H21	1.90	0.53
1:A:144:GLY:HA2	1:B:247:VAL:HG11	1.91	0.53
1:A:155:ILE:HD11	1:A:227:LEU:HD12	1.91	0.52
1:A:68:PRO:CD	2:A:301:EDO:C1	2.82	0.51
1:A:68:PRO:HD2	2:A:301:EDO:C1	2.42	0.50
1:A:38:ARG:HH12	1:A:65:MET:HE2	1.76	0.50
1:A:43:ASN:ND2	1:A:105:GLY:HA2	2.28	0.49
1:B:105:GLY:HA3	2:B:302:EDO:H11	1.95	0.49
1:B:121:LEU:CD2	1:B:123:VAL:HG22	2.43	0.48
1:B:38:ARG:CG	1:B:38:ARG:HH11	2.26	0.48
1:B:4:LEU:HD11	1:B:32:VAL:CG1	2.43	0.48
1:B:38:ARG:HG3	1:B:38:ARG:NH1	2.28	0.47
1:B:43:ASN:HD21	2:B:302:EDO:C2	2.28	0.46
1:B:237:HIS:HE1	4:B:475:HOH:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HG13	1:B:32:VAL:O	2.17	0.44
1:A:52:ARG:HH11	1:A:52:ARG:CG	2.14	0.44
1:A:111[B]:MET:HE2	1:A:229:VAL:HG23	1.99	0.44
1:A:180:HIS:C	1:A:182:ALA:H	2.26	0.43
1:B:105:GLY:N	2:B:302:EDO:H11	2.33	0.43
1:B:105:GLY:CA	2:B:302:EDO:H11	2.48	0.43
1:A:236:ALA:HA	1:A:239:VAL:HG12	2.01	0.43
1:B:208:ALA:O	2:B:301:EDO:O1	2.30	0.43
1:B:3:ILE:HD13	1:B:23:LEU:HD13	2.01	0.42
1:B:180:HIS:HE1	1:B:218:ASP:OD2	2.03	0.42
1:A:184:LYS:HD3	1:A:185:VAL:N	2.34	0.41
1:A:38:ARG:HB3	2:A:301:EDO:C2	2.49	0.41
1:B:8:ASP:OD2	2:B:302:EDO:C1	2.60	0.41
1:A:38:ARG:O	2:A:301:EDO:H22	2.22	0.40
1:B:1:MET:HE2	1:B:146:SER:HB2	2.02	0.40
1:A:36:ARG:HD2	1:A:65:MET:HE3	2.04	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	244/267 (91%)	235 (96%)	8 (3%)	1 (0%)	30	28
1	B	249/267 (93%)	242 (97%)	7 (3%)	0	100	100
All	All	493/534 (92%)	477 (97%)	15 (3%)	1 (0%)	43	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	VAL

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	191/214 (89%)	183 (96%)	8 (4%)	26	27
1	B	187/214 (87%)	180 (96%)	7 (4%)	30	31
All	All	378/428 (88%)	363 (96%)	15 (4%)	29	28

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

Mol	Chain	Res	Type
1	A	25	GLU
1	A	52	ARG
1	A	65	MET
1	A	111[A]	MET
1	A	111[B]	MET
1	A	147	ARG
1	A	184	LYS
1	A	222	VAL
1	B	5	LEU
1	B	25	GLU
1	B	38	ARG
1	B	123	VAL
1	B	152	THR
1	B	227	LEU
1	B	241	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	43	ASN
1	A	92	ASN
1	B	64	GLN
1	B	180	HIS
1	B	188	GLN

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 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	EDO	B	303	-	3,3,3	0.41	0	2,2,2	0.43	0
2	EDO	A	302	-	3,3,3	0.40	0	2,2,2	0.45	0
2	EDO	B	301	-	3,3,3	0.48	0	2,2,2	0.34	0
2	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.34	0
2	EDO	B	302	-	3,3,3	0.47	0	2,2,2	0.06	0
2	EDO	A	303	-	3,3,3	0.41	0	2,2,2	0.42	0
2	EDO	A	301	-	3,3,3	0.36	0	2,2,2	0.32	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
2	EDO	B	303	-	-	1/1/1/1	-
2	EDO	A	302	-	-	0/1/1/1	-
2	EDO	B	301	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	304	-	-	0/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	A	303	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	303	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
2	B	303	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	EDO	1	0
2	B	301	EDO	1	0
2	B	302	EDO	7	0
2	A	303	EDO	2	0
2	A	301	EDO	9	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	244/267 (91%)	0.71	34 (13%) 6 7	25, 46, 97, 121	4 (1%)
1	B	252/267 (94%)	0.90	22 (8%) 16 17	28, 54, 77, 96	2 (0%)
All	All	496/534 (92%)	0.81	56 (11%) 10 11	25, 51, 89, 121	6 (1%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	252	GLN	4.6
1	A	247	VAL	4.3
1	A	251	THR	3.9
1	B	205	LYS	3.7
1	A	191	PRO	3.7
1	A	100	ASP	3.5
1	B	152	THR	3.5
1	A	250	GLY	3.4
1	A	150	LEU	3.4
1	B	81	ARG	3.2
1	B	79	LEU	3.1
1	A	196	LEU	3.1
1	B	253	TRP	3.1
1	B	1	MET	3.1
1	A	249	VAL	3.1
1	A	244	LEU	3.1
1	B	150	LEU	2.8
1	A	248	GLY	2.8
1	A	198	TRP	2.8
1	A	194	ASN	2.8
1	A	236	ALA	2.8
1	A	235	SER	2.8
1	B	145	LEU	2.7
1	A	188	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	2.7
1	B	168	VAL	2.7
1	B	118	PHE	2.6
1	A	171	ILE	2.6
1	A	185	VAL	2.6
1	A	176	CYS	2.6
1	A	181	PRO	2.5
1	B	170	GLY	2.5
1	A	178[A]	SER	2.5
1	A	233	ALA	2.5
1	A	229	VAL	2.5
1	B	208	ALA	2.4
1	B	206	TYR	2.4
1	B	251	THR	2.4
1	A	190	ASP	2.4
1	A	239	VAL	2.4
1	A	152	THR	2.4
1	A	192	ARG	2.4
1	B	147	ARG	2.4
1	A	195	THR	2.4
1	B	209	GLY	2.3
1	A	102	ILE	2.3
1	B	78	ALA	2.2
1	B	249	VAL	2.2
1	A	209	GLY	2.2
1	B	250	GLY	2.1
1	A	243	TRP	2.1
1	A	199	ILE	2.1
1	A	197	TYR	2.1
1	B	2	ARG	2.1
1	A	238	ASP	2.0
1	B	174	THR	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	EDO	A	304	4/4	0.75	0.16	49,49,49,50	0
2	EDO	B	302	4/4	0.76	0.19	38,38,41,41	0
2	EDO	B	303	4/4	0.79	0.13	71,72,72,74	0
2	EDO	A	302	4/4	0.82	0.13	51,52,55,59	0
2	EDO	A	303	4/4	0.86	0.18	40,43,43,49	0
2	EDO	B	301	4/4	0.89	0.11	38,39,42,44	0
3	MG	B	304	1/1	0.91	0.11	47,47,47,47	0
3	MG	A	305	1/1	0.92	0.09	47,47,47,47	0
2	EDO	A	301	4/4	0.92	0.16	36,38,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.