



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:45 AM UTC

PDB ID : 5KSR / pdb_00005ksr
Title : Stationary phase survival protein E (SurE) from Xylella fastidiosa - XFSurE-TB (Tetramer Bigger).
Authors : Machado, A.T.P.; Fonseca, E.M.B.; Dos Reis, M.A.; Saraiva, A.M.; Dos Santos, C.A.; De Toledo, M.A.; Polikarpov, I.; De Souza, A.P.; De Aparicio, R.; Iulek, J.
Deposited on : 2016-07-09
Resolution : 1.96 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
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

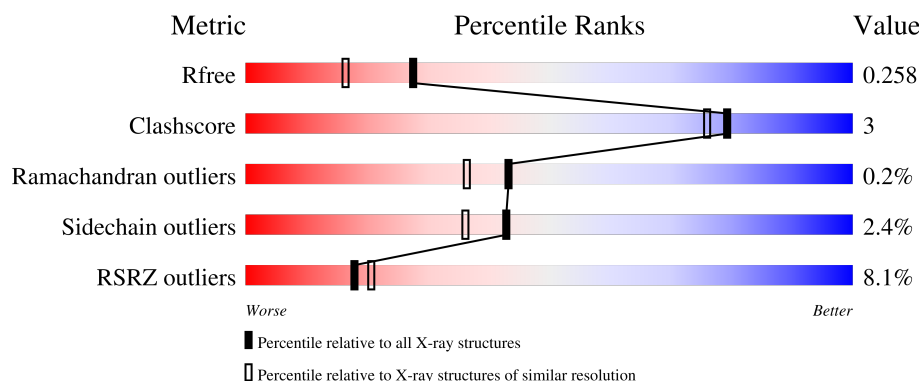
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	270	
1	B	270	
1	C	270	
1	D	270	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8554 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'-nucleotidase SurE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	10	3	0
			1956	1219	351	378	8			
1	B	254	Total	C	N	O	S	24	3	0
			1943	1212	346	377	8			
1	C	258	Total	C	N	O	S	43	6	0
			1999	1253	354	383	9			
1	D	259	Total	C	N	O	S	41	3	0
			1981	1233	354	386	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	263	LEU	-	expression tag	UNP Q9PF20
A	264	GLU	-	expression tag	UNP Q9PF20
A	265	HIS	-	expression tag	UNP Q9PF20
A	266	HIS	-	expression tag	UNP Q9PF20
A	267	HIS	-	expression tag	UNP Q9PF20
A	268	HIS	-	expression tag	UNP Q9PF20
A	269	HIS	-	expression tag	UNP Q9PF20
A	270	HIS	-	expression tag	UNP Q9PF20
B	263	LEU	-	expression tag	UNP Q9PF20
B	264	GLU	-	expression tag	UNP Q9PF20
B	265	HIS	-	expression tag	UNP Q9PF20
B	266	HIS	-	expression tag	UNP Q9PF20
B	267	HIS	-	expression tag	UNP Q9PF20
B	268	HIS	-	expression tag	UNP Q9PF20
B	269	HIS	-	expression tag	UNP Q9PF20
B	270	HIS	-	expression tag	UNP Q9PF20
C	263	LEU	-	expression tag	UNP Q9PF20
C	264	GLU	-	expression tag	UNP Q9PF20
C	265	HIS	-	expression tag	UNP Q9PF20
C	266	HIS	-	expression tag	UNP Q9PF20
C	267	HIS	-	expression tag	UNP Q9PF20

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Chain	Residue	Modelled	Actual	Comment	Reference
C	268	HIS	-	expression tag	UNP Q9PF20
C	269	HIS	-	expression tag	UNP Q9PF20
C	270	HIS	-	expression tag	UNP Q9PF20
D	263	LEU	-	expression tag	UNP Q9PF20
D	264	GLU	-	expression tag	UNP Q9PF20
D	265	HIS	-	expression tag	UNP Q9PF20
D	266	HIS	-	expression tag	UNP Q9PF20
D	267	HIS	-	expression tag	UNP Q9PF20
D	268	HIS	-	expression tag	UNP Q9PF20
D	269	HIS	-	expression tag	UNP Q9PF20
D	270	HIS	-	expression tag	UNP Q9PF20

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	171	Total 171	O 171	0	0
5	B	165	Total 165	O 165	0	0
5	C	168	Total 168	O 168	0	0
5	D	157	Total 157	O 157	0	0

L254	TRP
T255	PRO
A256	THR
H257	LEU
M258	GLU
D259	HIS
	HIS
	HIS
	HIS
	HIS
	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.34Å 84.17Å 87.31Å 90.00° 96.62° 90.00°	Depositor
Resolution (Å)	43.25 – 1.96 43.25 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.25-1.96) 99.5 (43.25-1.96)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.196 , 0.238 (Not available) , 0.258	Depositor DCC
R_{free} test set	4432 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8554	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.41% 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: IOD, CL, MN

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	1.31	4/2004 (0.2%)	1.12	6/2742 (0.2%)
1	B	1.29	3/1991 (0.2%)	1.12	3/2726 (0.1%)
1	C	1.22	2/2058 (0.1%)	1.07	3/2817 (0.1%)
1	D	1.18	1/2024 (0.0%)	1.08	6/2771 (0.2%)
All	All	1.25	10/8077 (0.1%)	1.10	18/11056 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	SER	CA-C	5.73	1.59	1.52
1	B	34	ALA	N-CA	5.67	1.51	1.45
1	A	86	ILE	N-CA	5.50	1.52	1.46
1	D	166	ASN	CA-C	5.41	1.59	1.52
1	A	167	VAL	N-CA	5.23	1.50	1.46
1	A	123	VAL	CA-CB	5.16	1.61	1.54
1	B	122	ALA	CA-CB	5.13	1.61	1.53
1	A	4	LEU	CA-C	5.11	1.58	1.52
1	C	77	THR	CA-CB	5.09	1.60	1.53
1	C	34	ALA	CA-C	5.00	1.57	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	GLY	N-CA-C	7.00	125.14	115.27
1	D	101	VAL	N-CA-C	7.00	117.14	110.42
1	B	120	ALA	N-CA-C	6.15	118.65	108.99
1	A	34	ALA	N-CA-C	6.08	115.30	108.25
1	D	190	ALA	CA-C-N	5.99	127.33	119.84
1	D	190	ALA	C-N-CA	5.99	127.33	119.84
1	C	34	ALA	N-CA-C	5.90	115.09	108.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	ALA	N-CA-C	5.87	118.79	108.75
1	D	120	ALA	N-CA-C	5.84	118.17	108.99
1	C	120	ALA	N-CA-C	5.84	118.15	108.99
1	B	34	ALA	N-CA-C	5.65	114.81	108.25
1	D	34	ALA	N-CA-C	5.64	114.79	108.25
1	A	102	ILE	N-CA-C	5.58	116.31	110.62
1	A	119	PRO	CA-C-O	-5.54	115.13	121.56
1	C	167	VAL	N-CA-C	5.39	114.03	107.61
1	D	192	CYS	N-CA-C	5.37	117.65	110.35
1	B	10	GLY	N-CA-C	5.32	118.69	111.72
1	A	10	GLY	N-CA-C	5.23	118.57	111.72

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	1956	0	1935	11	0
1	B	1943	0	1921	9	0
1	C	1999	0	1988	11	0
1	D	1981	0	1950	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	171	0	0	5	0
5	B	165	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	168	0	0	4	1
5	D	157	0	0	6	1
All	All	8554	0	7794	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 3.

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:99[B]:ASP:OD2	1:B:185:ASN:ND2	2.07	0.88
1:A:99[A]:ASP:OD2	1:A:185:ASN:ND2	2.12	0.83
4:B:503:CL:CL	5:B:692:HOH:O	2.41	0.74
1:A:114:ARG:NH1	1:A:159:ALA:HB1	2.09	0.68
1:B:139:GLU:OE2	5:B:601:HOH:O	2.13	0.67
1:D:185:ASN:ND2	5:D:605:HOH:O	2.28	0.67
1:A:39:ARG:NH1	5:A:604:HOH:O	2.28	0.66
1:A:134:GLN:N	5:A:606:HOH:O	2.31	0.62
1:A:114:ARG:HH12	1:A:159:ALA:HB1	1.63	0.62
1:B:215:ALA:O	5:B:602:HOH:O	2.15	0.61
1:A:186[A]:ARG:NH1	5:A:610:HOH:O	2.35	0.60
1:D:188:ARG:O	5:D:601:HOH:O	2.16	0.60
1:A:12:ASP:OD2	5:A:601:HOH:O	2.16	0.59
1:B:39:ARG:NH2	5:B:606:HOH:O	2.36	0.58
1:B:114:ARG:NH2	1:B:117:GLY:HA2	2.21	0.56
1:A:114:ARG:HG3	1:A:162:ILE:HG22	1.88	0.56
1:C:210:GLY:O	1:C:213:GLN:NE2	2.36	0.55
1:C:99[B]:ASP:OD2	1:C:185[B]:ASN:ND2	2.41	0.54
1:C:176:ARG:NH2	5:C:611:HOH:O	2.40	0.54
1:D:40:SER:HB3	5:D:675:HOH:O	2.07	0.54
1:D:25:ASN:ND2	5:D:614:HOH:O	2.44	0.50
1:A:212:GLU:H	1:A:212:GLU:CD	2.20	0.50
1:D:114[A]:ARG:NH1	1:D:159:ALA:HB1	2.28	0.49
1:D:57[B]:ILE:HD11	1:D:63:SER:HB2	1.94	0.48
1:D:153:LYS:NZ	5:D:612:HOH:O	2.37	0.47
1:C:48:LEU:O	5:C:601:HOH:O	2.20	0.47
1:A:31:MET:HE3	1:A:31:MET:HB3	1.83	0.46
1:B:40:SER:HB3	5:B:604:HOH:O	2.14	0.46
1:D:2:ARG:NH1	5:D:607:HOH:O	2.29	0.45
1:C:208:PRO:O	5:C:602:HOH:O	2.21	0.45
1:B:112:GLU:OE2	5:B:603:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:NH2	5:A:611:HOH:O	2.37	0.44
1:C:53:ARG:NE	5:C:609:HOH:O	2.38	0.44
1:B:135:ALA:HA	1:B:136:PRO:HD3	1.86	0.44
1:B:31:MET:HE3	1:B:31:MET:HB3	1.86	0.42
1:D:114[A]:ARG:CZ	1:D:159:ALA:HB1	2.50	0.42
1:C:162[B]:ILE:HD11	1:C:234:ILE:HD11	2.02	0.41
1:C:114:ARG:HB2	1:C:162[A]:ILE:HD11	2.01	0.41
1:C:190:ALA:HA	1:C:191:PRO:HD3	1.82	0.41
1:C:135:ALA:HA	1:C:136:PRO:HD3	1.82	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)
5:C:759:HOH:O	5:D:726:HOH:O[2_555]	2.19	0.01

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	254/270 (94%)	247 (97%)	7 (3%)	0	100	100
1	B	253/270 (94%)	244 (96%)	8 (3%)	1 (0%)	30	21
1	C	260/270 (96%)	251 (96%)	9 (4%)	0	100	100
1	D	259/270 (96%)	249 (96%)	9 (4%)	1 (0%)	30	21
All	All	1026/1080 (95%)	991 (97%)	33 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	191	PRO

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Mol	Chain	Res	Type
1	B	198	PRO

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	213/224 (95%)	208 (98%)	5 (2%)	44	38
1	B	212/224 (95%)	206 (97%)	6 (3%)	38	30
1	C	219/224 (98%)	211 (96%)	8 (4%)	30	20
1	D	215/224 (96%)	211 (98%)	4 (2%)	50	45
All	All	859/896 (96%)	836 (97%)	23 (3%)	43	32

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	37	ARG
1	A	114	ARG
1	A	162	ILE
1	A	227	THR
1	B	37	ARG
1	B	97	LEU
1	B	99[A]	ASP
1	B	99[B]	ASP
1	B	189	SER
1	B	227	THR
1	C	8	ASP
1	C	99[A]	ASP
1	C	99[B]	ASP
1	C	111	MET
1	C	162[A]	ILE
1	C	162[B]	ILE
1	C	192	CYS
1	C	227	THR
1	D	8	ASP

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Mol	Chain	Res	Type
1	D	114[A]	ARG
1	D	151	GLN
1	D	227	THR

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	164	ASN
1	B	96	ASN
1	D	92	ASN
1	D	151	GLN
1	D	173	GLN
1	D	174	GLN
1	D	195	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

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	255/270 (94%)	0.33	14 (5%)	30 36	15, 29, 55, 90	6 (2%)
1	B	254/270 (94%)	0.38	22 (8%)	16 18	14, 31, 56, 78	10 (3%)
1	C	258/270 (95%)	0.39	17 (6%)	24 28	13, 30, 60, 90	16 (6%)
1	D	259/270 (95%)	0.53	30 (11%)	9 11	16, 32, 69, 98	13 (5%)
All	All	1026/1080 (95%)	0.41	83 (8%)	18 21	13, 31, 60, 98	45 (4%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	260	TRP	7.8
1	B	116	LEU	6.5
1	C	158	PRO	5.4
1	A	259	ASP	5.2
1	A	159	ALA	4.5
1	A	116	LEU	4.5
1	D	116	LEU	4.5
1	D	132	GLY	4.4
1	D	256	ALA	4.4
1	D	131	GLU	4.1
1	B	129	TYR	4.1
1	D	254	LEU	4.0
1	C	159	ALA	4.0
1	D	40	SER	3.8
1	D	257	HIS	3.7
1	C	187	HIS	3.7
1	D	158	PRO	3.7
1	D	189	SER	3.5
1	D	259	ASP	3.5
1	C	191	PRO	3.5
1	D	191	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	42	ALA	3.4
1	B	119	PRO	3.4
1	A	189	SER	3.4
1	D	190	ALA	3.3
1	A	134	GLN	3.3
1	A	119	PRO	3.3
1	B	115	PHE	3.3
1	B	212	GLU	3.2
1	D	129	TYR	3.2
1	B	118	LEU	3.1
1	B	259	ASP	3.1
1	C	259	ASP	3.0
1	B	157	LEU	3.0
1	D	207	GLY	3.0
1	D	186	ARG	2.9
1	D	133	GLN	2.9
1	A	129	TYR	2.9
1	D	157	LEU	2.9
1	D	117	GLY	2.8
1	B	189	SER	2.8
1	B	187	HIS	2.7
1	A	118	LEU	2.7
1	C	254	LEU	2.7
1	B	159	ALA	2.7
1	C	129	TYR	2.7
1	B	257	HIS	2.6
1	B	114	ARG	2.6
1	D	130	ARG	2.5
1	C	39	ARG	2.5
1	D	185	ASN	2.5
1	A	187	HIS	2.5
1	C	189	SER	2.5
1	D	209	ALA	2.5
1	A	158	PRO	2.5
1	C	157	LEU	2.4
1	D	115	PHE	2.4
1	C	40	SER	2.4
1	B	57	ILE	2.4
1	D	187	HIS	2.4
1	A	115	PHE	2.3
1	C	154	THR	2.3
1	C	256	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	211	PRO	2.3
1	D	188	ARG	2.2
1	B	210	GLY	2.2
1	B	211	PRO	2.2
1	D	118	LEU	2.2
1	B	186	ARG	2.2
1	B	40	SER	2.2
1	A	39	ARG	2.2
1	B	154	THR	2.1
1	A	211	PRO	2.1
1	B	185	ASN	2.1
1	B	41	GLY	2.1
1	D	41	GLY	2.1
1	D	208	PRO	2.1
1	B	171	THR	2.0
1	A	117	GLY	2.0
1	C	210	GLY	2.0
1	D	119	PRO	2.0
1	D	211	PRO	2.0
1	D	154	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
4	CL	C	504	1/1	0.86	0.15	37,37,37,37	0
4	CL	D	503	1/1	0.89	0.11	36,36,36,36	0
4	CL	A	504	1/1	0.91	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	D	501	1/1	0.96	0.12	37,37,37,37	0
4	CL	B	503	1/1	0.96	0.08	31,31,31,31	0
2	MN	B	501	1/1	0.97	0.10	43,43,43,43	0
2	MN	A	501	1/1	0.98	0.08	41,41,41,41	0
3	IOD	A	503	1/1	0.98	0.04	39,39,39,39	1
2	MN	C	501	1/1	0.98	0.09	35,35,35,35	0
3	IOD	C	503	1/1	0.99	0.04	32,32,32,32	1
3	IOD	D	502	1/1	0.99	0.03	31,31,31,31	1
3	IOD	B	502	1/1	0.99	0.03	40,40,40,40	1
3	IOD	A	502	1/1	1.00	0.03	20,20,20,20	0
3	IOD	C	502	1/1	1.00	0.03	25,25,25,25	1

6.5 Other polymers [i](#)

There are no such residues in this entry.