



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 03:52 PM EDT

PDB ID : 5KST  
Title : Stationary phase Survival protein E (SurE) from *Xylella fastidiosa*- XfSurE-TSamp (Tetramer Smaller - crystallization with 3'AMP).  
Authors : Machado, A.T.P.; Fonseca, E.M.B.; Dos Reis, M.A.; Saraiva, A.M.; Dos Santos, C.A.; De Toledo, M.A.S.; Polikarpov, I.; De Souza, A.P.; Aparicio, R.; Iulek, J.  
Deposited on : 2016-07-09  
Resolution : 2.76 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

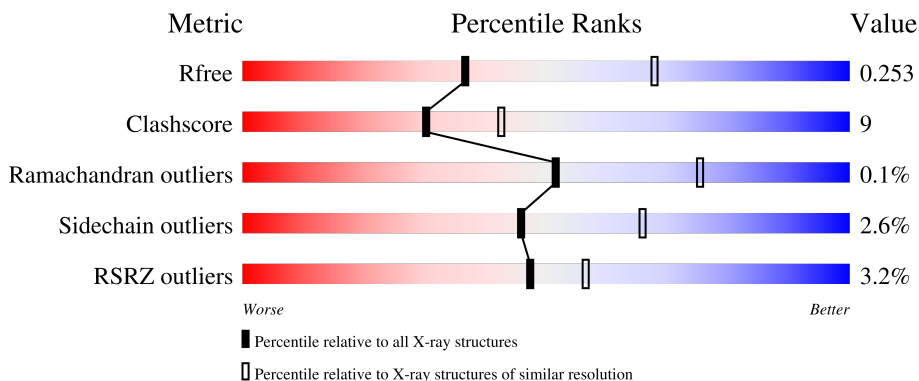
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 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))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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  $\geq 3$ , 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	 3% 76% 18% • 5%
1	B	270	 3% 78% 16% • 5%
1	C	270	 % 71% 22% • 6%
1	D	270	 5% 73% 20% • 6%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	IOD	C	502	-	-	X	-
3	IOD	D	603	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 8043 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
			Total	C	N	O	S			
1	A	257	Total 1953	C 1216	N 348	O 381	S 8	61	1	0
1	B	257	Total 1994	C 1240	N 358	O 387	S 9	23	6	0
1	C	254	Total 1930	C 1203	N 347	O 373	S 7	36	0	0
1	D	255	Total 1937	C 1207	N 347	O 375	S 8	66	0	0

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 (three-letter code: 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 (three-letter code: 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	1	Total I 1 1	0	0
3	D	2	Total I 2 2	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

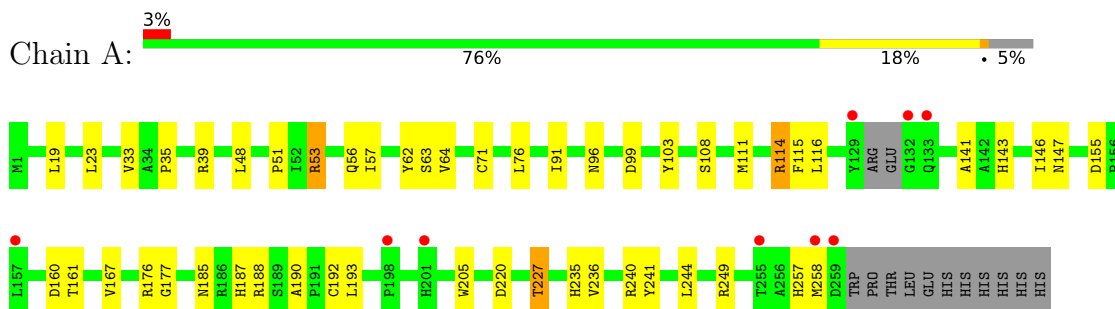
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	B	56	Total O 57 57	0	1
5	C	55	Total O 55 55	0	0
5	D	37	Total O 37 37	0	0

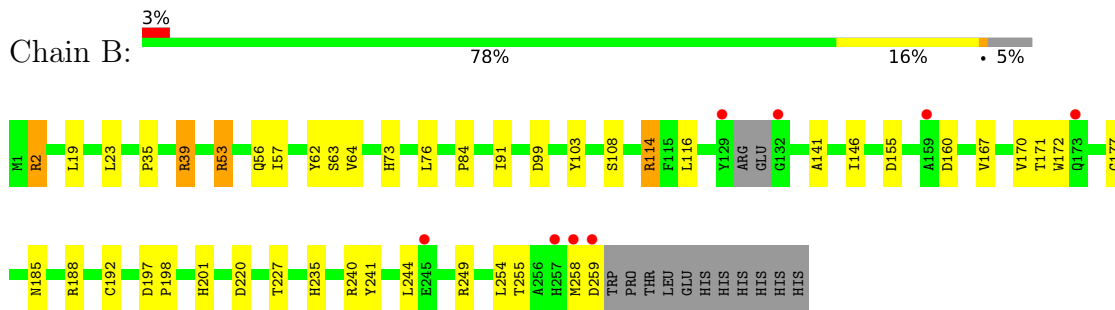
### 3 Residue-property plots [i](#)

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.

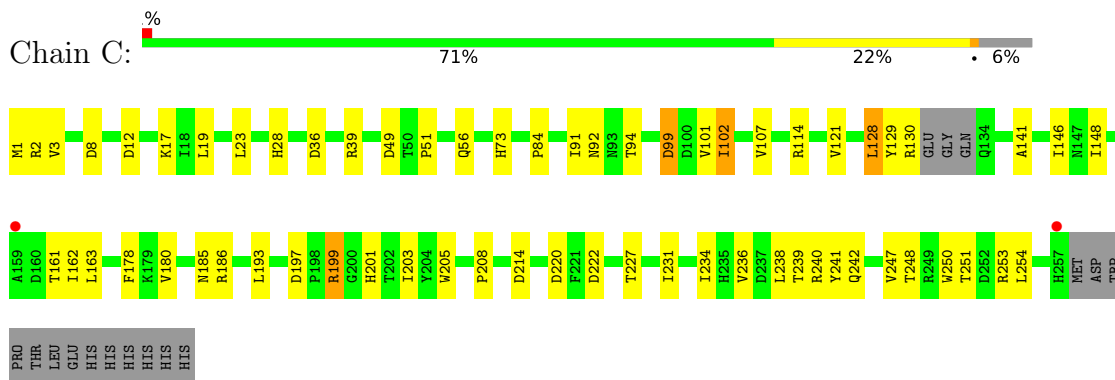
- Molecule 1: 5'-nucleotidase SurE



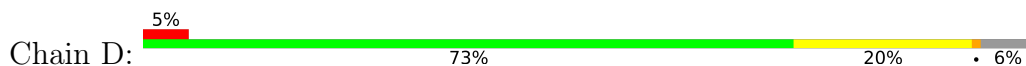
- Molecule 1: 5'-nucleotidase SurE

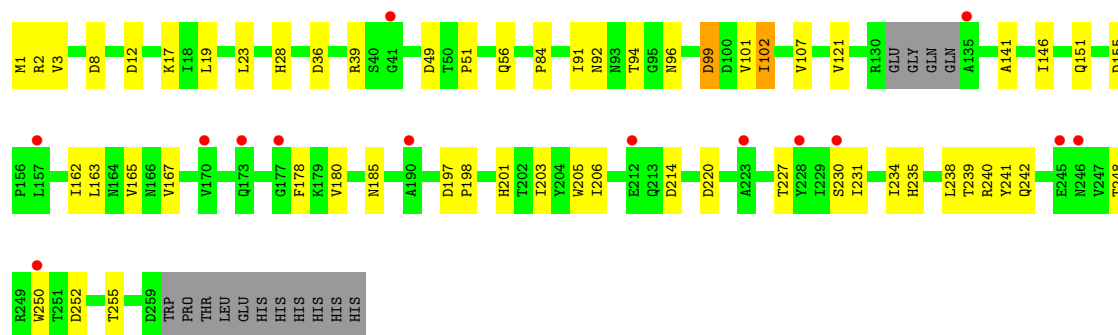


- Molecule 1: 5'-nucleotidase SurE



- Molecule 1: 5'-nucleotidase SurE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.00Å 78.21Å 82.16Å 90.00° 96.74° 90.00°	Depositor
Resolution (Å)	77.96 – 2.76 77.96 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.5 (77.96-2.76) 97.5 (77.96-2.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 2.77Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.197 , 0.248 0.200 , 0.253	Depositor DCC
$R_{free}$ test set	1255 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PO4, IOD, 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	0.29	0/1995	0.75	9/2731 (0.3%)
1	B	0.29	0/2036	0.75	9/2784 (0.3%)
1	C	0.28	0/1969	0.44	0/2696
1	D	0.27	0/1976	0.45	0/2705
All	All	0.28	0/7976	0.62	18/10916 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	B	53	ARG	NE-CZ-NH1	12.79	126.69	120.30
1	A	39	ARG	NE-CZ-NH2	-12.20	114.20	120.30
1	B	249	ARG	NE-CZ-NH2	-12.17	114.21	120.30
1	B	39	ARG	NE-CZ-NH1	-12.12	114.24	120.30
1	A	249	ARG	NE-CZ-NH1	-12.09	114.26	120.30
1	A	39	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	A	53	ARG	NE-CZ-NH1	-11.77	114.41	120.30
1	A	249	ARG	NE-CZ-NH2	11.77	126.19	120.30
1	B	249	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	A	53	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	B	39	ARG	NE-CZ-NH2	11.36	125.98	120.30
1	B	53	ARG	CD-NE-CZ	6.61	132.86	123.60
1	A	249	ARG	CD-NE-CZ	6.29	132.40	123.60
1	A	39	ARG	CD-NE-CZ	6.16	132.22	123.60
1	B	249	ARG	CD-NE-CZ	6.08	132.11	123.60
1	B	39	ARG	CD-NE-CZ	5.85	131.79	123.60
1	A	53	ARG	CD-NE-CZ	5.77	131.68	123.60

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	1953	0	1919	41	0
1	B	1994	0	1961	36	0
1	C	1930	0	1904	56	0
1	D	1937	0	1909	51	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	1	0
3	C	1	0	0	3	0
3	D	2	0	0	3	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
5	A	50	0	0	2	0
5	B	57	0	0	2	0
5	C	55	0	0	5	0
5	D	37	0	0	0	0
All	All	8043	0	7693	140	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 9.

All (140) 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:C:242:GLN:NE2	3:C:502:IOD:I	2.89	0.75
1:B:39:ARG:NH1	5:B:401:HOH:O	2.19	0.74
1:A:176:ARG:HG3	1:A:227:THR:HB	1.76	0.68
1:C:73:HIS:CD2	1:D:206:ILE:HD12	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ARG:NH1	1:C:49:ASP:O	2.28	0.67
1:B:57:ILE:HD11	1:B:63:SER:HB2	1.78	0.66
1:A:57:ILE:HD11	1:A:63:SER:HB2	1.77	0.65
1:D:242:GLN:HG3	3:D:603:IOD:I	2.68	0.64
1:C:186:ARG:NH1	5:C:604:HOH:O	2.22	0.64
1:A:188:ARG:HA	1:B:116:LEU:HD22	1.80	0.64
1:C:99:ASP:OD1	5:C:601:HOH:O	2.15	0.64
1:D:101:VAL:HG13	1:D:107:VAL:HG21	1.80	0.63
1:C:101:VAL:HG13	1:C:107:VAL:HG21	1.80	0.62
1:D:96:ASN:ND2	4:D:604:PO4:O4	2.20	0.62
1:B:2:ARG:HB3	1:B:84:PRO:HA	1.82	0.62
1:A:91:ILE:O	5:A:601:HOH:O	2.17	0.60
1:A:257:HIS:NE2	1:B:177:GLY:HA2	2.15	0.60
1:C:253:ARG:NE	1:D:155:ASP:OD2	2.34	0.60
1:A:177:GLY:HA3	1:B:255[B]:THR:HG23	1.82	0.60
1:C:248:THR:HA	1:D:180:VAL:HG21	1.84	0.59
1:A:116:LEU:HD22	1:B:188:ARG:HA	1.84	0.59
1:A:115:PHE:CE1	1:A:236:VAL:HG12	2.38	0.58
1:C:203:ILE:HB	1:D:51:PRO:HB2	1.85	0.58
1:A:257:HIS:CE1	1:B:177:GLY:HA2	2.38	0.58
1:C:23:LEU:HD23	1:C:146:ILE:HG22	1.86	0.57
1:C:242:GLN:OE1	3:C:502:IOD:I	2.93	0.57
1:D:23:LEU:HD23	1:D:146:ILE:HG22	1.86	0.56
1:C:180:VAL:HG21	1:D:248:THR:HA	1.86	0.56
1:D:185:ASN:HB2	1:D:214:ASP:HB3	1.88	0.56
1:D:241:TYR:N	3:D:603:IOD:I	3.10	0.55
1:A:48:LEU:O	1:C:199:ARG:NH1	2.39	0.55
1:A:141:ALA:HA	1:A:167:VAL:HG21	1.89	0.55
1:B:114:ARG:HD2	1:B:160:ASP:HA	1.88	0.55
1:C:148:ILE:HG23	1:D:250:TRP:CH2	2.42	0.55
1:C:36:ASP:OD1	1:C:39:ARG:NH1	2.25	0.54
1:B:141:ALA:HA	1:B:167:VAL:HG21	1.89	0.54
1:D:99:ASP:OD1	1:D:99:ASP:N	2.37	0.54
1:D:12:ASP:HA	1:D:17:LYS:HE3	1.89	0.54
1:C:238:LEU:HD11	1:D:102:ILE:HD12	1.90	0.54
1:A:53:ARG:HH11	1:D:49:ASP:HA	1.74	0.53
1:A:19:LEU:HB2	1:A:91:ILE:HG13	1.90	0.53
1:C:51:PRO:HB2	1:D:203:ILE:HB	1.91	0.53
1:C:242:GLN:CD	3:C:502:IOD:I	3.17	0.53
1:C:12:ASP:HA	1:C:17:LYS:HE3	1.89	0.53
1:C:240:ARG:HD2	1:D:235:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LEU:HB2	1:B:91:ILE:HG13	1.92	0.52
1:B:198:PRO:HB2	1:C:208:PRO:HD3	1.92	0.51
1:A:143:HIS:NE2	1:B:259[B]:ASP:O	2.44	0.50
1:B:254:LEU:HD23	1:B:258[B]:MET:HG3	1.94	0.49
1:C:247:VAL:HA	1:C:250:TRP:HB3	1.95	0.49
1:C:205:TRP:CH2	1:D:51:PRO:HD3	2.48	0.49
1:D:92:ASN:ND2	1:D:94:THR:O	2.46	0.48
1:A:114:ARG:HD2	1:A:160:ASP:HA	1.95	0.48
1:C:222:ASP:OD2	5:C:602:HOH:O	2.19	0.48
1:A:51:PRO:HD2	1:D:51:PRO:HD2	1.93	0.48
1:A:185:ASN:HB3	5:A:602:HOH:O	2.14	0.48
1:A:187:HIS:O	1:B:73:HIS:HE1	1.96	0.48
1:C:162:ILE:HD11	1:C:234:ILE:HD11	1.96	0.48
1:D:162:ILE:HD11	1:D:234:ILE:HD11	1.95	0.48
1:C:3:VAL:HG11	1:C:23:LEU:HD13	1.96	0.47
1:D:91:ILE:HD13	1:D:141:ALA:HB3	1.95	0.47
1:D:19:LEU:HB2	1:D:91:ILE:HG13	1.97	0.47
1:C:238:LEU:O	1:D:235:HIS:N	2.33	0.47
1:D:121:VAL:HG22	1:D:163:LEU:HB2	1.97	0.47
1:A:96:ASN:ND2	4:A:503:PO4:O4	2.36	0.47
1:C:19:LEU:HB2	1:C:91:ILE:HG13	1.95	0.47
1:B:91:ILE:HD13	1:B:141:ALA:HB3	1.97	0.46
1:C:51:PRO:HD3	1:D:205:TRP:CH2	2.51	0.46
1:C:91:ILE:HD13	1:C:141:ALA:HB3	1.97	0.46
1:D:2:ARG:HB2	1:D:84:PRO:HA	1.98	0.46
1:A:193:LEU:HD12	1:D:198:PRO:HB3	1.98	0.46
1:A:205:TRP:CG	1:D:198:PRO:HG2	2.51	0.46
1:C:121:VAL:HG22	1:C:163:LEU:HB2	1.97	0.46
1:B:185:ASN:HB3	5:B:422:HOH:O	2.16	0.46
1:C:161:THR:OG1	1:D:240:ARG:NH2	2.44	0.46
1:A:76:LEU:HD12	1:A:116:LEU:HD12	1.97	0.46
1:D:3:VAL:HG11	1:D:23:LEU:HD13	1.97	0.45
1:C:2:ARG:HB2	1:C:84:PRO:HA	1.98	0.45
1:C:254:LEU:HB2	1:D:151:GLN:HG2	1.96	0.45
1:D:242:GLN:N	3:D:603:IOD:I	3.09	0.45
1:C:128:LEU:HB2	1:C:130:ARG:HD2	1.99	0.45
1:A:56:GLN:HG3	1:A:62:TYR:CZ	2.52	0.45
1:B:241:TYR:HA	1:B:244:LEU:HG	1.99	0.45
1:C:178:PHE:HD2	1:C:231:ILE:HD11	1.82	0.45
1:A:114:ARG:HH11	1:A:161:THR:H	1.63	0.45
1:B:220:ASP:N	1:B:220:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TYR:HA	1:A:244:LEU:HG	2.00	0.44
1:A:51:PRO:CD	1:D:51:PRO:HD2	2.48	0.44
1:A:220:ASP:N	1:A:220:ASP:OD1	2.49	0.44
1:B:56:GLN:HG3	1:B:62:TYR:CZ	2.53	0.44
1:C:205:TRP:CZ2	1:D:51:PRO:HD3	2.52	0.44
1:A:91:ILE:HD13	1:A:141:ALA:HB3	1.99	0.44
1:A:103:TYR:OH	1:B:108:SER:HA	2.18	0.44
1:A:23:LEU:HD23	1:A:146:ILE:HG22	2.00	0.43
1:C:1:MET:HG2	1:C:28:HIS:ND1	2.33	0.43
1:C:92:ASN:ND2	1:C:94:THR:O	2.50	0.43
1:D:220:ASP:N	1:D:220:ASP:OD1	2.51	0.43
1:D:1:MET:HG2	1:D:28:HIS:ND1	2.33	0.43
1:A:205:TRP:CD2	1:D:198:PRO:HD2	2.53	0.43
1:B:76:LEU:HD12	1:B:116:LEU:HD12	1.99	0.43
1:C:148:ILE:HG23	1:D:250:TRP:HH2	1.82	0.43
1:A:108:SER:HA	1:B:103:TYR:OH	2.17	0.43
1:B:23:LEU:HD23	1:B:146:ILE:HG22	2.01	0.43
1:D:178:PHE:HD2	1:D:231:ILE:HD11	1.83	0.43
1:C:146:ILE:O	5:C:603:HOH:O	2.21	0.43
1:C:102:ILE:HD12	1:D:238:LEU:HD11	2.00	0.43
1:C:197:ASP:HB3	1:C:203:ILE:HD13	2.01	0.43
1:C:220:ASP:OD1	1:C:220:ASP:N	2.51	0.43
1:B:235:HIS:CE1	3:B:301:IOD:I	3.42	0.42
1:A:235:HIS:CE1	1:B:240:ARG:HD2	2.55	0.42
1:B:35:PRO:HA	1:B:64:VAL:O	2.19	0.42
1:D:197:ASP:HB3	1:D:203:ILE:HD13	2.01	0.42
1:A:240:ARG:HD2	1:B:235:HIS:CE1	2.54	0.42
1:B:170:VAL:HG23	1:B:171:THR:O	2.19	0.42
1:A:147:ASN:HD21	1:B:259[B]:ASP:HB3	1.83	0.42
1:A:257:HIS:HB3	1:B:172:TRP:HE1	1.85	0.42
1:C:251:THR:HA	1:C:254:LEU:HB3	2.02	0.42
1:A:190:ALA:O	1:B:73:HIS:NE2	2.53	0.42
1:C:185:ASN:HB3	1:C:214:ASP:HB3	2.02	0.42
1:C:197:ASP:OD1	1:C:201:HIS:N	2.53	0.42
1:A:35:PRO:HA	1:A:64:VAL:O	2.20	0.41
1:D:252:ASP:HA	1:D:255:THR:HG22	2.02	0.41
1:C:239:THR:HB	1:C:241:TYR:CE1	2.55	0.41
1:D:36:ASP:OD1	1:D:39:ARG:NH1	2.46	0.41
1:C:12:ASP:HB2	5:C:630:HOH:O	2.20	0.41
1:C:114:ARG:HG2	1:C:236:VAL:HG21	2.02	0.41
1:D:141:ALA:HA	1:D:167:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:PRO:HB3	1:C:193:LEU:HD12	2.03	0.41
1:C:51:PRO:HB3	1:D:205:TRP:CE2	2.55	0.41
1:B:201:HIS:CE1	1:C:129:TYR:HB2	2.55	0.41
1:A:33:VAL:HG12	1:A:71:CYS:HB3	2.02	0.41
1:B:197:ASP:HB2	1:B:198:PRO:HD2	2.02	0.41
1:C:231:ILE:HD13	1:D:250:TRP:HZ3	1.86	0.41
1:D:197:ASP:OD1	1:D:201:HIS:N	2.54	0.41
1:D:165:VAL:HA	1:D:230:SER:O	2.20	0.41
1:A:111:MET:SD	1:A:236:VAL:HG13	2.61	0.40
1:C:114:ARG:HD2	1:C:114:ARG:HA	1.81	0.40
1:D:239:THR:HB	1:D:241:TYR:CE1	2.56	0.40
1:C:247:VAL:O	1:C:251:THR:N	2.52	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	254/270 (94%)	245 (96%)	8 (3%)	1 (0%)	34	53
1	B	258/270 (96%)	245 (95%)	13 (5%)	0	100	100
1	C	250/270 (93%)	239 (96%)	11 (4%)	0	100	100
1	D	251/270 (93%)	239 (95%)	12 (5%)	0	100	100
All	All	1013/1080 (94%)	968 (96%)	44 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	MET

### 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	212/224 (95%)	208 (98%)	4 (2%)	57	73
1	B	216/224 (96%)	210 (97%)	6 (3%)	43	63
1	C	209/224 (93%)	202 (97%)	7 (3%)	38	58
1	D	210/224 (94%)	205 (98%)	5 (2%)	49	68
All	All	847/896 (94%)	825 (97%)	22 (3%)	46	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	A	155	ASP
1	A	192	CYS
1	A	227	THR
1	B	2	ARG
1	B	99	ASP
1	B	114	ARG
1	B	155	ASP
1	B	192	CYS
1	B	227	THR
1	C	8	ASP
1	C	56	GLN
1	C	99	ASP
1	C	102	ILE
1	C	128	LEU
1	C	199	ARG
1	C	227	THR
1	D	8	ASP
1	D	56	GLN
1	D	99	ASP
1	D	102	ILE
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	56	GLN
1	A	137	GLN
1	B	56	GLN
1	B	137	GLN
1	B	143	HIS
1	C	147	ASN
1	D	147	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	$\# Z  > 2$
4	PO4	C	503	2	4,4,4	0.90	0	6,6,6	0.51	0
4	PO4	D	604	2	4,4,4	0.92	0	6,6,6	0.42	0
4	PO4	A	503	2	4,4,4	0.84	0	6,6,6	0.40	0
4	PO4	B	303	2	4,4,4	0.90	0	6,6,6	0.49	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	604	PO4	1	0
4	A	503	PO4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	257/270 (95%)	0.33	9 (3%) 44 52	22, 44, 82, 119	16 (6%)
1	B	257/270 (95%)	0.39	8 (3%) 49 58	26, 45, 86, 127	5 (1%)
1	C	254/270 (94%)	0.23	2 (0%) 86 90	24, 48, 82, 101	7 (2%)
1	D	255/270 (94%)	0.55	14 (5%) 25 30	29, 57, 109, 133	17 (6%)
All	All	1023/1080 (94%)	0.37	33 (3%) 47 56	22, 49, 90, 133	45 (4%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	GLY	5.7
1	D	250	TRP	4.0
1	C	159	ALA	3.6
1	B	258[A]	MET	3.5
1	D	135	ALA	3.4
1	B	159	ALA	3.1
1	D	177	GLY	3.1
1	B	259[A]	ASP	2.9
1	B	132	GLY	2.9
1	A	133	GLN	2.8
1	B	129	TYR	2.7
1	D	157	LEU	2.5
1	D	170	VAL	2.5
1	C	257	HIS	2.5
1	B	257[A]	HIS	2.5
1	A	259	ASP	2.4
1	D	212	GLU	2.4
1	A	258	MET	2.3
1	D	41	GLY	2.3
1	D	230	SER	2.3
1	D	173	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	201	HIS	2.2
1	A	255	THR	2.2
1	D	228	TYR	2.2
1	D	246	ASN	2.2
1	D	245	GLU	2.1
1	A	198	PRO	2.1
1	D	190	ALA	2.1
1	A	129	TYR	2.1
1	B	245	GLU	2.0
1	D	223	ALA	2.0
1	A	157	LEU	2.0
1	B	173	GLN	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	IOD	A	504	1/1	0.89	0.11	83,83,83,83	1
3	IOD	B	301	1/1	0.89	0.10	165,165,165,165	1
3	IOD	C	502	1/1	0.95	0.17	113,113,113,113	1
3	IOD	D	603	1/1	0.95	0.09	78,78,78,78	1
2	MN	C	501	1/1	0.97	0.10	34,34,34,34	0
2	MN	D	602	1/1	0.98	0.06	49,49,49,49	0
2	MN	B	302	1/1	0.99	0.08	37,37,37,37	0
3	IOD	A	502	1/1	0.99	0.11	49,49,49,49	1
3	IOD	D	601	1/1	0.99	0.07	55,55,55,55	1
2	MN	A	501	1/1	0.99	0.08	39,39,39,39	0
4	PO4	A	503	5/5	0.99	0.13	38,40,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	B	303	5/5	0.99	0.10	33,36,36,37	0
4	PO4	C	503	5/5	0.99	0.11	37,37,38,38	0
4	PO4	D	604	5/5	0.99	0.13	53,53,54,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.