



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 03:36 AM GMT

PDB ID : 2UX1  
Title : IDENTIFICATION OF TWO ZINC-BINDING SITES IN THE STREPTOCOCCUS SUIS DPR PROTEIN  
Authors : Havukainen, H.; Kauko, A.; Pulliainen, A.T.; Haataja, S.; Meyer-Klaucke, W.; Finne, J.; Papageorgiou, A.C.  
Deposited on : 2007-03-26  
Resolution : 1.80 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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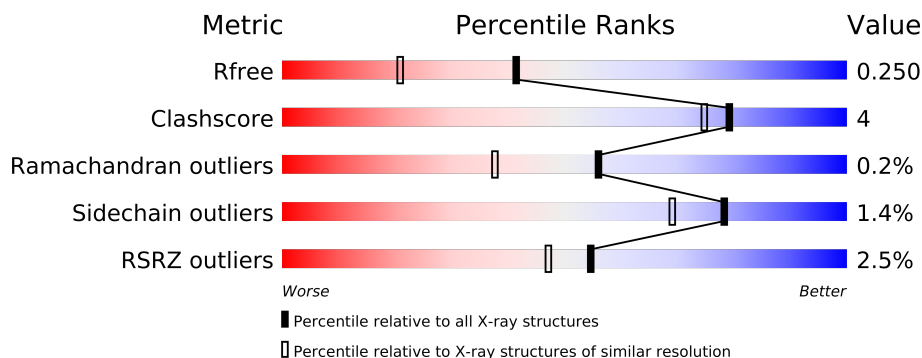
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
$R_{free}$	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	165	
1	B	165	
1	C	165	
1	D	165	
1	E	165	
1	F	165	
1	G	165	
1	H	165	
1	I	165	
1	J	165	
1	K	165	
1	L	165	

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	I	174	-	X
4	EPE	I	173	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15820 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA PROTECTION DURING STARVATION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	1	0
			1213	772	199	236	6			
1	B	151	Total	C	N	O	S	0	1	0
			1212	774	200	232	6			
1	C	151	Total	C	N	O	S	0	2	0
			1211	773	199	233	6			
1	D	152	Total	C	N	O	S	0	2	0
			1218	776	202	234	6			
1	E	150	Total	C	N	O	S	0	0	0
			1178	752	196	224	6			
1	F	152	Total	C	N	O	S	0	1	0
			1201	766	198	231	6			
1	G	165	Total	C	N	O	S	0	0	0
			1281	815	212	248	6			
1	H	152	Total	C	N	O	S	0	0	0
			1194	762	198	228	6			
1	I	153	Total	C	N	O	S	0	0	0
			1205	767	200	232	6			
1	J	152	Total	C	N	O	S	0	1	0
			1217	774	200	237	6			
1	K	152	Total	C	N	O	S	0	0	0
			1207	769	199	233	6			
1	L	152	Total	C	N	O	S	0	1	0
			1210	771	199	234	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
B	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
C	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
D	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
E	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
G	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
H	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
I	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
J	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
K	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9
L	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Zn 2 2	0	0
2	J	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	K	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	H	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	I	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	A	2	Total Zn 2 2	0	0
2	L	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

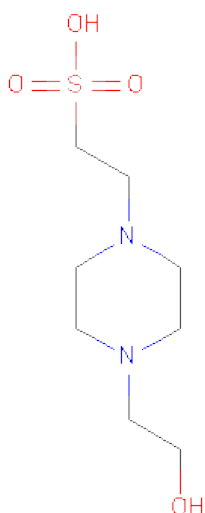
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Ca 1 1	0	0
3	I	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ca	0	0
			1	1		
3	K	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	I	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	J	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	K	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Cl	0	0
			1	1		
5	L	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

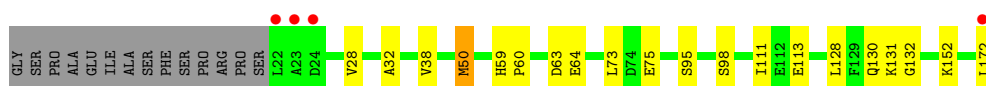
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	108	Total 108	O 108	0	0
6	B	98	Total 98	O 98	0	0
6	C	87	Total 87	O 87	0	0
6	D	133	Total 133	O 133	0	0
6	E	83	Total 83	O 83	0	0
6	F	110	Total 110	O 110	0	0
6	G	90	Total 90	O 90	0	0
6	H	99	Total 99	O 99	0	0
6	I	97	Total 97	O 97	0	0
6	J	90	Total 90	O 90	0	0
6	K	99	Total 99	O 99	0	0
6	L	89	Total 89	O 89	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

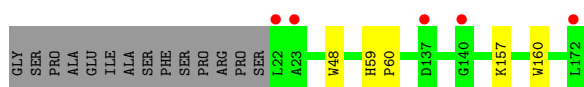
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain A: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain B: 



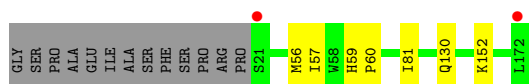
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain C: 



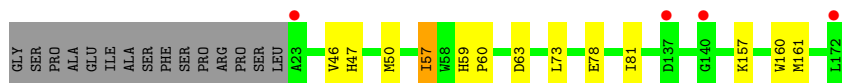
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain D: 



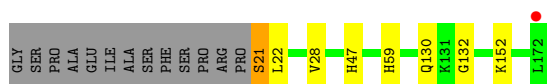
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain E: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain F: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain G: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain H: 



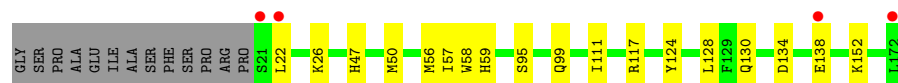
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain I: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain J: 



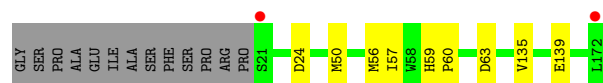
- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain K: 



- Molecule 1: DNA PROTECTION DURING STARVATION PROTEIN

Chain L: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.52Å 137.69Å 142.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 1.80 19.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.97-1.80) 99.9 (19.92-1.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.206 , 0.248 0.208 , 0.250	Depositor DCC
$R_{free}$ test set	8779 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.5	EDS
Estimated twinning fraction	0.048 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	2 of 189026 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EPE, CA, CL

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	0.55	0/1238	0.60	0/1673
1	B	0.59	0/1237	0.62	0/1671
1	C	0.51	0/1239	0.58	0/1675
1	D	0.58	0/1249	0.62	0/1687
1	E	0.47	0/1203	0.54	0/1628
1	F	0.53	0/1229	0.61	0/1663
1	G	0.51	0/1308	0.59	1/1770 (0.1%)
1	H	0.49	0/1219	0.61	0/1650
1	I	0.50	0/1230	0.57	0/1663
1	J	0.52	0/1242	0.59	0/1678
1	K	0.55	0/1232	0.58	0/1665
1	L	0.48	0/1238	0.54	0/1673
All	All	0.52	0/14864	0.59	1/20096 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	PRO	N-CA-CB	6.16	110.69	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1213	0	1166	15	0
1	B	1212	0	1178	3	0
1	C	1211	0	1172	10	0
1	D	1218	0	1182	5	0
1	E	1178	0	1127	13	0
1	F	1201	0	1151	4	0
1	G	1281	0	1213	11	0
1	H	1194	0	1142	11	0
1	I	1205	0	1153	11	0
1	J	1217	0	1172	9	0
1	K	1207	0	1164	9	0
1	L	1210	0	1169	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	D	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	E	15	0	17	0	0
4	I	15	0	17	1	0
4	J	15	0	17	0	0
4	K	15	0	17	0	0
5	H	1	0	0	0	0
5	L	1	0	0	3	0
6	A	108	0	0	5	0
6	B	98	0	0	1	0
6	C	87	0	0	1	0
6	D	133	0	0	0	0
6	E	83	0	0	1	0
6	F	110	0	0	0	1
6	G	90	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	99	0	0	2	0
6	I	97	0	0	2	0
6	J	90	0	0	0	0
6	K	99	0	0	1	1
6	L	89	0	0	2	0
All	All	15820	0	14057	100	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (100) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:57:ILE:HD11	1:E:57:ILE:HG21	1.36	1.03
5:L:173:CL:CL	6:L:2058:HOH:O	2.43	0.74
1:A:75:GLU:HG2	6:A:2036:HOH:O	1.87	0.74
1:C:56:MET:HB3	1:E:57:ILE:HD11	1.71	0.72
6:C:2079:HOH:O	5:L:173:CL:CL	2.44	0.71
1:H:146:ASP:OD2	6:H:2079:HOH:O	2.11	0.69
5:L:173:CL:CL	6:L:2056:HOH:O	2.47	0.68
1:A:50:MET:HG2	1:A:111:ILE:HD13	1.76	0.67
1:I:26:LYS:NZ	6:I:2005:HOH:O	2.29	0.66
1:C:56:MET:HB3	1:E:57:ILE:CD1	2.25	0.65
1:G:29:LEU:O	1:G:33:VAL:HG23	1.97	0.64
1:K:130:GLN:HB2	1:K:152:LYS:HE3	1.81	0.62
1:D:56:MET:HG2	1:G:57:ILE:HD11	1.84	0.59
1:A:131:LYS:NZ	6:A:2080:HOH:O	2.35	0.58
1:G:130:GLN:OE1	1:G:152:LYS:HE3	2.04	0.57
1:K:152:LYS:NZ	6:K:2082:HOH:O	2.38	0.56
1:L:24:ASP:HB3	1:L:135:VAL:CG1	2.35	0.56
1:G:157:LYS:HE3	6:G:2078:HOH:O	2.03	0.56
1:G:59:HIS:HB3	1:G:60:PRO:HD3	1.86	0.56
1:H:50:MET:HG3	1:H:111:ILE:HD13	1.88	0.55
1:D:56:MET:CG	1:G:57:ILE:HD11	2.36	0.55
1:A:50:MET:HG2	1:A:111:ILE:CD1	2.36	0.55
1:C:57:ILE:HD12	1:E:57:ILE:HD13	1.89	0.55
1:H:28:VAL:HG11	1:H:132:GLY:HA2	1.90	0.54
1:J:50:MET:HG3	1:J:111:ILE:CD1	2.37	0.54
1:J:47:HIS:CE1	1:J:59:HIS:CE1	2.96	0.53
1:A:113:GLU:OE1	6:A:2071:HOH:O	2.18	0.53
1:J:57:ILE:HG23	1:J:58:TRP:CD1	2.44	0.52
1:H:56:MET:HE1	1:K:161:MET:HB3	1.92	0.51
1:H:157:LYS:HD2	6:H:2085:HOH:O	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:24:ASP:HB3	1:L:135:VAL:HG11	1.93	0.50
1:E:57:ILE:HG22	1:L:57:ILE:HD13	1.93	0.50
1:I:117:ARG:O	1:I:121:VAL:HG23	2.12	0.50
1:G:56:MET:HE1	1:I:161:MET:HB3	1.94	0.50
1:C:135:VAL:O	1:C:139:GLU:HG3	2.12	0.50
1:K:126:ALA:O	1:K:152:LYS:HE2	2.12	0.49
1:D:130:GLN:OE1	1:D:152:LYS:HE3	2.13	0.49
1:H:21:SER:C	1:H:23:ALA:H	2.16	0.49
1:I:60:PRO:O	1:I:63:ASP:HB2	2.13	0.48
1:F:28:VAL:HG11	1:F:132:GLY:HA2	1.96	0.48
1:C:56:MET:HE1	1:E:161:MET:HB3	1.96	0.47
1:J:130:GLN:OE1	1:J:152:LYS:HE3	2.14	0.47
1:H:74:ASP:O	1:H:78:GLU:HG3	2.13	0.47
1:A:130:GLN:OE1	1:A:152:LYS:HE3	2.15	0.47
1:I:50:MET:HG3	1:I:111:ILE:CD1	2.45	0.47
1:K:130:GLN:HB2	1:K:152:LYS:CE	2.45	0.46
1:E:60:PRO:O	1:E:63:ASP:HB2	2.15	0.46
1:I:152:LYS:NZ	1:I:156:GLU:OE2	2.43	0.46
1:E:157:LYS:HZ2	1:E:160:TRP:HZ3	1.63	0.46
1:I:46:VAL:O	1:I:50:MET:HB2	2.16	0.46
1:B:48:TRP:HB3	1:D:81:ILE:HD11	1.98	0.46
1:C:58:TRP:CH2	1:L:56:MET:HE2	2.49	0.46
1:G:109:VAL:HG12	1:G:113:GLU:HB2	1.98	0.45
1:F:130:GLN:OE1	1:F:152:LYS:HE3	2.16	0.45
1:F:47:HIS:CE1	1:F:59:HIS:CE1	3.04	0.45
1:L:24:ASP:HB2	1:L:139:GLU:OE2	2.17	0.45
1:C:78:GLU:HA	1:C:81:ILE:HD12	1.99	0.45
1:A:28:VAL:HG11	1:A:132:GLY:HA2	1.99	0.44
1:L:24:ASP:HB3	1:L:135:VAL:HG13	1.98	0.44
1:E:46:VAL:O	1:E:50:MET:HB2	2.18	0.44
1:K:60:PRO:O	1:K:63:ASP:HB2	2.17	0.44
1:G:21:SER:O	1:G:23:ALA:N	2.49	0.43
1:B:157:LYS:HE3	6:B:2084:HOH:O	2.18	0.43
1:L:50:MET:HE1	1:L:59:HIS:N	2.32	0.43
1:A:32:ALA:HA	1:A:128:LEU:HD21	2.00	0.43
1:I:47:HIS:CE1	1:I:59:HIS:CE1	3.06	0.43
1:E:157:LYS:HE3	1:E:161:MET:HE3	1.99	0.43
1:J:22:LEU:O	1:J:26:LYS:HG3	2.18	0.43
1:F:21:SER:HB2	1:F:22:LEU:H	1.63	0.43
1:J:56:MET:HE2	1:J:56:MET:HB2	1.89	0.43
1:A:73:LEU:HD23	1:A:73:LEU:C	2.39	0.43
1:I:29:LEU:O	1:I:33:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:152:LYS:NZ	1:K:156:GLU:OE2	2.48	0.42
1:B:59:HIS:HB3	1:B:60:PRO:CD	2.49	0.42
1:D:59:HIS:HB3	1:D:60:PRO:CD	2.48	0.42
1:C:60:PRO:O	1:C:63:ASP:HB2	2.19	0.42
1:H:24:ASP:HB3	1:H:135:VAL:HG11	2.01	0.42
1:H:28:VAL:HG11	1:H:132:GLY:CA	2.50	0.42
1:A:64:GLU:OE2	6:A:2023:HOH:O	2.20	0.42
4:I:173:EPE:H32	6:I:2094:HOH:O	2.20	0.42
1:A:38:VAL:HG21	1:A:98:SER:CB	2.50	0.42
1:K:46:VAL:O	1:K:50:MET:HB2	2.20	0.42
1:E:157:LYS:NZ	6:E:2070:HOH:O	2.30	0.42
1:L:60:PRO:O	1:L:63:ASP:HB2	2.20	0.42
1:H:21:SER:C	1:H:23:ALA:N	2.74	0.41
1:A:59:HIS:HB3	1:A:60:PRO:CD	2.50	0.41
1:J:50:MET:HG3	1:J:111:ILE:HD13	2.01	0.41
1:I:50:MET:HG3	1:I:111:ILE:HD13	2.02	0.41
1:J:134:ASP:O	1:J:138:GLU:HG2	2.20	0.41
1:E:78:GLU:HA	1:E:81:ILE:HD12	2.01	0.41
1:A:172:LEU:HD11	1:I:82:THR:HG22	2.01	0.41
1:C:46:VAL:O	1:C:50:MET:HB2	2.21	0.41
1:A:131:LYS:NZ	6:A:2081:HOH:O	2.54	0.41
1:H:32:ALA:HA	1:H:128:LEU:HD21	2.03	0.41
1:J:99:GLN:HB2	1:J:124:TYR:OH	2.21	0.41
1:G:46:VAL:O	1:G:50:MET:HB2	2.21	0.41
1:K:32:ALA:HA	1:K:128:LEU:HD11	2.03	0.40
1:G:72:TYR:OH	1:G:154:SER:OG	2.23	0.40
1:A:60:PRO:O	1:A:63[B]:ASP:HB3	2.22	0.40
1:E:47:HIS:CE1	1:E:59:HIS:CE1	3.09	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	Distance(Å)	Clash(Å)
6:F:2068:HOH:O	6:K:2076:HOH:O[4_475]	1.78	0.42

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	B	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	C	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	D	152/165 (92%)	151 (99%)	1 (1%)	0	100	100
1	E	148/165 (90%)	147 (99%)	1 (1%)	0	100	100
1	F	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	G	163/165 (99%)	155 (95%)	4 (2%)	4 (2%)	9	1
1	H	150/165 (91%)	147 (98%)	3 (2%)	0	100	100
1	I	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	J	151/165 (92%)	150 (99%)	1 (1%)	0	100	100
1	K	150/165 (91%)	149 (99%)	1 (1%)	0	100	100
1	L	151/165 (92%)	149 (99%)	2 (1%)	0	100	100
All	All	1818/1980 (92%)	1796 (99%)	18 (1%)	4 (0%)	56	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	17	SER
1	G	19	ARG
1	G	20	PRO
1	G	22	LEU

### 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	129/140 (92%)	127 (98%)	2 (2%)	75	63
1	B	129/140 (92%)	128 (99%)	1 (1%)	89	85
1	C	129/140 (92%)	127 (98%)	2 (2%)	75	63
1	D	130/140 (93%)	129 (99%)	1 (1%)	89	85
1	E	122/140 (87%)	120 (98%)	2 (2%)	75	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	126/140 (90%)	125 (99%)	1 (1%)	89	85
1	G	132/140 (94%)	129 (98%)	3 (2%)	63	46
1	H	124/140 (89%)	123 (99%)	1 (1%)	89	85
1	I	126/140 (90%)	124 (98%)	2 (2%)	75	63
1	J	130/140 (93%)	127 (98%)	3 (2%)	63	46
1	K	128/140 (91%)	125 (98%)	3 (2%)	63	46
1	L	129/140 (92%)	129 (100%)	0	100	100
All	All	1534/1680 (91%)	1513 (99%)	21 (1%)	78	69

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	MET
1	A	95	SER
1	B	160	TRP
1	C	75	GLU
1	C	160	TRP
1	D	57	ILE
1	E	57	ILE
1	E	73	LEU
1	F	21	SER
1	G	57	ILE
1	G	95	SER
1	G	104	LEU
1	H	24	ASP
1	I	73	LEU
1	I	95	SER
1	J	95	SER
1	J	117	ARG
1	J	128	LEU
1	K	63	ASP
1	K	69	ILE
1	K	128	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	130	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 30 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	EPE	E	173	-	15,15,15	0.86	1 (6%)	20,20,20	1.84	6 (30%)
4	EPE	I	173	-	15,15,15	0.77	1 (6%)	20,20,20	2.16	6 (30%)
4	EPE	J	173	-	15,15,15	0.70	1 (6%)	20,20,20	2.10	4 (20%)
4	EPE	K	173	-	15,15,15	0.73	1 (6%)	20,20,20	2.26	6 (30%)

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
4	EPE	E	173	-	-	0/9/19/19	0/1/1/1
4	EPE	I	173	-	-	0/9/19/19	0/1/1/1
4	EPE	J	173	-	-	0/9/19/19	0/1/1/1
4	EPE	K	173	-	-	0/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	173	EPE	C10-S	3.02	1.82	1.77
4	K	173	EPE	C10-S	2.52	1.81	1.77
4	I	173	EPE	C10-S	2.47	1.81	1.77
4	J	173	EPE	C10-S	2.25	1.80	1.77

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	173	EPE	O1S-S-C10	7.42	113.16	106.81
4	I	173	EPE	O1S-S-C10	6.01	111.96	106.81
4	K	173	EPE	O1S-S-C10	5.73	111.72	106.81
4	K	173	EPE	C5-N4-C3	4.21	119.33	108.86
4	I	173	EPE	C5-N4-C3	4.19	119.26	108.86
4	E	173	EPE	O3S-S-C10	3.77	110.70	105.93
4	E	173	EPE	C5-N4-C3	3.63	117.88	108.86
4	J	173	EPE	C5-N4-C3	3.63	117.87	108.86
4	K	173	EPE	C7-N4-C3	3.55	120.48	111.32
4	K	173	EPE	C7-N4-C5	3.43	120.19	111.32
4	I	173	EPE	C7-N4-C3	3.20	119.59	111.32
4	K	173	EPE	O3S-S-C10	2.94	109.66	105.93
4	E	173	EPE	C7-N4-C3	2.89	118.79	111.32
4	I	173	EPE	C7-N4-C5	2.88	118.75	111.32
4	J	173	EPE	C7-N4-C3	2.80	118.55	111.32
4	E	173	EPE	C7-N4-C5	2.80	118.55	111.32
4	K	173	EPE	O2S-S-C10	-2.69	104.51	106.81
4	E	173	EPE	O2S-S-C10	2.63	109.06	106.81
4	J	173	EPE	C7-N4-C5	2.50	117.77	111.32
4	E	173	EPE	O1S-S-C10	2.48	108.93	106.81
4	I	173	EPE	O3S-S-C10	2.27	108.80	105.93
4	I	173	EPE	C9-N1-C2	-2.03	106.08	111.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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	151/165 (91%)	0.14	4 (2%) 53 46	24, 30, 40, 44	0
1	B	151/165 (91%)	0.12	5 (3%) 44 36	21, 28, 40, 53	0
1	C	151/165 (91%)	0.23	3 (1%) 62 56	25, 31, 41, 51	1 (0%)
1	D	152/165 (92%)	-0.01	2 (1%) 74 70	20, 26, 35, 43	0
1	E	150/165 (90%)	0.31	4 (2%) 52 44	28, 33, 44, 50	0
1	F	152/165 (92%)	0.11	1 (0%) 84 83	21, 26, 39, 48	0
1	G	165/165 (100%)	0.48	11 (6%) 17 12	24, 33, 51, 63	0
1	H	152/165 (92%)	0.16	4 (2%) 53 46	22, 30, 42, 55	0
1	I	153/165 (92%)	0.43	6 (3%) 37 30	23, 32, 46, 58	0
1	J	152/165 (92%)	0.28	4 (2%) 53 46	22, 30, 41, 50	0
1	K	152/165 (92%)	0.18	0 100 100	24, 29, 39, 41	0
1	L	152/165 (92%)	0.25	2 (1%) 74 70	25, 31, 41, 50	0
All	All	1833/1980 (92%)	0.23	46 (2%) 54 47	20, 30, 42, 63	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	20	PRO	6.9
1	G	18	PRO	6.9
1	B	23	ALA	6.3
1	C	23	ALA	6.3
1	G	19	ARG	6.1
1	G	20	PRO	5.3
1	G	21	SER	5.2
1	E	23	ALA	5.1
1	G	17	SER	5.0
1	I	22	LEU	4.6
1	H	22	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	G	137	ASP	4.5
1	B	22	LEU	4.4
1	A	22	LEU	4.2
1	G	172	LEU	4.1
1	L	21	SER	4.0
1	E	172	LEU	4.0
1	B	172	LEU	3.9
1	J	21	SER	3.8
1	C	22	LEU	3.8
1	J	22	LEU	3.8
1	H	23	ALA	3.6
1	D	172	LEU	3.4
1	J	172	LEU	3.3
1	L	172	LEU	3.3
1	G	10	PRO	3.3
1	C	172	LEU	3.2
1	A	172	LEU	3.1
1	I	172	LEU	3.1
1	J	138	GLU	3.1
1	I	21	SER	3.0
1	H	172	LEU	3.0
1	D	21	SER	3.0
1	H	21	SER	3.0
1	F	172	LEU	2.9
1	E	140	GLY	2.8
1	G	23	ALA	2.8
1	B	137	ASP	2.7
1	I	96	GLU	2.3
1	E	137	ASP	2.3
1	A	23	ALA	2.2
1	A	24	ASP	2.2
1	G	11	ALA	2.2
1	I	138	GLU	2.1
1	B	140	GLY	2.1
1	G	22	LEU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	EPE	I	173	15/15	0.17	3.36	39,41,44,46	10
3	CA	I	174	1/1	0.18	2.04	38,38,38,38	0
4	EPE	K	173	15/15	0.16	1.56	40,48,56,57	0
4	EPE	E	173	15/15	0.16	0.62	52,57,62,63	0
4	EPE	J	173	15/15	0.14	0.59	48,51,56,57	0
3	CA	H	174	1/1	0.11	-0.35	23,23,23,23	1
5	CL	L	173	1/1	0.09	-0.55	47,47,47,47	0
2	ZN	J	1173	1/1	0.06	-1.47	45,45,45,45	0
3	CA	D	173	1/1	0.07	-1.51	18,18,18,18	1
5	CL	H	173	1/1	0.07	-1.67	43,43,43,43	0
2	ZN	G	1173	1/1	0.08	-1.70	50,50,50,50	0
2	ZN	B	1174	1/1	0.06	-1.83	41,41,41,41	0
2	ZN	B	1173	1/1	0.03	-1.87	23,23,23,23	0
2	ZN	C	1173	1/1	0.02	-1.97	25,25,25,25	0
2	ZN	K	1174	1/1	0.02	-2.10	26,26,26,26	0
2	ZN	A	1173	1/1	0.06	-2.13	42,42,42,42	0
2	ZN	H	1173	1/1	0.06	-2.19	44,44,44,44	0
2	ZN	C	1174	1/1	0.05	-2.49	42,42,42,42	0
2	ZN	D	1174	1/1	0.02	-2.67	24,24,24,24	0
2	ZN	I	1174	1/1	0.02	-2.70	29,29,29,29	0
2	ZN	L	1174	1/1	0.07	-2.80	40,40,40,40	0
2	ZN	A	1174	1/1	0.03	-2.83	29,29,29,29	0
2	ZN	H	1174	1/1	0.03	-2.85	27,27,27,27	0
3	CA	K	174	1/1	0.04	-2.94	30,30,30,30	0
2	ZN	F	1174	1/1	0.02	-2.98	27,27,27,27	0
2	ZN	J	1174	1/1	0.03	-3.16	30,30,30,30	0
2	ZN	G	1174	1/1	0.02	-3.20	31,31,31,31	0
2	ZN	D	1173	1/1	0.04	-3.24	44,44,44,44	0
2	ZN	E	1174	1/1	0.06	-3.73	48,48,48,48	0
2	ZN	E	1173	1/1	0.03	-3.92	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	K	1173	1/1	0.03	-3.93	43,43,43,43	0
2	ZN	I	1173	1/1	0.04	-4.64	44,44,44,44	0
2	ZN	L	1173	1/1	0.02	-6.79	27,27,27,27	0
2	ZN	F	1173	1/1	0.07	-6.93	41,41,41,41	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.