

# Full wwPDB X-ray Structure Validation Report (i)

#### Nov 22, 2021 – 12:39 PM EST

PDB ID	:	7L6Z
Title	:	Crystal Structure of Peptidyl-Prolyl Cis-Trans Isomerasefrom (PpiB) Strepto-
		coccus pneumoniae R6
Authors	:	Minasov, G.; Shuvalova, L.; Kiryukhina, O.; Dubrovska, I.; Satchell, K.J.F.;
		Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2020-12-24
Resolution	:	1.88  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 (i) symbol.

The following versions of software and data (see references (1)) 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	:	2.23.2
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)	:	2.23.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.88 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.



Motria	Whole archive	Similar resolution			
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$			
$R_{free}$	130704	9470 (1.90-1.86)			
Clashscore	141614	10282 (1.90-1.86)			
Ramachandran outliers	138981	10152 (1.90-1.86)			
Sidechain outliers	138945	10152 (1.90-1.86)			
RSRZ outliers	127900	9303 (1.90-1.86)			

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 <=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	Δ	214	059/	E9/
		214	95% %	
1	В	214	92%	7%
1	С	214	95%	•
1	D	014	2%	
	D	214	98%	•
1	Ε	214	93%	7%



Contr	nued from	<i>i</i> previous	page	
Mol	Chain	Length	Quality of chain	
1	F	214	% 93%	7%
1	G	214	93%	6%
1	Н	214	<u>6%</u> 94%	5%
1	Ι	214	93%	6%
1	J	214	95%	5%

 $\alpha$ Jf nti



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18400 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	214	Total	С	Ν	Ο	Se	0	0	0
1		214	1672	1058	278	332	4	0	0	0
1	В	913	Total	$\mathbf{C}$	Ν	Ο	Se	0	9	0
	D	210	1682	1065	282	331	4	0		0
1	C	213	Total	$\mathbf{C}$	Ν	Ο	Se	0	1	0
1	U	210	1670	1059	277	330	4	0	Ĩ	0
1	а	914	Total	$\mathbf{C}$	Ν	Ο	Se	0	1	0
1	D	214	1681	1064	280	333	4		I	0
1	F	E 213	Total	$\mathbf{C}$	Ν	Ο	Se	0	3	0
-			1688	1069	280	335	4	0	5	0
1	F	913	Total	$\mathbf{C}$	Ν	Ο	Se	0	3	0
1	T,	210	1689	1069	281	335	4	0	5	0
1	G	913	Total	$\mathbf{C}$	Ν	Ο	Se	0	0	0
1	u	210	1662	1053	276	329	4	0	0	0
1	н	913	Total	$\mathbf{C}$	Ν	Ο	Se	0	1	0
1	11	210	1673	1059	280	330	4	0	Ĩ	0
1	Т	913	Total	$\mathbf{C}$	Ν	Ο	Se	0	0	0
	1	210	1662	1053	276	329	4	0	0	0
1	T	213	Total	C	Ν	0	Se	0	0	0
	J	210	1662	1053	276	329	4	0	0	0

• Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase.

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	60	MSE	-	initiating methionine	UNP Q8DQG5
А	268	GLU	-	expression tag	UNP Q8DQG5
А	269	ASN	-	expression tag	UNP Q8DQG5
А	270	LEU	-	expression tag	UNP Q8DQG5
А	271	TYR	-	expression tag	UNP Q8DQG5
А	272	PHE	-	expression tag	UNP Q8DQG5
А	273	GLN	-	expression tag	UNP Q8DQG5
В	60	MSE	-	initiating methionine	UNP Q8DQG5
B	268	GLU	_	expression tag	UNP Q8DQG5



Chain	Residue	Modelled	Actual Comment		Reference
В	269	ASN	-	expression tag	UNP Q8DQG5
В	270	LEU	-	expression tag	UNP Q8DQG5
В	271	TYR	-	expression tag	UNP Q8DQG5
В	272	PHE	-	expression tag	UNP Q8DQG5
В	273	GLN	-	expression tag	UNP Q8DQG5
С	60	MSE	-	initiating methionine	UNP Q8DQG5
С	268	GLU	-	expression tag	UNP Q8DQG5
C	269	ASN	-	expression tag	UNP Q8DQG5
С	270	LEU	-	expression tag	UNP Q8DQG5
С	271	TYR	-	expression tag	UNP Q8DQG5
С	272	PHE	-	expression tag	UNP Q8DQG5
С	273	GLN	-	expression tag	UNP Q8DQG5
D	60	MSE	-	initiating methionine	UNP Q8DQG5
D	268	GLU	-	expression tag	UNP Q8DQG5
D	269	ASN	-	expression tag	UNP Q8DQG5
D	270	LEU	-	expression tag	UNP Q8DQG5
D	271	TYR	-	expression tag	UNP Q8DQG5
D	272	PHE	-	expression tag	UNP Q8DQG5
D	273	GLN	-	expression tag	UNP Q8DQG5
Е	60	MSE	-	initiating methionine	UNP Q8DQG5
Е	268	GLU	-	expression tag	UNP Q8DQG5
Е	269	ASN	-	expression tag	UNP Q8DQG5
Е	270	LEU	-	expression tag	UNP Q8DQG5
Е	271	TYR	-	expression tag	UNP Q8DQG5
Е	272	PHE	-	expression tag	UNP Q8DQG5
Е	273	GLN	-	expression tag	UNP Q8DQG5
F	60	MSE	-	initiating methionine	UNP Q8DQG5
F	268	GLU	-	expression tag	UNP Q8DQG5
F	269	ASN	-	expression tag	UNP Q8DQG5
F	270	LEU	-	expression tag	UNP Q8DQG5
F	271	TYR	-	expression tag	UNP Q8DQG5
F	272	PHE	-	expression tag	UNP Q8DQG5
F	273	GLN	-	expression tag	UNP Q8DQG5
G	60	MSE	-	initiating methionine	UNP Q8DQG5
G	268	GLU	-	expression tag	UNP Q8DQG5
G	269	ASN	-	expression tag	UNP Q8DQG5
G	270	LEU	-	expression tag	UNP Q8DQG5
G	271	TYR	-	expression tag	UNP Q8DQG5
G	272	PHE	-	expression tag	UNP Q8DQG5
G	273	GLN	-	expression tag	UNP Q8DQG5
Н	60	MSE	-	initiating methionine	UNP Q8DQG5
Н	268	GLU	-	expression tag	UNP Q8DQG5



Chain	Residue	Modelled	Actual	Comment	Reference
Н	269	ASN	-	expression tag	UNP Q8DQG5
Н	270	LEU	-	expression tag	UNP Q8DQG5
Н	271	TYR	-	expression tag	UNP Q8DQG5
Н	272	PHE	-	expression tag	UNP Q8DQG5
Н	273	GLN	-	expression tag	UNP Q8DQG5
Ι	60	MSE	-	initiating methionine	UNP Q8DQG5
Ι	268	GLU	-	expression tag	UNP Q8DQG5
Ι	269	ASN	-	expression tag	UNP Q8DQG5
Ι	270	LEU	-	expression tag	UNP Q8DQG5
Ι	271	TYR	-	expression tag	UNP Q8DQG5
Ι	272	PHE	-	expression tag	UNP Q8DQG5
Ι	273	GLN	-	expression tag	UNP Q8DQG5
J	60	MSE	-	initiating methionine	UNP Q8DQG5
J	268	GLU	-	expression tag	UNP Q8DQG5
J	269	ASN	-	expression tag	UNP Q8DQG5
J	270	LEU	-	expression tag	UNP Q8DQG5
J	271	TYR	-	expression tag	UNP Q8DQG5
J	272	PHE	-	expression tag	UNP Q8DQG5
J	273	GLN	-	expression tag	UNP Q8DQG5

• Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Cl 3 3	0	1
2	В	2	Total Cl 2 2	0	0
2	D	1	Total Cl 1 1	0	0
2	Е	1	Total Cl 1 1	0	0
2	G	1	Total Cl 1 1	0	0

• Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 4	${ m C} 2$	O 2	0	0

• Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	С	1	Total 12	C 6	N 1	0 4	${ m S}$	0	0
4	С	1	Total	C 6	N 1	$\frac{1}{0}$	S 1	0	0



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Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
4	Л	1	Total	С	Ν	0	S	0	0
4	D	1	12	6	1	4	1	0	0
4	F	1	Total	С	Ν	0	$\mathbf{S}$	0	0
4	Ľ	1	12	6	1	4	1	0	0
4	F	1	Total	С	Ν	0	$\mathbf{S}$	0	0
4	Г	1	12	6	1	4	1	0	0
4	Б	1	Total	С	Ν	Ο	S	0	0
4	Г	1	12	6	1	4	1	0	0
4	Ц	1	Total	С	Ν	0	S	0	0
4	11	1	12	6	1	4	1	0	0
4	т	1	Total	С	Ν	0	S	0	0
4	J	1	12	6	1	4	1		0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	221	Total         O           226         226	0	5
5	В	188	Total O 190 190	0	2
5	С	189	Total O 189 189	0	0
5	D	193	Total O 196 196	0	3
5	Е	202	Total         O           206         206	0	6
5	F	175	Total O 179 179	0	4
5	G	116	Total O 118 118	0	2
5	Н	96	Total O 99 99	0	4
5	Ι	90	Total         O           90         90	0	0
5	J	58	Total         O           58         58	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: Peptidyl-prolyl cis-trans isomerase









## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	88.43Å 156.53Å 90.53Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $117.18^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{Posolution} \left( \overset{\circ}{\mathbf{A}} \right)$	29.97 - 1.88	Depositor
Resolution (A)	29.97 - 1.88	EDS
% Data completeness	98.9 (29.97-1.88)	Depositor
(in resolution range)	99.0 (29.97-1.88)	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	0.09	Depositor
$< I/\sigma(I) > 1$	$2.88 (at 1.88 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
P. P.	0.173 , $0.212$	Depositor
$n, n_{free}$	0.183 , $0.218$	DCC
$R_{free}$ test set	9021 reflections $(5.14\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	27.3	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , $41.5$	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18400	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 3.58% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: CL, MES, 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).

Mal	Chain	Bond	lengths	B	ond angles
INIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.66	0/1705	0.78	2/2296~(0.1%)
1	В	0.65	0/1715	0.78	2/2309~(0.1%)
1	С	0.63	0/1703	0.78	1/2295~(0.0%)
1	D	0.65	0/1714	0.76	1/2307~(0.0%)
1	Е	0.66	0/1721	0.76	0/2319
1	F	0.64	0/1722	0.75	0/2319
1	G	0.64	0/1695	0.76	2/2284~(0.1%)
1	Н	0.65	0/1706	0.76	1/2298~(0.0%)
1	Ι	0.66	0/1695	0.76	2/2284~(0.1%)
1	J	0.65	0/1695	0.72	1/2284~(0.0%)
All	All	0.65	0/17071	0.76	12/22995~(0.1%)

There are no bond length outliers.

All	(12)	$\operatorname{bond}$	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	231	MSE	CG-SE-CE	7.86	116.19	98.90
1	А	231	MSE	CG-SE-CE	7.80	116.06	98.90
1	Ι	231	MSE	CG-SE-CE	6.85	113.96	98.90
1	В	231	MSE	CG-SE-CE	6.84	113.95	98.90
1	G	60	MSE	CG-SE-CE	6.12	112.36	98.90
1	G	231	MSE	CG-SE-CE	6.04	112.18	98.90
1	А	60	MSE	CG-SE-CE	5.60	111.23	98.90
1	D	60	MSE	CG-SE-CE	5.55	111.10	98.90
1	Ι	60	MSE	CG-SE-CE	5.43	110.85	98.90
1	J	231	MSE	CG-SE-CE	5.24	110.44	98.90
1	В	170	MSE	CG-SE-CE	5.08	110.07	98.90
1	Н	231	MSE	CG-SE-CE	5.01	109.92	98.90

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	А	1672	0	1634	4	0
1	В	1682	0	1650	9	0
1	С	1670	0	1636	7	0
1	D	1681	0	1646	2	0
1	Е	1688	0	1648	9	0
1	F	1689	0	1650	12	0
1	G	1662	0	1626	8	0
1	Н	1673	0	1638	6	0
1	Ι	1662	0	1626	6	0
1	J	1662	0	1626	5	0
2	А	3	0	0	0	0
2	В	2	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	G	1	0	0	0	0
3	А	4	0	6	0	0
4	С	24	0	26	2	0
4	D	12	0	13	0	0
4	Е	12	0	13	0	0
4	F	24	0	26	5	0
4	Н	12	0	13	0	0
4	J	12	0	13	1	0
5	А	226	0	0	0	0
5	В	190	0	0	0	0
5	С	189	0	0	1	0
5	D	196	0	0	1	0
5	Е	206	0	0	0	0
5	F	179	0	0	2	0
5	G	118	0	0	1	0
5	Н	99	0	0	0	0
5	Ι	90	0	0	1	0
5	J	58	0	0	1	0
All	All	18400	0	16490	67	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 2.

All (67) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:H:163:ASN:HD22	1:H:186:ASN:HD21	1.24	0.86
1:H:149:LYS:HE2	1:H:149:LYS:H	1.46	0.79
1:F:168:LEU:HD11	1:F:183:PHE:CD2	2.29	0.66
1:E:168[A]:LEU:HD11	1:E:183:PHE:CD2	2.31	0.65
1:E:87:ILE:HD13	1:E:168[B]:LEU:HD21	1.79	0.65
1:F:269:ASN:O	4:F:301:MES:H62	1.97	0.65
1:F:269:ASN:O	4:F:301:MES:C6	2.49	0.61
1:H:168:LEU:HD11	1:H:183:PHE:CD1	2.40	0.56
1:J:114:THR:HG22	1:J:253:THR:HG22	1.87	0.56
1:H:242:LYS:HD2	1:H:246:ASP:HA	1.86	0.56
1:B:75:GLU:OE1	1:B:86[B]:ARG:NE	2.39	0.56
1:D:190:THR:HG23	5:D:534:HOH:O	2.05	0.55
1:D:242:LYS:HD2	1:D:246:ASP:HA	1.89	0.55
1:B:75:GLU:OE1	1:B:86[B]:ARG:CZ	2.54	0.55
1:B:270:LEU:HD21	1:I:221:HIS:CE1	2.41	0.54
1:B:168:LEU:HD11	1:B:183:PHE:CD2	2.42	0.54
1:E:168[A]:LEU:HG	1:E:224:PHE:CZ	2.44	0.52
1:F:195:LYS:O	1:F:196:LEU:HD23	2.10	0.52
1:B:75:GLU:OE1	1:B:86[B]:ARG:NH2	2.42	0.52
1:B:129:PRO:HB3	1:G:143:LYS:HE3	1.91	0.52
1:E:242:LYS:HD2	1:E:246:ASP:HA	1.90	0.52
1:C:269:ASN:O	4:C:301:MES:H51	2.10	0.51
1:E:271:TYR:O	1:E:272:PHE:HB2	2.11	0.50
1:C:125:GLN:HB3	5:C:509:HOH:O	2.12	0.49
1:B:242:LYS:HD2	1:B:246:ASP:HA	1.94	0.48
1:H:149:LYS:HE2	1:H:149:LYS:N	2.21	0.48
1:F:263:TYR:OH	4:F:301:MES:H31	2.13	0.48
1:A:168:LEU:HD11	1:A:183:PHE:CD2	2.49	0.47
1:J:110:TYR:HA	1:J:113:ILE:HD12	1.97	0.47
1:A:87:ILE:HG21	1:A:168:LEU:HD22	1.96	0.47
1:I:162:TYR:CE1	1:I:205:ILE:HG13	2.50	0.46
1:C:168:LEU:HD11	1:C:183:PHE:CD1	2.51	0.46
1:G:123:MSE:SE	1:G:125:GLN:CG	3.14	0.46
1:E:244:GLU:H	1:E:244:GLU:CD	2.18	0.46
1:F:168:LEU:CD1	1:F:183:PHE:CD2	2.99	0.46
1:A:242:LYS:HD2	1:A:246:ASP:HA	1.98	0.46
1:I:262:ASP:OD1	1:I:263:TYR:N	2.47	0.45



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:203:GLN:O	1:A:207:GLU:HG2	2.18	0.44
1:E:63:PRO:HB2	1:E:90:PHE:CE1	2.52	0.44
1:G:250:THR:HG23	5:G:483:HOH:O	2.18	0.44
1:F:171:ALA:O	1:F:221:HIS:CE1	2.71	0.44
1:F:145:LYS:NZ	5:F:404:HOH:O	2.48	0.43
4:F:301:MES:H32	5:F:472:HOH:O	2.18	0.43
1:G:63:PRO:HB2	1:G:90:PHE:CE1	2.53	0.43
1:C:123:MSE:HE1	1:C:125:GLN:HG3	2.01	0.43
1:H:198:THR:HG23	1:H:206:ILE:HD13	2.01	0.42
1:G:123:MSE:SE	1:G:125:GLN:HG3	2.68	0.42
1:G:172:ASN:HB2	1:G:178:THR:OG1	2.19	0.42
1:C:242:LYS:HD2	1:C:246:ASP:HA	2.02	0.42
1:I:172:ASN:HB2	1:I:178:THR:OG1	2.20	0.42
1:J:125:GLN:HB2	5:J:435:HOH:O	2.20	0.42
1:F:137[A]:GLN:OE1	1:F:141:HIS:CE1	2.73	0.41
1:G:168:LEU:HD11	1:G:183:PHE:CD2	2.54	0.41
1:I:87:ILE:HD13	1:I:168:LEU:HD21	2.02	0.41
1:F:197:PRO:HG2	1:F:200:LYS:CG	2.50	0.41
1:E:87:ILE:HG21	1:E:168[A]:LEU:HD22	2.03	0.41
1:B:171:ALA:O	1:B:221:HIS:ND1	2.54	0.41
1:C:267:SER:O	4:C:301:MES:H61	2.20	0.41
1:I:190:THR:HG23	5:I:330:HOH:O	2.20	0.41
1:J:74:ALA:HB3	1:J:89:LEU:HB2	2.02	0.41
1:E:110:TYR:HA	1:E:113:ILE:HD12	2.02	0.41
1:J:267:SER:HB3	4:J:301:MES:H71	2.03	0.41
1:F:171:ALA:O	1:F:221:HIS:ND1	2.55	0.40
1:C:123:MSE:SE	1:C:125:GLN:HG3	2.71	0.40
1:F:263:TYR:OH	4:F:301:MES:C3	2.69	0.40
1:B:110:TYR:HA	1:B:113:ILE:HD12	2.02	0.40
1:G:244:GLU:HA	1:G:244:GLU:OE1	2.20	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.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	212/214~(99%)	204~(96%)	8 (4%)	0	100	100
1	В	213/214~(100%)	204 (96%)	9~(4%)	0	100	100
1	С	212/214~(99%)	203~(96%)	9 (4%)	0	100	100
1	D	213/214~(100%)	206~(97%)	7(3%)	0	100	100
1	Е	214/214~(100%)	205~(96%)	9 (4%)	0	100	100
1	F	214/214~(100%)	207~(97%)	7 (3%)	0	100	100
1	G	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
1	Н	212/214~(99%)	201 (95%)	11 (5%)	0	100	100
1	Ι	211/214 (99%)	203~(96%)	8 (4%)	0	100	100
1	J	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
All	All	2123/2140 (99%)	2032 (96%)	91 (4%)	0	100	100

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	182/178~(102%)	180~(99%)	2(1%)	73	70
1	В	183/178~(103%)	181~(99%)	2(1%)	73	70
1	С	182/178~(102%)	181 (100%)	1 (0%)	88	88
1	D	183/178~(103%)	182 (100%)	1 (0%)	88	88
1	Ε	184/178~(103%)	182~(99%)	2(1%)	73	70
1	F	184/178~(103%)	183 (100%)	1 (0%)	88	88
1	G	181/178~(102%)	179~(99%)	2(1%)	73	70
1	Н	182/178~(102%)	180 (99%)	2 (1%)	73	70
1	Ι	181/178~(102%)	180 (99%)	1 (1%)	86	86



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	J	181/178~(102%)	180~(99%)	1 (1%)	86	86
All	All	1823/1780~(102%)	1808~(99%)	15 (1%)	81	80

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

Mol	Chain	Res	Type
1	А	123	MSE
1	А	158	THR
1	В	123	MSE
1	В	158	THR
1	С	123	MSE
1	D	123	MSE
1	Е	123	MSE
1	Е	158	THR
1	F	123	MSE
1	G	123	MSE
1	G	158	THR
1	Н	123	MSE
1	Н	149	LYS
1	Ι	123	MSE
1	J	123	MSE

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

Mol	Chain	Res	Type
1	Н	163	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 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
4	MES	Е	302	-	12,12,12	0.74	0	$14,\!16,\!16$	0.42	0
4	MES	С	302	-	12,12,12	0.74	0	8,16,16	0.22	0
4	MES	С	301	-	12,12,12	0.70	0	$14,\!16,\!16$	0.42	0
4	MES	D	302	-	12,12,12	0.73	0	14,16,16	0.44	0
3	EDO	А	303	-	3,3,3	0.09	0	2,2,2	0.22	0
4	MES	Н	301	-	12,12,12	0.75	0	14,16,16	0.45	0
4	MES	F	302	-	12,12,12	0.73	0	14,16,16	0.36	0
4	MES	F	301	-	12,12,12	0.72	0	14,16,16	0.47	0
4	MES	J	301	-	12,12,12	0.76	0	14,16,16	0.35	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
4	MES	Е	302	-	-	3/6/14/14	0/1/1/1
4	MES	С	301	-	-	2/6/14/14	0/1/1/1
4	MES	D	302	-	-	0/6/14/14	0/1/1/1
3	EDO	А	303	-	-	1/1/1/1	-
4	MES	Н	301	-	-	1/6/14/14	0/1/1/1
4	MES	F	302	-	-	4/6/14/14	0/1/1/1
4	MES	F	301	-	-	3/6/14/14	0/1/1/1
4	MES	J	301	-	_	3/6/14/14	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	Е	302	MES	N4-C7-C8-S
4	F	301	MES	C7-C8-S-O2S
4	F	301	MES	C7-C8-S-O3S
4	J	301	MES	C7-C8-S-O2S
4	F	302	MES	C7-C8-S-O3S
4	С	301	MES	C8-C7-N4-C5
4	Е	302	MES	C8-C7-N4-C3
4	Е	302	MES	C8-C7-N4-C5
4	J	301	MES	C7-C8-S-O3S
4	Н	301	MES	C7-C8-S-O3S
4	F	301	MES	C7-C8-S-O1S
4	F	302	MES	C7-C8-S-O1S
4	F	302	MES	C7-C8-S-O2S
4	J	301	MES	C7-C8-S-O1S
3	А	303	EDO	O1-C1-C2-O2
4	С	301	MES	C8-C7-N4-C3
4	F	302	MES	N4-C7-C8-S

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	301	MES	2	0
4	F	301	MES	5	0
4	J	301	MES	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,  $95^{th}$  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	$<$ <b>RSRZ</b> $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	210/214~(98%)	-0.26	0 100 100	17, 25, 41, 74	0
1	В	209/214~(97%)	-0.32	2 (0%) 82 83	18, 26, 47, 77	0
1	С	209/214~(97%)	-0.16	7 (3%) 46 47	20, 28, 47, 68	0
1	D	210/214~(98%)	-0.24	4 (1%) 66 68	21, 30, 48, 82	0
1	Е	209/214~(97%)	-0.20	5 (2%) 59 60	18, 29, 50, 66	0
1	F	209/214~(97%)	-0.14	2 (0%) 82 83	21, 31, 50, 84	0
1	G	209/214~(97%)	0.04	10 (4%) 30 32	24,  35,  67,  81	0
1	Н	209/214~(97%)	0.13	13 (6%) 20 22	28, 38, 61, 77	0
1	Ι	209/214~(97%)	0.21	9 (4%) 35 36	26, 41, 63, 91	0
1	J	209/214~(97%)	0.33	14 (6%) 17 19	30, 47, 72, 86	0
All	All	2092/2140~(97%)	-0.06	66 (3%) 47 49	17, 33, 60, 91	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	195	LYS	5.9
1	G	198	THR	4.7
1	J	272	PHE	4.6
1	В	272	PHE	4.6
1	С	198	THR	4.6
1	Ι	61	ASN	4.2
1	G	200	LYS	4.1
1	Ι	272	PHE	4.1
1	G	272	PHE	3.6
1	Н	61	ASN	3.5
1	Н	198	THR	3.5
1	Н	195	LYS	3.4
1	Ι	62	PHE	3.4



Mol	Chain	Res	Type	RSRZ
1	Н	272	PHE	3.4
1	J	244	GLU	3.3
1	Н	244	GLU	3.3
1	Ι	65	LEU	3.1
1	G	196	LEU	3.0
1	J	200	LYS	3.0
1	Ι	149	LYS	3.0
1	D	198	THR	3.0
1	Н	183	PHE	2.9
1	Н	199	SER	2.9
1	G	194	SER	2.9
1	С	185	ILE	2.9
1	Ι	160	TYR	2.9
1	J	199	SER	2.8
1	Ι	145	LYS	2.7
1	С	199	SER	2.7
1	D	273	GLN	2.7
1	G	244	GLU	2.7
1	J	61	ASN	2.7
1	J	149	LYS	2.7
1	J	201	TYR	2.7
1	Н	271	TYR	2.6
1	J	192	THR	2.6
1	J	168	LEU	2.6
1	С	197	PRO	2.5
1	J	71	GLU	2.5
1	С	168	LEU	2.5
1	J	198	THR	2.5
1	J	203	GLN	2.4
1	Н	168	LEU	2.4
1	G	241	GLU	2.4
1	С	167	ALA	2.3
1	E	167	ALA	2.3
1	E	168[A]	LEU	2.3
1	Ι	168	LEU	2.3
1	Н	184	PHE	2.2
1	С	200	LYS	2.2
1	J	194	SER	2.2
1	G	250	THR	2.2
1	F	227	VAL	2.2
1	D	200	LYS	2.2
1	G	199	SER	2.2



Mol	Chain	Res	Type	RSRZ
1	Ε	249	THR	2.2
1	Н	169	ALA	2.2
1	Н	146	THR	2.1
1	Н	194	SER	2.1
1	J	197	PRO	2.1
1	D	199	SER	2.1
1	G	197	PRO	2.1
1	Е	244	GLU	2.1
1	Ε	241	GLU	2.0
1	В	271	TYR	2.0
1	Ι	169	ALA	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,  $95^{th}$  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
3	EDO	A	303	4/4	0.68	0.21	$56,\!57,\!57,\!59$	0
4	MES	F	302	12/12	0.84	0.17	74,90,105,111	0
4	MES	E	302	12/12	0.86	0.15	59,66,77,86	0
4	MES	С	301	12/12	0.86	0.22	54,60,68,71	0
4	MES	F	301	12/12	0.87	0.27	63,66,83,90	0
4	MES	Н	301	12/12	0.89	0.17	58,66,69,70	0
4	MES	J	301	12/12	0.89	0.16	65,71,73,75	0
2	CL	А	302[B]	1/1	0.90	0.14	49,49,49,49	1
2	CL	А	302[A]	1/1	0.90	0.14	48,48,48,48	1
4	MES	С	302	12/12	0.91	0.20	72,97,124,127	0
4	MES	D	302	12/12	0.92	0.20	53,58,63,67	0
2	CL	D	301	1/1	0.94	0.07	53,53,53,53	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	CL	Е	301	1/1	0.95	0.11	44,44,44,44	0
2	CL	G	301	1/1	0.96	0.05	40,40,40,40	0
2	CL	В	302	1/1	0.96	0.12	$51,\!51,\!51,\!51$	0
2	CL	В	301	1/1	0.98	0.07	47,47,47,47	0
2	CL	А	301	1/1	0.98	0.09	36,36,36,36	0

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## 6.5 Other polymers (i)

There are no such residues in this entry.

