



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:06 PM EST

PDB ID : 4X9D  
Title : High-resolution structure of Hfq from *Methanococcus jannaschii* in complex with UMP  
Authors : Nikulin, A.D.; Tishchenko, S.V.; Nikonova, E.Y.; Murina, V.N.; Mihailina, A.O.; Lekontseva, N.V.  
Deposited on : 2014-12-11  
Resolution : 1.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

**i**

## X-RAY DIFFRACTION

A.



$R_{free}$
Clashscore
Ramachandran outliers
Sidechain outliers
RSRZ outliers

1	A	71
1	B	71
1	C	71
1	D	71
1	E	71
1	F	71

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PGE	E	102	-	-	-	X
3	SO4	A	102	-	-	-	X
3	SO4	F	102	-	-	-	X
5	U5P	A	104	-	-	-	X
5	U5P	B	104	-	-	-	X
5	U5P	C	104	-	-	-	X
5	U5P	D	101	-	-	-	X
5	U5P	E	104	-	-	X	X
5	U5P	F	104	-	-	-	X
7	PG4	C	101	-	-	-	X
9	PEG	F	101	-	-	-	X

## 2 Entry composition [i](#)

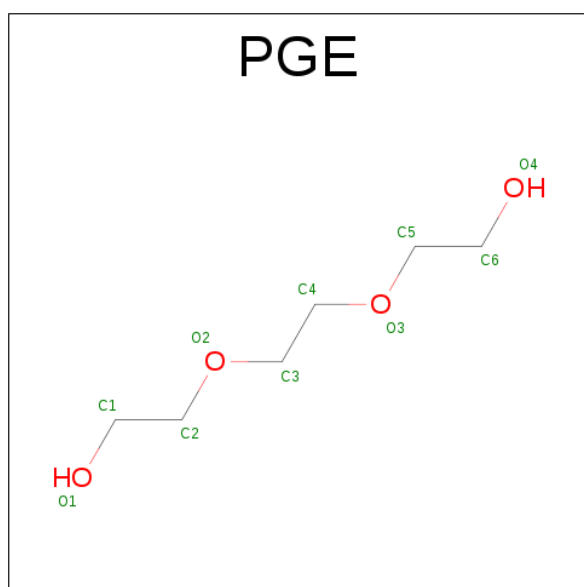
There are 10 unique types of molecules in this entry. The entry contains 3322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uncharacterized protein MJ1435.

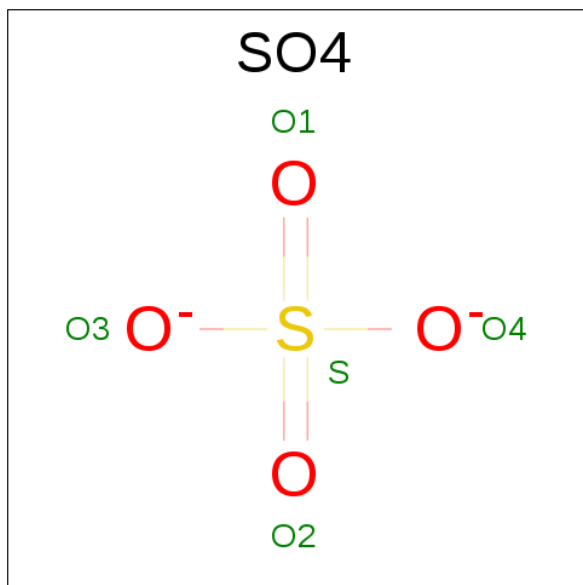
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	56	Total	C	N	O	S	0	5	0
			495	321	85	88	1			
1	B	58	Total	C	N	O	S	0	0	0
			478	309	82	86	1			
1	C	56	Total	C	N	O	S	0	0	0
			463	298	80	84	1			
1	D	59	Total	C	N	O	S	0	2	0
			499	324	87	87	1			
1	E	56	Total	C	N	O	S	0	2	0
			476	306	83	86	1			
1	F	57	Total	C	N	O	S	0	0	0
			470	303	81	85	1			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

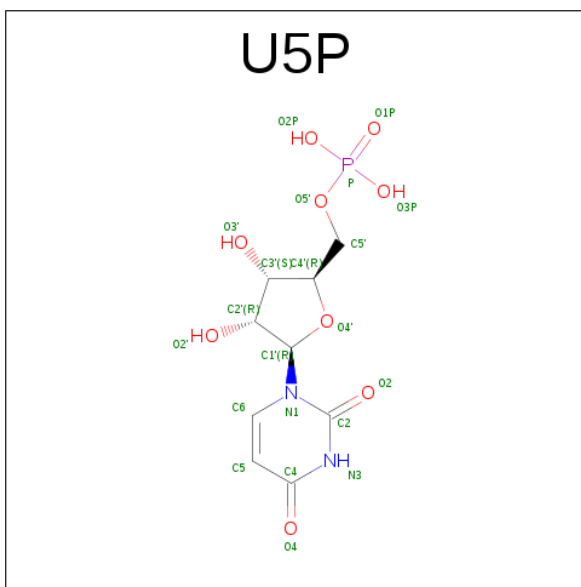


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

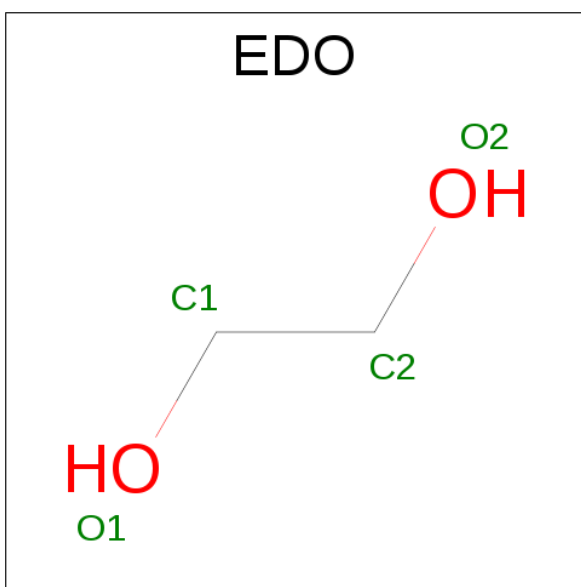
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		
4	A	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>2</sub>O<sub>9</sub>P).



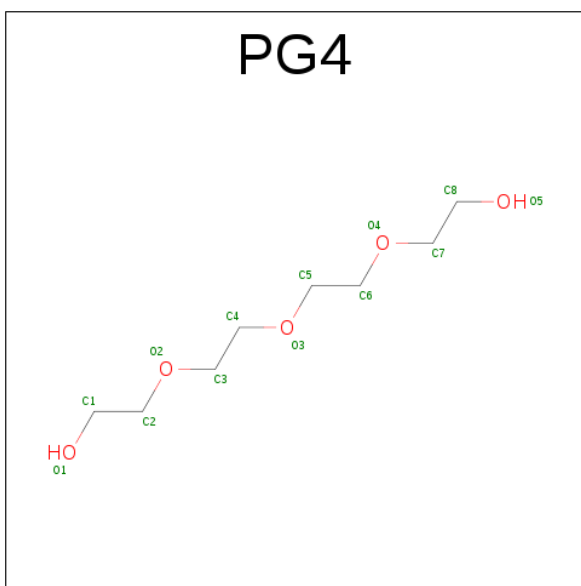
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
5	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
5	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
5	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
5	E	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
5	F	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).

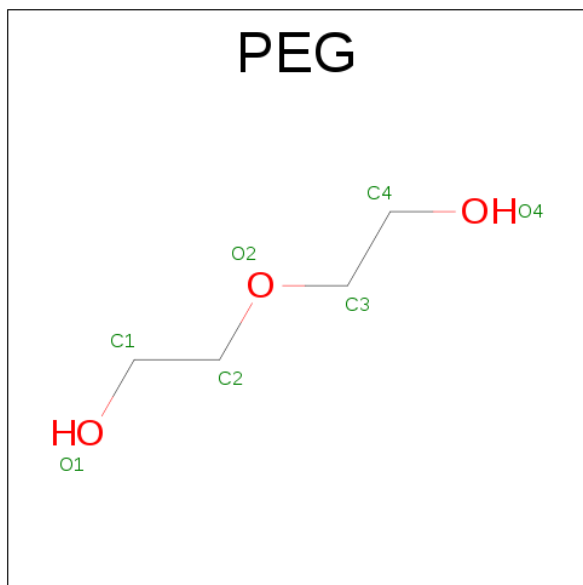


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			13	8	5		
7	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Cl 1 1	0	0
8	E	1	Total Cl 1 1	0	0

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	F	1	Total C O 7 4 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	28	Total O 28 28	0	0
10	B	39	Total O 39 39	0	0
10	C	41	Total O 41 41	0	0
10	D	38	Total O 38 38	0	0
10	E	50	Total O 50 50	0	0
10	F	45	Total O 45 45	0	0



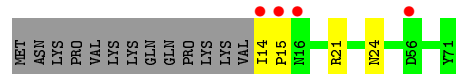
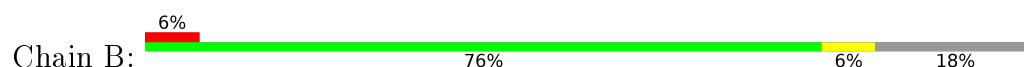
### 3 Residue-property plots [i](#)

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.

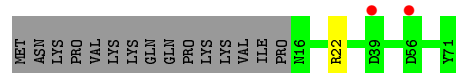
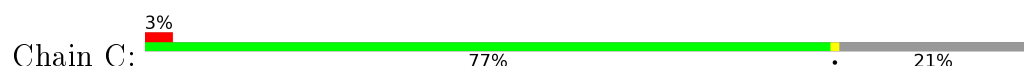
- Molecule 1: Uncharacterized protein MJ1435



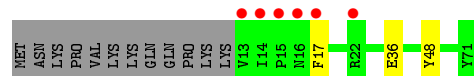
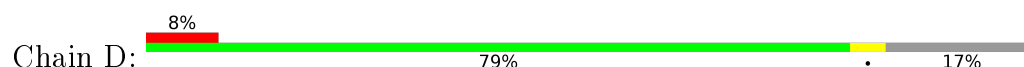
- Molecule 1: Uncharacterized protein MJ1435



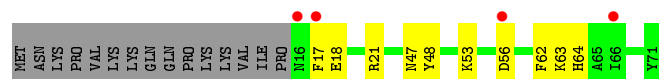
- Molecule 1: Uncharacterized protein MJ1435



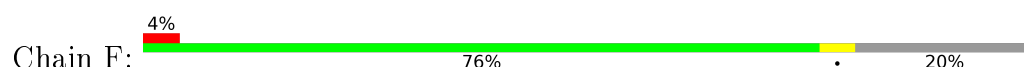
- Molecule 1: Uncharacterized protein MJ1435

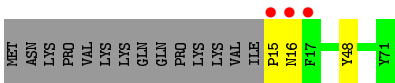


- Molecule 1: Uncharacterized protein MJ1435



- Molecule 1: Uncharacterized protein MJ1435





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.74Å 66.87Å 109.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.70 – 1.50 43.70 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.70-1.50) 99.5 (43.70-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.174 , 0.203 0.175 , 0.203	Depositor DCC
$R_{free}$ test set	3393 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3322	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: PGE, CL, NA, EDO, U5P, PG4, SO4, PEG

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	0.34	0/517	0.56	0/689
1	B	0.34	0/486	0.54	0/652
1	C	0.34	0/470	0.53	0/629
1	D	0.35	0/513	0.54	0/687
1	E	0.38	0/489	0.58	0/654
1	F	0.35	0/478	0.56	0/640
All	All	0.35	0/2953	0.55	0/3951

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	495	0	519	5	0
1	B	478	0	486	2	0
1	C	463	0	468	1	0
1	D	499	0	521	5	0
1	E	476	0	485	14	0
1	F	470	0	476	3	0
2	A	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	10	0	14	0	0
3	A	5	0	0	0	0
3	F	5	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	A	21	0	11	2	0
5	B	21	0	11	2	0
5	C	21	0	11	1	0
5	D	21	0	11	1	0
5	E	21	0	11	10	0
5	F	21	0	11	5	0
6	B	4	0	6	0	0
7	C	13	0	18	1	0
7	E	13	0	18	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
9	F	7	0	10	0	0
10	A	28	0	0	0	0
10	B	39	0	0	1	0
10	C	41	0	0	1	0
10	D	38	0	0	2	1
10	E	50	0	0	0	0
10	F	45	0	0	1	1
All	All	3322	0	3101	35	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 6.

All (35) 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:E:64:HIS:N	5:E:104:U5P:O3P	2.02	0.91
5:F:104:U5P:O2P	10:F:245:HOH:O	1.89	0.88
1:A:21[B]:ARG:NH2	1:A:47:ASN:OD1	2.11	0.83
1:E:48:TYR:HD1	5:E:104:U5P:H5'1	1.49	0.76
1:D:36:GLU:OE1	10:D:201:HOH:O	2.03	0.76
1:C:22:ARG:HD2	7:C:101:PG4:H51	1.69	0.73
5:B:104:U5P:O1P	10:B:239:HOH:O	2.08	0.71
1:E:63:LYS:N	5:E:104:U5P:O3P	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:HIS:ND1	5:E:104:U5P:O2P	2.25	0.68
5:C:104:U5P:O2	10:C:237:HOH:O	2.12	0.67
1:D:48:TYR:CG	5:E:104:U5P:H2'	2.33	0.63
1:E:48:TYR:CD1	5:E:104:U5P:H5'1	2.34	0.61
1:A:29[B]:LYS:HE2	1:A:37:VAL:HG11	1.82	0.61
1:D:48:TYR:CD1	5:E:104:U5P:H2'	2.37	0.59
5:E:104:U5P:O1P	5:F:104:U5P:O2'	2.15	0.58
1:F:48:TYR:HD1	5:F:104:U5P:H5'1	1.69	0.57
1:E:18:GLU:HG3	1:E:21[B]:ARG:HG3	1.92	0.52
1:E:48:TYR:HB3	5:E:104:U5P:O1P	2.11	0.51
1:B:21:ARG:O	1:B:24:ASN:HB2	2.12	0.50
1:D:17:PHE:HA	10:D:238:HOH:O	2.11	0.50
1:A:27[B]:LYS:HD2	1:A:40:ALA:O	2.12	0.50
1:A:53:LYS:HD2	1:A:57:ARG:O	2.12	0.49
1:E:18:GLU:H	1:E:21[B]:ARG:NH2	2.16	0.44
5:A:104:U5P:H6	5:A:104:U5P:O5'	2.19	0.43
1:E:21[A]:ARG:NH1	1:E:47:ASN:OD1	2.52	0.42
1:E:48:TYR:CD1	5:F:104:U5P:H2'	2.54	0.42
1:E:62:PHE:HB3	5:E:104:U5P:O3P	2.19	0.42
1:E:17:PHE:HA	1:E:21[B]:ARG:HH22	1.84	0.42
1:D:48:TYR:CE1	5:D:101:U5P:H6	2.54	0.42
1:E:53:LYS:HE3	1:E:56:ASP:HA	2.03	0.41
1:B:14:ILE:HB	1:B:15:PRO:HD2	2.01	0.41
1:E:47:ASN:OD1	1:F:15:PRO:HG3	2.21	0.41
1:F:15:PRO:HA	1:F:16:ASN:HA	1.64	0.41
5:A:104:U5P:HO3'	5:F:104:U5P:P	2.44	0.40
1:A:48:TYR:CD1	5:B:104:U5P:H2'	2.56	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)
10:D:203:HOH:O	10:F:210:HOH:O[1_455]	2.18	0.02

## 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	59/71 (83%)	59 (100%)	0	0	100	100
1	B	56/71 (79%)	56 (100%)	0	0	100	100
1	C	54/71 (76%)	54 (100%)	0	0	100	100
1	D	59/71 (83%)	57 (97%)	2 (3%)	0	100	100
1	E	56/71 (79%)	56 (100%)	0	0	100	100
1	F	55/71 (78%)	54 (98%)	1 (2%)	0	100	100
All	All	339/426 (80%)	336 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	54/64 (84%)	54 (100%)	0	100	100
1	B	51/64 (80%)	51 (100%)	0	100	100
1	C	49/64 (77%)	49 (100%)	0	100	100
1	D	54/64 (84%)	54 (100%)	0	100	100
1	E	51/64 (80%)	51 (100%)	0	100	100
1	F	50/64 (78%)	50 (100%)	0	100	100
All	All	309/384 (80%)	309 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	D	16	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 7 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	PGE	A	101	-	9,9,9	0.41	0	8,8,8	0.34	0
3	SO4	A	102	-	4,4,4	0.24	0	6,6,6	0.13	0
5	U5P	A	104	4	18,22,22	1.10	1 (5%)	23,33,33	2.73	3 (13%)
6	EDO	B	101	-	3,3,3	0.45	0	2,2,2	0.42	0
5	U5P	B	104	4	18,22,22	1.16	1 (5%)	23,33,33	2.86	3 (13%)
7	PG4	C	101	-	12,12,12	0.48	0	11,11,11	0.39	0
5	U5P	C	104	4	18,22,22	1.11	1 (5%)	23,33,33	2.60	3 (13%)
5	U5P	D	101	4	18,22,22	1.11	1 (5%)	23,33,33	2.74	2 (8%)
7	PG4	E	101	-	12,12,12	0.44	0	11,11,11	0.41	0
2	PGE	E	102	-	9,9,9	0.40	0	8,8,8	0.55	0
5	U5P	E	104	-	18,22,22	1.47	4 (22%)	23,33,33	3.01	5 (21%)
9	PEG	F	101	-	6,6,6	0.46	0	5,5,5	0.37	0
3	SO4	F	102	-	4,4,4	0.26	0	6,6,6	0.09	0
5	U5P	F	104	-	18,22,22	1.17	1 (5%)	23,33,33	2.74	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral



centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	A	101	-	-	0/7/7/7	0/0/0/0
3	SO4	A	102	-	-	0/0/0/0	0/0/0/0
5	U5P	A	104	4	-	0/6/26/26	0/2/2/2
6	EDO	B	101	-	-	0/1/1/1	0/0/0/0
5	U5P	B	104	4	-	0/6/26/26	0/2/2/2
7	PG4	C	101	-	-	0/10/10/10	0/0/0/0
5	U5P	C	104	4	-	0/6/26/26	0/2/2/2
5	U5P	D	101	4	-	0/6/26/26	0/2/2/2
7	PG4	E	101	-	-	0/10/10/10	0/0/0/0
2	PGE	E	102	-	-	0/7/7/7	0/0/0/0
5	U5P	E	104	-	-	0/6/26/26	0/2/2/2
9	PEG	F	101	-	-	0/4/4/4	0/0/0/0
3	SO4	F	102	-	-	0/0/0/0	0/0/0/0
5	U5P	F	104	-	-	0/6/26/26	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	104	U5P	P-O3P	-2.95	1.44	1.54
5	E	104	U5P	P-O2P	-2.51	1.46	1.54
5	E	104	U5P	C6-N1	2.34	1.38	1.35
5	A	104	U5P	C4-N3	2.76	1.38	1.33
5	F	104	U5P	C4-N3	2.99	1.38	1.33
5	D	101	U5P	C4-N3	3.01	1.38	1.33
5	C	104	U5P	C4-N3	3.05	1.38	1.33
5	B	104	U5P	C4-N3	3.12	1.38	1.33
5	E	104	U5P	C4-N3	3.19	1.38	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	104	U5P	C5-C4-N3	-3.65	114.31	123.28
5	D	101	U5P	C5-C4-N3	-3.60	114.43	123.28
5	A	104	U5P	C5-C4-N3	-3.58	114.49	123.28
5	E	104	U5P	C5-C4-N3	-3.51	114.66	123.28
5	F	104	U5P	C5-C4-N3	-3.51	114.67	123.28
5	C	104	U5P	C5-C4-N3	-3.46	114.80	123.28
5	E	104	U5P	O2P-P-O5'	-2.60	99.13	106.72
5	F	104	U5P	O2P-P-O1P	2.33	118.22	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	104	U5P	O2P-P-O1P	2.60	119.10	110.63
5	A	104	U5P	O3P-P-O2P	2.83	117.84	107.44
5	B	104	U5P	O3P-P-O2P	2.96	118.31	107.44
5	E	104	U5P	O5'-P-O1P	2.96	114.53	107.08
5	E	104	U5P	O3P-P-O5'	3.38	116.59	106.72
5	C	104	U5P	C4-N3-C2	11.44	126.26	114.21
5	A	104	U5P	C4-N3-C2	11.97	126.82	114.21
5	F	104	U5P	C4-N3-C2	12.10	126.96	114.21
5	D	101	U5P	C4-N3-C2	12.24	127.10	114.21
5	E	104	U5P	C4-N3-C2	12.48	127.36	114.21
5	B	104	U5P	C4-N3-C2	12.63	127.52	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	104	U5P	2	0
5	B	104	U5P	2	0
7	C	101	PG4	1	0
5	C	104	U5P	1	0
5	D	101	U5P	1	0
5	E	104	U5P	10	0
5	F	104	U5P	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	56/71 (78%)	0.21	4 (7%)	19 19	11, 18, 35, 53	0
1	B	58/71 (81%)	0.33	4 (6%)	20 20	11, 19, 39, 47	0
1	C	56/71 (78%)	0.05	2 (3%)	46 49	12, 17, 30, 41	0
1	D	59/71 (83%)	0.46	6 (10%)	9 8	11, 18, 40, 47	0
1	E	56/71 (78%)	0.26	4 (7%)	19 19	10, 14, 29, 52	0
1	F	57/71 (80%)	0.20	3 (5%)	30 31	10, 15, 33, 51	0
All	All	342/426 (80%)	0.25	23 (6%)	21 21	10, 17, 36, 53	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	15	PRO	9.2
1	E	16	ASN	6.9
1	D	17	PHE	6.6
1	A	17	PHE	6.1
1	B	14	ILE	6.0
1	D	13	VAL	5.2
1	A	16	ASN	4.5
1	F	16	ASN	4.5
1	C	56	ASP	4.2
1	D	15	PRO	4.2
1	D	16	ASN	4.1
1	B	15	PRO	4.0
1	A	56	ASP	3.9
1	D	14	ILE	3.1
1	A	21[A]	ARG	3.0
1	E	17	PHE	2.8
1	D	22	ARG	2.6
1	B	56	ASP	2.5
1	C	39	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	56	ASP	2.4
1	B	16	ASN	2.3
1	F	17	PHE	2.2
1	E	66	ILE	2.1

## 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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	U5P	C	104	21/21	0.38	0.48	25.90	25,31,41,48	21
5	U5P	E	104	21/21	0.77	0.36	10.88	13,30,35,39	21
7	PG4	C	101	13/13	0.72	0.23	10.80	35,38,45,45	0
5	U5P	B	104	21/21	0.77	0.30	10.10	32,38,45,58	4
5	U5P	F	104	21/21	0.60	0.28	7.13	20,29,47,58	21
5	U5P	A	104	21/21	0.84	0.19	5.80	23,32,43,51	17
9	PEG	F	101	7/7	0.76	0.20	3.81	32,35,43,48	0
2	PGE	E	102	10/10	0.88	0.12	3.81	19,24,31,39	0
3	SO4	A	102	5/5	0.76	0.30	3.65	36,38,46,46	5
3	SO4	F	102	5/5	0.89	0.24	2.59	32,38,43,46	5
5	U5P	D	101	21/21	0.74	0.27	2.53	28,34,38,44	17
7	PG4	E	101	13/13	0.88	0.12	1.67	18,28,33,39	0
6	EDO	B	101	4/4	0.82	0.18	1.14	35,36,43,49	0
2	PGE	A	101	10/10	0.88	0.11	-0.14	26,33,39,39	0
4	NA	B	102	1/1	0.97	0.12	-	29,29,29,29	0
8	CL	E	103	1/1	0.91	0.06	-	57,57,57,57	0
4	NA	C	102	1/1	0.99	0.04	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	A	103	1/1	0.99	0.05	-	22,22,22,22	0
4	NA	F	103	1/1	0.98	0.05	-	21,21,21,21	0
8	CL	C	103	1/1	0.89	0.18	-	56,56,56,56	0
4	NA	B	103	1/1	1.00	0.08	-	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.