



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:21 PM GMT

PDB ID : 3QSY  
Title : Recognition of the methionylated initiator tRNA by the translation initiation factor 2 in Archaea  
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Deposited on : 2011-02-22  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

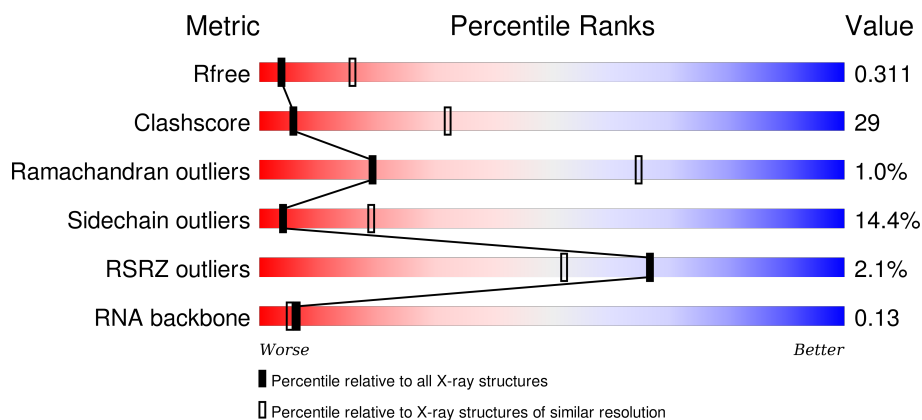
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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. 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	415	<div> <div>2%</div> <div>42%</div> <div>51%</div> <div>7%</div> </div>
2	B	89	<div> <div>3%</div> <div>52%</div> <div>37%</div> <div>11%</div> </div>
3	D	77	<div> <div>8%</div> <div>42%</div> <div>45%</div> <div>5%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5593 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 Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total	C	N	O	S	0	0	0
			3220	2063	549	595	13			

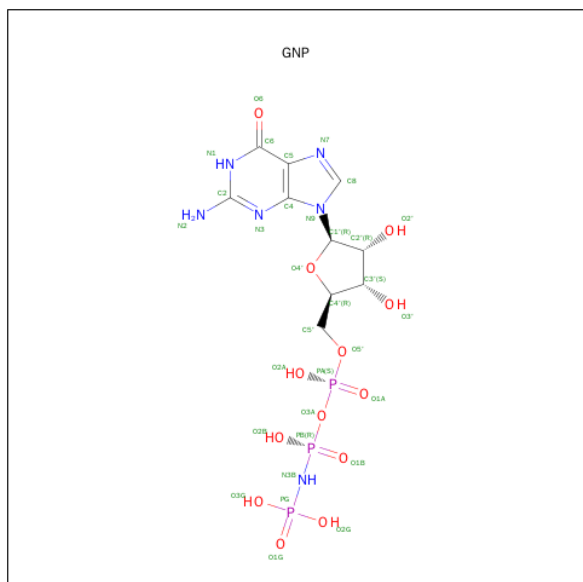
- Molecule 2 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	89	Total	C	N	O	S	0	0	0
			694	439	116	138	1			

- Molecule 3 is a RNA chain called tRNA.

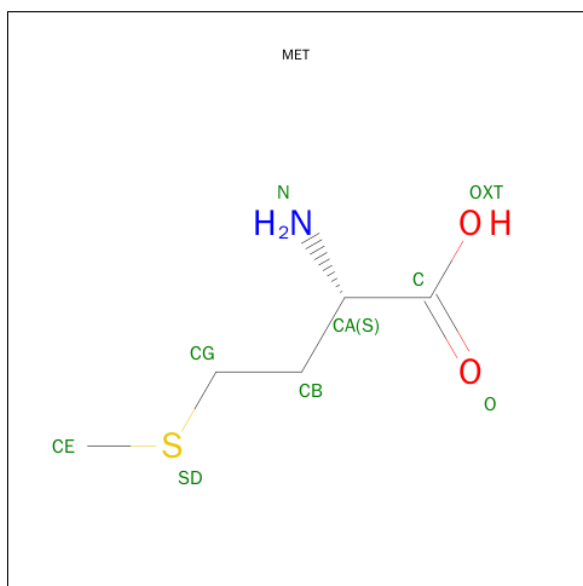
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula:  $C_{10}H_{17}N_6O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is METHIONINE (three-letter code: MET) (formula:  $C_5H_{11}NO_2S$ ).

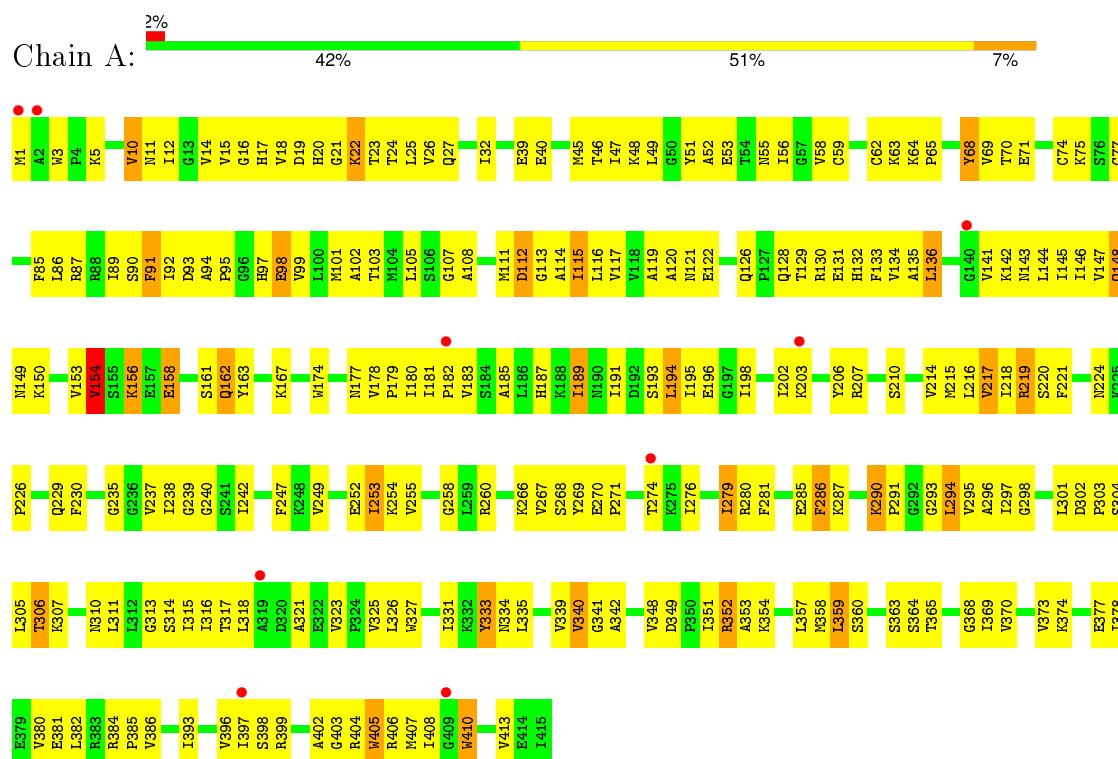


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

### 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 ( $\text{RSRZ} > 2$ ). 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: Translation initiation factor 2 subunit gamma



U60	C1
G61	G2
G62	C3
G63	G4
G64	G5
G65	G6
G66	G7
G67	G8
G68	G9
G69	G10
G70	A11
A71	G12
A72	C13
A73	G14
C74	G15
C75	C16
A76	C17
	U17A
	G18
	G19
	U20
	A21
	G22
	C23
	U24
	C25
	G26
	U27
	C28
	G29
	G30
	G31
	C32
	U33
	C34
	A35
	U36
	A37
	A38
	C39
	C40
	C41
	G42
	A43
	A44
	G45
	A46
	U47
	C48
	G49
	U50
	C51
	G52
	G53
	U54
	U55
	C56
	A57
	A58
	A59

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.68Å 93.68Å 220.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.95 – 3.20 14.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (14.95-3.20) 100.0 (14.95-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.97 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.278 , 0.302 0.293 , 0.311	Depositor DCC
$R_{free}$ test set	973 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtriage
Anisotropy	1.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.07 , 130.8	EDS
Estimated twinning fraction	0.500 for -h,-k,l 0.470 for -h,-k,l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18940 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5593	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GNP

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	0.36	0/3279	0.68	0/4440
2	B	0.32	0/699	0.63	0/942
3	D	0.54	0/1831	1.08	7/2853 (0.2%)
All	All	0.42	0/5809	0.84	7/8235 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	61	C	N1-C2-O2	5.65	122.29	118.90
3	D	68	C	N1-C2-O2	5.63	122.28	118.90
3	D	30	G	N3-C4-C5	-5.62	125.79	128.60
3	D	61	C	C5-C6-N1	5.42	123.71	121.00
3	D	30	G	N3-C4-N9	5.12	129.07	126.00

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	3220	0	3344	224	0
2	B	694	0	734	33	0
3	D	1639	0	836	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	32	0	13	6	0
5	D	8	0	8	5	0
All	All	5593	0	4935	302	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 29.

The worst 5 of 302 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:A:281:PHE:HB2	1:A:286:PHE:HB2	1.56	0.88
1:A:128:GLN:HA	1:A:131:GLU:HB3	1.56	0.85
1:A:130:ARG:HH22	1:A:340:VAL:HB	1.40	0.85
1:A:146:ILE:O	1:A:180:ILE:HA	1.75	0.85
1:A:99:VAL:HG11	3:D:71:C:H5'	1.59	0.84

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	413/415 (100%)	331 (80%)	77 (19%)	5 (1%)	16	60
2	B	87/89 (98%)	75 (86%)	12 (14%)	0	100	100
All	All	500/504 (99%)	406 (81%)	89 (18%)	5 (1%)	19	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	393	ILE

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Mol	Chain	Res	Type
1	A	154	VAL
1	A	10	VAL
1	A	279	ILE

### 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	Percentiles	
1	A	357/357 (100%)	311 (87%)	46 (13%)	5	24
2	B	80/80 (100%)	64 (80%)	16 (20%)	1	8
All	All	437/437 (100%)	375 (86%)	62 (14%)	4	19

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ARG
1	A	290	LYS
2	B	232	VAL
1	A	253	ILE
1	A	306	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	224	ASN
2	B	209	GLN
1	A	162	GLN
1	A	392	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	D	76/77 (98%)	52 (68%)	4 (5%)

5 of 52 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	D	2	G
3	D	3	C
3	D	6	G
3	D	8	U
3	D	9	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	D	23	C
3	D	40	C
3	D	44	A
3	D	74	C

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	GNP	A	501	-	28,34,34	1.94	5 (17%)	33,54,54	2.56	11 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	MET	D	77	3	6,7,8	0.31	0	4,7,9	0.90	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	GNP	A	501	-	-	0/12/38/38	0/3/3/3
5	MET	D	77	3	-	0/4/6/8	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	GNP	PB-O3A	-5.79	1.51	1.59
4	A	501	GNP	PB-O2B	-3.19	1.47	1.56
4	A	501	GNP	C8-N7	-2.08	1.30	1.34
4	A	501	GNP	C6-N1	3.43	1.39	1.33
4	A	501	GNP	PG-O1G	5.05	1.51	1.46

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	GNP	C5-C6-N1	-8.43	112.07	123.59
4	A	501	GNP	C4'-O4'-C1'	-5.12	104.09	109.72
4	A	501	GNP	O3G-PG-O1G	-3.76	103.48	113.49
4	A	501	GNP	PA-O3A-PB	-3.04	122.47	132.67
4	A	501	GNP	C2'-C1'-N9	-2.33	110.73	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	GNP	6	0
5	D	77	MET	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 [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	415/415 (100%)	-0.68	9 (2%)	65 50	42, 109, 331, 545	0
2	B	89/89 (100%)	-0.58	3 (3%)	49 34	41, 111, 284, 545	0
3	D	77/77 (100%)	-0.52	0	100 100	64, 113, 208, 345	0
All	All	581/581 (100%)	-0.64	12 (2%)	67 52	41, 110, 284, 545	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.9
1	A	319	ALA	3.8
2	B	183	ILE	3.5
1	A	182	PRO	2.8
1	A	274	THR	2.8

### 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( $\text{\AA}^2$ )	Q<0.9
5	MET	D	77	8/9	0.91	0.14	-0.41	30,37,111,127	0
4	GNP	A	501	32/32	0.94	0.10	-0.49	28,70,108,121	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.