



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:56 PM GMT

PDB ID : 4AZA  
Title : Improved eIF4E binding peptides by phage display guided design.  
Authors : Chew, W.Z.; Quah, S.T.; Verma, C.S.; Liu, Y.; Lane, D.P.; Brown, C.J.  
Deposited on : 2012-06-25  
Resolution : 2.16 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 (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

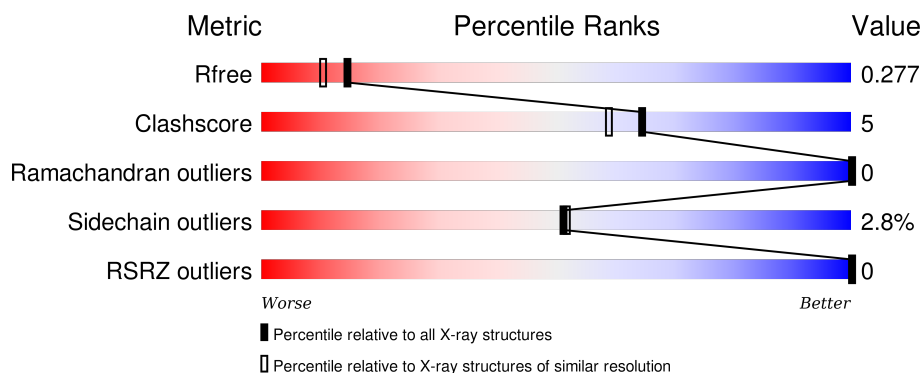
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.16 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	217	<div> <div>72%</div> <div>14%</div> <div>13%</div> </div>
1	C	217	<div> <div>78%</div> <div>7%</div> <div>14%</div> </div>
2	B	14	<div> <div>86%</div> <div>14%</div> </div>
2	D	14	<div> <div>93%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3604 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.

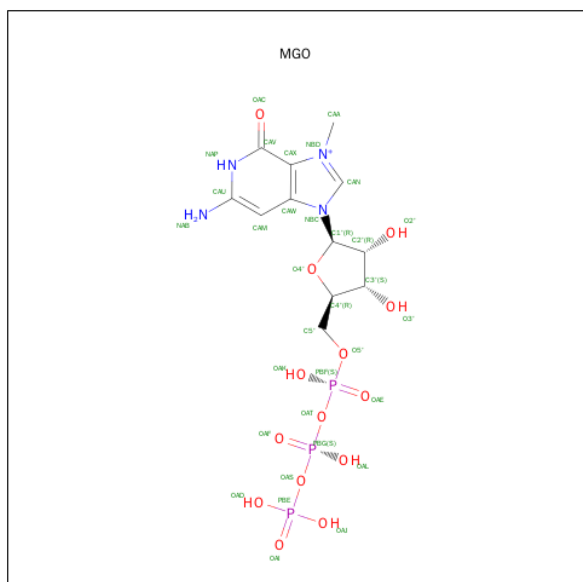
- Molecule 1 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1552	989	274	283	6			
1	C	186	Total	C	N	O	S	0	0	0
			1542	984	272	280	6			

- Molecule 2 is a protein called EIF4G1\_D5S PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	0	0	1
			113	75	21	17			
2	D	14	Total	C	N	O	0	0	1
			113	75	21	17			

- Molecule 3 is [[(2R,3S,4R,5R)-5-(6-AMINO-3-METHYL-4-OXO-5H-IMIDAZO[4,5-C]PYRIDIN-1-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL] PHOSPHONO HYDROGEN PHOSPHATE (three-letter code: MGO) (formula: C<sub>12</sub>H<sub>20</sub>N<sub>4</sub>O<sub>14</sub>P<sub>3</sub>).



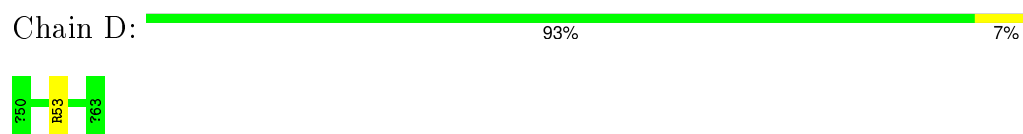
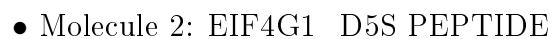
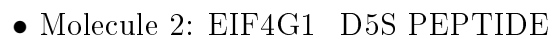
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			33	12	4	14	3		
3	C	1	Total	C	N	O	P	0	0
			33	12	4	14	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	7	Total	O	0	0
			7	7		
4	C	98	Total	O	0	0
			98	98		
4	D	3	Total	O	0	0
			3	3		



- Molecule 1: EUKARYOTIC TRANSLATION INITIATION FACTOR 4E



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.66 Å 38.17 Å 121.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.76 – 2.16 60.88 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.2 (121.76-2.16) 99.2 (60.88-2.16)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.16 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.233 , 0.279 0.233 , 0.277	Depositor DCC
$R_{free}$ test set	1542 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 9.7	EDS
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 30403 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: MGO, ACE, NH2

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	0.62	3/1591 (0.2%)	0.61	0/2150
1	C	0.60	2/1581 (0.1%)	0.57	0/2137
2	B	0.46	0/112	0.44	0/146
2	D	0.41	0/112	0.48	0/146
All	All	0.60	5/3396 (0.1%)	0.58	0/4579

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	TRP	CD2-CE2	5.51	1.48	1.41
1	A	102	TRP	CD2-CE2	5.41	1.47	1.41
1	C	166	TRP	CD2-CE2	5.06	1.47	1.41
1	A	130	TRP	CD2-CE2	5.04	1.47	1.41
1	C	102	TRP	CD2-CE2	5.03	1.47	1.41

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	1552	0	1515	22	0
1	C	1542	0	1507	12	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	113	0	118	2	0
2	D	113	0	118	1	0
3	A	33	0	16	1	0
3	C	33	0	16	0	0
4	A	110	0	0	6	0
4	B	7	0	0	0	0
4	C	98	0	0	6	1
4	D	3	0	0	0	0
All	All	3604	0	3290	34	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 5.

All (34) 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:177:THR:HG22	1:A:181:ARG:NH1	1.70	1.07
1:A:177:THR:HG22	1:A:181:ARG:HH12	1.38	0.87
1:A:177:THR:CG2	1:A:181:ARG:NH1	2.35	0.87
1:A:170:CYS:HB2	4:A:2085:HOH:O	1.82	0.79
1:A:143:ASP:HB2	4:A:2074:HOH:O	1.88	0.73
1:A:177:THR:CG2	1:A:181:ARG:HH12	2.00	0.70
1:C:143:ASP:HB2	4:C:2073:HOH:O	1.96	0.64
1:A:177:THR:HG21	4:A:2088:HOH:O	1.97	0.64
1:C:140:GLU:OE1	1:C:146:SER:HB2	1.98	0.63
1:A:47:PHE:HB2	1:A:63:ILE:HD11	1.82	0.62
1:A:140:GLU:OE1	1:A:146:SER:HB2	2.01	0.61
3:A:1218:MGO:HAM	4:A:2109:HOH:O	2.02	0.59
1:A:143:ASP:HA	2:B:53:ARG:CZ	2.36	0.56
1:A:214:ARG:HG3	4:A:2085:HOH:O	2.06	0.55
1:C:112:ARG:HG2	1:C:112:ARG:O	2.10	0.51
1:A:141:SER:OG	1:A:186:ARG:NH2	2.44	0.50
1:C:159:LYS:HG3	4:C:2081:HOH:O	2.12	0.49
1:A:63:ILE:HG22	1:A:64:SER:HB2	1.95	0.47
1:A:205:THR:HG22	1:A:205:THR:O	2.15	0.47
1:A:207:SER:HB2	1:C:144:ASP:OD2	2.15	0.47
1:A:63:ILE:HG22	1:A:64:SER:CB	2.45	0.47
1:C:48:PHE:CE1	1:C:59:ASN:HB2	2.51	0.46
1:A:131:LEU:O	1:A:135:LEU:HG	2.16	0.45
1:C:143:ASP:HA	2:D:53:ARG:HH11	1.81	0.45
1:A:40:GLN:HE22	2:B:51:LYS:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:HD3	4:A:2068:HOH:O	2.16	0.44
1:C:159:LYS:HG2	4:C:2079:HOH:O	2.18	0.43
1:C:185:GLU:HG2	4:C:2086:HOH:O	2.19	0.42
1:C:158:ALA:HA	4:C:2060:HOH:O	2.19	0.42
1:A:205:THR:O	1:A:205:THR:CG2	2.69	0.41
1:A:113:TRP:O	1:A:164:ALA:HA	2.21	0.41
1:A:60:LEU:HD21	1:A:100:PRO:HG2	2.02	0.40
1:C:30:ASN:HD22	1:C:33:HIS:CE1	2.39	0.40
1:C:112:ARG:HD2	4:C:2043:HOH:O	2.22	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)
1:C:27:GLU:O	4:C:2017:HOH:O[2_554]	2.15	0.05

## 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	184/217 (85%)	177 (96%)	7 (4%)	0	100	100
1	C	182/217 (84%)	176 (97%)	6 (3%)	0	100	100
2	B	12/14 (86%)	12 (100%)	0	0	100	100
2	D	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
All	All	390/462 (84%)	376 (96%)	14 (4%)	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	167/195 (86%)	160 (96%)	7 (4%)	36	34
1	C	166/195 (85%)	163 (98%)	3 (2%)	66	71
2	B	11/11 (100%)	11 (100%)	0	100	100
2	D	11/11 (100%)	11 (100%)	0	100	100
All	All	355/412 (86%)	345 (97%)	10 (3%)	51	52

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	61	ARG
1	A	80	GLN
1	A	148	ASP
1	A	174	GLU
1	A	192	LYS
1	A	198	GLN
1	C	112	ARG
1	C	148	ASP
1	C	198	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	ASN
1	C	33	HIS

### 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 ⓘ

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$
3	MGO	A	1218	-	28,35,35	1.96	9 (32%)	33,56,56	1.41	6 (18%)
3	MGO	C	1218	-	28,35,35	1.90	9 (32%)	33,56,56	1.39	6 (18%)

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
3	MGO	A	1218	-	-	0/18/38/38	0/3/3/3
3	MGO	C	1218	-	-	0/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1218	MGO	CAW-NBC	-4.16	1.33	1.38
3	A	1218	MGO	CAW-NBC	-4.05	1.33	1.38
3	A	1218	MGO	CAX-CAW	-3.69	1.34	1.44
3	C	1218	MGO	CAX-CAW	-3.61	1.34	1.44
3	C	1218	MGO	CAM-CAW	-3.30	1.33	1.40
3	A	1218	MGO	CAM-CAW	-3.18	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1218	MGO	CAV-CAX	-2.97	1.35	1.41
3	A	1218	MGO	CAV-CAX	-2.84	1.35	1.41
3	C	1218	MGO	PBE-OAD	2.17	1.62	1.54
3	C	1218	MGO	CAU-NAP	2.28	1.39	1.35
3	A	1218	MGO	PBE-OAD	2.30	1.63	1.54
3	A	1218	MGO	PBE-OAJ	2.46	1.63	1.54
3	C	1218	MGO	PBE-OAJ	2.64	1.64	1.54
3	A	1218	MGO	CAU-NAP	2.76	1.40	1.35
3	C	1218	MGO	O4'-C1'	3.02	1.45	1.41
3	A	1218	MGO	O4'-C1'	3.18	1.45	1.41
3	C	1218	MGO	CAV-NAP	3.91	1.40	1.33
3	A	1218	MGO	CAV-NAP	4.53	1.41	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1218	MGO	PBG-OAS-PBE	-3.97	119.36	132.67
3	A	1218	MGO	PBG-OAS-PBE	-3.54	120.79	132.67
3	A	1218	MGO	PBF-OAT-PBG	-2.99	124.34	132.73
3	C	1218	MGO	C2'-C1'-NBC	-2.93	109.82	114.29
3	C	1218	MGO	CAX-CAV-NAP	-2.92	119.59	123.59
3	A	1218	MGO	CAX-CAV-NAP	-2.81	119.75	123.59
3	C	1218	MGO	PBF-OAT-PBG	-2.32	126.20	132.73
3	A	1218	MGO	C2'-C1'-NBC	-2.20	110.93	114.29
3	C	1218	MGO	CAX-CAW-NBC	2.32	108.42	105.72
3	A	1218	MGO	CAX-CAW-NBC	2.42	108.54	105.72
3	C	1218	MGO	NAB-CAU-NAP	2.54	121.14	116.50
3	A	1218	MGO	NAB-CAU-NAP	2.88	121.75	116.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1218	MGO	1	0

## 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 [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(Å²)	Q<0.9	
1	A	188/217 (86%)	-0.55	0	100100	7, 12, 24, 37	0
1	C	186/217 (85%)	-0.62	0	100100	7, 11, 22, 31	0
2	B	12/14 (85%)	-0.36	0	100100	14, 16, 22, 26	0
2	D	12/14 (85%)	-0.45	0	100100	14, 15, 23, 27	0
All	All	398/462 (86%)	-0.57	0	100100	7, 12, 24, 37	0

There are no RSRZ outliers to report.

### 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
3	MGO	A	1218	33/33	0.96	0.10	0.41	10,11,20,21	0
3	MGO	C	1218	33/33	0.95	0.10	0.12	10,11,20,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.