



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:37 PM GMT

PDB ID : 3UG2  
Title : Crystal structure of the mutated EGFR kinase domain (G719S/T790M) in complex with gefitinib  
Authors : Parker, L.J.; Handa, N.; Yoshikawa, S.; Kukimoto-Niino, M.; Shirouzu, M.; Yokoyama, S.  
Deposited on : 2011-11-02  
Resolution : 2.50 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 (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

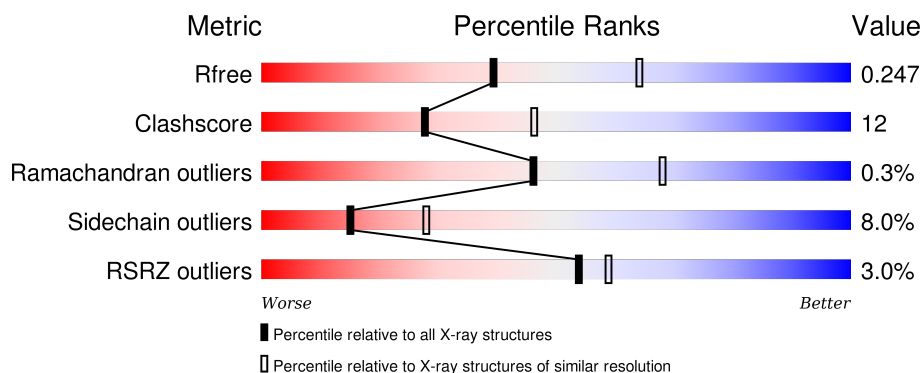
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	334	

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	IRE	A	1	-	-	-	X



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.

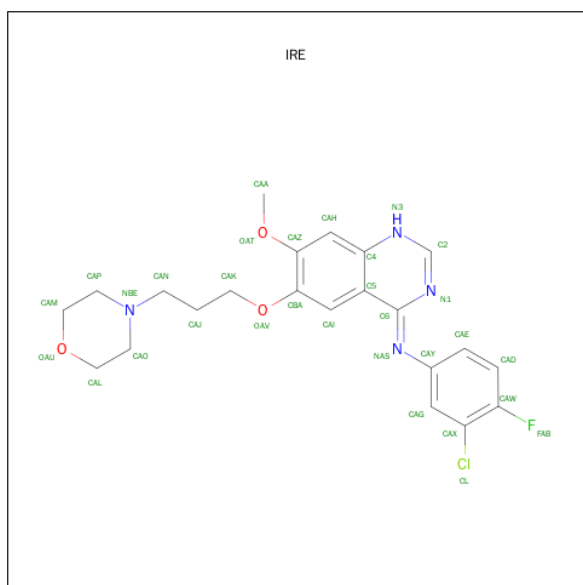
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	1	0
			2341	1506	391	425	19			

There are 8 discrepancies between the modelled and reference sequences:

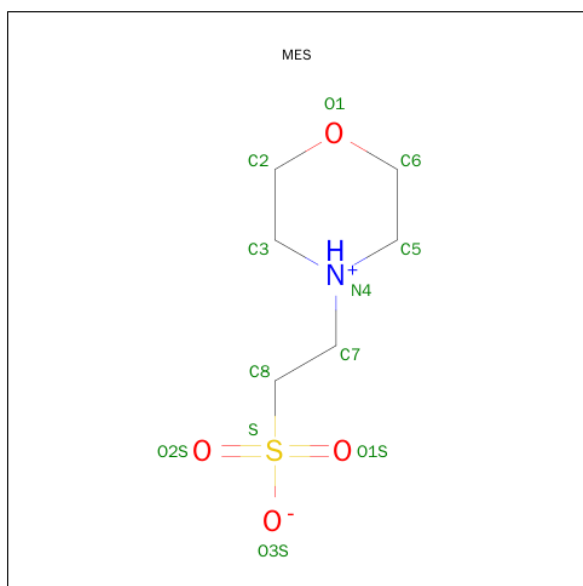
Chain	Residue	Modelled	Actual	Comment	Reference
A	689	GLY	-	EXPRESSION TAG	UNP P00533
A	690	ALA	-	EXPRESSION TAG	UNP P00533
A	691	MET	-	EXPRESSION TAG	UNP P00533
A	692	GLY	-	EXPRESSION TAG	UNP P00533
A	693	ILE	-	EXPRESSION TAG	UNP P00533
A	694	ARG	-	EXPRESSION TAG	UNP P00533
A	719	SER	GLY	ENGINEERED MUTATION	UNP P00533
A	790	MET	THR	ENGINEERED MUTATION	UNP P00533

- Molecule 2 is GEFITINIB (three-letter code: IRE) (formula:  $C_{22}H_{24}ClFN_4O_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			31	22	1	1	4	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

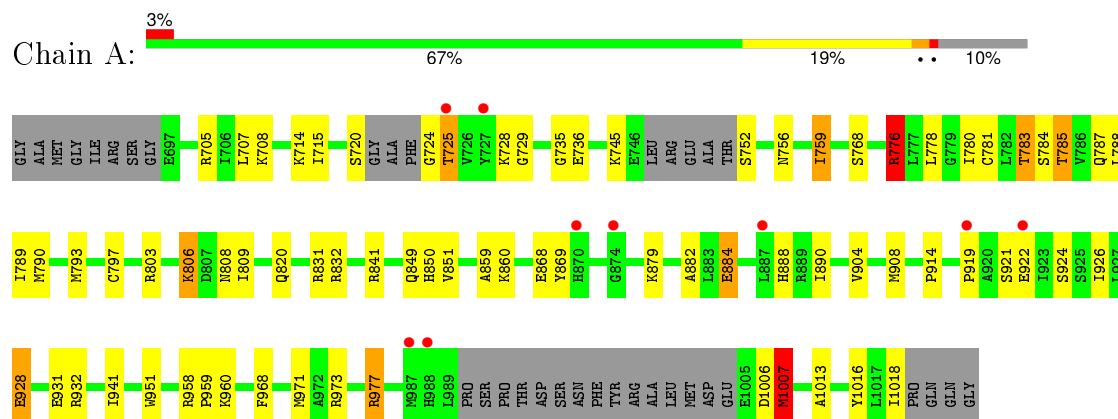
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		

### 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 ( $\text{RSRZ} > 2$ ). 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: Epidermal growth factor receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.68Å 143.68Å 143.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 2.50 45.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.45-2.50) 100.0 (45.43-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.249 0.184 , 0.247	Depositor DCC
$R_{free}$ test set	871 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.6	EDS
Estimated twinning fraction	0.028 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 17240 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2439	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IRE, MES

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	1.18	3/2392 (0.1%)	1.06	8/3245 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	776	ARG	CG-CD	5.58	1.66	1.51
1	A	728	LYS	CD-CE	5.51	1.65	1.51
1	A	797	CYS	CB-SG	-5.06	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	803	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	A	958	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	A	1007	MET	CG-SD-CE	6.49	110.59	100.20
1	A	958	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	977	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	735	GLY	N-CA-C	-5.85	98.47	113.10
1	A	841	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	832	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	2341	0	2327	56	0
2	A	31	0	24	2	0
3	A	12	0	12	0	0
4	A	55	0	0	2	0
All	All	2439	0	2363	56	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 12.

All (56) 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:919:PRO:HD2	1:A:922:GLU:OE1	1.56	1.04
1:A:783:THR:HG22	1:A:785:THR:O	1.57	1.01
1:A:724:GLY:O	1:A:725:THR:HG22	1.73	0.88
1:A:776:ARG:HH11	1:A:776:ARG:HG3	1.40	0.86
1:A:705:ARG:NH1	1:A:1018:ILE:HG21	1.90	0.86
1:A:793:MET:H	2:A:1:IRE:H3	1.22	0.86
1:A:776:ARG:CG	1:A:776:ARG:HH11	1.91	0.84
1:A:705:ARG:HH11	1:A:1018:ILE:HG21	1.41	0.84
1:A:888:HIS:O	1:A:890:ILE:HD12	1.87	0.74
1:A:882:ALA:HB1	1:A:884:GLU:OE2	1.94	0.68
1:A:820:GLN:NE2	1:A:851:VAL:H	1.93	0.67
1:A:776:ARG:CG	1:A:776:ARG:NH1	2.54	0.66
1:A:725:THR:HG23	1:A:725:THR:O	1.96	0.65
1:A:924:SER:O	1:A:928:GLU:HG3	1.99	0.63
1:A:724:GLY:O	1:A:725:THR:CG2	2.47	0.63
1:A:705:ARG:HH12	1:A:1018:ILE:HD13	1.63	0.62
1:A:919:PRO:CD	1:A:922:GLU:OE1	2.43	0.57
1:A:1006:ASP:O	1:A:1007:MET:CE	2.52	0.57
1:A:790:MET:HG3	2:A:1:IRE:CL	2.42	0.57
1:A:888:HIS:O	1:A:890:ILE:CD1	2.52	0.57
1:A:768:SER:O	1:A:831:ARG:NH2	2.38	0.57
1:A:820:GLN:HE22	1:A:851:VAL:H	1.53	0.56
1:A:715:ILE:HG12	1:A:729:GLY:HA2	1.86	0.56
1:A:707:LEU:HD12	1:A:789:ILE:HD13	1.88	0.55
1:A:1006:ASP:O	1:A:1007:MET:HE2	2.06	0.55
1:A:924:SER:O	1:A:928:GLU:CG	2.55	0.54
1:A:959:PRO:HB3	4:A:24:HOH:O	2.07	0.53
1:A:780:ILE:HG22	1:A:788:LEU:CD2	2.39	0.53

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:LYS:HD2	1:A:869:TYR:CZ	2.45	0.52
1:A:926:ILE:HG23	1:A:931:GLU:HB3	1.91	0.51
1:A:820:GLN:HE22	1:A:850:HIS:HA	1.76	0.51
1:A:931:GLU:O	1:A:932:ARG:HD3	2.12	0.50
1:A:860:LYS:HD2	1:A:869:TYR:CE1	2.46	0.50
1:A:904:VAL:O	1:A:908:MET:HG2	2.11	0.50
1:A:781:CYS:HB3	1:A:787:GLN:HB2	1.93	0.49
1:A:859:ALA:O	1:A:860:LYS:HE3	2.13	0.48
1:A:968:PHE:CD1	1:A:971:MET:CE	2.97	0.48
1:A:932:ARG:HE	1:A:951:TRP:HB3	1.79	0.47
1:A:831:ARG:NH2	4:A:49:HOH:O	2.47	0.47
1:A:745:LYS:O	1:A:787:GLN:HA	2.15	0.47
1:A:752:SER:O	1:A:756:ASN:ND2	2.40	0.46
1:A:705:ARG:NH1	1:A:1018:ILE:HD13	2.30	0.45
1:A:724:GLY:O	1:A:725:THR:CB	2.66	0.44
1:A:736:GLU:OE1	1:A:1016:TYR:OH	2.22	0.44
1:A:776:ARG:NH2	1:A:1016:TYR:O	2.50	0.44
1:A:968:PHE:CD1	1:A:971:MET:HE3	2.53	0.44
1:A:919:PRO:HD2	1:A:922:GLU:CD	2.34	0.43
1:A:888:HIS:CB	1:A:890:ILE:HD13	2.49	0.43
1:A:1006:ASP:O	1:A:1007:MET:HE3	2.19	0.42
1:A:714:LYS:NZ	1:A:787:GLN:HE22	2.17	0.42
1:A:780:ILE:HG22	1:A:788:LEU:HD22	2.00	0.41
1:A:778:LEU:HD21	1:A:1013:ALA:HB1	2.02	0.41
1:A:884:GLU:OE2	1:A:884:GLU:N	2.45	0.41
1:A:879:LYS:HD3	1:A:914:PRO:O	2.20	0.41
1:A:806:LYS:HE3	1:A:806:LYS:HB3	1.62	0.41
1:A:759:ILE:HA	1:A:759:ILE:HD12	1.64	0.41

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	292/334 (87%)	279 (96%)	12 (4%)	1 (0%)	46 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	725	THR

### 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	251/292 (86%)	231 (92%)	20 (8%)	15 28

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	708	LYS
1	A	720	SER
1	A	759	ILE
1	A	776	ARG
1	A	783	THR
1	A	784	SER
1	A	785	THR
1	A	806	LYS
1	A	808	ASN
1	A	809	ILE
1	A	849	GLN
1	A	868	GLU
1	A	884	GLU
1	A	921	SER
1	A	928	GLU
1	A	941	ILE
1	A	960	LYS
1	A	973	ARG
1	A	977	ARG
1	A	1007	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	787	GLN
1	A	808	ASN
1	A	816	ASN
1	A	820	GLN

### 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 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	$\# Z  > 2$
2	IRE	A	1	-	34,34,34	1.22	4 (11%)	43,46,46	3.05	16 (37%)
3	MES	A	1023	-	11,12,12	0.67	0	14,16,16	3.15	8 (57%)

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	IRE	A	1	-	-	0/11/21/21	0/4/4/4
3	MES	A	1023	-	-	0/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	IRE	CAY-NAS	-3.01	1.37	1.42
2	A	1	IRE	CAH-C4	-2.33	1.38	1.41
2	A	1	IRE	CAX-CL	2.39	1.79	1.73
2	A	1	IRE	CAI-CBA	3.04	1.42	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	IRE	N3-C2-N1	-12.15	119.59	128.89
2	A	1	IRE	CAW-CAX-CL	-4.12	116.28	120.06
2	A	1	IRE	FAB-CAW-CAX	-3.82	115.64	119.01
2	A	1	IRE	OAT-CAZ-CAH	-3.79	120.17	125.25
2	A	1	IRE	CAJ-CAN-NBE	-3.74	104.48	113.89
3	A	1023	MES	O2S-S-O1S	-2.53	104.27	113.48
3	A	1023	MES	O3S-S-O1S	-2.06	106.81	111.61
3	A	1023	MES	O3S-S-O2S	-2.01	106.92	111.61
3	A	1023	MES	O1S-S-C8	2.07	108.67	106.91
2	A	1	IRE	FAB-CAW-CAD	2.11	123.28	118.47
2	A	1	IRE	CAM-OAU-CAL	2.21	117.33	109.89
2	A	1	IRE	CAN-NBE-CAO	2.56	117.83	111.27
2	A	1	IRE	CAK-OAV-CBA	2.76	124.41	117.64
2	A	1	IRE	CAN-NBE-CAP	2.79	118.43	111.27
3	A	1023	MES	C7-N4-C3	2.89	118.67	111.27
2	A	1	IRE	OAT-CAZ-CBA	3.51	120.41	115.40
2	A	1	IRE	C6-NAS-CAY	3.63	127.81	121.22
3	A	1023	MES	C7-N4-C5	3.75	120.88	111.27
2	A	1	IRE	C2-N1-C6	3.76	122.20	113.47
2	A	1	IRE	CAG-CAX-CL	3.76	124.30	118.50
3	A	1023	MES	C5-N4-C3	5.32	120.42	108.90
2	A	1	IRE	C2-N3-C4	6.52	121.21	115.19
2	A	1	IRE	CAP-NBE-CAO	6.85	123.73	108.90
3	A	1023	MES	O2S-S-C8	7.80	113.56	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	IRE	2	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	299/334 (89%)	-0.02	9 (3%) 54 59	21, 36, 66, 81	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	988	HIS	4.0
1	A	727	TYR	3.1
1	A	874	GLY	3.1
1	A	987	MET	2.6
1	A	887	LEU	2.6
1	A	922	GLU	2.4
1	A	725	THR	2.4
1	A	870	HIS	2.1
1	A	919	PRO	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 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
2	IRE	A	1	31/31	0.90	0.24	2.11	16,26,51,52	31
3	MES	A	1023	12/12	0.97	0.21	0.82	40,42,44,45	12

## 6.5 Other polymers [i](#)

There are no such residues in this entry.