

Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 06:46 AM EDT

PDB ID : 6XGV

Title: Crystal Structure of KRAS-G13D (GMPPNP-bound) in complex with RAS-

binding domain (RBD) and cysteine-rich domain (CRD) of RAF1/CRAF

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Deposited on : 2020-06-18

Resolution : 2.11 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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 : 2.35.1

buster-report : 1.1.7 (2018)

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)

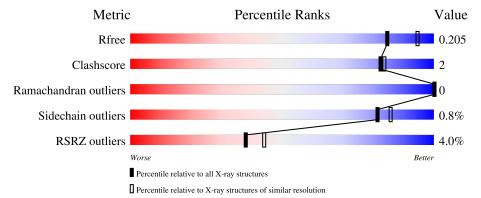
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.11 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	A	170	90%	9%	-
2	В	137	92%	6%	-



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 2566 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 GTPase KRas.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	168	Total 1331	C 832	N 228	O 264	S 7	1	0	0

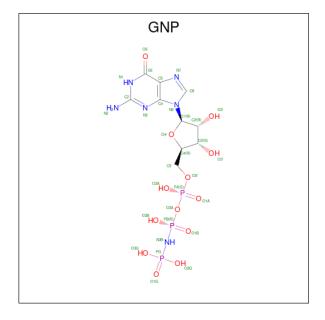
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	13	ASP	GLY	engineered mutation	UNP P01116

• Molecule 2 is a protein called RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
2	R	134	Total	As	С	N	О	S	5	1	0
	Б	104	1073	1	681	194	185	12	9	1	U

• Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).





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

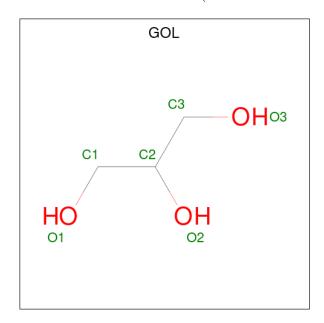
• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	В	2	Total Zn 2 2	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total C O 6 3 3	0	0
6	В	1	Total C O 6 3 3	0	0

• Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	В	1	Total Cl 1 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	46	Total O 46 46	0	0
8	В	67	Total O 67 67	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: GTPase KRas

Chain A:

90%

9%

Molecule 2: RAF proto-oncogene serine/threonine-protein kinase

Chain B:

92%

6%

6%

6%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants	132.75Å 132.75Å 89.48Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.36 - 2.11	Depositor
Resolution (A)	48.36 - 2.11	EDS
% Data completeness	99.6 (48.36-2.11)	Depositor
(in resolution range)	95.9 (48.36-2.11)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.28 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
D D.	0.184 , 0.204	Depositor
R, R_{free}	0.185 , 0.205	DCC
R_{free} test set	2000 reflections (7.32%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 44.3	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2566	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities 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: ZN, CAF, GNP, CL, MG, GOL

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.42	0/1351	0.60	0/1823	
2	В	0.51	0/1088	0.62	0/1467	
All	All	0.46	0/2439	0.61	0/3290	

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	1331	0	1304	9	0
2	В	1073	0	1058	3	0
3	A	32	0	13	1	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
5	В	2	0	0	0	0
6	В	12	0	16	1	0
7	В	1	0	0	0	0
8	A	46	0	0	0	0
8	В	67	0	0	0	0
All	All	2566	0	2391	12	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 (12) 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:101:LYS:HE2	1:A:107:GLU:HG2	1.82	0.61
1:A:13:ASP:H	3:A:201:GNP:HNB3	1.52	0.58
1:A:22:GLN:HG3	1:A:149:ARG:HG3	1.87	0.56
2:B:100:ARG:HD2	2:B:124:GLU:OE2	2.09	0.53
1:A:56:LEU:HD21	1:A:71:TYR:CG	2.47	0.49
1:A:72:MET:HB2	1:A:103:VAL:HG21	1.95	0.49
2:B:135:PRO:HA	6:B:201:GOL:H2	1.98	0.44
1:A:84:ILE:CD1	1:A:118:CYS:HA	2.48	0.44
1:A:134:ALA:HB1	1:A:139:ILE:O	2.19	0.42
1:A:84:ILE:HD11	1:A:118:CYS:HA	2.01	0.42
2:B:152:CYS:HB2	2:B:173:HIS:CE1	2.55	0.42
1:A:29:VAL:HG12	1:A:31:GLU:HG3	2.03	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.

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	166/170~(98%)	164 (99%)	2 (1%)	0	100	100	
2	В	132/137~(96%)	129 (98%)	3 (2%)	0	100	100	
All	All	298/307~(97%)	293 (98%)	5 (2%)	0	100	100	

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	Percer	ntiles
1	A	146/150 (97%)	146 (100%)	0	100	100
2	В	117/123 (95%)	115 (98%)	2 (2%)	60	66
All	All	263/273 (96%)	261 (99%)	2 (1%)	81	86

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	157	LYS
2	В	170	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is 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	Pog	Link	Bond lengths			Bond angles			
	Туре	Chain	rtes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CAF	В	95	2	3,9,10	0.86	0	1,12,14	2.95	1 (100%)



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	CAF	В	95	2	-	0/0/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
2	В	95	CAF	CA-CB-SG	-2.95	106.63	112.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	Mol Type Chain Res		Link	Bo	ond leng	$ ag{ths}$	Bond angles			
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	В	202	-	5,5,5	1.19	1 (20%)	5,5,5	1.27	1 (20%)
6	GOL	В	201	-	5,5,5	1.32	0	5,5,5	0.98	0
3	GNP	A	201	4	29,34,34	1.81	6 (20%)	33,54,54	2.13	9 (27%)

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
6	GOL	В	202	-	-	1/4/4/4	-
6	GOL	В	201	-	-	0/4/4/4	-
3	GNP	A	201	4	-	3/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
3	A	201	GNP	PB-O3A	4.38	1.64	1.59
3	A	201	GNP	PG-N3B	4.29	1.74	1.63
3	A	201	GNP	PG-O1G	3.89	1.52	1.46
3	A	201	GNP	C6-N1	3.44	1.39	1.33
3	A	201	GNP	PB-O1B	3.22	1.51	1.46
6	В	202	GOL	C3-C2	2.09	1.60	1.51
3	A	201	GNP	C5-C6	2.05	1.44	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	201	GNP	C5-C6-N1	-8.53	111.76	123.43
3	A	201	GNP	C2-N1-C6	5.77	125.10	115.93
3	A	201	GNP	N3-C2-N1	-2.67	123.66	127.22
3	A	201	GNP	C4-C5-C6	-2.35	118.56	120.80
3	A	201	GNP	C2-N3-C4	-2.20	112.84	115.36
3	A	201	GNP	O2G-PG-O1G	-2.16	108.03	113.45
6	В	202	GOL	O2-C2-C3	2.14	118.55	109.12
3	A	201	GNP	O1G-PG-N3B	2.10	114.86	111.77
3	A	201	GNP	O3G-PG-O1G	-2.08	108.23	113.45
3	A	201	GNP	O3A-PB-N3B	2.01	112.16	106.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	GNP	PB-N3B-PG-O1G
3	A	201	GNP	PA-O3A-PB-O1B
3	A	201	GNP	PA-O3A-PB-O2B
6	В	202	GOL	O2-C2-C3-O3

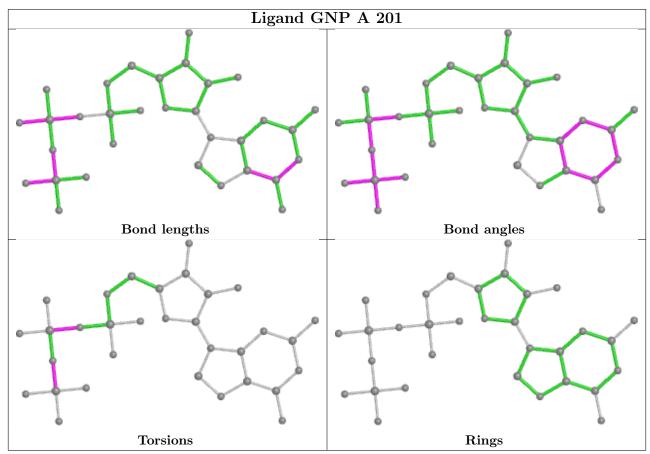
There are no ring outliers.



\circ			• 1	1 1	•	\circ	1			
2	monomers	are	invol	lved	ın	2	sho	ort	contact	ts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	В	201	GOL	1	0
3	A	201	GNP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	$\langle { m RSRZ} \rangle$	$\#\mathbf{RSRZ}>$	>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	A	168/170 (98%)	0.18	7 (4%) 36	42	38, 52, 83, 104	5 (2%)
2	В	132/137 (96%)	0.00	5 (3%) 40	46	36, 45, 76, 114	1 (0%)
All	All	300/307 (97%)	0.10	12 (4%) 38	44	36, 49, 81, 114	6 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32	TYR	4.2
1	A	71	TYR	3.6
1	A	65	SER	3.4
2	В	55	SER	3.3
1	A	63	GLU	2.8
2	В	147	LEU	2.6
1	A	62	GLU	2.3
2	В	103	HIS	2.3
2	В	107	GLY	2.2
1	A	66	ALA	2.2
1	A	148	THR	2.1
2	В	105	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	CAF	В	95	10/11	0.98	0.16	35,41,51,53	6



6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

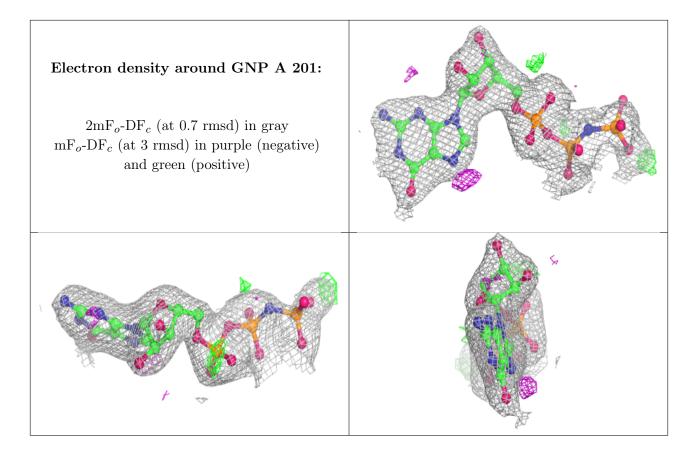
6.4 Ligands (i)

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
6	GOL	В	201	6/6	0.69	0.23	43,51,67,76	0
7	CL	В	203	1/1	0.77	0.11	82,82,82,82	0
6	GOL	В	202	6/6	0.86	0.24	39,41,48,53	6
5	ZN	A	203	1/1	0.96	0.04	68,68,68,68	1
3	GNP	A	201	32/32	0.97	0.12	44,49,58,61	2
4	MG	A	202	1/1	0.98	0.04	51,51,51,51	0
5	ZN	В	205	1/1	1.00	0.13	46,46,46,46	0
5	ZN	В	204	1/1	1.00	0.12	40,40,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

