



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 05:31 PM GMT

PDB ID : 4M1T  
Title : Crystal Structure of small molecule vinylsulfonamide 14 covalently bound to K-Ras G12C  
Authors : Ostrem, J.M.; Peters, U.; Sos, M.L.; Wells, J.A.; Shokat, K.M.  
Deposited on : 2013-08-04  
Resolution : 1.70 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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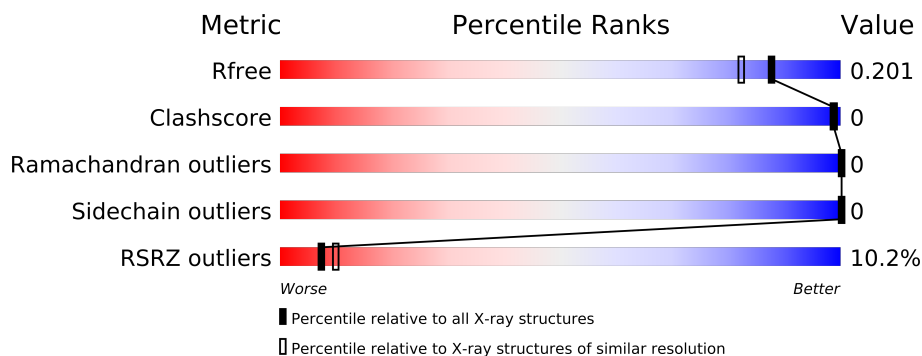
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 1.70 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))
$R_{free}$	66092	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	170	
1	B	170	
1	C	170	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7825 atoms, of which 3781 are hydrogens and 0 are deuterium.

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 K-Ras GTPase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	163	Total	C	H	N	O	S	0	3	0
			2579	813	1282	224	254	6			
1	B	162	Total	C	H	N	O	S	0	1	0
			2583	812	1289	227	250	5			
1	C	151	Total	C	H	N	O	S	0	2	0
			2361	748	1179	204	225	5			

There are 33 discrepancies between the modelled and reference sequences:

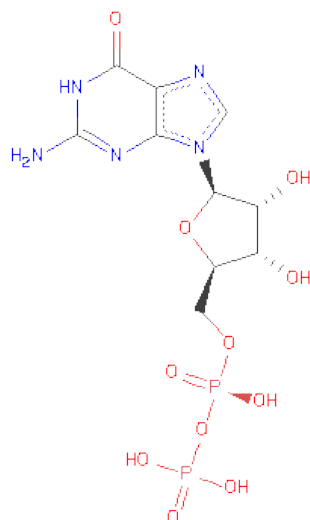
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP P01116
A	12	CYS	GLY	VARIANT	UNP P01116
A	51	SER	CYS	ENGINEERED MUTATION	UNP P01116
A	80	LEU	CYS	ENGINEERED MUTATION	UNP P01116
A	118	SER	CYS	ENGINEERED MUTATION	UNP P01116
A	151	GLY	ARG	SEE REMARK 999	UNP P01116
A	153	ASP	GLU	SEE REMARK 999	UNP P01116
A	165	LYS	GLN	SEE REMARK 999	UNP P01116
A	166	HIS	TYR	SEE REMARK 999	UNP P01116
A	167	LYS	ARG	SEE REMARK 999	UNP P01116
A	168	GLU	LEU	SEE REMARK 999	UNP P01116
B	0	GLY	-	EXPRESSION TAG	UNP P01116
B	12	CYS	GLY	VARIANT	UNP P01116
B	51	SER	CYS	ENGINEERED MUTATION	UNP P01116
B	80	LEU	CYS	ENGINEERED MUTATION	UNP P01116
B	118	SER	CYS	ENGINEERED MUTATION	UNP P01116
B	151	GLY	ARG	SEE REMARK 999	UNP P01116
B	153	ASP	GLU	SEE REMARK 999	UNP P01116
B	165	LYS	GLN	SEE REMARK 999	UNP P01116
B	166	HIS	TYR	SEE REMARK 999	UNP P01116
B	167	LYS	ARG	SEE REMARK 999	UNP P01116
B	168	GLU	LEU	SEE REMARK 999	UNP P01116
C	0	GLY	-	EXPRESSION TAG	UNP P01116

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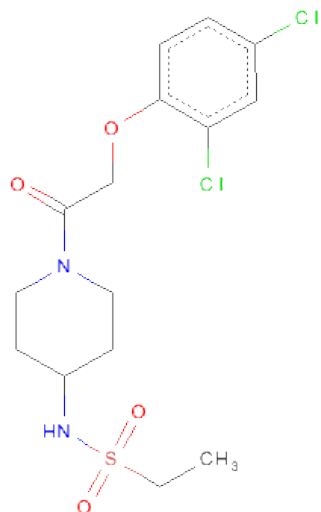
Chain	Residue	Modelled	Actual	Comment	Reference
C	12	CYS	GLY	VARIANT	UNP P01116
C	51	SER	CYS	ENGINEERED MUTATION	UNP P01116
C	80	LEU	CYS	ENGINEERED MUTATION	UNP P01116
C	118	SER	CYS	ENGINEERED MUTATION	UNP P01116
C	151	GLY	ARG	SEE REMARK 999	UNP P01116
C	153	ASP	GLU	SEE REMARK 999	UNP P01116
C	165	LYS	GLN	SEE REMARK 999	UNP P01116
C	166	HIS	TYR	SEE REMARK 999	UNP P01116
C	167	LYS	ARG	SEE REMARK 999	UNP P01116
C	168	GLU	LEU	SEE REMARK 999	UNP P01116

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			32	10	4	5	11	2		
2	B	1	Total	C	H	N	O	P	0	0
			32	10	4	5	11	2		
2	C	1	Total	C	H	N	O	P	0	0
			32	10	4	5	11	2		

- Molecule 3 is N-{1-[(2,4-DICHLOROPHENOXY)ACETYL]PIPERIDIN-4-YL}ETHANES ULFONAMIDE (three-letter code: 21M) (formula:  $C_{15}H_{20}Cl_2N_2O_4S$ ).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	Cl	H	N	O	S		
3	B	1	43	15	2	19	2	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	49	Total	O	0	0
			49	49		
4	C	43	Total	O	0	0
			43	43		

### 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 ( $RSRZ > 2$ ). 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: K-Ras GTPase

Chain A: 



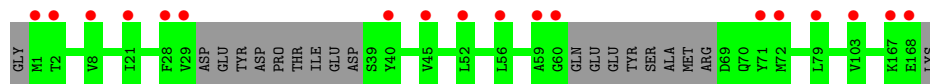
#### • Molecule 1: K-Ras GTPase

Chain B: 



#### • Molecule 1: K-Ras GTPase

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.17Å 83.48Å 85.75Å 90.00° 110.63° 90.00°	Depositor
Resolution (Å)	24.79 – 1.70 24.79 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.79-1.70) 96.4 (24.79-1.70)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 1.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1402)	Depositor
R, $R_{free}$	0.170 , 0.202 0.169 , 0.201	Depositor DCC
$R_{free}$ test set	1956 reflections (4.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 41.4	EDS
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48943 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7825	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 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 21M

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	0.31	0/1324	0.50	0/1783
1	B	0.29	0/1315	0.48	0/1770
1	C	0.28	0/1204	0.47	0/1623
All	All	0.29	0/3843	0.48	0/5176

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1297	1282	0	1	0
1	B	1294	1289	0	0	0
1	C	1182	1179	0	0	0
2	A	28	4	0	0	0
2	B	28	4	0	0	0
2	C	28	4	0	0	0
3	B	24	19	0	0	0
4	A	71	0	0	0	0
4	B	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	43	0	0	0	0
All	All	4044	3781	0	1	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 0.

All (1) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:PHE:HB2	1:A:89:SER:HG	1.83	0.44

There are no symmetry-related clashes.

## 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	162/170 (95%)	159 (98%)	3 (2%)	0	100	100
1	B	159/170 (94%)	156 (98%)	3 (2%)	0	100	100
1	C	147/170 (86%)	144 (98%)	3 (2%)	0	100	100
All	All	468/510 (92%)	459 (98%)	9 (2%)	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	142/150 (95%)	142 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	141/150 (94%)	141 (100%)	0	100	100
1	C	129/150 (86%)	129 (100%)	0	100	100
All	All	412/450 (92%)	412 (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	B	95	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	GDP	A	201	-	30,30,30	1.40	4 (13%)	44,47,47	3.20	7 (15%)
3	21M	B	201	1	25,25,25	2.01	10 (40%)	35,35,35	2.46	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GDP	B	202	-	30,30,30	1.39	3 (10%)	44,47,47	4.30	11 (25%)
2	GDP	C	201	-	30,30,30	1.47	5 (16%)	44,47,47	4.53	8 (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
2	GDP	A	201	-	-	0/16/32/32	0/1/3/3
3	21M	B	201	1	-	0/17/27/27	0/2/2/2
2	GDP	B	202	-	-	0/16/32/32	0/1/3/3
2	GDP	C	201	-	-	0/16/32/32	0/1/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	GDP	C4-N9	-4.36	1.31	1.37
2	C	201	GDP	C6-C5	4.34	1.48	1.41
3	B	201	21M	C08-N09	4.16	1.45	1.35
2	C	201	GDP	C4-N9	-3.82	1.32	1.37
2	A	201	GDP	C4-N9	-3.72	1.32	1.37
2	B	202	GDP	C6-C5	3.58	1.47	1.41
2	A	201	GDP	C6-C5	3.58	1.47	1.41
3	B	201	21M	O06-C05	3.37	1.44	1.37
3	B	201	21M	O17-S14	3.19	1.48	1.43
3	B	201	21M	O18-S14	3.15	1.48	1.43
2	B	202	GDP	C5-C4	3.09	1.47	1.40
2	C	201	GDP	C5-C4	2.99	1.47	1.40
2	A	201	GDP	C5-C4	2.86	1.47	1.40
3	B	201	21M	O21-C08	2.79	1.29	1.23
3	B	201	21M	C02-CL1	-2.67	1.68	1.74
3	B	201	21M	S14-N13	2.54	1.66	1.62
3	B	201	21M	C24-C02	2.47	1.42	1.38
2	A	201	GDP	C2-N2	2.31	1.36	1.32
2	C	201	GDP	C6-N1	-2.26	1.33	1.37
2	C	201	GDP	C2-N2	2.09	1.35	1.32
3	B	201	21M	O06-C07	-2.08	1.37	1.42
3	B	201	21M	C15-S14	-2.08	1.75	1.76

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	GDP	C6-C5-N7	27.93	137.90	134.14
2	B	202	GDP	C6-C5-N7	26.32	137.68	134.14
2	A	201	GDP	C6-C5-N7	18.44	136.62	134.14
3	B	201	21M	O18-S14-O17	-10.03	100.87	119.30
3	B	201	21M	C12-N13-S14	-6.21	112.85	121.93
2	A	201	GDP	N3-C4-N9	4.56	133.60	126.91
2	C	201	GDP	N3-C4-N9	4.51	133.53	126.91
2	C	201	GDP	C4-C5-N7	-4.44	105.72	109.52
2	C	201	GDP	C5-C4-N3	-4.29	119.73	125.94
2	B	202	GDP	C4-C5-N7	-4.21	105.92	109.52
2	B	202	GDP	C8-N9-C4	3.95	109.92	106.90
2	A	201	GDP	C8-N9-C4	3.94	109.91	106.90
2	C	201	GDP	C2-N3-C4	3.92	120.60	115.09
2	B	202	GDP	N3-C4-N9	3.65	132.27	126.91
3	B	201	21M	C16-C15-S14	3.64	119.08	113.18
2	A	201	GDP	C5-C4-N3	-3.64	120.67	125.94
2	A	201	GDP	C4-C5-N7	-3.40	106.61	109.52
3	B	201	21M	O17-S14-N13	3.20	110.95	106.95
2	C	201	GDP	C8-N9-C4	3.19	109.34	106.90
2	B	202	GDP	C5-C4-N3	-3.18	121.33	125.94
2	B	202	GDP	N2-C2-N3	-3.17	116.00	120.30
2	A	201	GDP	C2-N3-C4	2.91	119.18	115.09
3	B	201	21M	C15-S14-N13	2.84	113.22	107.26
2	B	202	GDP	C2-N3-C4	2.82	119.05	115.09
2	B	202	GDP	N2-C2-N1	2.81	120.95	117.86
2	A	201	GDP	C6-N1-C2	2.66	124.16	119.51
2	B	202	GDP	C6-N1-C2	2.58	124.02	119.51
2	B	202	GDP	C1'-N9-C4	-2.38	122.52	126.64
2	C	201	GDP	C6-N1-C2	2.21	123.37	119.51
2	B	202	GDP	O4'-C1'-N9	-2.17	106.42	108.44
2	C	201	GDP	C1'-N9-C4	-2.13	122.96	126.64
3	B	201	21M	O18-S14-N13	2.07	109.53	106.95
3	B	201	21M	O17-S14-C15	2.05	111.63	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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	163/170 (95%)	0.17	11 (6%) 17 21	15, 29, 56, 77	0
1	B	162/170 (95%)	0.42	20 (12%) 5 6	13, 32, 70, 91	0
1	C	151/170 (88%)	0.61	18 (11%) 5 7	15, 39, 68, 87	0
All	All	476/510 (93%)	0.39	49 (10%) 7 10	13, 33, 67, 91	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	29	VAL	12.1
1	B	29	VAL	5.9
1	A	103	VAL	5.6
1	C	103	VAL	5.3
1	B	103	VAL	5.2
1	B	64	TYR	5.2
1	B	60	GLY	5.0
1	C	60	GLY	5.0
1	C	59	ALA	4.9
1	C	71	TYR	4.8
1	B	105	ASP	4.6
1	B	106	SER	4.2
1	B	30	ASP	3.4
1	C	21	ILE	3.3
1	A	108	ASP	3.3
1	A	165	LYS	3.2
1	B	45	VAL	3.1
1	A	30	ASP	3.1
1	B	44	VAL	3.1
1	A	1	MET	3.0
1	A	36	ILE	3.0
1	C	168	GLU	3.0
1	B	107	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	50	THR	2.7
1	C	1	MET	2.7
1	A	107	GLU	2.6
1	B	168	GLU	2.6
1	B	37	GLU	2.5
1	C	28	PHE	2.5
1	C	72	MET	2.5
1	C	45	VAL	2.5
1	B	2	THR	2.4
1	B	1	MET	2.3
1	B	7	VAL	2.3
1	B	61	GLN	2.3
1	B	38	ASP	2.3
1	A	102	ARG	2.3
1	C	167	LYS	2.3
1	B	81	VAL	2.3
1	A	2	THR	2.3
1	A	74	THR	2.2
1	A	61	GLN	2.2
1	C	56	LEU	2.2
1	C	2	THR	2.1
1	C	52	LEU	2.1
1	C	79	LEU	2.1
1	C	8	VAL	2.1
1	B	167	LYS	2.1
1	C	40	TYR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	21M	B	201	24/24	0.14	-0.03	28,44,61,72	0
2	GDP	C	201	28/28	0.07	-0.37	18,27,40,42	0
2	GDP	B	202	28/28	0.06	-0.46	14,21,29,33	0
2	GDP	A	201	28/28	0.05	-0.60	15,20,28,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.