

Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 06:43 PM JST

PDB ID : 7YV1

Title: Human K-Ras G12D (GDP-bound) in complex with cyclic peptide inhibitor

LUNA18 and KA30L Fab

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Deposited on : 2022-08-18

Resolution : 1.45 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 : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

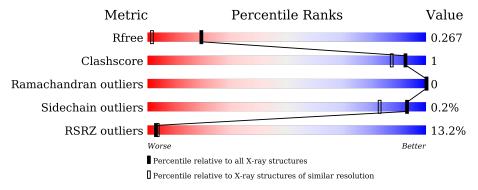
Validation Pipeline (wwPDB-VP) : 2.36

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 1.45 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	179	16%		• 6%
2	Н	225	17%		
3	L	214	97%		•
4	I	11	55%	36%	9%



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5857 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 Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total 1342	C 840	N 226	O 268	S 8	0	2	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P01116
A	-3	SER	-	expression tag	UNP P01116
A	-2	SER	-	expression tag	UNP P01116
A	-1	GLY	-	expression tag	UNP P01116
A	0	GLY	-	expression tag	UNP P01116
A	1	SER	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116

• Molecule 2 is a protein called KA30L Fab H-chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Н	222	Total 1669	C 1063	N 274	O 328	S 4	0	3	0

• Molecule 3 is a protein called KA30L Fab L-chain.

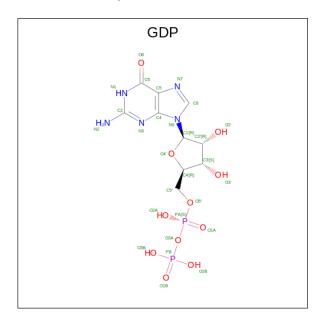
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	L	213	Total 1643	C 1026	N 273	O 339	S 5	0	5	0

• Molecule 4 is a protein called LUNA18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Т	11	Total	С	F	N	О	0	0	0
4	1	11	102	73	5	12	12	U	0	U



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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	Δ	1	Total	С	N	О	Р	0	0
	1	28	10	5	11	2	0		

• Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	243	Total O 243 243	0	0
7	Н	380	Total O 380 380	0	0
7	L	433	Total O 433 433	0	0
7	I	16	Total O 16 16	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: Isoform 2B of GTPase KRas Chain A: • Molecule 2: KA30L Fab H-chain Chain H: 98% • Molecule 3: KA30L Fab L-chain Chain L: 97% • Molecule 4: LUNA18 Chain I: 55% 36%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	65.62Å 90.37Å 116.81Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.41 - 1.45	Depositor
Resolution (A)	58.40 - 1.45	EDS
% Data completeness	80.0 (58.41-1.45)	Depositor
(in resolution range)	80.0 (58.40-1.45)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.81 (at 1.45Å)	Xtriage
Refinement program	BUSTER 2.11.8 (20-APR-2021)	Depositor
D D.	0.238 , 0.277	Depositor
R, R_{free}	0.233 , 0.267	DCC
R_{free} test set	4912 reflections $(5.02%)$	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 32.9	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	0.94	EDS
Total number of atoms	5857	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.35% 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: MLE, GDP, 7VN, 7W2, MAA, 02A, AC5, 7WC, 7VU, MG, SAR

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		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.42	0/1369	0.57	0/1850	
2	Н	0.42	0/1725	0.62	0/2359	
3	L	0.43	0/1692	0.60	0/2298	
4	I	0.18	0/14	0.53	0/16	
All	All	0.42	0/4800	0.60	0/6523	

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	1342	0	1305	4	0
2	Н	1669	0	1639	1	0
3	L	1643	0	1607	3	0
4	I	102	0	51	2	0
5	A	28	0	12	0	0
6	A	1	0	0	0	0
7	A	243	0	0	0	0
7	Н	380	0	0	0	0
7	I	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	433	0	0	0	0
All	All	5857	0	4614	10	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 1.

All (10) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ & \\ & & \\ &$	Clash overlap (Å)
1:A:24:ILE:HD12	1:A:42:LYS:HB2	1.72	0.70
1:A:84:ILE:HD13	1:A:123:ARG:HD3	1.76	0.66
4:I:3:MAA:HB1	4:I:4:02A:CA	2.38	0.54
1:A:94:HIS:CE1	1:A:95:HIS:CE1	2.99	0.51
3:L:145:LYS:HB3	3:L:197:THR:HB	1.94	0.50
3:L:22[B]:THR:HG22	3:L:72:THR:HG22	1.95	0.48
1:A:24:ILE:CD1	1:A:42:LYS:HB2	2.41	0.47
4:I:2:ILE:HA	4:I:3:MAA:HM1	1.76	0.44
2:H:33:TYR:CD2	2:H:100:ARG:HA	2.53	0.43
3:L:185:ASP:O	3:L:189:HIS:HD2	2.03	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	Percei	ntiles
1	A	$169/179\ (94\%)$	164 (97%)	5 (3%)	0	100	100
2	Н	$223/225\ (99\%)$	218 (98%)	5 (2%)	0	100	100
3	L	$216/214 \ (101\%)$	210 (97%)	6 (3%)	0	100	100
4	I	2/11 (18%)	2 (100%)	0	0	100	100
All	All	$610/629 \ (97\%)$	594 (97%)	16 (3%)	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	Percei	ntiles
1	A	148/156 (95%)	147 (99%)	1 (1%)	84	65
2	Н	191/195 (98%)	191 (100%)	0	100	100
3	L	191/188 (102%)	191 (100%)	0	100	100
4	I	2/2 (100%)	2 (100%)	0	100	100
All	All	532/541 (98%)	531 (100%)	1 (0%)	93	83

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	95	HIS
3	L	160	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)

9 non-standard protein/DNA/RNA residues 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	Tuno	Chain	Res	Link	Вс	ond leng	ths	В	ond ang	les
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AC5	I	9	4	6,8,9	0.75	0	5,11,13	1.13	1 (20%)
4	SAR	I	6	4	4,4,5	0.73	0	1,3,5	1.42	0
4	7VN	I	10	4	8,10,11	0.38	0	8,12,14	0.95	0
4	02A	I	4	4	4,6,7	0.83	0	2,7,9	3.04	1 (50%)
4	7WC	I	11	4	10,10,11	0.53	0	10,12,14	1.02	0
4	7VU	I	5	4	13,14,15	0.34	0	15,17,19	0.66	1 (6%)
4	7W2	I	7	4	17,18,19	0.39	0	21,26,28	0.42	0
4	MAA	I	3	4	4,5,6	0.57	0	1,5,7	0.16	0
4	MLE	I	1	4	7,8,9	0.41	0	6,9,11	0.85	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	AC5	I	9	4	-	0/2/12/15	0/1/1/1
4	SAR	I	6	4	-	1/1/2/3	-
4	7VN	I	10	4	-	2/6/15/17	0/1/1/1
4	02A	I	4	4	-	0/0/8/10	0/1/1/1
4	7WC	I	11	4	-	6/13/13/14	-
4	7VU	I	5	4	-	3/8/9/11	0/1/1/1
4	7W2	I	7	4	-	0/12/13/15	0/1/1/1
4	MAA	I	3	4	-	0/1/4/6	-
4	MLE	I	1	4	-	0/5/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	I	4	02A	C26-C27-CA	3.90	92.44	87.53
4	I	9	AC5	CG1-CB1-CA	-2.10	100.12	104.03
4	I	5	7VU	O-C-CA	-2.00	119.53	124.78

There are no chirality outliers.



All (12) torsion outliers are listed below	All (1	12)	torsion	outliers	are	listed	below
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Mol	Chain	Res	Type	Atoms
4	I	6	SAR	C-CA-N-CN
4	I	11	7WC	CA-CB-CG-OD1
4	I	5	7VU	CB-CA-N-C1
4	I	10	7VN	CB-CA-N-CN
4	I	10	7VN	O-C-CA-CB
4	I	11	7WC	CB-CA-N-CN
4	I	11	7WC	O-C-CA-N
4	I	11	7WC	O-C-CA-CB
4	I	11	7WC	N1-C-CA-CB
4	I	5	7VU	CA-CB-CG-CD1
4	I	5	7VU	C2-C1-N-CA
4	I	11	7WC	N1-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	4	02A	1	0
4	I	3	MAA	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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 Chair		n Res	Res Link		Bond lengths			Bond angles		
MIOI	Туре	Chain	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	GDP	A	201	6	24,30,30	0.85	0	30,47,47	0.67	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
5	GDP	A	201	6	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	<RSRZ $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	169/179 (94%)	1.38	28 (16%) 1 2	4, 11, 27, 34	0
2	Н	$222/225 \ (98\%)$	1.44	39 (17%) 1 1	5, 11, 25, 31	0
3	L	213/214 (99%)	1.09	13 (6%) 21 23	5, 9, 17, 25	0
4	I	2/11 (18%)	1.38	0 100 100	10, 10, 10, 10	0
All	All	606/629 (96%)	1.30	80 (13%) 3 4	4, 10, 25, 34	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Н	139	SER	6.4
1	A	122	SER	5.5
3	L	212	GLY	5.1
2	Н	222	SER	5.0
2	Н	211	ASN	5.0
2	Н	165	ALA	4.9
2	Н	197	GLY	4.9
1	A	1	SER	4.1
1	A	44	VAL	3.8
1	A	121	PRO	3.8
2	Н	198	THR	3.8
1	A	41	ARG	3.5
3	L	194	CYS	3.5
1	A	52	LEU	3.5
1	A	48	GLY	3.4
2	Н	136	LYS	3.4
1	A	127	THR	3.4
2	Н	9	PRO	3.3
1	A	125	VAL	3.2
1	A	2	THR	3.1
3	L	21	ILE	3.1

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Mol	nued fron Chain	$oxed{\mathbf{Res}}$	Type	RSRZ
2	Н	143	ALA	3.1
2	Н	196	LEU	3.0
1	A	118[A]	CYS	3.0
2	Н	206	ASN	3.0
2	Н	183	TYR	3.0
2	Н	141	GLY	2.9
1	A	168	GLU	2.9
2	Н	138	THR	2.9
2	Н	135	SER	2.9
1	A	7	VAL	2.7
	Н	140	GLY	2.7
1	A	131	GLN	2.7
1	A	4	TYR	2.6
1	A	123	ARG	2.6
2	Н	214	VAL	2.6
2	Н	142	THR	2.5
1	A	157	TYR	2.5
2	Н	1	GLN	2.5
2	Н	176	VAL	2.4
1	A	50	THR	2.4
2	Н	166	LEU	2.4
2	Н	205	VAL	2.4
3	L	88	CYS	2.4
3	L	202	SER	2.4
2	Н	75[A]	SER	2.3
2	Н	100	ARG	2.3
3	L	48	ILE	2.3
3	L	50	ALA	2.3
1	A	108	ASP	2.3
1	A	165	LYS	2.3
2	Н	170	VAL	2.3
2	Н	192	PRO	2.2
2	Н	199	GLN	2.2
1	A	149	ARG	2.2
2	Н	102	TRP	2.2
1	A	64	TYR	2.2
2	Н	93	VAL	2.2
1	A	126	ASP	2.2
2	Н	38	ILE	2.2
2	Н	212	THR	2.2
3	L	102	THR	2.2
3	L	73	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	56	LEU	2.1
2	Н	209	PRO	2.1
1	A	132	ASP	2.1
3	L	71	PHE	2.1
2	Н	131	LEU	2.1
1	A	24	ILE	2.1
2	Н	86	VAL	2.1
1	A	67[A]	MET	2.1
3	L	35	TRP	2.1
2	Н	163	SER	2.1
2	Н	129	PHE	2.1
3	L	96	LEU	2.1
2	Н	105	SER	2.0
2	Н	208	LYS	2.0
3	L	134	CYS	2.0
1	A	46	ILE	2.0
2	Н	194	SER	2.0

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	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
4	MLE	I	1	9/10	0.86	0.14	10,11,12,13	0
4	SAR	I	6	5/6	0.87	0.15	8,8,11,11	0
4	7WC	I	11	11/12	0.87	0.14	7,7,9,9	0
4	MAA	I	3	6/7	0.89	0.13	9,10,11,11	0
4	7VN	I	10	10/11	0.90	0.15	6,7,8,9	0
4	7W2	I	7	18/19	0.90	0.14	6,7,13,14	0
4	AC5	I	9	8/9	0.91	0.12	8,10,12,12	0
4	7VU	I	5	14/15	0.92	0.12	10,11,12,13	0
4	02A	I	4	6/7	0.92	0.13	11,12,12,12	0

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
5	GDP	A	201	28/28	0.95	0.12	4,7,9,11	0
6	MG	A	202	1/1	0.99	0.13	5,5,5,5	0

6.5 Other polymers (i)

There are no such residues in this entry.

