Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 08:13 pm GMT

PDB ID	:	1PLJ
Title	:	CRYSTALLOGRAPHIC STUDIES ON P21H-RAS USING SYNCHROTRON LAUE METHOD: IMPROVEMENT OF CRYSTAL QUALITY AND MONITORING OF THE GTPASE REACTION AT DIFFERENT TIME POINTS
Authors	:	Scheidig, A.; Sanchez-Llorente, A.; Lautwein, A.; Pai, E.F.; Corrie, J.E.T.; Reid, G.P.; Wittinghofer, A.; Goody, R.S.
Deposited on	:	1994-03-13
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:
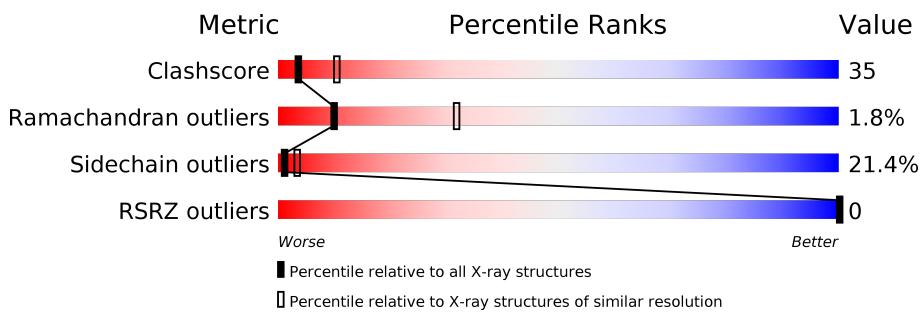
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		35
Ramachandran outliers		1.8%
Sidechain outliers		21.4%
RSRZ outliers		0

Worse　　　　*Better*

▍ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 >=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 <=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	166	33% 　 37% 　 18% · 8%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 1224 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 C-H-RAS P21 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total 1180	C 735	N 198	O 240	S 7	0	0	0
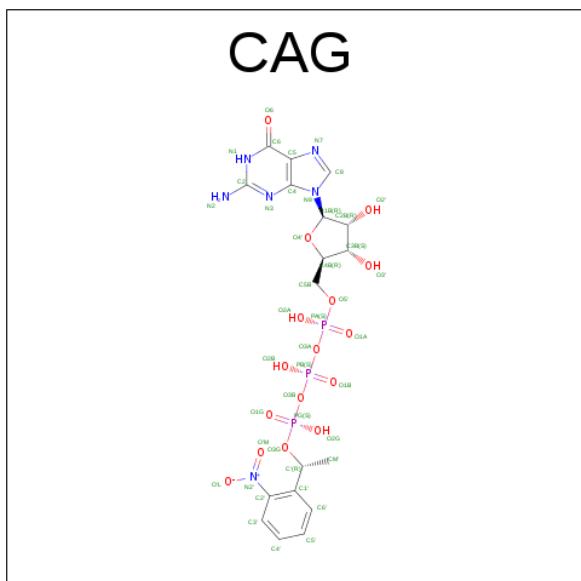
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	PRO	GLY	CONFLICT	UNP P01112

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is GUANOSINE 5'-TRIPHOSPHATE P3-[1-(2-NITROPHENYL)ETHYL ESTER] (three-letter code: CAG) (formula: $C_{18}H_{23}N_6O_{16}P_3$).
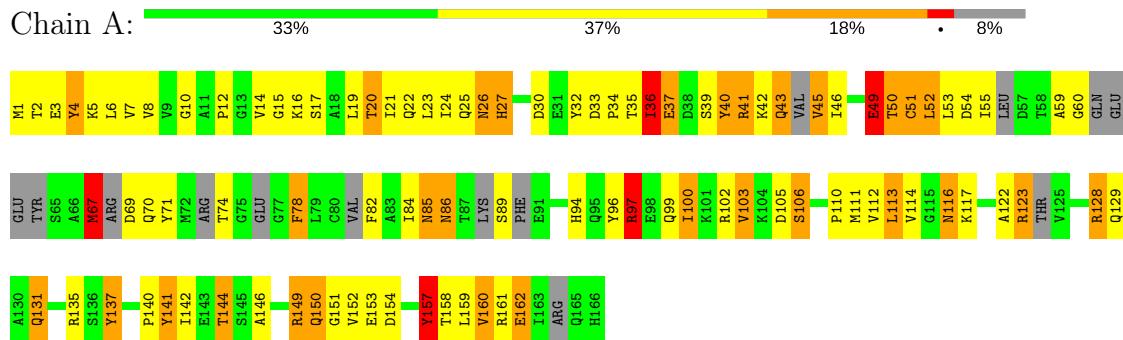
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	43	18	6	16	3	0	0

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 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: C-H-RAS P21 PROTEIN

Chain A:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	40.40Å 40.40Å 158.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 9.69 – 2.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.80) 56.4 (9.69-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.04 , 5.3	EDS
L-test for twinning[1]	$< |L| > = 0.24$, $< L^2 > = 0.09$	Xtriage
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
F_o,F_c correlation	0.67	EDS
Total number of atoms	1224	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Theoretical 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.14	1/1172 (0.1%)	1.93	36/1550 (2.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	VAL	CA-CB	6.14	1.67	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	TYR	CB-CG-CD1	12.63	128.58	121.00
1	A	157	TYR	CB-CG-CD2	-10.39	114.76	121.00
1	A	135	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	A	30	ASP	CB-CG-OD1	9.53	126.88	118.30
1	A	137	TYR	CB-CG-CD2	-9.27	115.44	121.00
1	A	37	GLU	CA-C-N	-8.83	97.78	117.20
1	A	135	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	36	ILE	CA-C-N	8.47	135.83	117.20
1	A	41	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	41	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	128	ARG	NE-CZ-NH2	7.91	124.25	120.30
1	A	67	MET	CG-SD-CE	7.40	112.04	100.20

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	70	GLN	CB-CG-CD	6.90	129.53	111.60
1	A	78	PHE	CA-C-N	-6.88	102.06	117.20
1	A	102	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	86	ASN	CA-C-N	-6.70	102.47	117.20
1	A	40	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	A	105	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	96	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	A	1	MET	CG-SD-CE	6.40	110.44	100.20
1	A	129	GLN	O-C-N	6.28	132.75	122.70
1	A	160	VAL	CG1-CB-CG2	-6.04	101.23	110.90
1	A	99	GLN	OE1-CD-NE2	-6.02	108.05	121.90
1	A	158	THR	OG1-CB-CG2	-6.00	96.20	110.00
1	A	106	SER	CA-C-N	-5.81	104.42	117.20
1	A	36	ILE	O-C-N	-5.67	113.63	122.70
1	A	37	GLU	O-C-N	5.66	131.75	122.70
1	A	122	ALA	CA-C-N	-5.59	104.89	117.20
1	A	49	GLU	CA-C-N	-5.57	104.94	117.20
1	A	162	GLU	O-C-N	5.54	131.56	122.70
1	A	26	ASN	CB-CG-ND2	5.46	129.80	116.70
1	A	137	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	123	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	157	TYR	CA-C-N	5.33	128.93	117.20
1	A	10	GLY	O-C-N	5.33	131.22	122.70
1	A	122	ALA	O-C-N	5.16	130.95	122.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	157	TYR	Sidechain
1	A	32	TYR	Sidechain
1	A	4	TYR	Sidechain
1	A	97	ARG	Sidechain

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	1180	0	1122	81	0
2	A	1	0	0	0	0
3	A	43	0	20	8	0
All	All	1224	0	1142	82	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 35.

All (82) 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:22:GLN:HG2	1:A:152:VAL:HG21	1.48	0.96
1:A:84:ILE:HD13	1:A:123:ARG:HB3	1.50	0.91
1:A:45:VAL:HG13	1:A:50:THR:HG23	1.59	0.82
1:A:39:SER:O	1:A:40:TYR:N	2.19	0.76
1:A:14:VAL:O	1:A:15:GLY:N	2.21	0.74
1:A:117:LYS:HG2	3:A:167:CAG:C6	2.18	0.73
1:A:22:GLN:O	1:A:23:LEU:N	2.23	0.72
1:A:51:CYS:SG	1:A:52:LEU:O	2.50	0.70
1:A:24:ILE:HD12	1:A:42:LYS:HB2	1.72	0.70
1:A:159:LEU:O	1:A:162:GLU:HB2	1.92	0.69
1:A:144:THR:HG22	1:A:151:GLY:O	1.93	0.68
1:A:33:ASP:O	1:A:34:PRO:N	2.27	0.68
1:A:69:ASP:HA	1:A:103:VAL:HG11	1.77	0.65
1:A:4:TYR:HD2	1:A:51:CYS:SG	2.19	0.65
1:A:117:LYS:HE2	3:A:167:CAG:C8	2.27	0.65
1:A:35:THR:HG22	1:A:59:ALA:HA	1.78	0.65
1:A:35:THR:CG2	1:A:59:ALA:HA	2.30	0.61
1:A:7:VAL:O	1:A:8:VAL:N	2.33	0.61
1:A:114:VAL:HG13	1:A:144:THR:OG1	1.99	0.61
1:A:51:CYS:SG	1:A:52:LEU:N	2.73	0.61
1:A:19:LEU:HD21	1:A:116:ASN:ND2	2.17	0.60
1:A:52:LEU:HD22	1:A:53:LEU:H	1.69	0.58
1:A:12:PRO:HG3	1:A:60:GLY:C	2.25	0.57
1:A:24:ILE:HD11	1:A:55:ILE:HD11	1.85	0.57
1:A:41:ARG:HA	1:A:53:LEU:O	2.05	0.56
1:A:20:THR:OG1	1:A:55:ILE:HG21	2.06	0.55
1:A:3:GLU:HG2	1:A:5:LYS:HG3	1.87	0.55
1:A:6:LEU:HD13	1:A:159:LEU:HD23	1.87	0.55
1:A:35:THR:HG21	3:A:167:CAG:O1G	2.07	0.55
1:A:14:VAL:CG2	1:A:16:LYS:HG3	2.38	0.54
1:A:15:GLY:HA2	3:A:167:CAG:PA	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:ND2	1:A:117:LYS:H	2.06	0.53
1:A:78:PHE:O	1:A:111:MET:HA	2.08	0.53
1:A:17:SER:HB2	3:A:167:CAG:O1A	2.09	0.52
1:A:19:LEU:HD21	1:A:116:ASN:HD21	1.75	0.51
1:A:85:ASN:H	1:A:85:ASN:HD22	1.58	0.51
1:A:131:GLN:OE1	1:A:141:TYR:HB3	2.11	0.51
1:A:22:GLN:NE2	1:A:146:ALA:O	2.44	0.51
1:A:8:VAL:CG1	1:A:16:LYS:HB3	2.40	0.51
1:A:4:TYR:CG	1:A:160:VAL:HG22	2.47	0.49
1:A:157:TYR:O	1:A:161:ARG:HG3	2.13	0.48
1:A:35:THR:HG22	1:A:59:ALA:CA	2.44	0.48
1:A:46:ILE:HD12	1:A:160:VAL:HG21	1.96	0.48
3:A:167:CAG:O3G	3:A:167:CAG:O'L	2.32	0.48
1:A:22:GLN:CG	1:A:152:VAL:HG21	2.33	0.48
1:A:21:ILE:O	1:A:25:GLN:HB2	2.14	0.47
1:A:23:LEU:HD13	1:A:153:GLU:HG2	1.97	0.47
1:A:6:LEU:HD22	1:A:159:LEU:CD2	2.45	0.47
1:A:82:PHE:CE1	1:A:84:ILE:HG22	2.49	0.47
1:A:6:LEU:HD22	1:A:159:LEU:HG	1.97	0.47
1:A:112:VAL:HG12	1:A:114:VAL:HG23	1.97	0.46
1:A:78:PHE:HB2	1:A:111:MET:CE	2.45	0.46
1:A:142:ILE:HG22	1:A:144:THR:HG23	1.96	0.46
1:A:78:PHE:HB2	1:A:111:MET:HE2	1.97	0.46
1:A:111:MET:HB2	1:A:111:MET:HE3	1.69	0.46
1:A:117:LYS:HG2	3:A:167:CAG:C5	2.45	0.46
1:A:16:LYS:HE2	1:A:16:LYS:HB2	1.79	0.45
1:A:14:VAL:O	1:A:15:GLY:CA	2.64	0.45
1:A:86:ASN:HB3	1:A:89:SER:OG	2.17	0.45
1:A:42:LYS:HG3	1:A:43:GLN:O	2.17	0.44
1:A:4:TYR:CD2	1:A:51:CYS:SG	3.06	0.44
1:A:36:ILE:HG13	1:A:37:GLU:N	2.33	0.44
1:A:52:LEU:HD22	1:A:53:LEU:N	2.31	0.44
1:A:94:HIS:HA	1:A:137:TYR:OH	2.18	0.44
1:A:21:ILE:HG22	1:A:27:HIS:O	2.18	0.43
1:A:4:TYR:CB	1:A:53:LEU:HD23	2.48	0.43
1:A:84:ILE:HD11	1:A:117:LYS:O	2.19	0.43
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.79	0.43
1:A:144:THR:HG22	1:A:151:GLY:C	2.39	0.43
1:A:14:VAL:O	1:A:117:LYS:HE3	2.19	0.42
1:A:46:ILE:HG12	1:A:157:TYR:CD2	2.54	0.42
1:A:84:ILE:HD13	1:A:123:ARG:CB	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HA	1:A:100:ILE:HD11	2.02	0.42
1:A:45:VAL:HA	1:A:49:GLU:O	2.19	0.41
1:A:12:PRO:HB2	3:A:167:CAG:H6'	2.03	0.41
1:A:149:ARG:HD3	1:A:149:ARG:HA	1.84	0.41
1:A:67:MET:O	1:A:71:TYR:CD2	2.74	0.41
1:A:6:LEU:HD22	1:A:159:LEU:CG	2.50	0.41
1:A:42:LYS:HD2	1:A:42:LYS:HA	1.76	0.41
1:A:46:ILE:HG12	1:A:157:TYR:CE2	2.56	0.41
1:A:110:PRO:HB3	1:A:162:GLU:HB3	2.02	0.41
1:A:4:TYR:HB2	1:A:51:CYS:SG	2.61	0.40

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	114/166 (69%)	98 (86%)	14 (12%)	2 (2%)	10	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	150	GLN

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	126/145 (87%)	99 (79%)	27 (21%)	1 3

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	20	THR
1	A	26	ASN
1	A	27	HIS
1	A	43	GLN
1	A	45	VAL
1	A	49	GLU
1	A	50	THR
1	A	51	CYS
1	A	52	LEU
1	A	54	ASP
1	A	67	MET
1	A	74	THR
1	A	85	ASN
1	A	97	ARG
1	A	100	ILE
1	A	103	VAL
1	A	106	SER
1	A	113	LEU
1	A	116	ASN
1	A	128	ARG
1	A	131	GLN
1	A	140	PRO
1	A	144	THR
1	A	149	ARG
1	A	150	GLN
1	A	154	ASP

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

Mol	Chain	Res	Type
1	A	85	ASN
1	A	116	ASN
1	A	166	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 ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	CAG	A	167	2	34,46,46	2.91	8 (23%)	33,71,71	1.71	5 (15%)

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	CAG	A	167	2	-	0/32/51/51	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	167	CAG	C4-N9	-8.95	1.35	1.47
3	A	167	CAG	C5-C6	-6.27	1.41	1.53
3	A	167	CAG	C2'-C1'	-3.52	1.36	1.40
3	A	167	CAG	C8-N9	-3.12	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	167	CAG	O3G-C'	-2.81	1.42	1.45
3	A	167	CAG	C6'-C1'	-2.70	1.36	1.39
3	A	167	CAG	C6-N1	2.96	1.38	1.33
3	A	167	CAG	O'M-N2'	9.86	1.40	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	167	CAG	O3B-PG-O3G	-2.67	97.28	102.05
3	A	167	CAG	C2B-C1B-N9	-2.48	106.92	113.34
3	A	167	CAG	O6-C6-N1	-2.16	119.82	122.70
3	A	167	CAG	O3G-C'-C1'	4.75	117.57	109.47
3	A	167	CAG	O6-C6-C5	4.91	129.07	119.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	167	CAG	8	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 ⓘ

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, 95th 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^2)	Q<0.9
1	A	152/166 (91%)	-1.59	0	100	100	2, 22, 51, 72	0

There are no RSRZ outliers to report.

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, 95th 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^2)	Q<0.9
3	CAG	A	167	43/43	0.99	0.06	-0.65	25,25,25,25	0
2	MG	A	168	1/1	1.00	0.05	-1.97	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.