



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:07 PM GMT

PDB ID : 1WQ1
Title : RAS-RASGAP COMPLEX
Authors : Scheffzek, K.; Ahmadian, M.R.; Kabsch, W.; Wiesmueller, L.; Lautwein, A.; Schmitz, F.; Wittinghofer, A.
Deposited on : 1997-07-03
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

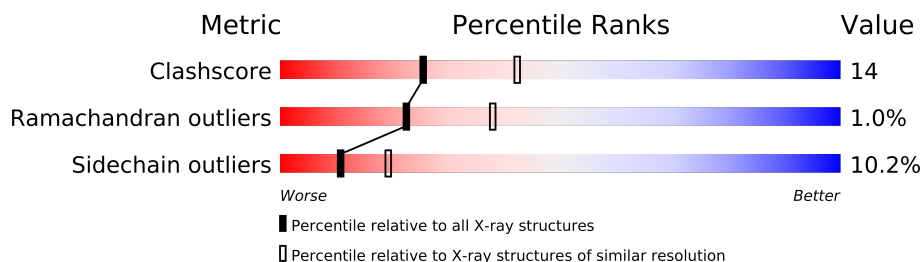
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 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))
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	R	166	
2	G	334	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3922 atoms, of which 0 are hydrogen 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 H-RAS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	166	Total	C	N	O	S	0	0	0
			1322	823	228	264	7			

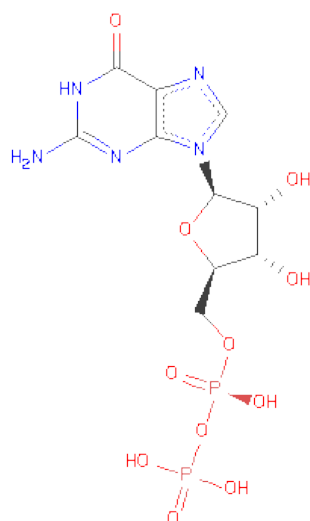
- Molecule 2 is a protein called P120GAP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	320	Total	C	N	O	S	0	0	0
			2532	1611	431	473	17			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

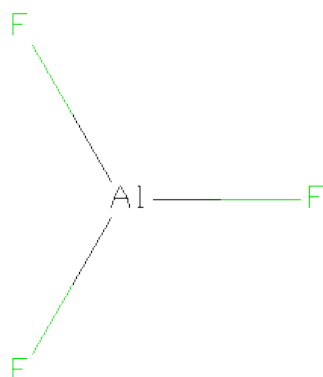
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	R	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	R	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	24	Total	O	0	0
			24	24		
6	R	11	Total	O	0	0
			11	11		

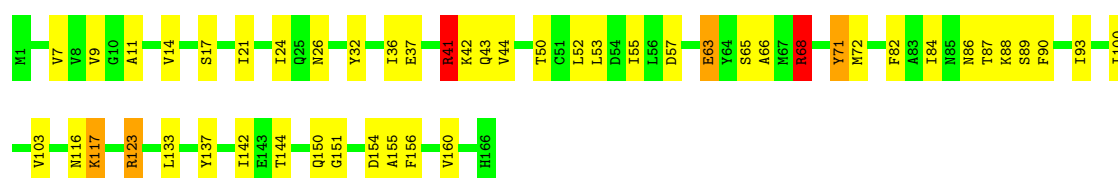
3 Residue-property plots

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.

Note EDS was not executed.

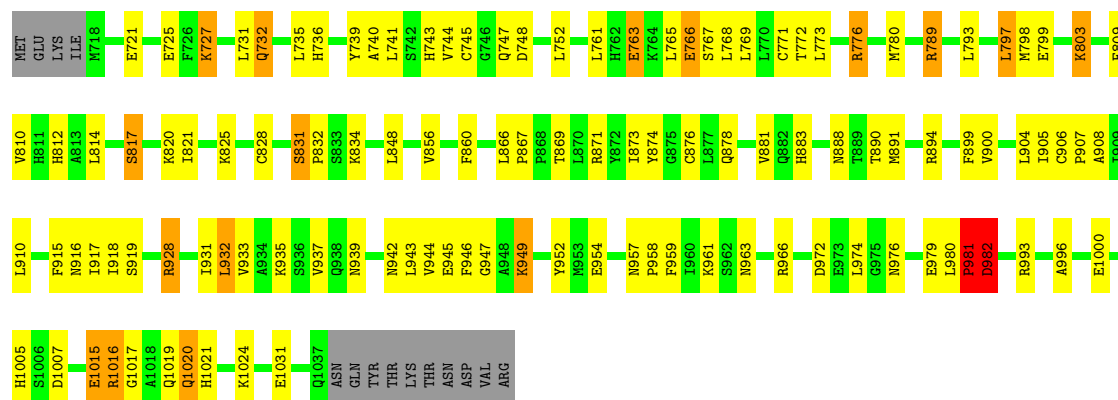
• Molecule 1: H-RAS

Chain R: 



• Molecule 2: P120GAP

Chain G: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.90Å 41.10Å 89.00Å 90.00° 108.40° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50	Depositor
% Data completeness (in resolution range)	77.3 (30.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.233 , 0.319	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3922	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, AF3

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	R	0.42	0/1341	0.56	1/1808 (0.1%)
2	G	0.46	1/2574 (0.0%)	0.55	2/3483 (0.1%)
All	All	0.45	1/3915 (0.0%)	0.55	3/5291 (0.1%)

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	R	0	4
2	G	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	981	PRO	C-O	8.20	1.39	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	982	ASP	N-CA-C	7.16	130.33	111.00
1	R	41	ARG	NE-CZ-NH1	-6.85	116.87	120.30
2	G	981	PRO	N-CA-C	6.57	129.17	112.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	981	PRO	Peptide
2	G	982	ASP	Mainchain
1	R	123	ARG	Sidechain
1	R	41	ARG	Sidechain
1	R	68	ARG	Sidechain
1	R	71	TYR	Sidechain

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	R	1322	0	1290	31	0
2	G	2532	0	2587	79	0
3	R	1	0	0	0	0
4	R	28	0	12	1	0
5	R	4	0	0	0	0
6	G	24	0	0	1	0
6	R	11	0	0	0	0
All	All	3922	0	3889	105	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 14.

All (105) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:761:LEU:HD23	2:G:766:GLU:HG2	1.59	0.84
2:G:739:TYR:CE1	2:G:773:LEU:HD12	2.15	0.81
2:G:832:PRO:HD3	2:G:952:TYR:HB3	1.68	0.76
1:R:41:ARG:HE	1:R:52:LEU:HD21	1.51	0.74
2:G:736:HIS:CD2	2:G:1019:GLN:HG2	2.28	0.69
1:R:84:ILE:HD12	1:R:123:ARG:HB2	1.78	0.65
2:G:957:ASN:HB3	2:G:961:LYS:NZ	2.14	0.63
2:G:866:LEU:HD21	2:G:874:TYR:HE2	1.66	0.60
2:G:957:ASN:N	2:G:958:PRO:HD2	2.17	0.60
2:G:727:LYS:HD3	2:G:731:LEU:HD11	1.83	0.60
1:R:72:MET:HE1	1:R:100:ILE:HG13	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:142:ILE:HD13	1:R:155:ALA:HA	1.83	0.60
2:G:799:GLU:O	2:G:803:LYS:HD3	2.01	0.59
2:G:946:PHE:H	2:G:957:ASN:HD21	1.49	0.59
2:G:810:VAL:HG13	2:G:814:LEU:HD22	1.84	0.59
2:G:776:ARG:NH1	2:G:780:MET:SD	2.75	0.59
2:G:810:VAL:O	2:G:814:LEU:HB2	2.03	0.58
1:R:42:LYS:HE2	1:R:44:VAL:CG1	2.33	0.58
1:R:21:ILE:HD11	2:G:949:LYS:HG2	1.86	0.57
2:G:803:LYS:HZ2	2:G:915:PHE:HZ	1.49	0.57
1:R:82:PHE:HB3	1:R:93:ILE:HD11	1.86	0.57
2:G:888:ASN:OD1	2:G:890:THR:HG22	2.04	0.57
2:G:980:LEU:HD12	2:G:981:PRO:HD2	1.86	0.56
1:R:32:TYR:HB2	2:G:894:ARG:NH1	2.21	0.56
2:G:739:TYR:CE1	2:G:776:ARG:HG3	2.40	0.56
2:G:928:ARG:HD2	2:G:932:LEU:HD22	1.89	0.55
2:G:957:ASN:HB3	2:G:961:LYS:HZ3	1.72	0.55
2:G:908:ALA:HB2	2:G:915:PHE:CE1	2.42	0.54
2:G:741:LEU:HA	2:G:744:VAL:HG22	1.89	0.54
2:G:798:MET:HG3	2:G:899:PHE:CE1	2.44	0.52
2:G:740:ALA:HA	2:G:743:HIS:HD2	1.74	0.52
2:G:996:ALA:O	2:G:1000:GLU:HG3	2.10	0.51
1:R:68:ARG:HA	1:R:71:TYR:CE2	2.47	0.50
2:G:767:SER:O	2:G:771:CYS:HB2	2.12	0.49
2:G:803:LYS:NZ	2:G:915:PHE:HZ	2.10	0.49
1:R:68:ARG:HG3	1:R:71:TYR:OH	2.13	0.49
2:G:1017:GLY:O	2:G:1020:GLN:HB2	2.12	0.49
2:G:732:GLN:HA	2:G:732:GLN:HE21	1.77	0.48
2:G:942:ASN:O	2:G:943:LEU:HB2	2.14	0.48
2:G:963:ASN:HD22	2:G:966:ARG:HD3	1.79	0.48
2:G:1016:ARG:HA	2:G:1020:GLN:HG3	1.94	0.48
2:G:735:LEU:HD12	2:G:772:THR:HB	1.95	0.48
4:R:167:GDP:H5''	2:G:789:ARG:NH2	2.28	0.48
2:G:856:VAL:HG12	2:G:860:PHE:CE2	2.49	0.48
2:G:918:ILE:HG13	2:G:919:SER:H	1.78	0.48
1:R:84:ILE:HD12	1:R:123:ARG:CB	2.43	0.47
1:R:116:ASN:O	1:R:117:LYS:HB2	2.13	0.47
2:G:761:LEU:HD23	2:G:766:GLU:CG	2.39	0.47
2:G:856:VAL:HG21	2:G:959:PHE:HZ	1.79	0.47
2:G:1015:GLU:O	2:G:1020:GLN:HG3	2.15	0.47
2:G:933:VAL:O	2:G:937:VAL:HG23	2.14	0.47
2:G:740:ALA:HA	2:G:743:HIS:CD2	2.50	0.47
2:G:789:ARG:NH2	6:G:220:HOH:O	2.46	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:873:ILE:O	2:G:876:CYS:HB2	2.15	0.47
2:G:900:VAL:O	2:G:905:ILE:HG12	2.15	0.46
2:G:904:LEU:HD12	2:G:915:PHE:HZ	1.80	0.46
1:R:65:SER:O	1:R:66:ALA:HB3	2.16	0.46
2:G:931:ILE:O	2:G:935:LYS:HG3	2.16	0.46
2:G:763:GLU:O	2:G:765:LEU:HG	2.16	0.46
2:G:745:CYS:SG	2:G:752:LEU:HD22	2.55	0.46
2:G:731:LEU:HD22	2:G:765:LEU:HD12	1.98	0.46
2:G:878:GLN:HA	2:G:881:VAL:HG22	1.97	0.46
2:G:735:LEU:HD11	2:G:769:LEU:HA	1.99	0.45
1:R:36:ILE:HG23	2:G:910:LEU:HD11	1.97	0.45
2:G:748:ASP:OD2	2:G:1005:HIS:HE1	1.99	0.45
1:R:156:PHE:O	1:R:160:VAL:HG23	2.17	0.45
2:G:810:VAL:HG12	2:G:917:ILE:HD11	1.99	0.45
2:G:773:LEU:CD2	2:G:797:LEU:HD23	2.47	0.45
2:G:831:SER:HB2	2:G:834:LYS:HB2	1.98	0.45
1:R:21:ILE:HD11	2:G:949:LYS:CG	2.46	0.45
1:R:24:ILE:HD11	1:R:55:ILE:HD12	1.99	0.45
2:G:809:PHE:HE2	2:G:905:ILE:HD11	1.81	0.45
1:R:144:THR:HA	1:R:150:GLN:O	2.17	0.45
1:R:87:THR:O	1:R:90:PHE:HB3	2.17	0.44
2:G:817:SER:O	2:G:821:ILE:HG13	2.18	0.44
2:G:793:LEU:HG	2:G:797:LEU:HD22	2.00	0.44
2:G:797:LEU:HA	2:G:797:LEU:HD12	1.79	0.43
2:G:828:CYS:HB3	2:G:848:LEU:HD13	2.00	0.43
1:R:133:LEU:HG	1:R:137:TYR:CE2	2.53	0.43
2:G:766:GLU:HG3	2:G:766:GLU:H	1.45	0.43
2:G:831:SER:HA	2:G:832:PRO:HD3	1.77	0.43
1:R:88:LYS:HE2	1:R:88:LYS:HB3	1.69	0.43
2:G:908:ALA:HB2	2:G:915:PHE:HE1	1.82	0.43
2:G:963:ASN:ND2	2:G:966:ARG:HH11	2.16	0.43
1:R:63:GLU:HG2	1:R:63:GLU:H	1.43	0.43
2:G:974:LEU:HA	2:G:974:LEU:HD12	1.80	0.42
2:G:809:PHE:CE2	2:G:905:ILE:HD11	2.54	0.42
1:R:72:MET:HB3	1:R:103:VAL:HG21	2.02	0.42
2:G:918:ILE:HG23	2:G:919:SER:N	2.35	0.42
1:R:144:THR:HG22	1:R:151:GLY:O	2.19	0.42
1:R:7:VAL:HG12	1:R:9:VAL:HG13	2.02	0.42
1:R:144:THR:HG22	1:R:151:GLY:C	2.40	0.42
1:R:11:ALA:O	1:R:14:VAL:HG22	2.20	0.42
2:G:980:LEU:HD12	2:G:981:PRO:CD	2.50	0.41
2:G:735:LEU:HB3	2:G:739:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:R:17:SER:HA	1:R:57:ASP:OD2	2.19	0.41
2:G:888:ASN:ND2	2:G:891:MET:HG2	2.34	0.41
2:G:980:LEU:HA	2:G:981:PRO:HD3	1.67	0.41
1:R:32:TYR:CD2	2:G:894:ARG:HD3	2.55	0.41
2:G:1021:HIS:HA	2:G:1024:LYS:HD2	2.03	0.41
2:G:906:CYS:HB2	2:G:907:PRO:HD3	2.03	0.41
1:R:86:ASN:OD1	1:R:89:SER:HB3	2.21	0.40
2:G:867:PRO:O	2:G:871:ARG:HG3	2.21	0.40
2:G:904:LEU:HD12	2:G:915:PHE:CZ	2.57	0.40
1:R:42:LYS:HG2	1:R:44:VAL:HG13	2.02	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	R	164/166 (99%)	154 (94%)	8 (5%)	2 (1%)	19	32
2	G	318/334 (95%)	294 (92%)	21 (7%)	3 (1%)	25	42
All	All	482/500 (96%)	448 (93%)	29 (6%)	5 (1%)	22	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	947	GLY
2	G	949	LYS
2	G	982	ASP
1	R	37	GLU
1	R	117	LYS

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	R	144/144 (100%)	136 (94%)	8 (6%)	30	51	
2	G	287/307 (94%)	251 (88%)	36 (12%)	7	12	
All	All	431/451 (96%)	387 (90%)	44 (10%)	11	19	

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	26	ASN
1	R	41	ARG
1	R	43	GLN
1	R	50	THR
1	R	53	LEU
1	R	63	GLU
1	R	68	ARG
1	R	154	ASP
2	G	721	GLU
2	G	725	GLU
2	G	727	LYS
2	G	732	GLN
2	G	747	GLN
2	G	763	GLU
2	G	766	GLU
2	G	768	LEU
2	G	776	ARG
2	G	789	ARG
2	G	797	LEU
2	G	803	LYS
2	G	812	HIS
2	G	817	SER
2	G	820	LYS
2	G	825	LYS
2	G	831	SER
2	G	869	THR
2	G	883	HIS
2	G	916	ASN
2	G	928	ARG
2	G	932	LEU
2	G	939	ASN
2	G	944	VAL
2	G	945	GLU

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Mol	Chain	Res	Type
2	G	954	GLU
2	G	972	ASP
2	G	976	ASN
2	G	979	GLU
2	G	981	PRO
2	G	993	ARG
2	G	1007	ASP
2	G	1015	GLU
2	G	1016	ARG
2	G	1020	GLN
2	G	1031	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	25	GLN
2	G	732	GLN
2	G	743	HIS
2	G	747	GLN
2	G	826	GLN
2	G	844	ASN
2	G	847	HIS
2	G	882	GLN
2	G	938	GLN
2	G	957	ASN
2	G	963	ASN
2	G	999	HIS
2	G	1005	HIS
2	G	1014	ASN
2	G	1037	GLN

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 ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
4	GDP	R	167	3,5	30,30,30	1.26	5 (16%)	44,47,47	4.04	5 (11%)
5	AF3	R	169	3,2,4,6	0,3,3	0.00	-	0,3,3	0.00	-

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	GDP	R	167	3,5	-	0/16/32/32	0/1/3/3
5	AF3	R	169	3,2,4,6	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	167	GDP	PB-O2B	-2.69	1.44	1.54
4	R	167	GDP	C8-N7	-2.60	1.29	1.34
4	R	167	GDP	C8-N9	-2.22	1.33	1.36
4	R	167	GDP	PA-O2A	-2.10	1.45	1.55
4	R	167	GDP	C2'-C1'	-2.05	1.50	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	167	GDP	C6-C5-N7	-25.38	130.72	134.14
4	R	167	GDP	C8-N9-C4	-4.55	103.43	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	167	GDP	C6-N1-C2	3.95	126.41	119.51
4	R	167	GDP	O4'-C1'-C2'	-2.27	103.29	106.77
4	R	167	GDP	O2B-PB-O1B	2.14	117.43	110.44

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.