



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:38 AM GMT

PDB ID : 2RGN  
Title : Crystal Structure of p63RhoGEF complex with Galpha-q and RhoA  
Authors : Shankaranarayanan, A.; Nance, M.R.; Tesmer, J.J.G.  
Deposited on : 2007-10-04  
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

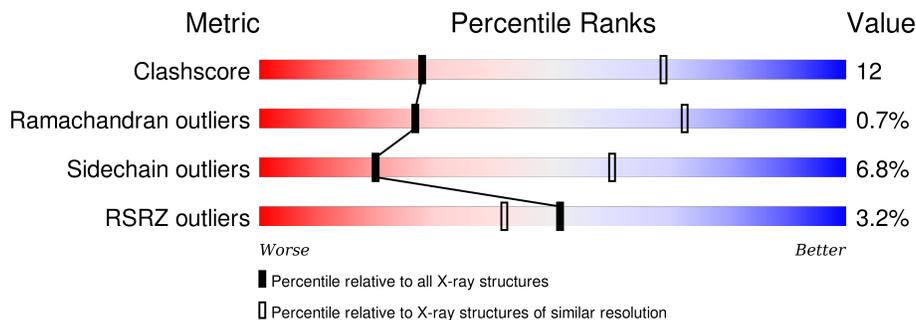
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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. 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  $\leq 5\%$ . 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	353	
1	D	353	
2	B	354	
2	E	354	
3	C	196	
3	F	196	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13529 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 Guanine nucleotide-binding protein G(q) subunit alpha, Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2680	1710	454	504	12	0	0	0
1	D	324	2680	1710	454	504	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	ARG	-	linker	UNP P10824
A	36	SER	-	linker	UNP P10824
D	35	ARG	-	linker	UNP P10824
D	36	SER	-	linker	UNP P10824

- Molecule 2 is a protein called RhoA/RAC/CDC42 exchange factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	327	2677	1697	472	492	16	0	0	0
2	E	326	2671	1694	471	490	16	0	0	0

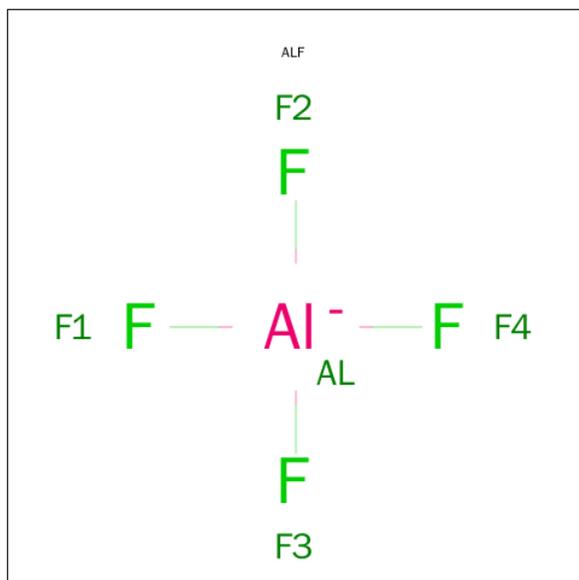
- Molecule 3 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	177	1408	891	238	269	10	0	0	0
3	F	168	1339	847	227	255	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P61586
C	-1	GLU	-	expression tag	UNP P61586
C	0	PHE	-	expression tag	UNP P61586
F	-2	GLY	-	expression tag	UNP P61586
F	-1	GLU	-	expression tag	UNP P61586
F	0	PHE	-	expression tag	UNP P61586

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $\text{AlF}_4$ ).

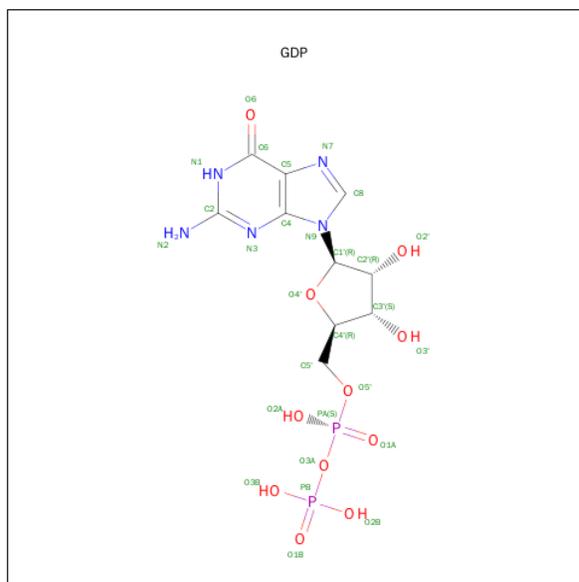


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
4	A	1	5	1	4	0	0
4	D	1	5	1	4	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	D	1	1	1	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$ ).

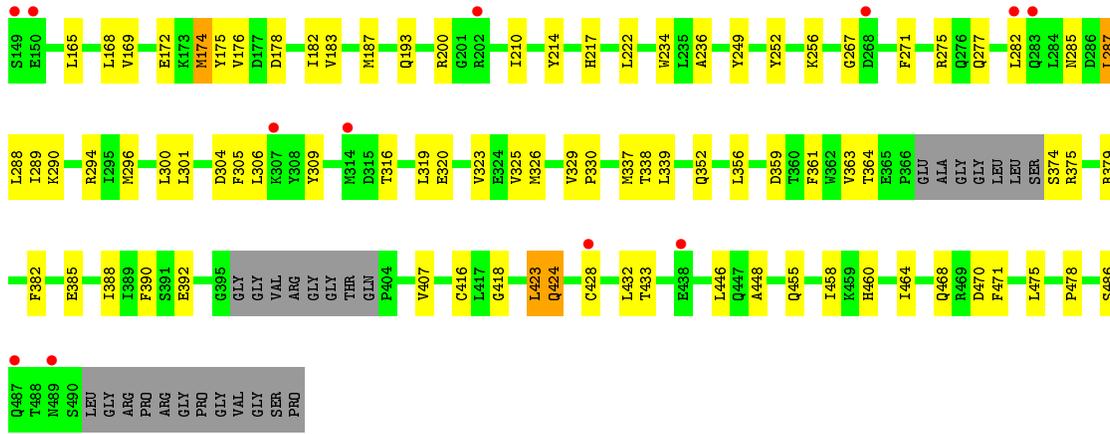


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

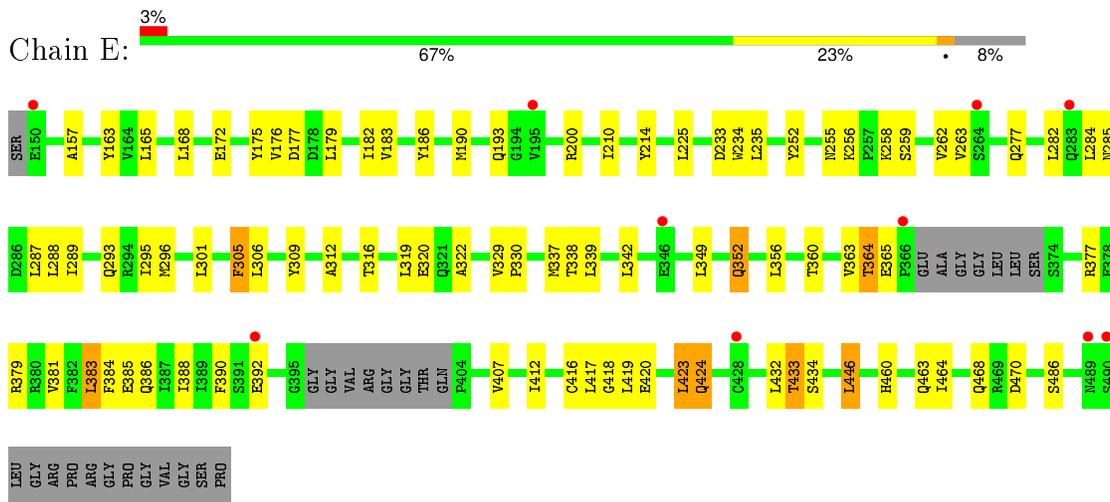
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	O	0	0
			3	3		
7	D	3	Total	O	0	0
			3	3		

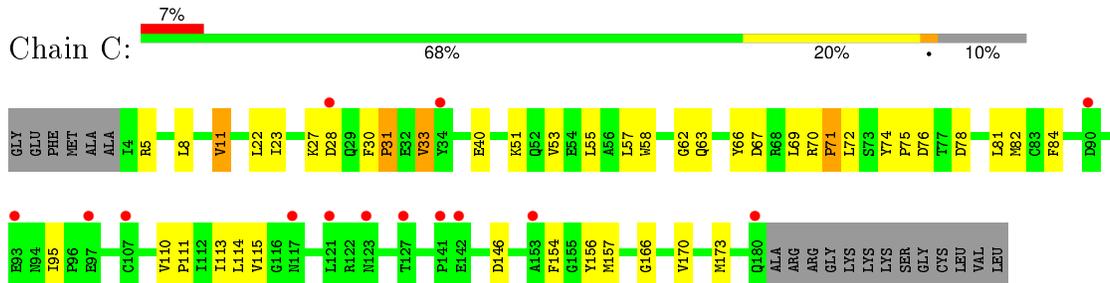




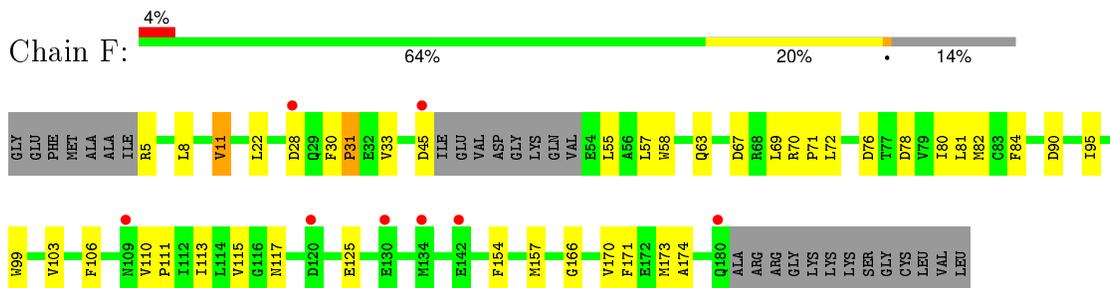
• Molecule 2: RhoA/RAC/CDC42 exchange factor



• Molecule 3: Transforming protein RhoA



• Molecule 3: Transforming protein RhoA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.19Å 68.06Å 138.02Å 80.87° 85.16° 87.09°	Depositor
Resolution (Å)	20.00 – 3.50 19.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-3.50) 91.9 (19.99-3.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.52Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.243 , 0.299 0.233 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	102.1	Xtrriage
Anisotropy	0.146	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 123.9	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Outliers	0 of 29080 reflections	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	144.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 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: GDP, ALF, MG

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	0.54	0/2737	0.64	0/3698
1	D	0.54	0/2737	0.63	0/3698
2	B	0.49	0/2728	0.59	0/3667
2	E	0.46	0/2722	0.57	0/3659
3	C	0.40	0/1436	0.53	0/1942
3	F	0.38	0/1366	0.52	0/1846
All	All	0.48	0/13726	0.59	0/18510

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	2680	0	2645	75	0
1	D	2680	0	2645	69	0
2	B	2677	0	2661	64	0
2	E	2671	0	2656	61	0
3	C	1408	0	1400	39	0
3	F	1339	0	1325	30	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	28	0	12	1	0
6	D	28	0	12	1	0
7	A	3	0	0	0	0
7	D	3	0	0	0	0
All	All	13529	0	13356	316	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 12.

The worst 5 of 316 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:153:LEU:HD11	1:A:157:THR:HG21	1.22	1.09
1:A:153:LEU:CD1	1:A:157:THR:HG21	1.91	1.00
1:A:259:ILE:HD11	1:A:269:VAL:HG11	1.58	0.85
1:A:78:LEU:HD13	1:A:184:VAL:HG21	1.60	0.82
1:D:78:LEU:HD13	1:D:184:VAL:HG21	1.60	0.81

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	322/353 (91%)	287 (89%)	34 (11%)	1 (0%)	46 84
1	D	322/353 (91%)	289 (90%)	32 (10%)	1 (0%)	46 84
2	B	321/354 (91%)	294 (92%)	26 (8%)	1 (0%)	46 84
2	E	320/354 (90%)	292 (91%)	27 (8%)	1 (0%)	46 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	175/196 (89%)	157 (90%)	14 (8%)	4 (2%)	8	48
3	F	164/196 (84%)	149 (91%)	12 (7%)	3 (2%)	11	53
All	All	1624/1806 (90%)	1468 (90%)	145 (9%)	11 (1%)	26	72

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	31	PRO
3	F	31	PRO
1	A	318	PRO
3	C	28	ASP
1	D	318	PRO

### 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	Percentiles	
1	A	297/321 (92%)	281 (95%)	16 (5%)	27	67
1	D	297/321 (92%)	272 (92%)	25 (8%)	14	50
2	B	288/304 (95%)	267 (93%)	21 (7%)	17	57
2	E	287/304 (94%)	263 (92%)	24 (8%)	14	50
3	C	156/169 (92%)	150 (96%)	6 (4%)	40	76
3	F	148/169 (88%)	140 (95%)	8 (5%)	27	67
All	All	1473/1588 (93%)	1373 (93%)	100 (7%)	20	60

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	68	SER
1	D	166	ARG
3	F	5	ARG
1	D	92	ARG
1	D	115	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	149	ASN
1	D	162	ASN
3	F	117	ASN
1	D	111	GLN
1	D	176	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z  > 2$
6	GDP	A	360	5,4	23,30,30	1.15	2 (8%)	30,47,47	1.81	6 (20%)
4	ALF	A	361	7,6	0,4,4	0.00	-	0,6,6	0.00	-
6	GDP	D	360	5,4	23,30,30	1.16	3 (13%)	30,47,47	1.82	7 (23%)
4	ALF	D	361	7,6	0,4,4	0.00	-	0,6,6	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
6	GDP	A	360	5,4	-	0/12/32/32	0/3/3/3
4	ALF	A	361	7,6	-	0/0/0/0	0/0/0/0
6	GDP	D	360	5,4	-	0/12/32/32	0/3/3/3
4	ALF	D	361	7,6	-	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)
6	D	360	GDP	C5-C4	2.42	1.46	1.40
6	D	360	GDP	O4'-C1'	2.68	1.44	1.41
6	A	360	GDP	C5-C4	2.87	1.47	1.40
6	D	360	GDP	C6-C5	3.10	1.47	1.41
6	A	360	GDP	C6-C5	3.27	1.47	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	360	GDP	C5-C6-N1	-4.34	117.66	123.59
6	A	360	GDP	C5-C6-N1	-3.99	118.13	123.59
6	A	360	GDP	C6-C5-C4	-3.49	116.73	120.90
6	D	360	GDP	N3-C2-N1	-3.34	122.36	127.44
6	A	360	GDP	N3-C2-N1	-3.30	122.42	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	360	GDP	1	0
6	D	360	GDP	1	0

## 5.7 Other polymers [i](#)

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 [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<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	324/353 (91%)	-0.14	3 (0%) 85 78	135, 143, 150, 158	0
1	D	324/353 (91%)	-0.04	6 (1%) 70 60	136, 144, 150, 158	0
2	B	327/354 (92%)	0.10	12 (3%) 45 36	138, 145, 150, 157	0
2	E	326/354 (92%)	0.09	10 (3%) 52 43	135, 145, 150, 157	0
3	C	177/196 (90%)	0.43	14 (7%) 15 13	143, 145, 147, 149	0
3	F	168/196 (85%)	0.27	8 (4%) 34 27	143, 146, 147, 149	0
All	All	1646/1806 (91%)	0.08	53 (3%) 51 42	135, 145, 149, 158	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	5.6
3	C	28	ASP	5.5
1	D	222	ASN	5.4
2	E	428	CYS	4.7
2	E	490	SER	4.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GDP	D	360	28/28	0.82	0.28	0.04	132,135,142,148	0
6	GDP	A	360	28/28	0.84	0.25	-0.24	133,134,139,145	0
4	ALF	A	361	5/5	0.83	0.25	-0.32	152,152,152,153	0
4	ALF	D	361	5/5	0.89	0.15	-1.85	151,152,153,154	0
5	MG	A	362	1/1	0.79	0.12	-2.78	148,148,148,148	0
5	MG	D	362	1/1	0.95	0.06	-	148,148,148,148	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.