



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 11:25 am GMT

PDB ID : 2ODE  
Title : Crystal structure of the heterodimeric complex of human RGS8 and activated Gi alpha 3  
Authors : Gileadi, C.; Soundararajan, M.; Turnbull, A.P.; Elkins, J.M.; Papagrigoriou, E.; Pike, A.C.W.; Bunkoczi, G.; Gorrec, F.; Umeano, C.; von Delft, F.; Weigelt, J.; Edwards, A.; Arrowsmith, C.H.; Sundstrom, M.; Doyle, D.A.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-12-22  
Resolution : 1.90 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

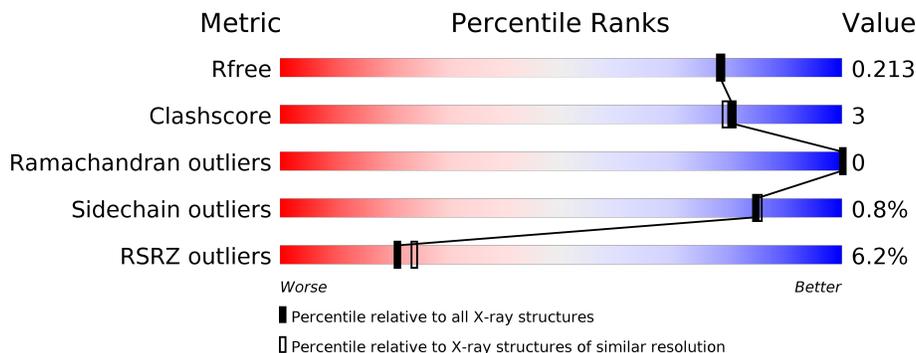
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	350	 8% 85% 5% 10%
1	C	350	 4% 83% 7% 9%
2	B	141	 3% 85% 6% 7%
2	D	141	 5% 77% 6% 18%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7749 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(k) subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	Total	C	N	O	S	0	2	0
			2508	1597	416	479	16			
1	C	317	Total	C	N	O	S	0	4	0
			2511	1599	417	478	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	EXPRESSION TAG	UNP P08754
A	3	MET	-	EXPRESSION TAG	UNP P08754
A	351	SER	-	EXPRESSION TAG	UNP P08754
C	2	SER	-	EXPRESSION TAG	UNP P08754
C	3	MET	-	EXPRESSION TAG	UNP P08754
C	351	SER	-	EXPRESSION TAG	UNP P08754

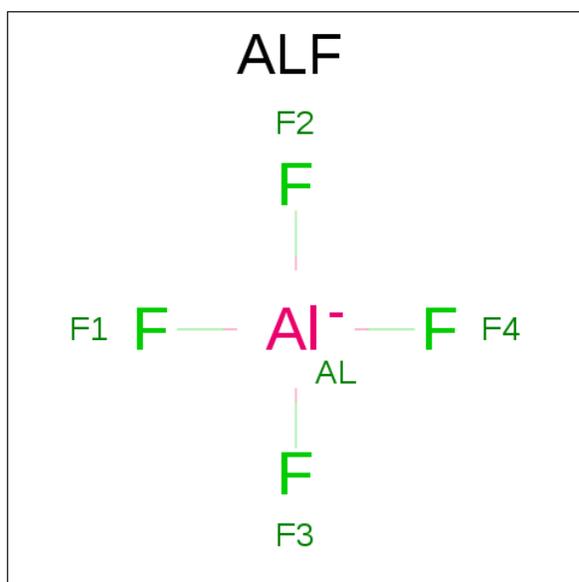
- Molecule 2 is a protein called Regulator of G-protein signaling 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	131	Total	C	N	O	S	0	3	0
			1064	677	175	208	4			
2	D	116	Total	C	N	O	S	0	1	0
			943	607	154	178	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	40	SER	-	EXPRESSION TAG	UNP P57771
B	41	MET	-	EXPRESSION TAG	UNP P57771
D	40	SER	-	EXPRESSION TAG	UNP P57771
D	41	MET	-	EXPRESSION TAG	UNP P57771

- Molecule 3 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula:  $AlF_4$ ).

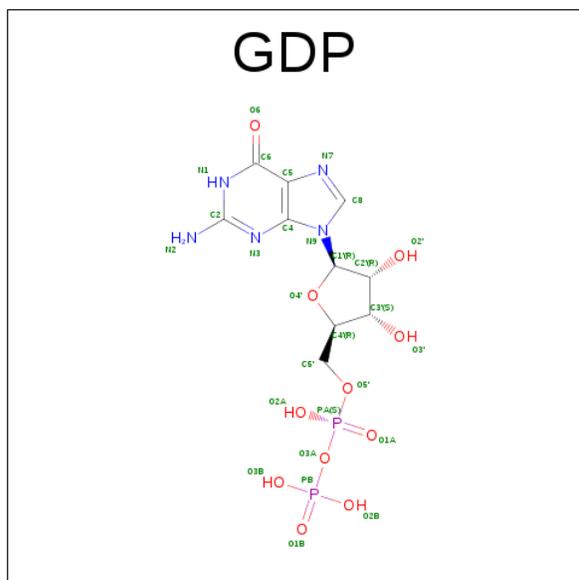


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
3	A	1	5	1	4	0	0
3	C	1	5	1	4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0
4	C	1	1	1	0	0

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

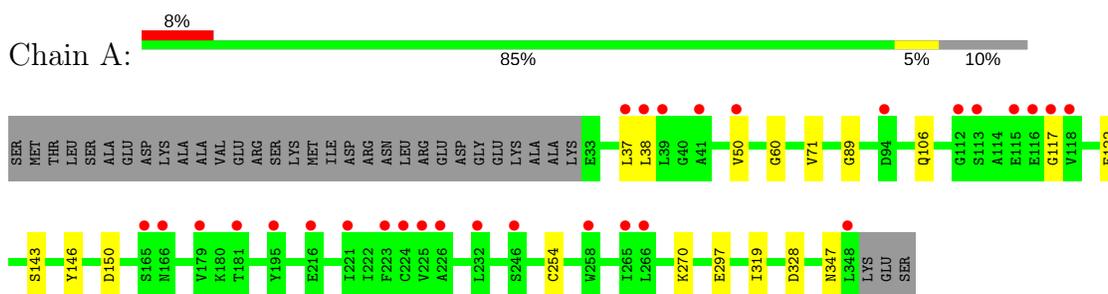
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	261	Total	O	0	0
			261	261		
6	B	99	Total	O	0	0
			99	99		
6	C	213	Total	O	0	0
			213	213		
6	D	82	Total	O	0	0
			82	82		

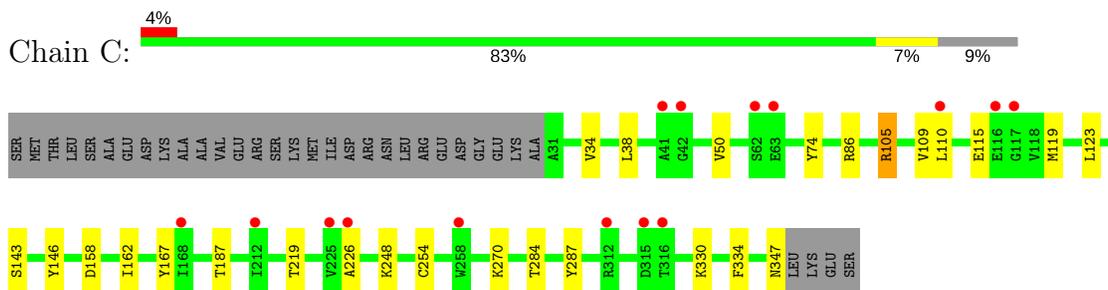
### 3 Residue-property plots [i](#)

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.

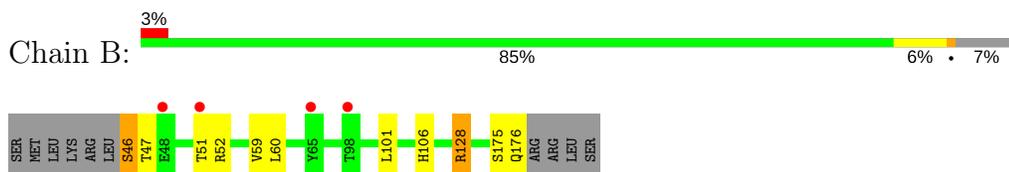
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha



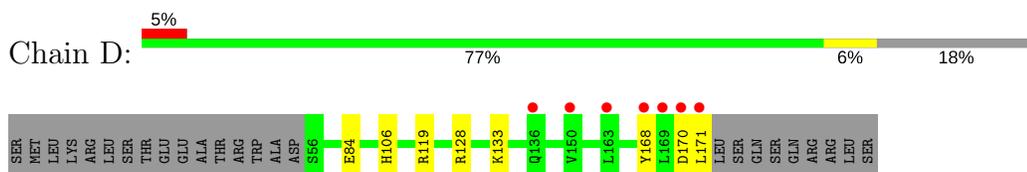
- Molecule 1: Guanine nucleotide-binding protein G(k) subunit alpha



- Molecule 2: Regulator of G-protein signaling 8



- Molecule 2: Regulator of G-protein signaling 8



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.84Å 130.22Å 68.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 1.90 29.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.40-1.90) 99.8 (29.41-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.180 , 0.211 0.184 , 0.213	Depositor DCC
$R_{free}$ test set	4021 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtrriage
Anisotropy	0.041	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.68	0/2559	0.68	1/3457 (0.0%)
1	C	0.69	1/2568 (0.0%)	0.71	1/3472 (0.0%)
2	B	0.74	1/1096 (0.1%)	0.75	2/1480 (0.1%)
2	D	0.74	0/967	0.72	2/1302 (0.2%)
All	All	0.70	2/7190 (0.0%)	0.71	6/9711 (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
2	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	254	CYS	CB-SG	-8.43	1.68	1.82
2	B	46	SER	CB-OG	6.18	1.50	1.42

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	128	ARG	NE-CZ-NH2	7.40	124.00	120.30
2	B	128	ARG	NE-CZ-NH1	7.35	123.98	120.30
2	B	128	ARG	NE-CZ-NH2	-7.18	116.71	120.30
2	D	128	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	328	ASP	CB-CG-OD1	5.30	123.07	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	170	ASP	Peptide

## 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	2508	0	2443	12	0
1	C	2511	0	2425	16	0
2	B	1064	0	997	10	0
2	D	943	0	897	5	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	28	0	12	0	0
5	C	28	0	12	0	0
6	A	261	0	0	6	0
6	B	99	0	0	3	0
6	C	213	0	0	3	0
6	D	82	0	0	3	0
All	All	7749	0	6786	43	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 3.

The worst 5 of 43 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)
2:B:47:THR:HG22	2:B:175:SER:OG	1.44	1.16
2:D:106:HIS:HE1	6:D:226:HOH:O	1.61	0.82
2:B:47:THR:HG23	2:B:176:GLN:HG3	1.74	0.70
2:B:106:HIS:HE1	6:B:268:HOH:O	1.77	0.68
2:B:52:ARG:HG3	2:B:59:VAL:HG11	1.82	0.62

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	316/350 (90%)	312 (99%)	4 (1%)	0	100	100
1	C	319/350 (91%)	314 (98%)	5 (2%)	0	100	100
2	B	132/141 (94%)	130 (98%)	2 (2%)	0	100	100
2	D	115/141 (82%)	113 (98%)	2 (2%)	0	100	100
All	All	882/982 (90%)	869 (98%)	13 (2%)	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	Percentiles	
1	A	268/308 (87%)	267 (100%)	1 (0%)	93	93
1	C	264/308 (86%)	260 (98%)	4 (2%)	70	67
2	B	112/128 (88%)	111 (99%)	1 (1%)	82	82
2	D	98/128 (77%)	98 (100%)	0	100	100
All	All	742/872 (85%)	736 (99%)	6 (1%)	85	85

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	105	ARG
1	C	347	ASN
1	C	115	GLU

*Continued on next page...*

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Mol	Chain	Res	Type
2	B	46	SER
1	C	158	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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$
5	GDP	A	1001	3,4	25,30,30	1.27	4 (16%)	26,47,47	1.99	5 (19%)
3	ALF	A	2001	5,4,6	0,4,4	0.00	-	0,6,6	0.00	-
5	GDP	C	1002	3,4	25,30,30	1.19	3 (12%)	26,47,47	2.03	6 (23%)
3	ALF	C	2002	5,4,6	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
5	GDP	A	1001	3,4	-	0/12/32/32	0/3/3/3
3	ALF	A	2001	5,4,6	-	0/0/0/0	0/0/0/0
5	GDP	C	1002	3,4	-	0/12/32/32	0/3/3/3
3	ALF	C	2002	5,4,6	-	0/0/0/0	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	GDP	C2'-C1'	-2.02	1.50	1.53
5	C	1002	GDP	C6-C5	2.22	1.45	1.41
5	C	1002	GDP	PB-O3A	2.24	1.63	1.60
5	A	1001	GDP	C5-C4	2.87	1.47	1.40
5	C	1002	GDP	C5-C4	2.88	1.47	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1002	GDP	C6-C5-C4	-5.74	115.14	120.84
5	A	1001	GDP	C5-C6-N1	-4.61	116.92	123.48
5	A	1001	GDP	C6-C5-C4	-4.46	116.41	120.84
5	C	1002	GDP	C5-C6-N1	-3.52	118.47	123.48
5	C	1002	GDP	N3-C2-N1	-2.98	123.11	127.46

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<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	316/350 (90%)	0.60	29 (9%) 10 11	29, 34, 42, 58	0
1	C	317/350 (90%)	0.53	15 (4%) 32 36	29, 34, 43, 56	0
2	B	131/141 (92%)	0.30	4 (3%) 49 53	30, 34, 40, 45	0
2	D	116/141 (82%)	0.32	7 (6%) 23 26	30, 34, 40, 44	0
All	All	880/982 (89%)	0.50	55 (6%) 21 24	29, 34, 43, 58	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	169	LEU	5.9
1	C	117	GLY	4.2
2	B	65	TYR	4.1
1	A	118	VAL	4.0
1	C	116	GLU	3.4

### 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( $\text{\AA}^2$ )	Q < 0.9
5	GDP	A	1001	28/28	0.97	0.08	-1.48	17,21,24,25	0
5	GDP	C	1002	28/28	0.98	0.06	-2.44	18,22,24,25	0
3	ALF	C	2002	5/5	0.98	0.05	-4.56	22,22,24,27	0
3	ALF	A	2001	5/5	0.98	0.05	-4.86	20,21,22,23	0
4	MG	A	3001	1/1	0.98	0.05	-4.95	20,20,20,20	0
4	MG	C	3002	1/1	0.96	0.06	-5.11	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.