



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1K5G  
Title : Crystal structure of Ran-GDP-AlFx-RanBP1-RanGAP complex  
Authors : Seewald, M.J.; Koerner, C.; Wittinghofer, A.; Vetter, I.R.  
Deposited on : 2001-10-10  
Resolution : 3.10 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

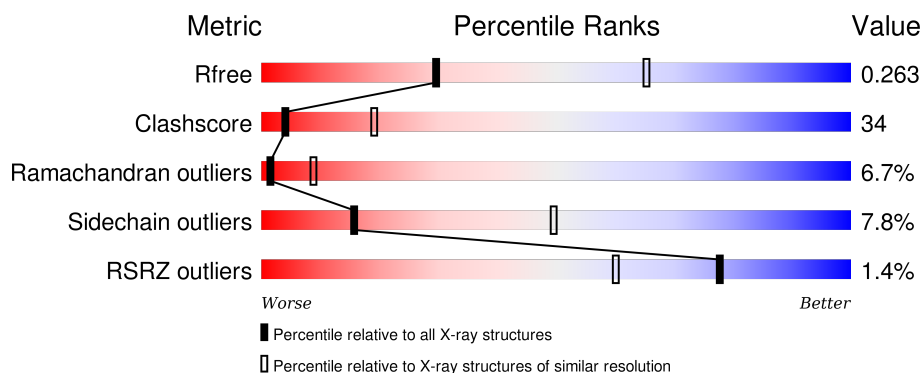
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	216	<div> <div>2%</div> <div>38% 49% 8% 5%</div> </div>
1	D	216	<div> <div>4%</div> <div>34% 52% 9% 5%</div> </div>
1	G	216	<div> <div>%</div> <div>35% 51% 8% 5%</div> </div>
1	J	216	<div> <div>%</div> <div>34% 51% 9% 5%</div> </div>
2	B	201	<div> <div>2%</div> <div>24% 40% 8% 27%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	201	
2	H	201	
2	K	201	
3	C	386	
3	F	386	
3	I	386	
3	L	386	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	A	1251	-	-	-	X
4	MG	D	2251	-	-	-	X
4	MG	G	3251	-	-	-	X
4	MG	J	4251	-	-	-	X
6	AF3	D	2252	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22396 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 GTP-binding nuclear protein RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	D	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	G	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	J	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	E	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	H	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	K	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			

- Molecule 3 is a protein called Ran GTPase activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	F	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	I	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	L	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			

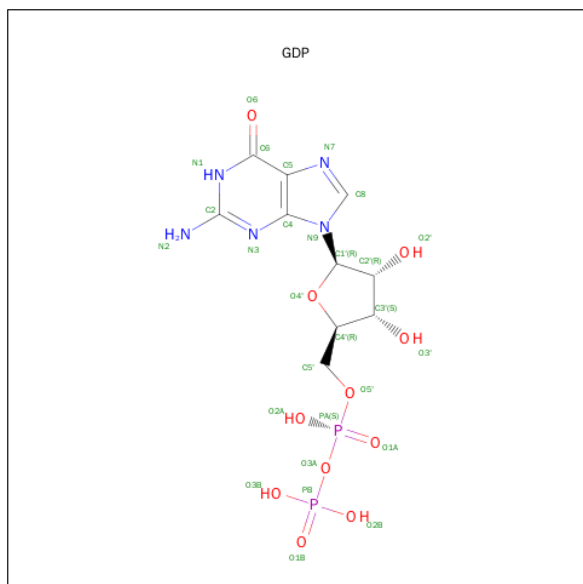
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	SER	SEE REMARK 999	UNP P41391
F	2	ALA	SER	SEE REMARK 999	UNP P41391
I	2	ALA	SER	SEE REMARK 999	UNP P41391
L	2	ALA	SER	SEE REMARK 999	UNP P41391

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

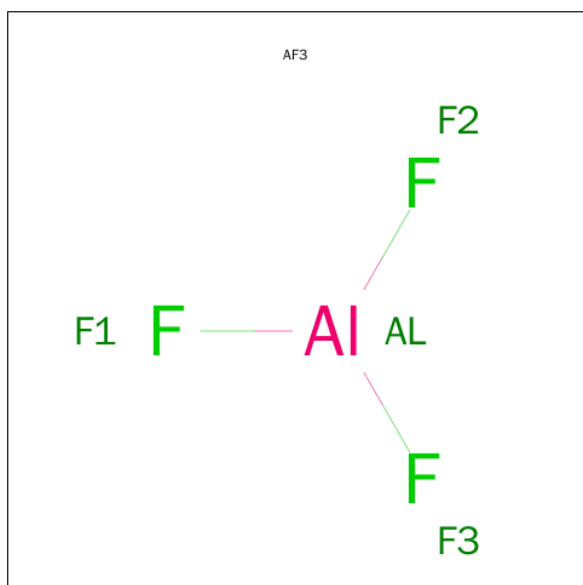
- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $\text{AlF}_3$ ).

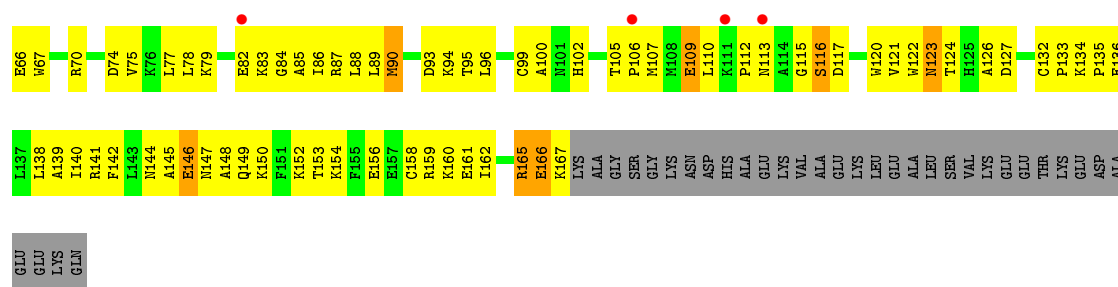


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	D	1	Total	Al	F	0	0
			4	1	3		
6	G	1	Total	Al	F	0	0
			4	1	3		
6	J	1	Total	Al	F	0	0
			4	1	3		

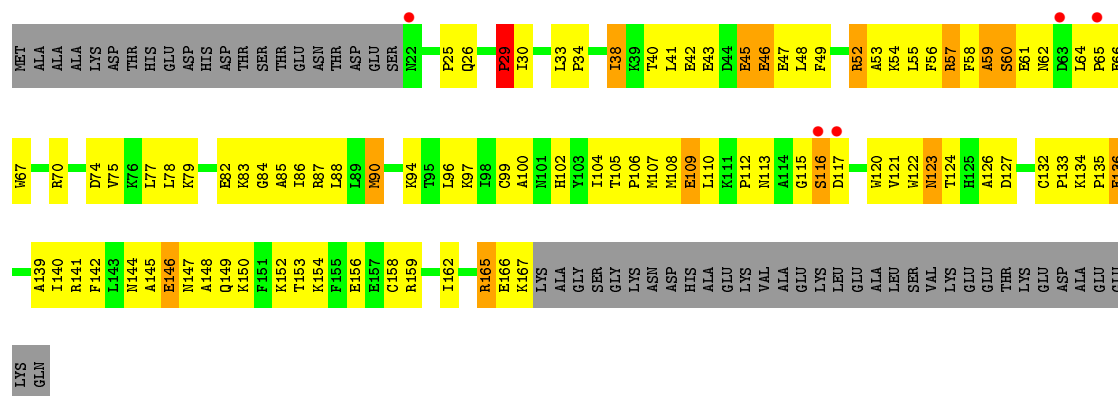




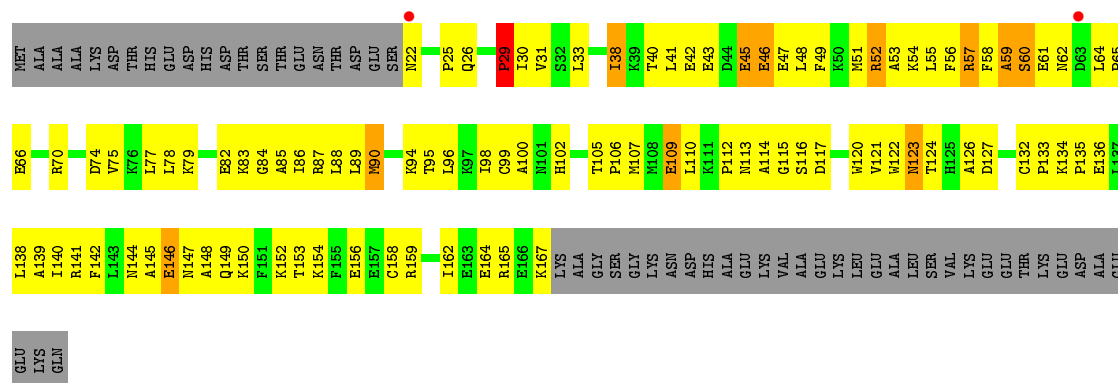
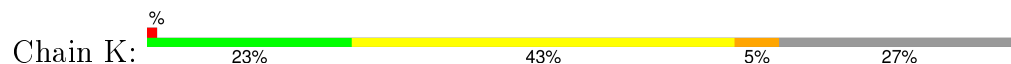




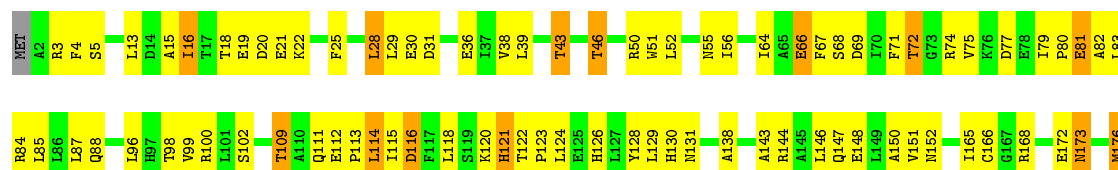
• Molecule 2: Ran-specific GTPase-activating protein

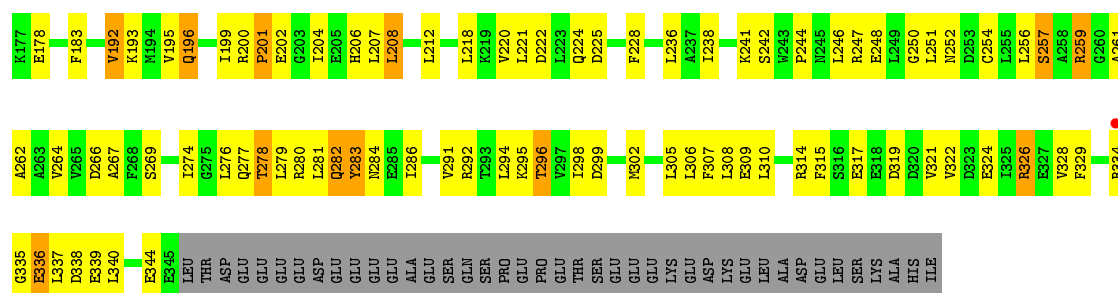


• Molecule 2: Ran-specific GTPase-activating protein



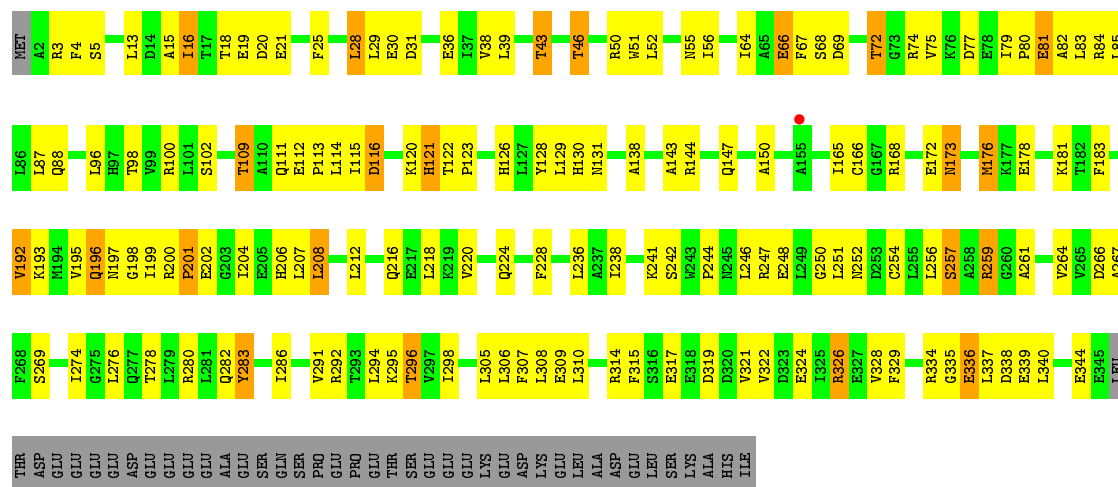
• Molecule 3: Ran GTPase activating protein 1





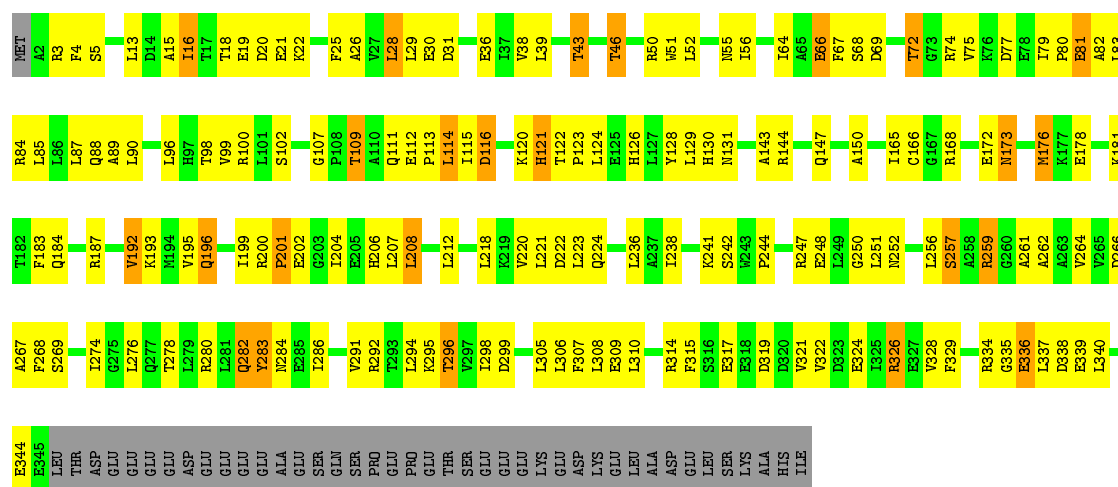
• Molecule 3: Ran GTPase activating protein 1

Chain F: 49% 34% 6% 11%



• Molecule 3: Ran GTPase activating protein 1

Chain I: 47% 36% 6% 11%



• Molecule 3: Ran GTPase activating protein 1

Chain L: 44% 39% 6% 11%

E324	L255	K177	R84
L325	L256	E178	L85
R326	S257	F183	L86
E327	A258	H186	L87
V328	R259		Q88
F329	G260		
	A261		L96
R334	A262	V192	R97
G335	A263	K193	T98
E336	V264	M194	V99
L337	V265	V195	R100
D338	D266	Q196	L101
E339	A267	N197	S102
L340	F268	G198	
	S269	I199	T109
E344	K270	R200	A110
E345		P201	Q111
LEU	I274	E202	E112
THR	G275	G203	P113
ASP	L276	L204	L114
GLU	D277	E205	I115
GLU	T278	R206	D116
GLU	L279	L207	F117
GLU	R280	L208	L118
ASP	L281		S119
GLU	Q282		K120
GLU	Y283	A213	V38
GLU	N284		H121
GLU	E285	Q216	T122
ALA	L286	E217	P123
GLU		L218	
SER	V291	K219	H126
GLN	R292	V220	L127
SER	T293	L221	Y128
PRO	L294	D222	L129
GLU	K295	L223	M51
PRO	T296	Q224	N131
GLU	V297	D225	L52
THR	L298		M55
SER	D299		L56
GLU		F228	
GLU	M302	S234	A143
GLU		A235	R144
LYS	L305	L236	A145
GLU	L306	A237	L146
ASP	F307	I238	Q147
LYS	L308		E148
GLU	E309	K241	L149
LEU	L310	S242	A150
ALA		V243	V151
ASP	R314	P244	
GLU	F315		L161
LEU	S316	R247	T64
SER	E317	E248	A65
LYS	L318	L249	B66
ALA	D319	G250	F67
HIS	R320	L251	S68
TLE	V321	N252	D69
	V322	D253	I70
	D323	C254	F71
			T72
			G73
			R74
			V75
			K76
			D77
			E78
			I79
			P80
			B81
			A82
			L83

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.93Å 102.57Å 118.85Å 71.67° 79.09° 67.81°	Depositor
Resolution (Å)	31.00 – 3.10 31.22 – 2.88	Depositor EDS
% Data completeness (in resolution range)	96.2 (31.00-3.10) 86.6 (31.22-2.88)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.250 , 0.269 0.224 , 0.263	Depositor DCC
$R_{free}$ test set	7166 reflections (11.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.8	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 88616 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	22396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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, 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	A	0.42	0/1693	0.67	0/2296
1	D	0.45	0/1693	0.68	0/2296
1	G	0.43	0/1693	0.67	0/2296
1	J	0.46	0/1693	0.69	0/2296
2	B	0.37	0/1242	0.63	0/1666
2	E	0.36	0/1242	0.62	0/1666
2	H	0.38	0/1242	0.62	0/1666
2	K	0.38	0/1242	0.63	0/1666
3	C	0.41	0/2737	0.68	0/3697
3	F	0.41	0/2737	0.68	0/3697
3	I	0.41	0/2737	0.67	0/3697
3	L	0.42	0/2737	0.69	0/3697
All	All	0.41	0/22688	0.67	0/30636

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	1652	0	1660	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1652	0	1659	141	0
1	G	1652	0	1659	140	0
1	J	1652	0	1660	145	0
2	B	1216	0	1208	117	0
2	E	1216	0	1208	118	0
2	H	1216	0	1208	107	0
2	K	1216	0	1208	110	0
3	C	2698	0	2733	166	0
3	F	2698	0	2733	143	0
3	I	2698	0	2733	162	0
3	L	2698	0	2733	164	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	28	0	12	5	0
5	D	28	0	12	5	0
5	G	28	0	12	5	0
5	J	28	0	12	4	0
6	A	4	0	0	0	0
6	D	4	0	0	0	0
6	G	4	0	0	0	0
6	J	4	0	0	0	0
All	All	22396	0	22450	1526	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 34.

The worst 5 of 1526 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)
3:I:259:ARG:NH1	3:I:259:ARG:HB3	1.68	1.07
3:F:259:ARG:HB3	3:F:259:ARG:NH1	1.69	1.06
3:L:259:ARG:NH1	3:L:259:ARG:HB3	1.71	1.04
3:C:259:ARG:HB3	3:C:259:ARG:NH1	1.73	1.04
3:I:259:ARG:HH11	3:I:259:ARG:HB3	1.20	1.03

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	204/216 (94%)	156 (76%)	27 (13%)	21 (10%)	1	4
1	D	204/216 (94%)	153 (75%)	29 (14%)	22 (11%)	0	3
1	G	204/216 (94%)	156 (76%)	28 (14%)	20 (10%)	1	4
1	J	204/216 (94%)	154 (76%)	28 (14%)	22 (11%)	0	3
2	B	144/201 (72%)	118 (82%)	14 (10%)	12 (8%)	1	6
2	E	144/201 (72%)	117 (81%)	15 (10%)	12 (8%)	1	6
2	H	144/201 (72%)	119 (83%)	14 (10%)	11 (8%)	1	7
2	K	144/201 (72%)	117 (81%)	18 (12%)	9 (6%)	2	10
3	C	342/386 (89%)	275 (80%)	54 (16%)	13 (4%)	4	22
3	F	342/386 (89%)	280 (82%)	48 (14%)	14 (4%)	3	20
3	I	342/386 (89%)	278 (81%)	50 (15%)	14 (4%)	3	20
3	L	342/386 (89%)	278 (81%)	50 (15%)	14 (4%)	3	20
All	All	2760/3212 (86%)	2201 (80%)	375 (14%)	184 (7%)	1	9

5 of 184 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	106	ARG
1	A	135	SER
1	A	179	MET
1	A	186	GLU

### 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	178/185 (96%)	164 (92%)	14 (8%)	15	49
1	D	178/185 (96%)	161 (90%)	17 (10%)	10	37
1	G	178/185 (96%)	163 (92%)	15 (8%)	14	46
1	J	178/185 (96%)	161 (90%)	17 (10%)	10	37
2	B	131/176 (74%)	117 (89%)	14 (11%)	8	31
2	E	131/176 (74%)	118 (90%)	13 (10%)	10	34
2	H	131/176 (74%)	117 (89%)	14 (11%)	8	31
2	K	131/176 (74%)	119 (91%)	12 (9%)	11	40
3	C	295/334 (88%)	277 (94%)	18 (6%)	23	59
3	F	295/334 (88%)	277 (94%)	18 (6%)	23	59
3	I	295/334 (88%)	277 (94%)	18 (6%)	23	59
3	L	295/334 (88%)	277 (94%)	18 (6%)	23	59
All	All	2416/2780 (87%)	2228 (92%)	188 (8%)	16	49

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	173	ASN
1	G	155	TYR
3	L	43	THR
3	F	192	VAL
1	G	18	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	224	GLN
2	H	123	ASN
3	L	147	GLN
3	F	252	ASN
1	G	145	GLN

### 5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	1250	4,6	23,30,30	1.62	3 (13%)	30,47,47	2.42	5 (16%)
6	AF3	A	1252	5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	D	2250	4,6	23,30,30	1.69	5 (21%)	30,47,47	2.39	5 (16%)
6	AF3	D	2252	5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	G	3250	4,6	23,30,30	1.63	4 (17%)	30,47,47	2.46	6 (20%)
6	AF3	G	3252	5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	J	4250	4,6	23,30,30	1.64	3 (13%)	30,47,47	2.48	7 (23%)
6	AF3	J	4252	5,4	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
5	GDP	A	1250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	A	1252	5,4	-	0/0/0/0	0/0/0/0
5	GDP	D	2250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	D	2252	5,4	-	0/0/0/0	0/0/0/0
5	GDP	G	3250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	G	3252	5,4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	J	4250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	J	4252	5,4	-	0/0/0/0	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4250	GDP	C8-N7	-3.02	1.28	1.34
5	A	1250	GDP	C8-N7	-2.80	1.29	1.34
5	G	3250	GDP	C8-N7	-2.78	1.29	1.34
5	D	2250	GDP	C8-N7	-2.67	1.29	1.34
5	D	2250	GDP	PA-O2A	-2.41	1.44	1.54

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3250	GDP	C5-C6-N1	-8.63	111.79	123.59
5	D	2250	GDP	C5-C6-N1	-8.51	111.95	123.59
5	J	4250	GDP	C5-C6-N1	-8.42	112.08	123.59
5	A	1250	GDP	C5-C6-N1	-8.40	112.10	123.59
5	J	4250	GDP	N3-C2-N1	-3.67	121.85	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1250	GDP	5	0
5	D	2250	GDP	5	0
5	G	3250	GDP	5	0
5	J	4250	GDP	4	0

## 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 ⓘ

### 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, 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	206/216 (95%)	-0.47	5 (2%) 62 39	21, 57, 156, 186	0
1	D	206/216 (95%)	-0.49	9 (4%) 38 17	13, 46, 161, 199	0
1	G	206/216 (95%)	-0.55	2 (0%) 84 69	14, 50, 159, 198	0
1	J	206/216 (95%)	-0.62	3 (1%) 76 58	11, 47, 148, 199	0
2	B	146/201 (72%)	-0.25	4 (2%) 58 34	43, 88, 148, 200	0
2	E	146/201 (72%)	0.05	7 (4%) 34 15	43, 100, 162, 195	0
2	H	146/201 (72%)	-0.22	5 (3%) 49 24	32, 80, 158, 187	0
2	K	146/201 (72%)	-0.29	2 (1%) 78 60	44, 80, 145, 188	0
3	C	344/386 (89%)	-0.72	1 (0%) 94 88	18, 48, 107, 144	0
3	F	344/386 (89%)	-0.82	1 (0%) 94 88	11, 47, 93, 143	0
3	I	344/386 (89%)	-0.74	0 100 100	15, 50, 100, 148	0
3	L	344/386 (89%)	-0.79	0 100 100	8, 43, 97, 150	0
All	All	2784/3212 (86%)	-0.57	39 (1%) 78 60	8, 55, 139, 200	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	PRO	7.2
2	H	63	ASP	5.2
1	D	188	VAL	3.8
1	D	195	ALA	3.8
1	A	206	THR	3.6

### 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 [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
4	MG	J	4251	1/1	0.89	0.40	13.55	33,33,33,33	0
4	MG	D	2251	1/1	0.63	0.30	9.39	45,45,45,45	0
4	MG	A	1251	1/1	0.91	0.39	8.23	31,31,31,31	0
4	MG	G	3251	1/1	0.86	0.37	8.01	44,44,44,44	0
6	AF3	D	2252	4/4	0.97	0.26	4.12	57,57,57,57	0
6	AF3	J	4252	4/4	0.98	0.24	1.54	57,57,57,57	0
6	AF3	A	1252	4/4	0.95	0.26	1.13	57,57,57,57	0
6	AF3	G	3252	4/4	0.97	0.19	0.42	57,57,57,57	0
5	GDP	A	1250	28/28	0.95	0.15	-0.51	43,43,43,43	0
5	GDP	G	3250	28/28	0.96	0.13	-0.64	35,35,35,35	0
5	GDP	J	4250	28/28	0.97	0.13	-0.72	29,29,29,29	0
5	GDP	D	2250	28/28	0.97	0.12	-0.78	31,31,31,31	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.