



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:04 AM GMT

PDB ID : 2ZET
Title : Crystal structure of the small GTPase Rab27B complexed with the Slp homology domain of Slac2-a/melanophilin
Authors : Kukimoto-Niino, M.; Sakamoto, A.; Kanno, E.; Hanawa-Suetsugu, K.; Terada, T.; Shirouzu, M.; Fukuda, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-12-17
Resolution : 3.00 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
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:

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

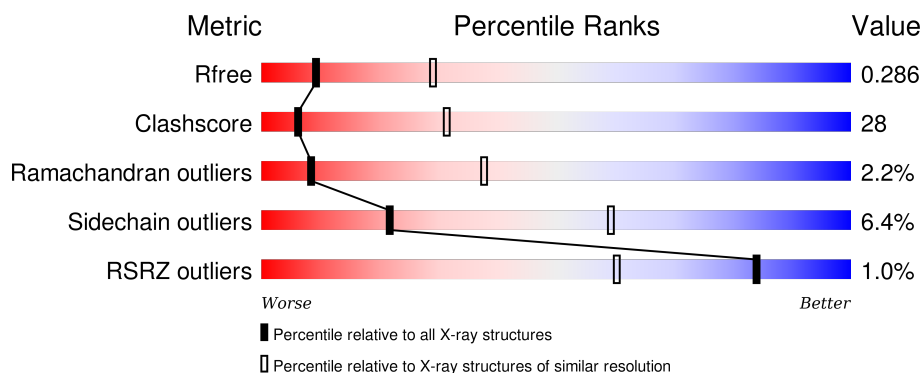
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	203	<div> <div>45%</div> <div>40%</div> <div>•</div> <div>11%</div> </div>
1	B	203	<div> <div>%</div> <div>41%</div> <div>40%</div> <div>5%</div> <div>14%</div> </div>
2	C	153	<div> <div>55%</div> <div>32%</div> <div>5%</div> <div>•</div> <div>8%</div> </div>
2	D	153	<div> <div>2%</div> <div>46%</div> <div>41%</div> <div>5%</div> <div>8%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5297 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 Ras-related protein Rab-27B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	Se	0	0	0
			1465	934	248	276	2	5			
1	B	174	Total	C	N	O	S	Se	0	0	0
			1423	910	239	267	2	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q99P58
A	0	SER	-	EXPRESSION TAG	UNP Q99P58
A	78	LEU	GLN	ENGINEERED	UNP Q99P58
B	-1	GLY	-	EXPRESSION TAG	UNP Q99P58
B	0	SER	-	EXPRESSION TAG	UNP Q99P58
B	78	LEU	GLN	ENGINEERED	UNP Q99P58

- Molecule 2 is a protein called Melanophilin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	141	Total	C	N	O	S		0	0	0
			1160	719	226	206	9				
2	D	141	Total	C	N	O	S		0	0	0
			1160	719	226	206	9				

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLY	-	EXPRESSION TAG	UNP Q91V27
C	-5	SER	-	EXPRESSION TAG	UNP Q91V27
C	-4	SER	-	EXPRESSION TAG	UNP Q91V27
C	-3	GLY	-	EXPRESSION TAG	UNP Q91V27
C	-2	SER	-	EXPRESSION TAG	UNP Q91V27
C	-1	SER	-	EXPRESSION TAG	UNP Q91V27

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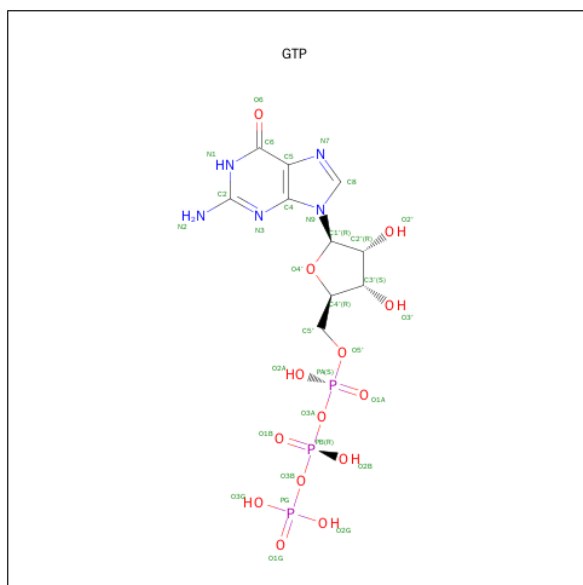
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	EXPRESSION TAG	UNP Q91V27
D	-6	GLY	-	EXPRESSION TAG	UNP Q91V27
D	-5	SER	-	EXPRESSION TAG	UNP Q91V27
D	-4	SER	-	EXPRESSION TAG	UNP Q91V27
D	-3	GLY	-	EXPRESSION TAG	UNP Q91V27
D	-2	SER	-	EXPRESSION TAG	UNP Q91V27
D	-1	SER	-	EXPRESSION TAG	UNP Q91V27
D	0	GLY	-	EXPRESSION TAG	UNP Q91V27

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 32 10 5 14 3	0	0
4	B	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	2	Total	Zn	0	0
			2	2		
5	C	2	Total	Zn	0	0
			2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

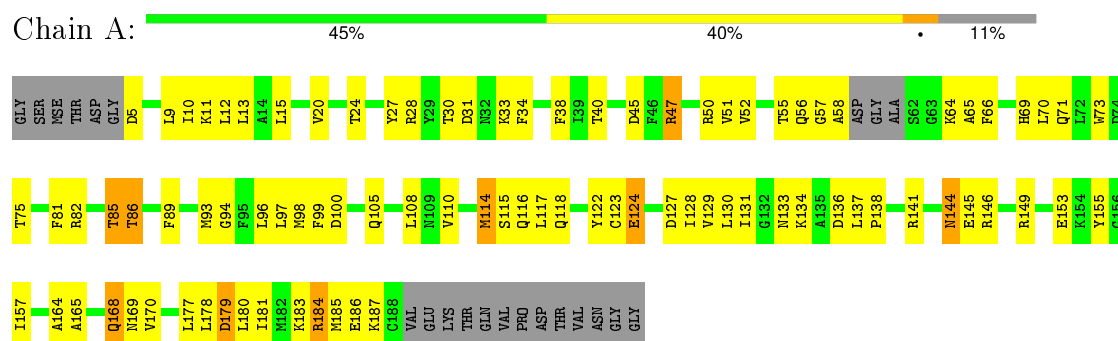
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	O	0	0
			1	1		
7	C	2	Total	O	0	0
			2	2		
7	B	1	Total	O	0	0
			1	1		
7	D	5	Total	O	0	0
			5	5		

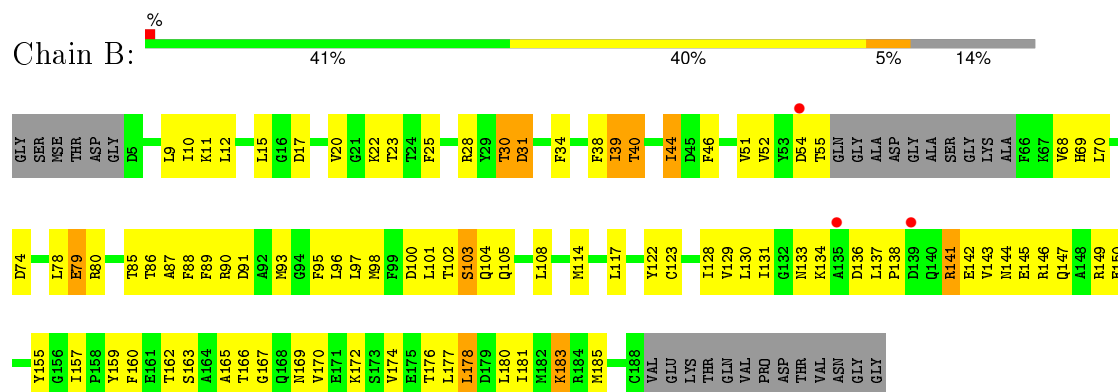
3 Residue-property plots

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.

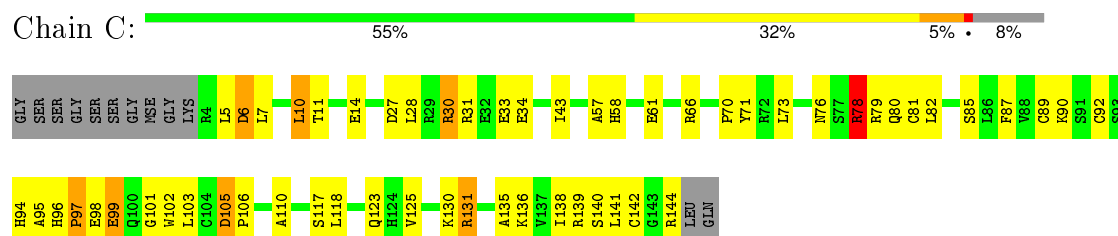
• Molecule 1: Ras-related protein Rab-27B



• Molecule 1: Ras-related protein Rab-27B

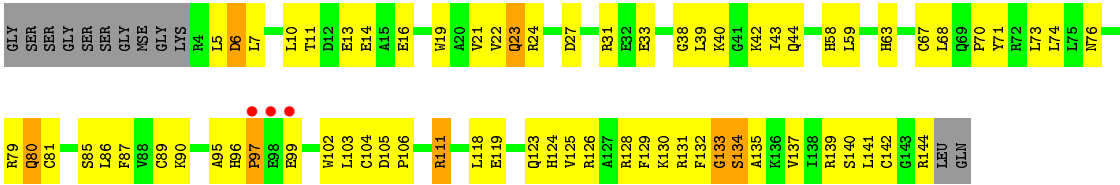


• Molecule 2: Melanophilin



• Molecule 2: Melanophilin





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	82.21Å 82.21Å 325.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.28 – 3.00 45.28 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.28-3.00) 99.9 (45.28-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.296 0.239 , 0.286	Depositor DCC
R_{free} test set	2311 reflections (9.87%)	DCC
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 23508 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5297	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GTP, MG, ZN, SO4

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	0.46	0/1487	0.63	0/1995
1	B	0.39	0/1445	0.59	0/1940
2	C	0.55	0/1182	0.70	0/1587
2	D	0.40	0/1182	0.64	0/1587
All	All	0.45	0/5296	0.64	0/7109

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	1465	0	1447	94	0
1	B	1423	0	1404	103	0
2	C	1160	0	1149	57	0
2	D	1160	0	1149	63	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	32	0	12	4	0
4	B	32	0	12	5	0
5	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	2	0	0	0	0
6	C	5	0	0	1	0
6	D	5	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	2	0	0	0	0
7	D	5	0	0	1	0
All	All	5297	0	5173	293	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 28.

The worst 5 of 293 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:82:ARG:HD2	1:A:116:GLN:HE21	1.27	0.97
2:C:135:ALA:O	2:C:138:ILE:HG22	1.66	0.94
1:A:185:MSE:HE3	2:C:118:LEU:HD21	1.47	0.92
2:D:40:LYS:O	2:D:44:GLN:HG3	1.80	0.81
1:B:162:THR:HG22	1:B:169:ASN:HB2	1.60	0.81

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	177/203 (87%)	155 (88%)	20 (11%)	2 (1%)	17	58
1	B	170/203 (84%)	152 (89%)	14 (8%)	4 (2%)	7	35
2	C	139/153 (91%)	117 (84%)	18 (13%)	4 (3%)	6	29
2	D	139/153 (91%)	121 (87%)	14 (10%)	4 (3%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	625/712 (88%)	545 (87%)	66 (11%)	14 (2%)	8	38

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	78	ARG
1	B	103	SER
2	C	99	GLU
1	B	40	THR
2	D	99	GLU

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	157/167 (94%)	146 (93%)	11 (7%)	19	55
1	B	154/167 (92%)	147 (96%)	7 (4%)	34	74
2	C	127/134 (95%)	118 (93%)	9 (7%)	18	54
2	D	127/134 (95%)	118 (93%)	9 (7%)	18	54
All	All	565/602 (94%)	529 (94%)	36 (6%)	22	59

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	80	GLN
1	B	30	THR
2	D	111	ARG
2	C	105	ASP
1	B	31	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
2	C	76	ASN
2	D	17	HIS
1	A	144	ASN
2	D	58	HIS

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 10 ligands modelled in this entry, 6 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	$\# Z > 2$
4	GTP	A	203	3	25,34,34	1.40	4 (16%)	34,54,54	2.06	8 (23%)
4	GTP	B	203	3	25,34,34	1.67	6 (24%)	34,54,54	2.10	10 (29%)
6	SO4	C	303	-	4,4,4	0.03	0	6,6,6	0.12	0
6	SO4	D	303	-	4,4,4	0.10	0	6,6,6	0.08	0

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	GTP	A	203	3	-	0/18/38/38	0/3/3/3
4	GTP	B	203	3	-	0/18/38/38	0/3/3/3
6	SO4	C	303	-	-	0/0/0/0	0/0/0/0
6	SO4	D	303	-	-	0/0/0/0	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	203	GTP	C6-C5	2.06	1.45	1.41
4	A	203	GTP	PG-O2G	2.06	1.62	1.54
4	B	203	GTP	PG-O2G	2.07	1.62	1.54
4	A	203	GTP	C2-N2	2.15	1.38	1.34
4	B	203	GTP	O4'-C1'	2.21	1.44	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	203	GTP	PB-O3B-PG	-6.35	111.36	132.67
4	B	203	GTP	PB-O3B-PG	-6.00	112.54	132.67
4	B	203	GTP	PA-O3A-PB	-4.82	119.19	132.73
4	B	203	GTP	N3-C2-N1	-4.44	120.68	127.44
4	A	203	GTP	PA-O3A-PB	-4.25	120.79	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	203	GTP	4	0
4	B	203	GTP	5	0
6	C	303	SO4	1	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 [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, 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	176/203 (86%)	-0.24	0 100 100	48, 67, 100, 117	0
1	B	169/203 (83%)	0.07	3 (1%) 71 43	46, 83, 114, 130	0
2	C	141/153 (92%)	-0.21	0 100 100	43, 68, 97, 121	0
2	D	141/153 (92%)	-0.19	3 (2%) 67 36	46, 68, 102, 128	0
All	All	627/712 (88%)	-0.14	6 (0%) 84 60	43, 72, 108, 130	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	ASP	3.9
2	D	98	GLU	3.0
1	B	135	ALA	2.4
2	D	99	GLU	2.3
1	B	54	ASP	2.2

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, 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(\AA^2)	Q<0.9
5	ZN	C	302	1/1	0.99	0.19	-0.28	61,61,61,61	0
4	GTP	B	203	32/32	0.90	0.18	-0.30	62,81,98,100	0
5	ZN	D	301	1/1	0.99	0.14	-0.49	70,70,70,70	0
4	GTP	A	203	32/32	0.97	0.15	-0.50	35,62,71,79	0
5	ZN	C	301	1/1	0.99	0.13	-0.64	64,64,64,64	0
5	ZN	D	302	1/1	0.99	0.15	-0.69	56,56,56,56	0
3	MG	B	202	1/1	0.99	0.23	-	42,42,42,42	0
6	SO4	C	303	5/5	0.95	0.16	-	80,84,92,92	0
6	SO4	D	303	5/5	0.97	0.16	-	82,82,88,88	0
3	MG	A	202	1/1	0.91	0.26	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.