

Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 11:01 AM JST

PDB ID : 6IYB

Title : Structure of human ORP1 ANK - Rab7 complex

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Deposited on : 2018-12-14

Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

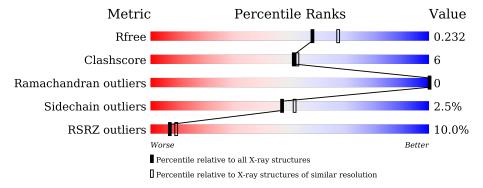
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.09 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	199	78%	8%		14%
1	С	199	74%	12%		14%
2	В	154	67%	0%	•	12%
2	D	154	78%	9%	•	12%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5225 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-7a.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	171		C 860		0	S	0	0	0
			1363	869	231	257	О			
1	C	171	Total	С	N	Ο	\mathbf{S}	0	0	0
1	O	1/1	1363	869	231	257	6			0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P51149
A	-3	SER	-	expression tag	UNP P51149
A	-2	ALA	-	expression tag	UNP P51149
A	-1	MET	-	expression tag	UNP P51149
A	0	GLY	-	expression tag	UNP P51149
A	1	SER	-	expression tag	UNP P51149
A	67	LEU	GLN	engineered mutation	UNP P51149
A	?	-	LEU	deletion	UNP P51149
С	-4	GLY	-	expression tag	UNP P51149
С	-3	SER	-	expression tag	UNP P51149
С	-2	ALA	-	expression tag	UNP P51149
С	-1	MET	-	expression tag	UNP P51149
С	0	GLY	-	expression tag	UNP P51149
С	1	SER	-	expression tag	UNP P51149
С	67	LEU	GLN	engineered mutation	UNP P51149
С	?	-	LEU	deletion	UNP P51149

• Molecule 2 is a protein called Oxysterol-binding protein-related protein 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	D	135	Total	С	N	О	S	0	0	0
2 B	139	1052	645	197	204	6	U		0	
9	D	195	Total	С	N	О	S	0	0	0
	D	135	1047	642	196	203	6	U		U



There are 12	discrepancies	hetween	the modelled	and	reference	segmences.
1 11010 arc 12	uisci cpancics	DCGWCCII	ine modelica	and	TOTOTOTICE	sequences.

Chain	Residue	Modelled	Actual	Comment	Reference
В	-1	GLY	-	expression tag	UNP Q9BXW6
В	0	SER	-	expression tag	UNP Q9BXW6
В	1	ALA	-	expression tag	UNP Q9BXW6
В	2	MET	-	expression tag	UNP Q9BXW6
В	3	GLY	-	expression tag	UNP Q9BXW6
В	4	SER	-	expression tag	UNP Q9BXW6
D	-1	GLY	-	expression tag	UNP Q9BXW6
D	0	SER	-	expression tag	UNP Q9BXW6
D	1	ALA	-	expression tag	UNP Q9BXW6
D	2	MET	-	expression tag	UNP Q9BXW6
D	3	GLY	-	expression tag	UNP Q9BXW6
D	4	SER	-	expression tag	UNP Q9BXW6

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

• Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



N	/Iol	Chain	Residues	Atoms				ZeroOcc	AltConf	
	1	Λ	1	Total	С	N	О	Р	0	0
	$\begin{array}{c c} 4 & A \\ \end{array}$	1	32	10	5	14	3	U		
	1	С	1	Total	С	N	О	Р	0	0
	4 C	1	32	10	5	14	3	U		

$\bullet\,$ Molecule 5 is water.

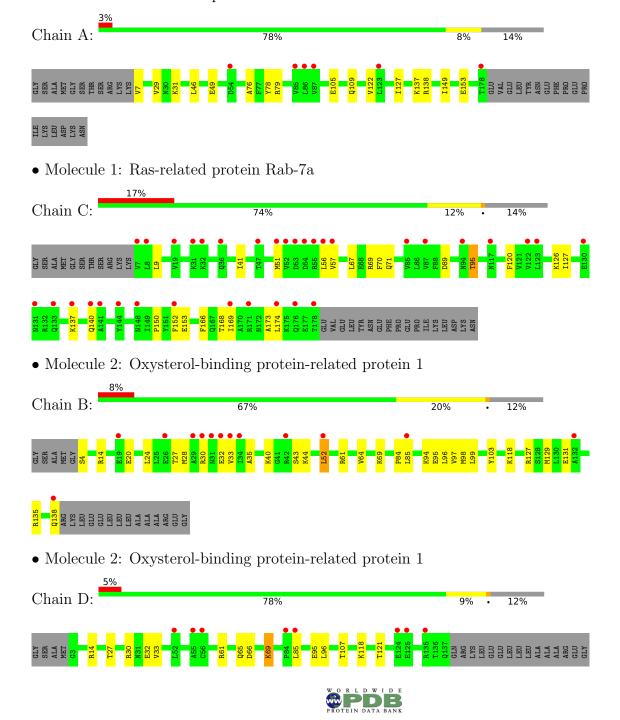
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	153	Total O 153 153	0	0
5	В	51	Total O 51 51	0	0
5	С	36	Total O 36 36	0	0
5	D	94	Total O 94 94	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Ras-related protein Rab-7a



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	55.14Å 117.22Å 130.48Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.29 - 2.09	Depositor
rtesolution (A)	26.29 - 2.09	EDS
% Data completeness	98.5 (26.29-2.09)	Depositor
(in resolution range)	95.5 (26.29-2.09)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	6.38 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
P. P.	0.195 , 0.232	Depositor
R, R_{free}	0.195 , 0.232	DCC
R_{free} test set	2545 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 56.9	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5225	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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

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		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.52	0/1389	0.62	0/1881	
1	С	0.35	0/1389	0.50	0/1881	
2	В	0.43	0/1065	0.57	0/1438	
2	D	0.43	0/1060	0.54	0/1431	
All	All	0.44	0/4903	0.56	0/6631	

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1363	0	1352	13	0
1	С	1363	0	1352	13	0
2	В	1052	0	1040	23	0
2	D	1047	0	1035	8	0
3	A	1	0	0	0	0
3	С	1	0	0	0	0
4	A	32	0	12	0	0
4	С	32	0	12	1	0
5	A	153	0	0	6	1



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	51	0	0	2	0
5	С	36	0	0	0	0
5	D	94	0	0	0	0
All	All	5225	0	4803	54	1

The all-atom clash score is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clash score for this structure is 6.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A 4 1	A 4 9	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
2:B:94:LYS:NZ	5:B:201:HOH:O	2.12	0.79
2:B:4:SER:N	5:B:202:HOH:O	2.16	0.77
2:B:30:ARG:NH1	2:B:32:GLU:OE2	2.18	0.76
1:A:78:TYR:OH	5:A:1401:HOH:O	2.03	0.76
1:A:29:VAL:HG21	1:A:46:LEU:HD11	1.71	0.72
2:D:61:ARG:NH1	2:D:65:GLN:OE1	2.25	0.69
1:A:105:GLU:OE2	5:A:1401:HOH:O	2.10	0.69
2:B:61:ARG:HA	2:B:96:LEU:HD21	1.74	0.69
1:A:49:GLU:OE2	5:A:1402:HOH:O	2.11	0.69
2:B:30:ARG:O	2:B:30:ARG:HG2	1.93	0.68
1:A:105:GLU:HB2	2:B:44:LYS:HG3	1.76	0.67
2:B:28:MET:HG2	2:B:35:ALA:HB3	1.77	0.65
2:B:52:LEU:HD13	2:B:84:PRO:HG2	1.78	0.63
2:B:131:GLU:OE2	2:B:135:ARG:NH2	2.30	0.63
2:B:61:ARG:HD3	2:B:95:GLU:OE1	2.01	0.60
1:A:105:GLU:OE2	2:B:44:LYS:HD2	2.01	0.60
1:C:127:ILE:HG21	1:C:153:GLU:HB3	1.84	0.58
2:D:27:THR:HG22	2:D:33:VAL:HG22	1.86	0.56
1:A:109:GLN:NE2	5:A:1403:HOH:O	2.39	0.56
2:D:61:ARG:HH12	2:D:65:GLN:CD	2.11	0.54
1:A:127:ILE:HG21	1:A:153:GLU:HB3	1.90	0.53
2:B:27:THR:HG22	2:B:33:VAL:HG22	1.91	0.53
2:B:98:MET:CE	2:B:129:MET:HG2	2.40	0.52
2:D:61:ARG:HA	2:D:96:LEU:HD21	1.94	0.49
2:D:66:ASP:O	2:D:69:LYS:HE3	2.12	0.49
2:B:94:LYS:H	2:B:94:LYS:HD2	1.77	0.49
1:A:122:VAL:HG23	1:A:149:ILE:HG21	1.96	0.48
2:B:69:LYS:HG2	2:B:103:TYR:OH	2.14	0.48
1:C:57:VAL:HG11	1:C:174:LEU:HD22	1.97	0.47
2:B:98:MET:HE1	2:B:129:MET:HG2	1.97	0.46



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A to a set		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \ (\mathring{\rm A})$	overlap (Å)
2:B:61:ARG:CD	2:B:95:GLU:OE1	2.64	0.46
1:C:67:LEU:O	1:C:71:GLN:HG3	2.16	0.46
2:D:30:ARG:NH2	2:D:32:GLU:OE1	2.50	0.45
1:C:166:PHE:HA	1:C:169:ILE:HD12	1.98	0.45
1:A:76:ALA:O	1:A:79:ARG:HG2	2.17	0.45
1:A:7:VAL:N	5:A:1407:HOH:O	2.49	0.45
1:A:137:LYS:HA	1:A:137:LYS:HD3	1.84	0.44
1:C:51:MET:HG2	1:C:56:LEU:HA	2.01	0.43
2:B:85:LEU:HD11	2:B:97:VAL:HG13	2.00	0.43
1:C:89:ASP:HB3	1:C:95:THR:HG21	2.00	0.43
2:B:118:LYS:HE2	2:B:118:LYS:HB3	1.87	0.42
2:B:20:GLU:OE1	2:B:20:GLU:N	2.39	0.42
2:B:40:LYS:HE3	1:C:69:ARG:HA	2.00	0.42
1:C:152:PHE:HZ	1:C:168:THR:HG1	1.65	0.41
2:B:30:ARG:HH11	2:B:32:GLU:CB	2.33	0.41
2:D:118:LYS:O	2:D:121:THR:HG22	2.21	0.41
2:D:85:LEU:HD21	2:D:107:THR:HG22	2.02	0.41
1:C:41:ILE:HA	1:C:70:PHE:HB3	2.03	0.41
2:B:64:VAL:HG12	2:B:99:LEU:HD23	2.03	0.41
1:C:9:LEU:HD13	1:C:173:ALA:HB3	2.03	0.41
1:A:138:ARG:NH1	5:A:1404:HOH:O	2.39	0.40
1:C:41:ILE:HG12	1:C:70:PHE:CD1	2.56	0.40
1:C:126:LYS:HG2	4:C:1302:GTP:C6	2.56	0.40
1:C:120:PHE:O	1:C:150:PRO:HD2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
5:A:1551:HOH:O	5:A:1553:HOH:O[4_445]	2.04	0.16

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	Perce	entiles
1	A	169/199~(85%)	164 (97%)	5 (3%)	0	100	100
1	С	169/199~(85%)	161 (95%)	8 (5%)	0	100	100
2	В	133/154 (86%)	132 (99%)	1 (1%)	0	100	100
2	D	133/154 (86%)	130 (98%)	3 (2%)	0	100	100
All	All	604/706 (86%)	587 (97%)	17 (3%)	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	148/173 (86%)	147 (99%)	1 (1%)	84 88		
1	C	148/173 (86%)	145 (98%)	3 (2%)	55 60		
2	В	112/124 (90%)	106 (95%)	6 (5%)	22 20		
2	D	111/124 (90%)	108 (97%)	3 (3%)	44 48		
All	All	519/594 (87%)	506 (98%)	13 (2%)	47 52		

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
2	В	14	ARG
2	В	24	LEU
2	В	43	SER
2	В	52	LEU
2	В	127	ARG
2	В	138	GLN
1	С	95	THR
1	С	137	LYS
1	С	140	GLN
2	D	14	ARG



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Mol	Chain	Res	Type
2	D	69	LYS
2	D	95	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	65	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are 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	Mal True Chair Day I		T inle	Bond lengths			Bond angles			
MIOI	Type Chain Res	Res	s Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	GTP	A	1302	3	26,34,34	1.05	2 (7%)	32,54,54	1.32	5 (15%)
4	GTP	С	1302	3	26,34,34	1.02	2 (7%)	32,54,54	1.35	6 (18%)

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.

ľ	Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
	4	GTP	A	1302	3	-	2/18/38/38	0/3/3/3
	4	GTP	С	1302	3	-	1/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
4	A	1302	GTP	C5-C6	-3.67	1.39	1.47
4	С	1302	GTP	C5-C6	-3.43	1.40	1.47
4	С	1302	GTP	C2-N3	2.26	1.38	1.33
4	A	1302	GTP	C2-N3	2.12	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	1302	GTP	C8-N7-C5	3.55	109.74	102.99
4	С	1302	GTP	C5-C6-N1	2.97	119.20	113.95
4	С	1302	GTP	C8-N7-C5	2.91	108.54	102.99
4	С	1302	GTP	C2-N1-C6	-2.59	120.34	125.10
4	С	1302	GTP	O3G-PG-O3B	2.50	113.03	104.64
4	A	1302	GTP	C5-C6-N1	2.25	117.93	113.95
4	A	1302	GTP	O6-C6-N1	-2.14	118.12	120.65
4	С	1302	GTP	PB-O3B-PG	-2.11	125.60	132.83
4	A	1302	GTP	PB-O3B-PG	-2.09	125.66	132.83
4	С	1302	GTP	PA-O3A-PB	-2.02	125.89	132.83
4	A	1302	GTP	O3G-PG-O3B	2.01	111.36	104.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1302	GTP	PA-O3A-PB-O1B
4	A	1302	GTP	PA-O3A-PB-O2B
4	С	1302	GTP	PA-O3A-PB-O2B

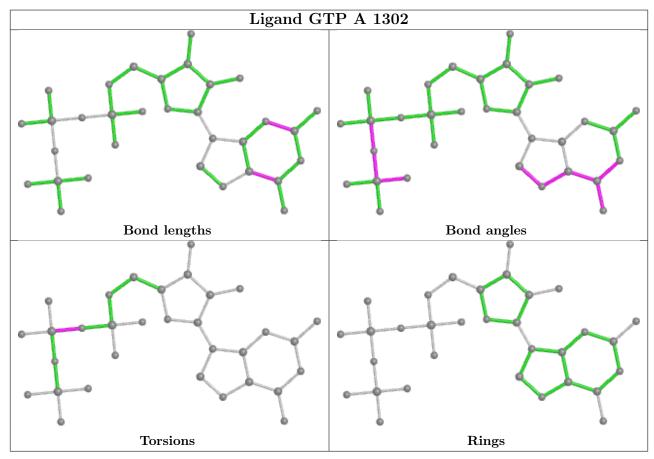
There are no ring outliers.

1 monomer is involved in 1 short contact:

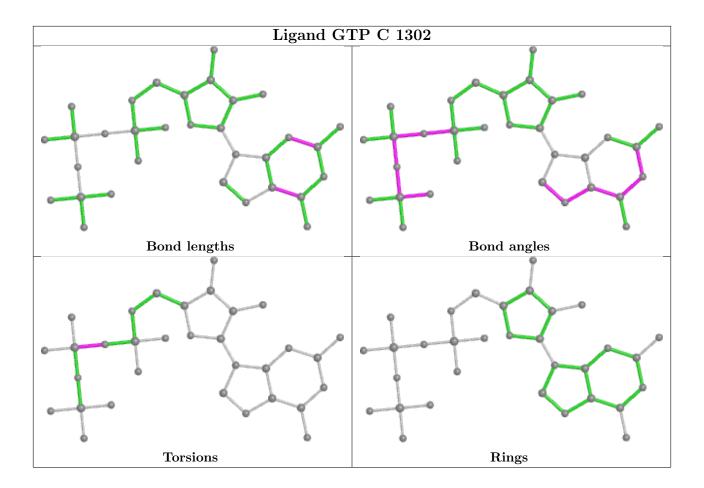
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	1302	GTP	1	0



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	171/199 (85%)	-0.07	6 (3%) 44 50	16, 26, 41, 58	0
1	С	171/199 (85%)	1.08	34 (19%) 1 1	34, 55, 90, 116	0
2	В	135/154 (87%)	0.53	13 (9%) 8 10	24, 42, 73, 89	0
2	D	135/154 (87%)	0.31	8 (5%) 22 27	22, 35, 56, 65	0
All	All	612/706 (86%)	0.47	61 (9%) 7 9	16, 38, 74, 116	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	56	LEU	10.5
2	В	34	ILE	6.4
1	С	7	VAL	6.2
1	С	55	ARG	6.2
1	С	52	VAL	6.1
1	С	53	ASP	6.0
1	С	54	ASP	5.8
1	С	178	THR	5.3
1	С	51	MET	4.9
1	С	144	TYR	4.7
2	В	32	GLU	4.7
1	С	130	GLU	4.5
1	С	57	VAL	4.5
2	В	31	ASN	4.3
1	С	123	LEU	4.3
2	В	30	ARG	4.1
2	В	33	VAL	3.8
1	С	137	LYS	3.8
1	С	8	LEU	3.7
1	С	174	LEU	3.5
2	В	29	ALA	3.5



 $Continued\ from\ previous\ page...$

Mol	Chain	m Res	Type	RSRZ
2	D	85	LEU	3.2
1	С	87	VAL	3.2
2	D	52	LEU	3.0
1	С	171	ARG	2.9
1	A	123	LEU	2.9
1	С	85	VAL	2.9
1	C C C	47	THR	2.8
1	С	140	GLN	2.8
2	В	138	GLN	2.8
1	A	86	LEU	2.7
1	С	131	ASN	2.7
2	D	56	CYS	2.7
2	D	125	GLU	2.7
2	D	84	PRO	2.6
1	С	148	ASN	2.6
1	A	87	VAL	2.6
1	С	31	LYS	2.4
1	С	133	GLN	2.4
1	С	32	LYS	2.4
1	A	85	VAL	2.4
1	С	152	PHE	2.3
2	В	19	GLU	2.3
2	В	132	ALA	2.3
1	A	178	THR	2.3
1	С	169	ILE	2.3
1	С	94	ASN	2.3
2	В	26	GLU	2.3
2	В	42	ARG	2.3
2	D	55	ALA	2.2
2	D	135	ARG	2.2
2	В	52	LEU	2.2
1	С	117	ASN	2.1
1	С	122	VAL	2.1
1	A	54	ASP	2.1
2	В	85	LEU	2.1
2	D	124	GLU	2.1
1	С	176	GLN	2.1
1	С	141	ALA	2.0
1	С	19	VAL	2.0
1	С	36	GLN	2.0



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 monosaccharides in this entry.

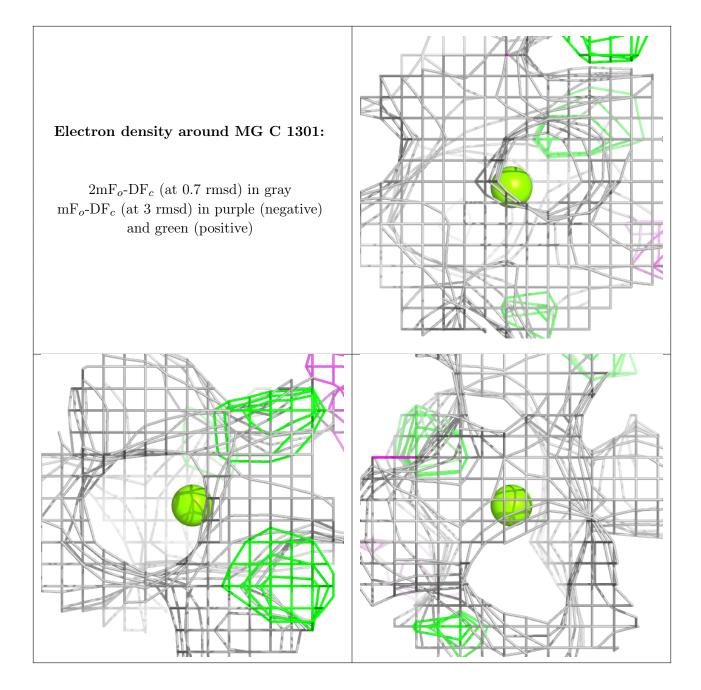
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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.

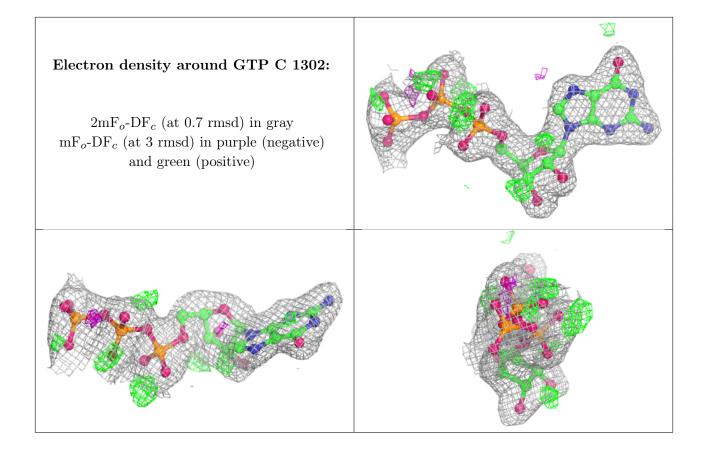
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	MG	С	1301	1/1	0.90	0.07	37,37,37,37	0
4	GTP	С	1302	32/32	0.97	0.10	28,44,50,51	0
3	MG	A	1301	1/1	0.98	0.08	18,18,18,18	0
4	GTP	A	1302	32/32	0.99	0.09	14,18,20,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





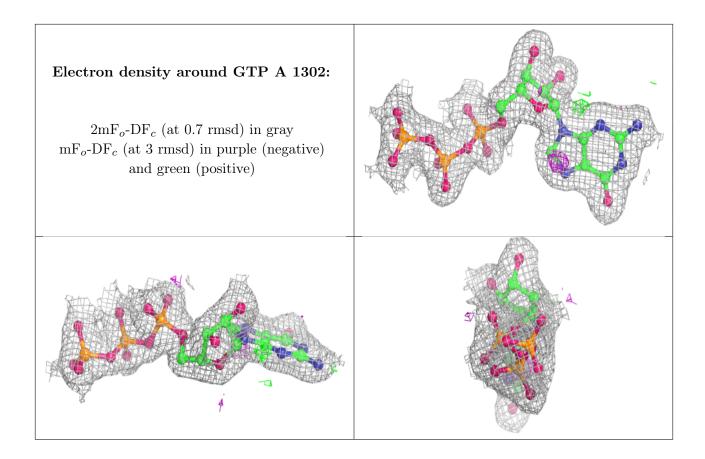






Electron density around MG A 1301: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_{o}\text{-}\mathrm{DF}_{c}$ (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.

