



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:22 PM GMT

PDB ID : 3WYF
Title : Crystal structure of Xpo1p-Yrb2p-Gsp1p-GTP complex
Authors : Koyama, M.; Shirai, N.; Matsuura, Y.
Deposited on : 2014-08-26
Resolution : 2.22 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

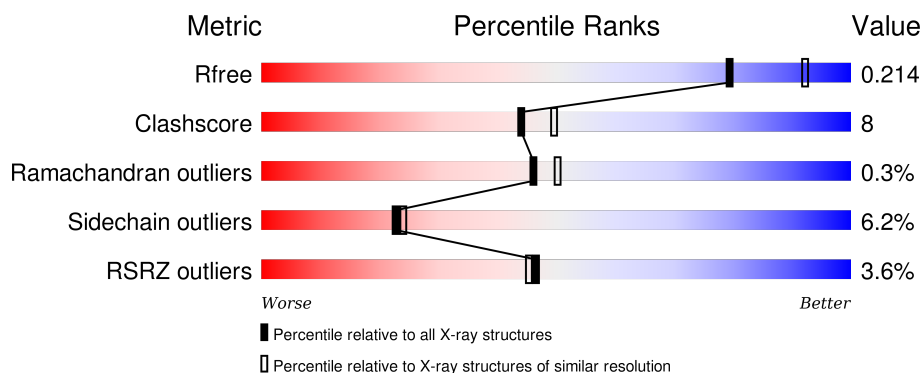
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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.



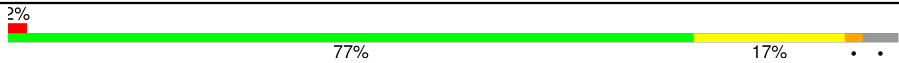
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	219	<div> <div>4%</div> <div>68% 16% • 14%</div> </div>
1	D	219	<div> <div>%</div> <div>65% 18% • 16%</div> </div>
2	B	238	<div> <div>11%</div> <div>43% 14% • 39%</div> </div>
2	E	238	<div> <div>7%</div> <div>35% 19% • • 40%</div> </div>
3	C	1049	<div> <div>3%</div> <div>81% 17% ••</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	1049	 A horizontal bar chart showing the quality of chain F. The bar is divided into segments: a small red segment at the beginning labeled '2%', a large green segment labeled '77%', a yellow segment labeled '17%', and a small grey segment at the end. Two small black dots are visible at the far right end of the bar.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22420 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 Gsp1p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1492	973	252	262	5			
1	D	185	Total	C	N	O	S	0	0	0
			1459	953	245	257	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LEU	GLN	ENGINEERED MUTATION	UNP E7KFU1
D	71	LEU	GLN	ENGINEERED MUTATION	UNP E7KFU1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1073	691	180	200	2			
2	E	142	Total	C	N	O	S	0	0	0
			1074	690	181	201	2			

- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1040	Total	C	N	O	S	0	0	0
			8322	5348	1361	1573	40			
3	F	1005	Total	C	N	O	S	0	0	0
			8046	5179	1316	1512	39			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	EXPRESSION TAG	UNP P30822
C	0	ALA	-	EXPRESSION TAG	UNP P30822

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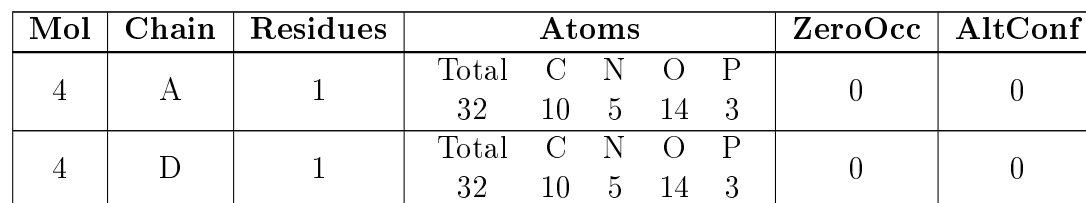
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	DELETION	UNP P30822
C	?	-	GLN	DELETION	UNP P30822
C	?	-	ARG	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	PRO	DELETION	UNP P30822
C	?	-	ALA	DELETION	UNP P30822
C	?	-	THR	DELETION	UNP P30822
C	?	-	GLU	DELETION	UNP P30822
C	?	-	MET	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	PRO	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	ILE	DELETION	UNP P30822
C	?	-	GLN	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	VAL	DELETION	UNP P30822
C	?	-	GLY	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	GLN	DELETION	UNP P30822
C	?	-	ALA	DELETION	UNP P30822
C	?	-	ILE	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	THR	DELETION	UNP P30822
C	?	-	GLY	DELETION	UNP P30822
C	?	-	SER	DELETION	UNP P30822
C	?	-	GLY	DELETION	UNP P30822
C	?	-	ALA	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	ASN	DELETION	UNP P30822
C	?	-	PRO	DELETION	UNP P30822
C	?	-	GLU	DELETION	UNP P30822
C	?	-	TYR	DELETION	UNP P30822
C	?	-	MET	DELETION	UNP P30822
C	?	-	LYS	DELETION	UNP P30822
C	?	-	ARG	DELETION	UNP P30822
C	?	-	PHE	DELETION	UNP P30822
F	-1	GLY	-	EXPRESSION TAG	UNP P30822
F	0	ALA	-	EXPRESSION TAG	UNP P30822
F	?	-	VAL	DELETION	UNP P30822
F	?	-	GLN	DELETION	UNP P30822
F	?	-	ARG	DELETION	UNP P30822

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	LEU	DELETION	UNP P30822
F	?	-	PRO	DELETION	UNP P30822
F	?	-	ALA	DELETION	UNP P30822
F	?	-	THR	DELETION	UNP P30822
F	?	-	GLU	DELETION	UNP P30822
F	?	-	MET	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	PRO	DELETION	UNP P30822
F	?	-	LEU	DELETION	UNP P30822
F	?	-	ILE	DELETION	UNP P30822
F	?	-	GLN	DELETION	UNP P30822
F	?	-	LEU	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	VAL	DELETION	UNP P30822
F	?	-	GLY	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	GLN	DELETION	UNP P30822
F	?	-	ALA	DELETION	UNP P30822
F	?	-	ILE	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	THR	DELETION	UNP P30822
F	?	-	GLY	DELETION	UNP P30822
F	?	-	SER	DELETION	UNP P30822
F	?	-	GLY	DELETION	UNP P30822
F	?	-	ALA	DELETION	UNP P30822
F	?	-	LEU	DELETION	UNP P30822
F	?	-	ASN	DELETION	UNP P30822
F	?	-	PRO	DELETION	UNP P30822
F	?	-	GLU	DELETION	UNP P30822
F	?	-	TYR	DELETION	UNP P30822
F	?	-	MET	DELETION	UNP P30822
F	?	-	LYS	DELETION	UNP P30822
F	?	-	ARG	DELETION	UNP P30822
F	?	-	PHE	DELETION	UNP P30822

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



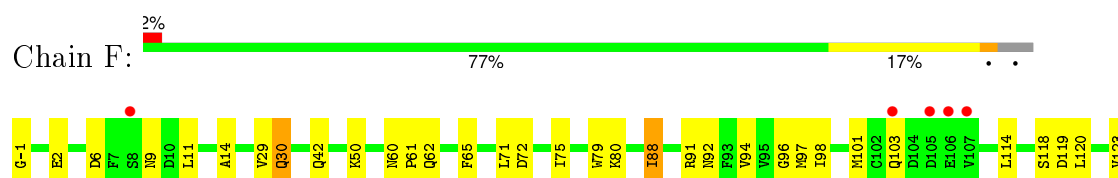
- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | A | 1 | Total Mg
1 1 | 0 | 0 |
| 5 | D | 1 | Total Mg
1 1 | 0 | 0 |

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 6 | A | 84 | Total O
84 84 | 0 | 0 |
| 6 | B | 11 | Total O
11 11 | 0 | 0 |
| 6 | C | 351 | Total O
351 351 | 0 | 0 |
| 6 | D | 86 | Total O
86 86 | 0 | 0 |
| 6 | E | 10 | Total O
10 10 | 0 | 0 |



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	346	Total	O	0	0
			346	346		



T1007	L877	V696	L536	Q124
S1008	L877	K697	D537	I125
A1017	A881	I698	L538	L126
L1018	A881	M713	T539	K127
Q1021	A892	L729	D546	Q128
F1028	F893	R733	V859	H134
I1039	K894	A734	N571	P135
D1054	R898	V735	G580	E136
LYS	V912	S736	I600	I138
GLU	E916	S737	Q604	P139
ASN	V921	H738	Q607	E140
ALA	P922	A741	R327	L141
LEU	I934	VAL	E331	N154
MET	E938	ALA	E334	K160
GLU	T939	GLU	Y346	E164
ASN	F940	LEU	Q349	Q173
ARG	V941	ILE	K352	N184
LEU	V942	ALA	R356	K188
GLU	L943	THR	I429	Q192
ARG	T944	LYS	R656	K195
GLU	D947	L759	S657	L201
LYS	H948	R760	V658	V211
ALA	K949	T761	A659	A212
LYS	S950	I762	R660	T213
ILE	S853	K763	N662	L214
GLY	K954	E765	R663	E215
LEU	Q955	I774	L664	R219
LEU	K961	N793	L665	Y226
LYS	L962	D798	Q670	I229
PRO	L965	K821	M674	I234
SER	K970	L832	T678	L235
GLU	V973	I833	I679	S245
ASP	V981	E681	V680	P246
ASP	Q982	V637	Q682	D247
ASP	Q983	T850	M686	L262
ASP	G984	F859	P687	K263
ASP	T985	Y860	T688	L264
ASP	Y994	L863	L689	P265
ASP	S1000	E868	I690	F278
ASP	F1003	K869	LEU	L283
ASP	P1004	H1005	ASP	
ASP	H1005	GLU	SER	
ASP	L1006	S870	GLU	
ASP			T695	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.49Å 155.95Å 149.82Å 90.00° 106.91° 90.00°	Depositor
Resolution (Å)	33.69 – 2.22 33.69 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.69-2.22) 99.0 (33.69-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.175 , 0.214 0.175 , 0.214	Depositor DCC
R_{free} test set	9411 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
Estimated twinning fraction	0.776 for H, K, L 0.224 for H, -K, -H-L 0.226 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.776 for H, K, L 0.224 for H, -K, -H-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 187295 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22420	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 2.88% 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

5.1 Standard geometry

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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	0/1531	0.87	1/2079 (0.0%)
1	D	0.72	0/1497	0.88	5/2033 (0.2%)
2	B	0.48	0/1082	0.75	0/1449
2	E	0.52	0/1082	0.85	3/1444 (0.2%)
3	C	0.68	0/8480	0.82	6/11503 (0.1%)
3	F	0.64	0/8202	0.78	1/11129 (0.0%)
All	All	0.66	0/21874	0.81	16/29637 (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	B	0	1
2	E	0	2
3	C	0	1
3	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	149	GLY	N-CA-C	-6.59	96.63	113.10
2	E	279	GLY	N-CA-C	-6.58	96.64	113.10
3	F	141	LEU	CA-CB-CG	6.50	130.26	115.30
1	D	142	ARG	NE-CZ-NH1	-6.12	117.24	120.30
2	E	292	LEU	CA-CB-CG	5.98	129.05	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	148	PHE	Peptide
3	C	376	GLU	Mainchain
2	E	148	PHE	Peptide
2	E	278	LYS	Peptide
3	F	687	PRO	Peptide

5.2 Too-close contacts

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	1492	0	1486	33	0
1	D	1459	0	1453	29	0
2	B	1073	0	1044	28	0
2	E	1074	0	1064	47	0
3	C	8322	0	8330	115	0
3	F	8046	0	8052	122	0
4	A	32	0	12	1	0
4	D	32	0	12	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	84	0	0	2	0
6	B	11	0	0	0	0
6	C	351	0	0	8	1
6	D	86	0	0	1	0
6	E	10	0	0	2	0
6	F	346	0	0	5	1
All	All	22420	0	21453	342	1

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 8.

The worst 5 of 342 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:280:PHE:O	2:B:286:SER:HB2	1.19	1.28
2:E:308:THR:HG21	2:E:313:THR:OG1	1.48	1.12
2:B:280:PHE:O	2:B:286:SER:CB	2.05	1.02
1:A:34:THR:OG1	1:A:36:GLU:HG2	1.65	0.97
3:C:1033:ARG:HG3	3:C:1033:ARG:HH11	1.30	0.96

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	Interatomic distance (Å)	Clash overlap (Å)
6:C:1274:HOH:O	6:F:1158:HOH:O[1_656]	2.17	0.03

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	185/219 (84%)	179 (97%)	6 (3%)	0	100	100
1	D	181/219 (83%)	171 (94%)	9 (5%)	1 (1%)	30	29
2	B	130/238 (55%)	115 (88%)	13 (10%)	2 (2%)	13	9
2	E	128/238 (54%)	112 (88%)	13 (10%)	3 (2%)	8	4
3	C	1038/1049 (99%)	1008 (97%)	29 (3%)	1 (0%)	56	64
3	F	999/1049 (95%)	958 (96%)	40 (4%)	1 (0%)	56	64
All	All	2661/3012 (88%)	2543 (96%)	110 (4%)	8 (0%)	46	50

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	312	GLU
2	E	323	LYS
3	F	681	GLU
2	B	105	LYS

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Mol	Chain	Res	Type
2	E	105	LYS

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	157/188 (84%)	150 (96%)	7 (4%)	34	40
1	D	153/188 (81%)	144 (94%)	9 (6%)	24	26
2	B	107/205 (52%)	92 (86%)	15 (14%)	4	3
2	E	109/205 (53%)	90 (83%)	19 (17%)	2	1
3	C	927/955 (97%)	882 (95%)	45 (5%)	31	35
3	F	900/955 (94%)	850 (94%)	50 (6%)	26	29
All	All	2353/2696 (87%)	2208 (94%)	145 (6%)	23	24

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1008	SER
2	E	211	SER
3	F	870	SER
1	D	10	VAL
1	D	159	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1057	ASN
2	E	219	ASN
3	F	867	ASN
3	C	1063	ASN
2	E	201	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GTP	A	301	5	25,34,34	1.47	4 (16%)	34,54,54	2.40	9 (26%)
4	GTP	D	301	5	25,34,34	1.43	4 (16%)	34,54,54	1.73	9 (26%)

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	301	5	-	0/18/38/38	0/3/3/3
4	GTP	D	301	5	-	0/18/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	GTP	PA-O2A	-2.60	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GTP	PG-O3G	-2.12	1.47	1.54
4	A	301	GTP	O4'-C1'	2.43	1.44	1.41
4	D	301	GTP	C5-C4	3.00	1.47	1.40
4	D	301	GTP	O4'-C1'	3.10	1.45	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	GTP	C5-C6-N1	-6.57	114.60	123.59
4	A	301	GTP	C4-C5-N7	-5.05	104.83	109.48
4	D	301	GTP	C4-C5-N7	-4.00	105.80	109.48
4	D	301	GTP	PA-O3A-PB	-3.92	121.73	132.73
4	A	301	GTP	C2'-C1'-N9	-3.70	108.64	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GTP	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	189/219 (86%)	0.13	8 (4%) 40 39	19, 32, 80, 108	0
1	D	185/219 (84%)	0.06	3 (1%) 74 73	22, 34, 61, 76	0
2	B	144/238 (60%)	1.12	25 (17%) 2 2	41, 69, 90, 104	0
2	E	142/238 (59%)	0.76	16 (11%) 7 6	34, 62, 91, 105	0
3	C	1040/1049 (99%)	0.01	27 (2%) 59 59	17, 36, 60, 98	0
3	F	1005/1049 (95%)	0.03	19 (1%) 70 68	18, 39, 65, 101	0
All	All	2705/3012 (89%)	0.13	98 (3%) 46 45	17, 39, 73, 108	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	271	VAL	8.2
1	A	187	PRO	7.0
2	B	281	THR	6.8
2	E	200	LEU	6.7
2	E	295	VAL	6.0

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 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(Å ²)	Q<0.9
4	GTP	A	301	32/32	0.98	0.11	-0.51	21,27,30,31	0
4	GTP	D	301	32/32	0.98	0.10	-0.76	23,28,34,38	0
5	MG	A	302	1/1	0.98	0.06	-2.81	24,24,24,24	0
5	MG	D	302	1/1	0.97	0.05	-4.01	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.