



# Full wwPDB X-ray Structure Validation Report

May 21, 2020 – 01:46 am BST

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 Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

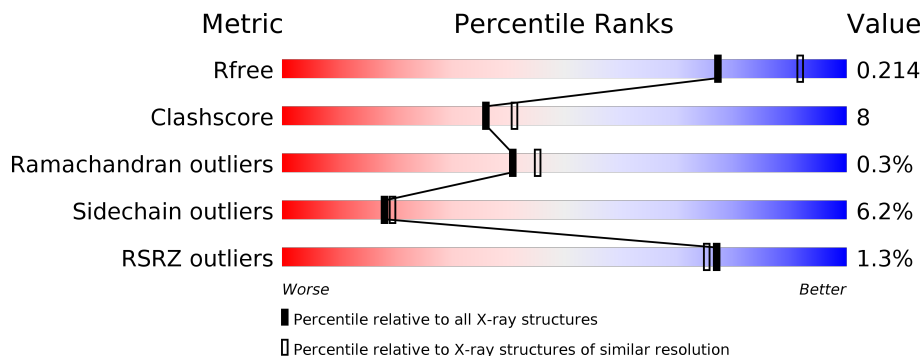
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (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  $\geq 3$ , 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  $\leq 5\%$ . 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	<p>2% 68% 16% 14%</p>
1	D	219	<p>65% 18% 16%</p>
2	B	238	<p>4% 43% 14% 39%</p>
2	E	238	<p>3% 35% 19% 40%</p>
3	C	1049	<p>81% 17%</p>
3	F	1049	<p>77% 17%</p>

## 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
			Total	C	N	O	S			
1	A	189	1492	973	252	262	5	0	0	0
1	D	185	1459	953	245	257	4	0	0	0

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
			Total	C	N	O	S			
2	B	144	1073	691	180	200	2	0	0	0
2	E	142	1074	690	181	201	2	0	0	0

- Molecule 3 is a protein called Exportin-1.

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

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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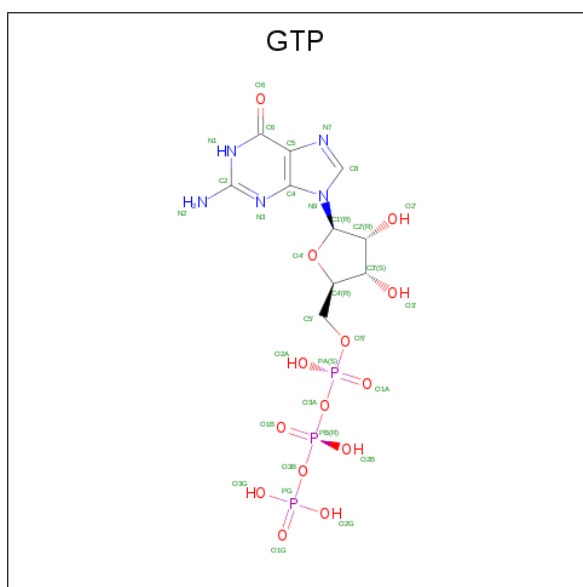
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	DELETION	UNP P30822
C	?	-	GLN	DELETION	UNP P30822
C	?	-	ARG	DELETION	UNP P30822
C	?	-	LEU	DELETION	UNP P30822
C	?	-	PRO	DELETION	UNP P30822
C	?	-	ALA	DELETION	UNP P30822
C	?	-	THR	DELETION	UNP P30822
C	?	-	GLU	DELETION	UNP P30822
C	?	-	MET	DELETION	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	
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

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

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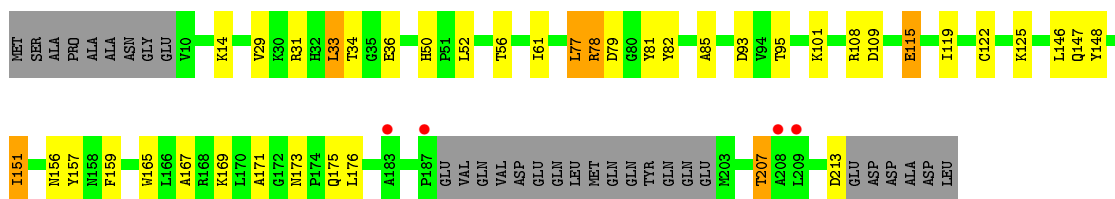
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	F	346	Total 346	O 346	0	0

### 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.

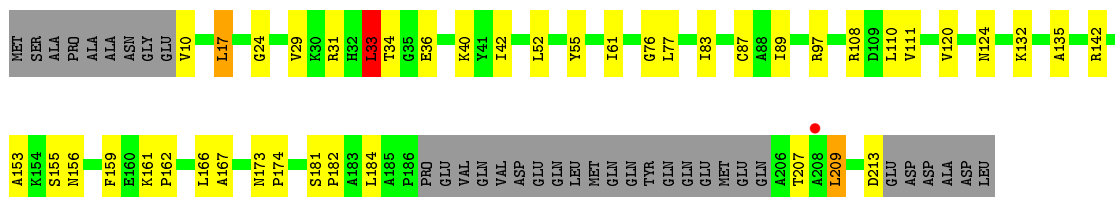
- Molecule 1: Gsp1p

Chain A:



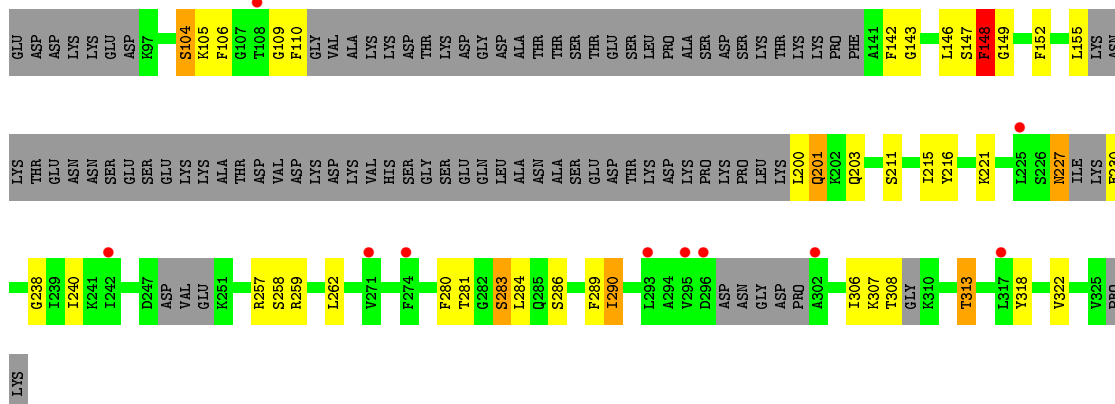
- Molecule 1: Gsp1p

Chain D:



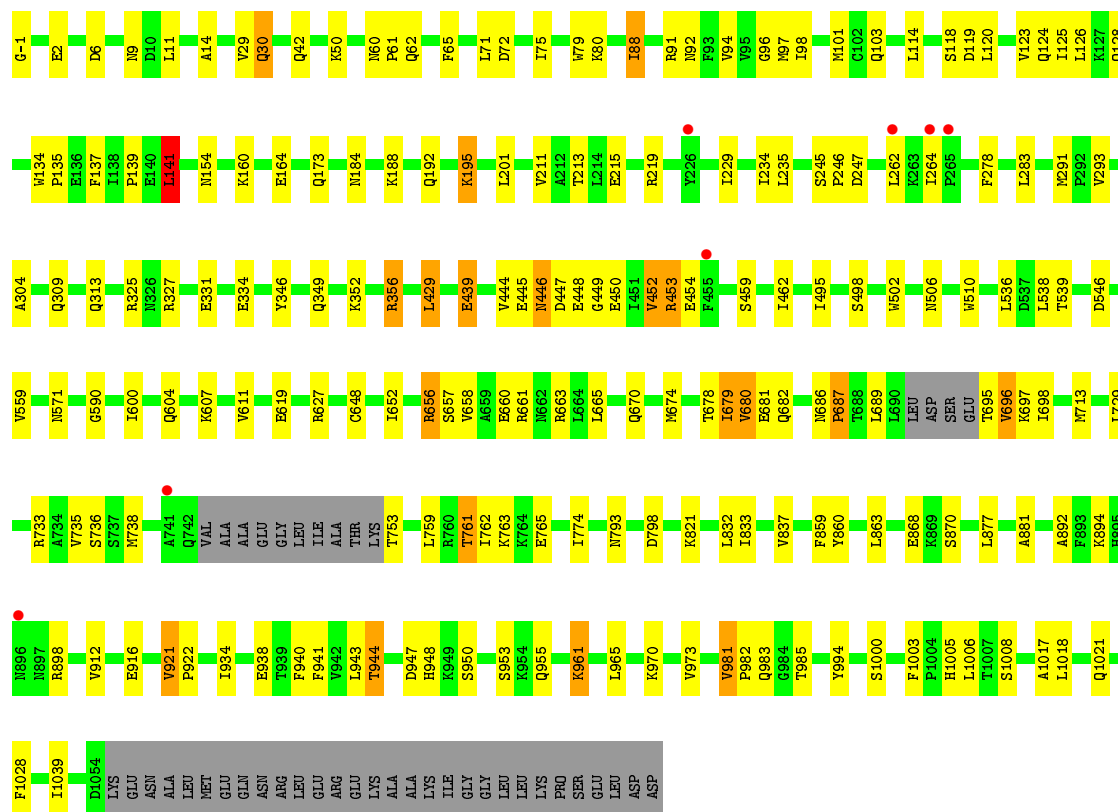
- Molecule 2: Ran-specific GTPase-activating protein 2

Chain B:









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 98.7 (33.69-2.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 21.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	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
Outliers	0 of 187295 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	22420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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: 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.

All (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
3	C	71	LEU	CA-CB-CG	5.90	128.86	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	D	17	LEU	CA-CB-CG	5.84	128.73	115.30
1	D	110	LEU	CB-CG-CD2	-5.59	101.50	111.00
3	C	428	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	108	ARG	NE-CZ-NH1	5.41	123.00	120.30
3	C	893	PHE	N-CA-CB	5.41	120.33	110.60
1	D	33	LEU	CA-CB-CG	5.29	127.48	115.30
3	C	428	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	C	748	LEU	CA-CB-CG	5.17	127.19	115.30
3	C	567	LYS	CD-CE-NZ	-5.16	99.83	111.70

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:D:209:LEU:HD23	1:D:209:LEU:H	1.28	0.96
1:A:207:THR:HG22	2:B:281:THR:H	1.33	0.92
1:D:55:TYR:HD1	2:E:206:LYS:HD3	1.34	0.91
1:D:174:PRO:HG3	3:F:304:ALA:HB3	1.53	0.91
2:E:308:THR:CG2	2:E:313:THR:OG1	2.20	0.89
3:C:264:ILE:HG22	3:C:325:ARG:NH2	1.88	0.87
2:B:283:SER:O	2:B:286:SER:HB3	1.78	0.84
3:F:-1:GLY:N	3:F:2:GLU:OE2	2.12	0.83
2:E:308:THR:HG21	2:E:313:THR:CB	2.10	0.81
3:F:695:THR:HA	3:F:698:ILE:HD13	1.60	0.81
3:F:763:LYS:NZ	3:F:798:ASP:OD2	2.14	0.81
2:B:152:PHE:O	2:B:155:LEU:HB2	1.80	0.80
3:C:236:GLU:HG2	6:C:1429:HOH:O	1.81	0.79
3:C:239:SER:HB2	3:C:281:ASN:HB2	1.67	0.77
2:B:290:ILE:HD11	2:B:318:TYR:HB2	1.65	0.77
3:C:270:LEU:O	3:C:274:GLN:HG3	1.85	0.77
3:C:981:VAL:HG11	3:C:985:THR:HB	1.66	0.76
3:C:446:ASN:HD21	3:C:450:GLU:H	1.33	0.76
1:D:34:THR:OG1	1:D:36:GLU:HG2	1.87	0.75
3:C:940:PHE:O	3:C:944:THR:HB	1.87	0.74
2:E:234:GLU:HB2	6:E:408:HOH:O	1.87	0.73
3:C:55:LEU:HB3	3:C:97:MET:HE3	1.69	0.73
2:E:308:THR:HG22	2:E:309:GLY:N	2.03	0.73
1:A:93:ASP:OD1	1:A:95:THR:HB	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:445:GLU:OE2	3:F:449:GLY:HA2	1.90	0.71
3:F:619:GLU:OE1	3:F:627:ARG:NH2	2.24	0.70
1:D:209:LEU:CD2	1:D:209:LEU:H	2.04	0.70
3:F:894:LYS:O	3:F:948:HIS:HE1	1.75	0.70
1:D:55:TYR:CD1	2:E:206:LYS:HD3	2.22	0.70
2:E:308:THR:CG2	2:E:309:GLY:N	2.55	0.70
1:D:61:ILE:HD13	1:D:167:ALA:HB1	1.75	0.69
1:A:56:THR:CG2	1:A:61:ILE:HD12	2.22	0.69
1:A:122:CYS:HB3	1:A:151:ILE:HD13	1.74	0.68
3:F:679:ILE:HD13	3:F:682:GLN:OE1	1.94	0.68
3:C:414:PRO:O	3:C:417:LYS:HB2	1.94	0.67
3:C:679:ILE:HD11	3:C:695:THR:HG23	1.76	0.67
3:F:940:PHE:O	3:F:944:THR:HB	1.94	0.67
3:C:446:ASN:ND2	3:C:450:GLU:H	1.93	0.67
3:F:184:ASN:O	3:F:188:LYS:HD3	1.94	0.66
1:D:209:LEU:HD23	1:D:209:LEU:N	2.06	0.66
2:E:275:THR:HG21	2:E:293:LEU:HD23	1.76	0.66
3:F:657:SER:OG	3:F:660:GLU:OE1	2.09	0.66
3:C:293:VAL:HG12	3:C:346:TYR:CE2	2.32	0.65
3:F:944:THR:HG23	3:F:1003:PHE:HZ	1.60	0.65
3:C:679:ILE:HD12	3:C:699:ILE:HD11	1.79	0.65
3:F:120:LEU:O	3:F:124:GLN:HG2	1.97	0.65
1:A:14:LYS:HG2	1:A:85:ALA:HA	1.79	0.64
3:C:981:VAL:CG1	3:C:985:THR:HB	2.26	0.64
3:C:936:VAL:HG11	3:C:995:LEU:HD21	1.78	0.63
1:D:155:SER:O	1:D:156:ASN:HB2	1.98	0.63
3:C:227:ARG:HG2	6:C:1422:HOH:O	1.98	0.63
3:C:29:VAL:O	3:C:33:GLN:HG3	1.99	0.63
1:A:56:THR:HG21	1:A:61:ILE:HD12	1.79	0.63
3:F:981:VAL:HG23	6:F:1255:HOH:O	1.98	0.62
3:C:918:MET:HE3	3:C:924:ALA:HB2	1.82	0.62
3:C:429:LEU:HD22	3:F:498:SER:HB2	1.81	0.62
3:F:264:ILE:HG22	3:F:325:ARG:NH2	2.15	0.61
1:D:31:ARG:HD3	1:D:156:ASN:OD1	2.00	0.61
3:F:30:GLN:HE21	3:F:30:GLN:H	1.47	0.61
3:F:88:ILE:HG23	3:F:92:ASN:ND2	2.15	0.61
2:B:142:PHE:CE2	3:C:52:ASP:HB3	2.36	0.61
3:C:981:VAL:HG11	3:C:985:THR:CB	2.31	0.61
3:F:912:VAL:HG13	3:F:965:LEU:HD11	1.84	0.60
3:C:981:VAL:CG1	3:C:985:THR:CB	2.80	0.60
1:D:29:VAL:HG12	1:D:33:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:219:ASN:HD21	2:E:259:ARG:HH21	1.48	0.59
3:F:453:ARG:NH1	3:F:454:GLU:O	2.36	0.58
3:F:14:ALA:O	6:F:1268:HOH:O	2.17	0.58
3:F:698:ILE:H	3:F:698:ILE:HD12	1.67	0.58
3:C:619:GLU:OE1	3:C:627:ARG:NH2	2.34	0.58
3:C:936:VAL:CG1	3:C:995:LEU:HD21	2.33	0.58
3:F:921:VAL:HG22	3:F:922:PRO:HD2	1.85	0.58
3:C:622:ILE:O	3:C:626:ILE:HG13	2.04	0.58
2:E:106:PHE:CD2	3:F:941:PHE:HD1	2.21	0.58
1:D:207:THR:CG2	2:E:281:THR:H	2.17	0.58
3:C:981:VAL:HG13	3:C:985:THR:OG1	2.04	0.57
3:F:309:GLN:O	3:F:313:GLN:HG3	2.04	0.57
3:C:211:VAL:O	3:C:215:GLU:HG2	2.05	0.57
2:E:308:THR:CG2	2:E:309:GLY:H	2.18	0.57
3:F:446:ASN:HD21	3:F:450:GLU:HB2	1.69	0.57
1:A:207:THR:HG22	2:B:281:THR:N	2.12	0.57
3:F:916:GLU:OE1	3:F:961:LYS:NZ	2.38	0.57
3:C:264:ILE:CG2	3:C:325:ARG:NH2	2.64	0.56
3:C:694:GLU:O	3:C:698:ILE:HG13	2.05	0.56
2:E:104:SER:C	2:E:106:PHE:H	2.07	0.56
2:B:148:PHE:O	3:C:96:GLY:HA3	2.06	0.56
2:E:143:GLY:HA2	2:E:146:LEU:HD12	1.86	0.56
3:C:959:LEU:O	3:C:963:ILE:HG13	2.06	0.56
3:F:898:ARG:NH1	3:F:950:SER:O	2.39	0.56
3:C:778:ARG:NH1	6:C:1356:HOH:O	2.39	0.55
3:F:944:THR:CG2	3:F:1003:PHE:HZ	2.19	0.55
1:A:29:VAL:HG12	1:A:33:LEU:HD22	1.89	0.55
2:B:240:ILE:CD1	2:B:306:ILE:HD13	2.37	0.55
3:F:119:ASP:OD2	3:F:154:ASN:ND2	2.39	0.55
1:D:181:SER:OG	6:D:456:HOH:O	2.11	0.55
3:F:445:GLU:HB3	6:F:1358:HOH:O	2.07	0.54
3:F:859:PHE:CE2	3:F:863:LEU:HD11	2.41	0.54
2:E:308:THR:HB	2:E:314:THR:OG1	2.07	0.54
3:F:439:GLU:HB3	3:F:462:ILE:HG12	1.90	0.54
3:C:1033:ARG:HG3	3:C:1033:ARG:NH1	2.09	0.54
3:C:55:LEU:HD22	3:C:97:MET:HE1	1.90	0.54
1:A:147:GLN:HE21	1:A:148:TYR:H	1.56	0.53
3:F:229:ILE:HD13	3:F:262:LEU:HD13	1.90	0.53
3:F:453:ARG:HG3	3:F:590:GLY:HA2	1.90	0.53
3:C:944:THR:CG2	3:C:1003:PHE:HZ	2.22	0.53
1:D:174:PRO:HG3	3:F:304:ALA:CB	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1033:ARG:CG	3:C:1033:ARG:HH11	2.12	0.53
3:C:235:LEU:HD21	3:C:259:VAL:HG11	1.91	0.53
1:A:157:TYR:CE2	3:C:458:GLU:HG2	2.45	0.52
3:C:570:TRP:CE2	3:C:614:GLN:HG3	2.43	0.52
3:F:506:ASN:HB3	3:F:510:TRP:CZ2	2.44	0.52
3:C:229:ILE:HD13	3:C:262:LEU:HD13	1.91	0.52
3:F:75:ILE:HD13	3:F:125:ILE:HG13	1.89	0.52
3:C:944:THR:HG23	3:C:1003:PHE:HZ	1.74	0.52
3:C:192:GLN:HG3	6:C:1395:HOH:O	2.07	0.52
2:E:146:LEU:O	2:E:149:GLY:HA3	2.09	0.52
3:C:264:ILE:HG22	3:C:325:ARG:HH22	1.72	0.52
3:C:-1:GLY:N	3:C:2:GLU:OE1	2.43	0.52
3:F:446:ASN:HD22	3:F:446:ASN:C	2.12	0.51
3:F:229:ILE:HG22	3:F:235:LEU:HG	1.92	0.51
3:F:349:GLN:HE22	3:F:352:LYS:NZ	2.08	0.51
1:A:56:THR:HG21	1:A:61:ILE:CD1	2.39	0.51
3:C:669:MET:O	3:C:672:PRO:HD2	2.10	0.51
3:C:282:THR:O	3:C:286:ILE:HG12	2.10	0.51
3:F:446:ASN:ND2	3:F:450:GLU:H	2.09	0.51
2:B:216:TYR:OH	2:B:313:THR:HG22	2.11	0.51
2:E:155:LEU:HD13	3:F:103:GLN:HE22	1.75	0.51
3:C:691:LEU:HD11	3:C:742:GLN:HE22	1.76	0.51
2:E:293:LEU:HD13	2:E:303:GLN:HG3	1.92	0.51
1:A:56:THR:HG23	1:A:61:ILE:HD12	1.91	0.51
1:A:165:TRP:CZ2	1:A:169:LYS:HE2	2.46	0.50
3:C:614:GLN:HE21	3:C:615:PRO:HD2	1.76	0.50
3:F:11:LEU:HB2	3:F:50:LYS:HD2	1.92	0.50
3:F:446:ASN:ND2	3:F:450:GLU:HB2	2.26	0.50
1:A:176:LEU:HD23	1:A:176:LEU:C	2.32	0.50
2:B:142:PHE:CZ	3:C:52:ASP:HB3	2.46	0.50
3:F:94:VAL:O	3:F:98:ILE:HG13	2.11	0.50
2:B:149:GLY:H	3:C:93:PHE:HA	1.75	0.50
2:B:109:GLY:O	2:B:110:PHE:HB2	2.11	0.50
3:C:327:ARG:O	3:C:331:GLU:HG3	2.11	0.50
3:C:443:VAL:HG13	3:C:451:ILE:CG2	2.41	0.50
2:E:308:THR:HG22	2:E:310:LYS:H	1.76	0.50
3:F:264:ILE:CG2	3:F:325:ARG:NH2	2.74	0.50
2:E:146:LEU:O	2:E:149:GLY:CA	2.60	0.50
3:F:160:LYS:HD2	3:F:219:ARG:CZ	2.41	0.50
2:B:238:GLY:HA3	2:B:257:ARG:O	2.12	0.50
3:C:964:SER:O	3:C:968:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:SER:C	2:B:106:PHE:H	2.16	0.49
2:E:275:THR:HB	2:E:293:LEU:HB2	1.94	0.49
1:A:213:ASP:OD1	2:B:221:LYS:NZ	2.43	0.49
3:C:565:PHE:HE2	3:C:572:PHE:CD2	2.30	0.49
2:E:308:THR:HG21	2:E:313:THR:HB	1.93	0.49
3:C:565:PHE:O	3:C:569:HIS:HD2	1.95	0.49
3:F:201:LEU:HD12	3:F:234:ILE:HD11	1.93	0.49
3:F:211:VAL:O	3:F:215:GLU:HG2	2.13	0.49
3:F:101:MET:HE1	3:F:114:LEU:HD21	1.95	0.49
3:F:658:VAL:HG22	3:F:661:ARG:HH22	1.78	0.49
1:A:101:LYS:HG2	1:A:101:LYS:O	2.12	0.48
1:A:33:LEU:HD13	1:A:52:LEU:HD12	1.95	0.48
3:C:466:LYS:O	3:C:470:GLU:HG3	2.13	0.48
2:E:275:THR:O	2:E:292:LEU:HB2	2.13	0.48
3:F:1018:LEU:HD22	3:F:1028:PHE:CE1	2.48	0.48
3:F:454:GLU:HG3	3:F:454:GLU:O	2.12	0.48
3:C:651:ILE:O	3:C:654:GLU:HB3	2.13	0.48
1:A:31:ARG:HD3	1:A:156:ASN:OD1	2.14	0.48
3:C:43:ASP:OD2	3:C:73:LYS:NZ	2.47	0.48
3:F:134:TRP:N	3:F:135:PRO:CD	2.76	0.48
1:A:61:ILE:HD11	1:A:176:LEU:HD11	1.95	0.48
3:F:600:ILE:O	3:F:604:GLN:HG3	2.13	0.48
3:C:789:GLU:O	3:C:793:ASN:HB2	2.14	0.48
3:C:885:PHE:O	3:C:889:ILE:HG13	2.13	0.48
3:C:372:ASP:HB2	6:C:1169:HOH:O	2.14	0.48
2:E:148:PHE:O	3:F:96:GLY:HA3	2.14	0.48
3:F:264:ILE:HG23	3:F:264:ILE:O	2.14	0.48
2:E:257:ARG:HA	2:E:263:LYS:O	2.14	0.48
3:F:6:ASP:OD2	3:F:9:ASN:ND2	2.47	0.48
3:C:599:PHE:O	3:C:603:VAL:HG13	2.13	0.48
3:F:160:LYS:O	3:F:164:GLU:HG3	2.13	0.47
3:C:4:ILE:HD11	3:C:37:ILE:HG22	1.96	0.47
3:C:443:VAL:HG13	3:C:451:ILE:HG23	1.96	0.47
3:F:79:TRP:CD1	3:F:128:GLN:HB3	2.50	0.47
3:F:859:PHE:CZ	3:F:863:LEU:HD11	2.48	0.47
3:C:112:LYS:HB2	6:C:1154:HOH:O	2.15	0.47
1:D:213:ASP:N	1:D:213:ASP:OD2	2.47	0.47
2:E:206:LYS:HA	2:E:206:LYS:HE3	1.95	0.47
3:C:570:TRP:CD2	3:C:614:GLN:HG3	2.49	0.47
2:E:319:ASN:O	2:E:323:LYS:HB2	2.14	0.47
3:F:860:TYR:CE1	3:F:892:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1018:LEU:HD22	3:C:1028:PHE:CE1	2.50	0.47
3:C:613:GLN:HE21	3:C:619:GLU:HA	1.79	0.47
3:F:349:GLN:HE22	3:F:352:LYS:HZ2	1.62	0.47
3:F:686:ASN:HB3	3:F:689:LEU:HD12	1.97	0.47
1:D:182:PRO:HB3	2:E:207:SER:O	2.15	0.46
2:B:143:GLY:HA2	2:B:146:LEU:HD12	1.96	0.46
3:C:130:TRP:CD1	3:C:131:PRO:HA	2.51	0.46
2:B:216:TYR:HH	2:B:313:THR:HG22	1.81	0.46
3:C:322:TYR:O	3:C:326:ASN:HB2	2.16	0.46
3:C:220:TYR:O	3:C:224:ILE:HG23	2.16	0.46
3:C:739:ILE:O	3:C:743:VAL:HG23	2.16	0.46
3:C:981:VAL:CG1	3:C:985:THR:OG1	2.63	0.46
3:F:860:TYR:CZ	3:F:892:ALA:HB2	2.51	0.46
3:F:934:ILE:O	3:F:938:GLU:HG2	2.15	0.46
1:D:97:ARG:NH1	1:D:132:LYS:HD3	2.31	0.46
3:F:648:CYS:O	3:F:652:ILE:HG13	2.15	0.46
3:C:937:SER:HB2	3:C:998:MET:SD	2.56	0.46
3:F:139:PRO:HG3	3:F:192:GLN:HE22	1.81	0.46
3:F:674:MET:O	3:F:678:THR:HG23	2.16	0.46
3:F:679:ILE:CG2	3:F:680:VAL:N	2.79	0.46
3:C:167:PHE:CE1	3:C:183:LYS:HG2	2.51	0.45
2:E:227:ASN:ND2	2:E:230:GLU:O	2.49	0.45
3:F:447:ASP:HA	6:F:1349:HOH:O	2.16	0.45
3:F:735:VAL:HG21	3:F:762:ILE:HD12	1.98	0.45
2:B:155:LEU:HD13	3:C:99:ILE:HD13	1.99	0.45
3:C:498:SER:HB2	3:F:429:LEU:HD22	1.97	0.45
2:E:292:LEU:HD22	2:E:304:TYR:HB2	1.98	0.45
3:F:981:VAL:CG1	3:F:985:THR:OG1	2.65	0.45
3:F:736:SER:HB3	3:F:798:ASP:OD1	2.16	0.45
1:A:125:LYS:HE2	4:A:301:GTP:C4	2.51	0.45
3:F:91:ARG:HG3	3:F:134:TRP:CH2	2.51	0.45
1:D:87:CYS:HB2	1:D:166:LEU:HD22	1.98	0.45
3:C:265:PRO:HD2	3:C:271:ILE:HD12	1.98	0.45
1:A:61:ILE:HD13	1:A:167:ALA:HB1	1.99	0.45
1:D:17:LEU:HD13	1:D:89:ILE:HB	1.99	0.45
2:B:149:GLY:N	3:C:93:PHE:HA	2.31	0.45
1:D:24:GLY:HA3	1:D:124:ASN:ND2	2.32	0.45
3:F:195:LYS:HB2	3:F:195:LYS:HE2	1.71	0.45
3:F:445:GLU:N	6:F:1358:HOH:O	2.35	0.45
2:E:148:PHE:CE2	3:F:97:MET:HG3	2.52	0.45
1:A:171:ALA:CB	2:B:201:GLN:HG3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:ILE:HB	3:C:189:GLU:OE2	2.17	0.45
3:C:669:MET:C	3:C:672:PRO:HD2	2.37	0.45
1:D:213:ASP:OD1	2:E:221:LYS:NZ	2.45	0.45
2:E:290:ILE:HG22	2:E:306:ILE:HB	1.99	0.45
3:F:1005:HIS:CD2	3:F:1005:HIS:H	2.35	0.45
3:F:774:ILE:O	3:F:821:LYS:HG2	2.17	0.45
2:B:258:SER:O	2:B:262:LEU:HA	2.17	0.44
3:C:55:LEU:HB3	3:C:97:MET:CE	2.44	0.44
3:F:293:VAL:HG12	3:F:346:TYR:CE2	2.53	0.44
3:F:729:LEU:O	3:F:733:ARG:HG3	2.16	0.44
1:A:77:LEU:HB2	1:A:81:TYR:CE1	2.53	0.44
2:E:308:THR:HG23	2:E:309:GLY:H	1.82	0.44
1:A:78:ARG:NH2	1:A:78:ARG:HG2	2.32	0.44
3:C:872:ALA:HA	3:C:875:LEU:HD12	2.00	0.44
3:F:502:TRP:CZ2	3:F:546:ASP:HB3	2.52	0.44
3:F:665:LEU:HD13	3:F:713:MET:SD	2.56	0.44
3:F:761:THR:O	3:F:765:GLU:HG2	2.18	0.44
3:C:1005:HIS:CE1	3:C:1039:ILE:O	2.70	0.44
3:F:445:GLU:HA	3:F:450:GLU:O	2.16	0.44
3:C:527:PHE:O	3:C:531:VAL:HG23	2.18	0.44
3:F:536:LEU:O	3:F:539:THR:HB	2.17	0.44
3:F:495:ILE:HD13	3:F:538:LEU:HG	2.00	0.44
1:A:115:GLU:HG3	6:A:452:HOH:O	2.17	0.44
3:C:1009:GLU:OE1	3:C:1009:GLU:N	2.51	0.44
3:C:971:ILE:HD13	3:C:975:LEU:HD21	2.00	0.44
3:F:1017:ALA:O	3:F:1021:GLN:HG3	2.18	0.44
3:C:824:HIS:CD2	3:C:824:HIS:H	2.35	0.43
3:F:994:TYR:C	3:F:994:TYR:CD2	2.91	0.43
3:C:493:ARG:HB3	3:C:499:GLU:HG3	2.00	0.43
2:E:217:GLN:HA	2:E:240:ILE:O	2.18	0.43
2:E:215:ILE:HD11	2:E:244:LYS:CB	2.48	0.43
3:F:696:VAL:CG2	3:F:759:LEU:HD23	2.48	0.43
3:C:1029:LYS:O	3:C:1033:ARG:HG2	2.18	0.43
3:C:445:GLU:N	6:C:1334:HOH:O	2.37	0.43
3:F:733:ARG:O	3:F:736:SER:HB2	2.18	0.43
1:A:33:LEU:HD21	1:A:50:HIS:HB3	2.00	0.43
3:C:326:ASN:O	3:C:329:LEU:HB2	2.18	0.43
2:E:155:LEU:CD1	3:F:103:GLN:NE2	2.82	0.43
3:F:88:ILE:HG23	3:F:92:ASN:HD22	1.84	0.43
3:C:966:VAL:HG21	3:C:991:LEU:HD22	2.01	0.43
1:D:83:ILE:HD11	3:F:65:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:229:ILE:HD13	3:F:262:LEU:CD1	2.47	0.43
3:C:691:LEU:HD11	3:C:742:GLN:NE2	2.33	0.43
3:F:916:GLU:OE2	3:F:970:LYS:HE2	2.18	0.43
2:B:240:ILE:CD1	2:B:306:ILE:CD1	2.97	0.43
3:C:686:ASN:ND2	3:C:688:THR:OG1	2.46	0.43
3:F:679:ILE:HG22	3:F:680:VAL:N	2.33	0.43
3:C:101:MET:HG2	3:C:107:VAL:HG11	2.01	0.43
1:D:29:VAL:HG12	1:D:33:LEU:CD2	2.47	0.43
1:A:78:ARG:HH21	1:A:78:ARG:HG2	1.84	0.42
1:A:82:TYR:CD1	1:A:82:TYR:N	2.86	0.42
2:B:227:ASN:HD22	2:B:230:GLU:N	2.17	0.42
3:F:877:LEU:HB3	3:F:881:ALA:HB3	2.01	0.42
3:F:981:VAL:HG13	3:F:982:PRO:O	2.18	0.42
1:A:78:ARG:HB3	1:A:79:ASP:H	1.49	0.42
1:D:40:LYS:HE2	1:D:42:ILE:HD11	2.01	0.42
3:F:123:VAL:HA	3:F:126:LEU:HD12	2.00	0.42
3:C:983:GLN:H	3:C:983:GLN:HG3	1.44	0.42
1:D:76:GLY:O	3:F:42:GLN:NE2	2.52	0.42
3:C:1033:ARG:CG	3:C:1033:ARG:NH1	2.78	0.42
3:F:327:ARG:O	3:F:331:GLU:HG3	2.20	0.42
3:F:60:ASN:HA	3:F:61:PRO:HD2	1.74	0.42
3:C:235:LEU:HA	3:C:235:LEU:HD23	1.71	0.41
3:C:435:MET:O	3:C:507:THR:HG22	2.20	0.41
3:C:755:LYS:O	3:C:759:LEU:HG	2.20	0.41
3:C:863:LEU:HA	3:C:863:LEU:HD23	1.87	0.41
3:F:448:GLU:HG3	3:F:450:GLU:OE1	2.19	0.41
3:C:771:GLU:HG2	3:C:817:THR:OG1	2.20	0.41
3:F:444:VAL:O	3:F:452:VAL:N	2.42	0.41
1:D:161:LYS:N	1:D:162:PRO:CD	2.84	0.41
3:C:532:ILE:HD13	3:C:532:ILE:HA	1.83	0.41
3:C:812:LEU:HB2	3:C:858:GLU:HB3	2.02	0.41
2:E:322:VAL:C	2:E:324:SER:N	2.74	0.41
1:A:173:ASN:OD1	1:A:175:GLN:HB2	2.19	0.41
3:C:330:LEU:HB2	3:C:340:LEU:HD13	2.02	0.41
3:C:506:ASN:HB3	3:C:510:TRP:CZ2	2.55	0.41
3:F:137:PHE:CZ	3:F:141:LEU:HG	2.56	0.41
3:F:245:SER:HA	3:F:246:PRO:HD3	1.84	0.41
3:F:283:LEU:HD13	3:F:283:LEU:HA	1.89	0.41
3:C:1040:LYS:HE3	6:C:1297:HOH:O	2.21	0.41
2:E:148:PHE:CZ	3:F:97:MET:HG3	2.55	0.41
2:B:289:PHE:CE2	2:B:307:LYS:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:656:ARG:HA	3:F:656:ARG:HD2	1.74	0.41
3:F:833:ILE:O	3:F:837:VAL:HG22	2.21	0.41
2:E:108:THR:HB	6:E:405:HOH:O	2.20	0.41
1:A:119:ILE:HB	1:A:146:LEU:HD22	2.02	0.41
3:C:1018:LEU:HD22	3:C:1028:PHE:CZ	2.55	0.41
3:F:293:VAL:HG12	3:F:346:TYR:CZ	2.55	0.41
1:A:108:ARG:NH1	6:A:463:HOH:O	2.54	0.41
3:C:761:THR:O	3:C:765:GLU:HG2	2.21	0.41
2:E:240:ILE:HG13	2:E:256:MET:HB2	2.03	0.41
3:C:322:TYR:C	3:C:322:TYR:CD2	2.94	0.40
3:C:60:ASN:HA	3:C:61:PRO:HD3	1.94	0.40
3:F:1006:LEU:HD11	3:F:1039:ILE:HG22	2.02	0.40
2:E:155:LEU:CD1	3:F:103:GLN:HE22	2.33	0.40
3:F:356:ARG:HB2	3:F:356:ARG:HE	1.65	0.40
2:B:104:SER:HB2	3:C:938:GLU:OE2	2.22	0.40
3:C:933:PHE:CD1	3:C:994:TYR:CD2	3.10	0.40
1:D:34:THR:O	2:E:235:ARG:HD2	2.21	0.40
2:E:212:GLU:OE2	2:E:243:ASN:HB3	2.21	0.40
2:E:148:PHE:HB2	3:F:96:GLY:C	2.42	0.40
3:F:982:PRO:O	3:F:985:THR:HG23	2.20	0.40
1:D:173:ASN:HA	1:D:174:PRO:HD3	1.81	0.40
2:E:258:SER:OG	2:E:261:ILE:HG23	2.22	0.40
3:F:687:PRO:HB2	3:F:738:MET:SD	2.61	0.40
2:B:146:LEU:O	2:B:149:GLY:HA3	2.21	0.40
1:D:31:ARG:HD2	1:D:153:ALA:O	2.22	0.40
3:F:943:LEU:HA	3:F:955:GLN:OE1	2.21	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	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%)	25	25
2	B	130/238 (55%)	115 (88%)	13 (10%)	2 (2%)	10	7
2	E	128/238 (54%)	112 (88%)	13 (10%)	3 (2%)	6	3
3	C	1038/1049 (99%)	1008 (97%)	29 (3%)	1 (0%)	51	60
3	F	999/1049 (95%)	958 (96%)	40 (4%)	1 (0%)	51	60
All	All	2661/3012 (88%)	2543 (96%)	110 (4%)	8 (0%)	41	45

All (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
2	E	105	LYS
3	C	172	GLU
1	D	135	ALA
2	B	215	ILE

### 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	157/188 (84%)	150 (96%)	7 (4%)	27	33
1	D	153/188 (81%)	144 (94%)	9 (6%)	19	22
2	B	107/205 (52%)	92 (86%)	15 (14%)	3	2
2	E	109/205 (53%)	90 (83%)	19 (17%)	2	1
3	C	927/955 (97%)	882 (95%)	45 (5%)	25	29
3	F	900/955 (94%)	850 (94%)	50 (6%)	21	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2353/2696 (87%)	2208 (94%)	145 (6%)	18	19

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	77	LEU
1	A	78	ARG
1	A	115	GLU
1	A	151	ILE
1	A	159	PHE
1	A	207	THR
2	B	104	SER
2	B	147	SER
2	B	148	PHE
2	B	200	LEU
2	B	201	GLN
2	B	203	GLN
2	B	211	SER
2	B	227	ASN
2	B	259	ARG
2	B	283	SER
2	B	284	LEU
2	B	290	ILE
2	B	308	THR
2	B	313	THR
2	B	322	VAL
3	C	71	LEU
3	C	82	LEU
3	C	84	ASN
3	C	88	ILE
3	C	105	ASP
3	C	136	GLU
3	C	186	MET
3	C	197	CYS
3	C	203	GLN
3	C	205	SER
3	C	207	SER
3	C	247	ASP
3	C	263	LYS
3	C	264	ILE
3	C	267	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	270	LEU
3	C	271	ILE
3	C	285	GLN
3	C	291	MET
3	C	364	ASP
3	C	446	ASN
3	C	453	ARG
3	C	456	VAL
3	C	459	SER
3	C	522	ASP
3	C	629	ILE
3	C	656	ARG
3	C	660	GLU
3	C	679	ILE
3	C	749	ILE
3	C	793	ASN
3	C	821	LYS
3	C	824	HIS
3	C	832	LEU
3	C	851	GLU
3	C	854	GLU
3	C	858	GLU
3	C	909	LEU
3	C	921	VAL
3	C	940	PHE
3	C	944	THR
3	C	981	VAL
3	C	983	GLN
3	C	1008	SER
3	C	1033	ARG
1	D	10	VAL
1	D	33	LEU
1	D	52	LEU
1	D	77	LEU
1	D	111	VAL
1	D	120	VAL
1	D	159	PHE
1	D	184	LEU
1	D	209	LEU
2	E	104	SER
2	E	148	PHE
2	E	154	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	203	GLN
2	E	206	LYS
2	E	211	SER
2	E	215	ILE
2	E	218	VAL
2	E	227	ASN
2	E	237	VAL
2	E	252	THR
2	E	259	ARG
2	E	280	PHE
2	E	286	SER
2	E	290	ILE
2	E	292	LEU
2	E	295	VAL
2	E	312	GLU
2	E	324	SER
3	F	29	VAL
3	F	30	GLN
3	F	62	GLN
3	F	71	LEU
3	F	72	ASP
3	F	80	LYS
3	F	88	ILE
3	F	118	SER
3	F	141	LEU
3	F	173	GLN
3	F	195	LYS
3	F	213	THR
3	F	247	ASP
3	F	278	PHE
3	F	291	MET
3	F	334	GLU
3	F	356	ARG
3	F	429	LEU
3	F	439	GLU
3	F	446	ASN
3	F	452	VAL
3	F	453	ARG
3	F	459	SER
3	F	559	VAL
3	F	571	ASN
3	F	607	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	F	611	VAL
3	F	656	ARG
3	F	663	ARG
3	F	670	GLN
3	F	679	ILE
3	F	680	VAL
3	F	696	VAL
3	F	697	LYS
3	F	753	THR
3	F	761	THR
3	F	793	ASN
3	F	832	LEU
3	F	868	GLU
3	F	870	SER
3	F	921	VAL
3	F	944	THR
3	F	947	ASP
3	F	953	SER
3	F	961	LYS
3	F	973	VAL
3	F	981	VAL
3	F	983	GLN
3	F	1000	SER
3	F	1008	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	84	ASN
1	A	147	GLN
1	A	158	ASN
2	B	201	GLN
2	B	203	GLN
2	B	269	GLN
3	C	35	GLN
3	C	49	GLN
3	C	192	GLN
3	C	285	GLN
3	C	446	ASN
3	C	569	HIS
3	C	613	GLN
3	C	614	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	639	GLN
3	C	686	ASN
3	C	742	GLN
3	C	824	HIS
3	C	867	ASN
3	C	948	HIS
3	C	983	GLN
3	C	1005	HIS
3	C	1057	ASN
3	C	1063	ASN
1	D	147	GLN
2	E	201	GLN
2	E	203	GLN
2	E	219	ASN
2	E	227	ASN
2	E	269	GLN
2	E	285	GLN
3	F	9	ASN
3	F	18	GLN
3	F	30	GLN
3	F	35	GLN
3	F	49	GLN
3	F	92	ASN
3	F	103	GLN
3	F	116	ASN
3	F	173	GLN
3	F	176	GLN
3	F	192	GLN
3	F	349	GLN
3	F	446	ASN
3	F	639	GLN
3	F	824	HIS
3	F	867	ASN
3	F	948	HIS
3	F	983	GLN
3	F	1005	HIS

### 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 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	D	301	5	26,34,34	1.45	4 (15%)	33,54,54	1.83	9 (27%)
4	GTP	A	301	5	26,34,34	1.47	4 (15%)	33,54,54	2.40	11 (33%)

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	D	301	5	-	6/18/38/38	0/3/3/3
4	GTP	A	301	5	-	5/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	GTP	C6-C5	4.21	1.48	1.41
4	A	301	GTP	C6-C5	4.18	1.48	1.41
4	D	301	GTP	O4'-C1'	2.90	1.45	1.41
4	A	301	GTP	C5-C4	2.74	1.48	1.40
4	D	301	GTP	PA-O2A	-2.44	1.43	1.55
4	D	301	GTP	C5-C4	2.40	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	GTP	O4'-C1'	2.29	1.44	1.41
4	A	301	GTP	PG-O3G	-2.01	1.47	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	GTP	C5-C6-N1	-6.45	114.60	123.43
4	A	301	GTP	C6-N1-C2	5.56	124.77	115.93
4	A	301	GTP	O4'-C1'-C2'	-4.77	99.95	106.93
4	A	301	GTP	C4-C5-N7	-4.38	104.83	109.40
4	D	301	GTP	C6-C5-C4	-3.65	117.32	120.80
4	D	301	GTP	C4-C5-N7	-3.46	105.80	109.40
4	D	301	GTP	C2-N3-C4	3.37	119.20	115.36
4	D	301	GTP	PA-O3A-PB	-3.23	121.73	132.83
4	A	301	GTP	N3-C2-N1	-3.15	123.03	127.22
4	A	301	GTP	O2G-PG-O1G	3.11	122.86	110.68
4	A	301	GTP	O3G-PG-O2G	3.05	119.31	107.64
4	D	301	GTP	C5-C6-N1	-2.92	119.44	123.43
4	A	301	GTP	C2-N3-C4	2.87	118.64	115.36
4	D	301	GTP	C1'-N9-C4	-2.79	121.73	126.64
4	D	301	GTP	O3B-PG-O1G	-2.78	95.75	111.19
4	A	301	GTP	PA-O3A-PB	-2.40	124.58	132.83
4	D	301	GTP	O3G-PG-O1G	2.18	119.21	110.68
4	A	301	GTP	C6-C5-C4	-2.13	118.76	120.80
4	A	301	GTP	O3B-PG-O1G	-2.11	99.47	111.19
4	D	301	GTP	O4'-C4'-C5'	-2.05	102.63	109.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

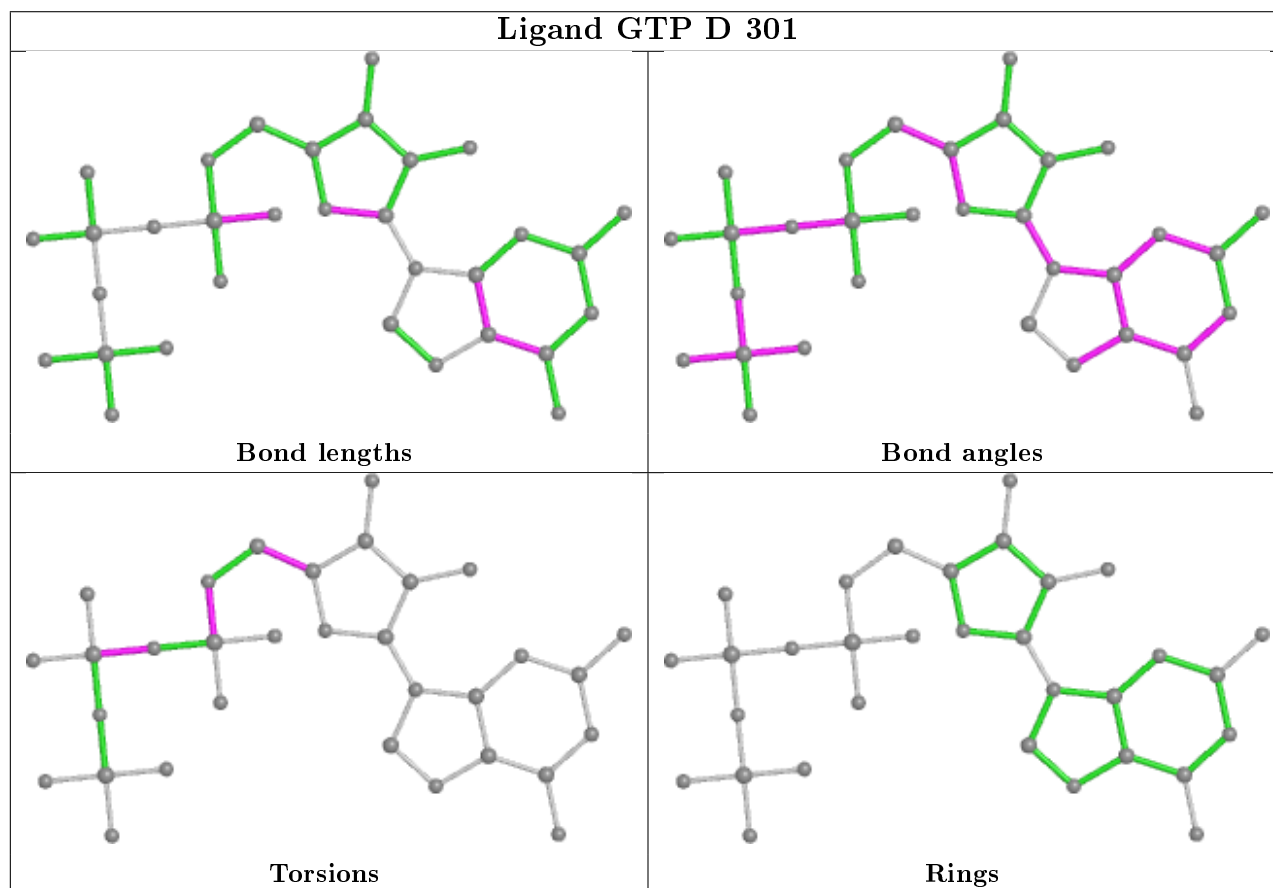
Mol	Chain	Res	Type	Atoms
4	D	301	GTP	C5'-O5'-PA-O3A
4	A	301	GTP	C5'-O5'-PA-O3A
4	D	301	GTP	O4'-C4'-C5'-O5'
4	D	301	GTP	C3'-C4'-C5'-O5'
4	D	301	GTP	PA-O3A-PB-O1B
4	D	301	GTP	C5'-O5'-PA-O1A
4	D	301	GTP	C5'-O5'-PA-O2A
4	A	301	GTP	C5'-O5'-PA-O2A
4	A	301	GTP	PG-O3B-PB-O1B
4	A	301	GTP	PA-O3A-PB-O1B
4	A	301	GTP	PA-O3A-PB-O2B

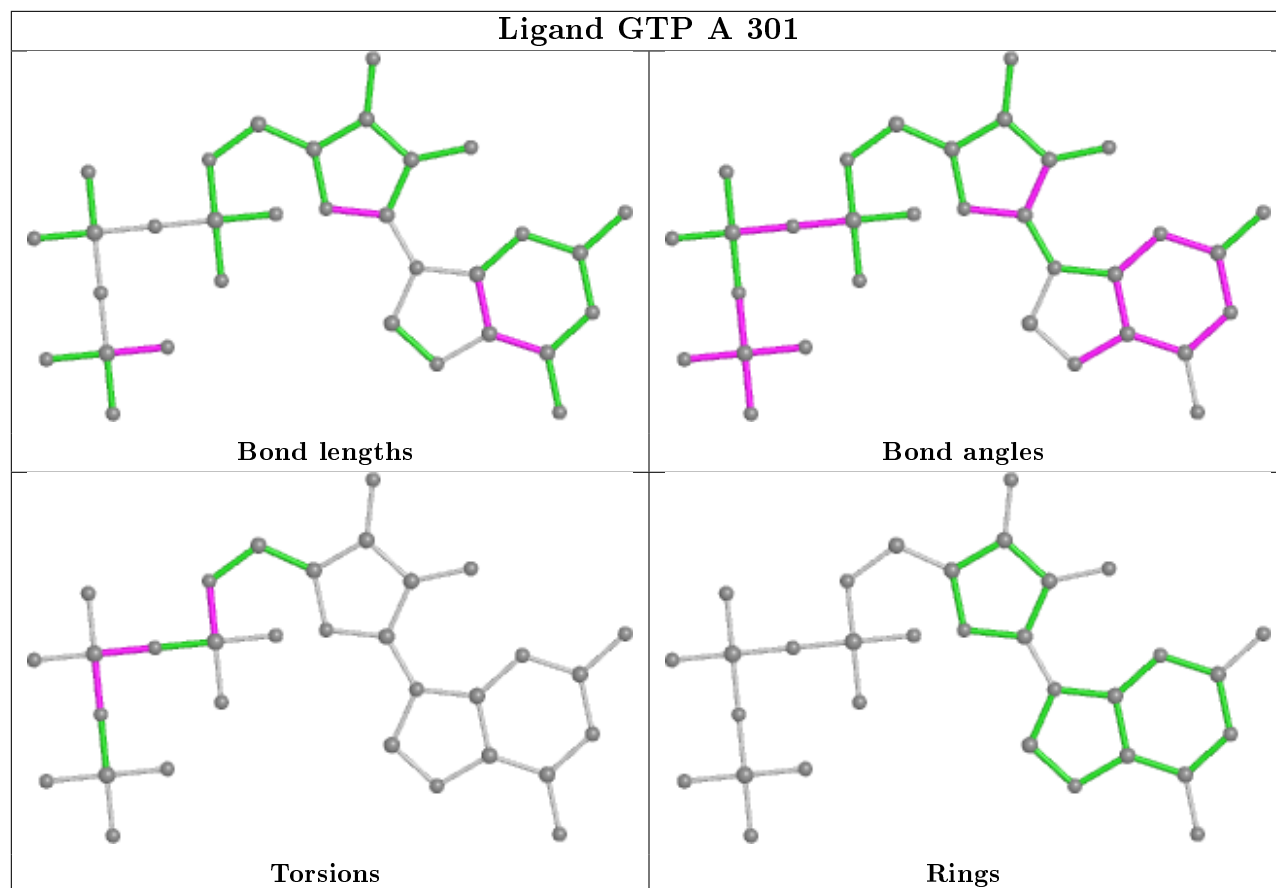
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	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 than 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

### 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	189/219 (86%)	-0.11	4 (2%) 63 61	19, 32, 80, 108	0
1	D	185/219 (84%)	-0.25	1 (0%) 91 90	22, 34, 61, 76	0
2	B	144/238 (60%)	0.47	10 (6%) 16 15	41, 69, 90, 104	0
2	E	142/238 (59%)	0.33	8 (5%) 24 23	34, 62, 91, 105	0
3	C	1040/1049 (99%)	-0.14	6 (0%) 89 88	17, 36, 60, 98	0
3	F	1005/1049 (95%)	-0.11	7 (0%) 87 86	18, 39, 65, 101	0
All	All	2705/3012 (89%)	-0.08	36 (1%) 77 75	17, 39, 73, 108	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	295	VAL	5.2
3	F	264	ILE	4.8
2	B	295	VAL	4.3
3	C	448	GLU	4.2
2	B	302	ALA	3.9
1	A	187	PRO	3.8
3	C	455	PHE	3.8
2	E	200	LEU	3.8
2	B	271	VAL	3.7
3	F	455	PHE	3.7
2	E	108	THR	3.7
2	B	296	ASP	3.7
3	C	1065	LEU	3.7
3	F	262	LEU	3.4
1	A	208	ALA	3.4
1	D	208	ALA	3.3
2	B	274	PHE	3.2
2	E	271	VAL	3.0
3	F	741	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	209	LEU	2.6
2	E	270	LEU	2.6
2	B	317	LEU	2.5
2	B	242	ILE	2.5
3	C	449	GLY	2.4
2	B	225	LEU	2.4
2	B	293	LEU	2.3
2	E	155	LEU	2.3
2	E	303	GLN	2.3
1	A	183	ALA	2.2
3	C	262	LEU	2.2
3	F	226	TYR	2.2
3	C	741	ALA	2.1
2	E	107	GLY	2.1
3	F	896	ASN	2.1
3	F	265	PRO	2.1
2	B	108	THR	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 carbohydrates in this entry.

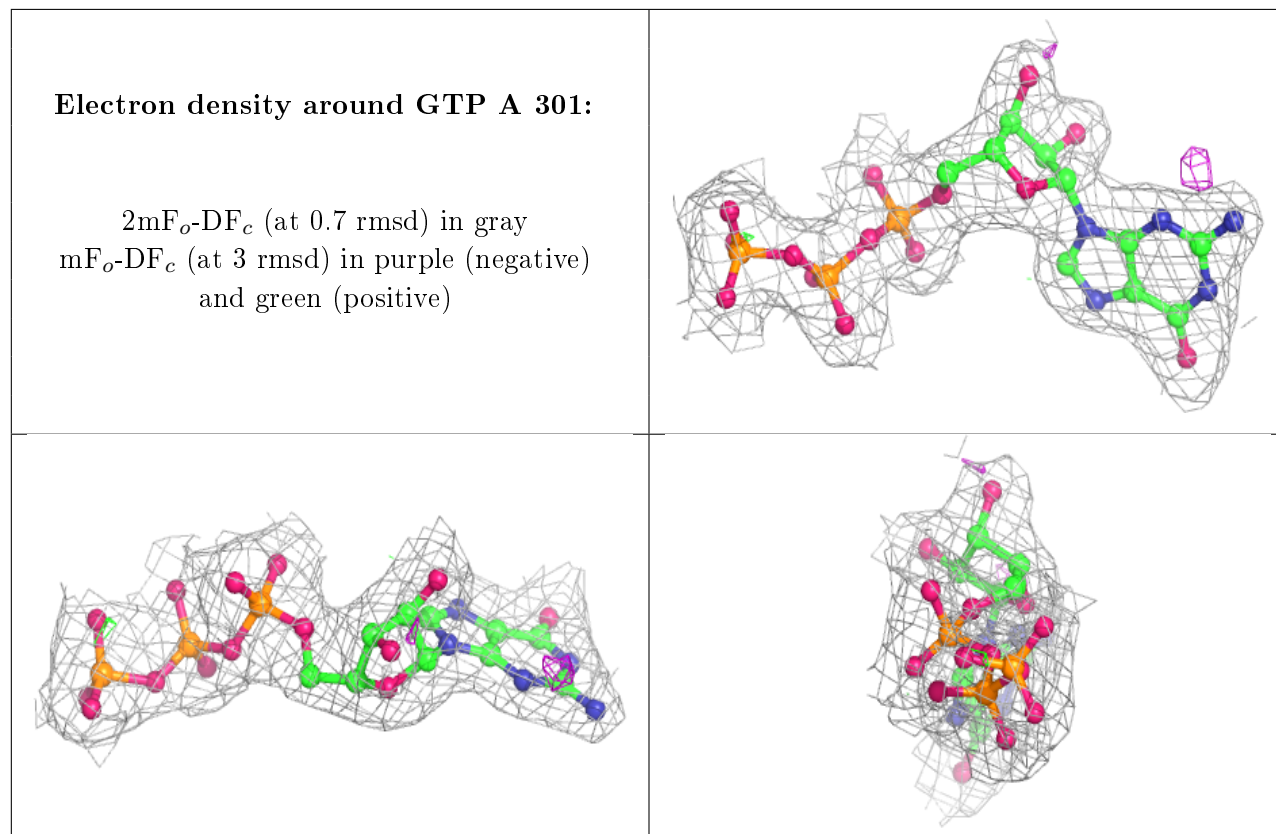
## 6.4 Ligands [i](#)

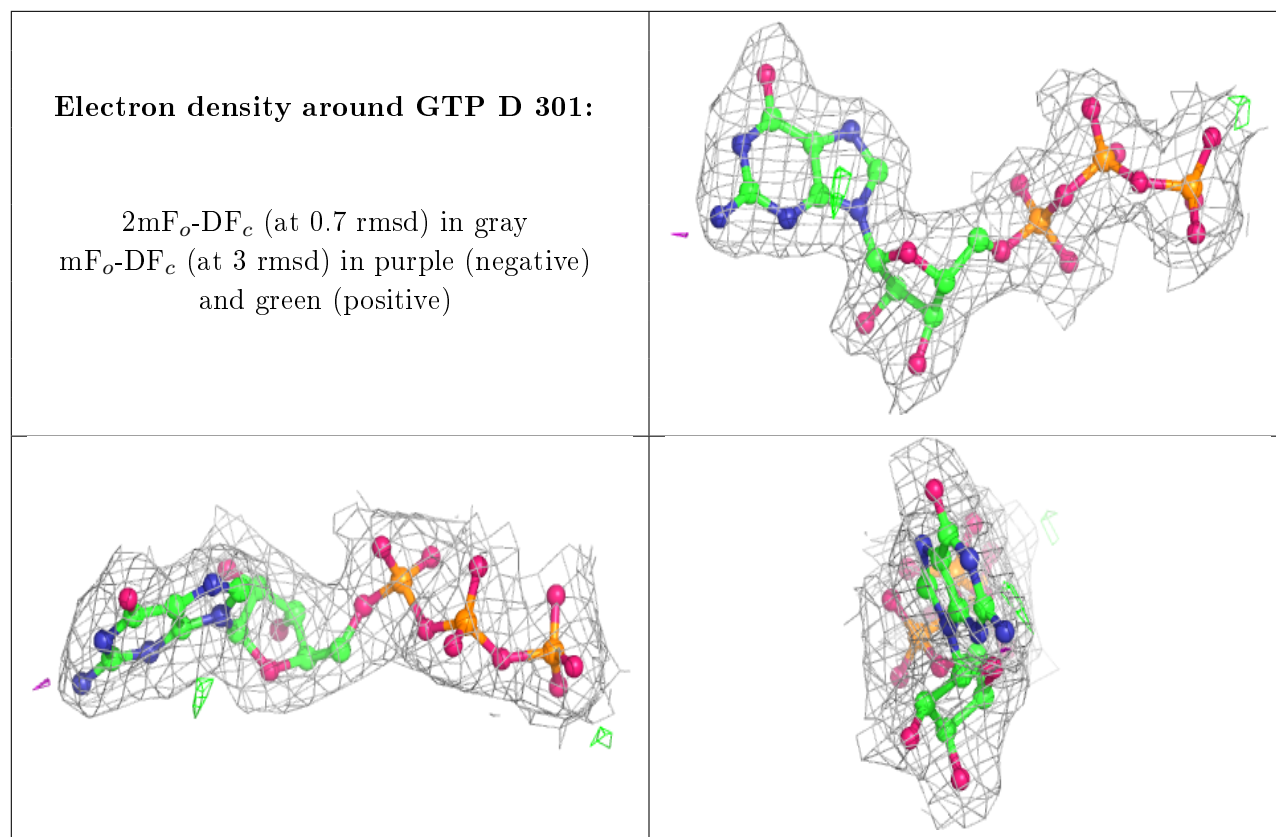
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	302	1/1	0.98	0.10	24,24,24,24	0
4	GTP	A	301	32/32	0.98	0.13	21,27,30,31	0
5	MG	D	302	1/1	0.99	0.08	27,27,27,27	0
4	GTP	D	301	32/32	0.99	0.12	23,28,34,38	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.