



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2024 – 07:20 AM EDT

PDB ID : 4PYG  
Title : Transglutaminase2 complexed with GTP  
Authors : Park, H.H.; Jang, T.H.  
Deposited on : 2014-03-27  
Resolution : 2.80 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

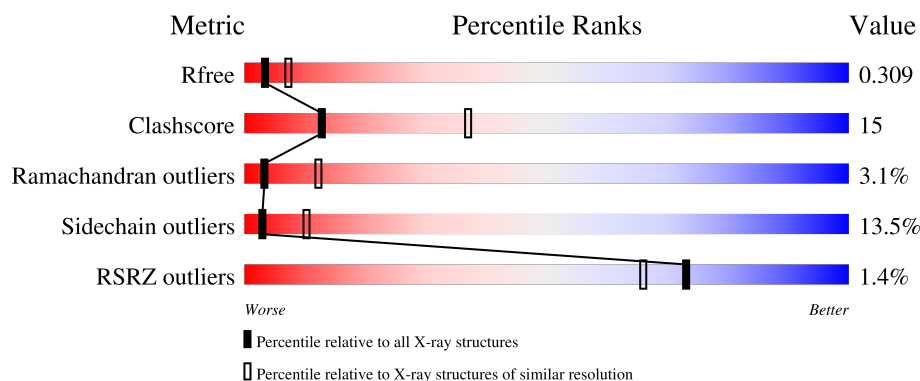
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	695	<div> <div></div> <div>65%</div> <div>27%</div> <div>6%</div> <div></div> </div>
1	B	695	<div> <div>2%</div> <div>60%</div> <div>32%</div> <div>7%</div> <div></div> </div>
1	E	695	<div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> <div></div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16462 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 Protein-glutamine gamma-glutamyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	685	Total	C	N	O	S	0	0	0
			5419	3424	933	1032	30			
1	B	685	Total	C	N	O	S	0	0	0
			5419	3424	933	1032	30			
1	E	685	Total	C	N	O	S	0	0	0
			5419	3424	933	1032	30			

There are 24 discrepancies between the modelled and reference sequences:

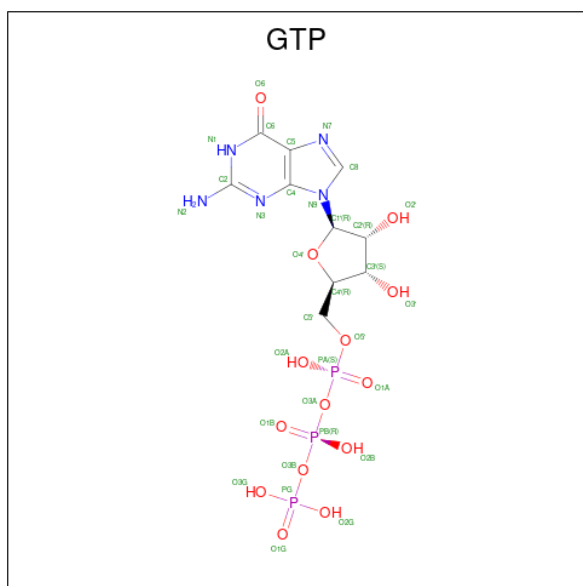
Chain	Residue	Modelled	Actual	Comment	Reference
A	688	LEU	-	expression tag	UNP P21980
A	689	GLU	-	expression tag	UNP P21980
A	690	HIS	-	expression tag	UNP P21980
A	691	HIS	-	expression tag	UNP P21980
A	692	HIS	-	expression tag	UNP P21980
A	693	HIS	-	expression tag	UNP P21980
A	694	HIS	-	expression tag	UNP P21980
A	695	HIS	-	expression tag	UNP P21980
B	688	LEU	-	expression tag	UNP P21980
B	689	GLU	-	expression tag	UNP P21980
B	690	HIS	-	expression tag	UNP P21980
B	691	HIS	-	expression tag	UNP P21980
B	692	HIS	-	expression tag	UNP P21980
B	693	HIS	-	expression tag	UNP P21980
B	694	HIS	-	expression tag	UNP P21980
B	695	HIS	-	expression tag	UNP P21980
E	688	LEU	-	expression tag	UNP P21980
E	689	GLU	-	expression tag	UNP P21980
E	690	HIS	-	expression tag	UNP P21980
E	691	HIS	-	expression tag	UNP P21980
E	692	HIS	-	expression tag	UNP P21980
E	693	HIS	-	expression tag	UNP P21980
E	694	HIS	-	expression tag	UNP P21980

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Chain	Residue	Modelled	Actual	Comment	Reference
E	695	HIS	-	expression tag	UNP P21980

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

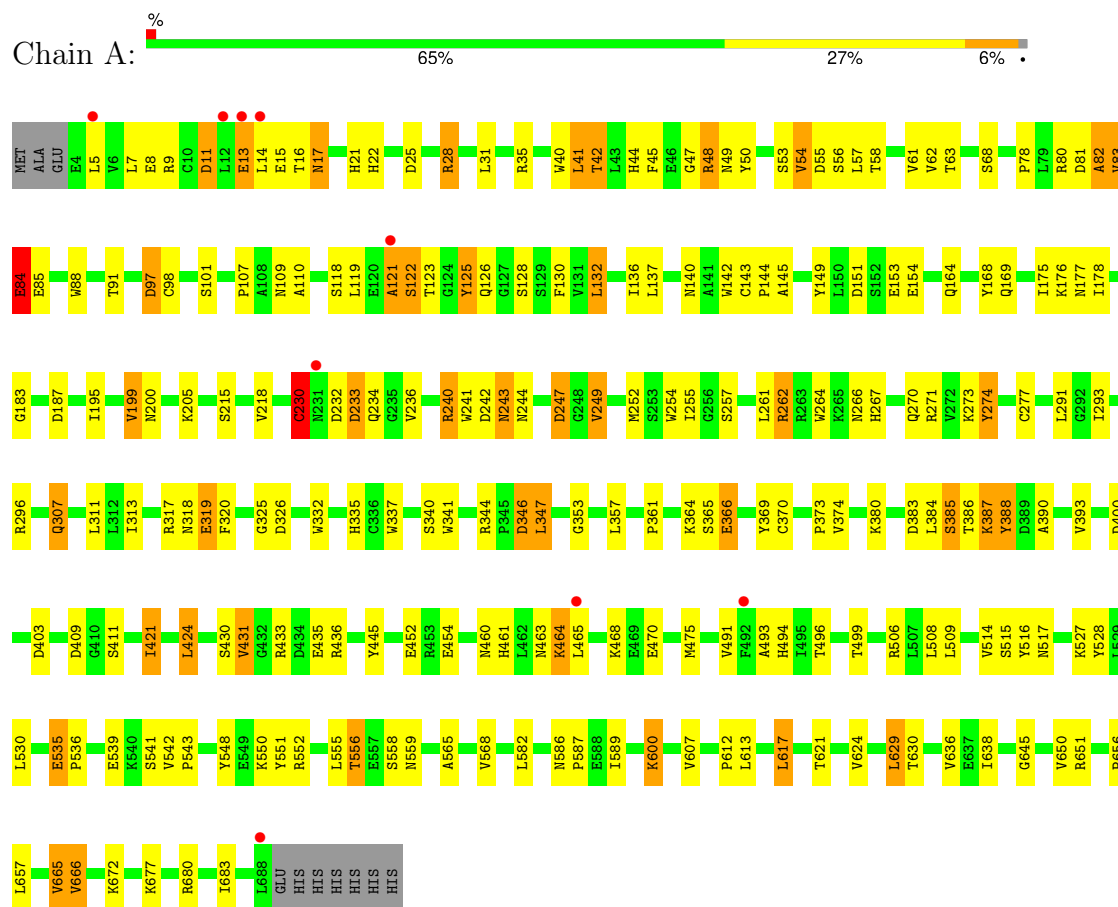
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	42	Total	O	0	0
			42	42		
3	E	33	Total	O	0	0
			33	33		

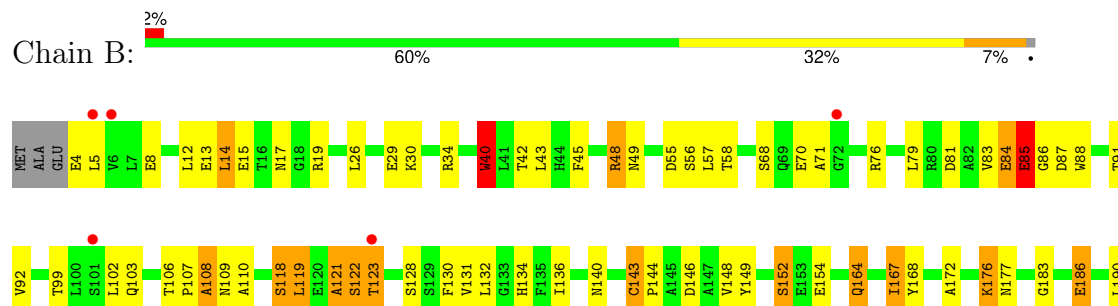
### 3 Residue-property plots

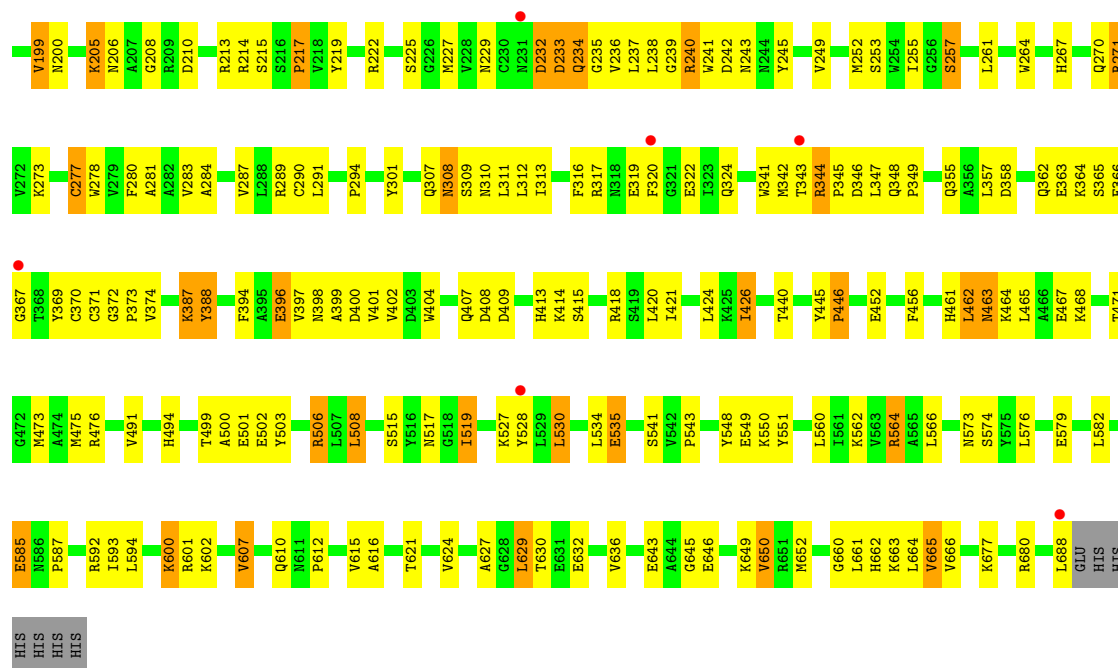
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein-glutamine gamma-glutamyltransferase 2

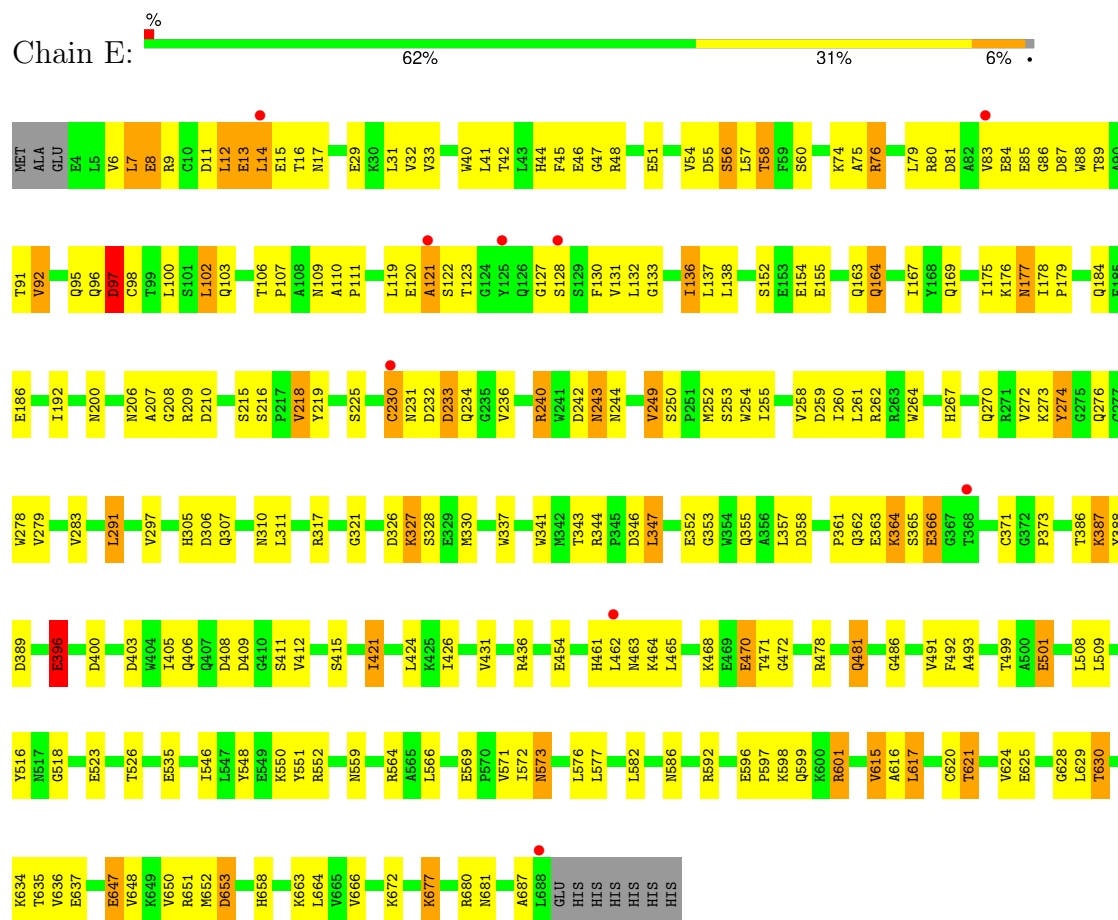


#### • Molecule 1: Protein-glutamine gamma-glutamyltransferase 2





• Molecule 1: Protein-glutamine gamma-glutamyltransferase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.55Å 216.22Å 165.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.92 – 2.80 39.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.92-2.80) 99.4 (39.92-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.88 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.236 , 0.319 0.230 , 0.309	Depositor DCC
$R_{free}$ test set	2961 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 30.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16462	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	0.68	1/5537 (0.0%)	0.80	3/7515 (0.0%)
1	B	0.65	0/5537	0.77	1/7515 (0.0%)
1	E	0.66	0/5537	0.76	0/7515
All	All	0.66	1/16611 (0.0%)	0.78	4/22545 (0.0%)

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
1	A	0	2
1	B	0	1
1	E	0	2
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	CYS	CB-SG	-5.28	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	LEU	CA-CB-CG	-5.99	101.53	115.30
1	A	424	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	5	LEU	CA-CB-CG	5.66	128.33	115.30
1	A	230	CYS	CA-CB-SG	5.20	123.35	114.00

There are no chirality outliers.



All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	LYS	Peptide
1	A	645	GLY	Peptide
1	B	645	GLY	Peptide
1	E	13	GLU	Peptide
1	E	273	LYS	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	5419	0	5312	146	0
1	B	5419	0	5312	187	0
1	E	5419	0	5312	165	0
2	A	32	0	12	1	0
2	B	32	0	12	1	0
2	E	32	0	12	0	0
3	A	34	0	0	1	0
3	B	42	0	0	5	0
3	E	33	0	0	0	0
All	All	16462	0	15972	483	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 15.

All (483) 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:346:ASP:OD1	1:A:387:LYS:HE3	1.50	1.10
1:A:463:ASN:O	1:A:464:LYS:HG2	1.57	1.04
1:E:55:ASP:HA	1:E:123:THR:OG1	1.64	0.95
1:E:344:ARG:HH21	1:E:387:LYS:HZ3	1.13	0.93
1:E:225:SER:HB2	1:E:357:LEU:HD23	1.48	0.92
1:A:14:LEU:HB2	1:A:17:ASN:HD21	1.36	0.90
1:A:344:ARG:HB3	1:A:347:LEU:HD11	1.54	0.88
1:E:421:ILE:HG13	1:E:424:LEU:HD21	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HD23	1:A:461:HIS:CD2	2.10	0.87
1:B:164:GLN:HG3	1:B:663:LYS:HB2	1.57	0.85
1:A:307:GLN:HE21	1:A:307:GLN:HA	1.41	0.85
1:E:87:ASP:HB3	1:E:107:PRO:HB3	1.57	0.85
1:E:344:ARG:HH21	1:E:387:LYS:NZ	1.73	0.85
1:E:267:HIS:O	1:E:270:GLN:HG2	1.77	0.84
1:B:241:TRP:CD1	1:B:517:ASN:ND2	2.46	0.82
1:B:452:GLU:HG2	1:B:456:PHE:CE1	2.15	0.81
1:A:344:ARG:HH21	1:A:387:LYS:NZ	1.78	0.81
1:A:311:LEU:HD23	1:A:461:HIS:HD2	1.47	0.79
1:B:320:PHE:CE1	1:B:528:TYR:CZ	2.70	0.79
1:E:186:GLU:OE1	1:E:258:VAL:HG21	1.84	0.78
1:B:615:VAL:HG12	1:B:616:ALA:H	1.49	0.77
1:B:210:ASP:OD2	1:B:219:TYR:OH	2.03	0.76
1:E:230:CYS:HB3	1:E:361:PRO:HB3	1.68	0.75
1:B:407:GLN:HE22	1:B:573:ASN:HD21	1.34	0.75
1:B:283:VAL:O	1:B:287:VAL:HG23	1.87	0.75
1:A:109:ASN:O	1:A:215:SER:HB2	1.85	0.74
1:B:508:LEU:HA	1:B:528:TYR:CD2	2.21	0.74
1:E:74:LYS:HE3	1:E:76:ARG:HD2	1.68	0.74
1:A:344:ARG:NH2	1:A:387:LYS:HZ1	1.85	0.74
1:A:320:PHE:HZ	1:B:528:TYR:CE1	2.06	0.73
1:E:344:ARG:NH2	1:E:387:LYS:HZ3	1.85	0.73
1:E:636:VAL:HG11	1:E:650:VAL:HG21	1.71	0.72
1:A:344:ARG:HH12	1:A:373:PRO:HB2	1.55	0.72
1:E:624:VAL:HG13	1:E:664:LEU:HD11	1.72	0.72
1:A:650:VAL:HG22	1:A:651:ARG:H	1.55	0.71
1:A:344:ARG:NH2	1:A:387:LYS:NZ	2.38	0.71
1:E:138:LEU:HD22	1:E:291:LEU:HA	1.72	0.71
1:E:240:ARG:HG3	1:E:274:TYR:CE1	2.25	0.71
1:A:232:ASP:O	1:A:271:ARG:NH1	2.18	0.71
1:B:373:PRO:O	1:B:388:TYR:HB2	1.89	0.71
1:B:320:PHE:HE1	1:B:528:TYR:CZ	2.07	0.71
1:B:358:ASP:HB3	1:B:371:CYS:HB2	1.70	0.71
1:E:615:VAL:HG12	1:E:616:ALA:H	1.56	0.70
1:B:119:LEU:HB3	1:B:132:LEU:HD11	1.72	0.70
1:B:348:GLN:HG2	3:B:832:HOH:O	1.92	0.70
1:B:607:VAL:HG23	1:B:650:VAL:HG12	1.74	0.70
1:A:320:PHE:CZ	1:B:528:TYR:CE1	2.81	0.69
1:A:344:ARG:HB3	1:A:347:LEU:CD1	2.23	0.69
1:A:506:ARG:HD2	1:B:530:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:GLN:HG3	1:E:663:LYS:HB2	1.74	0.69
1:B:508:LEU:HA	1:B:528:TYR:HD2	1.57	0.68
1:B:320:PHE:CD1	1:B:528:TYR:CZ	2.81	0.68
1:B:636:VAL:HG11	1:B:650:VAL:HG21	1.74	0.68
1:E:210:ASP:OD2	1:E:219:TYR:OH	2.12	0.68
1:A:255:ILE:HB	1:A:665:VAL:HG22	1.74	0.68
1:E:255:ILE:HG13	1:E:625:GLU:OE1	1.94	0.68
1:A:17:ASN:H	1:A:17:ASN:ND2	1.90	0.67
1:E:615:VAL:HG12	1:E:616:ALA:N	2.09	0.67
1:E:17:ASN:HD21	1:E:40:TRP:HB2	1.60	0.67
1:A:509:LEU:HD12	1:A:527:LYS:HB3	1.77	0.67
1:B:491:VAL:HG11	1:B:582:LEU:HD11	1.77	0.66
1:E:559:ASN:ND2	1:E:586:ASN:OD1	2.29	0.66
1:B:13:GLU:CD	1:B:13:GLU:H	1.98	0.66
1:B:680:ARG:NH2	1:E:154:GLU:OE1	2.28	0.65
1:E:122:SER:HA	1:E:127:GLY:HA2	1.78	0.65
1:B:154:GLU:OE1	1:E:680:ARG:NH2	2.30	0.64
1:E:57:LEU:HD22	1:E:119:LEU:HD11	1.79	0.64
1:A:168:TYR:CE2	1:A:436:ARG:HG3	2.32	0.64
1:B:592:ARG:HH21	1:B:594:LEU:HD21	1.62	0.64
1:B:587:PRO:HG3	1:B:612:PRO:HG3	1.79	0.64
1:B:243:ASN:HA	1:B:245:TYR:CZ	2.33	0.64
1:E:347:LEU:HD23	1:E:387:LYS:HD3	1.78	0.64
1:A:8:GLU:HB2	1:A:44:HIS:O	1.98	0.64
1:B:240:ARG:NH2	1:B:242:ASP:OD1	2.31	0.64
1:B:71:ALA:N	3:B:821:HOH:O	2.29	0.63
1:A:320:PHE:CZ	1:B:528:TYR:CD1	2.86	0.63
1:B:205:LYS:HG2	1:B:206:ASN:N	2.14	0.63
1:B:508:LEU:HD12	1:B:528:TYR:CD2	2.34	0.63
1:A:267:HIS:HB3	1:A:270:GLN:HE21	1.64	0.63
1:B:615:VAL:HG12	1:B:616:ALA:N	2.13	0.63
1:B:310:ASN:ND2	1:B:312:LEU:O	2.32	0.63
1:E:387:LYS:HG3	1:E:388:TYR:CE2	2.33	0.62
1:E:347:LEU:HD21	1:E:387:LYS:HZ2	1.63	0.62
1:B:467:GLU:HG2	1:B:468:LYS:N	2.15	0.62
1:E:305:HIS:O	1:E:307:GLN:N	2.32	0.62
1:B:320:PHE:CE1	1:B:528:TYR:CE2	2.87	0.62
1:B:222:ARG:HB2	1:B:373:PRO:HD3	1.79	0.62
1:E:167:ILE:HD12	1:E:297:VAL:HG11	1.81	0.62
1:A:347:LEU:HD12	1:A:347:LEU:N	2.14	0.62
1:B:144:PRO:HA	1:B:149:TYR:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PHE:HD1	1:B:528:TYR:HH	1.46	0.62
1:E:32:VAL:HG22	1:E:136:ILE:HG13	1.81	0.62
1:E:88:TRP:CZ3	1:E:106:THR:HG22	2.33	0.62
1:A:255:ILE:HB	1:A:665:VAL:CG2	2.30	0.61
1:B:344:ARG:NH2	1:B:387:LYS:NZ	2.48	0.61
1:E:177:ASN:HD22	1:E:177:ASN:H	1.48	0.61
1:B:311:LEU:HD23	1:B:461:HIS:CD2	2.35	0.61
1:B:320:PHE:HD1	1:B:528:TYR:OH	1.84	0.61
1:B:229:ASN:ND2	1:B:237:LEU:O	2.32	0.61
1:A:17:ASN:O	1:A:21:HIS:N	2.31	0.61
1:A:344:ARG:CZ	1:A:387:LYS:HZ1	2.13	0.61
1:A:78:PRO:HG2	1:A:80:ARG:HH11	1.65	0.60
1:A:463:ASN:O	1:A:464:LYS:CG	2.42	0.60
1:A:552:ARG:HH21	1:A:672:LYS:HE2	1.64	0.60
1:E:250:SER:HB3	1:E:253:SER:OG	2.01	0.60
1:E:615:VAL:CG1	1:E:616:ALA:H	2.15	0.60
1:B:235:GLY:O	1:B:264:TRP:NE1	2.34	0.60
1:E:347:LEU:HD21	1:E:387:LYS:NZ	2.16	0.60
1:A:307:GLN:HA	1:A:307:GLN:NE2	2.16	0.59
1:B:387:LYS:NZ	1:B:387:LYS:O	2.35	0.59
1:E:491:VAL:HG22	1:E:546:ILE:HD11	1.85	0.59
1:E:663:LYS:NZ	1:E:681:ASN:OD1	2.31	0.59
1:E:242:ASP:O	1:E:243:ASN:CB	2.51	0.59
1:E:598:LYS:HB2	1:E:601:ARG:HG2	1.84	0.59
1:A:293:ILE:HG22	1:A:340:SER:HB3	1.84	0.59
1:A:493:ALA:HB2	1:A:509:LEU:HD21	1.84	0.59
1:B:241:TRP:HD1	1:B:517:ASN:ND2	1.99	0.59
1:E:406:GLN:O	1:E:406:GLN:HG2	2.03	0.58
1:E:13:GLU:HB2	1:E:31:LEU:HD22	1.84	0.58
1:E:107:PRO:HG2	1:E:110:ALA:HB2	1.86	0.58
1:B:43:LEU:O	1:B:99:THR:HA	2.04	0.58
1:A:319:GLU:OE1	1:B:527:LYS:HA	2.03	0.58
1:E:599:GLN:HB3	1:E:687:ALA:HB2	1.86	0.58
1:E:305:HIS:C	1:E:307:GLN:H	2.07	0.57
1:A:17:ASN:H	1:A:17:ASN:HD22	1.49	0.57
1:B:344:ARG:NH2	1:B:387:LYS:HZ3	2.02	0.57
1:A:35:ARG:HA	1:A:137:LEU:HD11	1.86	0.57
1:A:514:VAL:O	1:A:556:THR:HG21	2.04	0.57
1:E:242:ASP:O	1:E:243:ASN:HB3	2.05	0.57
1:E:321:GLY:O	1:E:564:ARG:HD2	2.05	0.57
1:E:48:ARG:NH2	1:E:55:ASP:OD2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ARG:NH1	1:E:403:ASP:OD1	2.38	0.57
1:B:109:ASN:O	1:B:215:SER:HB2	2.05	0.56
1:A:48:ARG:NH2	1:A:55:ASP:OD2	2.38	0.56
1:B:548:TYR:HA	1:B:551:TYR:CE2	2.40	0.56
1:E:121:ALA:HB3	1:E:128:SER:HB3	1.86	0.56
1:A:508:LEU:O	1:A:565:ALA:HA	2.05	0.56
1:E:634:LYS:HE3	1:E:653:ASP:O	2.06	0.56
1:B:17:ASN:HD21	1:B:40:TRP:N	2.02	0.56
1:A:530:LEU:HD11	1:B:320:PHE:CZ	2.40	0.56
1:E:7:LEU:HD13	1:E:46:GLU:HB2	1.87	0.56
1:B:34:ARG:HB2	1:B:140:ASN:ND2	2.20	0.56
1:E:216:SER:OG	1:E:218:VAL:HG13	2.06	0.56
1:B:5:LEU:HD11	1:B:128:SER:HB2	1.86	0.56
1:A:650:VAL:HG22	1:A:651:ARG:N	2.18	0.56
1:B:281:ALA:O	1:B:284:ALA:HB3	2.06	0.56
1:A:364:LYS:O	1:A:366:GLU:N	2.38	0.55
1:E:109:ASN:O	1:E:215:SER:HB2	2.05	0.55
1:E:373:PRO:O	1:E:388:TYR:HB2	2.06	0.55
1:A:230:CYS:HB2	1:A:361:PRO:HB3	1.87	0.55
1:A:364:LYS:C	1:A:366:GLU:H	2.09	0.55
1:E:121:ALA:HB1	1:E:123:THR:HG22	1.88	0.55
1:A:195:ILE:O	1:A:199:VAL:HB	2.06	0.55
1:B:118:SER:HB3	1:B:131:VAL:HG22	1.88	0.55
1:B:121:ALA:O	1:B:122:SER:HB2	2.06	0.55
1:B:564:ARG:HB2	1:B:579:GLU:HG2	1.87	0.55
1:B:661:LEU:HD12	1:B:662:HIS:N	2.22	0.55
1:A:81:ASP:O	1:A:82:ALA:CB	2.54	0.55
1:B:232:ASP:O	1:B:271:ARG:NH1	2.40	0.55
1:E:86:GLY:O	1:E:87:ASP:HB2	2.07	0.55
1:E:344:ARG:HB3	1:E:347:LEU:HD12	1.88	0.55
1:E:358:ASP:HB3	1:E:371:CYS:HB2	1.88	0.55
1:E:56:SER:O	1:E:121:ALA:O	2.25	0.55
1:A:168:TYR:CE2	1:A:177:ASN:HB3	2.42	0.54
1:B:462:LEU:O	1:B:464:LYS:N	2.40	0.54
1:B:508:LEU:HB3	1:B:528:TYR:HE2	1.71	0.54
1:E:95:GLN:HG2	1:E:100:LEU:HD13	1.89	0.54
1:E:169:GLN:HB2	1:E:178:ILE:HD12	1.89	0.54
1:B:85:GLU:CD	1:B:86:GLY:H	2.09	0.54
1:E:51:GLU:O	1:E:55:ASP:HB2	2.08	0.54
1:B:14:LEU:HD13	1:B:40:TRP:HB3	1.88	0.54
1:B:320:PHE:CD1	1:B:528:TYR:OH	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LEU:HD23	1:B:387:LYS:HE3	1.90	0.54
1:E:279:VAL:O	1:E:283:VAL:HG23	2.07	0.54
1:A:421:ILE:HG13	1:A:424:LEU:HD21	1.89	0.54
1:B:40:TRP:HD1	1:B:103:GLN:HE21	1.56	0.54
1:E:347:LEU:HD22	1:E:386:THR:HG23	1.90	0.54
1:A:636:VAL:HG11	1:A:650:VAL:HG21	1.89	0.54
1:A:144:PRO:HA	1:A:149:TYR:CD1	2.43	0.53
1:B:148:VAL:HB	1:B:294:PRO:HD2	1.91	0.53
1:A:341:TRP:CZ3	1:A:353:GLY:HA2	2.43	0.53
1:B:217:PRO:HB2	1:B:342:MET:SD	2.48	0.53
1:B:357:LEU:HA	1:B:372:GLY:HA3	1.90	0.53
1:B:421:ILE:HG13	1:B:424:LEU:HD11	1.89	0.53
1:E:175:ILE:HG21	1:E:436:ARG:HD2	1.89	0.53
1:A:14:LEU:HD11	1:A:42:THR:HG22	1.90	0.53
1:B:121:ALA:HB1	1:B:123:THR:HG22	1.90	0.53
1:B:508:LEU:HB2	1:B:566:LEU:HB3	1.91	0.53
1:E:552:ARG:HH21	1:E:672:LYS:HE2	1.73	0.53
1:A:81:ASP:O	1:A:82:ALA:HB2	2.09	0.53
1:A:168:TYR:CZ	1:A:436:ARG:HG3	2.43	0.53
1:B:320:PHE:CD1	1:B:528:TYR:CE2	2.97	0.53
1:B:502:GLU:HG3	1:B:535:GLU:HG3	1.91	0.53
1:B:600:LYS:HG2	1:B:600:LYS:O	2.08	0.53
1:E:344:ARG:NH2	1:E:387:LYS:NZ	2.51	0.53
1:E:344:ARG:NH1	1:E:355:GLN:OE1	2.42	0.53
1:A:83:VAL:HG12	1:A:84:GLU:N	2.24	0.53
1:B:107:PRO:HB2	1:B:109:ASN:OD1	2.08	0.53
1:A:384:LEU:O	1:A:390:ALA:HB3	2.09	0.53
1:B:452:GLU:HG2	1:B:456:PHE:HE1	1.72	0.53
2:B:701:GTP:O1G	1:E:478:ARG:NH1	2.37	0.53
1:E:111:PRO:HA	1:E:215:SER:HA	1.91	0.53
1:A:169:GLN:OE1	1:A:178:ILE:HD13	2.09	0.52
1:A:514:VAL:HG22	1:A:515:SER:N	2.23	0.52
1:B:636:VAL:CG1	1:B:650:VAL:HG21	2.39	0.52
1:E:242:ASP:OD2	1:E:243:ASN:N	2.42	0.52
1:A:14:LEU:HB2	1:A:17:ASN:ND2	2.16	0.52
1:E:326:ASP:C	1:E:328:SER:H	2.12	0.52
1:A:475:MET:HA	1:A:494:HIS:O	2.09	0.52
1:B:643:GLU:HB2	1:B:646:GLU:HG2	1.91	0.52
1:E:615:VAL:CG1	1:E:616:ALA:N	2.72	0.52
1:A:240:ARG:NH2	1:A:242:ASP:OD1	2.43	0.52
1:B:369:TYR:CG	1:B:370:CYS:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:THR:HG22	1:B:500:ALA:N	2.24	0.52
1:B:515:SER:OG	1:B:519:ILE:HB	2.10	0.52
1:E:167:ILE:HG21	1:E:278:TRP:HB2	1.91	0.52
1:B:107:PRO:C	1:B:109:ASN:H	2.13	0.52
1:B:402:VAL:HG13	1:B:414:LYS:HE3	1.91	0.52
1:E:249:VAL:HG11	1:E:254:TRP:CH2	2.45	0.52
1:A:61:VAL:HG21	1:A:88:TRP:CZ3	2.45	0.52
1:A:107:PRO:HG2	1:A:110:ALA:HB2	1.92	0.52
1:B:85:GLU:C	1:B:87:ASP:H	2.14	0.52
1:B:502:GLU:HG3	1:B:535:GLU:HA	1.92	0.52
1:E:347:LEU:CD2	1:E:387:LYS:HD3	2.40	0.52
1:E:365:SER:HB2	1:E:366:GLU:OE2	2.10	0.51
1:B:227:MET:O	1:B:236:VAL:HG23	2.10	0.51
1:B:476:ARG:HH22	1:B:494:HIS:CD2	2.28	0.51
1:B:343:THR:O	1:B:345:PRO:HD3	2.10	0.51
1:A:530:LEU:HD22	1:B:530:LEU:HD11	1.92	0.51
1:A:311:LEU:CD2	1:A:461:HIS:HD2	2.22	0.51
1:B:213:ARG:C	1:B:215:SER:H	2.14	0.51
1:E:163:GLN:HA	1:E:184:GLN:HE22	1.76	0.51
1:E:236:VAL:HA	1:E:264:TRP:CD1	2.46	0.51
1:A:587:PRO:HD3	1:A:612:PRO:HG3	1.91	0.50
1:B:401:VAL:HG21	1:B:420:LEU:HD21	1.92	0.50
1:B:167:ILE:HG21	1:B:278:TRP:HB2	1.92	0.50
1:B:317:ARG:HA	1:B:322:GLU:O	2.12	0.50
1:B:316:PHE:CE2	1:B:404:TRP:CD1	3.00	0.50
1:E:470:GLU:C	1:E:472:GLY:H	2.15	0.50
1:E:87:ASP:HB3	1:E:107:PRO:CB	2.36	0.50
1:A:433:ARG:HB3	1:A:435:GLU:OE1	2.11	0.50
1:B:364:LYS:HE2	1:B:369:TYR:O	2.12	0.50
1:E:74:LYS:CE	1:E:76:ARG:HD2	2.37	0.50
1:E:344:ARG:HE	1:E:387:LYS:NZ	2.08	0.50
1:B:168:TYR:CE2	1:B:177:ASN:HB3	2.47	0.50
1:B:615:VAL:CG1	1:B:616:ALA:H	2.21	0.50
1:E:552:ARG:HH22	1:E:615:VAL:HG21	1.77	0.50
1:E:346:ASP:OD1	1:E:387:LYS:HE2	2.12	0.49
1:A:125:TYR:HD2	1:A:126:GLN:H	1.58	0.49
1:B:48:ARG:HG2	1:B:49:ASN:N	2.26	0.49
1:A:320:PHE:CZ	1:B:528:TYR:HE1	2.31	0.49
1:A:496:THR:HG23	1:A:539:GLU:HG2	1.94	0.49
1:E:51:GLU:N	1:E:55:ASP:OD1	2.38	0.49
1:A:8:GLU:HA	1:A:45:PHE:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:LEU:HD12	1:B:239:GLY:H	1.75	0.49
1:A:293:ILE:CG2	1:A:340:SER:HB3	2.42	0.49
1:B:257:SER:HB3	1:B:283:VAL:HG22	1.94	0.48
1:E:267:HIS:O	1:E:270:GLN:CG	2.57	0.48
1:A:369:TYR:CG	1:A:370:CYS:N	2.81	0.48
1:B:83:VAL:O	1:B:84:GLU:HB2	2.13	0.48
1:B:503:TYR:HB2	1:B:534:LEU:HB2	1.95	0.48
1:B:107:PRO:HD2	1:B:110:ALA:HB2	1.95	0.48
1:B:320:PHE:HE1	1:B:528:TYR:CE1	2.30	0.48
1:A:8:GLU:HB3	1:A:45:PHE:CD1	2.49	0.48
1:B:252:MET:O	1:B:677:LYS:NZ	2.47	0.48
1:E:647:GLU:HG3	1:E:648:VAL:N	2.27	0.48
1:A:242:ASP:O	1:A:243:ASN:HB3	2.13	0.48
1:E:630:THR:HG21	1:E:634:LYS:HE2	1.95	0.48
1:E:343:THR:HA	1:E:352:GLU:HB3	1.95	0.48
1:B:176:LYS:NZ	1:B:585:GLU:OE1	2.47	0.48
1:E:255:ILE:HG22	1:E:677:LYS:HE2	1.95	0.48
1:B:362:GLN:HB3	1:B:364:LYS:HG3	1.96	0.48
1:B:636:VAL:HG11	1:B:650:VAL:CG2	2.43	0.48
1:E:6:VAL:HG12	1:E:123:THR:HG21	1.96	0.47
1:A:528:TYR:HB2	1:B:320:PHE:CZ	2.49	0.47
1:E:79:LEU:HD11	1:E:92:VAL:HG12	1.96	0.47
1:B:277:CYS:HA	1:B:280:PHE:CD2	2.49	0.47
1:B:394:PHE:O	1:B:398:ASN:HB2	2.14	0.47
1:B:624:VAL:HG13	1:B:664:LEU:HD11	1.95	0.47
1:E:481:GLN:H	1:E:481:GLN:NE2	2.12	0.47
1:A:548:TYR:HA	1:A:551:TYR:CE2	2.50	0.47
1:B:87:ASP:HB3	1:B:107:PRO:HB3	1.96	0.47
2:A:701:GTP:O2G	2:A:701:GTP:O1A	2.32	0.47
1:E:33:VAL:HG23	1:E:137:LEU:CD1	2.44	0.47
1:E:305:HIS:O	1:E:307:GLN:HG2	2.13	0.47
1:E:471:THR:O	1:E:471:THR:HG22	2.14	0.47
1:B:600:LYS:O	1:B:600:LYS:CG	2.63	0.47
1:B:238:LEU:HD12	1:B:239:GLY:N	2.28	0.47
1:B:374:VAL:HB	1:B:388:TYR:O	2.15	0.47
1:E:206:ASN:O	1:E:208:GLY:N	2.47	0.47
1:E:647:GLU:HG3	1:E:648:VAL:H	1.79	0.47
1:B:344:ARG:HH21	1:B:387:LYS:NZ	2.13	0.47
1:A:586:ASN:HB3	1:A:587:PRO:HD2	1.96	0.47
1:B:344:ARG:NH1	1:B:355:GLN:OE1	2.48	0.47
1:E:501:GLU:H	1:E:501:GLU:HG2	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:THR:HG21	1:B:501:GLU:HG2	1.97	0.47
1:E:471:THR:O	1:E:471:THR:CG2	2.63	0.47
1:E:572:ILE:O	1:E:573:ASN:CB	2.63	0.47
1:B:172:ALA:HB2	1:B:301:TYR:HB3	1.97	0.46
1:E:508:LEU:HD23	1:E:566:LEU:HD23	1.96	0.46
1:A:13:GLU:H	1:A:13:GLU:CD	2.19	0.46
1:A:13:GLU:HB2	1:A:31:LEU:HD22	1.97	0.46
1:E:122:SER:CA	1:E:127:GLY:HA2	2.45	0.46
1:E:326:ASP:C	1:E:328:SER:N	2.68	0.46
1:E:386:THR:HG22	1:E:387:LYS:H	1.81	0.46
1:B:8:GLU:HA	1:B:45:PHE:HA	1.97	0.46
1:B:57:LEU:HD22	1:B:119:LEU:HD11	1.96	0.46
1:B:186:GLU:OE1	1:B:627:ALA:HB2	2.16	0.46
1:B:307:GLN:O	1:B:308:ASN:C	2.54	0.46
1:E:624:VAL:CG1	1:E:664:LEU:HD11	2.45	0.46
1:B:649:LYS:NZ	3:B:824:HOH:O	2.48	0.46
1:E:163:GLN:HG2	1:E:184:GLN:NE2	2.31	0.46
1:E:249:VAL:O	1:E:274:TYR:HB2	2.15	0.46
1:E:493:ALA:HB2	1:E:509:LEU:HD21	1.97	0.46
1:B:205:LYS:NZ	1:B:205:LYS:HB3	2.31	0.46
1:B:255:ILE:HB	1:B:665:VAL:HG22	1.97	0.46
1:A:296:ARG:O	1:A:296:ARG:CG	2.64	0.46
1:A:374:VAL:HG11	1:A:393:VAL:HG21	1.98	0.46
1:E:464:LYS:HA	1:E:465:LEU:HA	1.73	0.46
1:A:175:ILE:HG21	1:A:436:ARG:HD2	1.98	0.45
1:B:467:GLU:HG2	1:B:468:LYS:H	1.81	0.45
1:A:555:LEU:HD21	1:A:559:ASN:HA	1.98	0.45
1:A:629:LEU:HA	1:A:656:PRO:HB3	1.97	0.45
1:B:68:SER:C	3:B:821:HOH:O	2.54	0.45
1:E:344:ARG:HE	1:E:387:LYS:HZ1	1.64	0.45
1:A:14:LEU:HD13	1:A:40:TRP:HB3	1.98	0.45
1:B:134:HIS:N	3:B:828:HOH:O	2.49	0.45
1:B:143:CYS:HA	1:B:144:PRO:HD3	1.77	0.45
1:B:499:THR:CG2	1:B:501:GLU:HG2	2.46	0.45
1:E:596:GLU:HA	1:E:597:PRO:HD3	1.83	0.45
1:A:54:VAL:HG13	1:A:55:ASP:H	1.82	0.45
1:A:121:ALA:O	1:A:122:SER:CB	2.65	0.45
1:A:242:ASP:O	1:A:243:ASN:CB	2.64	0.45
1:A:262:ARG:O	1:A:266:ASN:HB2	2.16	0.45
1:A:657:LEU:HD12	1:A:657:LEU:N	2.31	0.45
1:A:241:TRP:CD1	1:A:517:ASN:ND2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ARG:HD2	1:B:344:ARG:HA	1.77	0.45
1:B:475:MET:HG3	1:B:494:HIS:O	2.16	0.45
1:E:12:LEU:HD22	1:E:14:LEU:HG	1.98	0.45
1:E:60:SER:HA	1:E:75:ALA:O	2.17	0.45
1:A:48:ARG:HH21	1:A:55:ASP:CG	2.19	0.45
1:B:8:GLU:OE2	1:B:130:PHE:CE1	2.70	0.45
1:B:183:GLY:O	1:B:186:GLU:HB2	2.17	0.45
1:B:660:GLY:O	1:B:662:HIS:CD2	2.70	0.45
1:E:387:LYS:HG3	1:E:388:TYR:CD2	2.51	0.45
1:E:650:VAL:HG22	1:E:651:ARG:H	1.82	0.45
1:B:320:PHE:HD1	1:B:528:TYR:CZ	2.30	0.45
1:B:373:PRO:O	1:B:388:TYR:CB	2.64	0.45
1:A:240:ARG:HG3	1:A:274:TYR:CE1	2.52	0.44
1:B:164:GLN:HG3	1:B:663:LYS:CB	2.38	0.44
1:B:199:VAL:O	1:B:199:VAL:HG13	2.17	0.44
1:E:8:GLU:HA	1:E:45:PHE:HA	1.99	0.44
1:E:647:GLU:CG	1:E:648:VAL:N	2.81	0.44
1:E:9:ARG:HE	1:E:44:HIS:HB3	1.81	0.44
1:A:153:GLU:HA	1:A:153:GLU:OE1	2.17	0.44
1:B:347:LEU:HD23	1:B:387:LYS:CE	2.47	0.44
1:A:140:ASN:OD1	1:A:142:TRP:HB2	2.18	0.44
1:A:344:ARG:NE	1:A:387:LYS:HZ1	2.15	0.44
1:A:380:LYS:HE2	1:A:445:TYR:CE1	2.53	0.44
1:A:347:LEU:HD12	1:A:347:LEU:H	1.81	0.44
1:A:514:VAL:HG22	1:A:515:SER:O	2.18	0.44
1:B:408:ASP:OD1	1:B:409:ASP:N	2.49	0.44
1:E:95:GLN:HG2	1:E:100:LEU:CD1	2.48	0.44
1:E:252:MET:O	1:E:677:LYS:NZ	2.50	0.44
1:A:249:VAL:HG22	1:A:254:TRP:CE2	2.53	0.44
1:A:267:HIS:O	1:A:270:GLN:HG2	2.17	0.44
1:A:307:GLN:HG3	1:A:313:ILE:HD11	2.00	0.44
1:E:97:ASP:HB3	1:E:98:CYS:H	1.64	0.44
1:E:634:LYS:HB2	1:E:652:MET:HE2	1.99	0.44
1:A:387:LYS:HE2	1:A:388:TYR:CE2	2.52	0.44
1:B:289:ARG:O	1:B:290:CYS:C	2.56	0.44
1:A:13:GLU:CD	1:A:13:GLU:N	2.71	0.43
1:A:49:ASN:OD1	1:A:50:TYR:N	2.48	0.43
1:B:242:ASP:OD2	1:B:242:ASP:C	2.56	0.43
1:E:58:THR:HG23	1:E:120:GLU:HG3	2.00	0.43
1:E:330:MET:HB2	1:E:518:GLY:HA3	2.00	0.43
1:E:33:VAL:HG23	1:E:137:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:TRP:CZ3	1:E:353:GLY:HA2	2.53	0.43
1:A:491:VAL:HG11	1:A:582:LEU:HD11	2.00	0.43
1:B:348:GLN:HA	1:B:349:PRO:HD3	1.80	0.43
1:B:342:MET:CG	1:B:355:GLN:HG3	2.49	0.43
1:A:552:ARG:HH21	1:A:672:LYS:CE	2.31	0.43
1:B:267:HIS:O	1:B:270:GLN:HG2	2.19	0.43
1:E:406:GLN:O	1:E:406:GLN:CG	2.66	0.43
1:A:121:ALA:O	1:A:122:SER:HB2	2.18	0.43
1:A:629:LEU:HD12	1:A:656:PRO:HB3	2.01	0.43
1:B:26:LEU:HD11	1:B:190:LEU:HB2	2.00	0.43
1:B:152:SER:HB2	1:E:592:ARG:HH21	1.84	0.43
1:B:462:LEU:HB3	1:B:463:ASN:H	1.65	0.43
1:E:152:SER:OG	1:E:155:GLU:HG3	2.18	0.43
1:A:11:ASP:OD1	1:A:41:LEU:HD21	2.18	0.43
1:A:22:HIS:CE1	1:A:142:TRP:CD1	3.07	0.43
1:A:638:ILE:HD12	1:A:638:ILE:N	2.33	0.43
1:B:471:THR:HG22	1:B:471:THR:O	2.19	0.43
1:E:307:GLN:O	1:E:310:ASN:HB2	2.18	0.43
1:E:337:TRP:HB2	1:E:357:LEU:O	2.18	0.43
1:A:318:ASN:OD1	1:A:320:PHE:HB2	2.18	0.42
1:B:560:LEU:HA	1:B:582:LEU:O	2.19	0.42
1:E:178:ILE:HA	1:E:179:PRO:HD2	1.81	0.42
1:A:47:GLY:O	1:A:98:CYS:SG	2.76	0.42
1:A:613:LEU:HD12	1:A:617:LEU:CD1	2.49	0.42
1:B:445:TYR:O	1:B:446:PRO:O	2.36	0.42
1:E:192:ILE:HG23	1:E:264:TRP:HZ3	1.84	0.42
1:E:403:ASP:O	1:E:415:SER:HB3	2.19	0.42
1:A:542:VAL:HA	1:A:543:PRO:HD3	1.79	0.42
1:A:335:HIS:CD2	1:A:337:TRP:CE3	3.07	0.42
1:B:424:LEU:HD23	1:B:424:LEU:HA	1.79	0.42
1:B:464:LYS:HA	1:B:465:LEU:HA	1.67	0.42
1:E:255:ILE:CG2	1:E:677:LYS:HE2	2.50	0.42
1:B:48:ARG:HG2	1:B:49:ASN:O	2.20	0.42
1:B:426:ILE:HG13	1:B:440:THR:HA	2.01	0.42
1:B:506:ARG:HB3	1:B:530:LEU:HD23	2.01	0.42
1:B:527:LYS:NZ	1:B:543:PRO:O	2.34	0.42
1:E:365:SER:C	1:E:366:GLU:HG3	2.39	0.42
1:A:548:TYR:HA	1:A:551:TYR:CZ	2.54	0.42
1:B:57:LEU:O	1:B:79:LEU:N	2.46	0.42
1:B:108:ALA:HB1	1:B:146:ASP:HA	2.01	0.42
1:A:143:CYS:O	1:A:145:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HA	1:A:264:TRP:CD1	2.55	0.42
1:A:535:GLU:HG3	1:A:536:PRO:HD3	2.02	0.42
1:B:593:ILE:O	1:E:154:GLU:HG3	2.20	0.42
1:E:259:ASP:O	1:E:260:ILE:C	2.58	0.42
1:E:362:GLN:O	1:E:364:LYS:N	2.51	0.42
1:A:607:VAL:HG11	1:A:666:VAL:HG21	2.01	0.42
1:B:421:ILE:CG1	1:B:424:LEU:HD11	2.49	0.42
1:E:86:GLY:O	1:E:87:ASP:CB	2.68	0.42
1:E:628:GLY:HA2	1:E:658:HIS:ND1	2.34	0.42
1:B:56:SER:O	1:B:57:LEU:HD23	2.19	0.42
1:E:177:ASN:H	1:E:177:ASN:ND2	2.15	0.42
1:A:296:ARG:O	1:A:296:ARG:HG2	2.20	0.41
1:A:320:PHE:HZ	1:B:528:TYR:CD1	2.30	0.41
1:E:337:TRP:CZ3	1:E:396:GLU:HG2	2.55	0.41
1:E:405:ILE:O	1:E:412:VAL:HA	2.19	0.41
1:B:13:GLU:CD	1:B:13:GLU:N	2.71	0.41
1:A:13:GLU:HG2	3:A:826:HOH:O	2.20	0.41
1:A:233:ASP:O	1:A:271:ARG:NH1	2.53	0.41
1:A:530:LEU:CD1	1:B:506:ARG:HH21	2.33	0.41
1:B:413:HIS:CE1	1:B:573:ASN:HD22	2.37	0.41
1:E:264:TRP:HB2	1:E:272:VAL:HG23	2.01	0.41
1:E:364:LYS:HB3	1:E:365:SER:H	1.54	0.41
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.93	0.41
1:B:344:ARG:CG	1:B:344:ARG:HH11	2.33	0.41
1:E:79:LEU:HD13	1:E:102:LEU:HD22	2.02	0.41
1:E:621:THR:HG23	1:E:637:GLU:HG3	2.02	0.41
1:A:230:CYS:CB	1:A:361:PRO:HB3	2.50	0.41
1:B:233:ASP:HB2	1:B:234:GLN:H	1.68	0.41
1:A:57:LEU:HB3	1:A:119:LEU:HD11	2.03	0.41
1:A:119:LEU:HB3	1:A:132:LEU:HD13	2.02	0.41
1:A:317:ARG:NH1	1:A:403:ASP:OD1	2.52	0.41
1:A:319:GLU:OE2	1:B:528:TYR:O	2.38	0.41
1:B:294:PRO:HG2	1:B:341:TRP:HB3	2.01	0.41
1:B:366:GLU:HB2	1:B:367:GLY:H	1.73	0.41
1:B:119:LEU:HB3	1:B:132:LEU:CD1	2.48	0.41
1:E:83:VAL:HG12	1:E:89:THR:HG21	2.02	0.41
1:E:492:PHE:CD1	1:E:492:PHE:N	2.88	0.41
1:E:548:TYR:HA	1:E:551:TYR:CE2	2.56	0.41
1:A:187:ASP:O	1:A:262:ARG:NH2	2.54	0.41
1:A:332:TRP:HZ3	1:A:516:TYR:HH	1.67	0.41
1:A:589:ILE:HD13	1:A:666:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:TRP:CZ3	1:B:106:THR:HG22	2.56	0.41
1:B:236:VAL:HA	1:B:264:TRP:CD1	2.56	0.41
1:B:316:PHE:O	1:B:324:GLN:HB2	2.21	0.41
1:E:169:GLN:OE1	1:E:178:ILE:HD13	2.21	0.41
1:E:462:LEU:HB3	1:E:463:ASN:H	1.70	0.41
1:E:486:GLY:HA2	1:E:548:TYR:CD1	2.56	0.41
1:E:617:LEU:HB3	1:E:620:CYS:SG	2.60	0.41
1:B:362:GLN:HB3	1:B:364:LYS:CG	2.51	0.41
1:B:629:LEU:HD22	1:B:662:HIS:HB2	2.03	0.41
1:E:305:HIS:HA	1:E:396:GLU:OE1	2.21	0.41
1:A:506:ARG:CZ	1:A:568:VAL:HG11	2.50	0.40
1:E:83:VAL:CG1	1:E:89:THR:HG21	2.50	0.40
1:E:164:GLN:HG3	1:E:663:LYS:H	1.85	0.40
1:A:252:MET:CE	1:A:558:SER:OG	2.70	0.40
1:E:635:THR:O	1:E:636:VAL:HG23	2.21	0.40
1:A:335:HIS:CD2	1:A:337:TRP:HE3	2.39	0.40
1:E:131:VAL:HG12	1:E:133:GLY:H	1.86	0.40
1:A:154:GLU:HG2	1:A:431:VAL:CG2	2.51	0.40
1:A:247:ASP:OD1	1:A:247:ASP:N	2.48	0.40
1:A:387:LYS:HG3	1:A:388:TYR:CG	2.56	0.40
1:A:154:GLU:HG2	1:A:431:VAL:HG23	2.03	0.40
1:B:48:ARG:NH2	1:B:55:ASP:OD1	2.55	0.40
1:B:252:MET:HG2	1:B:278:TRP:CZ2	2.57	0.40
1:E:346:ASP:OD1	1:E:387:LYS:CE	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	683/695 (98%)	605 (89%)	54 (8%)	24 (4%)	<b>3</b> <b>10</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	683/695 (98%)	582 (85%)	81 (12%)	20 (3%)	3	13
1	E	683/695 (98%)	595 (87%)	69 (10%)	19 (3%)	4	14
All	All	2049/2085 (98%)	1782 (87%)	204 (10%)	63 (3%)	3	12

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	82	ALA
1	A	122	SER
1	A	233	ASP
1	A	274	TYR
1	A	365	SER
1	A	464	LYS
1	A	470	GLU
1	A	600	LYS
1	B	233	ASP
1	B	399	ALA
1	B	463	ASN
1	E	230	CYS
1	E	243	ASN
1	E	274	TYR
1	E	306	ASP
1	E	573	ASN
1	A	9	ARG
1	A	83	VAL
1	A	84	GLU
1	A	183	GLY
1	A	325	GLY
1	B	108	ALA
1	B	122	SER
1	B	208	GLY
1	B	214	ARG
1	B	232	ASP
1	B	446	PRO
1	B	462	LEU
1	B	519	ILE
1	E	14	LEU
1	E	327	LYS
1	E	364	LYS
1	E	571	VAL

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Mol	Chain	Res	Type
1	A	16	THR
1	A	28	ARG
1	A	121	ALA
1	A	243	ASN
1	A	383	ASP
1	B	84	GLU
1	B	85	GLU
1	B	121	ALA
1	E	97	ASP
1	E	121	ALA
1	E	232	ASP
1	E	233	ASP
1	E	396	GLU
1	A	388	TYR
1	B	40	TRP
1	B	388	TYR
1	B	396	GLU
1	E	207	ALA
1	A	366	GLU
1	A	385	SER
1	B	14	LEU
1	B	217	PRO
1	B	363	GLU
1	E	84	GLU
1	E	363	GLU
1	A	97	ASP
1	A	430	SER
1	E	615	VAL
1	E	47	GLY

### 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	595/605 (98%)	515 (87%)	80 (13%)	3	10
1	B	595/605 (98%)	514 (86%)	81 (14%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	595/605 (98%)	515 (87%)	80 (13%)	3	10
All	All	1785/1815 (98%)	1544 (86%)	241 (14%)	3	10

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	ASP
1	A	13	GLU
1	A	15	GLU
1	A	17	ASN
1	A	25	ASP
1	A	28	ARG
1	A	41	LEU
1	A	42	THR
1	A	48	ARG
1	A	53	SER
1	A	56	SER
1	A	58	THR
1	A	62	VAL
1	A	63	THR
1	A	68	SER
1	A	84	GLU
1	A	85	GLU
1	A	91	THR
1	A	97	ASP
1	A	101	SER
1	A	118	SER
1	A	123	THR
1	A	125	TYR
1	A	128	SER
1	A	130	PHE
1	A	132	LEU
1	A	136	ILE
1	A	151	ASP
1	A	164	GLN
1	A	176	LYS
1	A	199	VAL
1	A	200	ASN
1	A	205	LYS
1	A	218	VAL
1	A	230	CYS

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Mol	Chain	Res	Type
1	A	234	GLN
1	A	240	ARG
1	A	244	ASN
1	A	247	ASP
1	A	249	VAL
1	A	257	SER
1	A	261	LEU
1	A	262	ARG
1	A	291	LEU
1	A	307	GLN
1	A	319	GLU
1	A	326	ASP
1	A	346	ASP
1	A	347	LEU
1	A	357	LEU
1	A	385	SER
1	A	386	THR
1	A	387	LYS
1	A	400	ASP
1	A	409	ASP
1	A	411	SER
1	A	421	ILE
1	A	431	VAL
1	A	452	GLU
1	A	454	GLU
1	A	460	ASN
1	A	465	LEU
1	A	468	LYS
1	A	499	THR
1	A	535	GLU
1	A	541	SER
1	A	550	LYS
1	A	556	THR
1	A	600	LYS
1	A	617	LEU
1	A	621	THR
1	A	624	VAL
1	A	629	LEU
1	A	630	THR
1	A	665	VAL
1	A	666	VAL
1	A	677	LYS

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Mol	Chain	Res	Type
1	A	680	ARG
1	A	683	ILE
1	B	4	GLU
1	B	12	LEU
1	B	15	GLU
1	B	19	ARG
1	B	29	GLU
1	B	30	LYS
1	B	40	TRP
1	B	42	THR
1	B	48	ARG
1	B	58	THR
1	B	70	GLU
1	B	76	ARG
1	B	81	ASP
1	B	85	GLU
1	B	91	THR
1	B	92	VAL
1	B	102	LEU
1	B	118	SER
1	B	119	LEU
1	B	123	THR
1	B	136	ILE
1	B	143	CYS
1	B	152	SER
1	B	164	GLN
1	B	167	ILE
1	B	176	LYS
1	B	186	GLU
1	B	199	VAL
1	B	200	ASN
1	B	205	LYS
1	B	225	SER
1	B	234	GLN
1	B	240	ARG
1	B	249	VAL
1	B	253	SER
1	B	257	SER
1	B	261	LEU
1	B	271	ARG
1	B	273	LYS
1	B	277	CYS

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Mol	Chain	Res	Type
1	B	291	LEU
1	B	308	ASN
1	B	309	SER
1	B	313	ILE
1	B	319	GLU
1	B	344	ARG
1	B	346	ASP
1	B	365	SER
1	B	387	LYS
1	B	396	GLU
1	B	397	VAL
1	B	400	ASP
1	B	415	SER
1	B	418	ARG
1	B	426	ILE
1	B	473	MET
1	B	506	ARG
1	B	508	LEU
1	B	535	GLU
1	B	541	SER
1	B	549	GLU
1	B	550	LYS
1	B	562	LYS
1	B	564	ARG
1	B	574	SER
1	B	576	LEU
1	B	585	GLU
1	B	600	LYS
1	B	601	ARG
1	B	602	LYS
1	B	607	VAL
1	B	610	GLN
1	B	621	THR
1	B	629	LEU
1	B	630	THR
1	B	632	GLU
1	B	650	VAL
1	B	652	MET
1	B	665	VAL
1	B	666	VAL
1	B	688	LEU
1	E	7	LEU

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Mol	Chain	Res	Type
1	E	8	GLU
1	E	11	ASP
1	E	12	LEU
1	E	15	GLU
1	E	16	THR
1	E	29	GLU
1	E	41	LEU
1	E	42	THR
1	E	54	VAL
1	E	56	SER
1	E	58	THR
1	E	76	ARG
1	E	80	ARG
1	E	81	ASP
1	E	85	GLU
1	E	91	THR
1	E	92	VAL
1	E	96	GLN
1	E	97	ASP
1	E	102	LEU
1	E	103	GLN
1	E	130	PHE
1	E	132	LEU
1	E	136	ILE
1	E	164	GLN
1	E	176	LYS
1	E	177	ASN
1	E	200	ASN
1	E	209	ARG
1	E	218	VAL
1	E	231	ASN
1	E	233	ASP
1	E	234	GLN
1	E	240	ARG
1	E	244	ASN
1	E	249	VAL
1	E	261	LEU
1	E	262	ARG
1	E	276	GLN
1	E	291	LEU
1	E	311	LEU
1	E	327	LYS

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Mol	Chain	Res	Type
1	E	347	LEU
1	E	366	GLU
1	E	387	LYS
1	E	389	ASP
1	E	396	GLU
1	E	400	ASP
1	E	408	ASP
1	E	409	ASP
1	E	411	SER
1	E	421	ILE
1	E	426	ILE
1	E	431	VAL
1	E	454	GLU
1	E	461	HIS
1	E	468	LYS
1	E	470	GLU
1	E	481	GLN
1	E	499	THR
1	E	501	GLU
1	E	516	TYR
1	E	523	GLU
1	E	526	THR
1	E	535	GLU
1	E	550	LYS
1	E	569	GLU
1	E	576	LEU
1	E	577	LEU
1	E	582	LEU
1	E	601	ARG
1	E	617	LEU
1	E	621	THR
1	E	629	LEU
1	E	630	THR
1	E	647	GLU
1	E	653	ASP
1	E	666	VAL
1	E	677	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN

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Mol	Chain	Res	Type
1	A	126	GLN
1	A	234	GLN
1	A	270	GLN
1	A	307	GLN
1	B	17	ASN
1	B	243	ASN
1	B	276	GLN
1	B	461	HIS
1	B	573	ASN
1	E	17	ASN
1	E	164	GLN
1	E	177	ASN
1	E	231	ASN
1	E	234	GLN
1	E	307	GLN
1	E	413	HIS
1	E	481	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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
2	GTP	A	701	-	29,34,34	1.89	3 (10%)	35,54,54	1.77	8 (22%)
2	GTP	E	701	-	29,34,34	1.83	5 (17%)	35,54,54	1.80	8 (22%)
2	GTP	B	701	-	29,34,34	1.73	3 (10%)	35,54,54	1.93	14 (40%)

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
2	GTP	A	701	-	-	3/18/38/38	0/3/3/3
2	GTP	E	701	-	-	3/18/38/38	0/3/3/3
2	GTP	B	701	-	-	1/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	GTP	C5-C6	-6.60	1.34	1.47
2	E	701	GTP	C5-C6	-6.54	1.34	1.47
2	A	701	GTP	C5-C6	-6.49	1.34	1.47
2	A	701	GTP	PB-O3A	-3.98	1.55	1.59
2	B	701	GTP	C5-C4	-3.70	1.33	1.43
2	A	701	GTP	C5-C4	-3.53	1.34	1.43
2	E	701	GTP	C5-C4	-3.32	1.34	1.43
2	B	701	GTP	C2'-C3'	-3.10	1.45	1.53
2	E	701	GTP	PB-O3A	-2.73	1.56	1.59
2	E	701	GTP	O4'-C1'	2.17	1.43	1.40
2	E	701	GTP	PG-O2G	-2.05	1.47	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GTP	O4'-C1'-N9	-4.26	103.09	108.75
2	B	701	GTP	C8-N7-C5	3.81	109.04	102.55
2	E	701	GTP	O2A-PA-O3A	3.77	117.45	107.27
2	E	701	GTP	C2-N1-C6	-3.69	118.36	125.11
2	B	701	GTP	O3A-PB-O1B	-3.55	100.02	110.70
2	A	701	GTP	O3B-PG-O1G	-3.48	92.71	111.04
2	A	701	GTP	C2-N1-C6	-3.23	119.20	125.11
2	A	701	GTP	C8-N7-C5	3.12	107.87	102.55
2	B	701	GTP	O2A-PA-O3A	3.12	115.71	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	GTP	C8-N7-C5	2.92	107.53	102.55
2	A	701	GTP	C5-C6-N1	2.82	119.46	114.07
2	B	701	GTP	O3'-C3'-C2'	-2.82	102.79	111.82
2	B	701	GTP	N1-C2-N3	-2.78	118.22	123.32
2	B	701	GTP	O3B-PG-O1G	-2.78	96.42	111.04
2	E	701	GTP	O2B-PB-O3A	-2.68	100.02	107.27
2	E	701	GTP	N2-C2-N1	2.66	122.37	116.76
2	B	701	GTP	C2-N1-C6	-2.63	120.30	125.11
2	B	701	GTP	C5-C6-N1	2.62	119.06	114.07
2	A	701	GTP	O2A-PA-O3A	2.61	114.34	107.27
2	A	701	GTP	N1-C2-N3	-2.61	118.54	123.32
2	E	701	GTP	O3B-PG-O1G	-2.57	97.52	111.04
2	E	701	GTP	C5-C6-N1	2.57	118.97	114.07
2	E	701	GTP	O3A-PA-O1A	-2.27	103.87	110.70
2	B	701	GTP	O6-C6-N1	-2.25	117.94	120.62
2	B	701	GTP	O2B-PB-O3A	2.22	113.28	107.27
2	B	701	GTP	O3G-PG-O2G	2.19	116.01	107.80
2	B	701	GTP	O2'-C2'-C3'	-2.16	104.89	111.82
2	A	701	GTP	O3G-PG-O2G	2.16	115.90	107.80
2	B	701	GTP	O3G-PG-O3B	2.16	111.87	104.64
2	B	701	GTP	O4'-C1'-N9	2.11	111.55	108.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	GTP	C5'-O5'-PA-O1A
2	E	701	GTP	C5'-O5'-PA-O1A
2	A	701	GTP	C5'-O5'-PA-O3A
2	A	701	GTP	C5'-O5'-PA-O2A
2	E	701	GTP	C5'-O5'-PA-O3A
2	E	701	GTP	C5'-O5'-PA-O2A
2	B	701	GTP	PB-O3B-PG-O1G

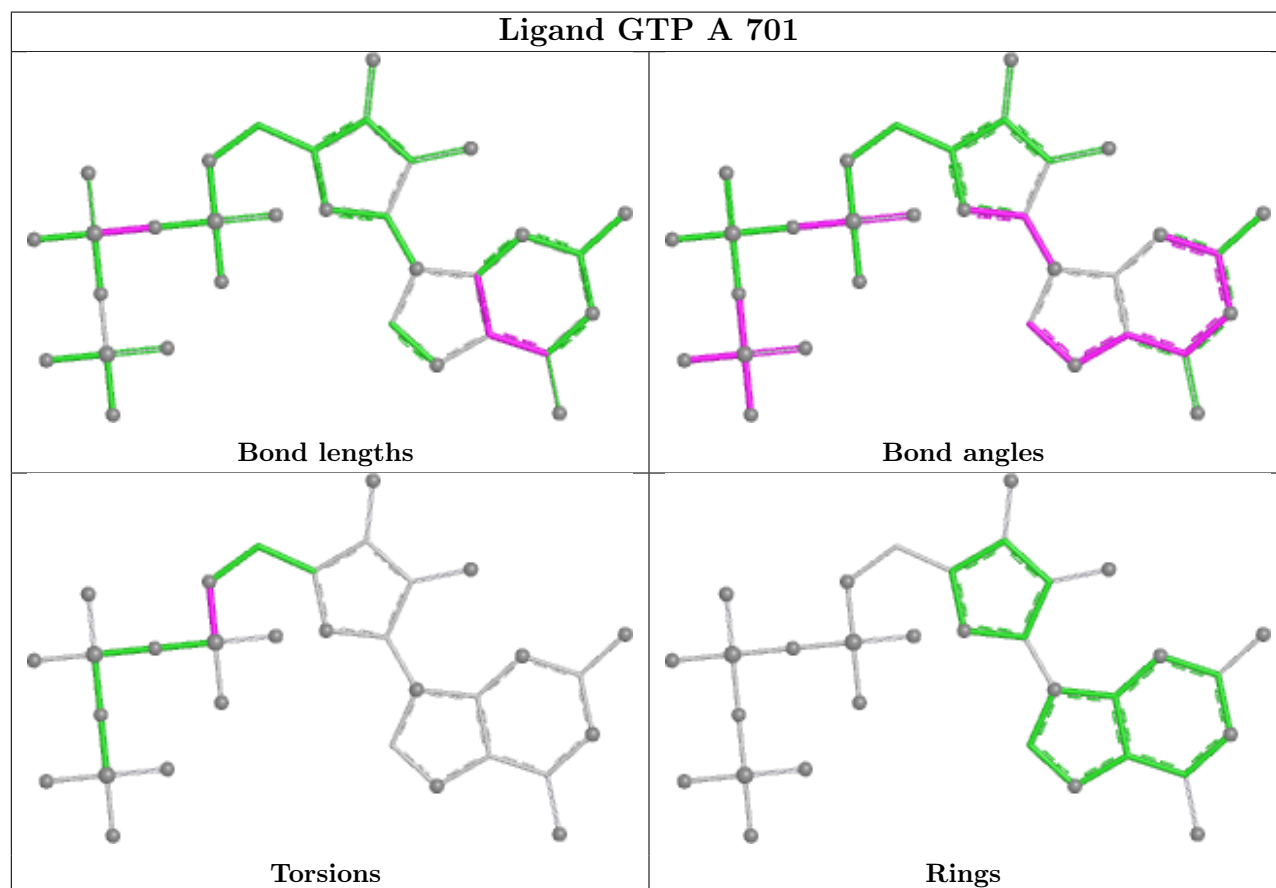
There are no ring outliers.

2 monomers are involved in 2 short contacts:

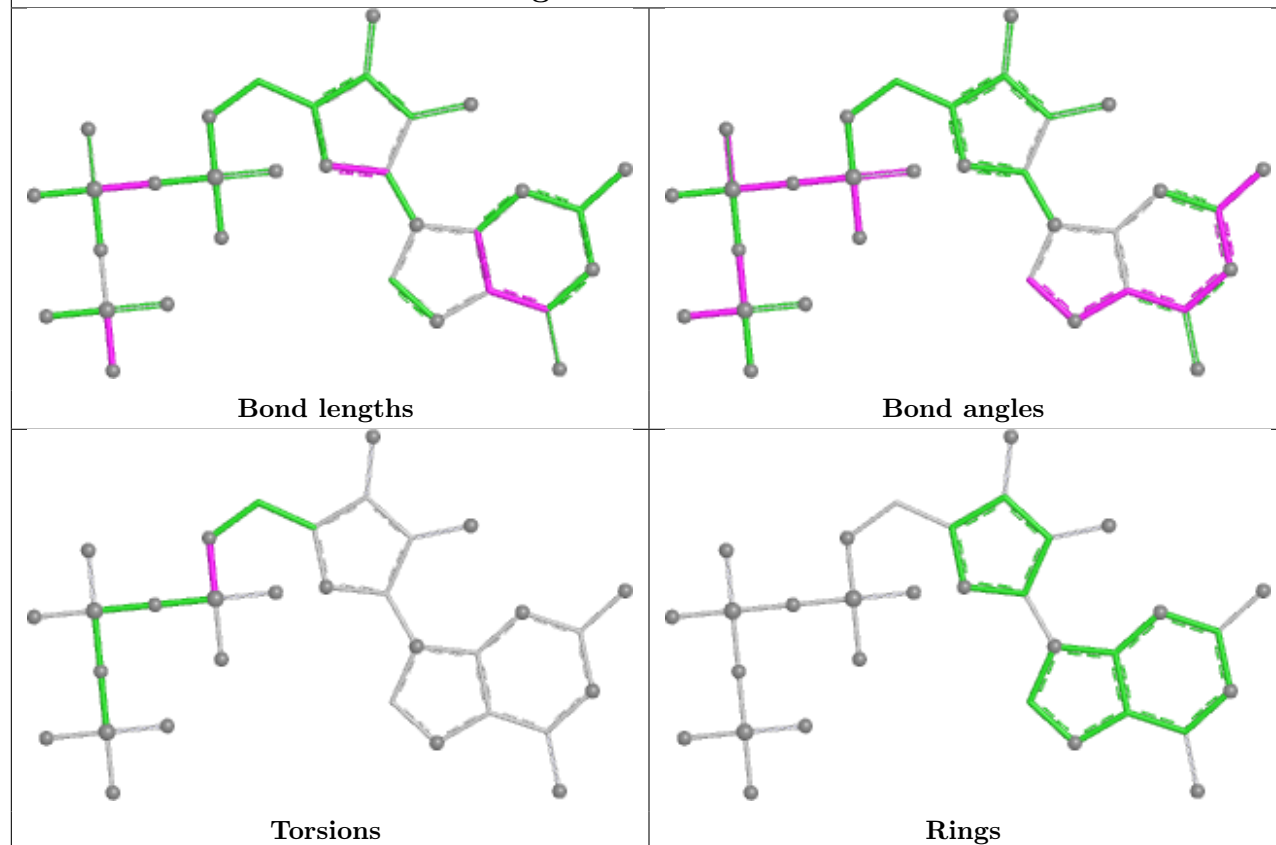
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GTP	1	0
2	B	701	GTP	1	0



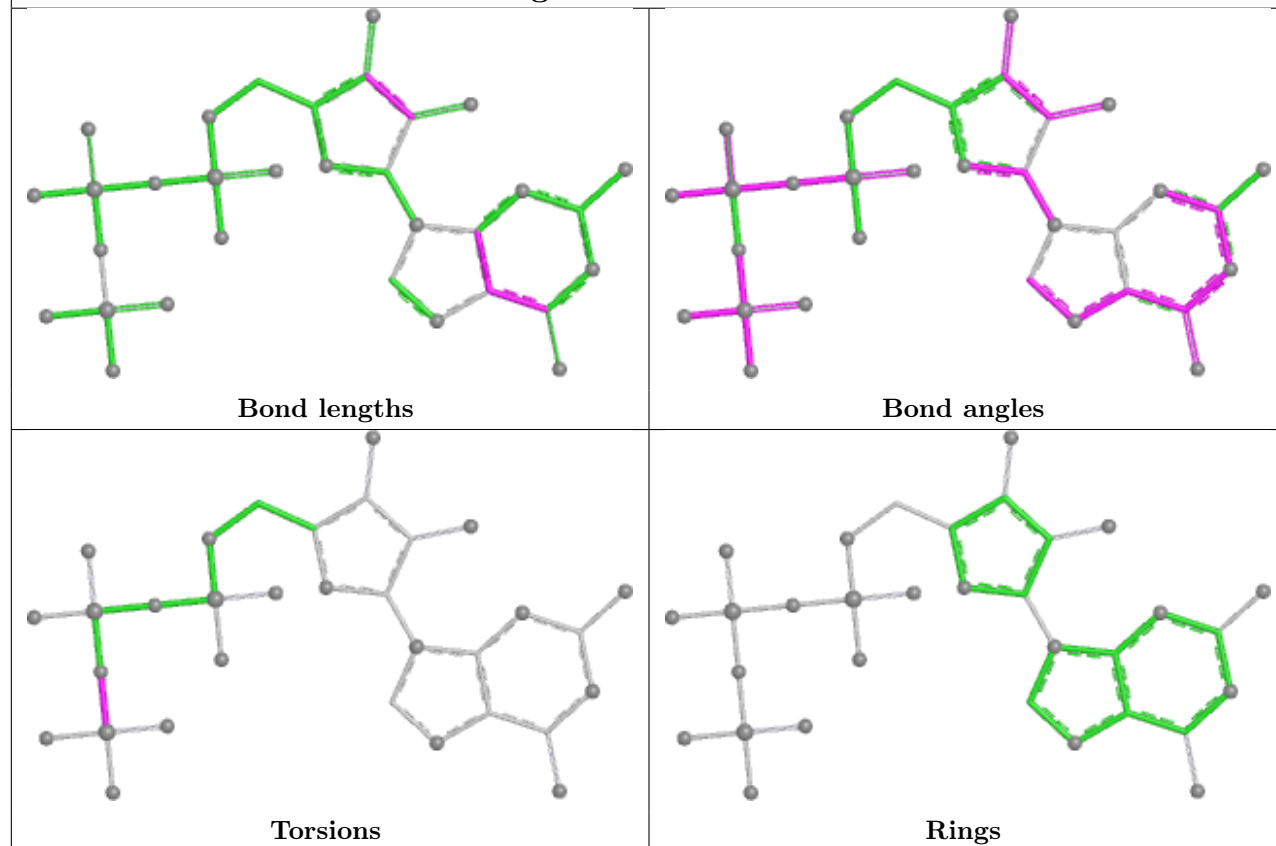
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



## Ligand GTP E 701



## Ligand GTP B 701



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	685/695 (98%)	-0.23	9 (1%) 74 67	41, 66, 99, 121	0
1	B	685/695 (98%)	-0.02	11 (1%) 70 63	44, 78, 119, 135	0
1	E	685/695 (98%)	-0.03	9 (1%) 74 67	43, 77, 106, 126	0
All	All	2055/2085 (98%)	-0.10	29 (1%) 73 66	41, 73, 113, 135	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	528	TYR	4.4
1	E	688	LEU	4.2
1	A	465	LEU	3.5
1	A	121	ALA	3.5
1	E	121	ALA	3.3
1	E	230	CYS	3.2
1	A	231	ASN	3.0
1	E	368	THR	2.9
1	B	6	VAL	2.9
1	B	688	LEU	2.9
1	E	14	LEU	2.8
1	E	128	SER	2.7
1	B	72	GLY	2.6
1	A	492	PHE	2.6
1	B	123	THR	2.6
1	B	101	SER	2.6
1	A	12	LEU	2.4
1	B	231	ASN	2.3
1	E	462	LEU	2.3
1	B	5	LEU	2.2
1	A	688	LEU	2.2
1	B	343	THR	2.2
1	E	125	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	13	GLU	2.1
1	E	83	VAL	2.1
1	B	367	GLY	2.1
1	B	320	PHE	2.1
1	A	14	LEU	2.1
1	A	5	LEU	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](#)

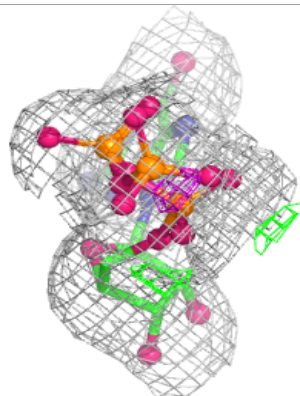
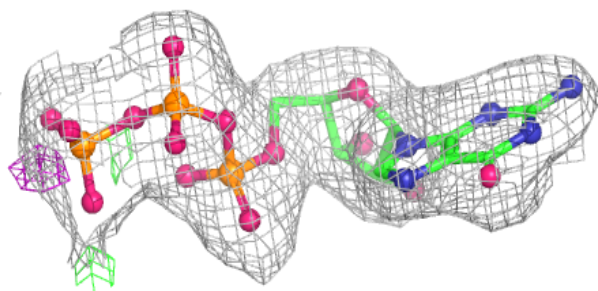
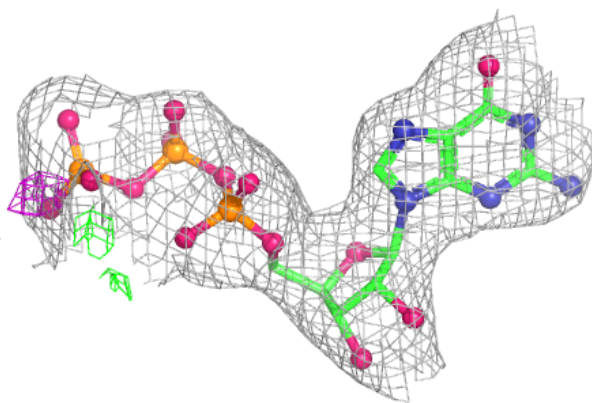
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GTP	B	701	32/32	0.92	0.07	63,67,79,80	0
2	GTP	A	701	32/32	0.93	0.06	45,53,80,81	0
2	GTP	E	701	32/32	0.94	0.06	45,63,75,75	0

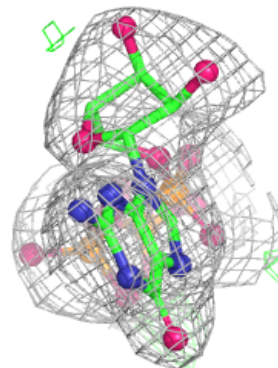
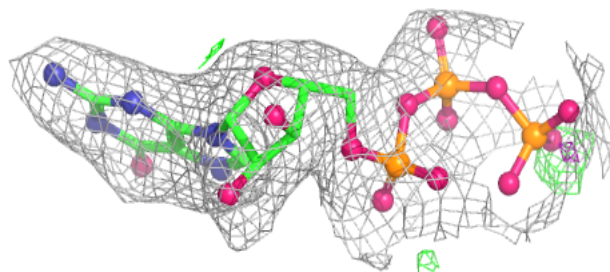
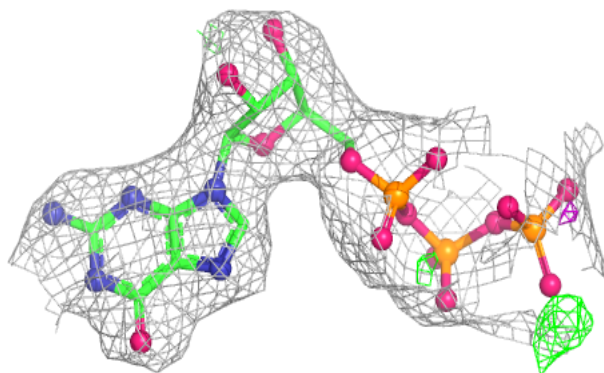
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

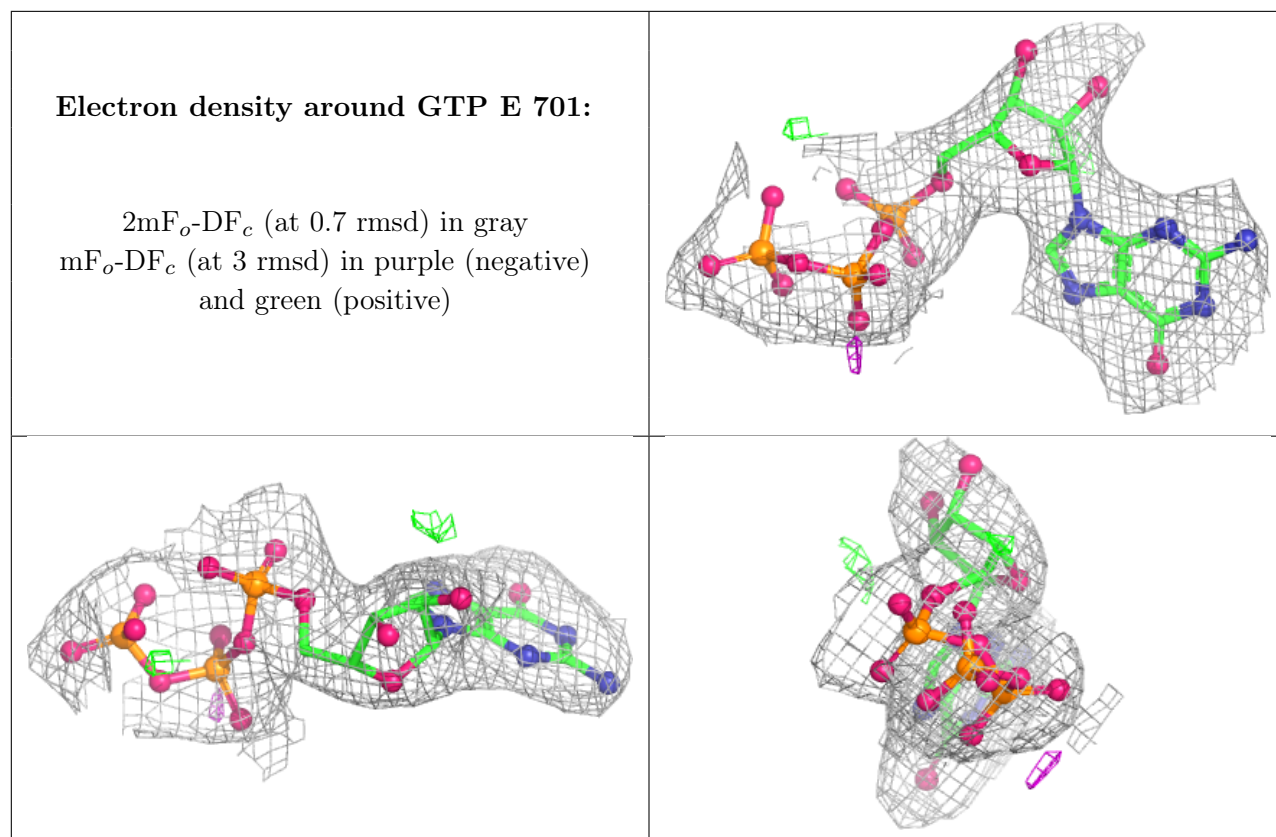
**Electron density around GTP B 701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around GTP A 701:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.