



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:11 AM UTC

PDB ID : 4FWT / pdb_00004fwt
Title : Complex structure of viral RNA polymerase form III
Authors : Takeshita, D.; Tomita, K.
Deposited on : 2012-07-02
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

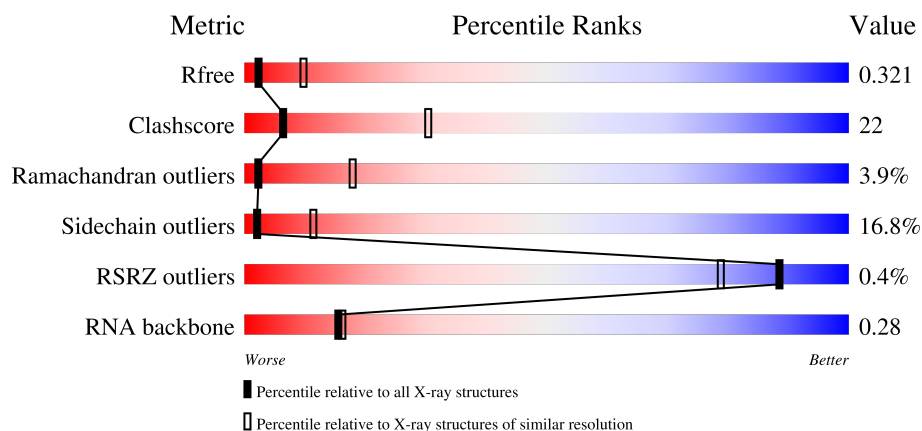
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

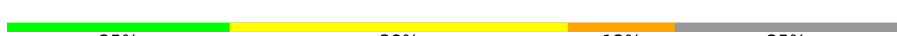
The reported resolution of this entry is 3.20 Å.

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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1289	
2	G	8	
3	T	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GTP	A	2501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9582 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 Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1203	Total	C	N	O	S	0	0	0
			9287	5865	1605	1772	45			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	HIS	-	linker	UNP P0A6P3
A	1284	HIS	-	expression tag	UNP Q8LTE0
A	1285	HIS	-	expression tag	UNP Q8LTE0
A	1286	HIS	-	expression tag	UNP Q8LTE0
A	1287	HIS	-	expression tag	UNP Q8LTE0
A	1288	HIS	-	expression tag	UNP Q8LTE0
A	1289	HIS	-	expression tag	UNP Q8LTE0

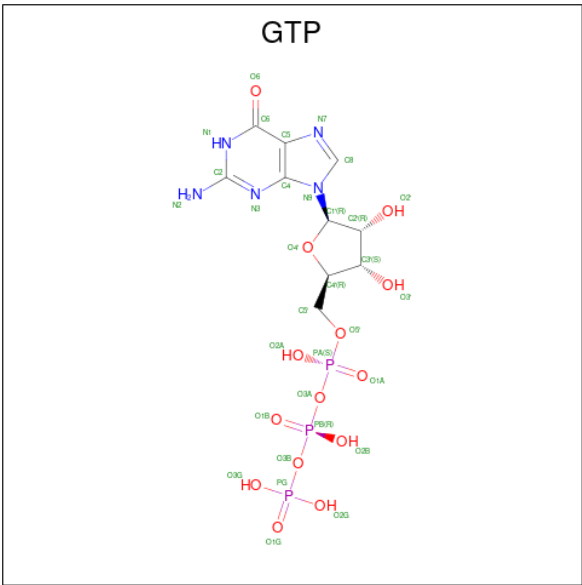
- Molecule 2 is a RNA chain called RNA (5'-R(*C*CP*CP*UP*AP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	P	0	0	1
			122	55	19	42	6			

- Molecule 3 is a RNA chain called RNA (5'-R(*GP*GP*GP*UP*AP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	6	Total	C	N	O	P	0	0	0
			131	59	27	40	5			

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		

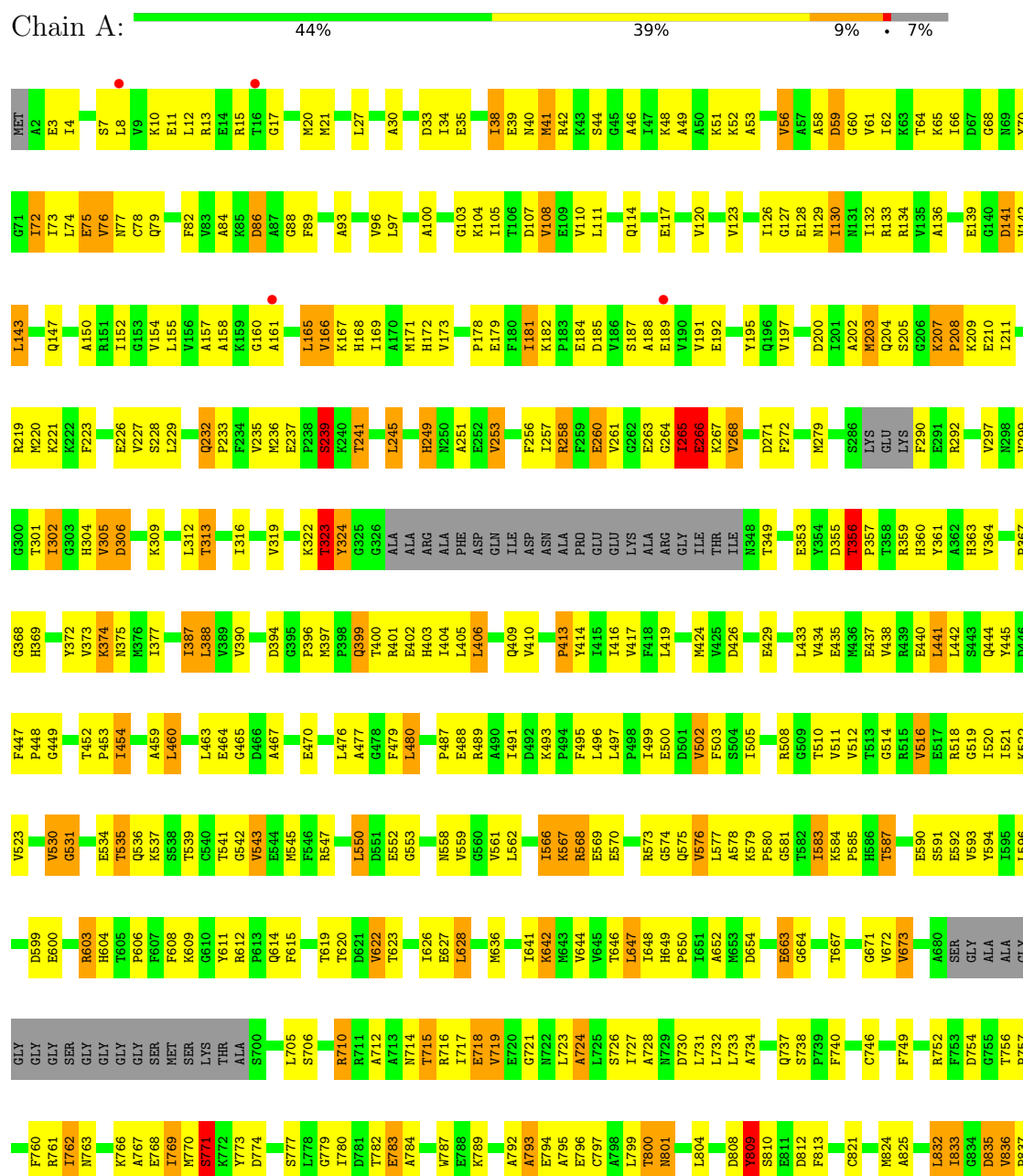
- Molecule 6 is water.

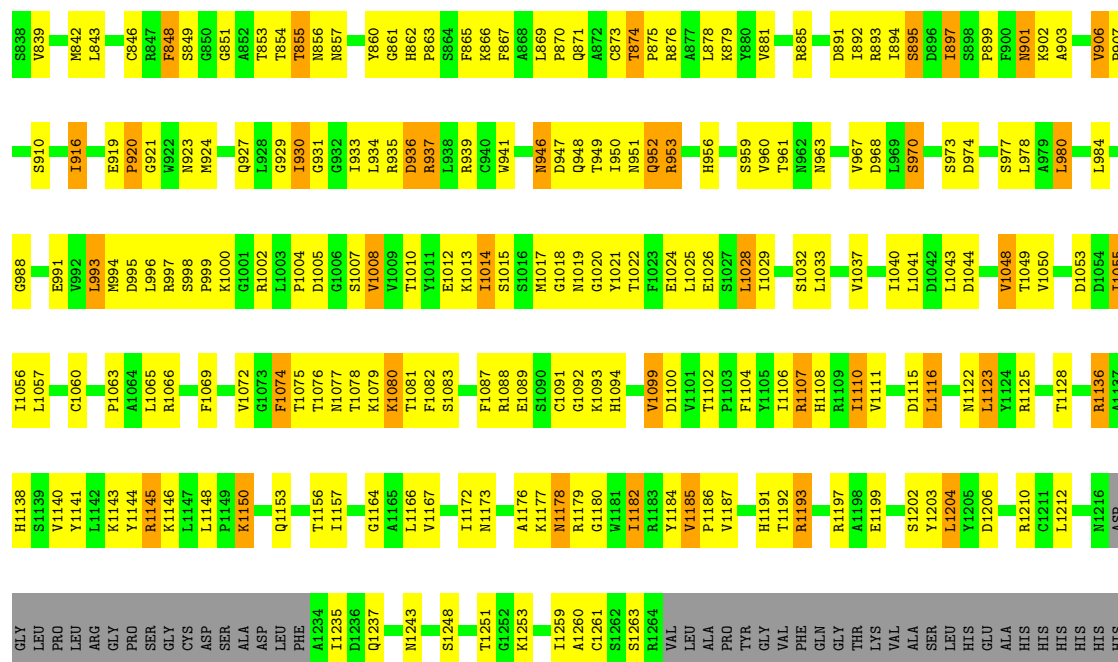
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		

3 Residue-property plots

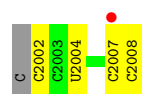
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Elongation factor Ts, Elongation factor Tu, LINKER, Q beta replicase

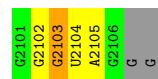
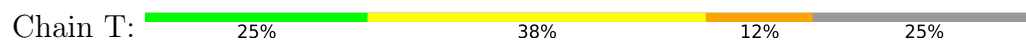




- Molecule 2: RNA (5'-R(*C*CP*CP*UP*AP*CP*CP*C)-3')



- Molecule 3: RNA (5'-R(*GP*GP*GP*UP*AP*GP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	137.51Å 255.05Å 100.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-3.20) 89.8 (20.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.245 , 0.314 0.246 , 0.321	Depositor DCC
R_{free} test set	1472 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 17.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9582	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: CA, 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	0.63	2/9456 (0.0%)	1.05	34/12787 (0.3%)
2	G	0.81	1/134 (0.7%)	0.46	0/206
3	T	0.40	0/147	0.40	0/229
All	All	0.63	3/9737 (0.0%)	1.03	34/13222 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	GLU	CA-C	8.25	1.63	1.52
2	G	2002	C	O3'-P	-7.89	1.49	1.61
1	A	266	GLU	C-O	6.61	1.32	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	GLU	N-CA-CB	-11.68	90.75	110.49
1	A	862	HIS	CA-C-N	8.61	130.60	119.84
1	A	862	HIS	C-N-CA	8.61	130.60	119.84
1	A	738	SER	CA-C-N	8.11	128.55	120.52
1	A	738	SER	C-N-CA	8.11	128.55	120.52
1	A	783	GLU	N-CA-C	-7.86	103.00	114.39
1	A	356	THR	N-CA-C	-7.74	101.26	108.22
1	A	649	HIS	CA-C-N	7.64	129.39	119.84
1	A	649	HIS	C-N-CA	7.64	129.39	119.84
1	A	266	GLU	N-CA-C	7.25	126.24	110.80
1	A	266	GLU	CA-C-O	6.83	130.28	120.51
1	A	1153	GLN	N-CA-C	-6.72	106.28	114.75
1	A	268	VAL	N-CA-C	-6.57	98.15	108.86
1	A	648	ILE	N-CA-C	6.43	117.18	110.62
1	A	953	ARG	N-CA-C	-6.42	104.36	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1193	ARG	N-CA-C	-6.38	100.83	110.28
1	A	559	VAL	N-CA-C	6.34	116.55	108.82
1	A	1261	CYS	N-CA-C	6.13	116.37	108.34
1	A	936	ASP	N-CA-C	-6.12	104.69	111.36
1	A	952	GLN	N-CA-C	-6.10	106.82	114.56
1	A	239	SER	N-CA-C	-6.05	104.88	112.93
1	A	849	SER	N-CA-C	5.87	118.06	108.55
1	A	853	THR	N-CA-C	-5.69	101.50	109.69
1	A	251	ALA	N-CA-C	5.68	117.88	109.69
1	A	260	GLU	N-CA-C	-5.68	101.28	109.29
1	A	1243	ASN	CA-C-N	5.58	125.53	119.78
1	A	1243	ASN	C-N-CA	5.58	125.53	119.78
1	A	604	HIS	N-CA-C	-5.50	106.45	112.72
1	A	1237	GLN	N-CA-C	-5.24	106.84	114.12
1	A	160	GLY	N-CA-C	-5.19	108.06	115.64
1	A	1243	ASN	N-CA-C	5.16	117.10	110.39
1	A	268	VAL	N-CA-CB	5.15	121.46	111.93
1	A	910	SER	N-CA-C	-5.13	107.02	113.28
1	A	253	VAL	CB-CA-C	-5.04	106.05	111.59

There are no chirality outliers.

There are no planarity outliers.

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	9287	0	9273	411	0
2	G	122	0	64	5	0
3	T	131	0	67	3	0
4	A	32	0	12	11	0
5	A	2	0	0	0	0
6	A	8	0	0	0	0
All	All	9582	0	9416	417	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 22.

All (417) 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:265:ILE:O	1:A:265:ILE:CG2	2.05	1.01
1:A:1094:HIS:H	1:A:1102:THR:HG22	1.27	0.97
1:A:1018:GLY:H	4:A:2501:GTP:HN21	1.02	0.91
1:A:265:ILE:O	1:A:265:ILE:HG22	1.69	0.90
1:A:264:GLY:C	1:A:266:GLU:H	1.80	0.89
1:A:710:ARG:O	1:A:714:ASN:ND2	2.05	0.88
1:A:1018:GLY:N	4:A:2501:GTP:HN21	1.71	0.88
1:A:491:ILE:HG23	1:A:520:ILE:HD11	1.59	0.85
1:A:1018:GLY:H	4:A:2501:GTP:N2	1.75	0.84
1:A:356:THR:HG22	1:A:359:ARG:H	1.42	0.84
1:A:558:ASN:HB3	1:A:1210:ARG:HD3	1.61	0.81
1:A:593:VAL:HG12	1:A:671:GLY:HA3	1.64	0.80
1:A:226:GLU:O	1:A:232:GLN:NE2	2.14	0.79
1:A:768:GLU:O	1:A:771:SER:OG	2.00	0.79
1:A:1050:VAL:HG13	1:A:1055:ILE:HG22	1.67	0.76
1:A:949:THR:HG22	1:A:953:ARG:HD3	1.67	0.76
1:A:523:VAL:HG12	1:A:542:GLY:HA2	1.66	0.76
1:A:961:THR:HG22	1:A:963:ASN:H	1.50	0.75
1:A:178:PRO:HG3	1:A:229:LEU:HD13	1.66	0.75
1:A:387:ILE:HD11	1:A:476:LEU:HD11	1.68	0.75
1:A:839:VAL:HA	1:A:842:MET:HB3	1.69	0.74
1:A:65:LYS:HB2	1:A:97:LEU:HD11	1.69	0.73
1:A:265:ILE:O	1:A:265:ILE:HG23	1.87	0.73
1:A:1206:ASP:OD1	1:A:1210:ARG:NH1	2.22	0.73
1:A:401:ARG:HB3	1:A:441:LEU:HD21	1.71	0.73
1:A:467:ALA:HA	1:A:470:GLU:HB2	1.71	0.72
1:A:505:ILE:HB	1:A:508:ARG:HB2	1.70	0.72
1:A:167:LYS:HG2	1:A:171:MET:HE3	1.70	0.72
1:A:797:CYS:O	1:A:801:ASN:ND2	2.19	0.72
1:A:1092:GLY:HA3	2:G:2007:C:H4'	1.71	0.71
1:A:372:TYR:CE1	1:A:410:VAL:HG21	2.26	0.71
1:A:724:ALA:HB1	1:A:770:MET:HE1	1.71	0.71
1:A:530:VAL:HG22	1:A:652:ALA:HB2	1.72	0.70
1:A:301:THR:HA	1:A:387:ILE:HG22	1.73	0.70
1:A:377:ILE:HG23	1:A:671:GLY:HA2	1.74	0.70
1:A:550:LEU:HD13	1:A:550:LEU:H	1.55	0.70
1:A:264:GLY:C	1:A:266:GLU:N	2.48	0.70
1:A:158:ALA:HA	1:A:253:VAL:HA	1.74	0.69
1:A:951:ASN:HD22	1:A:1049:THR:HG22	1.58	0.69
1:A:867:PHE:HB3	1:A:1204:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:ASN:HA	3:T:2103:G:H4'	1.74	0.68
1:A:543:VAL:HG13	1:A:561:VAL:HG22	1.73	0.68
1:A:1015:SER:HB3	1:A:1022:THR:OG1	1.94	0.67
1:A:792:ALA:HA	1:A:795:ALA:HB3	1.77	0.67
1:A:21:MET:HG3	1:A:424:MET:O	1.95	0.67
1:A:836:VAL:HG22	1:A:837:PRO:HD2	1.76	0.66
1:A:510:THR:OG1	1:A:566:ILE:O	2.07	0.66
1:A:970:SER:HB2	1:A:1075:THR:HG23	1.78	0.66
2:G:2007:C:O2	3:T:2102:G:N2	2.19	0.66
1:A:854:THR:HG22	1:A:920:PRO:HA	1.78	0.65
1:A:442:LEU:HD12	1:A:452:THR:HG21	1.78	0.65
1:A:592:GLU:HG2	1:A:642:LYS:HG2	1.79	0.65
1:A:1094:HIS:N	1:A:1102:THR:HG22	2.08	0.65
1:A:56:VAL:HG11	1:A:267:LYS:HD3	1.79	0.64
1:A:264:GLY:O	1:A:266:GLU:N	2.28	0.64
1:A:953:ARG:O	1:A:956:HIS:HB3	1.97	0.64
1:A:968:ASP:H	1:A:1081:THR:HG22	1.63	0.63
1:A:62:ILE:HD11	1:A:260:GLU:O	1.99	0.63
1:A:1077:ASN:O	1:A:1081:THR:HG23	1.98	0.63
1:A:304:HIS:HD2	1:A:306:ASP:H	1.46	0.62
1:A:502:VAL:O	1:A:1197:ARG:NH1	2.31	0.62
1:A:846:CYS:SG	1:A:929:GLY:HA3	2.39	0.62
1:A:301:THR:HB	1:A:363:HIS:NE2	2.15	0.62
1:A:594:TYR:OH	1:A:600:GLU:OE1	2.10	0.62
1:A:740:PHE:CE2	1:A:746:CYS:HA	2.34	0.62
1:A:165:LEU:O	1:A:168:HIS:N	2.32	0.62
1:A:76:VAL:HG11	1:A:93:ALA:HB1	1.82	0.61
1:A:611:TYR:HB3	1:A:626:ILE:HD11	1.82	0.61
1:A:860:TYR:HA	1:A:865:PHE:HD1	1.64	0.61
1:A:1083:SER:O	1:A:1088:ARG:NH1	2.33	0.61
1:A:499:ILE:HD12	1:A:512:VAL:HG11	1.81	0.61
1:A:590:GLU:HG3	1:A:644:VAL:HG22	1.83	0.61
1:A:717:ILE:HD12	1:A:718:GLU:H	1.64	0.61
1:A:663:GLU:HG3	1:A:1182:ILE:HD12	1.83	0.61
1:A:835:ASP:OD2	1:A:835:ASP:N	2.22	0.60
1:A:312:LEU:O	1:A:316:ILE:HG13	2.00	0.60
1:A:614:GLN:HA	1:A:623:THR:HA	1.82	0.60
1:A:1164:GLY:HA3	1:A:1187:VAL:HB	1.84	0.60
1:A:322:LYS:NZ	1:A:470:GLU:OE2	2.27	0.60
1:A:615:PHE:N	1:A:622:VAL:O	2.33	0.60
1:A:93:ALA:HA	1:A:96:VAL:HG12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:MET:H	1:A:394:ASP:HA	1.68	0.59
1:A:923:ASN:HB3	1:A:927:GLN:HE21	1.67	0.59
1:A:304:HIS:CD2	1:A:306:ASP:H	2.20	0.59
1:A:935:ARG:NH2	1:A:1024:GLU:OE1	2.36	0.58
1:A:530:VAL:HG13	1:A:576:VAL:HG22	1.85	0.58
1:A:369:HIS:NE2	1:A:406:LEU:HD23	2.19	0.58
1:A:62:ILE:HG23	1:A:74:LEU:O	2.03	0.58
1:A:851:GLY:HA2	1:A:861:GLY:HA3	1.85	0.58
1:A:752:ARG:NH1	1:A:754:ASP:OD1	2.37	0.57
1:A:949:THR:CG2	1:A:953:ARG:HD3	2.33	0.57
1:A:951:ASN:ND2	1:A:1049:THR:HG22	2.20	0.57
1:A:534:GLU:O	1:A:536:GLN:N	2.37	0.57
1:A:155:LEU:O	1:A:257:ILE:N	2.26	0.57
1:A:70:TYR:OH	1:A:100:ALA:O	2.22	0.57
1:A:769:ILE:HG12	1:A:1106:ILE:HG12	1.84	0.57
1:A:885:ARG:NH1	1:A:892:ILE:H	2.03	0.57
1:A:1026:GLU:OE2	4:A:2501:GTP:O2'	2.19	0.57
1:A:1069:PHE:HA	1:A:1072:VAL:HG22	1.87	0.57
1:A:1100:ASP:OD1	1:A:1102:THR:HG23	2.04	0.57
1:A:404:ILE:HD12	1:A:441:LEU:HD22	1.87	0.57
1:A:372:TYR:HE1	1:A:410:VAL:HG11	1.69	0.56
1:A:373:VAL:C	1:A:375:ASN:H	2.13	0.56
1:A:609:LYS:HA	1:A:628:LEU:HD23	1.87	0.56
4:A:2501:GTP:O4'	2:G:2008:C:H2'	2.05	0.56
1:A:417:VAL:HB	1:A:454:ILE:HD13	1.87	0.56
1:A:61:VAL:HG13	1:A:84:ALA:HB1	1.88	0.56
1:A:773:TYR:HA	1:A:1107:ARG:O	2.05	0.56
1:A:369:HIS:CD2	1:A:406:LEU:HD23	2.41	0.56
1:A:732:LEU:HD13	1:A:766:LYS:HE2	1.88	0.56
1:A:61:VAL:HG22	1:A:89:PHE:HE1	1.71	0.56
1:A:1141:TYR:O	1:A:1145:ARG:HB2	2.05	0.56
1:A:267:LYS:HG3	1:A:268:VAL:H	1.70	0.55
1:A:59:ASP:O	1:A:77:ASN:HB2	2.06	0.55
1:A:78:CYS:HB3	1:A:89:PHE:CE2	2.41	0.55
1:A:899:PRO:HB2	1:A:999:PRO:HG2	1.87	0.55
1:A:107:ASP:HB3	1:A:110:VAL:HG23	1.87	0.55
1:A:734:ALA:O	1:A:1136:ARG:HB2	2.07	0.55
1:A:760:PHE:O	1:A:763:ASN:N	2.40	0.55
1:A:878:LEU:HD13	1:A:897:ILE:HD11	1.88	0.55
1:A:12:LEU:HD22	1:A:27:LEU:HD13	1.88	0.55
1:A:901:ASN:HD22	1:A:901:ASN:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:MET:HG2	1:A:608:PHE:CZ	2.42	0.54
1:A:1087:PHE:O	1:A:1088:ARG:NH2	2.39	0.54
1:A:404:ILE:HD13	1:A:442:LEU:HD23	1.89	0.54
1:A:723:LEU:HD23	1:A:1110:ILE:HG12	1.89	0.54
1:A:134:ARG:NH1	1:A:263:GLU:OE2	2.41	0.54
1:A:782:THR:OG1	1:A:783:GLU:N	2.40	0.54
1:A:208:PRO:HD2	1:A:211:ILE:HG13	1.90	0.54
1:A:1185:VAL:HG12	1:A:1186:PRO:HD2	1.90	0.54
1:A:8:LEU:HG	1:A:11:GLU:HB2	1.90	0.53
1:A:396:PRO:HG3	1:A:437:GLU:O	2.08	0.53
1:A:192:GLU:HA	1:A:195:TYR:HB3	1.89	0.53
1:A:545:MET:HE3	1:A:550:LEU:HD11	1.90	0.53
1:A:824:MET:HE1	1:A:1040:ILE:HD13	1.90	0.53
1:A:902:LYS:NZ	1:A:1002:ARG:HH12	2.06	0.53
1:A:74:LEU:HD21	1:A:96:VAL:HG13	1.91	0.53
1:A:272:PHE:CZ	1:A:313:THR:HG21	2.43	0.53
1:A:309:LYS:O	1:A:313:THR:HG22	2.08	0.53
1:A:290:PHE:N	1:A:292:ARG:HH21	2.06	0.53
1:A:836:VAL:HG23	1:A:988:GLY:HA3	1.90	0.53
1:A:1074:PHE:N	1:A:1074:PHE:CD2	2.76	0.52
1:A:919:GLU:OE2	1:A:998:SER:HB2	2.08	0.52
1:A:927:GLN:OE1	1:A:1020:GLY:N	2.33	0.52
1:A:271:ASP:OD1	1:A:272:PHE:N	2.42	0.52
1:A:757:PRO:HB3	1:A:1099:VAL:HG11	1.92	0.52
1:A:496:LEU:HD11	1:A:576:VAL:HB	1.90	0.52
1:A:821:CYS:HA	1:A:824:MET:HE3	1.92	0.52
1:A:152:ILE:HG12	1:A:260:GLU:HG3	1.90	0.52
1:A:60:GLY:HA3	1:A:77:ASN:HB2	1.91	0.51
1:A:400:THR:HA	1:A:403:HIS:ND1	2.24	0.51
1:A:426:ASP:OD1	1:A:426:ASP:N	2.44	0.51
1:A:793:ALA:HB1	1:A:974:ASP:HB3	1.93	0.51
1:A:1136:ARG:H	1:A:1136:ARG:HD3	1.74	0.51
1:A:38:ILE:HA	1:A:41:MET:HG3	1.92	0.51
1:A:128:GLU:O	1:A:130:ILE:N	2.43	0.51
1:A:931:GLY:O	1:A:1024:GLU:HG2	2.10	0.51
1:A:946:ASN:OD1	1:A:946:ASN:N	2.43	0.51
1:A:20:MET:HE3	1:A:20:MET:HA	1.93	0.51
1:A:809:TYR:HE1	1:A:812:ASP:HA	1.76	0.51
1:A:1156:THR:O	1:A:1173:ASN:ND2	2.43	0.51
1:A:40:ASN:O	1:A:44:SER:OG	2.27	0.51
1:A:724:ALA:O	1:A:727:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:GLU:HB2	1:A:924:MET:HG2	1.93	0.51
1:A:497:LEU:HD12	1:A:516:VAL:HB	1.93	0.50
1:A:870:PRO:HB2	1:A:895:SER:HB3	1.93	0.50
1:A:73:ILE:HG12	1:A:74:LEU:H	1.76	0.50
1:A:267:LYS:NZ	1:A:268:VAL:O	2.45	0.50
1:A:749:PHE:CD1	1:A:767:ALA:HB2	2.47	0.50
1:A:1116:LEU:HB3	1:A:1148:LEU:HD21	1.92	0.50
1:A:1150:LYS:HD2	1:A:1150:LYS:H	1.75	0.50
1:A:267:LYS:CG	1:A:268:VAL:H	2.24	0.50
1:A:581:GLY:HA2	1:A:584:LYS:HE2	1.92	0.50
1:A:1077:ASN:ND2	1:A:1080:LYS:HD3	2.27	0.50
1:A:712:ALA:O	1:A:715:THR:HB	2.12	0.50
1:A:784:ALA:HA	1:A:787:TRP:HD1	1.77	0.50
1:A:857:ASN:O	1:A:860:TYR:N	2.42	0.50
1:A:951:ASN:HD22	1:A:1049:THR:CG2	2.25	0.50
1:A:1192:THR:HB	1:A:1248:SER:HB3	1.94	0.50
1:A:187:SER:C	1:A:189:GLU:H	2.19	0.50
1:A:495:PHE:HA	1:A:519:GLY:HA3	1.94	0.50
1:A:949:THR:C	1:A:951:ASN:H	2.20	0.50
1:A:388:LEU:HB3	1:A:417:VAL:HG22	1.93	0.49
1:A:531:GLY:HA3	1:A:575:GLN:HG2	1.93	0.49
1:A:1104:PHE:HZ	1:A:1123:LEU:HD12	1.75	0.49
1:A:499:ILE:HD11	1:A:577:LEU:HB2	1.93	0.49
1:A:856:ASN:ND2	1:A:865:PHE:O	2.42	0.49
1:A:512:VAL:HG21	1:A:577:LEU:HD22	1.94	0.49
1:A:606:PRO:HB3	1:A:636:MET:HG2	1.94	0.49
1:A:82:PHE:HE1	1:A:406:LEU:HB2	1.78	0.49
1:A:435:GLU:HA	1:A:438:VAL:HG12	1.94	0.49
1:A:842:MET:HE1	1:A:930:ILE:HG22	1.95	0.49
1:A:447:PHE:O	1:A:449:GLY:N	2.39	0.49
1:A:591:SER:OG	1:A:592:GLU:N	2.46	0.49
1:A:48:LYS:O	1:A:51:LYS:HB3	2.13	0.49
1:A:1191:HIS:CD2	1:A:1192:THR:H	2.31	0.49
1:A:62:ILE:O	1:A:147:GLN:NE2	2.45	0.49
1:A:567:LYS:HG3	1:A:570:GLU:OE1	2.13	0.49
1:A:1017:MET:HG2	4:A:2501:GTP:C2	2.48	0.49
1:A:583:ILE:HD11	1:A:652:ALA:C	2.38	0.48
1:A:930:ILE:HG13	1:A:931:GLY:N	2.28	0.48
1:A:980:LEU:CD1	1:A:1072:VAL:HB	2.43	0.48
1:A:521:ILE:O	1:A:553:GLY:N	2.36	0.48
1:A:534:GLU:O	1:A:536:GLN:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ASN:HB3	1:A:1210:ARG:HB3	1.95	0.48
1:A:930:ILE:HA	1:A:933:ILE:HG22	1.95	0.48
4:A:2501:GTP:C8	2:G:2008:C:C4	3.00	0.48
1:A:356:THR:CG2	1:A:359:ARG:H	2.20	0.48
1:A:1066:ARG:HH22	1:A:1078:THR:HG22	1.79	0.48
1:A:500:GLU:OE1	1:A:1210:ARG:NH2	2.46	0.48
1:A:1191:HIS:HB3	1:A:1251:THR:OG1	2.14	0.48
1:A:142:VAL:HG11	1:A:161:ALA:O	2.14	0.48
1:A:821:CYS:O	1:A:825:ALA:N	2.38	0.48
1:A:1037:VAL:O	1:A:1040:ILE:HG22	2.13	0.48
1:A:1050:VAL:HA	1:A:1055:ILE:HA	1.95	0.48
1:A:405:LEU:HB2	1:A:445:TYR:HE2	1.78	0.48
1:A:723:LEU:O	1:A:727:ILE:HG13	2.14	0.48
1:A:319:VAL:O	1:A:323:THR:OG1	2.31	0.47
1:A:460:LEU:HA	1:A:463:LEU:HD12	1.96	0.47
1:A:568:ARG:HH11	1:A:1199:GLU:CD	2.23	0.47
1:A:923:ASN:HB3	1:A:927:GLN:NE2	2.27	0.47
1:A:72:ILE:HD12	1:A:136:ALA:O	2.15	0.47
1:A:46:ALA:HA	1:A:49:ALA:HB3	1.96	0.47
1:A:956:HIS:O	1:A:959:SER:OG	2.27	0.47
1:A:977:SER:HB2	1:A:980:LEU:H	1.80	0.47
1:A:126:ILE:HG23	1:A:399:GLN:NE2	2.30	0.47
1:A:356:THR:HG22	1:A:359:ARG:N	2.22	0.47
1:A:1173:ASN:HB3	1:A:1176:ALA:HB2	1.97	0.47
1:A:272:PHE:HZ	1:A:313:THR:HG21	1.79	0.47
1:A:103:GLY:O	1:A:105:ILE:N	2.48	0.46
1:A:477:ALA:HA	1:A:480:LEU:HD23	1.97	0.46
1:A:377:ILE:CG2	1:A:671:GLY:HA2	2.44	0.46
1:A:585:PRO:HA	1:A:652:ALA:HA	1.97	0.46
1:A:361:TYR:CE1	1:A:480:LEU:HB3	2.50	0.46
1:A:459:ALA:O	1:A:463:LEU:HG	2.16	0.46
1:A:172:HIS:CE1	1:A:232:GLN:HG2	2.51	0.46
1:A:179:GLU:H	1:A:227:VAL:HG23	1.80	0.46
1:A:716:ARG:HE	1:A:716:ARG:HB2	1.63	0.46
1:A:919:GLU:HG3	1:A:1019:ASN:HA	1.98	0.46
1:A:301:THR:HG22	1:A:364:VAL:O	2.16	0.46
1:A:219:ARG:HH22	1:A:223:PHE:HB2	1.80	0.46
1:A:832:LEU:HG	1:A:941:TRP:NE1	2.30	0.46
1:A:933:ILE:O	1:A:937:ARG:HB2	2.16	0.46
1:A:1000:LYS:HE3	1:A:1010:THR:HG22	1.96	0.46
1:A:1018:GLY:N	4:A:2501:GTP:N2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:OE1	1:A:42:ARG:NH2	2.49	0.46
1:A:324:TYR:CE1	1:A:357:PRO:HD3	2.51	0.46
1:A:493:LYS:HD3	1:A:518:ARG:HD3	1.98	0.46
1:A:664:GLY:HA3	1:A:1260:ALA:HB3	1.97	0.46
1:A:980:LEU:HD13	1:A:1072:VAL:HB	1.97	0.46
1:A:202:ALA:HB1	1:A:207:LYS:HD2	1.98	0.46
1:A:377:ILE:HD12	1:A:592:GLU:O	2.16	0.46
1:A:440:GLU:O	1:A:444:GLN:HG3	2.16	0.46
1:A:719:VAL:HG21	1:A:723:LEU:HD13	1.98	0.46
1:A:1143:LYS:HA	1:A:1146:LYS:HE2	1.97	0.46
1:A:15:ARG:NH1	1:A:38:ILE:HD13	2.31	0.46
1:A:103:GLY:O	1:A:105:ILE:HG13	2.16	0.46
1:A:191:VAL:O	1:A:220:MET:HE1	2.16	0.46
1:A:503:PHE:CD1	1:A:1203:TYR:HD2	2.34	0.46
1:A:808:ASP:O	1:A:810:SER:N	2.49	0.46
1:A:34:ILE:O	1:A:38:ILE:HG23	2.17	0.45
1:A:237:GLU:C	1:A:239:SER:H	2.23	0.45
1:A:947:ASP:OD1	1:A:949:THR:HB	2.16	0.45
1:A:993:LEU:O	1:A:997:ARG:HB3	2.17	0.45
1:A:58:ALA:HA	1:A:265:ILE:HG21	1.98	0.45
1:A:219:ARG:NH2	1:A:223:PHE:HB2	2.32	0.45
1:A:416:ILE:HG23	1:A:453:PRO:HG2	1.97	0.45
1:A:647:LEU:H	1:A:647:LEU:HG	1.52	0.45
1:A:1122:ASN:OD1	1:A:1125:ARG:NH2	2.48	0.45
1:A:800:THR:O	1:A:804:LEU:HB2	2.17	0.45
1:A:948:GLN:HB2	1:A:1091:CYS:SG	2.57	0.45
1:A:1033:LEU:O	1:A:1037:VAL:HG23	2.15	0.45
1:A:143:LEU:HA	1:A:157:ALA:HA	1.97	0.45
1:A:228:SER:O	1:A:232:GLN:HB2	2.17	0.45
1:A:522:LYS:HA	1:A:552:GLU:HA	1.98	0.45
1:A:723:LEU:HD23	1:A:1110:ILE:CG1	2.46	0.45
1:A:848:PHE:HD2	1:A:867:PHE:CZ	2.34	0.45
1:A:3:GLU:HG2	1:A:426:ASP:OD2	2.16	0.45
1:A:372:TYR:HE1	1:A:410:VAL:HG21	1.77	0.45
1:A:476:LEU:O	1:A:480:LEU:HD22	2.17	0.45
1:A:1057:LEU:HD13	1:A:1065:LEU:HD22	1.99	0.45
4:A:2501:GTP:C4'	2:G:2008:C:H2'	2.47	0.45
1:A:487:PRO:O	1:A:489:ARG:N	2.50	0.45
1:A:715:THR:O	1:A:715:THR:HG22	2.17	0.45
1:A:573:ARG:NH2	1:A:619:THR:O	2.50	0.44
1:A:626:ILE:HD12	1:A:626:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:866:LYS:HA	1:A:871:GLN:HE21	1.82	0.44
1:A:1055:ILE:C	1:A:1056:ILE:HD12	2.42	0.44
1:A:1082:PHE:CD1	1:A:1087:PHE:HD1	2.36	0.44
1:A:1157:ILE:O	1:A:1167:VAL:HA	2.18	0.44
1:A:514:GLY:HA2	1:A:1210:ARG:NH2	2.32	0.44
1:A:927:GLN:HA	1:A:996:LEU:HD23	1.99	0.44
1:A:937:ARG:HD2	1:A:937:ARG:HA	1.86	0.44
1:A:182:LYS:HB2	1:A:185:ASP:OD2	2.17	0.44
1:A:184:GLU:OE1	1:A:184:GLU:N	2.50	0.44
1:A:734:ALA:HB1	1:A:1136:ARG:O	2.18	0.44
1:A:727:ILE:HG12	1:A:1144:TYR:CE2	2.53	0.44
1:A:612:ARG:HB3	1:A:1180:GLY:HA3	2.00	0.44
1:A:1082:PHE:CE1	1:A:1087:PHE:CD1	3.06	0.44
1:A:952:GLN:HB3	1:A:1091:CYS:HB2	1.99	0.44
1:A:1017:MET:HG2	4:A:2501:GTP:N3	2.33	0.44
1:A:120:VAL:HA	1:A:123:VAL:HG12	2.00	0.44
1:A:511:VAL:HB	1:A:562:LEU:HD23	1.99	0.44
1:A:579:LYS:HG3	1:A:580:PRO:HD2	1.99	0.44
1:A:796:GLU:O	1:A:799:LEU:N	2.50	0.44
1:A:949:THR:O	1:A:951:ASN:N	2.51	0.44
1:A:1178:ASN:OD1	1:A:1178:ASN:N	2.50	0.44
1:A:1179:ARG:HB2	1:A:1184:TYR:CD2	2.53	0.43
1:A:873:CYS:SG	1:A:874:THR:N	2.91	0.43
1:A:997:ARG:HD2	1:A:1014:ILE:O	2.19	0.43
1:A:355:ASP:OD1	1:A:360:HIS:ND1	2.40	0.43
1:A:369:HIS:CE1	1:A:406:LEU:HD23	2.53	0.43
1:A:1002:ARG:HG3	1:A:1008:VAL:HG12	2.00	0.43
1:A:304:HIS:CD2	1:A:305:VAL:N	2.87	0.43
1:A:1025:LEU:O	1:A:1029:ILE:HG12	2.18	0.43
4:A:2501:GTP:H5''	4:A:2501:GTP:O2B	2.18	0.43
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.85	0.43
1:A:726:SER:HG	1:A:1144:TYR:HH	1.58	0.43
1:A:833:ILE:HD13	1:A:833:ILE:HA	1.85	0.43
1:A:968:ASP:N	1:A:1081:THR:HG22	2.32	0.43
1:A:64:THR:HG22	1:A:73:ILE:HG13	2.01	0.43
1:A:205:SER:HB2	1:A:207:LYS:HG2	2.00	0.43
1:A:1005:ASP:C	1:A:1007:SER:H	2.26	0.43
1:A:500:GLU:CD	1:A:1210:ARG:HH22	2.26	0.43
1:A:574:GLY:HA3	1:A:620:THR:HG22	2.00	0.43
1:A:13:ARG:HH22	1:A:396:PRO:HD2	1.83	0.43
1:A:413:PRO:HB2	1:A:414:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1082:PHE:CE1	1:A:1087:PHE:HD1	2.37	0.43
1:A:229:LEU:HD12	1:A:229:LEU:HA	1.80	0.43
1:A:413:PRO:HB2	1:A:414:TYR:HD1	1.84	0.43
1:A:1048:VAL:HG22	1:A:1057:LEU:HB2	2.00	0.43
1:A:233:PRO:HA	1:A:241:THR:HA	2.01	0.42
1:A:1125:ARG:H	1:A:1125:ARG:HG3	1.66	0.42
1:A:35:GLU:O	1:A:39:GLU:HG2	2.18	0.42
1:A:86:ASP:CG	1:A:88:GLY:H	2.27	0.42
1:A:302:ILE:HG23	1:A:388:LEU:HD23	2.01	0.42
1:A:869:LEU:HA	1:A:870:PRO:HD2	1.76	0.42
1:A:906:VAL:HG23	1:A:907:PRO:HD2	2.00	0.42
1:A:126:ILE:HG22	1:A:127:GLY:N	2.33	0.42
1:A:368:GLY:O	1:A:372:TYR:N	2.52	0.42
1:A:728:ALA:O	1:A:732:LEU:HG	2.20	0.42
1:A:200:ASP:O	1:A:204:GLN:HB2	2.20	0.42
1:A:260:GLU:HG2	1:A:261:VAL:H	1.84	0.42
1:A:297:VAL:HG12	1:A:299:VAL:HG13	2.02	0.42
1:A:1156:THR:HA	1:A:1166:LEU:O	2.19	0.42
1:A:108:VAL:O	1:A:111:LEU:HD23	2.20	0.42
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.89	0.42
1:A:1019:ASN:HB3	1:A:1022:THR:OG1	2.20	0.42
1:A:1197:ARG:HD2	1:A:1202:SER:OG	2.20	0.42
1:A:495:PHE:CZ	1:A:521:ILE:HB	2.55	0.42
1:A:642:LYS:HB3	1:A:642:LYS:HE2	1.60	0.42
1:A:737:GLN:HG3	1:A:762:ILE:CG2	2.50	0.42
1:A:978:LEU:HA	1:A:978:LEU:HD23	1.80	0.42
1:A:1177:LYS:HD3	1:A:1177:LYS:HA	1.81	0.42
1:A:876:ARG:NH2	1:A:995:ASP:OD2	2.53	0.42
1:A:27:LEU:HA	1:A:30:ALA:HB3	2.02	0.42
1:A:503:PHE:CG	1:A:1203:TYR:HB2	2.55	0.42
1:A:902:LYS:HZ2	1:A:1002:ARG:HH12	1.67	0.42
1:A:1110:ILE:HD12	1:A:1115:ASP:HB2	2.02	0.42
1:A:260:GLU:HB3	1:A:263:GLU:CD	2.45	0.41
1:A:316:ILE:O	1:A:316:ILE:HG22	2.20	0.41
1:A:373:VAL:C	1:A:375:ASN:N	2.78	0.41
1:A:568:ARG:HH12	1:A:1197:ARG:HH11	1.68	0.41
1:A:181:ILE:HG23	1:A:185:ASP:OD1	2.20	0.41
1:A:405:LEU:O	1:A:409:GLN:HB2	2.20	0.41
1:A:568:ARG:NH1	1:A:1197:ARG:HH11	2.18	0.41
1:A:870:PRO:HB3	1:A:893:ARG:HB3	2.02	0.41
1:A:169:ILE:O	1:A:173:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLN:NE2	1:A:399:GLN:H	2.19	0.41
1:A:603:ARG:H	1:A:603:ARG:HG3	1.42	0.41
1:A:374:LYS:HG3	1:A:594:TYR:CE1	2.55	0.41
1:A:453:PRO:C	1:A:454:ILE:HG12	2.44	0.41
1:A:1028:LEU:O	1:A:1032:SER:HB2	2.20	0.41
1:A:35:GLU:O	1:A:38:ILE:HG12	2.20	0.41
1:A:73:ILE:HB	1:A:155:LEU:HD23	2.01	0.41
1:A:111:LEU:HA	1:A:114:GLN:HB3	2.02	0.41
1:A:166:VAL:HA	1:A:169:ILE:HG13	2.02	0.41
1:A:10:LYS:HG3	1:A:11:GLU:N	2.36	0.41
1:A:82:PHE:O	1:A:402:GLU:HG3	2.20	0.41
1:A:266:GLU:HB3	1:A:267:LYS:H	1.53	0.41
1:A:545:MET:HE3	1:A:545:MET:HB2	1.99	0.41
1:A:737:GLN:HG3	1:A:762:ILE:HG21	2.03	0.41
3:T:2103:G:H2'	3:T:2104:U:O4'	2.20	0.41
1:A:730:ASP:OD2	1:A:1143:LYS:NZ	2.52	0.41
1:A:855:THR:OG1	1:A:871:GLN:OE1	2.30	0.41
1:A:74:LEU:HB2	1:A:97:LEU:HD23	2.02	0.41
1:A:245:LEU:O	1:A:245:LEU:HD22	2.20	0.41
1:A:550:LEU:H	1:A:550:LEU:CD1	2.30	0.41
1:A:710:ARG:NH1	1:A:1253:LYS:HD3	2.36	0.41
1:A:731:LEU:O	1:A:734:ALA:HB3	2.21	0.41
1:A:749:PHE:HD1	1:A:767:ALA:HB2	1.85	0.41
1:A:760:PHE:O	1:A:761:ARG:C	2.63	0.41
1:A:870:PRO:HA	1:A:893:ARG:HB2	2.02	0.41
1:A:75:GLU:HG3	1:A:133:ARG:HE	1.86	0.41
1:A:731:LEU:HD13	1:A:1140:VAL:HG21	2.03	0.41
1:A:903:ALA:O	1:A:1004:PRO:HD3	2.21	0.41
1:A:1021:TYR:CD1	1:A:1021:TYR:C	2.99	0.41
1:A:203:MET:HE3	1:A:207:LYS:O	2.20	0.40
1:A:719:VAL:HG12	1:A:721:GLY:H	1.86	0.40
1:A:1000:LYS:HB3	1:A:1000:LYS:HE2	1.89	0.40
1:A:13:ARG:O	1:A:17:GLY:N	2.54	0.40
1:A:356:THR:HG23	1:A:357:PRO:HD2	2.04	0.40
1:A:792:ALA:C	1:A:794:GLU:N	2.78	0.40
1:A:874:THR:OG1	1:A:899:PRO:HA	2.21	0.40
1:A:991:GLU:O	1:A:994:MET:N	2.55	0.40
1:A:1060:CYS:O	1:A:1063:PRO:HD2	2.21	0.40
1:A:245:LEU:O	1:A:249:HIS:HB2	2.21	0.40
1:A:263:GLU:C	1:A:265:ILE:H	2.29	0.40
1:A:449:GLY:O	1:A:452:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PRO:HB2	1:A:479:PHE:CD2	2.56	0.40
1:A:496:LEU:HD13	1:A:578:ALA:HB2	2.04	0.40
1:A:154:VAL:HG12	1:A:258:ARG:CB	2.51	0.40
1:A:587:THR:HA	1:A:647:LEU:HD11	2.03	0.40
1:A:591:SER:HB2	1:A:673:VAL:HA	2.03	0.40
1:A:596:LEU:HD12	1:A:600:GLU:HB3	2.02	0.40
1:A:1013:LYS:HB3	1:A:1013:LYS:HE2	1.81	0.40
1:A:1079:LYS:HA	1:A:1079:LYS:HD3	1.79	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	1193/1289 (93%)	995 (83%)	152 (13%)	46 (4%)	2 18

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	129	ASN
1	A	209	LYS
1	A	324	TYR
1	A	464	GLU
1	A	488	GLU
1	A	535	THR
1	A	777	SER
1	A	809	TYR
1	A	53	ALA
1	A	104	LYS
1	A	141	ASP
1	A	265	ILE

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Mol	Chain	Res	Type
1	A	266	GLU
1	A	374	LYS
1	A	641	ILE
1	A	801	ASN
1	A	895	SER
1	A	921	GLY
1	A	950	ILE
1	A	1107	ARG
1	A	1263	SER
1	A	68	GLY
1	A	208	PRO
1	A	323	THR
1	A	413	PRO
1	A	771	SER
1	A	779	GLY
1	A	863	PRO
1	A	465	GLY
1	A	724	ALA
1	A	780	ILE
1	A	793	ALA
1	A	813	PHE
1	A	150	ALA
1	A	188	ALA
1	A	448	PRO
1	A	879	LYS
1	A	1111	VAL
1	A	531	GLY
1	A	875	PRO
1	A	367	PRO
1	A	650	PRO
1	A	566	ILE
1	A	916	ILE
1	A	920	PRO

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	995/1060 (94%)	828 (83%)	167 (17%)	2 11

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	33	ASP
1	A	38	ILE
1	A	41	MET
1	A	52	LYS
1	A	56	VAL
1	A	59	ASP
1	A	66	ILE
1	A	72	ILE
1	A	75	GLU
1	A	76	VAL
1	A	79	GLN
1	A	86	ASP
1	A	108	VAL
1	A	117	GLU
1	A	130	ILE
1	A	132	ILE
1	A	139	GLU
1	A	141	ASP
1	A	143	LEU
1	A	165	LEU
1	A	166	VAL
1	A	181	ILE
1	A	197	VAL
1	A	203	MET
1	A	207	LYS
1	A	210	GLU
1	A	221	LYS
1	A	232	GLN
1	A	235	VAL
1	A	239	SER
1	A	241	THR
1	A	245	LEU
1	A	249	HIS
1	A	256	PHE
1	A	258	ARG
1	A	265	ILE
1	A	266	GLU

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Mol	Chain	Res	Type
1	A	279	MET
1	A	302	ILE
1	A	305	VAL
1	A	306	ASP
1	A	313	THR
1	A	323	THR
1	A	349	THR
1	A	353	GLU
1	A	356	THR
1	A	387	ILE
1	A	388	LEU
1	A	390	VAL
1	A	397	MET
1	A	399	GLN
1	A	406	LEU
1	A	419	LEU
1	A	429	GLU
1	A	433	LEU
1	A	434	VAL
1	A	441	LEU
1	A	454	ILE
1	A	460	LEU
1	A	480	LEU
1	A	502	VAL
1	A	516	VAL
1	A	530	VAL
1	A	535	THR
1	A	537	LYS
1	A	539	THR
1	A	541	THR
1	A	543	VAL
1	A	547	ARG
1	A	550	LEU
1	A	567	LYS
1	A	568	ARG
1	A	569	GLU
1	A	576	VAL
1	A	583	ILE
1	A	587	THR
1	A	599	ASP
1	A	603	ARG
1	A	622	VAL

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Mol	Chain	Res	Type
1	A	627	GLU
1	A	628	LEU
1	A	642	LYS
1	A	646	THR
1	A	647	LEU
1	A	654	ASP
1	A	663	GLU
1	A	667	THR
1	A	672	VAL
1	A	673	VAL
1	A	705	LEU
1	A	706	SER
1	A	710	ARG
1	A	715	THR
1	A	718	GLU
1	A	719	VAL
1	A	733	LEU
1	A	756	THR
1	A	762	ILE
1	A	769	ILE
1	A	771	SER
1	A	774	ASP
1	A	789	LYS
1	A	800	THR
1	A	809	TYR
1	A	832	LEU
1	A	833	ILE
1	A	835	ASP
1	A	836	VAL
1	A	843	LEU
1	A	848	PHE
1	A	855	THR
1	A	874	THR
1	A	881	VAL
1	A	891	ASP
1	A	894	ILE
1	A	897	ILE
1	A	901	ASN
1	A	906	VAL
1	A	916	ILE
1	A	930	ILE
1	A	934	LEU

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Mol	Chain	Res	Type
1	A	936	ASP
1	A	937	ARG
1	A	939	ARG
1	A	946	ASN
1	A	960	VAL
1	A	967	VAL
1	A	970	SER
1	A	973	SER
1	A	980	LEU
1	A	984	LEU
1	A	993	LEU
1	A	1008	VAL
1	A	1012	GLU
1	A	1014	ILE
1	A	1028	LEU
1	A	1041	LEU
1	A	1043	LEU
1	A	1044	ASP
1	A	1048	VAL
1	A	1053	ASP
1	A	1055	ILE
1	A	1074	PHE
1	A	1076	THR
1	A	1080	LYS
1	A	1089	GLU
1	A	1093	LYS
1	A	1099	VAL
1	A	1108	HIS
1	A	1110	ILE
1	A	1116	LEU
1	A	1123	LEU
1	A	1128	THR
1	A	1136	ARG
1	A	1138	HIS
1	A	1145	ARG
1	A	1150	LYS
1	A	1172	ILE
1	A	1178	ASN
1	A	1182	ILE
1	A	1185	VAL
1	A	1193	ARG
1	A	1204	LEU

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Mol	Chain	Res	Type
1	A	1212	LEU
1	A	1235	ILE
1	A	1259	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	55	ASN
1	A	148	HIS
1	A	196	GLN
1	A	369	HIS
1	A	737	GLN
1	A	763	ASN
1	A	814	ASN
1	A	901	ASN
1	A	951	ASN
1	A	952	GLN
1	A	963	ASN
1	A	1108	HIS
1	A	1191	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	4/8 (50%)	1 (25%)	0
3	T	5/8 (62%)	2 (40%)	0
All	All	9/16 (56%)	3 (33%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2004	U
3	T	2103	G
3	T	2105	A

There are no RNA pucker outliers to report.

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GTP	A	2501	5	33,34,34	1.66	5 (15%)	50,54,54	1.78	11 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	2501	5	-	8/22/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2501	GTP	PB-O3B	5.28	1.65	1.59
4	A	2501	GTP	PA-O3A	4.79	1.64	1.59
4	A	2501	GTP	PB-O3A	3.62	1.63	1.59
4	A	2501	GTP	C5-N7	-2.30	1.34	1.39
4	A	2501	GTP	C5-C4	2.09	1.44	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2501	GTP	C5-C4-N3	-5.03	120.38	128.39
4	A	2501	GTP	C2-N3-C4	4.63	120.27	112.30
4	A	2501	GTP	O3A-PA-O1A	3.16	120.21	110.70
4	A	2501	GTP	N9-C4-N3	3.05	132.05	125.95
4	A	2501	GTP	C2'-C1'-N9	-3.01	104.86	113.25
4	A	2501	GTP	O2B-PB-O3B	2.94	115.22	107.27
4	A	2501	GTP	C6-C5-N7	2.52	134.88	130.29
4	A	2501	GTP	C4-C5-N7	-2.52	106.68	110.67
4	A	2501	GTP	N2-C2-N1	2.48	122.00	116.76
4	A	2501	GTP	O6-C6-C5	-2.29	120.47	126.53
4	A	2501	GTP	C8-N7-C5	2.03	107.87	104.26

There are no chirality outliers.

All (8) torsion outliers are listed below:

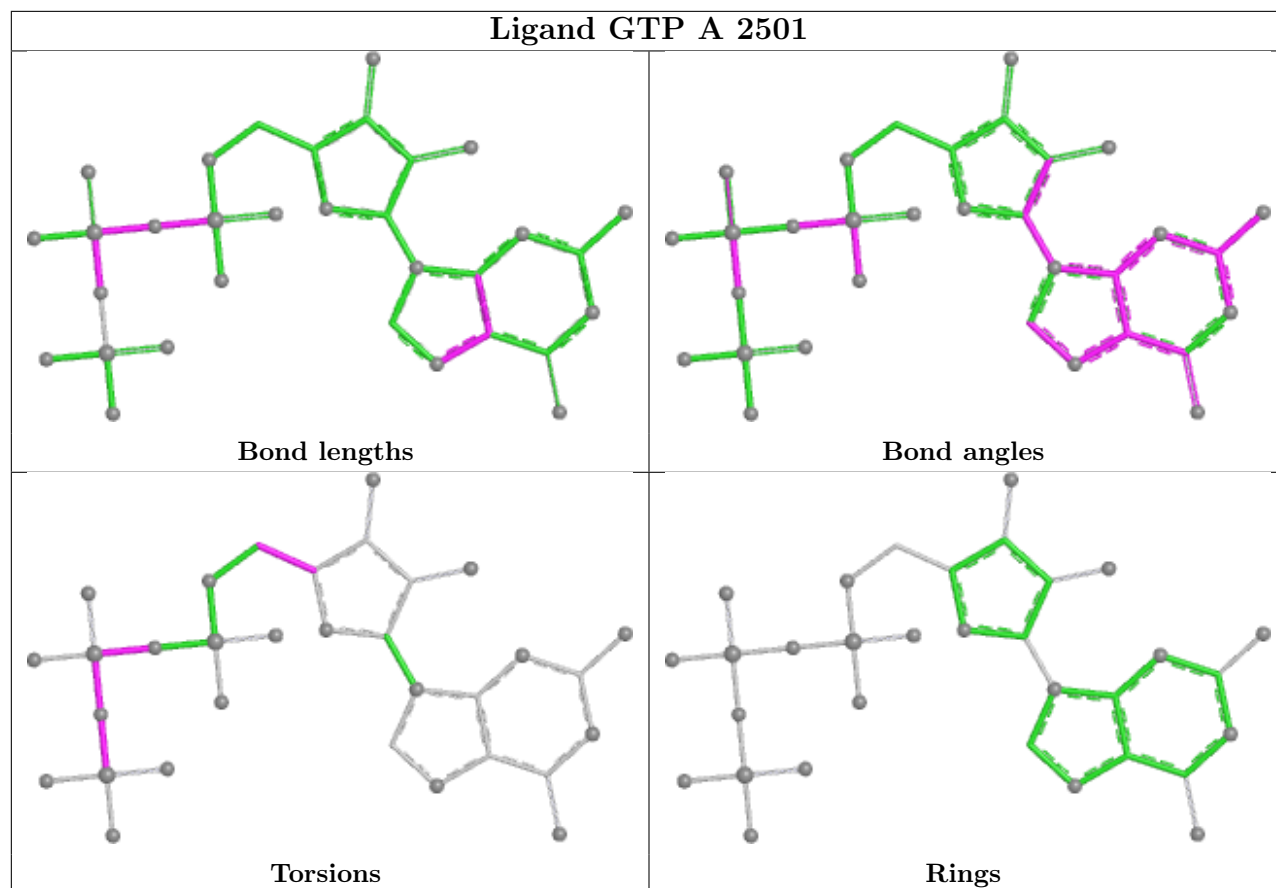
Mol	Chain	Res	Type	Atoms
4	A	2501	GTP	O4'-C4'-C5'-O5'
4	A	2501	GTP	C3'-C4'-C5'-O5'
4	A	2501	GTP	PB-O3B-PG-O1G
4	A	2501	GTP	PA-O3A-PB-O1B
4	A	2501	GTP	PB-O3B-PG-O2G
4	A	2501	GTP	PB-O3B-PG-O3G
4	A	2501	GTP	PG-O3B-PB-O2B
4	A	2501	GTP	PG-O3B-PB-O3A

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2501	GTP	11	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1203/1289 (93%)	-0.49	4 (0%) 90 81	46, 94, 142, 200	0
2	G	7/8 (87%)	1.11	1 (14%) 6 5	139, 187, 216, 222	0
3	T	6/8 (75%)	-0.13	0 100 100	126, 164, 171, 181	0
All	All	1216/1305 (93%)	-0.47	5 (0%) 88 79	46, 94, 145, 222	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	2007	C	3.4
1	A	161	ALA	2.4
1	A	16	THR	2.3
1	A	8	LEU	2.0
1	A	189	GLU	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](#)

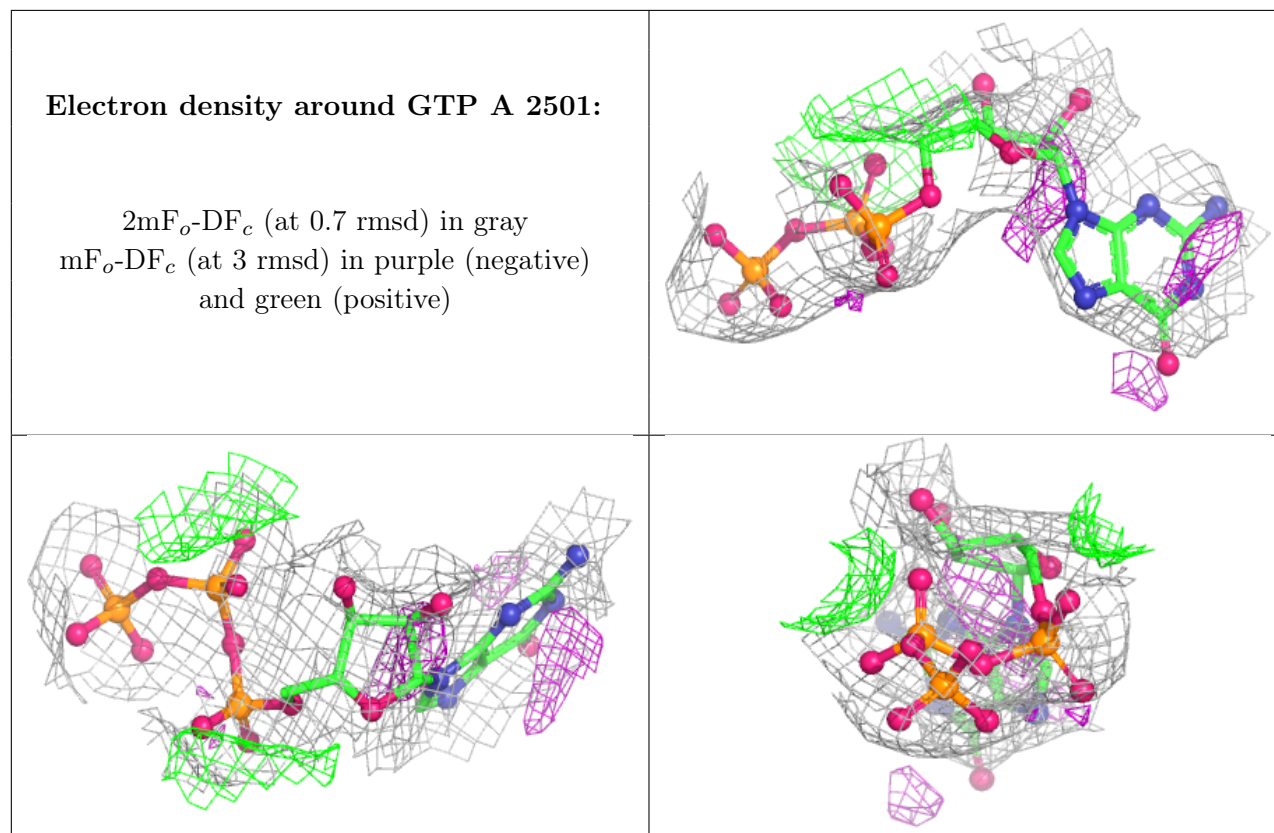
There are no oligosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GTP	A	2501	32/32	0.88	0.09	96,111,122,126	0
5	CA	A	2502	1/1	0.97	0.04	86,86,86,86	0
5	CA	A	2503	1/1	0.99	0.14	67,67,67,67	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.