Full wwPDB X-ray Structure Validation Report (i)

Feb 10, 2024 – 07:30 PM EST

PDB ID	:	2R7W
Title	:	Crystal Structure of Rotavirus SA11 VP1/RNA (UGUGACC)/mRNA 5'-CAP (m7GpppG) complex
Authors	:	Lu, X.; Harrison, S.C.; Tao, Y.J.; Patton, J.T.; Nibert, M.L.
Deposited on	:	2007-09-10
Resolution	:	2.60 Å(reported)

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

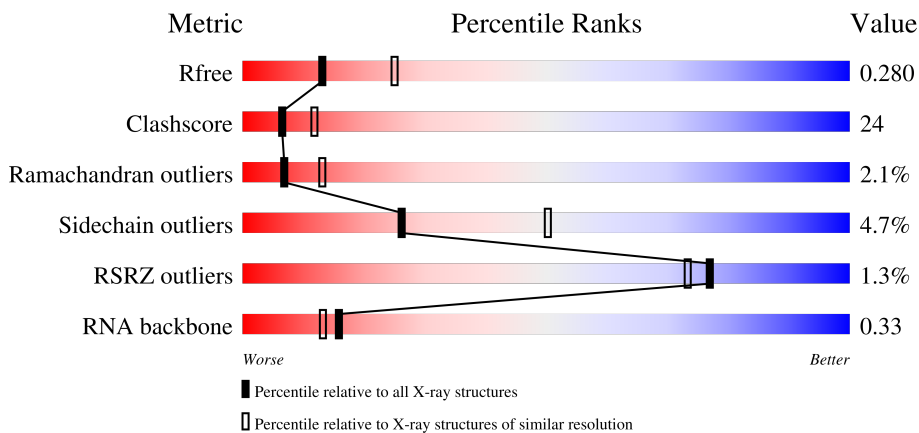|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.60 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	Percentile Ranks	Value
Rfree		0.280
Clashscore		24
Ramachandran outliers		2.1%
Sidechain outliers		4.7%
RSRZ outliers		1.3%
RNA backbone		0.33

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	7	29% 71%
2	A	1095	.% 56% 38% · ·

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GTP	A	1201	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8876 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 RNA chain called RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	7	Total 145	C 66	N 25	O 48	P 6	0	0	0

- Molecule 2 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	1073	Total 8699	C 5579	N 1448	O 1634	S 38	0	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).
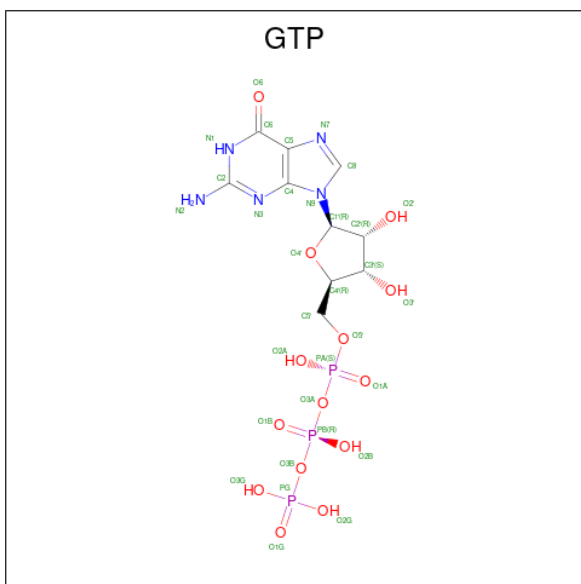
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 5	O 14	P 3	0	0

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.
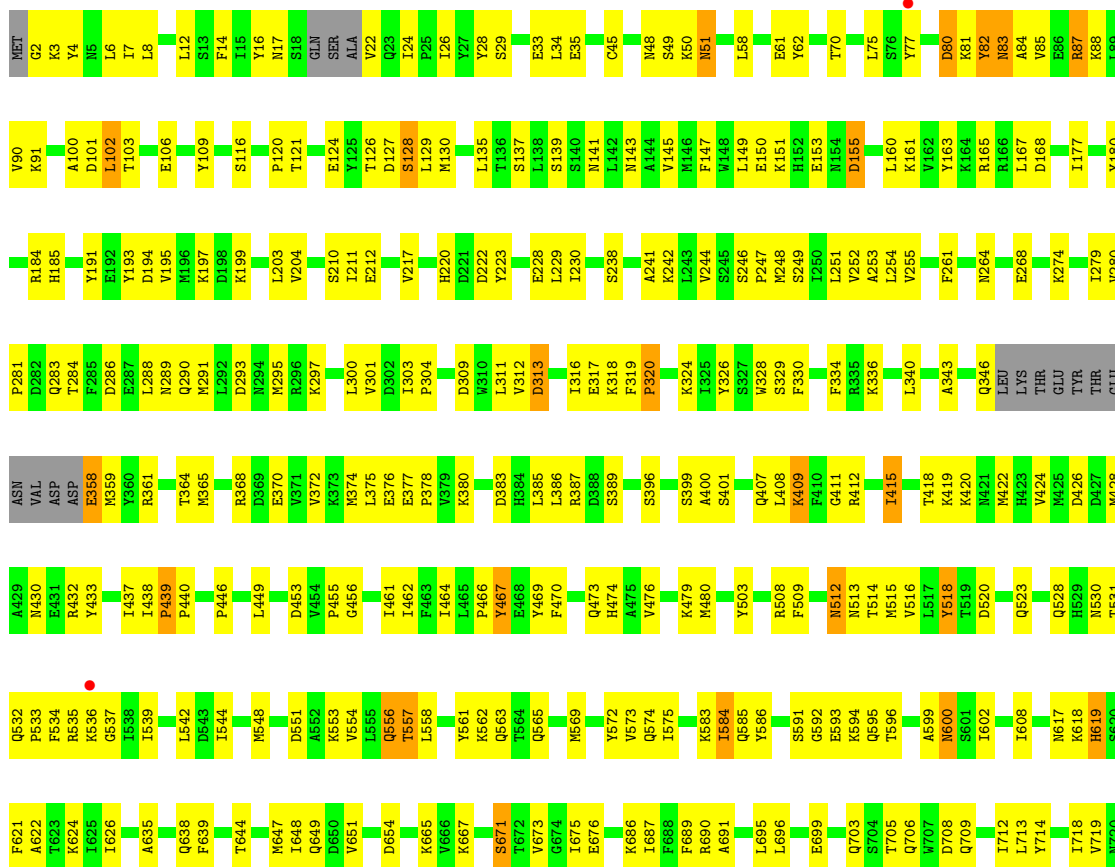
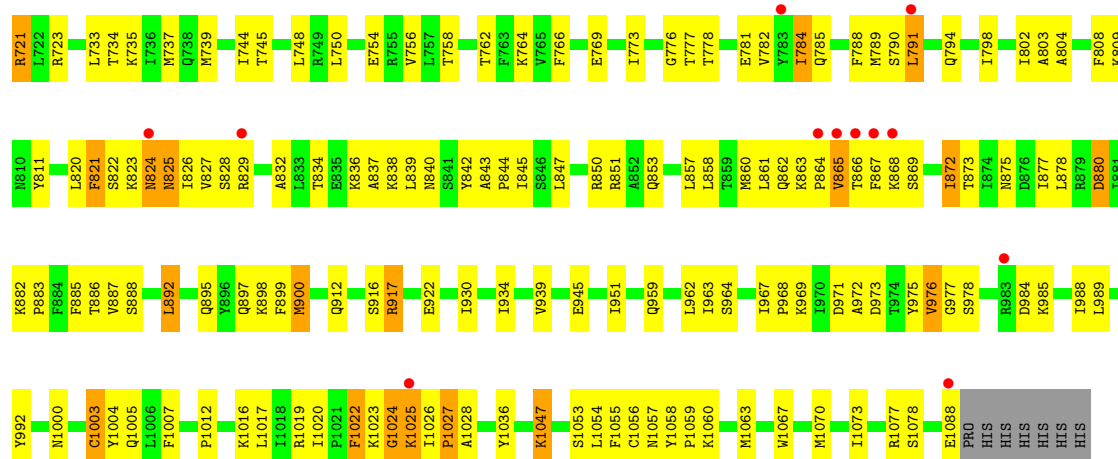- Molecule 1: RNA (5'-R(*UP*GP*UP*GP*AP*CP*C)-3')

Chain X:
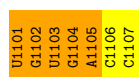
- Molecule 2: RNA-dependent RNA polymerase

Chain A:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	76.35Å　　112.75Å　　143.79Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	50.00　–　2.60 40.59　–　2.60	Depositor EDS
% Data completeness (in resolution range)	84.5 (50.00-2.60) 84.5 (40.59-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241　,　0.290 0.230　,　0.280	Depositor DCC
R_{free} test set	3030 reflections (7.88%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.2	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8876	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	X	0.52	0/161	0.91	0/249
2	A	0.45	1/8870 (0.0%)	0.62	0/11989
All	All	0.45	1/9031 (0.0%)	0.63	0/12238

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	CYS	CB-SG	-6.15	1.71	1.82

There are no bond angle outliers.

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	X	145	0	77	17	0
2	A	8699	0	8793	413	0
3	A	32	0	12	25	0
All	All	8876	0	8882	423	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 24.

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PROTEIN DATA BANK

All (423) 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:A:82:TYR:CD2	3:A:1201:GTP:H3'	1.42	1.53
2:A:82:TYR:CB	3:A:1201:GTP:H5'	1.00	1.48
2:A:82:TYR:CB	3:A:1201:GTP:C5'	1.97	1.40
2:A:82:TYR:HB2	3:A:1201:GTP:C5'	1.58	1.24
2:A:185:HIS:CE1	3:A:1201:GTP:O1A	1.94	1.19
2:A:82:TYR:HB3	3:A:1201:GTP:C5'	1.67	1.16
2:A:82:TYR:HD2	3:A:1201:GTP:C3'	1.60	1.14
2:A:82:TYR:CD2	3:A:1201:GTP:C3'	2.30	1.13
2:A:520:ASP:HB3	2:A:667:LYS:HG2	1.36	1.08
2:A:385:LEU:HD23	2:A:479:LYS:HE2	1.37	1.06
2:A:82:TYR:CG	3:A:1201:GTP:H3'	1.95	1.00
2:A:101:ASP:OD1	2:A:103:THR:HG22	1.62	0.99
2:A:82:TYR:HB3	3:A:1201:GTP:H5'	1.01	0.98
2:A:82:TYR:CG	3:A:1201:GTP:H5'	2.00	0.97
2:A:185:HIS:HE1	3:A:1201:GTP:O1A	1.41	0.97
2:A:865:VAL:HG22	2:A:866:THR:H	1.27	0.97
2:A:556:GLN:HA	2:A:556:GLN:HE21	1.29	0.93
2:A:82:TYR:HB3	3:A:1201:GTP:C3'	1.99	0.92
2:A:866:THR:HG22	2:A:867:PHE:H	1.35	0.91
1:X:1105:A:H5'	2:A:400:ALA:HB1	1.54	0.90
2:A:82:TYR:HB3	3:A:1201:GTP:C4'	2.01	0.90
2:A:824:ASN:ND2	2:A:827:VAL:HB	1.90	0.86
2:A:503:TYR:HB2	2:A:687:ILE:HD13	1.59	0.85
2:A:283:GLN:OE1	2:A:649:GLN:HG3	1.77	0.84
2:A:24:ILE:HB	2:A:75:LEU:HB2	1.60	0.83
2:A:82:TYR:HA	3:A:1201:GTP:C2	2.14	0.82
2:A:82:TYR:HB2	3:A:1201:GTP:H5'	0.82	0.81
2:A:892:LEU:HD22	2:A:1017:LEU:HD11	1.64	0.80
2:A:438:ILE:HD12	2:A:563:GLN:HB3	1.62	0.80
2:A:254:LEU:HD23	2:A:280:VAL:HG21	1.64	0.78
2:A:865:VAL:HG22	2:A:866:THR:N	1.98	0.78
2:A:248:MET:HE3	2:A:248:MET:O	1.84	0.77
2:A:161:LYS:O	2:A:165:ARG:HG3	1.85	0.77
2:A:708:ASP:O	2:A:712:ILE:HG13	1.84	0.77
2:A:87:ARG:O	2:A:90:VAL:HG22	1.86	0.76
2:A:82:TYR:HB3	3:A:1201:GTP:H3'	1.64	0.76
2:A:82:TYR:HA	3:A:1201:GTP:N3	2.00	0.75
2:A:386:LEU:O	2:A:557:THR:HG21	1.86	0.75
2:A:82:TYR:CB	3:A:1201:GTP:H3'	2.15	0.75
2:A:446:PRO:HG2	2:A:583:LYS:HD3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:945:GLU:HG2	2:A:992:TYR:HE1	1.52	0.74
2:A:84:ALA:HB1	2:A:88:LYS:NZ	2.03	0.73
2:A:217:VAL:HG13	2:A:222:ASP:HB2	1.70	0.73
2:A:866:THR:HG22	2:A:867:PHE:N	2.04	0.73
2:A:286:ASP:O	2:A:290:GLN:HG3	1.88	0.73
2:A:820:LEU:H	2:A:820:LEU:HD23	1.52	0.73
2:A:824:ASN:HD21	2:A:827:VAL:HB	1.51	0.73
2:A:461:ILE:HD11	2:A:586:TYR:CZ	2.24	0.73
2:A:573:VAL:HG12	2:A:575:ILE:HG13	1.68	0.73
1:X:1105:A:H5'	2:A:400:ALA:CB	2.18	0.72
2:A:622:ALA:HB3	2:A:638:GLN:HB3	1.72	0.72
2:A:520:ASP:CB	2:A:667:LYS:HG2	2.17	0.71
2:A:777:THR:HG21	2:A:882:LYS:HE3	1.70	0.71
2:A:878:LEU:HD22	2:A:1036:TYR:HD1	1.54	0.71
2:A:50:LYS:HG2	2:A:50:LYS:O	1.92	0.70
2:A:823:LYS:HE3	2:A:825:ASN:HD22	1.57	0.69
2:A:553:LYS:O	2:A:557:THR:HG22	1.93	0.69
2:A:618:LYS:HD2	2:A:654:ASP:OD2	1.93	0.69
2:A:744:ILE:HD13	2:A:748:LEU:HD22	1.75	0.69
2:A:804:ALA:HA	2:A:809:LYS:HE3	1.74	0.69
2:A:1019:ARG:HD2	2:A:1053:SER:OG	1.93	0.69
2:A:343:ALA:O	2:A:346:GLN:HG3	1.92	0.69
2:A:473:GLN:HG2	2:A:561:TYR:CE1	2.28	0.68
2:A:1059:PRO:O	2:A:1063:MET:HG3	1.93	0.68
2:A:102:LEU:HD22	2:A:102:LEU:H	1.57	0.68
2:A:972:ALA:O	2:A:976:VAL:HG23	1.93	0.68
2:A:324:LYS:O	2:A:328:TRP:HD1	1.78	0.67
1:X:1105:A:C5'	2:A:400:ALA:HB1	2.25	0.67
2:A:820:LEU:HB2	2:A:964:SER:O	1.93	0.67
2:A:419:LYS:HB2	2:A:422:MET:HG3	1.78	0.66
2:A:851:ARG:HH11	2:A:851:ARG:HG2	1.60	0.66
2:A:177:ILE:HD13	2:A:203:LEU:HD11	1.77	0.66
2:A:886:THR:OG1	2:A:1055:PHE:HB3	1.95	0.66
2:A:975:TYR:O	2:A:977:GLY:N	2.29	0.66
2:A:309:ASP:O	2:A:312:VAL:HG22	1.96	0.65
2:A:778:THR:O	2:A:782:VAL:HG23	1.96	0.65
2:A:82:TYR:HD2	3:A:1201:GTP:H3'	0.87	0.65
2:A:882:LYS:HB3	2:A:883:PRO:HD3	1.77	0.65
2:A:253:ALA:HB1	2:A:671:SER:HB2	1.79	0.65
2:A:885:PHE:CE1	2:A:1056:CYS:HB2	2.31	0.65
2:A:377:GLU:HB2	2:A:378:PRO:HD3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:212:GLU:HB2	2:A:696:LEU:HD12	1.79	0.65
2:A:385:LEU:HD23	2:A:479:LYS:CE	2.19	0.64
2:A:120:PRO:HD2	2:A:124:GLU:OE2	1.98	0.64
2:A:824:ASN:OD1	2:A:828:SER:HB2	1.97	0.64
2:A:528:GLN:O	2:A:531:THR:HG22	1.98	0.64
1:X:1104:G:H5'	2:A:401:SER:HB2	1.80	0.64
2:A:191:TYR:CE2	2:A:204:VAL:HG11	2.32	0.64
2:A:667:LYS:HG3	2:A:667:LYS:O	1.98	0.64
2:A:976:VAL:O	2:A:976:VAL:HG12	1.98	0.63
2:A:3:LYS:HA	2:A:6:LEU:HD23	1.80	0.63
2:A:789:MET:HE1	2:A:873:THR:HG21	1.80	0.63
2:A:165:ARG:HE	2:A:220:HIS:HA	1.63	0.62
2:A:865:VAL:CG2	2:A:866:THR:H	2.05	0.62
2:A:346:GLN:HG2	2:A:586:TYR:CE1	2.35	0.62
2:A:644:THR:OG1	2:A:647:MET:HG3	2.00	0.62
2:A:8:LEU:HD13	2:A:737:MET:HG2	1.82	0.62
2:A:264:ASN:HD21	2:A:268:GLU:HG3	1.65	0.61
2:A:180:TYR:HB3	2:A:199:LYS:HG3	1.82	0.61
2:A:781:GLU:O	2:A:785:GLN:HG3	2.00	0.61
2:A:556:GLN:HE21	2:A:556:GLN:CA	2.06	0.61
2:A:821:PHE:N	2:A:821:PHE:CD2	2.68	0.61
2:A:84:ALA:HB1	2:A:88:LYS:HZ1	1.65	0.60
2:A:897:GLN:N	2:A:897:GLN:OE1	2.34	0.60
2:A:165:ARG:NE	2:A:220:HIS:HA	2.15	0.60
2:A:608:ILE:HD13	2:A:626:ILE:HG23	1.83	0.60
2:A:1023:LYS:O	2:A:1060:LYS:HG2	2.02	0.60
2:A:530:ASN:O	2:A:533:PRO:HD2	2.02	0.59
2:A:823:LYS:HE3	2:A:825:ASN:ND2	2.18	0.59
2:A:185:HIS:NE2	3:A:1201:GTP:O1A	2.33	0.59
2:A:558:LEU:O	2:A:558:LEU:HD23	2.03	0.58
2:A:135:LEU:HD22	2:A:709:GLN:NE2	2.19	0.58
2:A:312:VAL:HG23	2:A:313:ASP:OD2	2.04	0.58
2:A:518:TYR:H	2:A:518:TYR:HD2	1.48	0.58
1:X:1106:C:H2'	1:X:1107:C:O4'	2.04	0.58
2:A:1024:GLY:O	2:A:1025:LYS:CB	2.51	0.58
2:A:210:SER:OG	2:A:230:ILE:HG23	2.04	0.58
2:A:438:ILE:CD1	2:A:563:GLN:HB3	2.33	0.58
2:A:719:VAL:HG12	2:A:723:ARG:HD2	1.86	0.58
2:A:473:GLN:HE21	2:A:594:LYS:HB3	1.69	0.58
2:A:794:GLN:HG2	2:A:853:GLN:OE1	2.03	0.58
2:A:1023:LYS:HD2	2:A:1058:TYR:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:967:ILE:HD12	2:A:967:ILE:N	2.18	0.57
2:A:83:ASN:O	2:A:85:VAL:N	2.34	0.57
2:A:82:TYR:CG	3:A:1201:GTP:C5'	2.75	0.57
2:A:312:VAL:HG23	2:A:313:ASP:N	2.20	0.57
2:A:744:ILE:HD13	2:A:748:LEU:CD2	2.34	0.57
1:X:1103:U:O2'	1:X:1104:G:P	2.63	0.57
2:A:744:ILE:HD11	2:A:750:LEU:HB2	1.87	0.57
2:A:385:LEU:CD2	2:A:479:LYS:HE2	2.24	0.57
2:A:821:PHE:N	2:A:821:PHE:HD2	2.03	0.56
2:A:80:ASP:O	2:A:81:LYS:HG3	2.05	0.56
2:A:279:ILE:HG22	2:A:648:ILE:HD12	1.85	0.56
2:A:516:VAL:HG21	2:A:675:ILE:CG2	2.35	0.56
2:A:193:TYR:CE2	2:A:197:LYS:HD2	2.40	0.56
2:A:368:ARG:O	2:A:372:VAL:HG23	2.05	0.56
2:A:794:GLN:HG2	2:A:853:GLN:CD	2.26	0.56
2:A:82:TYR:HA	3:A:1201:GTP:C4	2.41	0.56
2:A:514:THR:HG22	2:A:638:GLN:HA	1.87	0.56
2:A:82:TYR:HE1	2:A:184:ARG:HD2	1.70	0.56
2:A:984:ASP:O	2:A:988:ILE:HG12	2.06	0.56
2:A:532:GLN:HG3	2:A:536:LYS:HE3	1.88	0.56
2:A:1000:ASN:O	2:A:1005:GLN:HB3	2.06	0.56
2:A:647:MET:O	2:A:651:VAL:HG23	2.05	0.55
2:A:824:ASN:CG	2:A:828:SER:HB2	2.27	0.55
2:A:798:ILE:O	2:A:802:ILE:HG22	2.06	0.55
2:A:88:LYS:HA	2:A:91:LYS:HE2	1.88	0.55
2:A:313:ASP:OD2	2:A:313:ASP:N	2.38	0.55
2:A:318:LYS:HB2	2:A:318:LYS:NZ	2.22	0.55
2:A:470:PHE:HE1	2:A:594:LYS:HD3	1.71	0.55
2:A:261:PHE:CD2	2:A:899:PHE:HB3	2.42	0.55
2:A:857:LEU:O	2:A:861:LEU:HD13	2.06	0.55
2:A:866:THR:CG2	2:A:867:PHE:H	2.13	0.55
2:A:851:ARG:HG2	2:A:851:ARG:NH1	2.22	0.55
2:A:14:PHE:CE2	2:A:147:PHE:HB2	2.41	0.55
2:A:244:VAL:CG1	2:A:329:SER:HB3	2.36	0.55
2:A:383:ASP:O	2:A:387:ARG:HG3	2.07	0.54
2:A:261:PHE:HD2	2:A:899:PHE:HB3	1.71	0.54
2:A:776:GLY:HA3	2:A:785:GLN:NE2	2.22	0.54
2:A:1020:ILE:O	2:A:1020:ILE:HG22	2.08	0.54
2:A:428:MET:HE1	2:A:811:TYR:HD1	1.72	0.54
2:A:721:ARG:HH11	2:A:721:ARG:CG	2.20	0.54
2:A:85:VAL:HG21	2:A:139:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:VAL:C	2:A:304:PRO:HD2	2.27	0.54
2:A:784:ILE:HG23	2:A:788:PHE:CE2	2.43	0.54
2:A:217:VAL:HG13	2:A:222:ASP:CB	2.36	0.54
2:A:721:ARG:HH11	2:A:721:ARG:HG3	1.72	0.53
2:A:100:ALA:O	2:A:102:LEU:HD22	2.09	0.53
2:A:407:GLN:O	2:A:408:LEU:HD23	2.08	0.53
2:A:361:ARG:O	2:A:365:MET:HG2	2.08	0.53
2:A:470:PHE:CE1	2:A:594:LYS:HD3	2.44	0.53
2:A:518:TYR:CD2	2:A:518:TYR:N	2.76	0.53
1:X:1103:U:O2'	1:X:1104:G:H5"	2.08	0.53
2:A:735:LYS:O	2:A:739:MET:HG3	2.08	0.53
2:A:6:LEU:N	2:A:6:LEU:HD22	2.24	0.53
2:A:150:GLU:O	2:A:153:GLU:HB2	2.09	0.53
2:A:803:ALA:HA	2:A:808:PHE:CD2	2.43	0.53
2:A:58:LEU:N	2:A:58:LEU:HD22	2.23	0.53
2:A:102:LEU:HD22	2:A:102:LEU:N	2.24	0.53
2:A:843:ALA:HB3	2:A:844:PRO:HD3	1.91	0.53
2:A:135:LEU:HD22	2:A:709:GLN:HE21	1.73	0.53
2:A:301:VAL:O	2:A:304:PRO:HD2	2.09	0.53
2:A:428:MET:CE	2:A:811:TYR:HD1	2.22	0.53
2:A:462:ILE:HG23	2:A:591:SER:O	2.09	0.53
2:A:419:LYS:HB2	2:A:422:MET:CG	2.39	0.52
2:A:249:SER:HB3	2:A:676:GLU:OE1	2.09	0.52
2:A:375:LEU:C	2:A:378:PRO:HD2	2.30	0.52
2:A:917:ARG:NH1	2:A:1004:TYR:O	2.43	0.52
2:A:437:ILE:O	2:A:439:PRO:HD3	2.09	0.52
2:A:826:ILE:O	2:A:829:ARG:HG2	2.09	0.52
2:A:33:GLU:HG3	2:A:34:LEU:H	1.74	0.52
2:A:872:ILE:HG22	2:A:1073:ILE:HA	1.90	0.52
2:A:295:MET:O	2:A:300:LEU:HB2	2.10	0.52
2:A:428:MET:HG2	2:A:433:TYR:CB	2.40	0.52
2:A:820:LEU:C	2:A:821:PHE:HD2	2.13	0.52
2:A:1003:CYS:SG	2:A:1007:PHE:CZ	3.03	0.52
2:A:199:LYS:H	2:A:199:LYS:HD2	1.75	0.51
2:A:281:PRO:HG2	2:A:284:THR:OG1	2.10	0.51
2:A:428:MET:HG2	2:A:433:TYR:CG	2.45	0.51
2:A:880:ASP:O	2:A:883:PRO:HD2	2.10	0.51
2:A:330:PHE:CE1	2:A:690:ARG:CZ	2.94	0.51
2:A:420:LYS:O	2:A:424:VAL:HG23	2.10	0.51
2:A:756:VAL:HG13	2:A:788:PHE:CZ	2.46	0.51
2:A:842:TYR:CE2	2:A:844:PRO:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:733:LEU:O	2:A:737:MET:HE2	2.11	0.51
2:A:82:TYR:CE1	2:A:184:ARG:HD2	2.45	0.50
2:A:129:LEU:HD22	2:A:336:LYS:O	2.11	0.50
2:A:303:ILE:HB	2:A:304:PRO:HD3	1.93	0.50
2:A:689:PHE:HB2	2:A:723:ARG:HG2	1.92	0.50
2:A:473:GLN:NE2	2:A:595:GLN:HG2	2.26	0.50
2:A:824:ASN:HB3	2:A:828:SER:HB2	1.91	0.50
2:A:556:GLN:HA	2:A:556:GLN:NE2	2.11	0.50
2:A:744:ILE:HG22	2:A:745:THR:HG23	1.93	0.50
2:A:90:VAL:HG23	2:A:91:LYS:N	2.25	0.50
2:A:399:SER:HB3	2:A:838:LYS:HB3	1.94	0.50
2:A:535:ARG:HH11	2:A:565:GLN:HE22	1.60	0.50
2:A:975:TYR:C	2:A:977:GLY:H	2.15	0.50
2:A:22:VAL:HG22	2:A:77:TYR:HB2	1.93	0.49
2:A:542:LEU:HD11	2:A:561:TYR:HD2	1.77	0.49
2:A:242:LYS:O	2:A:246:SER:HB2	2.12	0.49
2:A:515:MET:HG2	2:A:639:PHE:HE2	1.76	0.49
2:A:248:MET:HE2	2:A:252:VAL:CG1	2.42	0.49
2:A:255:VAL:HG11	2:A:316:ILE:HB	1.93	0.49
2:A:968:PRO:HG2	2:A:971:ASP:OD2	2.11	0.49
2:A:1028:ALA:HB1	2:A:1070:MET:HE2	1.95	0.49
2:A:319:PHE:N	2:A:320:PRO:CD	2.75	0.49
2:A:667:LYS:O	2:A:667:LYS:CG	2.60	0.49
2:A:255:VAL:O	2:A:673:VAL:HG21	2.12	0.49
2:A:476:VAL:O	2:A:480:MET:HG3	2.13	0.49
2:A:358:GLU:OE2	2:A:359:MET:HG2	2.13	0.49
2:A:516:VAL:HG21	2:A:675:ILE:HG21	1.95	0.49
2:A:544:ILE:O	2:A:548:MET:HG3	2.13	0.49
2:A:887:VAL:HG22	2:A:1054:LEU:HD11	1.94	0.49
2:A:1026:ILE:HD11	2:A:1067:TRP:CG	2.47	0.49
2:A:449:LEU:HD21	2:A:573:VAL:HG11	1.95	0.49
2:A:185:HIS:H	2:A:185:HIS:CD2	2.29	0.48
2:A:762:THR:HA	2:A:1077:ARG:O	2.13	0.48
2:A:165:ARG:HD3	2:A:223:TYR:CB	2.43	0.48
2:A:288:LEU:HD21	2:A:311:LEU:HD11	1.94	0.48
2:A:340:LEU:O	2:A:340:LEU:HD12	2.13	0.48
2:A:687:ILE:HG22	2:A:899:PHE:O	2.13	0.48
2:A:449:LEU:CD2	2:A:573:VAL:HG11	2.43	0.48
2:A:246:SER:N	2:A:247:PRO:CD	2.77	0.48
2:A:534:PHE:HZ	2:A:599:ALA:HB1	1.77	0.48
2:A:565:GLN:O	2:A:569:MET:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1105:A:C5	2:A:462:ILE:HD13	2.49	0.48
2:A:87:ARG:H	2:A:87:ARG:HG2	1.41	0.48
2:A:617:ASN:N	2:A:617:ASN:HD22	2.09	0.48
2:A:744:ILE:CD1	2:A:748:LEU:HD22	2.43	0.48
2:A:241:ALA:HB3	2:A:456:GLY:HA2	1.95	0.48
2:A:687:ILE:HG23	2:A:900:MET:HG3	1.96	0.48
2:A:860:MET:HE3	2:A:860:MET:HB2	1.65	0.48
2:A:534:PHE:CZ	2:A:599:ALA:HB1	2.49	0.48
2:A:24:ILE:HD12	2:A:45:CYS:HB3	1.94	0.47
2:A:279:ILE:O	2:A:648:ILE:HD12	2.14	0.47
2:A:512:ASN:C	2:A:512:ASN:HD22	2.16	0.47
2:A:126:THR:OG1	2:A:128:SER:HB3	2.14	0.47
2:A:858:LEU:O	2:A:862:GLN:HG3	2.14	0.47
2:A:141:ASN:O	2:A:145:VAL:HG23	2.15	0.47
2:A:370:GLU:O	2:A:374:MET:HG3	2.14	0.47
2:A:28:TYR:CE2	2:A:70:THR:HB	2.50	0.47
2:A:4:TYR:HB3	2:A:754:GLU:OE1	2.15	0.47
2:A:228:GLU:OE1	2:A:303:ILE:HG13	2.14	0.47
2:A:244:VAL:HG12	2:A:329:SER:HB3	1.96	0.47
2:A:364:THR:HG23	2:A:537:GLY:CA	2.44	0.47
2:A:378:PRO:O	2:A:383:ASP:HB2	2.15	0.47
2:A:608:ILE:HD11	2:A:635:ALA:HB2	1.95	0.47
2:A:791:LEU:HD23	2:A:791:LEU:N	2.30	0.47
2:A:832:ALA:O	2:A:836:LYS:HG3	2.15	0.47
2:A:539:ILE:HG23	2:A:562:LYS:HE3	1.97	0.47
1:X:1103:U:O2'	1:X:1104:G:C5'	2.63	0.47
2:A:12:LEU:HD22	2:A:16:TYR:HE2	1.79	0.47
3:A:1201:GTP:O2A	3:A:1201:GTP:O1B	2.33	0.47
2:A:824:ASN:CB	2:A:828:SER:HB2	2.45	0.46
2:A:248:MET:HE1	2:A:251:LEU:HB2	1.98	0.46
2:A:137:SER:HB2	2:A:185:HIS:CD2	2.51	0.46
2:A:744:ILE:HB	2:A:748:LEU:HD22	1.97	0.46
2:A:449:LEU:HD13	2:A:573:VAL:HG13	1.98	0.46
2:A:551:ASP:HB3	2:A:554:VAL:HB	1.97	0.46
2:A:769:GLU:HG2	2:A:1047:LYS:NZ	2.31	0.46
2:A:962:LEU:O	2:A:967:ILE:HD13	2.16	0.46
2:A:312:VAL:HG23	2:A:313:ASP:H	1.80	0.46
2:A:102:LEU:H	2:A:102:LEU:CD2	2.25	0.46
2:A:161:LYS:O	2:A:165:ARG:NH1	2.48	0.45
2:A:744:ILE:CG1	2:A:748:LEU:HD22	2.46	0.45
2:A:33:GLU:HG3	2:A:34:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:ASP:O	2:A:103:THR:N	2.50	0.45
2:A:412:ARG:O	2:A:412:ARG:HG2	2.16	0.45
2:A:466:PRO:HD2	2:A:469:TYR:CD2	2.52	0.45
2:A:24:ILE:HG22	2:A:26:ILE:HD11	1.97	0.45
2:A:617:ASN:N	2:A:617:ASN:ND2	2.65	0.45
2:A:1023:LYS:HB3	2:A:1060:LYS:HG2	1.98	0.45
1:X:1101:U:O2'	1:X:1102:G:P	2.75	0.45
2:A:621:PHE:HA	2:A:638:GLN:O	2.17	0.45
2:A:959:GLN:NE2	2:A:973:ASP:OD1	2.50	0.45
2:A:127:ASP:O	2:A:129:LEU:N	2.50	0.45
2:A:1023:LYS:NZ	2:A:1057:ASN:HA	2.32	0.45
2:A:376:GLU:HG2	2:A:380:LYS:HE2	1.98	0.45
2:A:703:GLN:CD	2:A:703:GLN:N	2.69	0.45
1:X:1102:G:O2'	1:X:1103:U:P	2.75	0.45
2:A:168:ASP:OD2	2:A:223:TYR:OH	2.27	0.45
2:A:509:PHE:CD2	2:A:624:LYS:HB3	2.51	0.45
2:A:758:THR:HG22	2:A:766:PHE:O	2.16	0.45
1:X:1101:U:O4	2:A:415:ILE:HG13	2.16	0.45
2:A:409:LYS:HB2	2:A:409:LYS:NZ	2.32	0.45
2:A:50:LYS:O	2:A:51:ASN:OD1	2.35	0.44
1:X:1101:U:O2'	1:X:1102:G:OP1	2.32	0.44
2:A:49:SER:C	2:A:51:ASN:H	2.20	0.44
2:A:145:VAL:HG21	2:A:211:ILE:HG23	1.99	0.44
2:A:512:ASN:HD22	2:A:513:ASN:N	2.15	0.44
2:A:769:GLU:HG2	2:A:1047:LYS:HZ2	1.82	0.44
2:A:248:MET:HE2	2:A:252:VAL:HG13	2.00	0.44
2:A:837:ALA:O	2:A:840:ASN:ND2	2.49	0.44
2:A:734:THR:HA	2:A:737:MET:CE	2.48	0.44
2:A:945:GLU:HG2	2:A:992:TYR:CE1	2.41	0.44
2:A:1012:PRO:O	2:A:1016:LYS:HG3	2.18	0.44
2:A:193:TYR:CZ	2:A:197:LYS:HD2	2.53	0.44
2:A:324:LYS:O	2:A:328:TRP:CD1	2.63	0.44
2:A:464:ILE:O	2:A:464:ILE:HG22	2.17	0.44
1:X:1103:U:O2'	1:X:1104:G:OP2	2.35	0.44
2:A:163:TYR:CE2	2:A:167:LEU:HD22	2.53	0.44
2:A:930:ILE:O	2:A:934:ILE:HG13	2.17	0.44
2:A:161:LYS:HG2	2:A:165:ARG:CZ	2.48	0.43
2:A:473:GLN:HE22	2:A:593:GLU:HB3	1.83	0.43
2:A:248:MET:HG2	2:A:326:TYR:CD1	2.53	0.43
2:A:556:GLN:CA	2:A:556:GLN:NE2	2.77	0.43
2:A:195:VAL:O	2:A:199:LYS:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:453:ASP:HB2	2:A:699:GLU:HG3	2.00	0.43
2:A:619:HIS:ND1	2:A:619:HIS:N	2.66	0.43
2:A:691:ALA:HB2	2:A:723:ARG:HB3	1.99	0.43
2:A:785:GLN:OE1	2:A:875:ASN:ND2	2.51	0.43
2:A:898:LYS:HE2	2:A:912:GLN:NE2	2.33	0.43
2:A:165:ARG:HE	2:A:220:HIS:CA	2.29	0.43
2:A:424:VAL:HG22	2:A:467:TYR:CD2	2.53	0.43
2:A:473:GLN:HE22	2:A:595:GLN:H	1.65	0.43
2:A:572:TYR:CE1	2:A:585:GLN:HB2	2.53	0.43
2:A:719:VAL:CG1	2:A:723:ARG:HD2	2.49	0.43
2:A:790:SER:HB3	2:A:791:LEU:HD23	1.99	0.43
2:A:409:LYS:H	2:A:409:LYS:HZ2	1.65	0.43
2:A:8:LEU:HA	2:A:737:MET:SD	2.59	0.43
2:A:248:MET:CE	2:A:251:LEU:HB2	2.48	0.43
2:A:877:ILE:O	2:A:880:ASP:HB2	2.19	0.43
2:A:293:ASP:O	2:A:297:LYS:HG2	2.19	0.43
2:A:145:VAL:CG2	2:A:211:ILE:HG23	2.49	0.43
1:X:1105:A:C6	2:A:462:ILE:HD13	2.54	0.42
2:A:408:LEU:HD22	2:A:426:ASP:CG	2.39	0.42
2:A:449:LEU:HD22	2:A:573:VAL:CG1	2.49	0.42
2:A:721:ARG:CG	2:A:721:ARG:NH1	2.78	0.42
2:A:824:ASN:HB3	2:A:825:ASN:H	1.65	0.42
2:A:116:SER:HB3	2:A:197:LYS:HG3	2.02	0.42
2:A:523:GLN:HB2	2:A:665:LYS:O	2.19	0.42
2:A:28:TYR:CE1	2:A:784:ILE:HG12	2.53	0.42
2:A:473:GLN:HE22	2:A:595:GLN:HG2	1.84	0.42
2:A:430:ASN:C	2:A:432:ARG:H	2.23	0.42
2:A:473:GLN:HA	2:A:561:TYR:CD1	2.55	0.42
2:A:764:LYS:HZ1	2:A:773:ILE:HG23	1.84	0.42
2:A:887:VAL:HG12	2:A:888:SER:N	2.35	0.42
2:A:764:LYS:NZ	2:A:773:ILE:HG23	2.35	0.42
2:A:24:ILE:HG22	2:A:26:ILE:CD1	2.49	0.42
2:A:317:GLU:N	2:A:317:GLU:OE1	2.52	0.42
2:A:409:LYS:HB2	2:A:409:LYS:HZ3	1.85	0.42
2:A:516:VAL:N	2:A:671:SER:O	2.52	0.42
2:A:473:GLN:NE2	2:A:595:GLN:H	2.17	0.42
2:A:584:ILE:HD12	2:A:585:GLN:C	2.40	0.42
2:A:803:ALA:HA	2:A:808:PHE:CE2	2.55	0.42
2:A:1058:TYR:HA	2:A:1059:PRO:HD3	1.86	0.42
1:X:1103:U:O2'	1:X:1104:G:O5'	2.38	0.42
2:A:784:ILE:HD13	2:A:784:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:839:LEU:HB3	2:A:845:ILE:HD12	2.00	0.42
2:A:989:LEU:HD11	2:A:1070:MET:HE3	2.02	0.42
2:A:428:MET:HG2	2:A:433:TYR:HB2	2.01	0.42
2:A:695:LEU:HG	2:A:713:LEU:CD1	2.50	0.41
2:A:847:LEU:HD23	2:A:850:ARG:NH1	2.35	0.41
2:A:951:ILE:HG13	2:A:985:LYS:HG2	2.02	0.41
2:A:963:ILE:HD11	2:A:969:LYS:HG2	2.01	0.41
2:A:853:GLN:NE2	2:A:853:GLN:HA	2.35	0.41
2:A:29:SER:OG	2:A:34:LEU:HD23	2.19	0.41
2:A:283:GLN:OE1	2:A:649:GLN:CG	2.59	0.41
2:A:149:LEU:O	2:A:163:TYR:HE1	2.04	0.41
2:A:291:MET:O	2:A:295:MET:HG3	2.20	0.41
2:A:396:SER:HG	2:A:474:HIS:CE1	2.38	0.41
2:A:439:PRO:HA	2:A:440:PRO:HD3	1.85	0.41
2:A:665:LYS:HA	2:A:665:LYS:HD3	1.88	0.41
2:A:82:TYR:CD2	3:A:1201:GTP:O3'	2.69	0.41
2:A:161:LYS:HE3	2:A:161:LYS:HB2	1.97	0.41
2:A:289:ASN:HD22	2:A:289:ASN:HA	1.73	0.41
2:A:135:LEU:HD13	2:A:709:GLN:HE22	1.85	0.41
2:A:446:PRO:HB2	2:A:574:GLN:CG	2.51	0.41
2:A:532:GLN:CB	2:A:533:PRO:HD3	2.51	0.41
2:A:847:LEU:O	2:A:851:ARG:HG3	2.21	0.41
2:A:3:LYS:O	2:A:7:ILE:HG12	2.21	0.41
2:A:61:GLU:OE2	2:A:62:TYR:CE2	2.74	0.41
2:A:424:VAL:HG22	2:A:467:TYR:CE2	2.55	0.41
2:A:820:LEU:HD13	2:A:824:ASN:ND2	2.35	0.41
2:A:1026:ILE:HD11	2:A:1067:TRP:CD1	2.56	0.41
2:A:84:ALA:HB1	2:A:88:LYS:HZ2	1.82	0.41
2:A:370:GLU:HG2	2:A:602:ILE:HG23	2.03	0.41
2:A:703:GLN:CD	2:A:703:GLN:H	2.24	0.41
2:A:714:TYR:CZ	2:A:718:ILE:HD11	2.56	0.41
2:A:22:VAL:CG2	2:A:77:TYR:HB2	2.51	0.40
2:A:155:ASP:O	2:A:160:LEU:HD13	2.21	0.40
2:A:389:SER:OG	2:A:557:THR:HB	2.20	0.40
2:A:520:ASP:HB2	2:A:667:LYS:HE2	2.03	0.40
2:A:539:ILE:CG2	2:A:562:LYS:HE3	2.51	0.40
2:A:596:THR:O	2:A:600:ASN:HB2	2.21	0.40
2:A:705:THR:O	2:A:709:GLN:HG3	2.21	0.40
2:A:967:ILE:N	2:A:967:ILE:CD1	2.83	0.40
1:X:1107:C:OP1	2:A:594:LYS:NZ	2.49	0.40
2:A:2:GLY:HA2	2:A:754:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:VAL:HG23	2:A:91:LYS:H	1.86	0.40
2:A:147:PHE:O	2:A:151:LYS:HG2	2.21	0.40
2:A:762:THR:HA	2:A:1078:SER:HB3	2.02	0.40
2:A:135:LEU:HB3	2:A:706:GLN:HG2	2.03	0.40
2:A:334:PHE:CE2	2:A:455:PRO:HD3	2.57	0.40
2:A:834:THR:O	2:A:838:LYS:HG3	2.22	0.40
2:A:1022:PHE:O	2:A:1022:PHE:CG	2.74	0.40
2:A:165:ARG:HD3	2:A:223:TYR:HB2	2.03	0.40
2:A:686:LYS:HD2	2:A:899:PHE:HA	2.03	0.40
2:A:714:TYR:O	2:A:718:ILE:HG12	2.21	0.40
2:A:1024:GLY:O	2:A:1025:LYS:HB3	2.20	0.40
2:A:109:TYR:CD1	2:A:129:LEU:HD13	2.57	0.40
2:A:283:GLN:HG3	2:A:284:THR:N	2.36	0.40
2:A:976:VAL:O	2:A:976:VAL:CG1	2.68	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	
2	A	1067/1095 (97%)	951 (89%)	94 (9%)	22 (2%)	7	13

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	102	LEU
2	A	976	VAL
2	A	978	SER
2	A	1025	LYS
2	A	106	GLU
2	A	128	SER
2	A	822	SER

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Mol	Chain	Res	Type
2	A	825	ASN
2	A	865	VAL
2	A	1027	PRO
2	A	869	SER
2	A	82	TYR
2	A	439	PRO
2	A	592	GLY
2	A	51	ASN
2	A	83	ASN
2	A	238	SER
2	A	864	PRO
2	A	274	LYS
2	A	411	GLY
2	A	863	LYS
2	A	1024	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	
2	A	975/996 (98%)	929 (95%)	46 (5%)	26	50

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	17	ASN
2	A	35	GLU
2	A	48	ASN
2	A	80	ASP
2	A	87	ARG
2	A	121	THR
2	A	130	MET
2	A	143	ASN
2	A	155	ASP
2	A	194	ASP
2	A	229	LEU

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Mol	Chain	Res	Type
2	A	313	ASP
2	A	320	PRO
2	A	358	GLU
2	A	409	LYS
2	A	415	ILE
2	A	418	THR
2	A	467	TYR
2	A	508	ARG
2	A	512	ASN
2	A	518	TYR
2	A	556	GLN
2	A	557	THR
2	A	584	ILE
2	A	600	ASN
2	A	619	HIS
2	A	671	SER
2	A	721	ARG
2	A	784	ILE
2	A	791	LEU
2	A	821	PHE
2	A	824	ASN
2	A	868	LYS
2	A	872	ILE
2	A	880	ASP
2	A	892	LEU
2	A	895	GLN
2	A	900	MET
2	A	916	SER
2	A	917	ARG
2	A	922	GLU
2	A	939	VAL
2	A	1022	PHE
2	A	1027	PRO
2	A	1047	LYS
2	A	1088	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	36	ASN
2	A	48	ASN
2	A	63	ASN

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Mol	Chain	Res	Type
2	A	143	ASN
2	A	185	HIS
2	A	289	ASN
2	A	294	ASN
2	A	308	GLN
2	A	473	GLN
2	A	512	ASN
2	A	528	GLN
2	A	556	GLN
2	A	563	GLN
2	A	565	GLN
2	A	574	GLN
2	A	617	ASN
2	A	646	GLN
2	A	653	ASN
2	A	698	ASN
2	A	709	GLN
2	A	810	ASN
2	A	824	ASN
2	A	825	ASN
2	A	853	GLN
2	A	875	ASN
2	A	895	GLN
2	A	912	GLN
2	A	959	GLN
2	A	1034	HIS
2	A	1057	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	7/7 (100%)	4 (57%)	3 (42%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	1102	G
1	X	1103	U
1	X	1104	G
1	X	1105	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1101	U
1	X	1102	G
1	X	1103	U

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\#|Z| > 2$
3	GTP	A	1201	-	26,34,34	1.10	2 (7%)	32,54,54	1.66	7 (21%)

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
3	GTP	A	1201	-	-	4/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	GTP	C5-C6	-3.95	1.39	1.47
3	A	1201	GTP	C2-N3	2.21	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1201	GTP	PB-O3B-PG	-3.59	120.50	132.83
3	A	1201	GTP	PA-O3A-PB	-3.58	120.53	132.83
3	A	1201	GTP	C3'-C2'-C1'	3.24	105.86	100.98
3	A	1201	GTP	C5-C6-N1	3.22	119.63	113.95
3	A	1201	GTP	C8-N7-C5	3.02	108.75	102.99
3	A	1201	GTP	C2-N1-C6	-2.87	119.81	125.10
3	A	1201	GTP	O6-C6-C5	-2.13	120.20	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	GTP	C4'-C5'-O5'-PA
3	A	1201	GTP	O4'-C4'-C5'-O5'
3	A	1201	GTP	C3'-C4'-C5'-O5'
3	A	1201	GTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	GTP	25	0

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

Ligand GTP A 1201

Bond lengths

Bond angles

Torsions

Rings
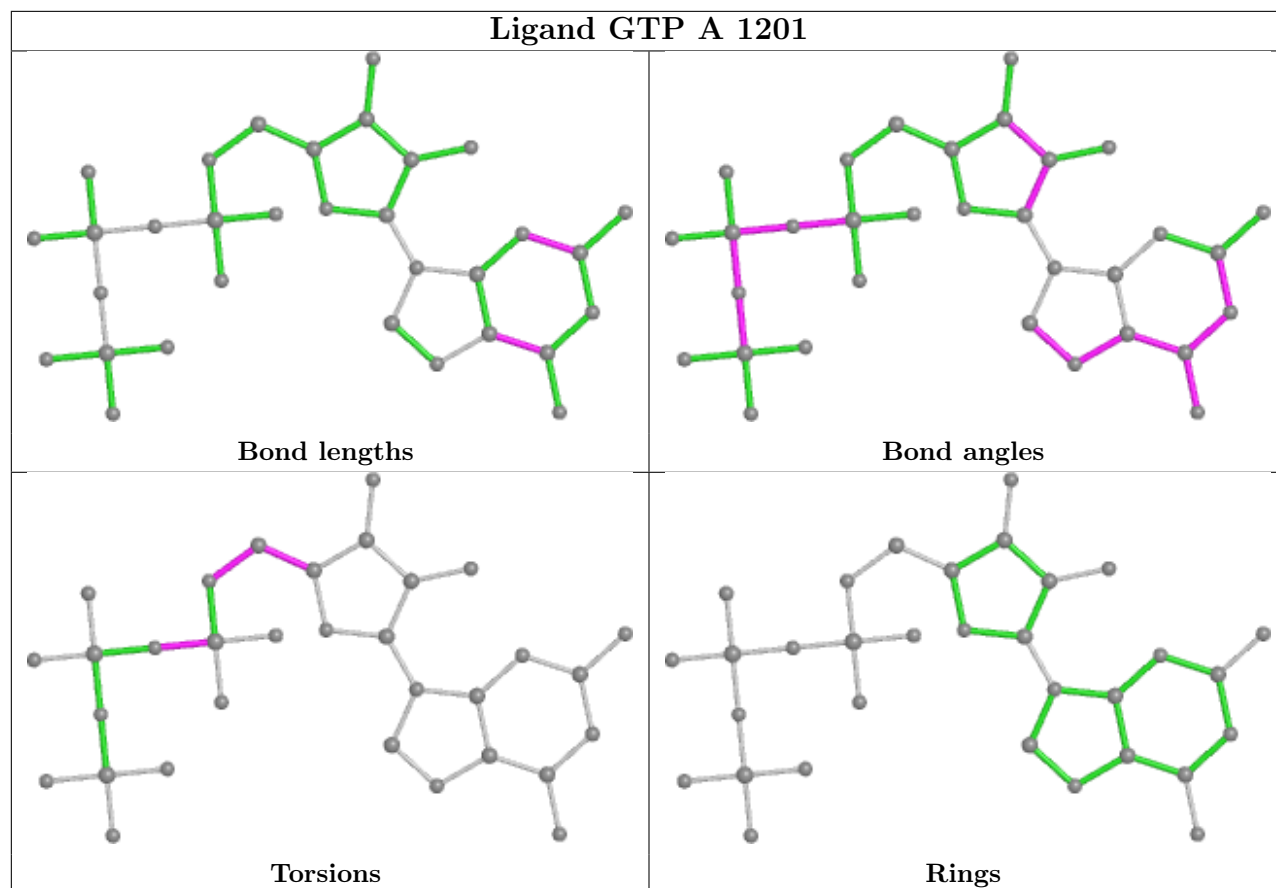
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	X	7/7 (100%)	-0.05	0	100	100	50, 64, 77, 81	0
2	A	1073/1095 (97%)	-0.08	14 (1%)	77	73	17, 51, 81, 124	0
All	All	1080/1102 (98%)	-0.08	14 (1%)	77	73	17, 51, 81, 124	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	867	PHE	4.5
2	A	824	ASN	4.3
2	A	864	PRO	3.4
2	A	865	VAL	3.3
2	A	1088	GLU	2.9
2	A	868	LYS	2.9
2	A	866	THR	2.6
2	A	77	TYR	2.5
2	A	783	TYR	2.5
2	A	983	ARG	2.4
2	A	1025	LYS	2.3
2	A	791	LEU	2.3
2	A	536	LYS	2.2
2	A	829	ARG	2.1

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

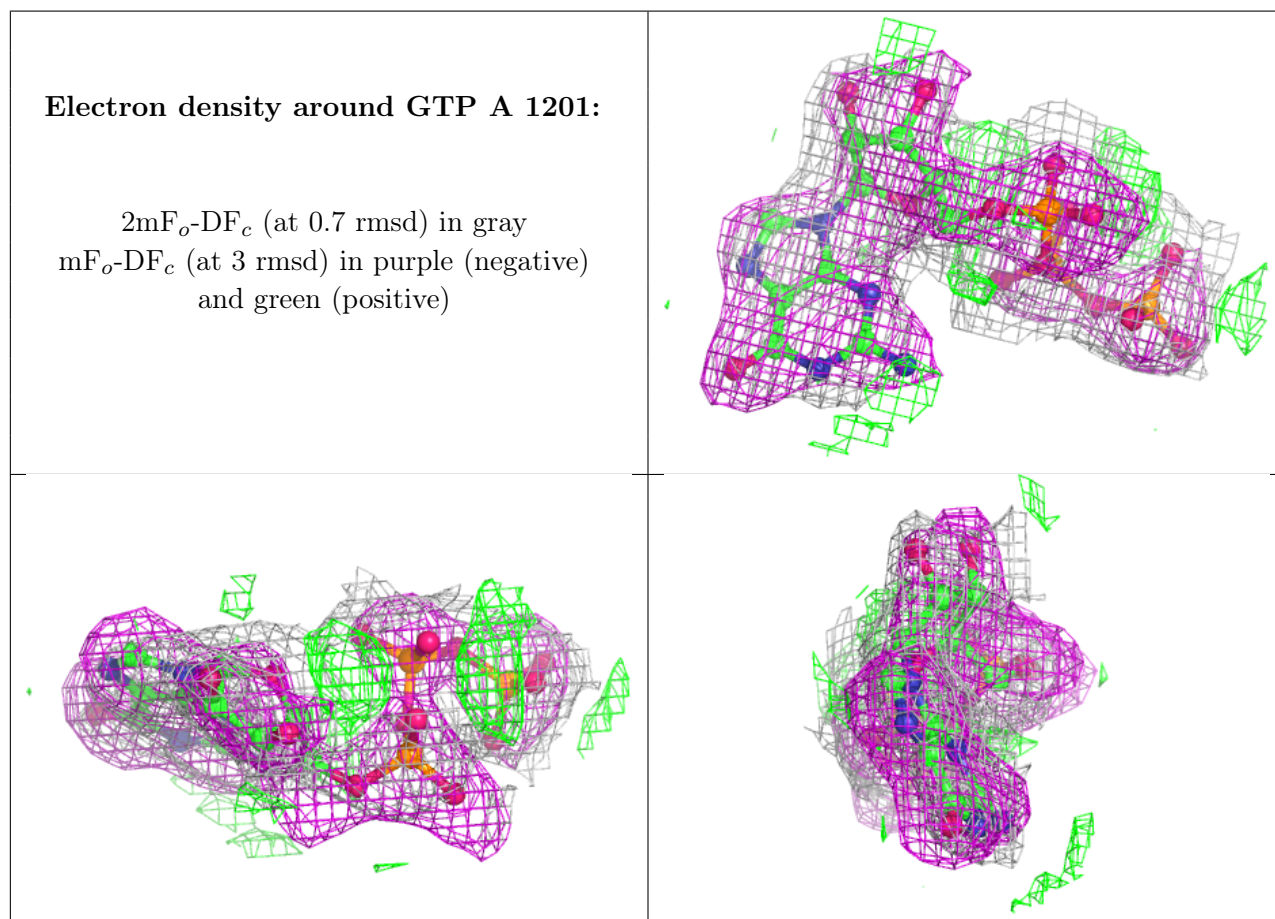There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
3	GTP	A	1201	32/32	0.81	0.32	20,20,20,20	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 A 1201:

$2mF_o$-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 ⓘ

There are no such residues in this entry.