



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:57 AM UTC

PDB ID : 5E6M / pdb_00005e6m
Title : Crystal structure of human wild type GlyRS bound with tRNAGly
Authors : Xie, W.; Qin, X.; Deng, X.; Chen, L.; Liu, Y.
Deposited on : 2015-10-10
Resolution : 2.93 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

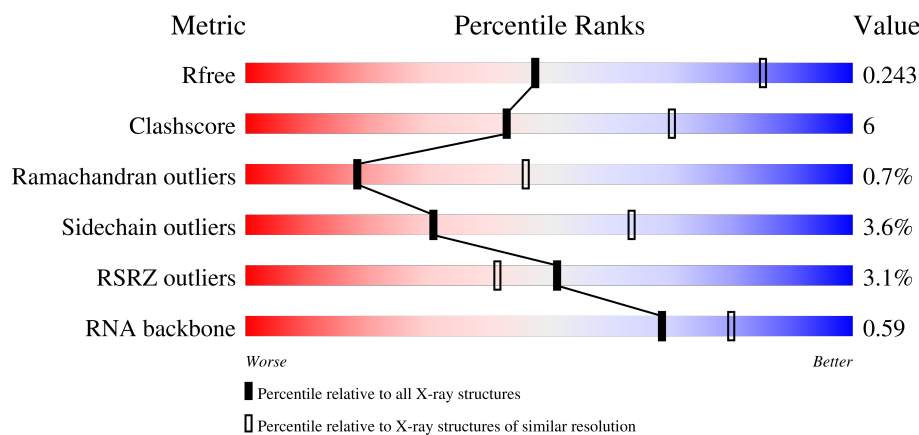
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)
RNA backbone	3983	1016 (3.12-2.72)

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	693	3% 61% 12% • 25%
1	B	693	3% 61% 11% • 27%
2	C	74	72% 24% •
2	E	74	66% 28% 5%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11178 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 Glycine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			3993	2541	696	738	18			
1	B	506	Total	C	N	O	S	0	0	0
			3892	2478	675	722	17			

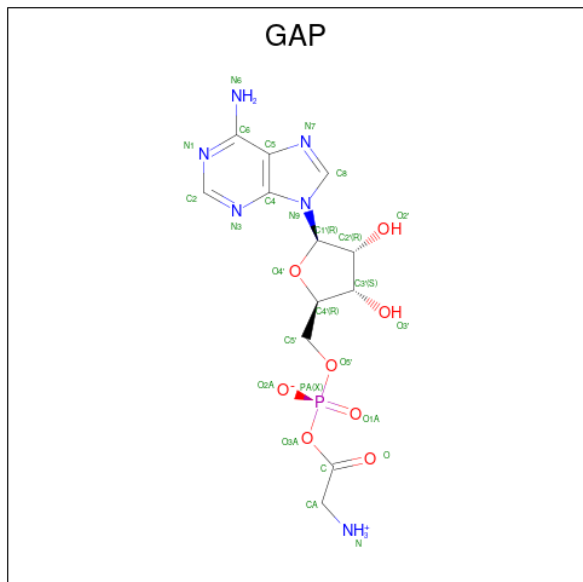
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	686	LEU	-	expression tag	UNP P41250
A	687	GLU	-	expression tag	UNP P41250
A	688	HIS	-	expression tag	UNP P41250
A	689	HIS	-	expression tag	UNP P41250
A	690	HIS	-	expression tag	UNP P41250
A	691	HIS	-	expression tag	UNP P41250
A	692	HIS	-	expression tag	UNP P41250
A	693	HIS	-	expression tag	UNP P41250
B	686	LEU	-	expression tag	UNP P41250
B	687	GLU	-	expression tag	UNP P41250
B	688	HIS	-	expression tag	UNP P41250
B	689	HIS	-	expression tag	UNP P41250
B	690	HIS	-	expression tag	UNP P41250
B	691	HIS	-	expression tag	UNP P41250
B	692	HIS	-	expression tag	UNP P41250
B	693	HIS	-	expression tag	UNP P41250

- Molecule 2 is a RNA chain called tRNA(Gly).

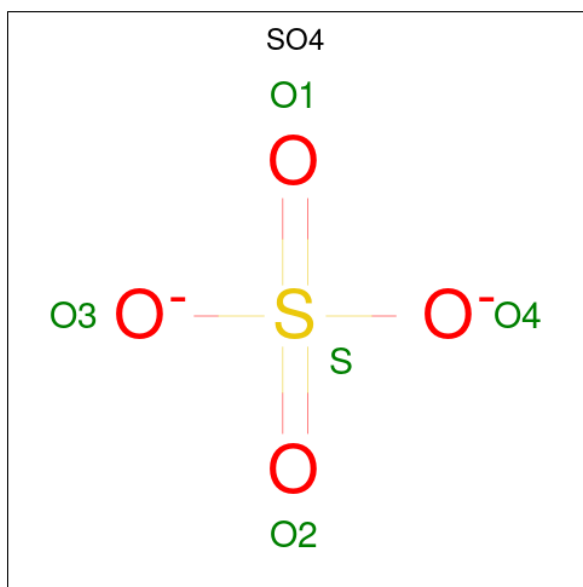
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	74	Total	C	N	O	P	0	0	0
			1580	700	273	531	76			
2	E	74	Total	C	N	O	P	0	0	0
			1580	700	273	531	76			

- Molecule 3 is GLYCYL-ADENOSINE-5'-PHOSPHATE (CCD ID: GAP) (formula: $C_{12}H_{17}N_6O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	12	6	8	1		
3	B	1	Total	C	N	O	P	0	0
			27	12	6	8	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



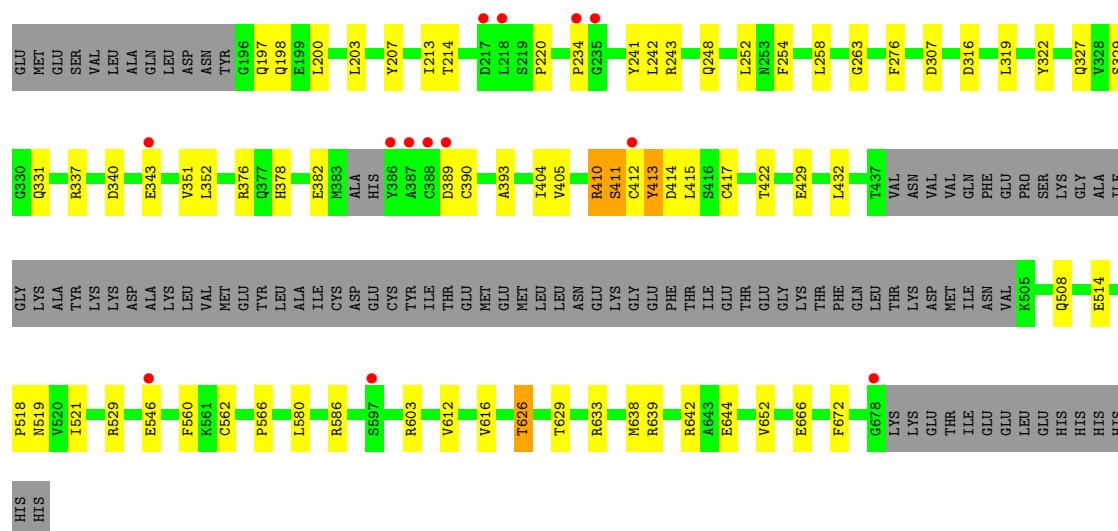
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Ni 1 1	0	0
5	E	1	Total Ni 1 1	0	0

- Molecule 6 is water.

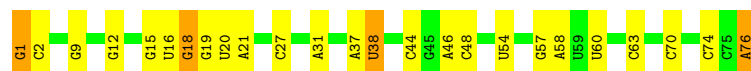
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O 22 22	0	0
6	B	24	Total O 24 24	0	0
6	C	17	Total O 17 17	0	0
6	E	9	Total O 9 9	0	0



- Molecule 2: tRNA(Gly)



- Molecule 2: tRNA(Gly)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	206.86Å 122.20Å 84.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.93 49.56 – 2.93	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.56-2.93) 95.9 (49.56-2.93)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.243 0.197 , 0.243	Depositor DCC
R_{free} test set	2283 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	68.5	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11178	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: GAP, GTP, NI, SO4

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	0.34	0/4078	0.81	2/5524 (0.0%)
1	B	0.35	0/3981	0.79	6/5400 (0.1%)
2	C	0.14	0/1726	0.28	0/2687
2	E	0.14	0/1726	0.28	0/2687
All	All	0.30	0/11511	0.68	8/16298 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	GLY	CA-C-N	6.52	127.99	119.84
1	A	233	GLY	C-N-CA	6.52	127.99	119.84
1	B	626	THR	CA-C-N	-6.12	112.19	119.84
1	B	626	THR	C-N-CA	-6.12	112.19	119.84
1	B	152	VAL	N-CA-C	5.87	116.65	110.72
1	B	220	PRO	O-C-N	5.34	123.77	121.31
1	B	97	GLY	CA-C-N	5.23	124.68	119.24
1	B	97	GLY	C-N-CA	5.23	124.68	119.24

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	3993	0	3826	62	0
1	B	3892	0	3703	44	0
2	C	1580	0	798	13	0
2	E	1580	0	798	18	0
3	A	27	0	17	2	0
3	B	27	0	17	1	0
4	A	5	0	0	1	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	A	22	0	0	2	0
6	B	24	0	0	4	0
6	C	17	0	0	0	0
6	E	9	0	0	1	0
All	All	11178	0	9159	124	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 6.

All (124) 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:C:54:U:H3	2:C:58:A:H2	1.13	0.97
1:B:140:HIS:HD2	2:C:76:A:H8	1.35	0.73
2:E:12:G:N7	6:E:201:HOH:O	2.22	0.72
1:B:629:THR:HA	1:B:644:GLU:HA	1.72	0.71
2:E:54:U:H3	2:E:58:A:H2	1.37	0.71
1:A:570:ASN:HB3	1:A:572:GLU:OE2	1.90	0.71
1:B:69:LYS:NZ	1:B:546:GLU:OE1	2.25	0.70
1:B:389:ASP:OD2	6:B:801:HOH:O	2.11	0.69
1:A:410:ARG:NH1	1:A:522:GLU:OE2	2.28	0.67
1:B:629:THR:HG22	1:B:644:GLU:HB3	1.77	0.67
1:A:654:ASP:HB3	1:A:660:ILE:HG12	1.78	0.65
1:A:234:PRO:HG3	2:C:1:GTP:H5'	1.79	0.65
1:A:140:HIS:HD2	2:E:76:A:H8	1.44	0.64
1:B:200:LEU:HA	1:B:203:LEU:HD12	1.80	0.63
1:B:150:LYS:H	1:B:151:ASP:HA	1.63	0.63
2:E:21:A:H61	2:E:46:A:H2'	1.66	0.61
3:B:701:GAP:N	6:B:802:HOH:O	2.31	0.60
1:B:128:MET:HE2	1:B:243:ARG:HH21	1.68	0.58
2:E:18:G:O2'	2:E:57:G:N2	2.27	0.58
1:B:112:ARG:HG2	1:B:116:ILE:HD12	1.85	0.57
1:B:316:ASP:OD1	1:B:337:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ARG:NH2	1:B:382:GLU:OE1	2.40	0.55
1:B:411:SER:O	1:B:519:ASN:HA	2.07	0.55
1:A:112:ARG:NH2	1:A:123:GLU:OE2	2.36	0.54
1:A:599:SER:OG	2:E:38:U:OP2	2.26	0.54
2:E:58:A:O2'	2:E:60:U:OP2	2.21	0.54
1:A:639:ARG:NH2	1:A:666:GLU:OE2	2.40	0.54
1:B:393:ALA:HB3	1:B:405:VAL:HB	1.89	0.54
1:A:67:ARG:NH1	2:E:70:C:OP1	2.35	0.53
1:A:390:CYS:SG	6:A:820:HOH:O	2.58	0.53
1:A:79:PHE:HA	1:A:99:VAL:HG23	1.91	0.53
1:A:132:GLU:HG3	1:A:241:TYR:HE2	1.74	0.53
1:B:140:HIS:HD2	2:C:76:A:C8	2.21	0.53
1:A:280:ILE:HG22	1:B:234:PRO:HB3	1.91	0.52
1:A:112:ARG:HG2	1:A:116:ILE:HD12	1.92	0.52
1:A:564:VAL:HG22	1:A:580:LEU:HD23	1.92	0.52
1:A:410:ARG:NH2	1:A:414:ASP:OD2	2.43	0.51
1:A:277:ARG:HD2	2:E:76:A:C6	2.44	0.51
2:E:18:G:HO2'	2:E:57:G:H22	1.56	0.51
2:E:15:G:H2'	2:E:16:U:C6	2.46	0.50
2:C:58:A:H8	2:C:60:U:C6	2.29	0.50
1:A:576:PHE:HE2	1:A:623:VAL:HG12	1.78	0.49
1:B:429:GLU:OE1	2:E:44:C:O2'	2.24	0.49
1:A:619:ASP:OD2	1:A:642:ARG:NH1	2.46	0.49
1:A:140:HIS:CD2	2:E:76:A:H8	2.29	0.48
1:A:392:ASP:HB3	1:A:403:GLU:HG3	1.94	0.48
1:A:46:ALA:O	1:A:50:VAL:HG23	2.14	0.48
1:B:560:PHE:HB2	1:B:612:VAL:HG22	1.95	0.48
1:A:86:ILE:HG23	1:B:422:THR:HG21	1.96	0.48
1:A:576:PHE:CE2	1:A:623:VAL:HG12	2.49	0.48
1:B:151:ASP:OD1	1:B:152:VAL:N	2.46	0.47
1:A:512:TYR:CG	2:C:43:G:H4'	2.49	0.47
1:B:351:VAL:HG11	1:B:521:ILE:HG13	1.96	0.47
1:B:378:HIS:HB2	1:B:390:CYS:HB3	1.96	0.47
1:B:562:CYS:HB2	1:B:652:VAL:HG11	1.95	0.47
2:E:58:A:H8	2:E:60:U:C6	2.33	0.47
1:B:119:GLU:HB2	1:B:121:ILE:HG13	1.96	0.46
1:B:404:ILE:HG22	1:B:529:ARG:HB3	1.96	0.46
1:A:629:THR:HG22	1:A:644:GLU:HA	1.97	0.46
1:B:410:ARG:O	1:B:411:SER:C	2.57	0.46
1:A:404:ILE:HG22	1:A:529:ARG:HB3	1.97	0.46
2:E:1:GTP:H8	2:E:1:GTP:O5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:HD21	1:B:514:GLU:HB3	1.98	0.46
1:A:16:ALA:O	1:A:20:GLN:HG3	2.16	0.46
1:B:254:PHE:CZ	1:B:518:PRO:HG2	2.51	0.46
1:A:316:ASP:OD1	1:A:337:ARG:NH1	2.48	0.46
1:B:337:ARG:HB3	1:B:340:ASP:HB2	1.98	0.46
1:A:274:ASN:ND2	4:A:702:SO4:O3	2.49	0.45
1:A:560:PHE:HB2	1:A:612:VAL:HG22	1.96	0.45
1:A:308:HIS:HA	1:A:309:PRO:HD3	1.83	0.45
1:A:563:SER:HB3	1:A:612:VAL:HG11	1.98	0.45
1:A:621:ASP:N	1:A:621:ASP:OD1	2.48	0.45
1:B:633:ARG:NH2	1:B:638:MET:HG2	2.32	0.45
2:C:9:G:H1'	2:C:45:G:H2'	1.99	0.45
1:A:569:GLN:H	1:A:569:GLN:HG3	1.54	0.45
2:E:1:GTP:H2'	2:E:2:C:C6	2.52	0.45
1:A:531:MET:HE3	1:A:531:MET:HB2	1.77	0.44
1:B:242:LEU:HB3	1:B:276:PHE:CD1	2.52	0.44
1:A:644:GLU:O	1:A:647:GLU:HG2	2.18	0.44
1:A:24:VAL:O	1:A:28:LYS:HG3	2.18	0.44
1:A:61:LYS:N	1:A:62:ASP:HA	2.32	0.44
1:A:296:GLU:OE2	3:A:701:GAP:HA2	2.17	0.44
1:B:258:LEU:HG	1:B:263:GLY:HA2	1.99	0.44
1:A:602:ARG:NH1	2:E:27:C:OP2	2.51	0.44
1:A:63:ASP:O	1:A:63:ASP:OD1	2.36	0.44
2:C:49:C:H2'	2:C:50:C:C6	2.53	0.44
1:B:322:TYR:CZ	1:B:327:GLN:HG2	2.52	0.43
1:A:431:PRO:HA	1:A:513:VAL:HG12	2.00	0.43
1:A:74:LEU:HD13	1:A:80:TYR:HE2	1.83	0.43
1:A:99:VAL:HG22	6:A:804:HOH:O	2.18	0.43
1:B:412:CYS:HB2	6:B:823:HOH:O	2.18	0.43
1:A:56:LEU:O	1:A:60:PRO:HD3	2.19	0.43
1:B:203:LEU:O	1:B:207:TYR:HD1	2.02	0.43
1:A:283:ARG:NH2	2:E:1:GTP:O6	2.51	0.43
1:A:572:GLU:H	1:A:572:GLU:CD	2.25	0.43
3:A:701:GAP:H8	3:A:701:GAP:O5'	2.18	0.42
1:A:619:ASP:OD1	1:A:622:THR:OG1	2.28	0.42
1:B:580:LEU:HD21	1:B:616:VAL:HG11	2.01	0.42
1:A:369:SER:HA	1:A:370:PRO:HD3	1.82	0.42
1:B:213:ILE:O	1:B:214:THR:OG1	2.31	0.42
1:B:639:ARG:NH2	1:B:666:GLU:OE2	2.46	0.42
1:A:109:GLN:O	1:A:113:GLN:HG3	2.19	0.42
1:B:410:ARG:NH2	6:B:802:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:HB2	1:A:287:ILE:HB	2.02	0.41
1:B:329:SER:HB2	1:B:331:GLN:HG2	2.02	0.41
1:A:411:SER:OG	1:A:412:CYS:N	2.44	0.41
1:B:642:ARG:HH21	1:B:672:PHE:HE1	1.67	0.41
1:A:633:ARG:NH2	1:A:638:MET:HG2	2.35	0.41
1:B:135:LEU:HD12	1:B:241:TYR:HB2	2.03	0.41
1:A:247:ALA:N	1:A:296:GLU:OE1	2.53	0.41
1:A:281:SER:OG	1:A:283:ARG:NH2	2.28	0.41
2:C:49:C:H2'	2:C:50:C:H6	1.85	0.41
1:A:410:ARG:HH11	1:A:522:GLU:CD	2.29	0.41
1:A:131:PRO:HG2	1:A:134:VAL:HG23	2.03	0.41
1:B:413:TYR:O	1:B:417:CYS:N	2.30	0.41
2:C:22:U:H2'	2:C:23:C:O4'	2.20	0.41
1:A:264:LYS:HA	1:A:264:LYS:HD3	1.86	0.40
1:A:429:GLU:OE2	2:C:44:C:O2'	2.36	0.40
1:B:566:PRO:O	1:B:603:ARG:NH1	2.45	0.40
1:B:248:GLN:O	1:B:252:LEU:HG	2.21	0.40
1:A:420:ARG:O	1:A:420:ARG:HD2	2.22	0.40
2:C:8:U:H5'	2:C:49:C:OP2	2.21	0.40
1:A:70:MET:HE2	1:A:70:MET:HB3	1.95	0.40
2:C:15:G:H2'	2:C:16:U:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	509/693 (73%)	490 (96%)	16 (3%)	3 (1%)	21	50
1	B	498/693 (72%)	472 (95%)	22 (4%)	4 (1%)	16	43
All	All	1007/1386 (73%)	962 (96%)	38 (4%)	7 (1%)	18	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	SER
1	A	413	TYR
1	B	150	LYS
1	B	411	SER
1	B	413	TYR
1	A	234	PRO
1	B	197	GLN

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	407/600 (68%)	391 (96%)	16 (4%)	28	61
1	B	399/600 (66%)	386 (97%)	13 (3%)	33	65
All	All	806/1200 (67%)	777 (96%)	29 (4%)	31	63

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	27	LEU
1	A	28	LYS
1	A	56	LEU
1	A	64	ILE
1	A	86	ILE
1	A	136	LYS
1	A	246	THR
1	A	306	LYS
1	A	334	ARG
1	A	410	ARG
1	A	569	GLN
1	A	572	GLU
1	A	621	ASP
1	A	623	VAL
1	A	646	SER

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Mol	Chain	Res	Type
1	B	65	VAL
1	B	128	MET
1	B	198	GLN
1	B	307	ASP
1	B	319	LEU
1	B	343	GLU
1	B	352	LEU
1	B	410	ARG
1	B	414	ASP
1	B	415	LEU
1	B	508	GLN
1	B	586	ARG
1	B	626	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	318	HIS
1	A	540	HIS
1	A	547	GLN
1	A	657	ASN
1	B	109	GLN
1	B	113	GLN
1	B	216	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	72/74 (97%)	7 (9%)	0
2	E	72/74 (97%)	11 (15%)	0
All	All	144/148 (97%)	18 (12%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	9	G
2	C	12	G
2	C	18	G
2	C	37	A

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Mol	Chain	Res	Type
2	C	38	U
2	C	48	C
2	C	76	A
2	E	9	G
2	E	18	G
2	E	19	G
2	E	20	U
2	E	31	A
2	E	37	A
2	E	38	U
2	E	48	C
2	E	63	C
2	E	74	C
2	E	76	A

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues 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	E	1	2	33,34,34	2.74	14 (42%)	50,54,54	2.03	11 (22%)
2	GTP	C	1	2	33,34,34	2.74	12 (36%)	50,54,54	2.04	12 (24%)

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	E	1	2	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GTP	C	1	2	-	4/22/38/38	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	GTP	O6-C6	9.55	1.41	1.23
2	E	1	GTP	O6-C6	9.53	1.41	1.23
2	C	1	GTP	C2-N2	4.82	1.45	1.34
2	E	1	GTP	C2-N2	4.77	1.45	1.34
2	C	1	GTP	C2'-C3'	-4.66	1.40	1.53
2	C	1	GTP	C5-N7	-4.34	1.30	1.39
2	E	1	GTP	C5-N7	-4.21	1.30	1.39
2	E	1	GTP	C2'-C3'	-3.89	1.42	1.53
2	E	1	GTP	C8-N9	-3.71	1.29	1.37
2	C	1	GTP	C8-N9	-3.62	1.29	1.37
2	E	1	GTP	O4'-C4'	-3.54	1.37	1.45
2	E	1	GTP	PB-O3A	-3.27	1.56	1.59
2	C	1	GTP	PB-O3A	-3.16	1.56	1.59
2	C	1	GTP	C8-N7	-2.95	1.24	1.32
2	E	1	GTP	C8-N7	-2.89	1.24	1.32
2	C	1	GTP	C5-C4	2.86	1.46	1.38
2	E	1	GTP	C5-C4	2.80	1.46	1.38
2	C	1	GTP	O3'-C3'	-2.70	1.36	1.43
2	C	1	GTP	O4'-C4'	-2.68	1.39	1.45
2	E	1	GTP	PA-O3A	-2.23	1.57	1.59
2	E	1	GTP	O5'-C5'	-2.15	1.36	1.44
2	E	1	GTP	C4-N9	2.12	1.43	1.38
2	E	1	GTP	C6-N1	-2.11	1.34	1.38
2	C	1	GTP	C4-N9	2.06	1.43	1.38
2	E	1	GTP	O3'-C3'	-2.03	1.37	1.43
2	C	1	GTP	C6-N1	-2.01	1.35	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	GTP	N9-C4-N3	6.10	138.15	125.95
2	C	1	GTP	N9-C4-N3	6.09	138.13	125.95
2	E	1	GTP	C5-C4-N3	-5.91	118.98	128.39
2	C	1	GTP	C5-C4-N3	-5.54	119.57	128.39
2	E	1	GTP	C8-N7-C5	5.31	113.71	104.26
2	C	1	GTP	C8-N7-C5	5.05	113.26	104.26
2	E	1	GTP	C2-N3-C4	4.53	120.09	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	GTP	C2-N3-C4	4.26	119.63	112.30
2	E	1	GTP	C4-C5-N7	-4.02	104.30	110.67
2	E	1	GTP	C6-C5-N7	3.92	137.42	130.29
2	C	1	GTP	C6-C5-N7	3.64	136.92	130.29
2	C	1	GTP	C4-C5-N7	-3.61	104.95	110.67
2	C	1	GTP	O5'-C5'-C4'	3.35	120.40	108.99
2	C	1	GTP	C3'-C2'-C1'	2.92	106.99	101.46
2	E	1	GTP	C2-N1-C6	-2.75	120.11	125.11
2	E	1	GTP	O5'-C5'-C4'	2.71	118.21	108.99
2	E	1	GTP	C5-C6-N1	2.56	119.77	113.25
2	E	1	GTP	O6-C6-C5	-2.51	119.92	126.53
2	C	1	GTP	C2-N1-C6	-2.45	120.66	125.11
2	C	1	GTP	C5-C6-N1	2.43	119.45	113.25
2	C	1	GTP	O6-C6-C5	-2.40	120.19	126.53
2	E	1	GTP	C1'-N9-C8	2.13	132.79	126.73
2	C	1	GTP	O4'-C4'-C3'	2.07	109.26	105.15

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	GTP	C5'-O5'-PA-O3A
2	C	1	GTP	C5'-O5'-PA-O1A
2	E	1	GTP	C5'-O5'-PA-O2A
2	E	1	GTP	O4'-C4'-C5'-O5'
2	E	1	GTP	C5'-O5'-PA-O3A
2	E	1	GTP	C5'-O5'-PA-O1A
2	C	1	GTP	PB-O3A-PA-O2A
2	C	1	GTP	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	GTP	3	0
2	C	1	GTP	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	SO4	A	702	-	4,4,4	0.71	0	6,6,6	0.19	0
3	GAP	B	701	-	28,29,29	1.35	4 (14%)	39,43,43	1.88	9 (23%)
3	GAP	A	701	-	28,29,29	1.42	4 (14%)	39,43,43	1.87	7 (17%)

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	GAP	B	701	-	-	3/15/33/33	0/3/3/3
3	GAP	A	701	-	-	3/15/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	GAP	C5-C4	4.94	1.47	1.39
3	B	701	GAP	C5-C4	4.62	1.47	1.39
3	A	701	GAP	C5-C6	3.03	1.49	1.41
3	B	701	GAP	C5-C6	2.79	1.48	1.41
3	A	701	GAP	C8-N7	2.65	1.36	1.31
3	B	701	GAP	C5-N7	-2.32	1.34	1.39
3	B	701	GAP	C8-N7	2.23	1.36	1.31
3	A	701	GAP	C5-N7	-2.16	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	GAP	C5-C4-N3	-6.14	118.26	126.72
3	B	701	GAP	C5-C4-N3	-5.98	118.48	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	GAP	N3-C4-N9	4.72	135.20	127.17
3	A	701	GAP	N3-C4-N9	4.24	134.38	127.17
3	A	701	GAP	C4-C5-N7	-4.07	105.93	110.58
3	A	701	GAP	C2-N3-C4	3.82	121.15	111.83
3	B	701	GAP	C2-N3-C4	3.78	121.07	111.83
3	B	701	GAP	C4-C5-N7	-3.64	106.42	110.58
3	B	701	GAP	N3-C2-N1	-3.26	123.65	128.58
3	A	701	GAP	N3-C2-N1	-3.09	123.91	128.58
3	B	701	GAP	C5-N7-C8	2.77	107.80	103.45
3	A	701	GAP	C5-N7-C8	2.74	107.75	103.45
3	B	701	GAP	C4-N9-C8	2.71	108.59	105.74
3	A	701	GAP	C6-C5-N7	2.24	136.41	132.09
3	B	701	GAP	N9-C8-N7	-2.16	110.87	113.94
3	B	701	GAP	C6-C5-N7	2.14	136.22	132.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	GAP	O-C-CA-N
3	A	701	GAP	O3A-C-CA-N
3	B	701	GAP	O-C-CA-N
3	B	701	GAP	O3A-C-CA-N
3	A	701	GAP	C-O3A-PA-O1A
3	B	701	GAP	C-O3A-PA-O1A

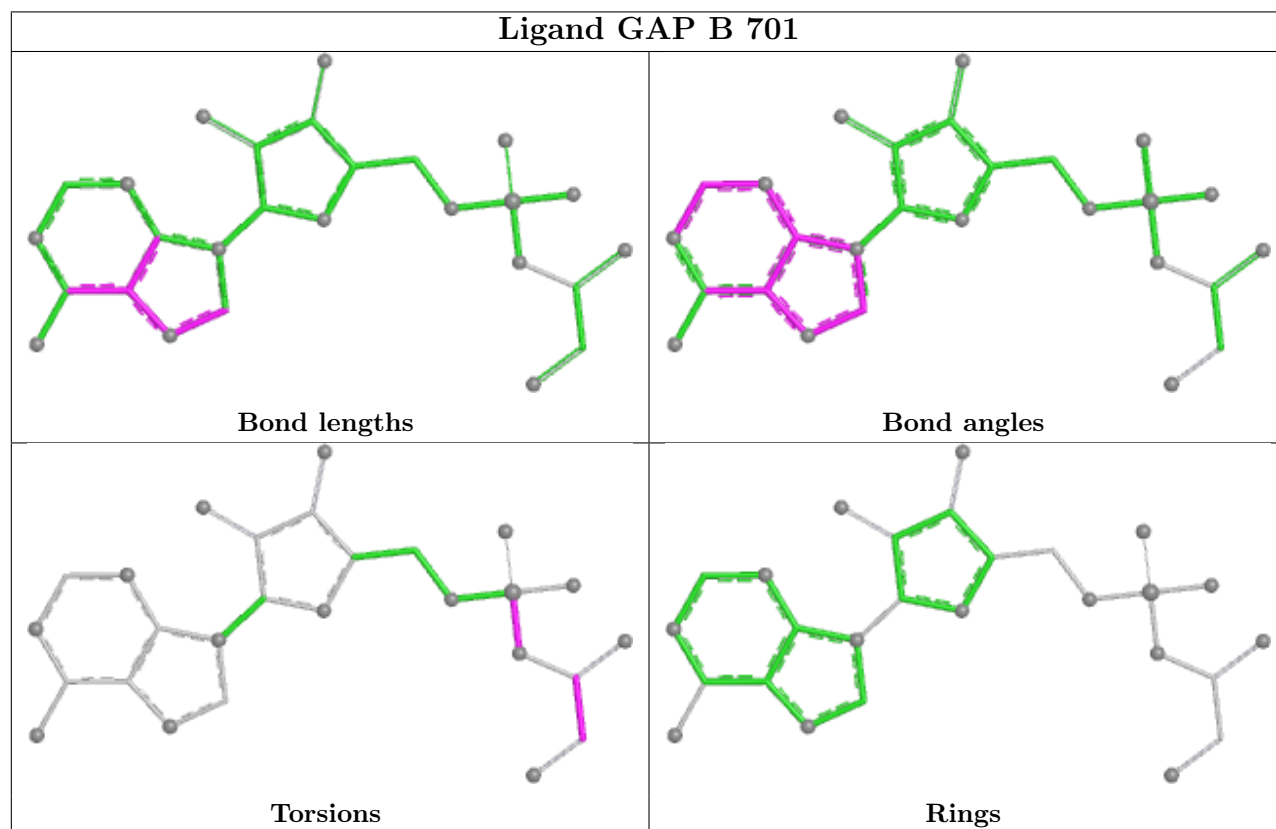
There are no ring outliers.

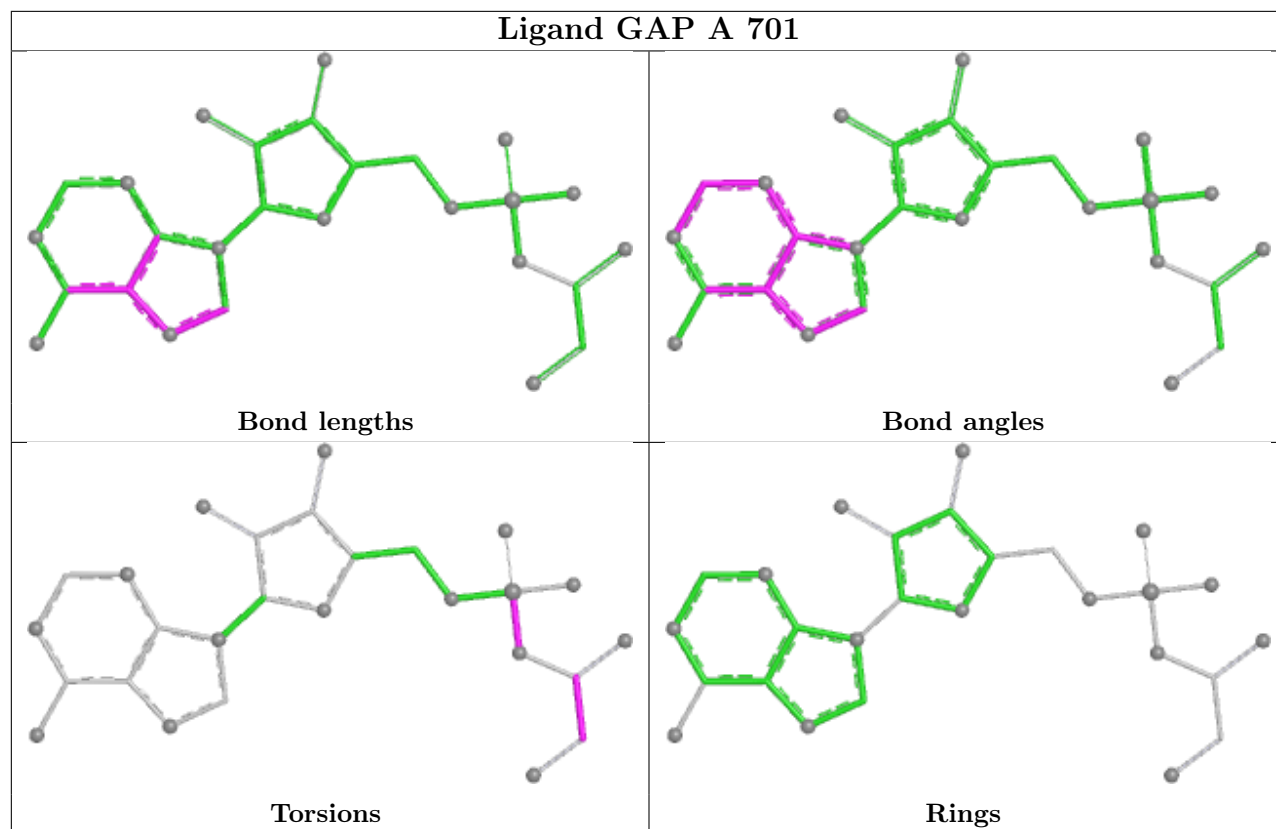
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	SO4	1	0
3	B	701	GAP	1	0
3	A	701	GAP	2	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	519/693 (74%)	0.03	18 (3%) 47 38	32, 56, 108, 137	0
1	B	506/693 (73%)	0.08	18 (3%) 46 37	36, 58, 107, 136	0
2	C	73/74 (98%)	-0.31	0 100 100	44, 57, 91, 96	0
2	E	73/74 (98%)	-0.24	0 100 100	45, 69, 99, 111	0
All	All	1171/1534 (76%)	0.01	36 (3%) 51 41	32, 58, 107, 137	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	678	GLY	5.8
1	A	234	PRO	5.3
1	A	147	PHE	4.8
1	B	64	ILE	4.4
1	B	386	TYR	4.3
1	A	40	ALA	4.0
1	A	237	ASN	4.0
1	A	37	VAL	3.7
1	A	41	VAL	3.4
1	A	677	THR	3.4
1	B	234	PRO	3.0
1	B	146	ASP	2.9
1	B	151	ASP	2.9
1	B	343	GLU	2.7
1	B	150	LYS	2.6
1	B	217	ASP	2.6
1	A	678	GLY	2.5
1	A	62	ASP	2.5
1	A	38	ASP	2.5
1	A	436	LYS	2.4
1	B	387	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	546	GLU	2.3
1	B	153	LYS	2.2
1	A	60	PRO	2.2
1	A	7	GLU	2.2
1	B	218	LEU	2.2
1	B	412	CYS	2.2
1	B	597	SER	2.2
1	B	235	GLY	2.1
1	B	388	CYS	2.1
1	A	577	VAL	2.1
1	A	43	GLU	2.1
1	A	675	GLN	2.0
1	A	145	ALA	2.0
1	B	389	ASP	2.0
1	A	146	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	GTP	C	1	32/32	0.77	0.17	98,111,156,183	0
2	GTP	E	1	32/32	0.79	0.14	84,111,147,159	0

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(Å ²)	Q<0.9
4	SO4	A	702	5/5	0.90	0.14	89,91,105,145	0

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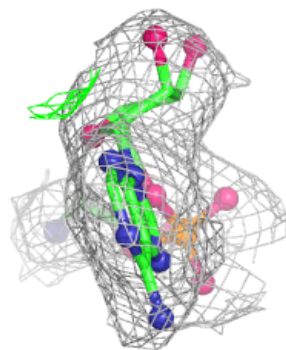
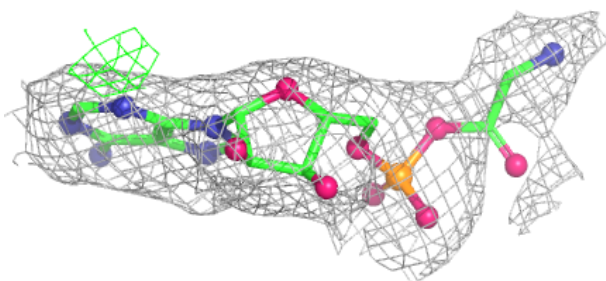
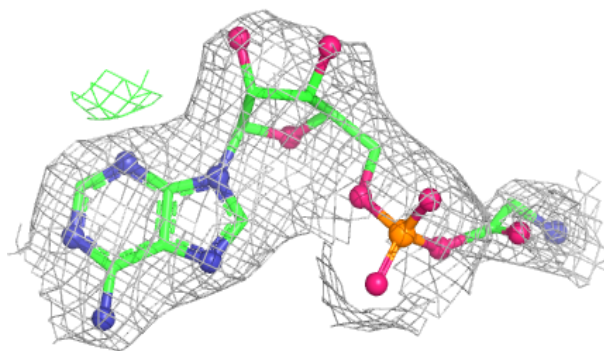
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NI	E	101	1/1	0.93	0.09	115,115,115,115	0
5	NI	C	101	1/1	0.95	0.07	89,89,89,89	0
3	GAP	B	701	27/27	0.95	0.08	40,50,87,109	0
3	GAP	A	701	27/27	0.96	0.07	34,53,82,95	0

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.

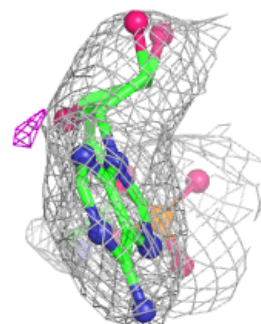
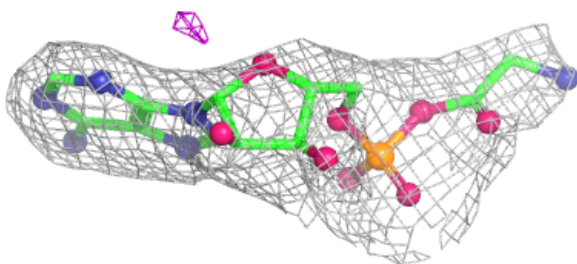
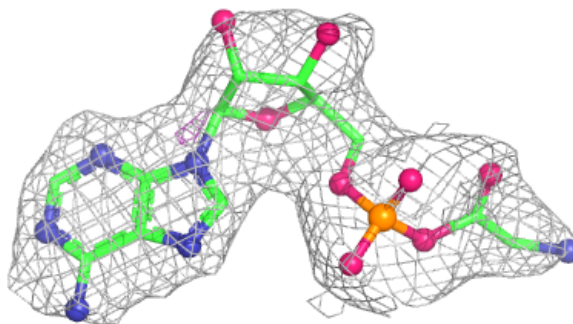
Electron density around GAP B 701:

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 GAP 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.