



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:43 AM EDT

PDB ID : 8Y1T / pdb_00008y1t
Title : CRYSTAL STRUCTURE OF TRYPANOSOMA BRUCEI GAMBIENSE GLYCEROL KINASE COMPLEX WITH ADP and G3P
Authors : Balogun, E.O.; Inaoka, D.K.; Ichinose, M.; Chishima, T.; Harada, S.; Kita, K.; Shiba, T.
Deposited on : 2024-01-25
Resolution : 2.40 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

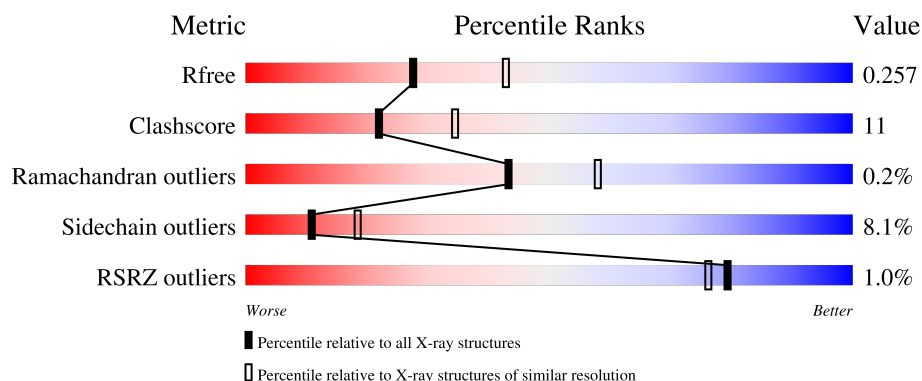
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	518	79% 18% ..
1	B	518	74% 21% ...

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7989 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.

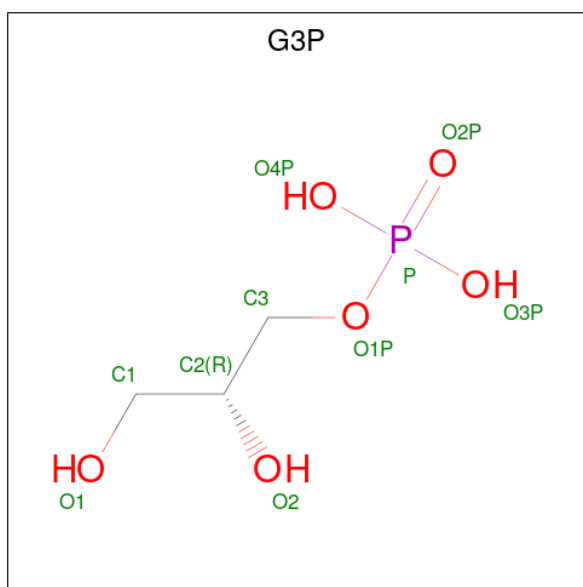
- Molecule 1 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			3956	2496	695	732	33			
1	B	514	Total	C	N	O	S	0	0	0
			3956	2496	695	732	33			

There are 12 discrepancies between the modelled and reference sequences:

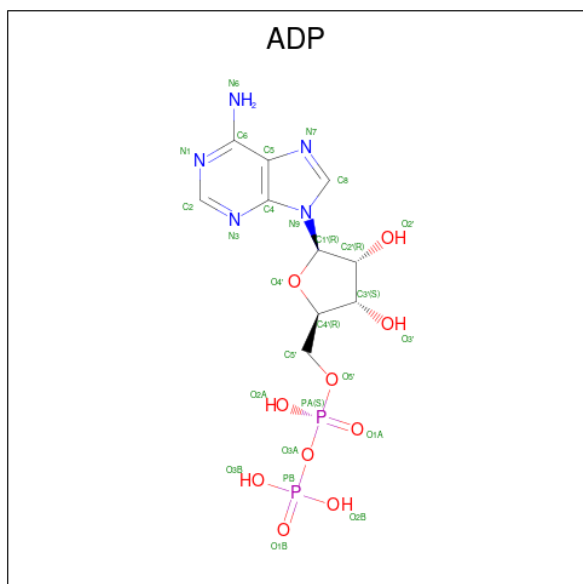
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP D3KVM3
A	-4	ILE	-	expression tag	UNP D3KVM3
A	-3	ASP	-	expression tag	UNP D3KVM3
A	-2	PRO	-	expression tag	UNP D3KVM3
A	-1	PHE	-	expression tag	UNP D3KVM3
A	0	THR	-	expression tag	UNP D3KVM3
B	-5	GLY	-	expression tag	UNP D3KVM3
B	-4	ILE	-	expression tag	UNP D3KVM3
B	-3	ASP	-	expression tag	UNP D3KVM3
B	-2	PRO	-	expression tag	UNP D3KVM3
B	-1	PHE	-	expression tag	UNP D3KVM3
B	0	THR	-	expression tag	UNP D3KVM3

- Molecule 2 is SN-GLYCEROL-3-PHOSPHATE (CCD ID: G3P) (formula: $C_3H_9O_6P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃) (labeled as "Ligand of Interest" by depositor).

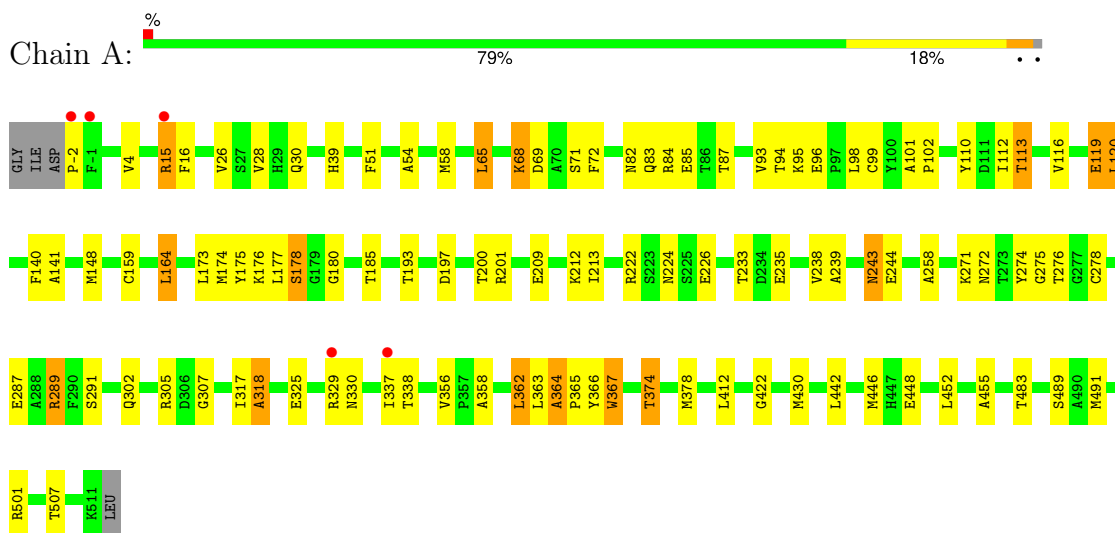


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

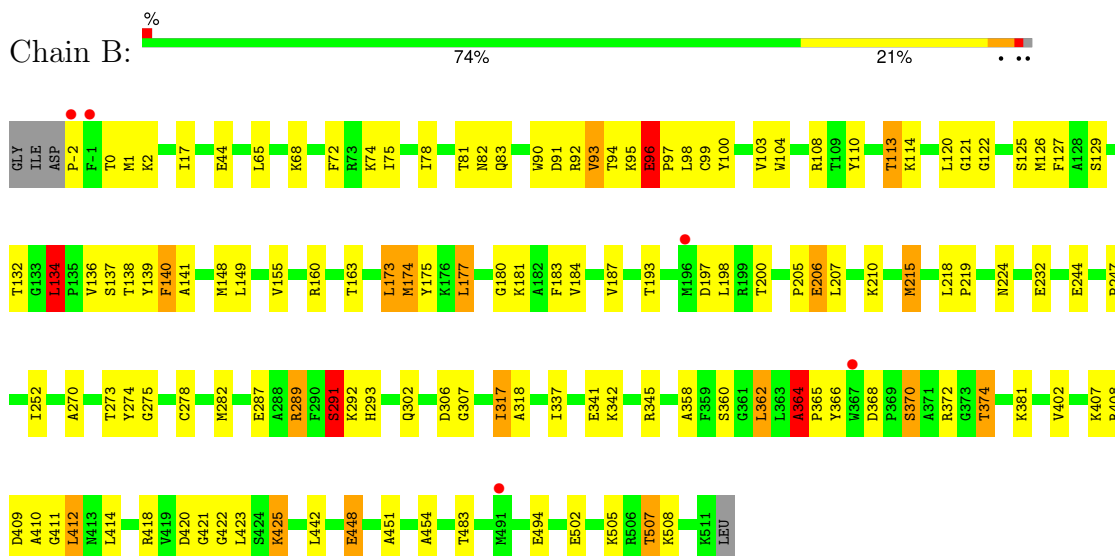
3 Residue-property plots [i](#)

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: Glycerol kinase



• Molecule 1: Glycerol kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.56Å 121.74Å 154.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.40 19.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.86-2.40) 99.7 (19.86-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.192 , 0.250 0.207 , 0.257	Depositor DCC
R_{free} test set	2326 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7989	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G3P, GOL, MG, ADP

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	1.05	0/4037	1.04	14/5463 (0.3%)
1	B	0.99	1/4037 (0.0%)	1.10	25/5463 (0.5%)
All	All	1.02	1/8074 (0.0%)	1.07	39/10926 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	364	ALA	C-N	7.44	1.39	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	GLY	N-CA-C	-11.21	89.47	112.34
1	B	291	SER	N-CA-C	8.22	122.31	109.07
1	A	235	GLU	N-CA-C	7.10	118.66	111.07
1	B	74	LYS	N-CA-C	6.94	118.73	108.60
1	A	82	ASN	N-CA-C	6.86	119.49	109.07
1	A	-2	PRO	N-CA-CB	6.84	110.52	103.00
1	B	82	ASN	N-CA-C	6.80	119.10	108.96
1	A	140	PHE	N-CA-C	6.73	119.99	110.23
1	B	318	ALA	N-CA-C	6.64	118.60	111.36
1	A	291	SER	N-CA-C	6.61	119.70	109.07
1	B	207	LEU	N-CA-C	6.52	118.47	111.36
1	B	83	GLN	N-CA-C	-6.47	100.26	109.96
1	B	139	TYR	N-CA-C	6.39	118.24	111.28
1	B	364	ALA	CA-C-N	-6.37	113.61	121.00
1	B	364	ALA	C-N-CA	-6.37	113.61	121.00
1	B	275	GLY	N-CA-C	-6.36	99.97	111.16
1	B	140	PHE	N-CA-C	6.25	119.54	110.28
1	B	134	LEU	N-CA-C	6.25	119.58	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLU	N-CA-C	6.10	118.01	111.36
1	B	-2	PRO	N-CA-CB	6.08	109.69	103.00
1	A	318	ALA	N-CA-C	6.06	117.96	111.36
1	B	198	LEU	N-CA-C	5.87	117.35	111.07
1	B	134	LEU	CA-C-N	-5.83	114.60	120.31
1	B	134	LEU	C-N-CA	-5.83	114.60	120.31
1	B	307	GLY	CA-C-N	-5.79	113.82	119.78
1	B	307	GLY	C-N-CA	-5.79	113.82	119.78
1	B	507	THR	N-CA-C	5.68	120.21	113.28
1	A	378	MET	N-CA-C	5.58	118.36	110.50
1	A	307	GLY	CA-C-N	-5.40	114.20	119.76
1	A	307	GLY	C-N-CA	-5.40	114.20	119.76
1	A	68	LYS	N-CA-C	5.39	119.96	113.17
1	B	96	GLU	CA-C-N	-5.37	114.39	119.76
1	B	96	GLU	C-N-CA	-5.37	114.39	119.76
1	B	218	LEU	CA-C-N	-5.24	115.33	120.52
1	B	218	LEU	C-N-CA	-5.24	115.33	120.52
1	A	39	HIS	CA-C-N	-5.17	114.43	119.76
1	A	39	HIS	C-N-CA	-5.17	114.43	119.76
1	B	132	THR	N-CA-C	5.16	119.58	113.12
1	A	164	LEU	N-CA-C	5.04	117.78	109.76

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	3956	0	3962	69	0
1	B	3956	0	3962	101	0
2	A	10	0	7	0	0
3	A	27	0	12	4	0
3	B	27	0	12	1	0
4	A	1	0	0	0	0
5	B	12	0	16	0	0
All	All	7989	0	7971	170	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 11.

All (170) 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:B:278:CYS:HB2	1:B:317:ILE:CG2	1.67	1.23
1:A:364:ALA:HB1	1:A:365:PRO:CD	1.69	1.22
1:B:205:PRO:HA	1:B:215:MET:HE1	1.21	1.19
1:A:15:ARG:HD2	1:A:30:GLN:NE2	1.63	1.12
1:A:364:ALA:CB	1:A:365:PRO:HD2	1.84	1.08
1:A:364:ALA:HB1	1:A:365:PRO:HD2	1.36	1.06
1:B:90:TRP:HA	1:B:98:LEU:HD13	1.38	1.05
1:B:278:CYS:HB2	1:B:317:ILE:HG23	1.08	1.05
1:B:205:PRO:CA	1:B:215:MET:HE1	1.86	1.05
1:B:113:THR:HG23	1:B:114:LYS:HE3	1.40	1.02
1:A:364:ALA:CB	1:A:365:PRO:CD	2.34	1.00
1:B:206:GLU:N	1:B:206:GLU:OE2	1.94	1.00
1:A:275:GLY:HA3	3:A:602:ADP:O1B	1.63	0.99
1:B:113:THR:CG2	1:B:114:LYS:HE3	1.93	0.98
1:A:15:ARG:HD2	1:A:30:GLN:HE21	0.83	0.98
1:A:15:ARG:CD	1:A:30:GLN:HE21	1.76	0.98
1:A:364:ALA:HB1	1:A:365:PRO:HD3	1.48	0.95
1:B:278:CYS:CB	1:B:317:ILE:HG23	1.97	0.94
1:A:174:MET:O	1:A:178:SER:HB2	1.68	0.93
1:B:114:LYS:HA	1:B:114:LYS:HE2	1.49	0.92
1:B:278:CYS:CB	1:B:317:ILE:CG2	2.50	0.88
1:B:205:PRO:HA	1:B:215:MET:CE	2.04	0.85
1:A:110:TYR:O	1:A:113:THR:HG22	1.77	0.84
1:B:197:ASP:OD1	1:B:200:THR:HG23	1.77	0.83
1:B:110:TYR:O	1:B:113:THR:HG22	1.80	0.81
1:B:44:GLU:HG2	1:B:100:TYR:HB3	1.65	0.79
1:A:325:GLU:HG3	1:A:329:ARG:HE	1.49	0.77
1:B:422:GLY:O	1:B:425:LYS:HG3	1.85	0.76
1:A:329:ARG:HD2	1:A:330:ASN:OD1	1.84	0.76
1:B:94:THR:C	1:B:95:LYS:HG2	2.11	0.76
1:A:325:GLU:O	1:A:329:ARG:HG2	1.88	0.73
1:B:90:TRP:CA	1:B:98:LEU:HD13	2.17	0.73
1:B:113:THR:HG23	1:B:114:LYS:CE	2.17	0.73
1:A:99:CYS:SG	1:A:148:MET:HE2	2.29	0.72
1:B:205:PRO:CB	1:B:215:MET:HE1	2.18	0.72
1:A:325:GLU:O	1:A:329:ARG:CG	2.38	0.72
1:B:91:ASP:HB3	1:B:94:THR:OG1	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:HD11	1:B:78:ILE:HG13	1.74	0.69
1:B:291:SER:HA	1:B:409:ASP:OD1	1.92	0.69
1:A:364:ALA:HB3	1:A:365:PRO:HD2	1.70	0.69
1:B:68:LYS:HE2	3:B:603:ADP:H5'2	1.75	0.68
1:B:278:CYS:HB2	1:B:317:ILE:HG22	1.70	0.68
1:B:114:LYS:HE2	1:B:114:LYS:CA	2.23	0.67
1:B:91:ASP:OD1	1:B:93:VAL:N	2.28	0.66
1:A:83:GLN:O	1:A:83:GLN:HG3	1.94	0.66
1:B:273:THR:HG23	1:B:420:ASP:OD2	1.96	0.65
1:B:364:ALA:HB1	1:B:402:VAL:HG22	1.78	0.65
1:B:141:ALA:HB3	1:B:193:THR:HA	1.79	0.65
1:A:275:GLY:CA	3:A:602:ADP:O1B	2.43	0.64
1:B:287:GLU:OE2	1:B:289:ARG:NH2	2.31	0.63
1:B:364:ALA:HB1	1:B:365:PRO:CD	2.28	0.62
1:A:374:THR:HG21	1:A:507:THR:HA	1.80	0.62
1:B:17:ILE:HD13	1:B:448:GLU:CG	2.29	0.62
1:B:502:GLU:OE2	1:B:505:LYS:NZ	2.33	0.62
1:B:206:GLU:O	1:B:210:LYS:HB2	2.00	0.61
1:A:224:ASN:HD22	1:A:302:GLN:H	1.49	0.61
1:B:125:SER:O	1:B:136:VAL:HG23	2.00	0.61
1:B:113:THR:HG22	1:B:114:LYS:HE3	1.81	0.61
1:A:141:ALA:HB3	1:A:193:THR:HA	1.82	0.60
1:B:99:CYS:SG	1:B:148:MET:HE3	2.41	0.60
1:B:374:THR:CG2	1:B:507:THR:HG22	2.31	0.60
1:A:87:THR:O	1:A:101:ALA:HB1	2.02	0.59
1:B:274:TYR:O	1:B:421:GLY:HA3	2.01	0.59
1:B:407:LYS:O	1:B:411:GLY:N	2.36	0.58
1:A:287:GLU:HG2	1:A:289:ARG:HH21	1.67	0.58
1:B:292:LYS:N	1:B:409:ASP:OD1	2.31	0.58
1:B:293:HIS:CD2	1:B:409:ASP:OD2	2.57	0.57
1:A:318:ALA:HB2	1:A:363:LEU:HD11	1.86	0.57
1:A:222:ARG:HD3	1:A:305:ARG:NH1	2.19	0.57
1:A:356:VAL:HG11	1:A:507:THR:HG21	1.87	0.57
1:B:270:ALA:HB3	1:B:414:LEU:HD11	1.86	0.57
1:B:91:ASP:OD1	1:B:94:THR:N	2.31	0.57
1:A:272:ASN:HD21	1:A:278:CYS:HB3	1.70	0.56
1:B:197:ASP:OD1	1:B:200:THR:CG2	2.52	0.56
1:B:364:ALA:CB	1:B:365:PRO:CD	2.83	0.56
1:A:69:ASP:OD1	1:A:71:SER:OG	2.21	0.56
1:B:293:HIS:HD2	1:B:409:ASP:OD2	1.88	0.56
1:A:120:LEU:HD23	1:A:120:LEU:N	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LYS:CE	1:B:114:LYS:CA	2.85	0.55
1:B:17:ILE:HD13	1:B:448:GLU:HG2	1.89	0.55
1:A:325:GLU:O	1:A:329:ARG:HG3	2.06	0.54
1:B:91:ASP:N	1:B:98:LEU:HD11	2.22	0.54
1:B:44:GLU:HG2	1:B:100:TYR:CB	2.35	0.54
1:A:287:GLU:HG2	1:A:289:ARG:NH2	2.22	0.54
1:B:81:THR:HA	1:B:252:ILE:O	2.08	0.53
1:B:364:ALA:HB1	1:B:365:PRO:HD3	1.90	0.53
1:A:159:CYS:HB2	1:A:164:LEU:HD22	1.89	0.53
1:A:15:ARG:NH2	1:A:28:VAL:HG21	2.24	0.52
1:A:65:LEU:HD13	1:A:72:PHE:CG	2.45	0.52
1:B:98:LEU:N	1:B:98:LEU:CD1	2.73	0.52
1:A:358:ALA:HB2	1:A:362:LEU:HD13	1.92	0.52
1:B:374:THR:HG23	1:B:507:THR:HG22	1.91	0.52
1:B:287:GLU:O	1:B:287:GLU:HG3	2.09	0.51
1:A:112:ILE:O	1:A:116:VAL:HG23	2.10	0.51
1:B:224:ASN:HD22	1:B:302:GLN:H	1.59	0.51
1:B:372:ARG:O	1:B:374:THR:HG22	2.11	0.51
1:B:126:MET:HE3	1:B:129:SER:CB	2.42	0.50
1:A:276:THR:N	3:A:602:ADP:O1B	2.42	0.50
1:B:96:GLU:HG3	1:B:97:PRO:HD2	1.93	0.49
1:A:325:GLU:HG3	1:A:329:ARG:NE	2.23	0.49
1:B:17:ILE:HD12	1:B:451:ALA:CB	2.41	0.49
1:A:102:PRO:HD3	1:A:148:MET:HE3	1.93	0.49
1:B:174:MET:HE3	1:B:184:VAL:HG23	1.95	0.49
1:B:91:ASP:N	1:B:98:LEU:CD1	2.75	0.49
1:B:374:THR:HG21	1:B:507:THR:HG22	1.94	0.48
1:B:75:ILE:HD11	1:B:78:ILE:CG1	2.41	0.48
1:B:1:MET:HG3	1:B:2:LYS:N	2.27	0.48
1:B:99:CYS:HG	1:B:148:MET:HE3	1.76	0.48
1:A:325:GLU:HG3	1:A:329:ARG:HG2	1.94	0.48
1:B:44:GLU:OE1	1:B:108:ARG:NH1	2.40	0.48
1:A:51:PHE:CE1	1:A:176:LYS:HB3	2.48	0.48
1:A:274:TYR:CZ	1:A:430:MET:HE1	2.48	0.48
1:B:410:ALA:O	1:B:412:LEU:HD12	2.13	0.48
1:B:423:LEU:HD23	1:B:423:LEU:HA	1.73	0.47
1:A:209:GLU:O	1:A:212:LYS:CD	2.62	0.47
1:A:200:THR:O	1:A:201:ARG:HB2	2.14	0.47
1:A:422:GLY:HA3	3:A:602:ADP:H5'2	1.96	0.47
1:A:222:ARG:HG2	1:A:305:ARG:HH12	1.78	0.47
1:A:374:THR:CG2	1:A:507:THR:HG22	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:THR:HG23	1:A:507:THR:HG22	1.96	0.47
1:B:205:PRO:HB3	1:B:215:MET:HE1	1.95	0.47
1:A:4:VAL:HG11	1:A:455:ALA:O	2.15	0.47
1:A:54:ALA:O	1:A:58:MET:HG3	2.15	0.46
1:A:274:TYR:CE1	1:A:430:MET:HE1	2.50	0.46
1:A:84:ARG:O	1:A:85:GLU:HB2	2.14	0.46
1:B:94:THR:O	1:B:95:LYS:CB	2.62	0.46
1:A:175:TYR:CE1	1:A:180:GLY:HA2	2.50	0.46
1:A:119:GLU:C	1:A:120:LEU:HD23	2.40	0.45
1:A:362:LEU:O	1:A:367:TRP:HA	2.16	0.45
1:A:446:MET:CE	1:A:452:LEU:HD22	2.46	0.45
1:A:233:THR:O	1:A:239:ALA:HB2	2.16	0.45
1:B:94:THR:O	1:B:95:LYS:CG	2.65	0.45
1:B:368:ASP:OD1	1:B:370:SER:HB2	2.17	0.45
1:A:238:VAL:HG13	1:A:239:ALA:N	2.32	0.45
1:B:134:LEU:HD13	1:B:140:PHE:CD1	2.52	0.44
1:B:92:ARG:HB2	1:B:163:THR:O	2.17	0.44
1:B:358:ALA:HB2	1:B:362:LEU:CD1	2.48	0.44
1:A:258:ALA:HB3	1:A:271:LYS:HE2	2.00	0.44
1:B:103:VAL:O	1:B:104:TRP:C	2.61	0.44
1:B:126:MET:HE3	1:B:126:MET:HB3	1.69	0.43
1:A:222:ARG:HD3	1:A:226:GLU:OE1	2.17	0.43
1:B:448:GLU:OE1	1:B:448:GLU:HA	2.18	0.43
1:B:98:LEU:N	1:B:98:LEU:HD12	2.33	0.43
1:B:374:THR:HG21	1:B:507:THR:HA	2.00	0.43
1:B:94:THR:O	1:B:95:LYS:HG2	2.18	0.42
1:A:197:ASP:O	1:A:201:ARG:N	2.45	0.42
1:A:94:THR:C	1:A:95:LYS:CG	2.92	0.42
1:B:282:MET:HE2	1:B:414:LEU:CD1	2.49	0.42
1:B:120:LEU:C	1:B:122:GLY:N	2.73	0.42
1:B:274:TYR:O	1:B:421:GLY:CA	2.65	0.42
1:B:121:GLY:HA2	1:B:127:PHE:CG	2.55	0.42
1:B:341:GLU:OE2	1:B:345:ARG:NH2	2.53	0.42
1:B:75:ILE:CD1	1:B:78:ILE:HG13	2.47	0.41
1:A:16:PHE:CD2	1:A:58:MET:HA	2.55	0.41
1:A:26:VAL:O	1:A:68:LYS:HE3	2.20	0.41
1:B:90:TRP:C	1:B:98:LEU:HD13	2.45	0.41
1:B:81:THR:HB	1:B:454:ALA:HB2	2.01	0.41
1:B:183:PHE:CD2	1:B:219:PRO:HA	2.56	0.41
1:B:287:GLU:CD	1:B:289:ARG:NH2	2.79	0.41
1:A:209:GLU:O	1:A:212:LYS:HD2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:HD22	1:A:243:ASN:HA	1.71	0.41
1:B:278:CYS:SG	1:B:317:ILE:CG2	3.09	0.41
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.93	0.41
1:B:99:CYS:SG	1:B:148:MET:CE	3.09	0.41
1:A:222:ARG:CG	1:A:305:ARG:HH12	2.35	0.40
1:B:181:LYS:NZ	1:B:232:GLU:OE2	2.25	0.40
1:B:149:LEU:HD23	1:B:155:VAL:HG12	2.04	0.40
1:B:173:LEU:O	1:B:177:LEU:HB2	2.22	0.40
1:B:175:TYR:CE1	1:B:180:GLY:HA2	2.57	0.40
1:B:358:ALA:CB	1:B:362:LEU:HD13	2.51	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	512/518 (99%)	492 (96%)	19 (4%)	1 (0%)	43	58
1	B	512/518 (99%)	484 (94%)	27 (5%)	1 (0%)	43	58
All	All	1024/1036 (99%)	976 (95%)	46 (4%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ALA
1	B	364	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	420/425 (99%)	391 (93%)	29 (7%)	14	24
1	B	420/425 (99%)	381 (91%)	39 (9%)	8	14
All	All	840/850 (99%)	772 (92%)	68 (8%)	11	18

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	65	LEU
1	A	93	VAL
1	A	96	GLU
1	A	98	LEU
1	A	113	THR
1	A	120	LEU
1	A	173	LEU
1	A	177	LEU
1	A	178	SER
1	A	185	THR
1	A	213	ILE
1	A	243	ASN
1	A	244	GLU
1	A	289	ARG
1	A	317	ILE
1	A	337	ILE
1	A	338	THR
1	A	362	LEU
1	A	366	TYR
1	A	367	TRP
1	A	374	THR
1	A	412	LEU
1	A	442	LEU
1	A	448	GLU
1	A	483	THR
1	A	489	SER
1	A	491	MET
1	A	501	ARG
1	B	0	THR
1	B	65	LEU
1	B	72	PHE
1	B	93	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	96	GLU
1	B	113	THR
1	B	134	LEU
1	B	137	SER
1	B	138	THR
1	B	160	ARG
1	B	173	LEU
1	B	174	MET
1	B	177	LEU
1	B	187	VAL
1	B	206	GLU
1	B	215	MET
1	B	244	GLU
1	B	247	PRO
1	B	289	ARG
1	B	291	SER
1	B	306	ASP
1	B	317	ILE
1	B	337	ILE
1	B	342	LYS
1	B	360	SER
1	B	362	LEU
1	B	366	TYR
1	B	370	SER
1	B	374	THR
1	B	381	LYS
1	B	408	ARG
1	B	412	LEU
1	B	418	ARG
1	B	425	LYS
1	B	442	LEU
1	B	448	GLU
1	B	483	THR
1	B	494	GLU
1	B	508	LYS

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	23	GLN
1	A	29	HIS
1	A	30	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	224	ASN
1	A	243	ASN
1	A	272	ASN
1	B	30	GLN
1	B	151	ASN
1	B	224	ASN
1	B	272	ASN
1	B	293	HIS
1	B	302	GLN
1	B	336	HIS
1	B	386	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z > 2$
3	ADP	A	602	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
5	GOL	B	601	-	5,5,5	0.51	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	603	-	28,29,29	1.61	5 (17%)	43,45,45	1.89	10 (23%)
2	G3P	A	601	-	9,9,9	0.54	0	10,12,12	1.08	1 (10%)
5	GOL	B	602	-	5,5,5	0.47	0	5,5,5	1.03	0

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	ADP	A	602	-	-	3/16/32/32	0/3/3/3
5	GOL	B	601	-	-	0/4/4/4	-
3	ADP	B	603	-	-	0/16/32/32	0/3/3/3
2	G3P	A	601	-	-	2/8/8/8	-
5	GOL	B	602	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ADP	C5-C4	4.70	1.47	1.39
3	B	603	ADP	C5-N7	-3.36	1.32	1.39
3	B	603	ADP	C5-C4	3.25	1.44	1.39
3	B	603	ADP	C8-N9	-3.05	1.32	1.37
3	B	603	ADP	C4-N9	-2.90	1.31	1.37
3	A	602	ADP	C5-C6	2.79	1.48	1.41
3	A	602	ADP	C8-N7	2.40	1.36	1.31
3	B	603	ADP	C5-C6	2.37	1.47	1.41
3	A	602	ADP	C5-N7	-2.24	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	ADP	C5-C4-N3	-6.05	118.38	126.72
3	A	602	ADP	C5-C4-N3	-5.85	118.66	126.72
3	A	602	ADP	N3-C4-N9	4.60	134.99	127.17
3	B	603	ADP	N3-C4-N9	4.41	134.67	127.17
3	B	603	ADP	C4-C5-N7	-4.15	105.83	110.58
3	B	603	ADP	C2-N3-C4	3.79	121.09	111.83
3	A	602	ADP	C2-N3-C4	3.70	120.87	111.83
3	A	602	ADP	C4-C5-N7	-3.47	106.61	110.58
3	A	602	ADP	N3-C2-N1	-3.21	123.72	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	ADP	N3-C2-N1	-2.87	124.23	128.58
3	B	603	ADP	C5-N7-C8	2.85	107.93	103.45
3	A	602	ADP	C4-N9-C8	2.61	108.47	105.74
3	A	602	ADP	C3'-C2'-C1'	2.56	106.31	101.46
3	B	603	ADP	C4-N9-C8	2.55	108.42	105.74
3	A	602	ADP	C5-N7-C8	2.52	107.42	103.45
3	B	603	ADP	C6-C5-N7	2.46	136.84	132.09
3	B	603	ADP	O3'-C3'-C2'	-2.43	104.03	111.82
3	B	603	ADP	N9-C8-N7	-2.16	110.87	113.94
2	A	601	G3P	O3P-P-O4P	2.10	115.68	107.80
3	A	602	ADP	C6-C5-N7	2.08	136.09	132.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	ADP	C5'-O5'-PA-O1A
2	A	601	G3P	O2-C2-C3-O1P
2	A	601	G3P	C1-C2-C3-O1P
5	B	602	GOL	C1-C2-C3-O3
5	B	602	GOL	O2-C2-C3-O3
3	A	602	ADP	O4'-C4'-C5'-O5'
3	A	602	ADP	C3'-C4'-C5'-O5'

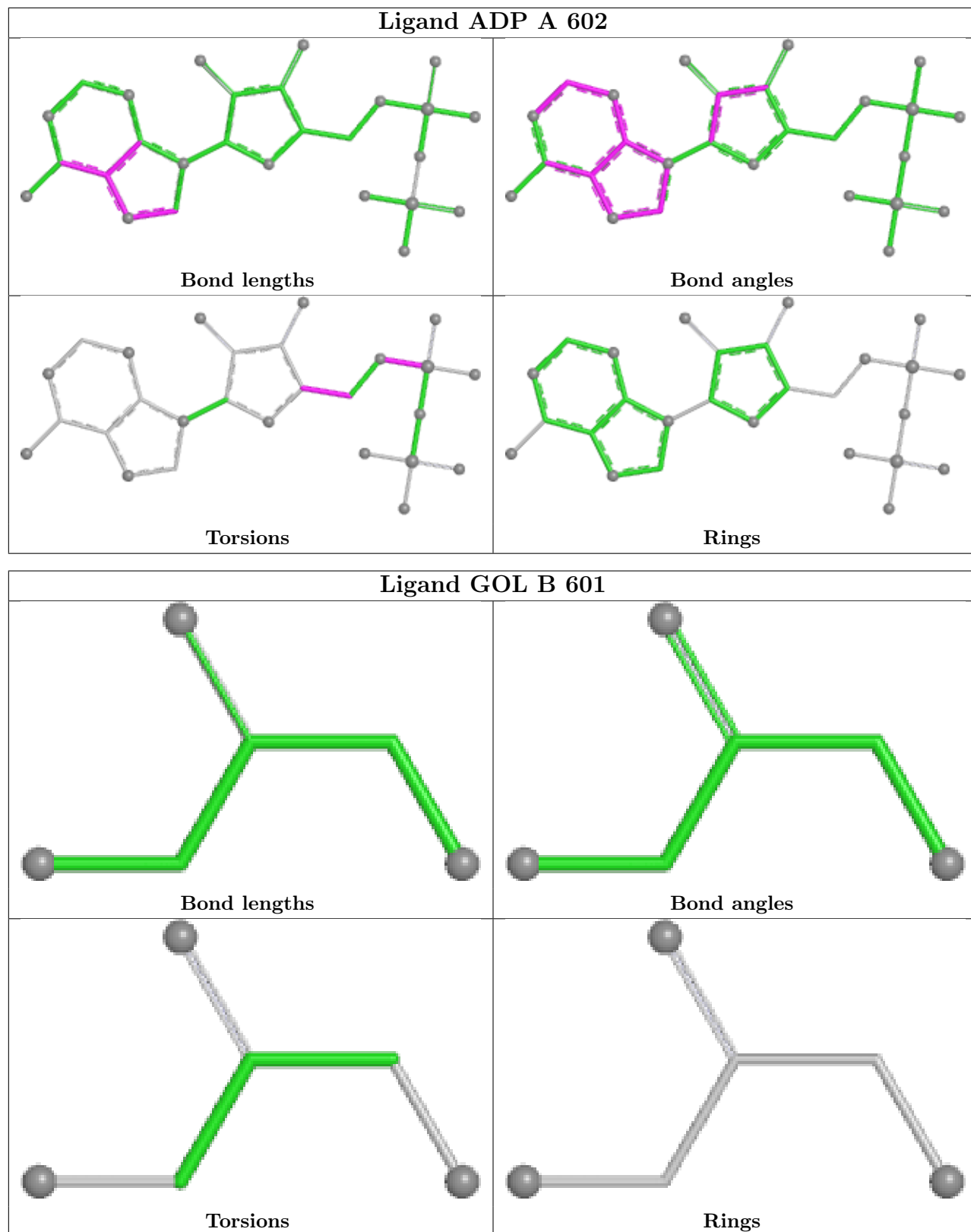
There are no ring outliers.

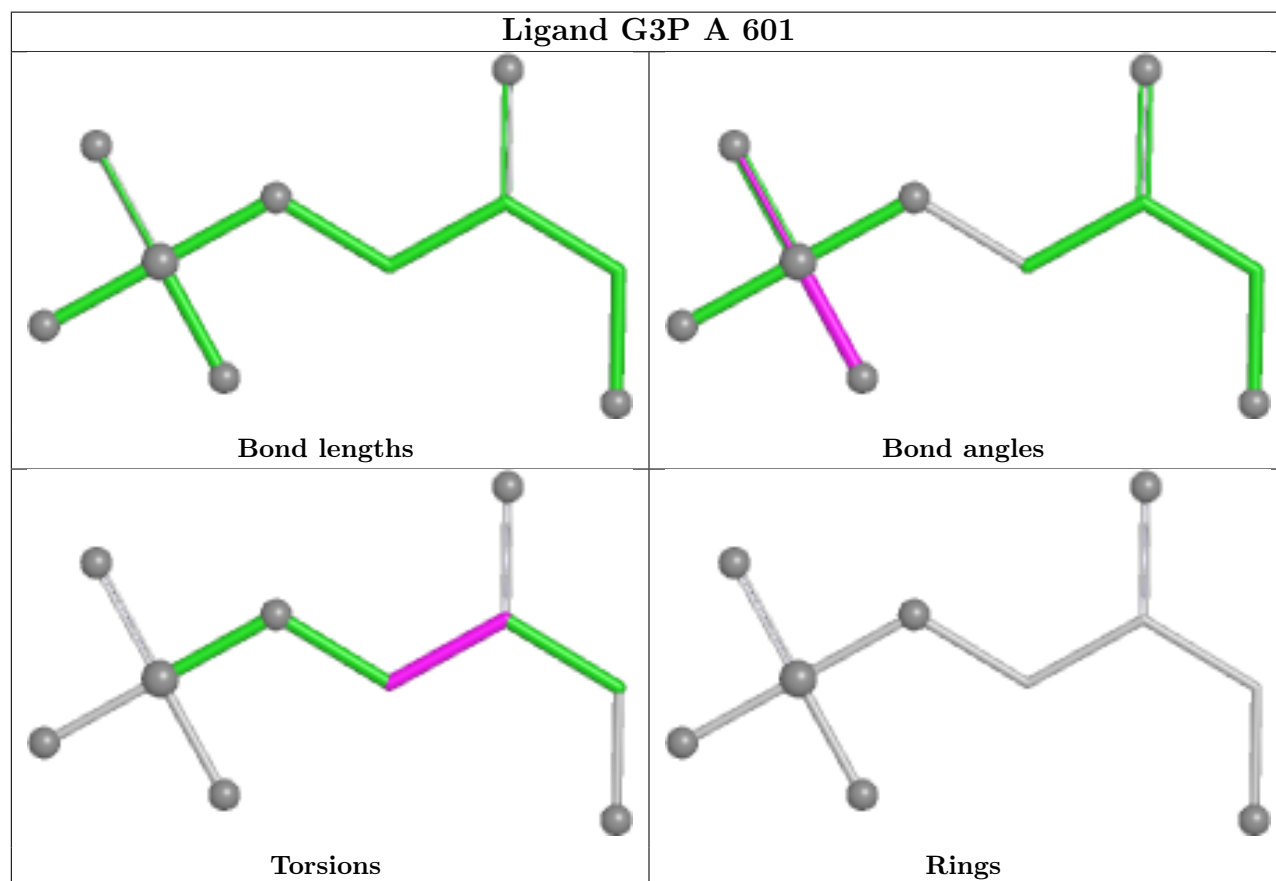
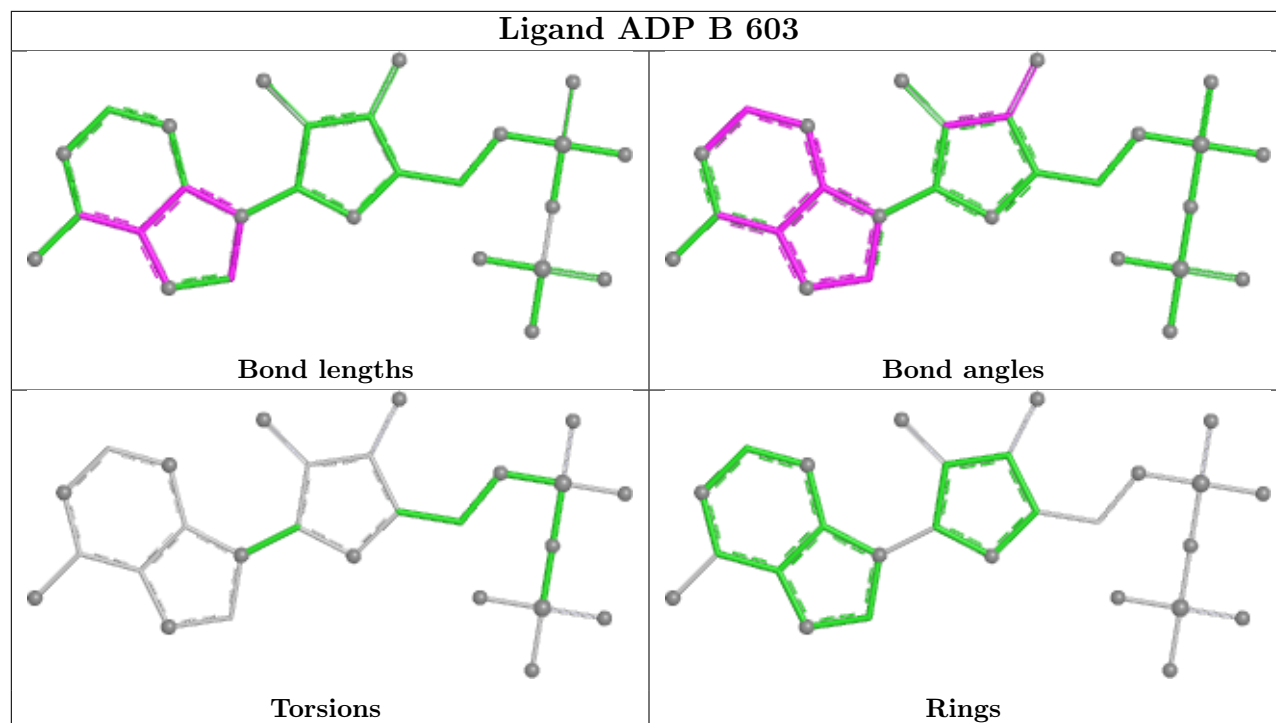
2 monomers are involved in 5 short contacts:

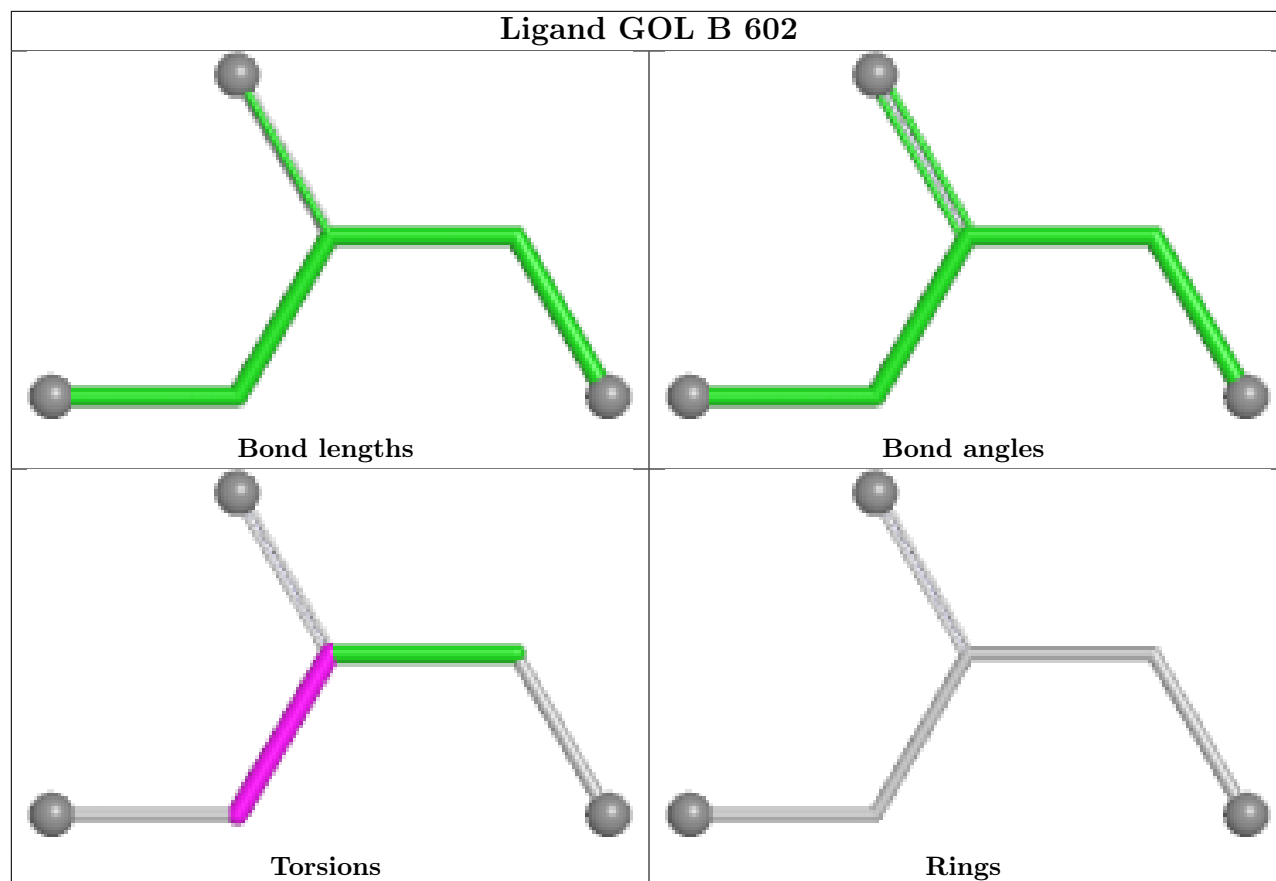
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	ADP	4	0
3	B	603	ADP	1	0

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

equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	514/518 (99%)	-0.20	5 (0%) 79 76	30, 66, 89, 117	0
1	B	514/518 (99%)	-0.05	5 (0%) 79 76	30, 75, 107, 136	0
All	All	1028/1036 (99%)	-0.12	10 (0%) 79 76	30, 70, 103, 136	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-2	PRO	3.3
1	B	-1	PHE	2.8
1	A	329	ARG	2.5
1	A	337	ILE	2.5
1	A	15	ARG	2.4
1	B	-2	PRO	2.4
1	B	367	TRP	2.4
1	A	-1	PHE	2.3
1	B	491	MET	2.1
1	B	196	MET	2.1

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](#)

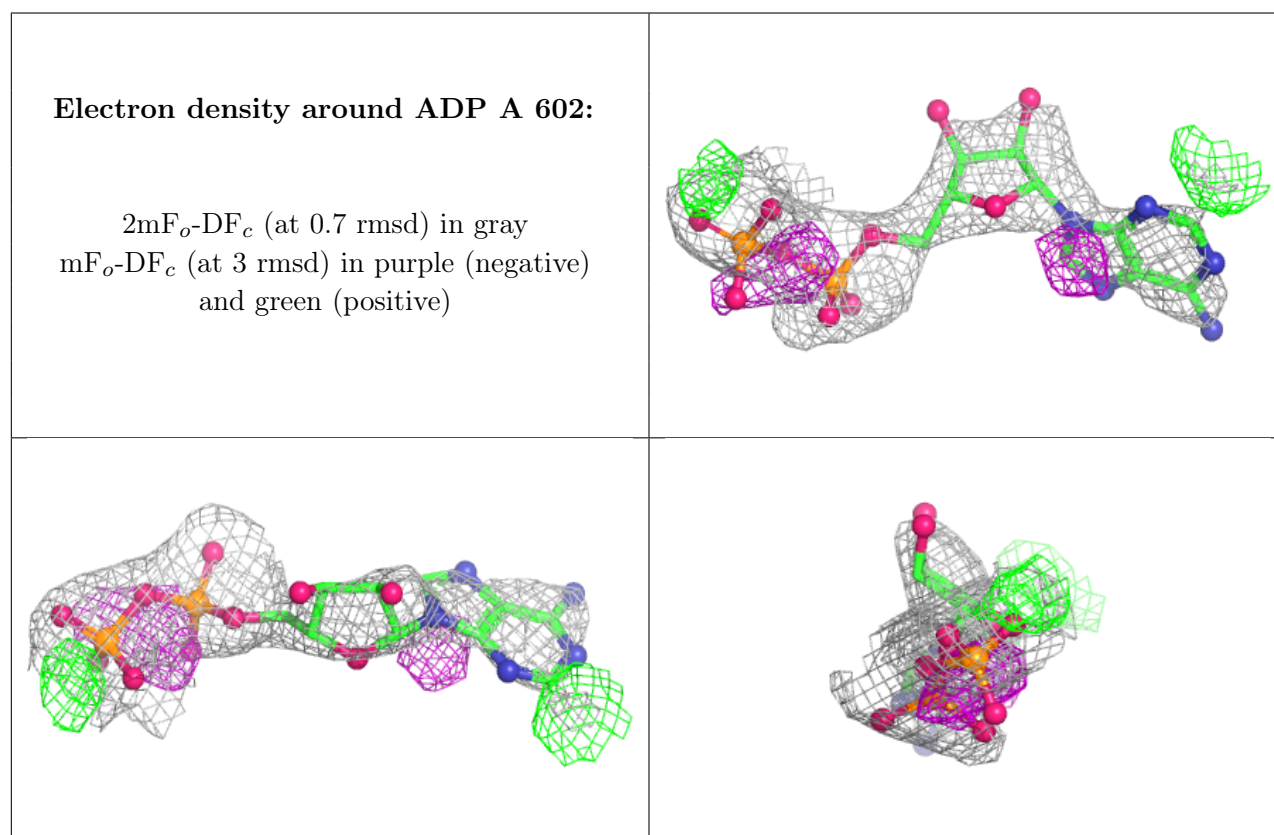
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

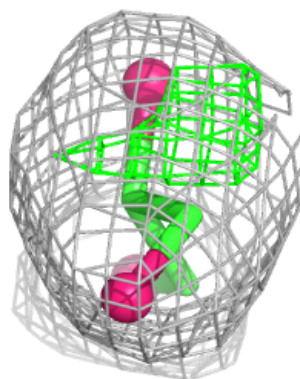
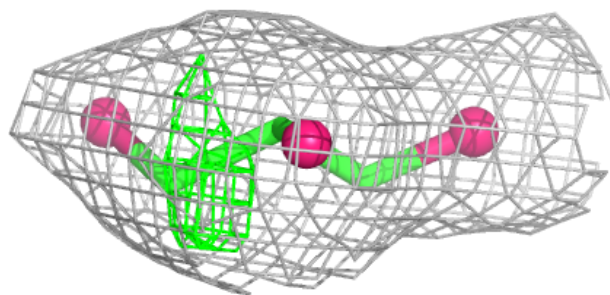
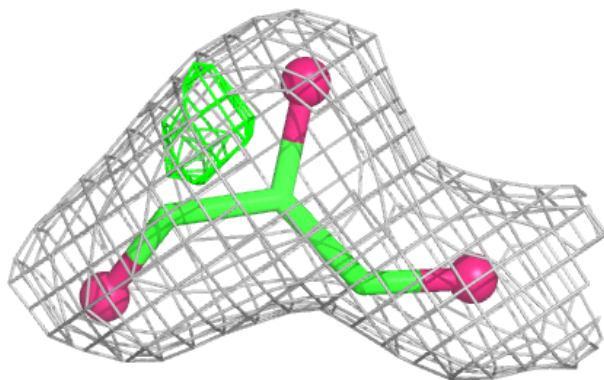
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	A	602	27/27	0.71	0.16	92,100,106,115	27
5	GOL	B	602	6/6	0.78	0.16	77,82,84,89	0
2	G3P	A	601	10/10	0.80	0.14	85,97,118,124	0
4	MG	A	603	1/1	0.86	0.27	92,92,92,92	0
3	ADP	B	603	27/27	0.91	0.08	61,67,112,118	0
5	GOL	B	601	6/6	0.95	0.08	63,68,69,72	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.

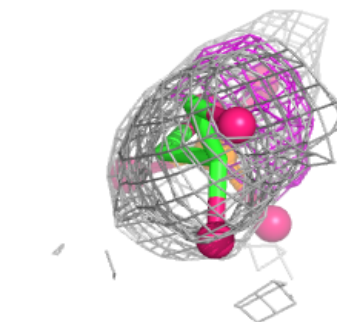
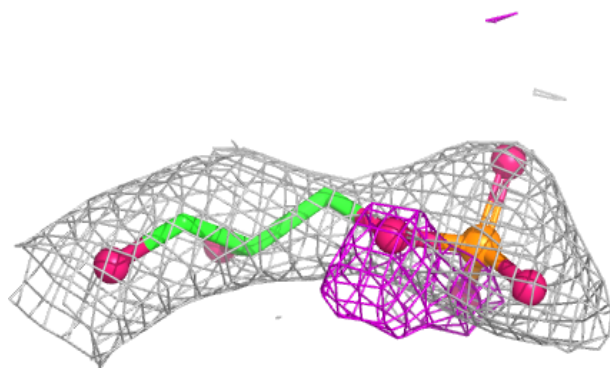
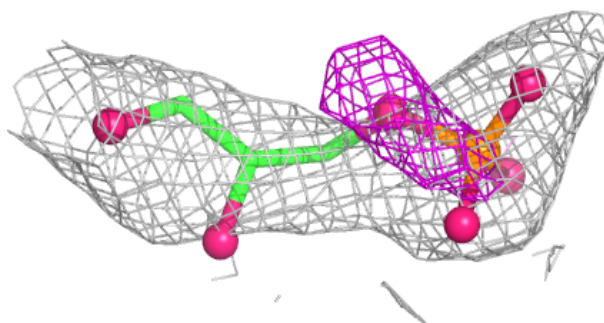


Electron density around GOL B 602:

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

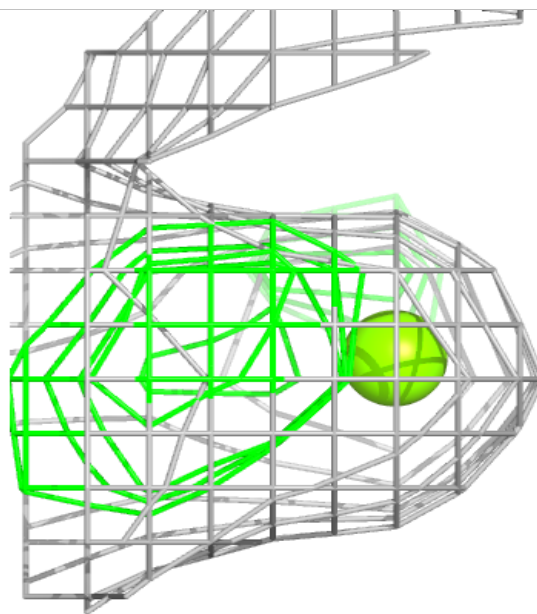
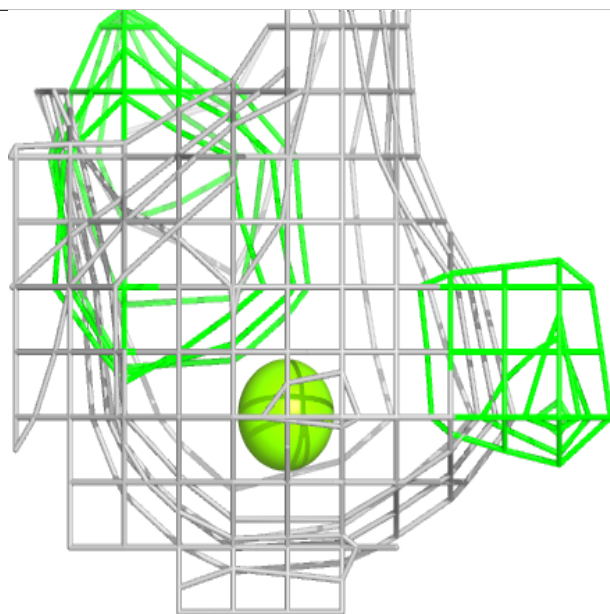
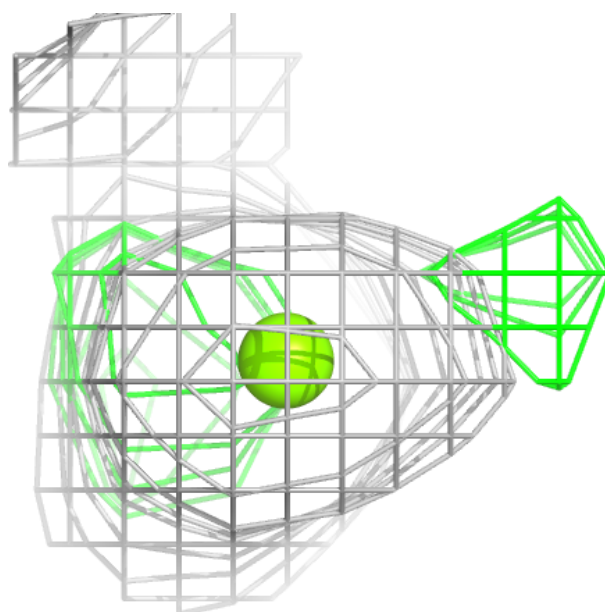
**Electron density around G3P A 601:**

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



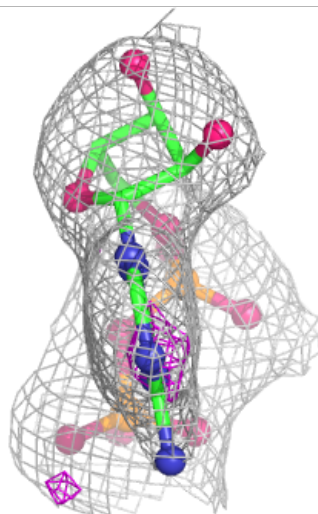
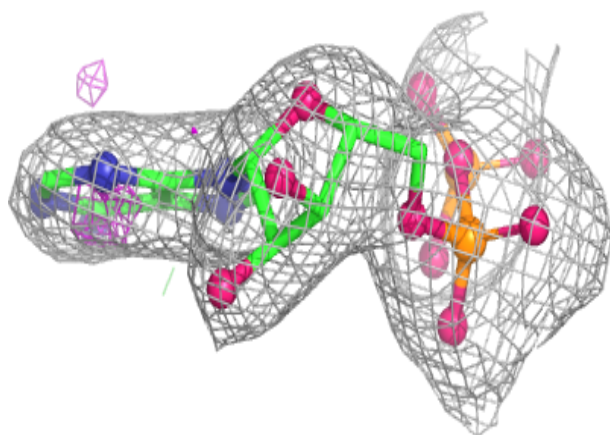
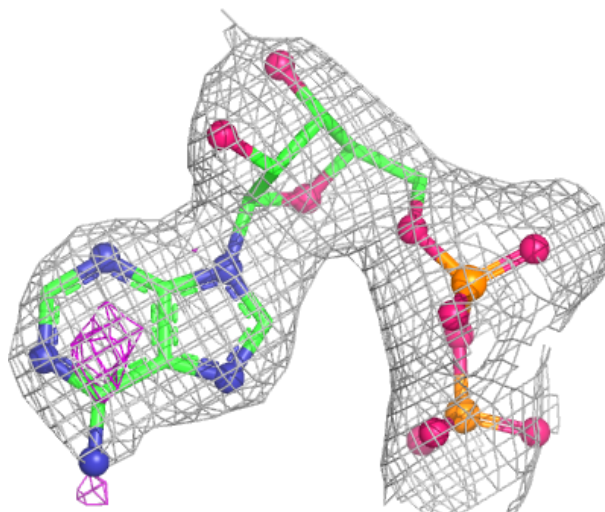
Electron density around MG A 603:

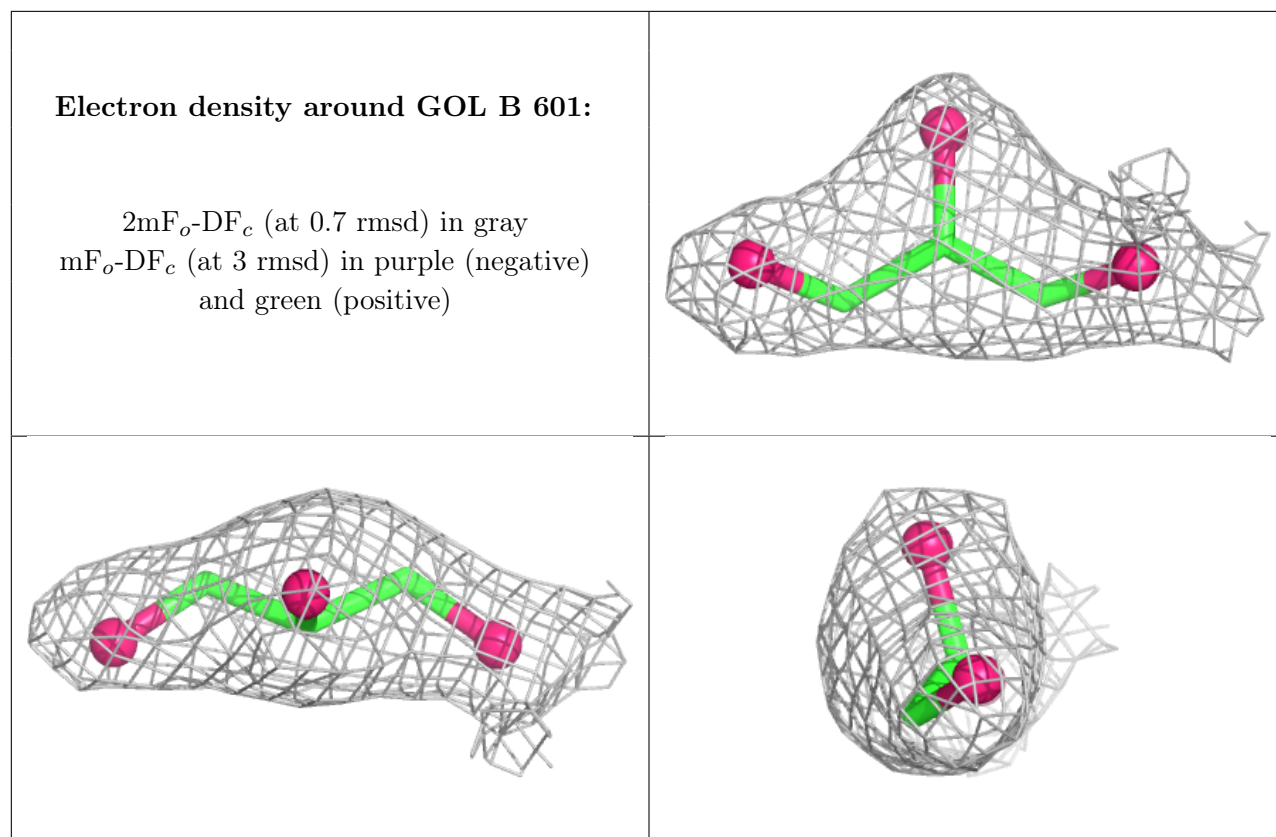
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ADP B 603:

$2mF_o-DF_c$ (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.