



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:13 AM UTC

PDB ID : 5KWK / pdb_00005kwk
Title : The structure of Arabidopsis thaliana FUT1 in complex with GDP
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2016-07-18
Resolution : 1.90 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

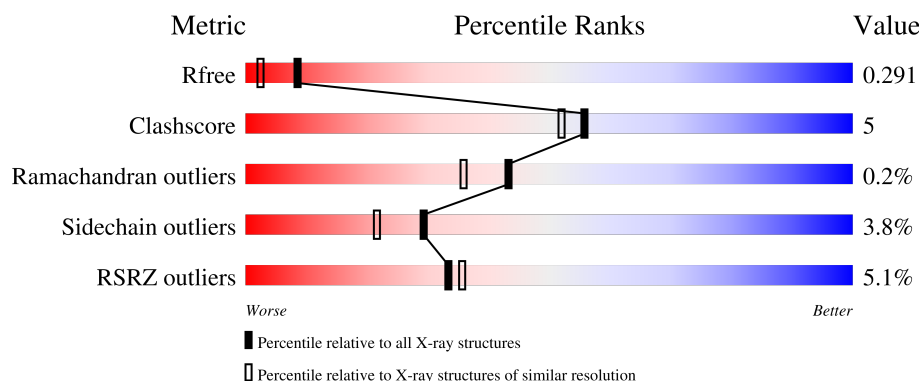
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	476	4% 69% 20% 8%
1	B	476	5% 73% 22% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8696 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.

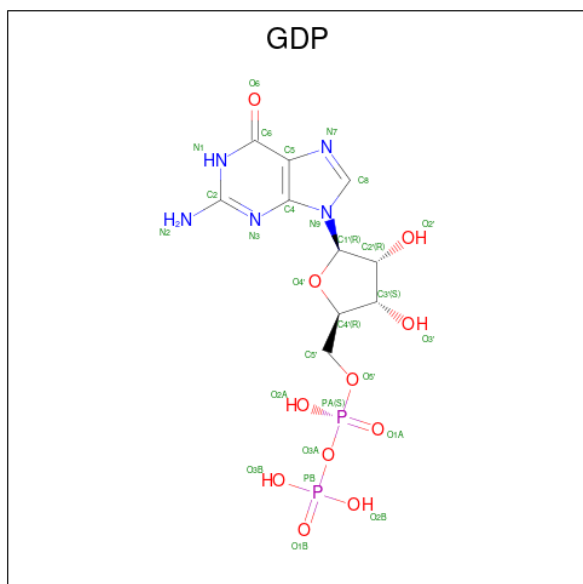
- Molecule 1 is a protein called Galactoside 2-alpha-L-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	17	0
			3673	2358	616	676	23			
1	B	457	Total	C	N	O	S	0	15	0
			3789	2433	630	703	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLY	-	expression tag	UNP Q9SWH5
B	83	GLY	-	expression tag	UNP Q9SWH5

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



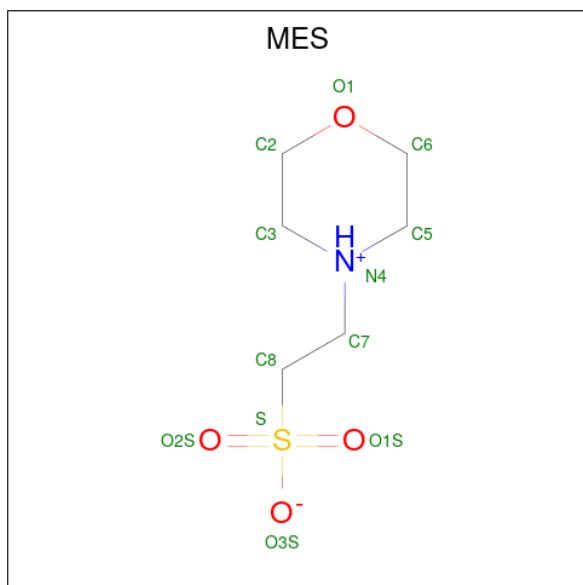
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	541	Total	O	0	29
			570	570		
6	B	491	Total	O	0	15
			506	506		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.93Å 113.10Å 87.78Å 90.00° 105.01° 90.00°	Depositor
Resolution (Å)	84.78 – 1.90 84.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (84.78-1.90) 97.8 (84.78-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.223 , 0.289 0.227 , 0.291	Depositor DCC
R_{free} test set	3790 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.003 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8696	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: GOL, GDP, EDO, MES

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	1.63	50/3776 (1.3%)	1.33	11/5115 (0.2%)
1	B	1.68	54/3897 (1.4%)	1.32	14/5283 (0.3%)
All	All	1.65	104/7673 (1.4%)	1.32	25/10398 (0.2%)

All (104) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	LEU	C-O	-13.45	1.08	1.24
1	A	364	GLN	C-O	9.88	1.35	1.24
1	B	185	ARG	C-O	9.06	1.34	1.24
1	A	414	LEU	C-O	8.96	1.34	1.24
1	A	443	VAL	C-O	-8.84	1.14	1.24
1	A	304	VAL	CA-CB	8.82	1.58	1.54
1	A	479	SER	CA-C	8.48	1.63	1.52
1	B	303	PHE	C-O	8.43	1.35	1.24
1	B	212	ASP	CA-C	7.97	1.63	1.52
1	A	198	LEU	C-O	-7.77	1.13	1.24
1	B	326	THR	N-CA	7.62	1.55	1.46
1	B	331	LEU	CA-C	7.62	1.62	1.52
1	A	217	GLU	CA-C	-7.40	1.44	1.52
1	B	196	ALA	C-O	7.39	1.32	1.24
1	A	338	PRO	CA-C	7.23	1.61	1.52
1	B	334	TYR	C-O	-7.12	1.15	1.24
1	A	313	PHE	N-CA	7.04	1.54	1.46
1	B	485	GLY	CA-C	6.90	1.60	1.51
1	B	359	GLU	C-O	6.90	1.32	1.23
1	A	463	ALA	CA-CB	-6.88	1.42	1.53
1	A	293	PRO	CA-C	6.82	1.62	1.52
1	A	327	VAL	CA-CB	-6.74	1.46	1.54
1	B	381	GLN	N-CA	6.60	1.54	1.46
1	A	414	LEU	CA-C	-6.40	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	302	TYR	N-CA	-6.39	1.38	1.46
1	A	337	HIS	C-O	-6.34	1.17	1.24
1	A	362	GLY	C-O	6.32	1.31	1.23
1	A	511	SER	C-O	-6.32	1.16	1.24
1	B	297	VAL	C-O	-6.30	1.17	1.24
1	A	215	PHE	CA-CB	6.29	1.64	1.53
1	A	173	TYR	CA-C	-6.27	1.45	1.52
1	B	487	VAL	C-O	-6.26	1.17	1.24
1	B	474	ASP	C-O	6.25	1.31	1.24
1	A	194	LEU	C-O	-6.25	1.16	1.24
1	B	152	SER	N-CA	6.25	1.53	1.46
1	A	428	SER	N-CA	-6.21	1.38	1.46
1	B	143	HIS	N-CA	6.20	1.53	1.46
1	A	465	ALA	C-O	-6.20	1.17	1.24
1	B	422	TYR	CA-CB	6.19	1.63	1.53
1	A	325	ALA	C-O	-6.18	1.15	1.24
1	B	522	PHE	CA-CB	6.17	1.60	1.53
1	B	515	ALA	CA-C	6.11	1.60	1.52
1	B	189	LEU	CA-C	6.08	1.60	1.52
1	B	282	CYS	N-CA	6.07	1.52	1.45
1	B	325	ALA	N-CA	6.02	1.54	1.46
1	A	488	ALA	C-O	6.01	1.31	1.24
1	A	302	TYR	N-CA	-5.99	1.39	1.46
1	A	379	MET	N-CA	5.98	1.53	1.46
1	B	364	GLN	CA-CB	5.94	1.60	1.53
1	B	316	GLU	C-O	-5.87	1.17	1.24
1	A	416	THR	C-O	5.85	1.31	1.24
1	B	364	GLN	C-O	5.84	1.31	1.24
1	B	498	ILE	C-O	-5.82	1.17	1.24
1	A	364	GLN	N-CA	5.81	1.53	1.46
1	B	477	VAL	CA-C	5.80	1.59	1.52
1	A	511	SER	CA-C	-5.79	1.45	1.52
1	A	347	THR	C-O	-5.72	1.17	1.24
1	B	311	PRO	C-O	5.71	1.30	1.23
1	B	184	ASN	N-CA	-5.70	1.39	1.46
1	A	193	PHE	N-CA	-5.67	1.39	1.46
1	B	444	HIS	C-O	5.67	1.30	1.24
1	A	548	CYS	CA-C	-5.66	1.45	1.52
1	B	218	PRO	CA-C	5.66	1.60	1.52
1	B	299	THR	CA-C	5.65	1.59	1.52
1	A	184	ASN	CA-C	-5.59	1.45	1.52
1	B	348	ARG	C-O	5.57	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	335	LEU	CB-CG	5.56	1.64	1.53
1	B	431	TRP	N-CA	5.54	1.53	1.46
1	A	114	ARG	N-CA	5.52	1.52	1.46
1	B	414	LEU	CA-C	-5.50	1.46	1.52
1	B	103	ALA	C-O	5.42	1.30	1.23
1	B	199	THR	N-CA	5.40	1.52	1.46
1	B	215	PHE	CA-CB	5.38	1.62	1.53
1	A	505	ARG	N-CA	5.35	1.54	1.46
1	B	459	HIS	CA-C	5.35	1.59	1.52
1	B	323	GLN	CA-C	-5.34	1.46	1.52
1	A	195	TYR	C-O	5.33	1.30	1.24
1	A	550	ASP	CA-CB	5.30	1.61	1.53
1	A	342	VAL	CA-CB	5.28	1.61	1.54
1	A	224	TRP	CA-C	-5.27	1.45	1.52
1	A	201	ARG	C-O	5.27	1.30	1.23
1	B	484	PHE	N-CA	-5.26	1.40	1.46
1	A	427	LYS	N-CA	5.26	1.52	1.46
1	B	309	LEU	N-CA	-5.26	1.39	1.46
1	A	303	PHE	N-CA	5.25	1.52	1.46
1	A	468	TYR	CA-C	5.25	1.59	1.52
1	A	189	LEU	N-CA	-5.23	1.40	1.46
1	B	313	PHE	C-O	-5.23	1.18	1.24
1	A	329	HIS	N-CA	5.22	1.52	1.46
1	B	349	TYR	C-O	-5.22	1.18	1.24
1	A	441	ILE	N-CA	-5.21	1.40	1.46
1	B	467	MET	N-CA	5.21	1.52	1.46
1	A	292	VAL	CA-C	5.20	1.57	1.53
1	B	203	LEU	CA-C	5.20	1.59	1.52
1	A	512	CYS	CA-C	-5.15	1.46	1.52
1	B	350	TYR	CA-CB	5.14	1.61	1.53
1	B	186	ILE	CA-C	5.13	1.59	1.52
1	A	367	VAL	CA-CB	-5.13	1.47	1.53
1	A	525	PRO	CA-C	5.12	1.56	1.52
1	B	490	GLY	N-CA	5.06	1.52	1.45
1	A	553	TRP	N-CA	-5.03	1.40	1.46
1	B	310	ILE	N-CA	-5.03	1.41	1.46
1	B	131	TYR	CA-C	5.02	1.59	1.52
1	B	302	TYR	CA-C	5.01	1.59	1.52

All (25) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ILE	N-CA-C	7.14	117.28	110.42
1	A	270	VAL	N-CA-C	-6.62	102.84	110.05
1	A	144	LYS	N-CA-C	6.14	117.97	111.28
1	B	212	ASP	N-CA-CB	-6.11	100.16	110.49
1	A	519	GLU	CA-C-N	5.99	125.90	119.85
1	A	519	GLU	C-N-CA	5.99	125.90	119.85
1	A	339	THR	N-CA-C	-5.98	103.05	110.41
1	B	126	TYR	N-CA-C	5.95	117.99	108.41
1	B	292	VAL	CA-C-N	-5.80	112.59	119.84
1	B	292	VAL	C-N-CA	-5.80	112.59	119.84
1	B	421	GLY	N-CA-C	5.67	119.75	112.83
1	B	314	ASP	N-CA-C	5.59	117.05	111.07
1	A	387	GLN	N-CA-C	5.50	117.08	111.14
1	A	441	ILE	N-CA-C	5.48	115.85	108.17
1	B	556	LYS	N-CA-C	5.48	117.51	109.24
1	A	534	THR	N-CA-CB	-5.40	102.64	111.66
1	A	552	SER	N-CA-C	5.38	118.94	112.38
1	B	552	SER	N-CA-C	5.33	117.85	111.71
1	B	523	HIS	N-CA-C	5.31	117.98	111.82
1	B	393	PRO	N-CA-C	5.17	119.16	111.41
1	B	314	ASP	CB-CG-OD1	5.16	130.27	118.40
1	A	182	LEU	N-CA-C	5.14	117.28	111.11
1	B	187	LEU	CA-C-O	-5.09	115.47	120.82
1	A	519	GLU	N-CA-C	5.05	117.47	110.20
1	B	495	LYS	CB-CA-C	5.01	115.13	110.17

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	3673	0	3540	36	0
1	B	3789	0	3654	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	12	1	0
2	B	28	0	12	0	0
3	A	12	0	13	0	0
3	B	12	0	13	0	0
4	A	40	0	60	3	0
4	B	32	0	48	0	0
5	A	6	0	8	0	0
6	A	570	0	0	5	0
6	B	506	0	0	3	0
All	All	8696	0	7360	70	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 5.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200[A]:ASP:OD2	6:A:706[A]:HOH:O	1.74	1.04
1:A:222[B]:MET:HE1	6:A:1011[B]:HOH:O	1.58	1.01
1:B:494:LEU:C	1:B:518[B]:MET:HG2	2.03	0.83
1:A:388[A]:LYS:NZ	1:A:389:GLU:OE2	2.23	0.66
1:B:127[B]:LYS:N	1:B:127[B]:LYS:HD3	2.11	0.66
1:B:341[A]:GLN:O	1:B:341[A]:GLN:NE2	2.31	0.63
1:A:185:ARG:NH1	1:A:211:MET:SD	2.71	0.63
1:A:250:MET:HE1	1:A:262:LEU:HD21	1.82	0.60
1:A:534:THR:HG21	6:B:791:HOH:O	2.02	0.59
1:B:356[B]:HIS:H	1:B:356[B]:HIS:CD2	2.21	0.58
1:B:127[B]:LYS:N	1:B:127[B]:LYS:CD	2.67	0.57
1:B:495:LYS:N	1:B:518[B]:MET:HG2	2.19	0.57
1:A:325:ALA:HB3	4:A:605:EDO:H22	1.87	0.57
1:B:495:LYS:HB2	1:B:518[B]:MET:HG3	1.87	0.56
1:A:109[A]:ASP:OD1	1:A:110:SER:N	2.39	0.56
1:B:99:GLY:HA3	1:B:127[A]:LYS:HE2	1.87	0.55
1:A:130[A]:SER:HB2	4:A:606[A]:EDO:H12	1.89	0.55
1:B:264:HIS:HA	1:B:294:TRP:O	2.07	0.54
1:A:131:TYR:CD1	1:A:319[B]:LYS:HE3	2.42	0.54
1:A:229:ASP:O	1:A:230:PHE:C	2.51	0.54
1:A:440:ILE:C	1:A:441:ILE:HD13	2.33	0.53
1:B:423:ALA:HB2	1:B:445:GLN:HE21	1.74	0.52
1:B:425:ASN:O	1:B:428[A]:SER:OG	2.26	0.52
1:A:342:VAL:HG11	1:A:464:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108[B]:GLU:H	1:B:108[B]:GLU:CD	2.18	0.51
1:B:242:GLU:OE1	6:B:713:HOH:O	2.19	0.51
1:A:176:TRP:CH2	1:A:178:SER:HA	2.46	0.50
1:B:99:GLY:HA3	1:B:127[A]:LYS:CE	2.41	0.50
1:B:163:GLU:HG2	1:B:245:ARG:NH2	2.26	0.50
1:A:408:PRO:HD3	6:A:1066:HOH:O	2.13	0.48
1:B:172[A]:LYS:HB3	1:B:201:ARG:HG2	1.96	0.48
1:B:172[B]:LYS:N	1:B:172[B]:LYS:HD3	2.29	0.48
1:A:424:GLU:OE2	4:A:608:EDO:O2	2.31	0.47
1:A:144:LYS:HA	1:A:222[A]:MET:HG3	1.97	0.47
1:A:184:ASN:ND2	1:A:483:THR:HG21	2.30	0.47
1:A:409:LYS:HG2	1:A:439:GLU:HG2	1.97	0.47
1:B:356[B]:HIS:CD2	1:B:356[B]:HIS:N	2.83	0.47
1:B:165:ILE:HD11	1:B:293:PRO:CG	2.45	0.47
1:B:165:ILE:CD1	1:B:263:SER:HA	2.45	0.46
1:B:428[A]:SER:OG	1:B:429:MET:N	2.48	0.46
1:A:94:SER:N	6:A:733:HOH:O	2.50	0.45
1:B:341[A]:GLN:NE2	1:B:341[A]:GLN:C	2.74	0.45
1:A:188:SER:HB2	1:A:299:THR:HG23	1.99	0.45
1:A:480:ALA:HB1	1:A:550:ASP:HB2	1.98	0.45
1:B:304:VAL:HB	1:B:305:PRO:HD3	1.99	0.44
1:B:127[A]:LYS:HD3	1:B:128:PRO:HD2	1.99	0.44
1:B:546:ARG:NH2	6:B:731:HOH:O	2.50	0.44
1:A:95:ASP:N	1:A:95:ASP:OD1	2.49	0.44
1:B:165:ILE:HG23	1:B:167:GLY:O	2.18	0.44
1:A:546:ARG:NH1	6:A:738:HOH:O	2.51	0.43
1:A:441:ILE:HD13	1:A:441:ILE:N	2.34	0.43
1:B:425:ASN:C	1:B:428[A]:SER:HG	2.26	0.43
1:A:481:TRP:CZ3	1:A:551:ILE:HD12	2.53	0.43
1:B:106:PHE:CD2	1:B:114:ARG:HD3	2.53	0.43
1:A:411:LYS:HB2	1:A:441:ILE:HD12	1.99	0.43
1:A:194:LEU:HD21	1:A:317:LEU:HD21	2.01	0.42
1:A:480:ALA:O	1:A:481:TRP:HB2	2.19	0.42
1:A:374:PRO:HG3	1:A:419:ASN:OD1	2.20	0.42
1:A:460:ASN:HD22	1:A:460:ASN:HA	1.68	0.42
1:B:116[B]:GLN:HE21	1:B:116[B]:GLN:HA	1.85	0.41
1:B:165:ILE:HD12	1:B:263:SER:HA	2.03	0.41
1:A:107:ASP:OD2	1:A:110:SER:HB3	2.20	0.41
1:B:342:VAL:HG11	1:B:464:LEU:HD23	2.01	0.41
1:A:418:LEU:HD21	2:A:601:GDP:C4	2.56	0.41
1:A:179:PHE:O	1:A:185:ARG:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:ND1	1:B:300:ASP:OD2	2.48	0.41
1:A:544:HIS:O	1:A:557:LEU:HA	2.21	0.41
1:A:267:LEU:HD11	1:A:295:LEU:HD13	2.03	0.40
1:B:285:ASP:O	1:B:289:ILE:HG13	2.22	0.40
1:B:230:PHE:HA	1:B:231:PRO:HD3	1.85	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	447/476 (94%)	431 (96%)	15 (3%)	1 (0%)	43	36
1	B	468/476 (98%)	451 (96%)	16 (3%)	1 (0%)	43	36
All	All	915/952 (96%)	882 (96%)	31 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	180	SER
1	A	255	VAL

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	406/423 (96%)	383 (94%)	23 (6%)	18	11
1	B	418/423 (99%)	401 (96%)	17 (4%)	27	19
All	All	824/846 (97%)	784 (95%)	40 (5%)	29	14

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	108	GLU
1	A	116	GLN
1	A	141	LYS
1	A	155	LYS
1	A	174	VAL
1	A	200[A]	ASP
1	A	200[B]	ASP
1	A	222[A]	MET
1	A	222[B]	MET
1	A	273	TYR
1	A	319[A]	LYS
1	A	319[B]	LYS
1	A	341[A]	GLN
1	A	341[B]	GLN
1	A	351[A]	GLU
1	A	351[B]	GLU
1	A	354	LEU
1	A	356[A]	HIS
1	A	356[B]	HIS
1	A	398	LEU
1	A	460	ASN
1	A	546	ARG
1	B	121[A]	ARG
1	B	121[B]	ARG
1	B	127[A]	LYS
1	B	127[B]	LYS
1	B	165	ILE
1	B	273	TYR
1	B	301	ASN
1	B	318	ASN
1	B	341[A]	GLN
1	B	341[B]	GLN
1	B	355[A]	SER
1	B	355[B]	SER

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Mol	Chain	Res	Type
1	B	360	LYS
1	B	398	LEU
1	B	399	VAL
1	B	409	LYS
1	B	531	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	276	HIS
1	A	323	GLN
1	A	445	GLN
1	A	448	GLN
1	A	460	ASN
1	A	504	ASN
1	B	444	HIS
1	B	445	GLN
1	B	452	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GDP	A	601	-	29,30,30	1.44	4 (13%)	45,47,47	1.70	10 (22%)
4	EDO	B	607	-	3,3,3	0.39	0	2,2,2	0.33	0
2	GDP	B	601	-	29,30,30	1.31	4 (13%)	45,47,47	1.82	9 (20%)
4	EDO	A	603	-	3,3,3	0.26	0	2,2,2	0.58	0
4	EDO	A	609[B]	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	A	606[B]	-	3,3,3	0.52	0	2,2,2	0.23	0
3	MES	A	602	-	12,12,12	2.20	1 (8%)	15,16,16	1.06	1 (6%)
4	EDO	A	605	-	3,3,3	0.37	0	2,2,2	0.82	0
4	EDO	B	606	-	3,3,3	0.55	0	2,2,2	0.80	0
4	EDO	B	605	-	3,3,3	0.40	0	2,2,2	0.19	0
4	EDO	B	608	-	3,3,3	0.25	0	2,2,2	0.50	0
4	EDO	A	610	-	3,3,3	0.45	0	2,2,2	0.32	0
4	EDO	B	603	-	3,3,3	0.35	0	2,2,2	0.39	0
4	EDO	A	607	-	3,3,3	0.39	0	2,2,2	0.34	0
4	EDO	B	604	-	3,3,3	0.36	0	2,2,2	0.57	0
4	EDO	A	608	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	B	609	-	3,3,3	0.49	0	2,2,2	0.16	0
4	EDO	A	609[A]	-	3,3,3	0.54	0	2,2,2	0.40	0
4	EDO	A	604	-	3,3,3	0.37	0	2,2,2	0.67	0
4	EDO	A	606[A]	-	3,3,3	0.43	0	2,2,2	0.41	0
3	MES	B	602	-	12,12,12	2.34	1 (8%)	15,16,16	1.26	1 (6%)
4	EDO	B	610	-	3,3,3	0.45	0	2,2,2	0.20	0
5	GOL	A	611	-	5,5,5	0.27	0	5,5,5	0.21	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
2	GDP	A	601	-	-	6/16/32/32	0/3/3/3
4	EDO	B	607	-	-	1/1/1/1	-
2	GDP	B	601	-	-	4/16/32/32	0/3/3/3
4	EDO	A	603	-	-	1/1/1/1	-
4	EDO	A	609[B]	-	-	1/1/1/1	-
4	EDO	A	606[B]	-	-	0/1/1/1	-
3	MES	A	602	-	-	1/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	605	-	-	1/1/1/1	-
4	EDO	B	606	-	-	0/1/1/1	-
4	EDO	B	605	-	-	1/1/1/1	-
4	EDO	B	608	-	-	0/1/1/1	-
4	EDO	A	610	-	-	1/1/1/1	-
4	EDO	B	603	-	-	1/1/1/1	-
4	EDO	A	607	-	-	1/1/1/1	-
4	EDO	B	604	-	-	1/1/1/1	-
4	EDO	A	608	-	-	1/1/1/1	-
4	EDO	B	609	-	-	0/1/1/1	-
4	EDO	A	609[A]	-	-	1/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	A	606[A]	-	-	1/1/1/1	-
3	MES	B	602	-	-	0/6/14/14	0/1/1/1
4	EDO	B	610	-	-	0/1/1/1	-
5	GOL	A	611	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	MES	C8-S	-7.89	1.66	1.77
3	A	602	MES	C8-S	-7.38	1.67	1.77
2	A	601	GDP	PA-O3A	5.09	1.65	1.59
2	B	601	GDP	PA-O3A	3.94	1.63	1.59
2	A	601	GDP	C6-N1	-2.63	1.33	1.38
2	A	601	GDP	C4-N9	-2.44	1.31	1.38
2	B	601	GDP	C5-N7	-2.39	1.34	1.39
2	B	601	GDP	C4-N9	-2.36	1.32	1.38
2	B	601	GDP	C5-C4	2.35	1.45	1.38
2	A	601	GDP	C5-N7	-2.18	1.34	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GDP	C2-N3-C4	5.45	121.69	112.30
2	B	601	GDP	C5-C4-N3	-5.00	120.44	128.39
2	A	601	GDP	C2-N3-C4	4.12	119.40	112.30
2	A	601	GDP	C5-C4-N3	-4.11	121.85	128.39
2	B	601	GDP	N9-C4-N3	3.86	133.67	125.95
2	A	601	GDP	N9-C4-N3	3.72	133.40	125.95
3	B	602	MES	O3S-S-C8	3.50	112.85	106.00
2	A	601	GDP	O6-C6-C5	-3.46	117.40	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GDP	C6-C5-N7	3.15	136.02	130.29
2	B	601	GDP	O3B-PB-O3A	2.92	114.41	104.64
2	B	601	GDP	N2-C2-N1	2.83	122.72	116.76
2	A	601	GDP	C6-C5-N7	2.81	135.40	130.29
2	B	601	GDP	O6-C6-C5	-2.68	119.45	126.53
3	A	602	MES	O1S-S-C8	2.54	110.57	106.73
2	A	601	GDP	O3'-C3'-C4'	2.54	118.38	111.08
2	A	601	GDP	C6-C5-C4	-2.22	115.49	118.83
2	B	601	GDP	O3A-PB-O1B	-2.16	99.66	111.04
2	A	601	GDP	O6-C6-N1	2.16	124.17	120.11
2	A	601	GDP	N2-C2-N1	2.15	121.31	116.76
2	A	601	GDP	C8-N9-C4	2.08	109.93	106.03
2	B	601	GDP	C6-C5-C4	-2.02	115.78	118.83

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	GDP	PA-O3A-PB-O2B
2	B	601	GDP	PB-O3A-PA-O5'
5	A	611	GOL	C1-C2-C3-O3
4	A	610	EDO	O1-C1-C2-O2
4	B	604	EDO	O1-C1-C2-O2
3	A	602	MES	N4-C7-C8-S
4	A	608	EDO	O1-C1-C2-O2
2	A	601	GDP	PA-O3A-PB-O1B
2	A	601	GDP	O4'-C4'-C5'-O5'
4	A	603	EDO	O1-C1-C2-O2
2	A	601	GDP	PB-O3A-PA-O5'
2	A	601	GDP	C3'-C4'-C5'-O5'
4	A	609[B]	EDO	O1-C1-C2-O2
2	A	601	GDP	C4'-C5'-O5'-PA
2	B	601	GDP	C4'-C5'-O5'-PA
5	A	611	GOL	O2-C2-C3-O3
4	A	606[A]	EDO	O1-C1-C2-O2
2	B	601	GDP	O4'-C4'-C5'-O5'
4	A	609[A]	EDO	O1-C1-C2-O2
4	A	605	EDO	O1-C1-C2-O2
4	A	607	EDO	O1-C1-C2-O2
4	B	603	EDO	O1-C1-C2-O2
4	B	607	EDO	O1-C1-C2-O2
2	B	601	GDP	PA-O3A-PB-O3B

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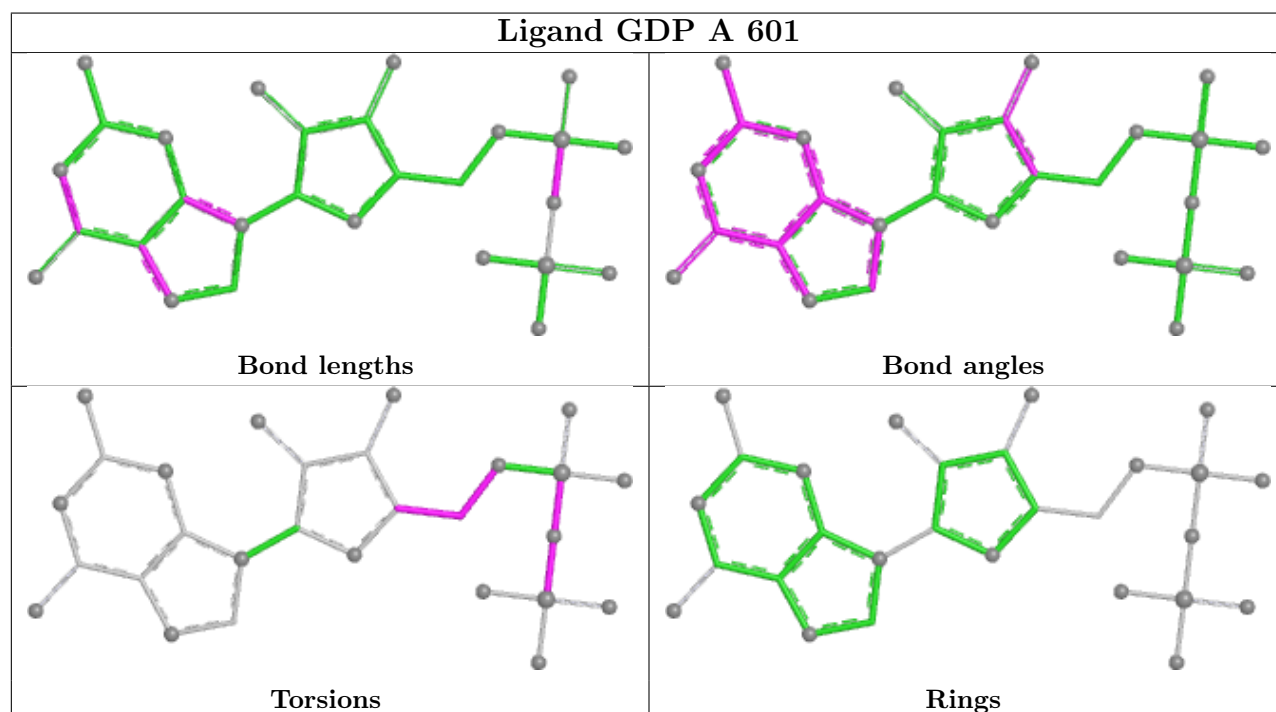
Mol	Chain	Res	Type	Atoms
4	B	605	EDO	O1-C1-C2-O2

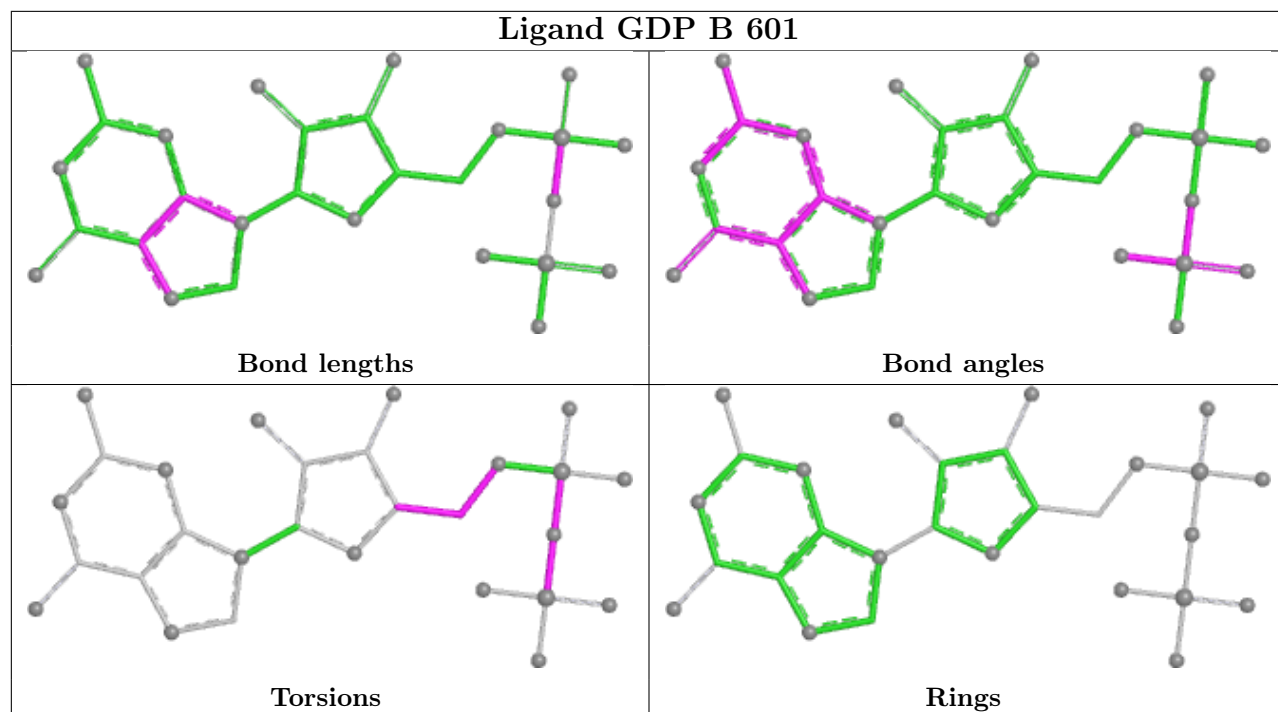
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	GDP	1	0
4	A	605	EDO	1	0
4	A	608	EDO	1	0
4	A	606[A]	EDO	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

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(Å ²)	Q<0.9
1	A	440/476 (92%)	0.39	21 (4%) 35 38	10, 21, 46, 75	17 (3%)
1	B	457/476 (96%)	0.47	25 (5%) 30 32	9, 21, 47, 71	16 (3%)
All	All	897/952 (94%)	0.43	46 (5%) 33 36	9, 21, 47, 75	33 (3%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	256	ILE	6.1
1	B	398	LEU	5.5
1	B	399	VAL	5.4
1	A	398	LEU	5.2
1	A	256	ILE	4.9
1	A	119[A]	HIS	4.1
1	B	454	THR	3.9
1	B	260	GLY	3.8
1	B	165	ILE	3.7
1	A	406	ASN	3.6
1	A	407	THR	3.6
1	B	258	THR	3.5
1	B	407	THR	3.5
1	A	118	VAL	3.4
1	B	255	VAL	3.3
1	A	408	PRO	3.3
1	A	261	THR	3.2
1	B	356[A]	HIS	3.2
1	A	162	GLN	3.1
1	A	356[A]	HIS	3.1
1	B	167	GLY	2.9
1	A	255	VAL	2.8
1	A	117	SER	2.7
1	B	257	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	94	SER	2.6
1	B	166	ASP	2.6
1	B	259	GLU	2.5
1	A	161[A]	ASP	2.5
1	B	397	THR	2.4
1	A	160	LEU	2.4
1	B	238	GLY	2.4
1	A	116	GLN	2.3
1	A	397	THR	2.3
1	A	459	HIS	2.3
1	A	468	TYR	2.3
1	A	123	PRO	2.2
1	B	527[A]	PHE	2.2
1	B	254	GLN	2.2
1	B	163	GLU	2.2
1	B	161	ASP	2.1
1	B	235	GLN	2.1
1	B	456	LYS	2.1
1	A	458	MET	2.1
1	B	234	ASP	2.1
1	B	451	TYR	2.0
1	B	162	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	610	4/4	0.63	0.25	26,26,27,27	4

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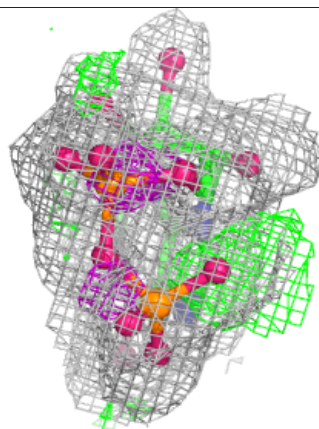
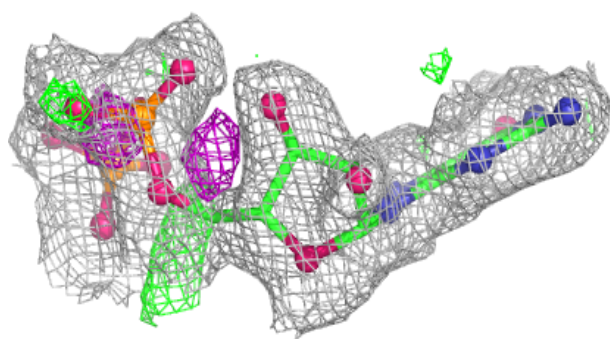
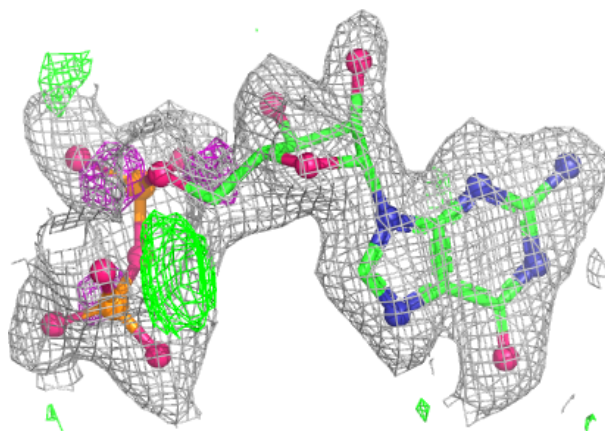
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	606[B]	4/4	0.69	0.23	30,30,31,31	4
4	EDO	A	609[A]	4/4	0.69	0.16	34,34,34,35	4
4	EDO	A	609[B]	4/4	0.69	0.16	30,31,32,33	4
4	EDO	A	606[A]	4/4	0.69	0.23	31,31,32,32	4
4	EDO	A	608	4/4	0.70	0.21	36,37,38,39	4
4	EDO	A	607	4/4	0.70	0.26	33,33,34,35	4
4	EDO	B	608	4/4	0.73	0.28	25,27,27,31	4
4	EDO	A	604	4/4	0.74	0.26	27,27,27,29	4
4	EDO	A	605	4/4	0.76	0.22	27,29,29,30	4
4	EDO	B	610	4/4	0.77	0.22	47,47,48,48	4
4	EDO	B	603	4/4	0.79	0.22	27,28,30,30	4
5	GOL	A	611	6/6	0.79	0.26	29,30,31,31	6
3	MES	A	602	12/12	0.80	0.24	38,40,43,43	12
4	EDO	B	607	4/4	0.81	0.17	42,44,45,46	0
4	EDO	B	609	4/4	0.83	0.16	56,59,61,63	0
4	EDO	B	604	4/4	0.84	0.15	38,42,42,44	0
2	GDP	A	601	28/28	0.85	0.12	18,30,45,50	0
4	EDO	A	603	4/4	0.86	0.24	18,22,22,25	4
4	EDO	B	605	4/4	0.87	0.15	35,36,36,39	0
2	GDP	B	601	28/28	0.87	0.12	20,27,41,47	0
4	EDO	B	606	4/4	0.88	0.12	24,26,28,28	0
3	MES	B	602	12/12	0.88	0.17	34,38,40,40	12

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.

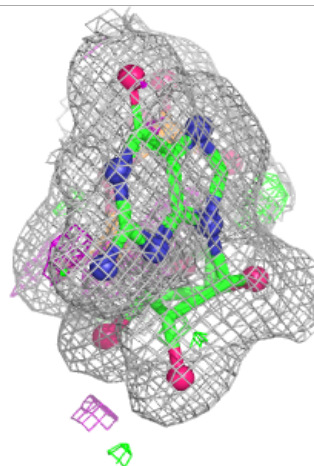
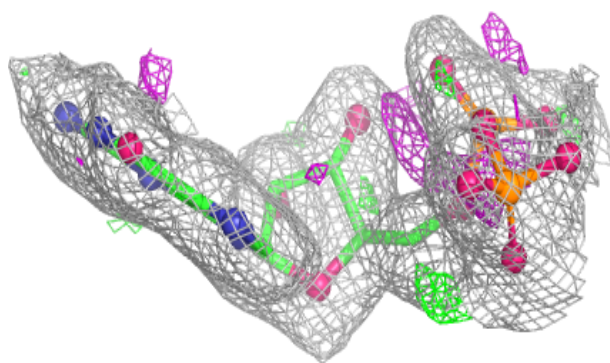
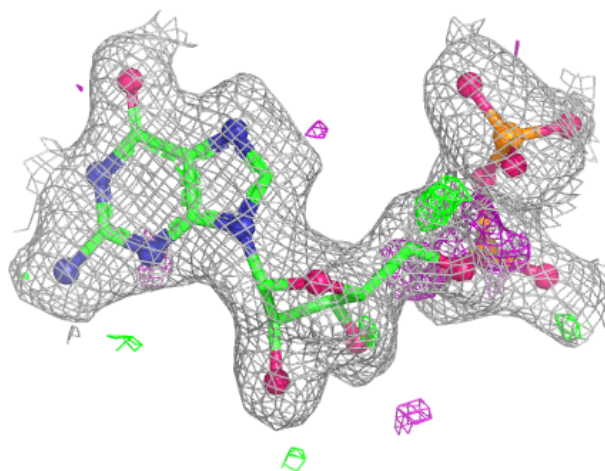
Electron density around GDP A 601:

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



Electron density around GDP B 601:

$2mF_o-DF_c$ (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.