



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:28 AM UTC

PDB ID : 3MOE / pdb_00003moe
Title : The structure of rat cytosolic PEPCK mutant A467G in complex with Beta-Sulfo pyruvate and GTP
Authors : Johnson, T.A.; Holyoak, T.
Deposited on : 2010-04-22
Resolution : 1.25 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

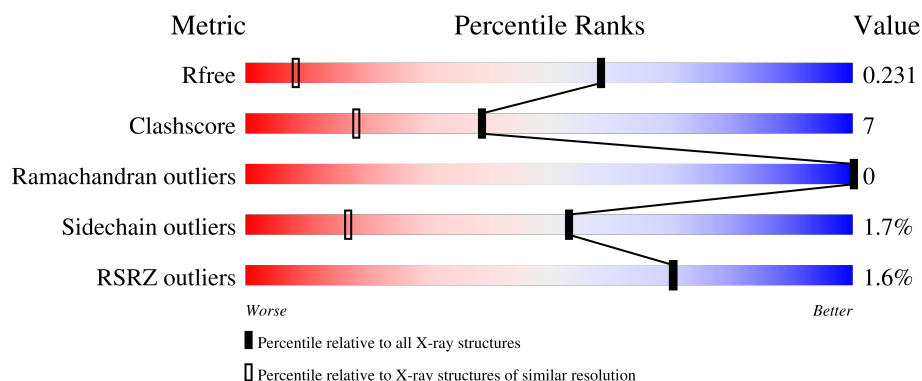
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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	624	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	1PE	A	1300	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	EDO	A	1401	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5758 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.

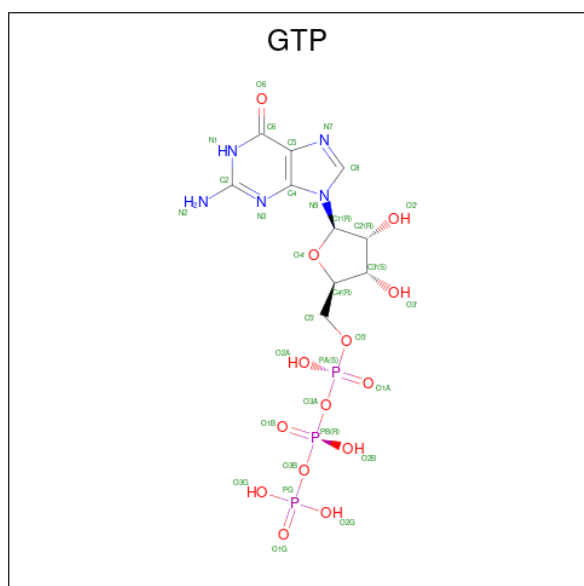
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	618	5051	3248	858	910	35	0	33	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P07379
A	0	SER	-	expression tag	UNP P07379
A	467	GLY	ALA	engineered mutation	UNP P07379

- Molecule 2 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

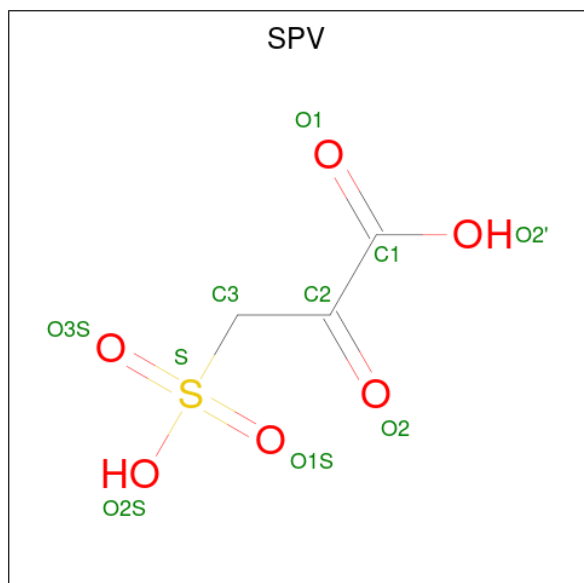
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	Mn		0	0
			2	2			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

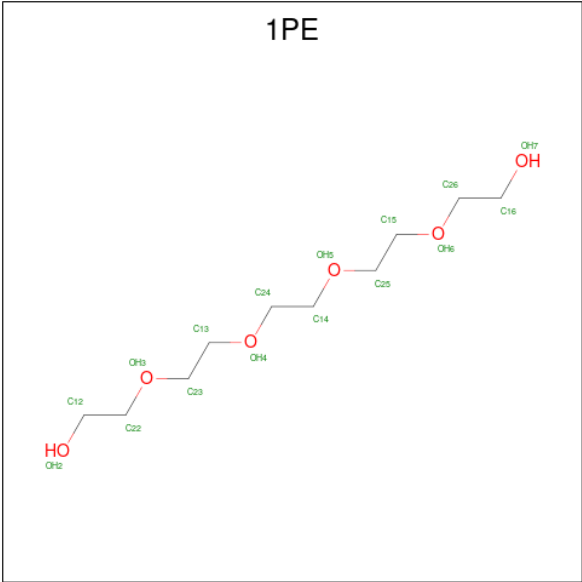
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Na		0	0
			1	1			

- Molecule 5 is SULFOPYRUVATE (CCD ID: SPV) (formula: C₃H₄O₆S).



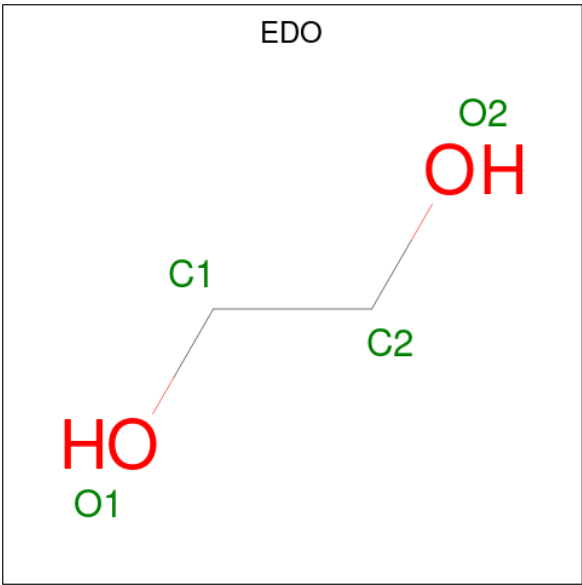
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			10	3	6	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	A	1	Total	C	O	0	0
			5	3	2		
6	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

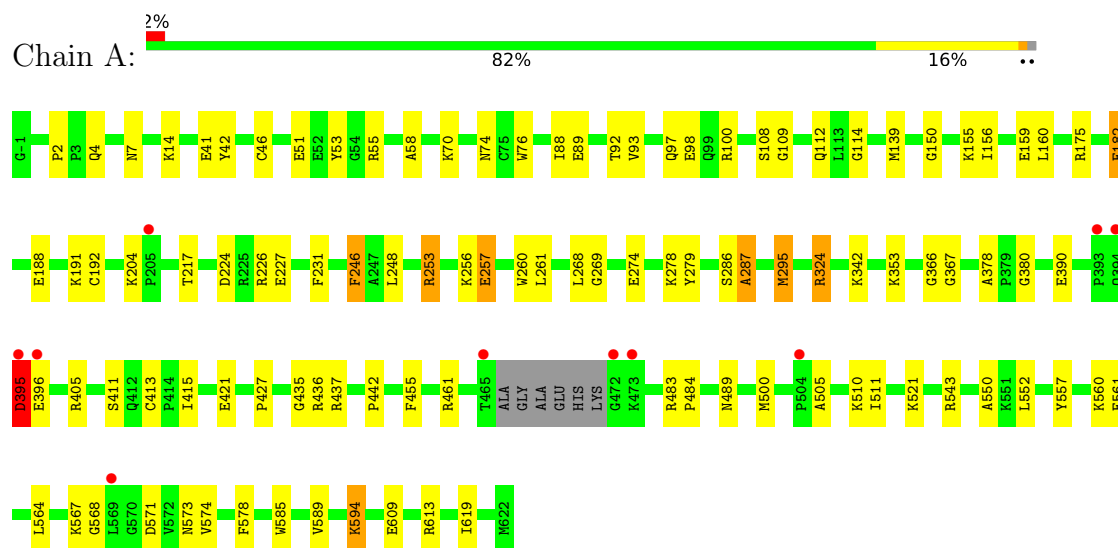
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	620	Total	O	0	0
			620	620		

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: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.32Å 119.12Å 60.05Å 90.00° 111.19° 90.00°	Depositor
Resolution (Å)	20.57 – 1.25 20.57 – 1.25	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.57-1.25) 95.0 (20.57-1.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.148 , 0.174 (Not available) , 0.231	Depositor DCC
R_{free} test set	7657 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5758	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: 1PE, SPV, GTP, EDO, NA, MN

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	1.67	39/5275 (0.7%)	1.40	22/7133 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	MET	SD-CE	-11.94	1.49	1.79
1	A	435	GLY	N-CA	8.60	1.54	1.44
1	A	295	MET	CA-CB	8.16	1.64	1.53
1	A	4	GLN	CA-C	-7.97	1.42	1.52
1	A	573	ASN	C-O	7.38	1.32	1.23
1	A	552	LEU	C-O	6.43	1.31	1.23
1	A	505	ALA	CA-CB	6.31	1.62	1.54
1	A	594	LYS	CE-NZ	6.30	1.68	1.49
1	A	109	GLY	N-CA	6.21	1.49	1.44
1	A	93	VAL	CA-C	-6.18	1.45	1.52
1	A	53	TYR	C-O	-5.93	1.17	1.24
1	A	287	ALA	CA-CB	5.91	1.62	1.53
1	A	413	CYS	CB-SG	-5.77	1.62	1.81
1	A	560	LYS	C-O	-5.71	1.15	1.23
1	A	274	GLU	N-CA	5.70	1.52	1.46
1	A	411	SER	C-O	5.62	1.31	1.24
1	A	353	LYS	CB-CG	-5.58	1.35	1.52
1	A	564	LEU	N-CA	5.57	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	GLY	N-CA	5.53	1.48	1.44
1	A	108	SER	N-CA	5.53	1.53	1.46
1	A	92	THR	N-CA	5.52	1.52	1.46
1	A	46	CYS	CA-C	-5.50	1.45	1.52
1	A	564	LEU	CB-CG	-5.46	1.42	1.53
1	A	378	ALA	C-N	5.36	1.40	1.33
1	A	279	TYR	C-O	5.33	1.30	1.23
1	A	260	TRP	CA-CB	5.24	1.62	1.53
1	A	109	GLY	C-O	5.22	1.28	1.23
1	A	427	PRO	C-O	5.18	1.28	1.23
1	A	427	PRO	CA-C	-5.17	1.47	1.52
1	A	269	GLY	CA-C	-5.12	1.48	1.52
1	A	489	ASN	C-O	5.12	1.30	1.24
1	A	114	GLY	N-CA	5.11	1.50	1.45
1	A	204	LYS	N-CA	5.04	1.50	1.45
1	A	405	ARG	CA-C	-5.03	1.46	1.52
1	A	455	PHE	N-CA	5.03	1.52	1.46
1	A	510	LYS	C-O	5.02	1.29	1.23
1	A	182	GLU	C-O	5.02	1.30	1.24
1	A	278	LYS	C-O	5.01	1.29	1.23
1	A	175	ARG	CG-CD	-5.01	1.37	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	GLY	CA-C-O	6.86	126.96	119.55
1	A	421	GLU	CB-CA-C	-6.76	100.07	111.02
1	A	88	ILE	CB-CA-C	6.13	117.90	111.09
1	A	139	MET	CG-SD-CE	-5.90	87.92	100.90
1	A	324	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	A	568	GLY	N-CA-C	-5.72	107.78	115.21
1	A	2	PRO	CB-CA-C	-5.58	105.93	111.17
1	A	436	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	257[A]	GLU	N-CA-C	-5.46	105.49	111.82
1	A	257[B]	GLU	N-CA-C	-5.46	105.49	111.82
1	A	58	ALA	CA-C-O	-5.44	115.11	120.82
1	A	489	ASN	N-CA-CB	-5.30	101.13	109.51
1	A	395	ASP	N-CA-C	-5.28	102.58	110.23
1	A	461	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	A	561	GLU	N-CA-C	-5.14	102.78	110.23
1	A	160	LEU	O-C-N	-5.11	117.50	123.27
1	A	366	GLY	CA-C-N	-5.07	117.41	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	GLY	C-N-CA	-5.07	117.41	122.69
1	A	2	PRO	N-CA-CB	5.07	105.86	103.22
1	A	7	ASN	N-CA-C	-5.06	104.28	110.61
1	A	253	ARG	CA-CB-CG	-5.04	104.03	114.10
1	A	442	PRO	N-CD-CG	-5.03	95.66	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150[A]	GLY	Peptide

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	5051	0	5097	67	1
2	A	32	0	12	1	0
3	A	2	0	0	0	0
4	A	1	0	0	0	0
5	A	10	0	2	0	0
6	A	26	0	32	10	0
7	A	16	0	24	9	0
8	A	620	0	0	16	2
All	All	5758	0	5167	70	2

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 7.

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:594:LYS:CE	1:A:594:LYS:NZ	1.68	1.51
1:A:342:LYS:HG3	8:A:1163:HOH:O	1.30	1.24
1:A:42[B]:TYR:HE2	8:A:1243:HOH:O	1.32	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LYS:HE2	8:A:1012:HOH:O	1.62	0.97
1:A:286[A]:SER:OG	8:A:1176:HOH:O	1.81	0.95
1:A:574:VAL:HG13	1:A:578[B]:PHE:CD2	2.01	0.95
1:A:42[B]:TYR:OH	8:A:1224:HOH:O	1.83	0.91
6:A:1301:1PE:H121	8:A:1105:HOH:O	1.73	0.89
1:A:585:TRP:O	1:A:589[B]:VAL:HG23	1.78	0.83
1:A:100[B]:ARG:HG2	1:A:100[B]:ARG:HH11	1.51	0.75
1:A:609:GLU:OE2	1:A:613[B]:ARG:NH2	2.19	0.74
1:A:156:ILE:H	7:A:1401:EDO:H22	1.52	0.73
1:A:589[B]:VAL:HG21	1:A:619[B]:ILE:CD1	2.20	0.72
1:A:437:ARG:HH21	7:A:1403:EDO:H22	1.55	0.72
1:A:390:GLU:HG3	8:A:1169:HOH:O	1.89	0.71
1:A:574:VAL:HG13	1:A:578[B]:PHE:HD2	1.56	0.70
1:A:589[B]:VAL:HG21	1:A:619[B]:ILE:HD12	1.72	0.69
1:A:574:VAL:HG13	1:A:578[B]:PHE:CE2	2.29	0.68
1:A:100[B]:ARG:HG2	1:A:100[B]:ARG:NH1	2.09	0.67
1:A:55[A]:ARG:NH2	8:A:1064:HOH:O	2.29	0.64
1:A:543[A]:ARG:HH22	7:A:1400:EDO:H21	1.61	0.64
1:A:155[B]:LYS:HA	7:A:1401:EDO:H11	1.80	0.63
1:A:511:ILE:H	6:A:1301:1PE:C23	2.11	0.63
1:A:42[B]:TYR:CE2	8:A:1243:HOH:O	2.20	0.62
1:A:14[A]:LYS:NZ	6:A:1300:1PE:H242	2.15	0.61
1:A:14[B]:LYS:HE2	6:A:1300:1PE:H242	1.83	0.60
1:A:574:VAL:CG1	1:A:578[B]:PHE:CD2	2.82	0.60
1:A:188:GLU:O	7:A:1401:EDO:H21	2.01	0.60
1:A:589[B]:VAL:CG2	1:A:619[B]:ILE:CD1	2.80	0.59
1:A:437:ARG:HH21	7:A:1403:EDO:C2	2.15	0.58
1:A:226:ARG:HB2	8:A:1207:HOH:O	2.03	0.58
1:A:156:ILE:H	7:A:1401:EDO:C2	2.15	0.57
1:A:224:ASP:OD1	1:A:253:ARG:NH2	2.37	0.57
1:A:287:ALA:HA	2:A:1100:GTP:O2A	2.04	0.57
1:A:14[B]:LYS:HE2	6:A:1300:1PE:H251	1.86	0.56
1:A:483[B]:ARG:HB3	1:A:484:PRO:HD3	1.87	0.56
1:A:14[A]:LYS:HZ2	6:A:1300:1PE:H242	1.70	0.55
1:A:155[A]:LYS:HA	7:A:1401:EDO:H11	1.89	0.53
1:A:550:ALA:HB1	1:A:557:TYR:HB3	1.92	0.52
1:A:574:VAL:CG1	1:A:578[B]:PHE:HD2	2.20	0.52
1:A:191:LYS:HB2	1:A:227[A]:GLU:HG2	1.95	0.49
1:A:182:GLU:OE1	8:A:981:HOH:O	2.20	0.49
1:A:14[A]:LYS:NZ	6:A:1300:1PE:H251	2.28	0.48
1:A:74:ASN:ND2	1:A:76:TRP:HE1	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:GLU:O	1:A:613[A]:ARG:HG3	2.14	0.47
1:A:613[B]:ARG:CZ	8:A:1208:HOH:O	2.63	0.46
1:A:543[A]:ARG:HH22	7:A:1400:EDO:C2	2.28	0.46
1:A:159:GLU:HA	1:A:192:CYS:HB2	1.99	0.44
1:A:217:THR:HA	1:A:231:PHE:O	2.17	0.44
1:A:543[A]:ARG:HA	1:A:543[A]:ARG:HD2	1.82	0.43
1:A:268:LEU:C	1:A:268:LEU:HD12	2.44	0.43
1:A:100[B]:ARG:NH1	1:A:100[B]:ARG:CG	2.70	0.42
1:A:246:PHE:C	1:A:246:PHE:CD1	2.97	0.42
1:A:395:ASP:N	1:A:395:ASP:OD1	2.52	0.42
1:A:609:GLU:OE2	1:A:613[B]:ARG:CZ	2.67	0.42
1:A:594:LYS:NZ	1:A:594:LYS:CD	2.68	0.42
1:A:14[A]:LYS:HE2	8:A:1152:HOH:O	2.20	0.41
1:A:257[A]:GLU:OE2	8:A:1080:HOH:O	2.21	0.41
1:A:324:ARG:HH11	1:A:324:ARG:HD3	1.59	0.41
6:A:1300:1PE:H242	6:A:1300:1PE:H251	1.82	0.41
1:A:97[B]:GLN:OE1	1:A:98[B]:GLU:HG2	2.21	0.41
6:A:1300:1PE:H122	8:A:1179:HOH:O	2.20	0.41
1:A:261:LEU:HD11	1:A:500[A]:MET:SD	2.61	0.41
1:A:295:MET:HA	1:A:415:ILE:HD11	2.02	0.40
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.93	0.40
1:A:41[B]:GLU:OE2	8:A:1171:HOH:O	2.22	0.40
1:A:89:GLU:OE2	1:A:483[B]:ARG:NH1	2.46	0.40
1:A:589[B]:VAL:CG2	1:A:619[B]:ILE:HD13	2.51	0.40
1:A:14[B]:LYS:NZ	6:A:1300:1PE:H131	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41[A]:GLU:OE2	8:A:1206:HOH:O[2_545]	2.08	0.12
8:A:1206:HOH:O	8:A:1224:HOH:O[2_555]	2.11	0.09

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	647/624 (104%)	628 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	549/520 (106%)	539 (98%)	10 (2%)	51	15

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLU
1	A	70	LYS
1	A	112[A]	GLN
1	A	112[B]	GLN
1	A	246	PHE
1	A	395	ASP
1	A	396	GLU
1	A	521	LYS
1	A	567	LYS
1	A	571	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	HIS
1	A	74	ASN
1	A	297	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\# Z > 2$
7	EDO	A	1400	-	3,3,3	0.35	0	2,2,2	1.11	0
6	1PE	A	1300	-	15,15,15	0.92	0	14,14,14	1.31	1 (7%)
7	EDO	A	1402	-	3,3,3	0.27	0	2,2,2	0.86	0
5	SPV	A	1200	3	9,9,9	3.71	3 (33%)	12,13,13	1.28	1 (8%)
6	1PE	A	1301	-	4,4,15	0.88	0	3,3,14	1.50	0
2	GTP	A	1100	3	33,34,34	1.58	6 (18%)	50,54,54	1.50	9 (18%)
7	EDO	A	1403	-	3,3,3	0.63	0	2,2,2	0.56	0
6	1PE	A	1302	-	4,4,15	0.87	0	3,3,14	0.28	0
7	EDO	A	1401	-	3,3,3	0.57	0	2,2,2	1.17	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
7	EDO	A	1400	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	A	1300	-	-	7/13/13/13	-
7	EDO	A	1402	-	-	1/1/1/1	-
5	SPV	A	1200	3	-	0/8/9/9	-
6	1PE	A	1301	-	-	1/2/2/13	-
2	GTP	A	1100	3	-	1/22/38/38	0/3/3/3
7	EDO	A	1403	-	-	1/1/1/1	-
6	1PE	A	1302	-	-	2/2/2/13	-
7	EDO	A	1401	-	-	1/1/1/1	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1200	SPV	C2-C1	-9.44	1.39	1.53
5	A	1200	SPV	C3-C2	4.78	1.61	1.52
2	A	1100	GTP	PB-O3A	3.47	1.63	1.59
2	A	1100	GTP	C2-N1	-3.01	1.30	1.37
2	A	1100	GTP	PA-O2A	-2.86	1.42	1.55
2	A	1100	GTP	C1'-N9	-2.53	1.40	1.47
2	A	1100	GTP	PG-O3G	-2.19	1.46	1.54
2	A	1100	GTP	C2-N2	2.16	1.39	1.34
5	A	1200	SPV	O2-C2	2.14	1.27	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1100	GTP	C4-C5-N7	-3.50	105.13	110.67
2	A	1100	GTP	C5-C4-N9	3.37	111.70	105.66
2	A	1100	GTP	O4'-C1'-C2'	-3.06	100.08	106.62
6	A	1300	1PE	OH5-C25-C15	3.05	124.27	110.35
2	A	1100	GTP	C8-N9-C4	-2.40	101.53	106.03
2	A	1100	GTP	C2'-C3'-C4'	-2.40	97.98	102.61
2	A	1100	GTP	C3'-C2'-C1'	2.29	105.80	101.46
2	A	1100	GTP	O3A-PB-O1B	-2.20	104.08	110.70
2	A	1100	GTP	N9-C4-N3	-2.05	121.85	125.95
2	A	1100	GTP	C6-C5-C4	2.01	121.85	118.83
5	A	1200	SPV	O1-C1-C2	-2.00	119.32	121.81

There are no chirality outliers.

All (15) torsion outliers are listed below:

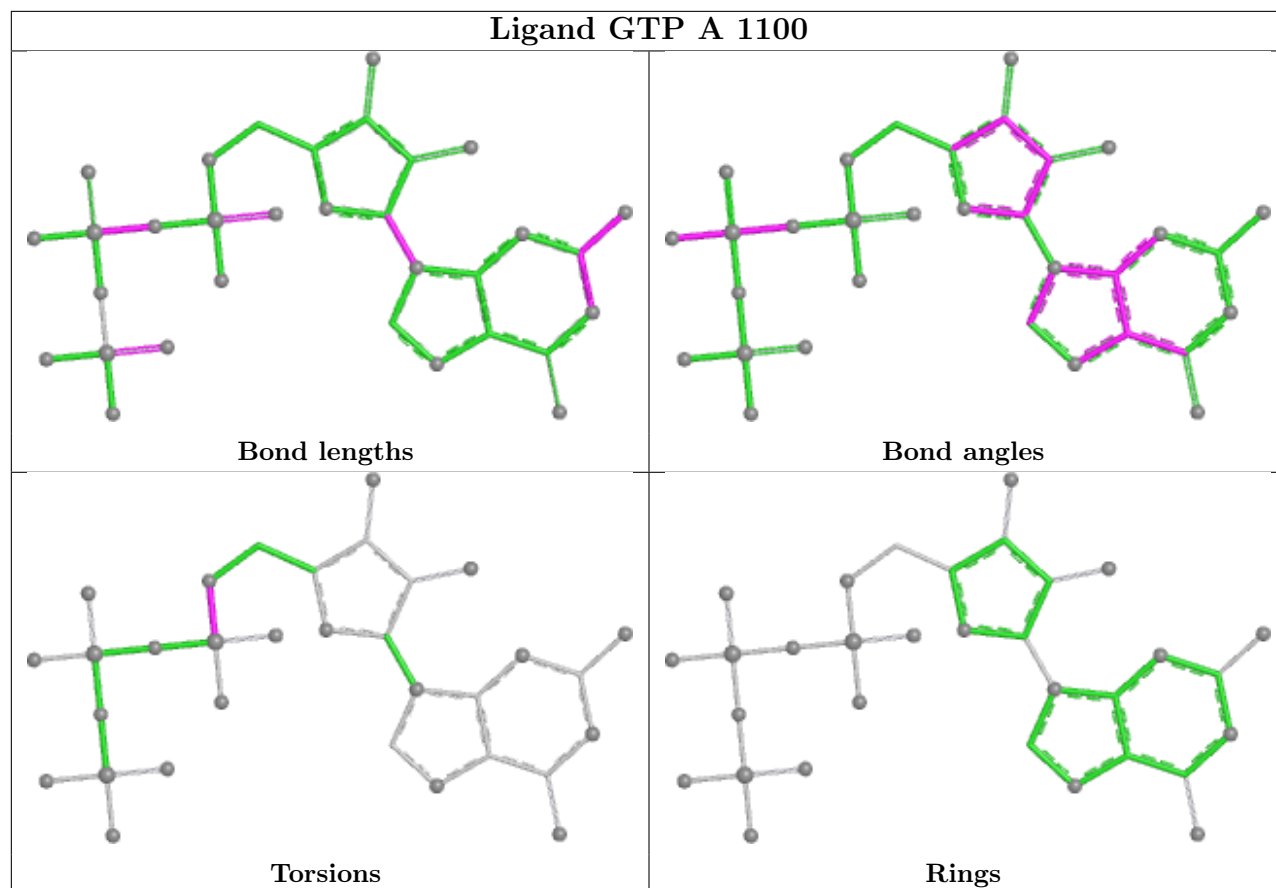
Mol	Chain	Res	Type	Atoms
6	A	1300	1PE	C23-C13-OH4-C24
6	A	1300	1PE	OH6-C15-C25-OH5
6	A	1300	1PE	OH7-C16-C26-OH6
6	A	1302	1PE	OH2-C12-C22-OH3
7	A	1400	EDO	O1-C1-C2-O2
7	A	1403	EDO	O1-C1-C2-O2
7	A	1401	EDO	O1-C1-C2-O2
6	A	1302	1PE	C12-C22-OH3-C23
6	A	1300	1PE	OH4-C13-C23-OH3
2	A	1100	GTP	C5'-O5'-PA-O1A
6	A	1301	1PE	C12-C22-OH3-C23
6	A	1300	1PE	C13-C23-OH3-C22
7	A	1402	EDO	O1-C1-C2-O2
6	A	1300	1PE	OH5-C14-C24-OH4
6	A	1300	1PE	C16-C26-OH6-C15

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1400	EDO	2	0
6	A	1300	1PE	8	0
6	A	1301	1PE	2	0
2	A	1100	GTP	1	0
7	A	1403	EDO	2	0
7	A	1401	EDO	5	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	618/624 (99%)	-0.12	10 (1%) 70 70	2, 7, 21, 52	34 (5%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	PRO	3.8
1	A	394	GLN	3.2
1	A	465	THR	3.0
1	A	569	LEU	3.0
1	A	395	ASP	2.6
1	A	473	LYS	2.5
1	A	205	PRO	2.3
1	A	393	PRO	2.3
1	A	472	GLY	2.2
1	A	396	GLU	2.2

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

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

6.3 Carbohydrates [i](#)

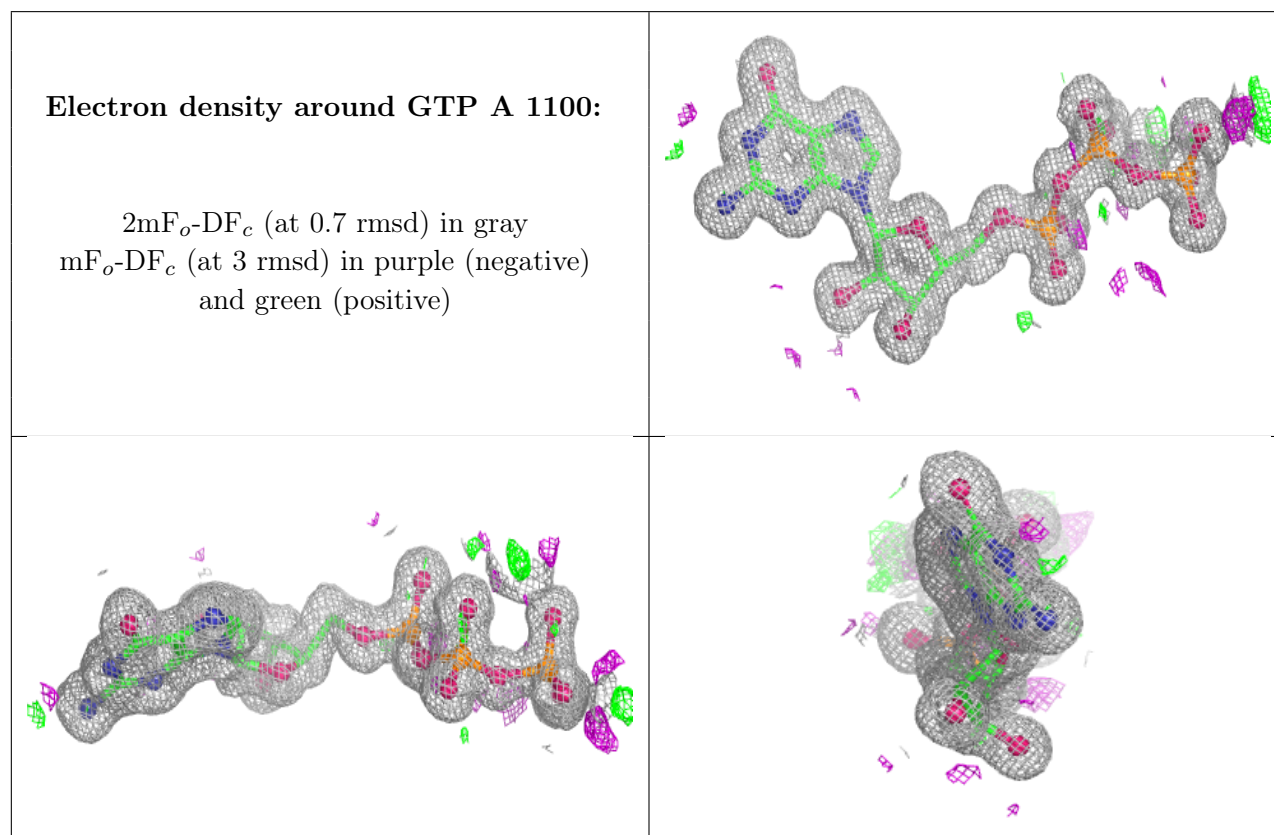
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1PE	A	1302	5/16	0.70	0.20	42,46,49,52	0
6	1PE	A	1300	16/16	0.82	0.14	24,44,58,62	0
7	EDO	A	1402	4/4	0.83	0.12	42,43,43,45	0
7	EDO	A	1400	4/4	0.90	0.09	37,39,40,42	0
6	1PE	A	1301	5/16	0.91	0.09	11,22,25,36	0
7	EDO	A	1401	4/4	0.92	0.09	29,30,32,32	0
4	NA	A	800	1/1	0.93	0.07	22,22,22,22	1
7	EDO	A	1403	4/4	0.93	0.08	18,26,28,36	0
5	SPV	A	1200	10/10	0.99	0.03	10,11,11,12	0
2	GTP	A	1100	32/32	0.99	0.04	9,10,13,14	0
3	MN	A	701	1/1	1.00	0.03	10,10,10,10	0
3	MN	A	700	1/1	1.00	0.03	10,10,10,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.