Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 09:58 PM EST

PDB ID	:	3DTB
Title	:	The structure of rat cytosolic PEPCK in complex with phosphoglycolate and GDP
Authors	:	Sullivan, S.M.; Holyoak, T.
Deposited on	:	2008-07-14
Resolution	:	1.30 Å(reported)

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

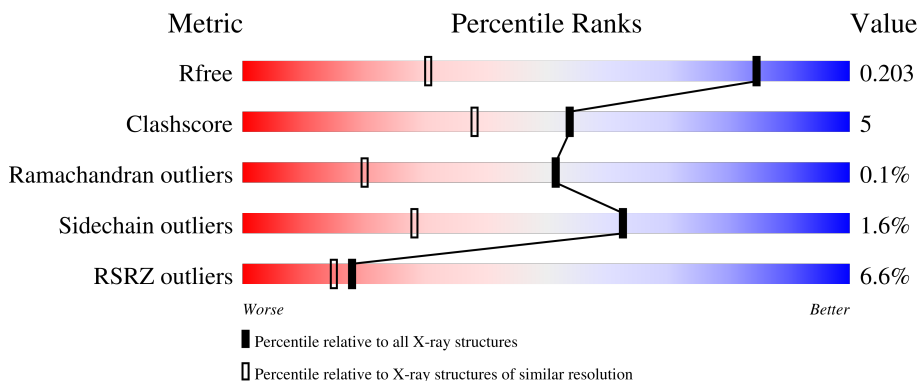|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1   Overall quality at a glance   ⓘ

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

The reported resolution of this entry is 1.30 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}	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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

Mol	Chain	Length	Quality of chain
1	A	624	6% ... 90% ... 8% ..
1	B	624	7% ... 88% ... 10% .

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
7	1PE	A	1000	-	-	X	-

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 11713 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.
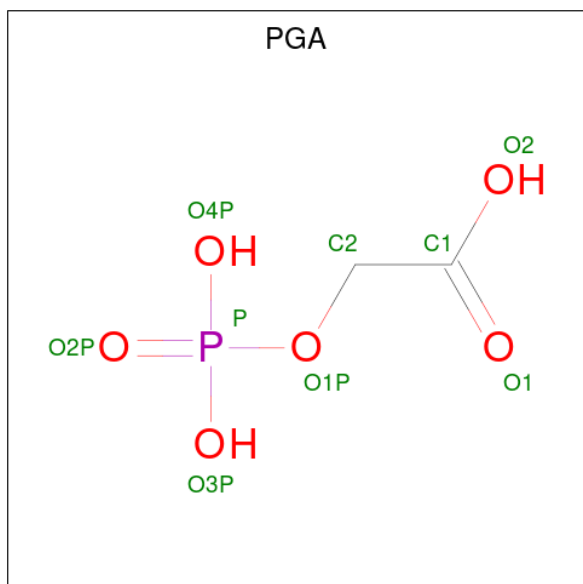
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	41	0
			5078	3269	859	917	33			
1	B	612	Total	C	N	O	S	0	26	0
			4972	3200	845	895	32			

There are 4 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
B	-1	GLY	-	expression tag	UNP P07379
B	0	SER	-	expression tag	UNP P07379

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$).

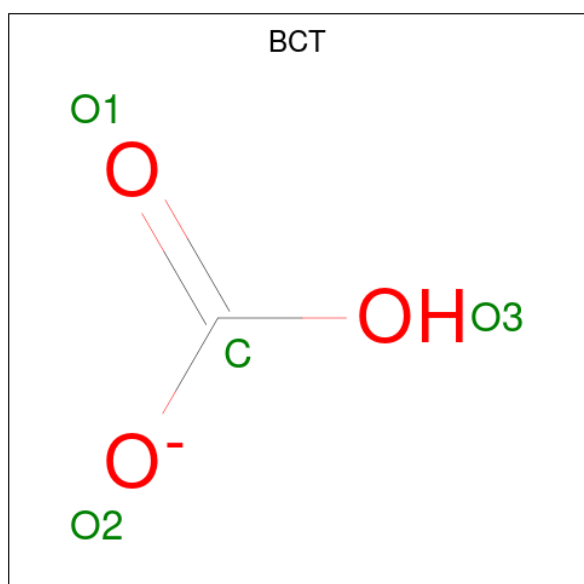| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 9	C 2	O 6	P 1	0	0
2	B	1	Total 9	C 2	O 6	P 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 1	O 3	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).
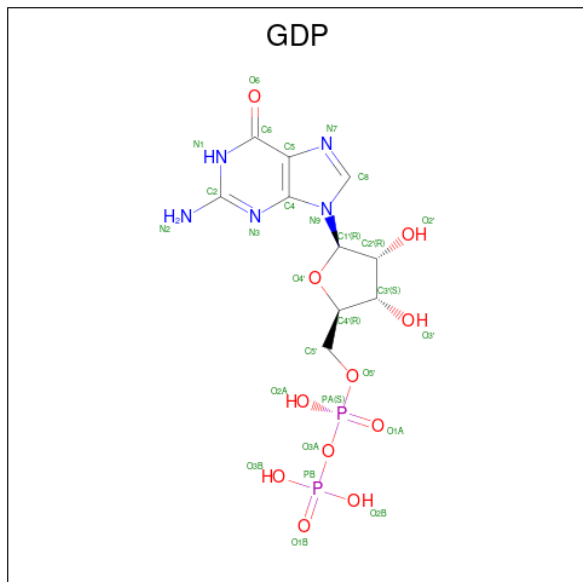

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

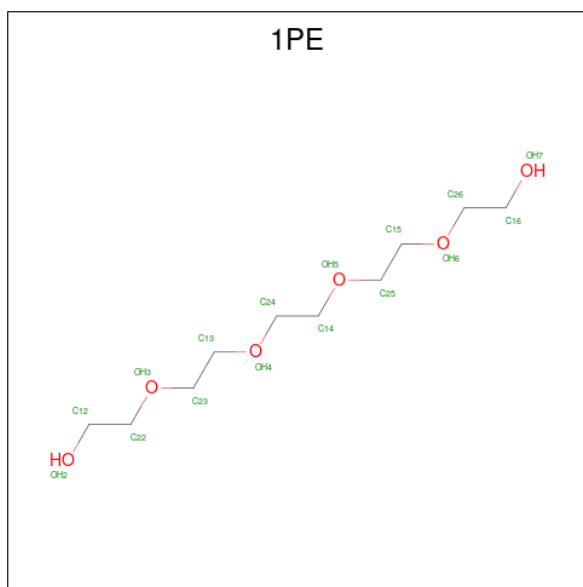- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 10	C 6	O 4	0	0
7	A	1	Total 10	C 6	O 4	0	0

- Molecule 8 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
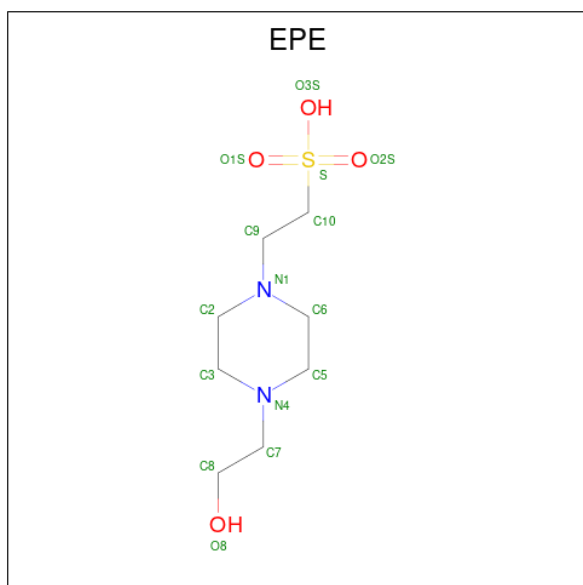

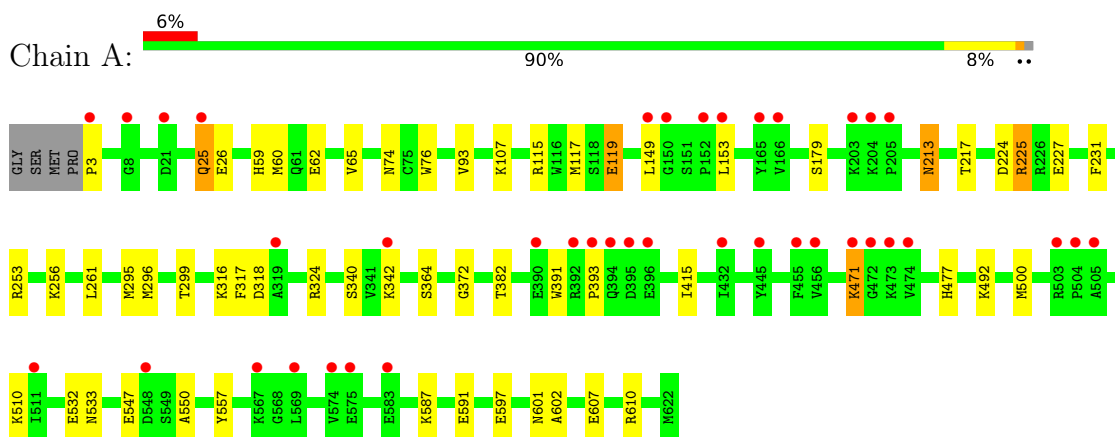| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total 15	C 8	N 2	O 4	S 1	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	791	Total 791	O 791	0	0
9	B	753	Total 753	O 753	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphoenolpyruvate carboxykinase, cytosolic [GTP]

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4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.15Å 119.68Å 86.85Å 90.00° 107.05° 90.00°	Depositor
Resolution (Å)	28.83 – 1.30 28.84 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (28.83-1.30) 97.7 (28.84-1.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.193 0.178 , 0.203	Depositor DCC
R_{free} test set	14703 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11713	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0407e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, BCT, PGA, EPE, MN, NA, 1PE

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	0.60	0/5333	0.73	1/7211 (0.0%)
1	B	0.60	0/5179	0.75	9/7000 (0.1%)
All	All	0.60	0/10512	0.74	10/14211 (0.1%)

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	B	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	461	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	139	MET	CG-SD-CE	-6.50	89.79	100.20
1	B	246	PHE	CB-CG-CD2	-6.28	116.40	120.80
1	B	47	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	436	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	B	7[A]	ASN	O-C-N	-5.25	114.28	123.20
1	B	7[B]	ASN	O-C-N	-5.25	114.28	123.20
1	B	437	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	246	PHE	CB-CG-CD1	5.13	124.39	120.80
1	A	225	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7[A]	ASN	Peptide
1	B	7[B]	ASN	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	5078	0	5166	66	0
1	B	4972	0	5016	42	1
2	A	9	0	2	0	0
2	B	9	0	2	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
6	A	28	0	12	0	0
6	B	28	0	12	1	0
7	A	20	0	26	9	0
8	A	15	0	18	2	0
9	A	791	0	0	10	2
9	B	753	0	0	13	1
All	All	11713	0	10254	108	3

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 (108) 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:324[A]:ARG:NH2	9:A:3844:HOH:O	1.63	1.26
1:A:364[B]:SER:OG	1:A:382[B]:THR:CG2	1.88	1.22
1:B:203:LYS:HE3	9:B:1343:HOH:O	1.40	1.20
1:A:224[A]:ASP:OD2	9:A:3727:HOH:O	1.64	1.12
1:A:364[B]:SER:OG	1:A:382[B]:THR:HG23	1.42	1.10
1:A:256[A]:LYS:HE3	9:A:3865:HOH:O	1.58	1.03
1:A:316:LYS:HZ3	7:A:1000:1PE:H231	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601[B]:ASN:HD22	1:A:602:ALA:H	0.97	0.95
1:A:364[B]:SER:OG	1:A:382[B]:THR:HG22	1.66	0.93
1:A:93[B]:VAL:HG11	1:A:117:MET:HB2	1.52	0.91
1:B:51:GLU:HG2	9:B:1851:HOH:O	1.68	0.90
1:A:317:PHE:HE2	1:A:500[B]:MET:CE	1.87	0.87
1:A:601[B]:ASN:ND2	1:A:602:ALA:H	1.69	0.87
1:A:253:ARG:NH1	9:A:3738:HOH:O	2.08	0.86
1:A:364[B]:SER:HG	1:A:382[B]:THR:HG23	1.41	0.84
1:B:155[A]:LYS:HE2	1:B:254:LEU:HD13	1.61	0.83
1:A:340[B]:SER:OG	1:A:372:GLY:O	1.98	0.81
1:A:149:LEU:HD21	1:A:179[B]:SER:HB3	1.63	0.80
1:A:342:LYS:HG2	9:A:3608:HOH:O	1.82	0.79
1:B:9:LEU:HG	9:B:1577:HOH:O	1.85	0.77
1:B:49:SER:OG	1:B:51:GLU:HG3	1.84	0.77
1:B:226[B]:ARG:HD3	9:B:1582:HOH:O	1.85	0.76
1:A:149:LEU:HD21	1:A:179[A]:SER:HB2	1.67	0.75
1:A:316:LYS:NZ	7:A:1000:1PE:H122	2.03	0.74
1:A:317:PHE:HE2	1:A:500[B]:MET:HE3	1.54	0.72
1:A:93[B]:VAL:HG11	1:A:117:MET:CB	2.19	0.72
1:A:299[B]:THR:HG21	1:A:532:GLU:OE1	1.90	0.72
1:A:93[B]:VAL:HG22	1:A:115[B]:ARG:HD3	1.73	0.71
1:B:609[B]:GLU:OE1	1:B:613[B]:ARG:NE	2.23	0.71
1:A:317:PHE:HE2	1:A:500[B]:MET:HE2	1.54	0.70
1:A:153:LEU:HD13	7:A:1000:1PE:H232	1.73	0.69
1:B:155[A]:LYS:HE2	1:B:254:LEU:CD1	2.25	0.65
1:A:317:PHE:CE2	1:A:500[B]:MET:HE3	2.34	0.63
1:A:607[B]:GLU:HG2	1:A:610:ARG:NH2	2.15	0.61
1:B:203:LYS:HE2	9:B:1220:HOH:O	2.01	0.60
1:A:601[B]:ASN:ND2	1:A:602:ALA:N	2.47	0.59
1:A:601[B]:ASN:HD22	1:A:602:ALA:N	1.82	0.59
1:A:317:PHE:CE2	1:A:500[B]:MET:CE	2.78	0.58
1:A:317:PHE:CE2	1:A:500[B]:MET:HE2	2.37	0.58
1:A:316:LYS:NZ	7:A:1000:1PE:H242	2.19	0.58
1:A:119:GLU:CG	1:A:225:ARG:HH22	2.16	0.57
1:A:316:LYS:HZ1	7:A:1000:1PE:H122	1.68	0.57
1:A:119:GLU:HG2	1:A:225:ARG:HH22	1.70	0.56
1:A:256[A]:LYS:NZ	1:A:492[A]:LYS:HB3	2.20	0.56
1:B:547[A]:GLU:HG2	1:B:549:SER:HB3	1.88	0.56
1:B:476[B]:MET:HE3	9:B:1633:HOH:O	2.04	0.56
1:A:382[B]:THR:HG23	9:A:3614:HOH:O	2.06	0.55
1:B:272:ASN:HD21	1:B:276:LYS:HZ2	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:HIS:HD2	1:B:62:GLU:OE1	1.90	0.55
1:A:60[B]:MET:HG2	1:A:65[B]:VAL:HG21	1.89	0.55
1:B:271:THR:HB	1:B:304:LYS:HD3	1.90	0.54
1:B:272:ASN:HD21	1:B:276:LYS:NZ	2.06	0.54
1:A:261:LEU:HD11	1:A:500[B]:MET:SD	2.48	0.54
1:A:510[B]:LYS:HG3	9:A:4069:HOH:O	2.08	0.54
1:B:483[B]:ARG:CD	9:B:1777:HOH:O	2.56	0.53
1:A:107:LYS:NZ	1:A:601[A]:ASN:OD1	2.39	0.53
1:B:264:HIS:CD2	1:B:290[A]:LYS:NZ	2.77	0.52
1:B:292[B]:ASN:ND2	9:B:1275:HOH:O	2.42	0.52
1:A:74:ASN:ND2	1:A:76:TRP:HE1	2.08	0.52
1:B:41[B]:GLU:OE1	9:B:1843:HOH:O	2.18	0.52
1:A:364[B]:SER:HG	1:A:382[B]:THR:CG2	2.04	0.52
1:A:316:LYS:NZ	7:A:1000:1PE:H231	2.12	0.52
1:A:316:LYS:HZ3	7:A:1000:1PE:H122	1.75	0.51
1:B:88[B]:ILE:H	1:B:238:ASN:HD21	1.55	0.51
1:B:88[A]:ILE:H	1:B:238:ASN:HD21	1.56	0.51
1:A:107:LYS:HG3	1:A:601[A]:ASN:ND2	2.25	0.51
1:B:547[A]:GLU:HG3	9:B:1416:HOH:O	2.11	0.51
1:A:597:GLU:O	1:A:601[B]:ASN:HB3	2.12	0.50
1:B:296:MET:HE1	1:B:533:ASN:HB2	1.93	0.50
1:A:227:GLU:OE1	8:A:3380:EPE:H91	2.12	0.50
1:B:483[A]:ARG:NE	9:B:1633:HOH:O	2.21	0.50
1:B:613[B]:ARG:HG3	9:B:1623:HOH:O	2.12	0.49
1:A:59:HIS:O	1:A:62[A]:GLU:HB2	2.11	0.49
1:B:483[A]:ARG:HB3	1:B:484:PRO:HD3	1.94	0.49
1:B:609[B]:GLU:OE1	1:B:613[B]:ARG:CZ	2.60	0.48
1:A:3:PRO:HA	9:A:3709:HOH:O	2.13	0.48
1:A:471:LYS:HE3	9:A:3463:HOH:O	2.15	0.47
1:B:391:TRP:CH2	1:B:393:PRO:HA	2.50	0.46
1:A:295:MET:HA	1:A:415[A]:ILE:HD11	1.97	0.46
1:A:25[B]:GLN:HG2	1:A:26:GLU:N	2.29	0.46
1:A:119:GLU:CD	1:A:225:ARG:HH12	2.20	0.45
1:A:391:TRP:CH2	1:A:393:PRO:HA	2.51	0.45
1:B:550:ALA:HB1	1:B:557:TYR:HB3	1.99	0.45
1:B:483[B]:ARG:HD3	9:B:1777:HOH:O	2.15	0.45
1:A:477:HIS:HE2	1:A:591:GLU:CD	2.20	0.45
1:A:550:ALA:HB1	1:A:557:TYR:HB3	1.99	0.44
1:B:295:MET:HA	1:B:415:ILE:HD11	1.99	0.44
1:B:74:ASN:ND2	1:B:76:TRP:HE1	2.15	0.44
1:A:318:ASP:OD2	1:A:324[B]:ARG:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LYS:HZ2	7:A:1000:1PE:H242	1.81	0.43
1:B:464:ALA:HB2	1:B:476[B]:MET:SD	2.58	0.43
1:B:336:ALA:HB3	1:B:337:PRO:HD3	2.00	0.43
1:A:213:ASN:C	1:A:213:ASN:HD22	2.22	0.43
1:A:93[B]:VAL:HG22	1:A:115[B]:ARG:CD	2.45	0.42
1:A:316:LYS:HZ3	7:A:1000:1PE:H242	1.85	0.42
1:B:59:HIS:O	1:B:62:GLU:HB2	2.19	0.42
1:B:569:LEU:HD23	1:B:569:LEU:HA	1.77	0.42
1:B:292[A]:ASN:ND2	6:B:800:GDP:H2'	2.35	0.42
1:A:510[B]:LYS:HG2	9:A:4116:HOH:O	2.20	0.41
8:A:3380:EPE:H81	8:A:3380:EPE:H52	1.31	0.41
1:A:107:LYS:O	1:B:507:LYS:NZ	2.53	0.41
1:B:217:THR:HA	1:B:231:PHE:O	2.20	0.41
1:B:266:LEU:C	1:B:266:LEU:HD12	2.41	0.41
1:A:296:MET:HE2	1:A:533:ASN:HB2	2.03	0.41
1:A:256[A]:LYS:HZ2	1:A:492[A]:LYS:HB3	1.84	0.41
1:B:520:ASP:OD1	1:B:524[B]:LYS:HE2	2.21	0.41
1:A:217:THR:HA	1:A:231:PHE:O	2.21	0.40
1:B:515:ASN:ND2	1:B:517:PHE:H	2.19	0.40

All (3) 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)
9:A:3767:HOH:O	9:A:3942:HOH:O[2_645]	2.00	0.20
1:B:63:GLU:OE2	9:B:1710:HOH:O[2_554]	2.13	0.07
9:A:3814:HOH:O	9:A:4111:HOH:O[2_655]	2.18	0.02

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	659/624 (106%)	643 (98%)	16 (2%)	0	100	100
1	B	634/624 (102%)	622 (98%)	11 (2%)	1 (0%)	47	19
All	All	1293/1248 (104%)	1265 (98%)	27 (2%)	1 (0%)	51	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	558/520 (107%)	550 (99%)	8 (1%)	67	34
1	B	539/520 (104%)	529 (98%)	10 (2%)	57	20
All	All	1097/1040 (106%)	1079 (98%)	18 (2%)	62	28

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25[A]	GLN
1	A	25[B]	GLN
1	A	119	GLU
1	A	213	ASN
1	A	471	LYS
1	A	547	GLU
1	A	587[A]	LYS
1	A	587[B]	LYS
1	B	4	GLN
1	B	9	LEU
1	B	110	GLN
1	B	213	ASN
1	B	246	PHE
1	B	253	ARG
1	B	394	GLN

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Mol	Chain	Res	Type
1	B	473	LYS
1	B	521	LYS
1	B	575	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	112	GLN
1	A	208	ASN
1	A	213	ASN
1	A	238	ASN
1	A	297	ASN
1	A	320	GLN
1	A	322	ASN
1	A	515	ASN
1	B	4	GLN
1	B	36	GLN
1	B	59	HIS
1	B	74	ASN
1	B	110	GLN
1	B	213	ASN
1	B	238	ASN
1	B	272	ASN
1	B	297	ASN
1	B	352	GLN
1	B	515	ASN
1	B	522	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\#|Z| > 2$
6	GDP	A	800	3	24,30,30	0.85	1 (4%)	30,47,47	1.06	2 (6%)
2	PGA	A	900	3	8,8,8	1.25	1 (12%)	10,11,11	1.31	1 (10%)
5	BCT	A	1044	-	2,3,3	0.49	0	2,3,3	0.96	0
7	1PE	A	1000	-	9,9,15	0.42	0	8,8,14	0.69	0
8	EPE	A	3380	-	15,15,15	1.87	1 (6%)	18,20,20	2.69	7 (38%)
2	PGA	B	900	3	8,8,8	0.96	0	10,11,11	1.46	1 (10%)
6	GDP	B	800	3	24,30,30	0.93	1 (4%)	30,47,47	1.02	0
7	1PE	A	1101	-	9,9,15	0.50	0	8,8,14	0.24	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
6	GDP	A	800	3	-	0/12/32/32	0/3/3/3
2	PGA	A	900	3	-	3/6/6/6	-
7	1PE	A	1000	-	-	3/7/7/13	-
8	EPE	A	3380	-	-	7/9/19/19	0/1/1/1
2	PGA	B	900	3	-	0/6/6/6	-
6	GDP	B	800	3	-	0/12/32/32	0/3/3/3
7	1PE	A	1101	-	-	6/7/7/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	3380	EPE	C10-S	-6.89	1.67	1.77
6	B	800	GDP	C6-N1	-2.86	1.33	1.37
6	A	800	GDP	C6-N1	-2.10	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	PGA	O1P-C2	-2.10	1.41	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	3380	EPE	C5-N4-C3	5.97	122.27	108.83
8	A	3380	EPE	C6-N1-C2	5.00	120.07	108.83
8	A	3380	EPE	C9-N1-C2	4.34	122.34	111.23
8	A	3380	EPE	O1S-S-C10	3.92	111.63	106.92
8	A	3380	EPE	C7-N4-C5	3.19	119.39	111.23
2	B	900	PGA	O1P-C2-C1	2.77	114.72	110.54
8	A	3380	EPE	C7-N4-C3	2.68	118.10	111.23
2	A	900	PGA	O1P-P-O2P	-2.46	99.58	106.47
8	A	3380	EPE	C9-N1-C6	2.42	117.43	111.23
6	A	800	GDP	C3'-C2'-C1'	2.28	104.42	100.98
6	A	800	GDP	N2-C2-N3	-2.02	115.81	119.74

There are no chirality outliers.

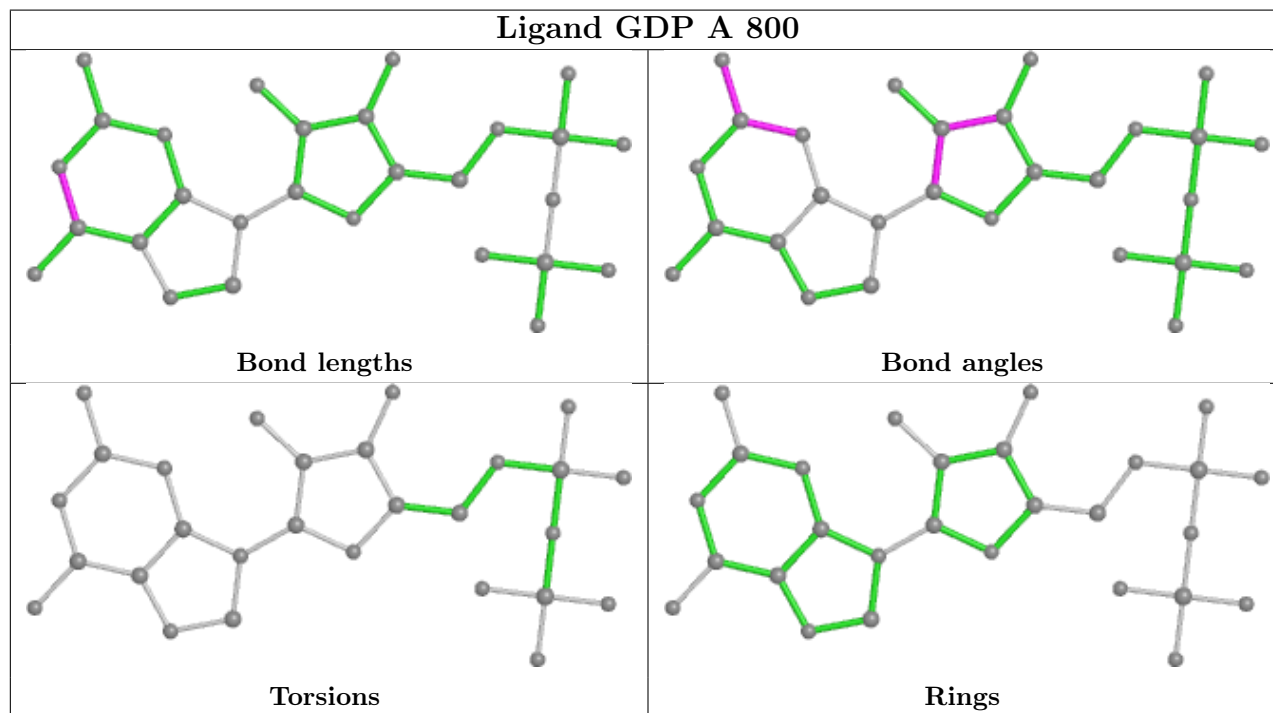All (19) torsion outliers are listed below:

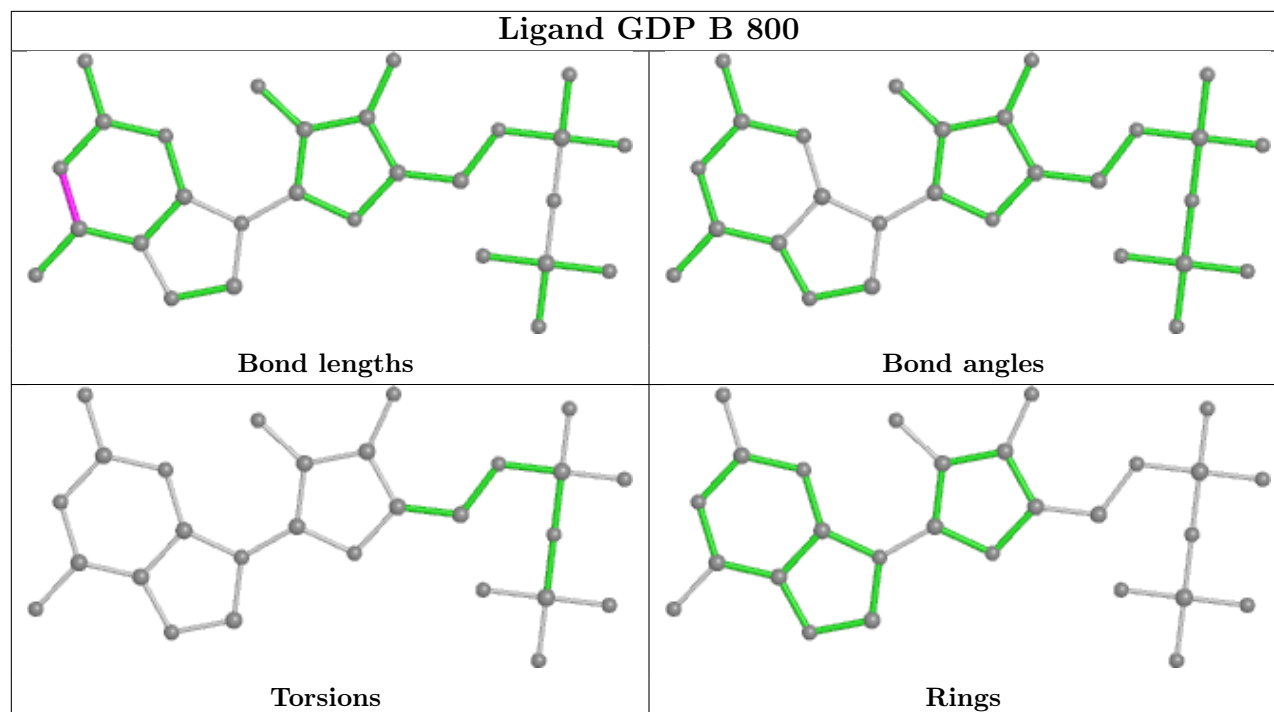| Mol	Chain	Res	Type	Atoms
2	A	900	PGA	C2-O1P-P-O2P
2	A	900	PGA	C2-O1P-P-O3P
2	A	900	PGA	C2-O1P-P-O4P
8	A	3380	EPE	C10-C9-N1-C2
8	A	3380	EPE	C8-C7-N4-C5
8	A	3380	EPE	C9-C10-S-O1S
7	A	1101	1PE	OH4-C13-C23-OH3
8	A	3380	EPE	N4-C7-C8-O8
8	A	3380	EPE	C9-C10-S-O3S
7	A	1101	1PE	OH5-C14-C24-OH4
7	A	1101	1PE	C13-C23-OH3-C22
7	A	1101	1PE	C23-C13-OH4-C24
7	A	1101	1PE	OH2-C12-C22-OH3
8	A	3380	EPE	C9-C10-S-O2S
7	A	1101	1PE	C12-C22-OH3-C23
7	A	1000	1PE	C12-C22-OH3-C23
7	A	1000	1PE	C23-C13-OH4-C24
8	A	3380	EPE	C10-C9-N1-C6
7	A	1000	1PE	OH4-C13-C23-OH3

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1000	1PE	9	0
8	A	3380	EPE	2	0
6	B	800	GDP	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GDP A 800

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP B 800

Bond lengths

Bond angles

Torsions

Rings

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	620/624 (99%)	0.39	39 (6%)	20	17	4, 8, 17, 32	0
1	B	612/624 (98%)	0.45	42 (6%)	16	14	4, 9, 19, 35	0
All	All	1232/1248 (98%)	0.42	81 (6%)	18	15	4, 8, 18, 35	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394	GLN	9.4
1	A	504	PRO	9.2
1	A	394	GLN	8.6
1	A	393	PRO	7.8
1	B	396	GLU	7.3
1	B	395	ASP	6.1
1	B	504	PRO	6.0
1	A	205	PRO	5.8
1	B	393	PRO	5.5
1	A	396	GLU	5.5
1	B	392	ARG	4.9
1	B	205	PRO	4.6
1	A	149	LEU	4.4
1	A	152	PRO	4.4
1	B	571	ASP	4.0
1	B	8	GLY	3.9
1	B	575	GLU	3.8
1	B	150	GLY	3.8
1	B	3	PRO	3.7
1	B	397	GLU	3.7
1	A	392	ARG	3.6
1	B	473	LYS	3.4
1	B	432	ILE	3.4
1	B	380	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	3	PRO	3.2
1	B	9	LEU	3.2
1	B	521	LYS	3.1
1	B	390	GLU	3.1
1	B	569	LEU	3.0
1	A	150	GLY	2.9
1	B	391	TRP	2.9
1	A	432	ILE	2.9
1	B	595[A]	TYR	2.9
1	A	575	GLU	2.9
1	B	7[A]	ASN	2.8
1	A	25[A]	GLN	2.8
1	A	319	ALA	2.8
1	A	204	LYS	2.7
1	A	395	ASP	2.7
1	B	379	PRO	2.7
1	A	472	GLY	2.7
1	B	570	GLY	2.7
1	A	8	GLY	2.7
1	A	471	LYS	2.6
1	B	583	GLU	2.6
1	A	569	LEU	2.6
1	A	474	VAL	2.6
1	A	583	GLU	2.5
1	B	502	HIS	2.5
1	A	456	VAL	2.5
1	B	522	ASN	2.5
1	A	574	VAL	2.5
1	A	505	ALA	2.5
1	B	165	TYR	2.4
1	A	567	LYS	2.4
1	B	389	LYS	2.4
1	B	505	ALA	2.4
1	B	166	VAL	2.4
1	B	319	ALA	2.3
1	A	445	TYR	2.3
1	A	511	ILE	2.3
1	A	390	GLU	2.3
1	A	503[A]	ARG	2.3
1	B	25	GLN	2.2
1	A	548[A]	ASP	2.2
1	B	456	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	342	LYS	2.2
1	A	473	LYS	2.2
1	B	203	LYS	2.2
1	A	153	LEU	2.1
1	A	166	VAL	2.1
1	B	561	GLU	2.1
1	B	480	PHE	2.1
1	A	203	LYS	2.1
1	B	433	PHE	2.1
1	B	51	GLU	2.1
1	B	100	ARG	2.0
1	A	165	TYR	2.0
1	A	21[A]	ASP	2.0
1	A	455	PHE	2.0
1	B	377	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
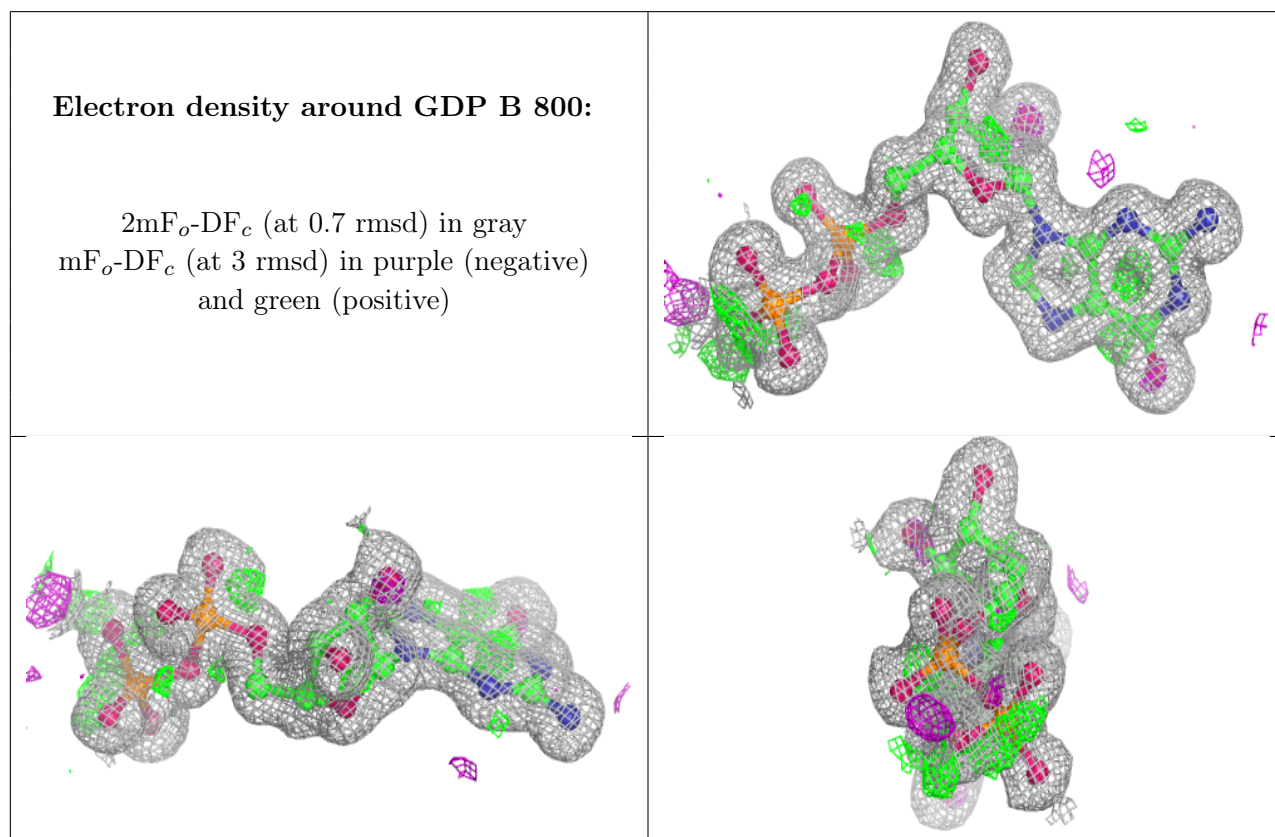
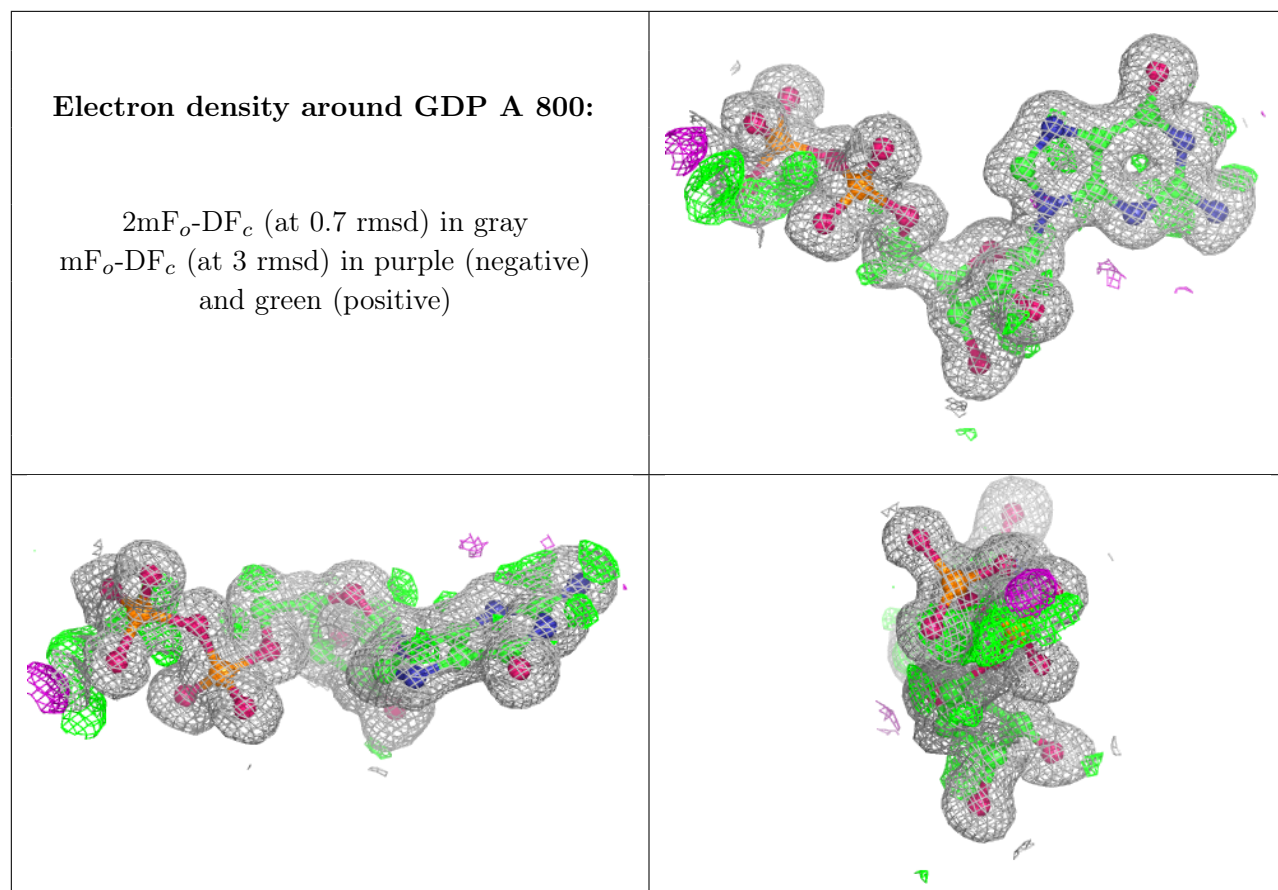| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	1PE	A	1101	10/16	0.68	0.20	38,39,40,40	0
8	EPE	A	3380	15/15	0.80	0.18	18,20,22,24	15
7	1PE	A	1000	10/16	0.85	0.18	9,14,20,22	0
5	BCT	A	1044	4/4	0.92	0.25	13,14,15,17	0
4	NA	A	1100	1/1	0.96	0.12	14,14,14,14	0
4	NA	B	1100	1/1	0.97	0.10	13,13,13,13	0
2	PGA	B	900	9/9	0.97	0.08	6,9,11,13	9
6	GDP	B	800	28/28	0.97	0.06	4,8,9,11	28

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PGA	A	900	9/9	0.98	0.06	4,5,6,6	9
6	GDP	A	800	28/28	0.98	0.06	2,4,5,5	28
3	MN	B	701	1/1	0.99	0.02	7,7,7,7	1
3	MN	A	700	1/1	1.00	0.04	4,4,4,4	0
3	MN	A	701	1/1	1.00	0.02	5,5,5,5	1
3	MN	B	700	1/1	1.00	0.03	5,5,5,5	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 GDP B 800:

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

Electron density around GDP A 800:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.