



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:41 PM UTC

PDB ID : 3DTB / pdb_00003dtb
Title : The structure of rat cytosolic PEPCCK in complex with phosphoglycolate and GDP
Authors : Sullivan, S.M.; Holyoak, T.
Deposited on : 2008-07-14
Resolution : 1.30 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

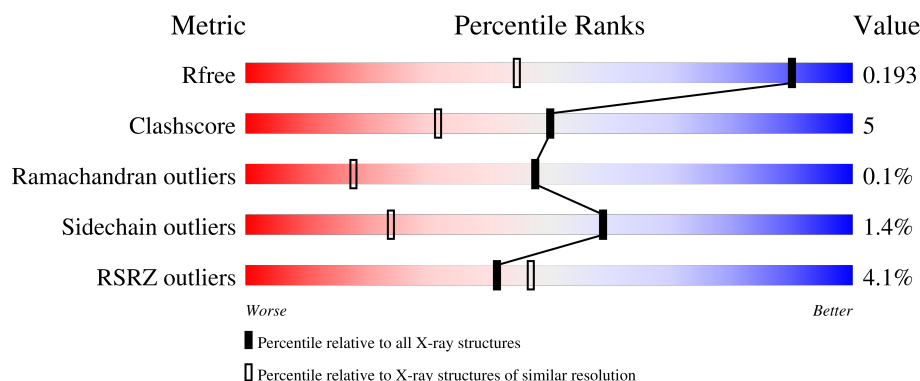
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (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 $\leq 5\%$. 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	4% 90% 9% .
1	B	624	4% 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 [i](#)

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.

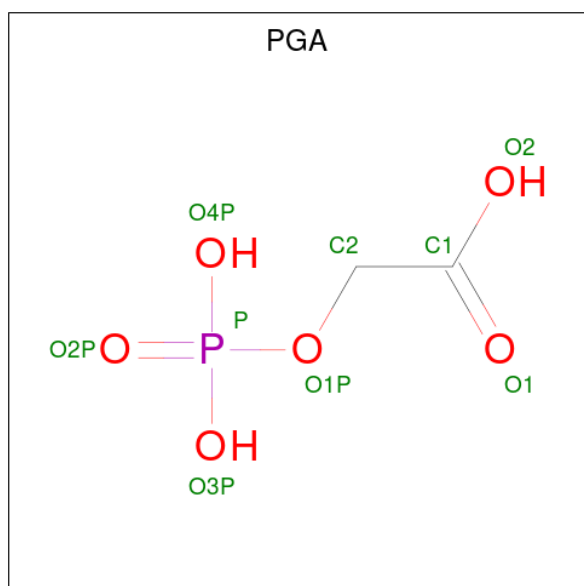
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

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 (CCD ID: PGA) (formula: $C_2H_5O_6P$).



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

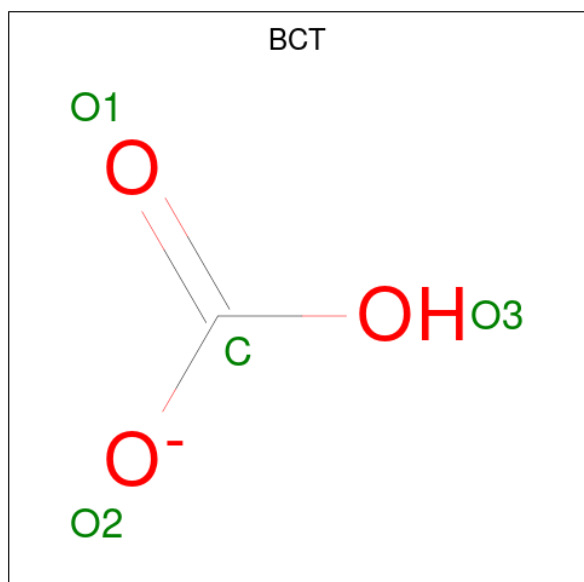
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	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		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



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

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- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected in a diphosphate chain, with the first phosphate linked to the 5' carbon of the ribose and the second phosphate linked to the first. The structure is labeled with various atoms and bonds, including the nitrogenous base, the sugar, and the phosphate groups.

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

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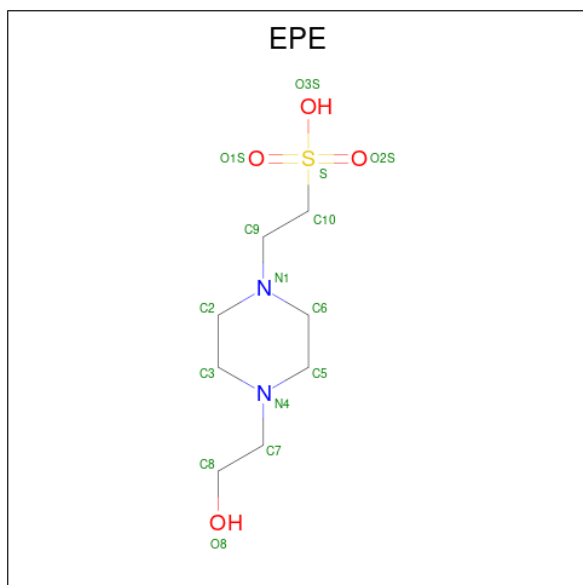
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			10	6	4		

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

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



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

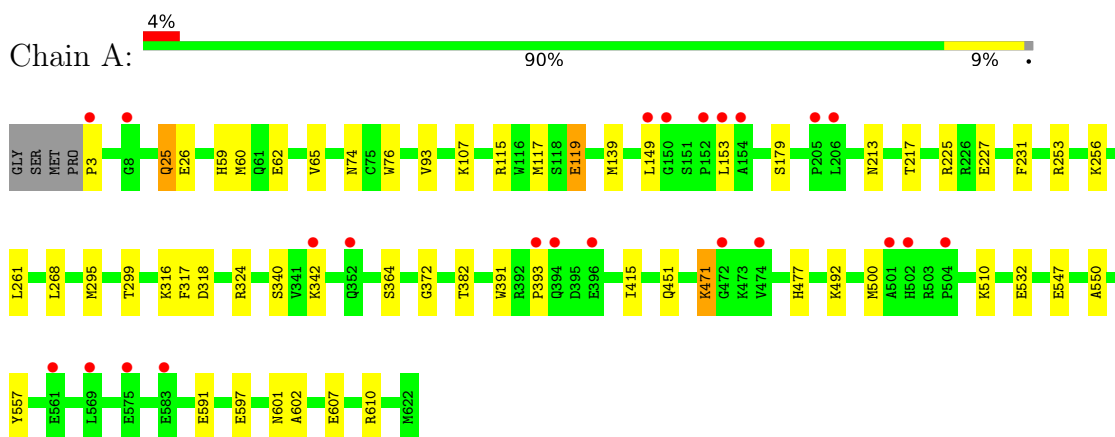
- Molecule 9 is water.

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

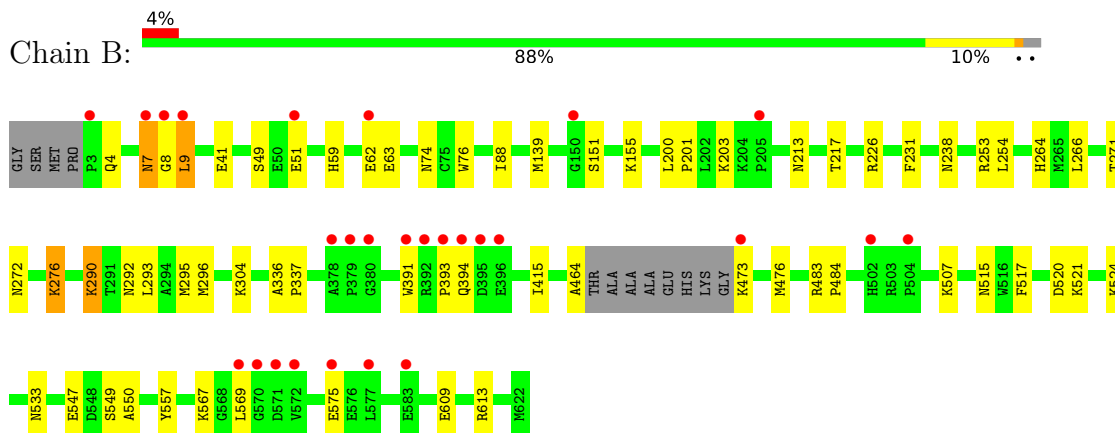
3 Residue-property plots

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]



- 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	62.15Å 119.68Å 86.85Å 90.00° 107.05° 90.00°	Depositor
Resolution (Å)	28.83 – 1.30 28.83 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (28.83-1.30) 97.9 (28.83-1.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.193 0.171 , 0.193	Depositor DCC
R_{free} test set	14703 reflections (4.93%)	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)	0.38 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

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: GDP, MN, EPE, PGA, NA, BCT, 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	0.70	1/5333 (0.0%)	0.81	0/7211
1	B	0.72	1/5179 (0.0%)	0.84	4/7000 (0.1%)
All	All	0.71	2/10512 (0.0%)	0.82	4/14211 (0.0%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	MET	SD-CE	-10.49	1.53	1.79
1	A	139	MET	SD-CE	-5.01	1.67	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	SER	N-CA-C	6.82	118.30	109.64
1	B	7[A]	ASN	O-C-N	-6.54	114.28	122.19
1	B	7[B]	ASN	O-C-N	-6.54	114.28	122.19
1	B	139	MET	CG-SD-CE	-5.05	89.79	100.90

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	64	0
1	B	4972	0	5016	44	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	7	0
8	A	15	0	18	2	0
9	A	791	0	0	9	2
9	B	753	0	0	11	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: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	1.31	0.95
1:A:601[B]:ASN:HD22	1:A:602:ALA:H	0.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:317:PHE:HE2	1:A:500[B]:MET:HE3	1.40	0.85
1:A:364[B]:SER:HG	1:A:382[B]:THR:HG23	1.42	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:316:LYS:HZ1	7:A:1000:1PE:H122	1.51	0.75
1:A:149:LEU:HD21	1:A:179[A]:SER:HB2	1.67	0.75
1:A:317:PHE:CE2	1:A:500[B]:MET:HE3	2.22	0.75
1:A:316:LYS:NZ	7:A:1000:1PE:H122	2.03	0.74
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: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:316:LYS:NZ	7:A:1000:1PE:H231	2.12	0.63
1:A:607[B]:GLU:HG2	1:A:610:ARG:NH2	2.15	0.61
1:B:293:LEU:HD12	1:B:296:MET:HE3	1.83	0.60
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:316:LYS:HZ3	7:A:1000:1PE:H242	1.69	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: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:A:256[A]:LYS:HZ1	1:A:492[A]:LYS:HB3	1.71	0.56
1:A:317:PHE:HE2	1:A:500[B]:MET:HE2	1.68	0.56
1:A:382[B]:THR:HG23	9:A:3614:HOH:O	2.06	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:A:107:LYS:NZ	1:A:601[A]:ASN:OD1	2.39	0.53
1:A:364[B]:SER:HG	1:A:382[B]:THR:CG2	2.03	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: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:B:476[B]:MET:HE3	9:B:1633:HOH:O	2.12	0.50
1:A:597:GLU:O	1:A:601[B]:ASN:HB3	2.12	0.50
1:A:119:GLU:CD	1:A:225:ARG:HH12	2.20	0.50
1:A:227:GLU:OE1	8:A:3380:EPE:H91	2.12	0.50
1:A:477:HIS:HE2	1:A:591:GLU:CD	2.20	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:213:ASN:C	1:A:213:ASN:HD22	2.22	0.47
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:B:266:LEU:C	1:B:266:LEU:HD12	2.41	0.46
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: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
1:B:200:LEU:HA	1:B:201:PRO:C	2.43	0.43
1:B:296:MET:HE2	1:B:533:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93[B]:VAL:HG22	1:A:115[B]:ARG:CD	2.45	0.42
1:B:59:HIS:O	1:B:62:GLU:HB2	2.19	0.42
1:B:272:ASN:HD21	1:B:276:LYS:HZ2	1.67	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:A:268:LEU:C	1:A:268:LEU:HD12	2.46	0.41
1:B:520:ASP:OD1	1:B:524[B]:LYS:HE2	2.21	0.41
1:A:317:PHE:CE2	1:A:500[B]:MET:HE2	2.50	0.41
1:B:213:ASN:C	1:B:213:ASN:HD22	2.28	0.41
1:B:293:LEU:CD1	1:B:296:MET:HE3	2.49	0.41
1:A:451[A]:GLN:H	1:A:451[A]:GLN:CD	2.29	0.40
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%)	43	17
All	All	1293/1248 (104%)	1265 (98%)	27 (2%)	1 (0%)	48	18

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%)	553 (99%)	5 (1%)	70	42
1	B	539/520 (104%)	528 (98%)	11 (2%)	48	12
All	All	1097/1040 (106%)	1081 (98%)	16 (2%)	59	21

All (16) 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	471	LYS
1	A	547	GLU
1	B	4	GLN
1	B	9	LEU
1	B	253	ARG
1	B	276	LYS
1	B	290[A]	LYS
1	B	290[B]	LYS
1	B	394	GLN
1	B	473	LYS
1	B	521	LYS
1	B	567	LYS

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Mol	Chain	Res	Type
1	B	575	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	208	ASN
1	A	213	ASN
1	A	320	GLN
1	A	352	GLN
1	A	388	ASN
1	A	502	HIS
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	352	GLN
1	B	515	ASN

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 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$
2	PGA	B	900	3	8,8,8	0.87	0	10,11,11	1.43	2 (20%)
8	EPE	A	3380	-	15,15,15	1.91	1 (6%)	19,20,20	2.58	7 (36%)
6	GDP	B	800	3	29,30,30	1.36	4 (13%)	45,47,47	1.46	6 (13%)
2	PGA	A	900	3	8,8,8	1.20	0	10,11,11	1.32	1 (10%)
7	1PE	A	1101	-	9,9,15	0.50	0	8,8,14	0.24	0
7	1PE	A	1000	-	9,9,15	0.42	0	8,8,14	0.68	0
5	BCT	A	1044	-	3,3,3	0.46	0	2,3,3	1.02	0
6	GDP	A	800	3	29,30,30	1.07	3 (10%)	45,47,47	1.26	5 (11%)

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	PGA	B	900	3	-	0/6/6/6	-
8	EPE	A	3380	-	-	7/9/19/19	0/1/1/1
6	GDP	B	800	3	-	0/16/32/32	0/3/3/3
2	PGA	A	900	3	-	3/6/6/6	-
7	1PE	A	1101	-	-	6/7/7/13	-
7	1PE	A	1000	-	-	2/7/7/13	-
6	GDP	A	800	3	-	0/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	3380	EPE	C10-S	-7.04	1.67	1.77
6	B	800	GDP	PA-O3A	4.38	1.64	1.59
6	A	800	GDP	C5-C4	3.03	1.47	1.38
6	B	800	GDP	C5-C4	3.02	1.47	1.38
6	B	800	GDP	C6-N1	-2.80	1.33	1.38
6	A	800	GDP	C5-N7	-2.28	1.34	1.39
6	A	800	GDP	C6-N1	-2.19	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	800	GDP	C4-N9	-2.12	1.32	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	3380	EPE	C5-N4-C3	6.23	122.27	108.84
8	A	3380	EPE	C6-N1-C2	5.21	120.07	108.84
8	A	3380	EPE	C9-N1-C2	4.17	122.34	111.24
6	B	800	GDP	N9-C4-N3	4.13	134.21	125.95
6	B	800	GDP	C5-C4-N3	-4.12	121.84	128.39
6	A	800	GDP	C6-C5-N7	3.48	136.63	130.29
6	B	800	GDP	C2-N3-C4	3.28	117.95	112.30
8	A	3380	EPE	O1S-S-C10	3.24	111.63	106.73
8	A	3380	EPE	C7-N4-C5	3.06	119.39	111.24
6	A	800	GDP	C5-C4-N3	-2.86	123.84	128.39
2	B	900	PGA	O1P-C2-C1	2.77	114.72	110.54
8	A	3380	EPE	C7-N4-C3	2.57	118.10	111.24
2	A	900	PGA	O1P-P-O2P	-2.54	99.58	106.44
6	B	800	GDP	C6-C5-N7	2.51	134.86	130.29
8	A	3380	EPE	C9-N1-C6	2.32	117.43	111.24
6	A	800	GDP	N9-C4-N3	2.25	130.46	125.95
6	A	800	GDP	C2-N3-C4	2.24	116.15	112.30
6	B	800	GDP	C8-N9-C4	2.21	110.16	106.03
6	A	800	GDP	C6-C5-C4	-2.18	115.55	118.83
6	B	800	GDP	C6-C5-C4	-2.07	115.72	118.83
2	B	900	PGA	O1P-P-O2P	-2.04	100.91	106.44

There are no chirality outliers.

All (18) 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
8	A	3380	EPE	C9-C10-S-O2S

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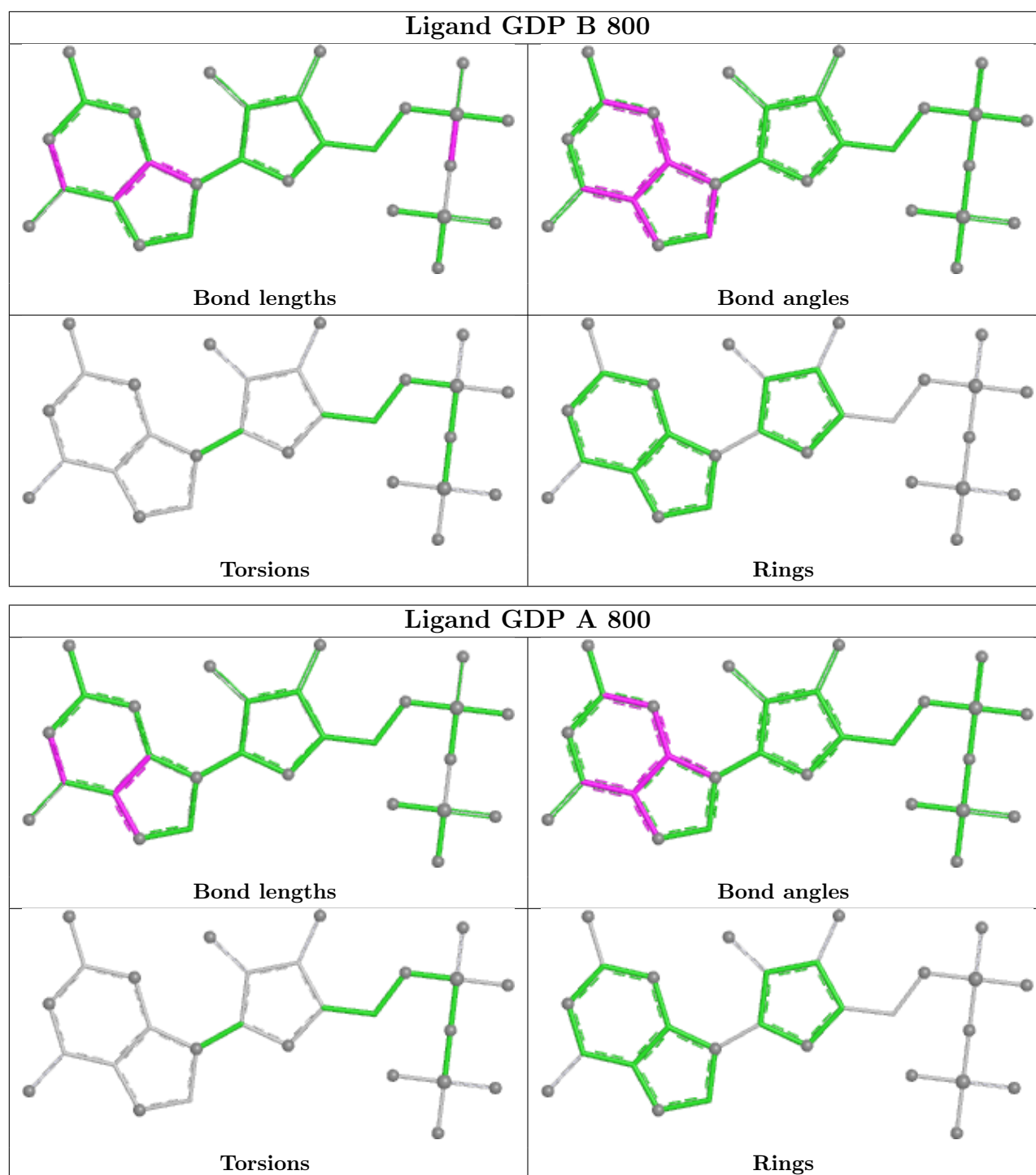
Mol	Chain	Res	Type	Atoms
7	A	1101	1PE	C13-C23-OH3-C22
7	A	1101	1PE	C23-C13-OH4-C24
7	A	1101	1PE	OH2-C12-C22-OH3
7	A	1101	1PE	C12-C22-OH3-C23
8	A	3380	EPE	C10-C9-N1-C6
7	A	1000	1PE	C12-C22-OH3-C23
7	A	1000	1PE	C23-C13-OH4-C24

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	3380	EPE	2	0
6	B	800	GDP	1	0
7	A	1000	1PE	7	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	620/624 (99%)	0.08	23 (3%)	45 50	3, 8, 17, 32	41 (6%)
1	B	612/624 (98%)	0.23	27 (4%)	39 44	4, 9, 19, 35	26 (4%)
All	All	1232/1248 (98%)	0.15	50 (4%)	41 47	3, 8, 18, 35	67 (5%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	GLY	5.4
1	A	504	PRO	5.3
1	A	152	PRO	4.4
1	B	396	GLU	4.2
1	A	393	PRO	4.1
1	A	205	PRO	4.0
1	B	394	GLN	4.0
1	B	570	GLY	3.8
1	A	394	GLN	3.7
1	A	396	GLU	3.5
1	B	150	GLY	3.4
1	B	395	ASP	3.3
1	B	205	PRO	3.2
1	B	379	PRO	3.1
1	B	504	PRO	3.1
1	B	3	PRO	3.1
1	B	575	GLU	3.1
1	B	7[A]	ASN	3.1
1	B	380	GLY	3.0
1	A	149	LEU	3.0
1	A	472	GLY	2.9
1	B	9	LEU	2.9
1	B	569	LEU	2.9
1	B	473	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	3	PRO	2.7
1	A	342	LYS	2.6
1	A	8	GLY	2.6
1	B	571	ASP	2.6
1	B	393	PRO	2.5
1	B	62	GLU	2.5
1	B	502	HIS	2.5
1	A	583	GLU	2.4
1	A	575	GLU	2.3
1	B	583	GLU	2.3
1	A	474	VAL	2.3
1	A	150	GLY	2.3
1	B	392	ARG	2.3
1	B	378	ALA	2.3
1	A	502	HIS	2.3
1	A	569	LEU	2.3
1	A	352	GLN	2.3
1	B	51	GLU	2.2
1	B	391	TRP	2.2
1	A	206	LEU	2.2
1	B	572	VAL	2.1
1	A	153	LEU	2.1
1	B	577	LEU	2.1
1	A	501	ALA	2.1
1	A	154	ALA	2.0
1	A	561	GLU	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](#)

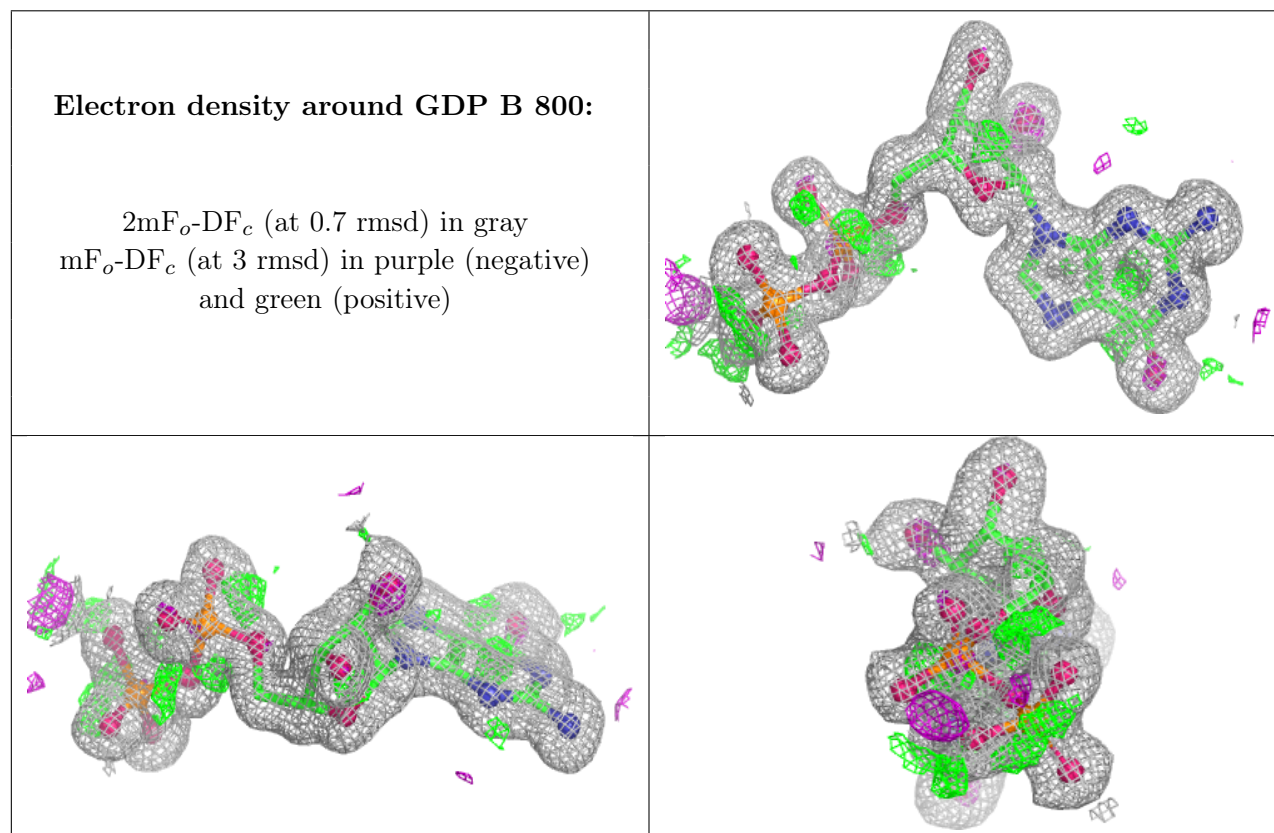
There are no oligosaccharides in this entry.

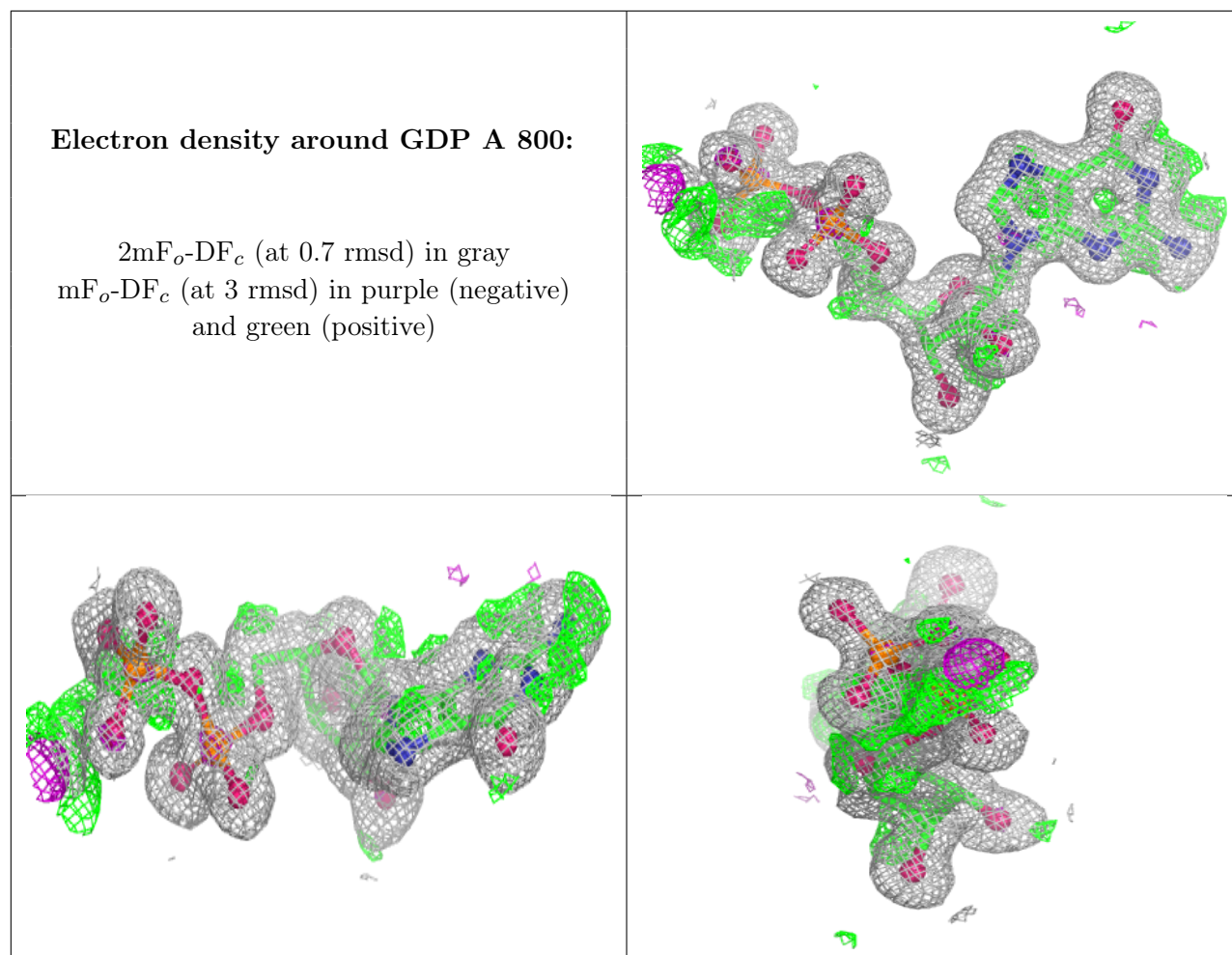
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
7	1PE	A	1101	10/16	0.75	0.15	38,39,40,40	0
8	EPE	A	3380	15/15	0.80	0.15	18,20,22,24	15
7	1PE	A	1000	10/16	0.85	0.10	9,14,20,22	0
5	BCT	A	1044	4/4	0.90	0.26	13,14,15,17	0
4	NA	A	1100	1/1	0.95	0.16	14,14,14,14	0
4	NA	B	1100	1/1	0.96	0.13	13,13,13,13	0
6	GDP	B	800	28/28	0.97	0.06	4,8,9,11	28
2	PGA	B	900	9/9	0.97	0.07	6,9,11,13	9
2	PGA	A	900	9/9	0.98	0.06	4,5,6,6	9
6	GDP	A	800	28/28	0.98	0.05	2,4,5,5	28
3	MN	B	701	1/1	0.99	0.06	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	0.07	5,5,5,5	1
3	MN	B	700	1/1	1.00	0.09	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.