



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:37 PM UTC

PDB ID : 7L3V / pdb_00007l3v
Title : PEPCK MMQX structure 120ms post-mixing with oxaloacetic acid
Authors : Clinger, J.A.; Moreau, D.W.; McLeod, M.J.; Holyoak, T.; Thorne, R.E.
Deposited on : 2020-12-18
Resolution : 1.98 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

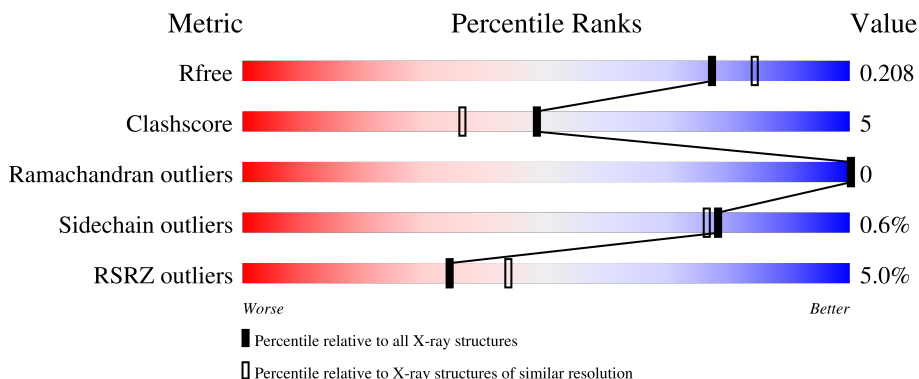
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	5% 84% 12% ...

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
4	PEP	A	903	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9924 atoms, of which 4694 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.

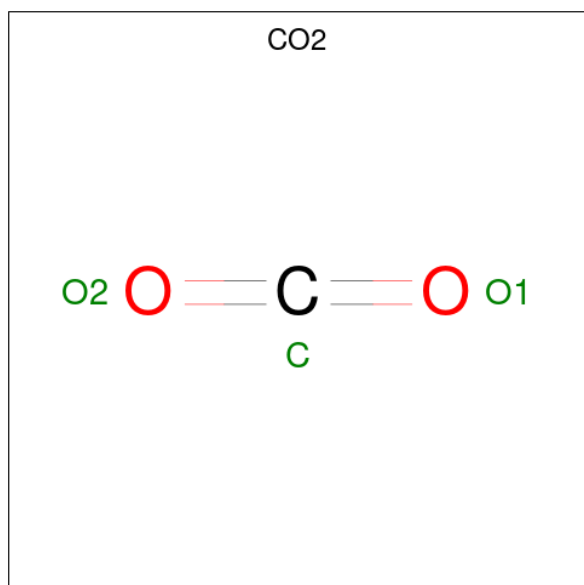
- Molecule 1 is a protein called Phosphoenolpyruvate carboxykinase, cytosolic [GTP].

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	601	9446	3045	4694	812	863	32	0	14	0

There are 2 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

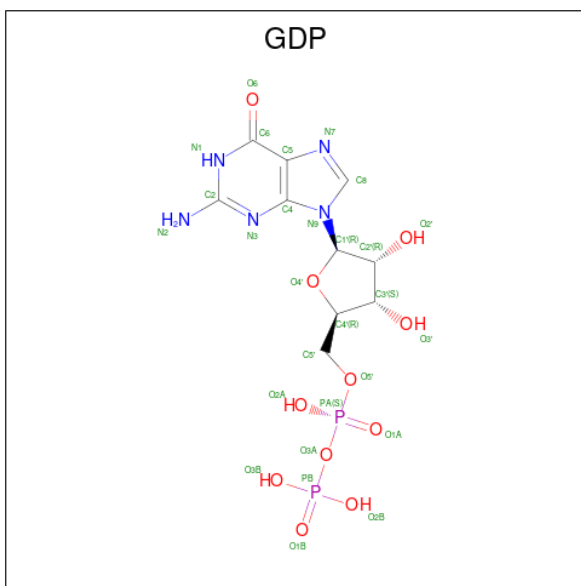
- Molecule 2 is CARBON DIOXIDE (CCD ID: CO2) (formula: CO₂).



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

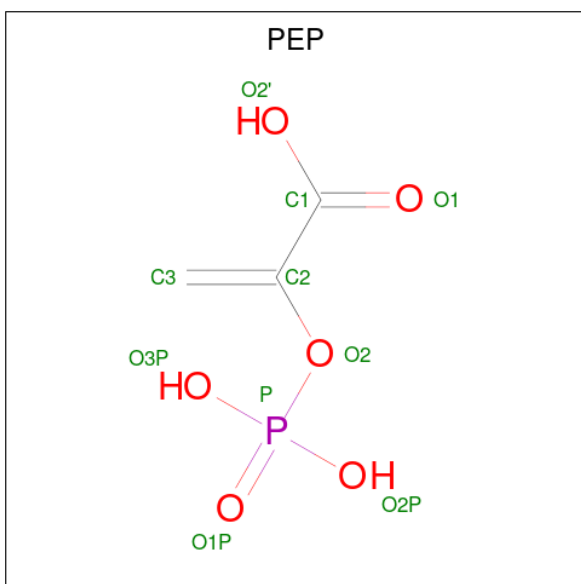
- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂)

(labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total 4	Mn 4	0	0

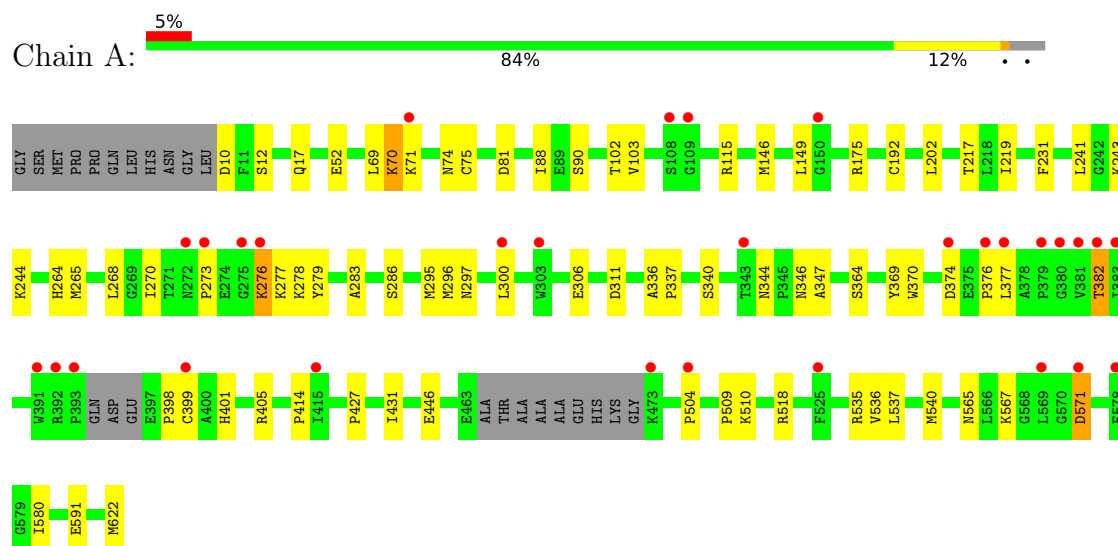
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	431	Total 433	O 433	0	2

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]



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.16Å 118.79Å 61.31Å 90.00° 107.25° 90.00°	Depositor
Resolution (Å)	41.67 – 1.98 41.67 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.67-1.98) 99.7 (41.67-1.98)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.186 , 0.206 0.192 , 0.208	Depositor DCC
R_{free} test set	2203 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9924	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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: GDP, PEP, MN, CO2

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	8/4933 (0.2%)	0.73	14/6678 (0.2%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	LYS	C-N	-17.40	1.08	1.33
1	A	401	HIS	C-N	11.98	1.49	1.33
1	A	71	LYS	C-N	-9.21	1.20	1.33
1	A	277	LYS	C-O	-9.13	1.12	1.23
1	A	146	MET	SD-CE	-5.80	1.65	1.79
1	A	273	PRO	C-O	-5.66	1.16	1.24
1	A	398	PRO	C-O	-5.38	1.17	1.23
1	A	401	HIS	C-O	-5.28	1.17	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	HIS	O-C-N	-11.99	108.95	121.30
1	A	70	LYS	O-C-N	-7.93	112.08	122.39
1	A	277	LYS	CA-C-O	-7.17	112.75	121.36
1	A	401	HIS	CA-C-N	6.64	126.59	119.28
1	A	401	HIS	C-N-CA	6.64	126.59	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	PRO	CA-C-N	6.19	133.37	121.54
1	A	504	PRO	C-N-CA	6.19	133.37	121.54
1	A	71	LYS	CA-C-N	-6.03	112.31	122.92
1	A	71	LYS	C-N-CA	-6.03	112.31	122.92
1	A	401	HIS	N-CA-CB	5.71	118.94	109.98
1	A	376	PRO	O-C-N	-5.66	116.82	122.98
1	A	571	ASP	CB-CA-C	5.50	120.41	112.05
1	A	146	MET	CG-SD-CE	5.42	112.82	100.90
1	A	382	THR	CA-CB-OG1	-5.10	101.96	109.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	70	LYS	Mainchain

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	4752	4694	4646	48	1
2	A	3	0	0	0	0
3	A	28	0	12	1	0
4	A	10	0	2	7	0
5	A	4	0	0	1	0
6	A	433	0	0	13	3
All	All	5230	4694	4660	52	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 (52) 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:295:MET:O	6:A:1001:HOH:O	1.92	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:903:PEP:O1	5:A:906:MN:MN	1.42	0.77
1:A:364:SER:OG	1:A:382:THR:OG1	2.03	0.75
1:A:286:SER:OG	6:A:1002:HOH:O	2.07	0.73
1:A:297:ASN:O	6:A:1003:HOH:O	2.08	0.72
1:A:10:ASP:O	6:A:1004:HOH:O	2.10	0.70
1:A:115[A]:ARG:NE	6:A:1008:HOH:O	2.22	0.69
1:A:536:VAL:HG12	1:A:540:MET:HE3	1.78	0.65
1:A:518:ARG:O	6:A:1005:HOH:O	2.16	0.60
1:A:115[B]:ARG:NH2	6:A:1014:HOH:O	2.35	0.60
1:A:286:SER:OG	4:A:903:PEP:O2'	2.21	0.58
1:A:296:MET:HE1	1:A:537:LEU:HD12	1.88	0.55
1:A:405:ARG:NH2	4:A:903:PEP:H32	2.21	0.55
1:A:405:ARG:HH22	4:A:903:PEP:H32	1.70	0.55
1:A:565:ASN:OD1	1:A:567:LYS:HG2	2.07	0.53
1:A:295:MET:HE1	1:A:347:ALA:HB2	1.92	0.51
1:A:202:LEU:HD22	6:A:1311:HOH:O	2.11	0.50
1:A:431:ILE:HD12	1:A:509:PRO:HG2	1.93	0.50
1:A:17:GLN:NE2	1:A:52:GLU:OE1	2.44	0.50
1:A:268:LEU:C	1:A:268:LEU:HD12	2.37	0.49
3:A:902:GDP:H5''	6:A:1361:HOH:O	2.13	0.48
1:A:565:ASN:OD1	1:A:567:LYS:HE3	2.14	0.47
1:A:295:MET:HE3	1:A:344:ASN:HD21	1.79	0.47
1:A:295:MET:CE	1:A:347:ALA:HB2	2.45	0.47
1:A:580:ILE:HG22	1:A:622:MET:HE1	1.95	0.47
1:A:102:THR:HG22	1:A:103:VAL:HG13	1.96	0.47
1:A:370:TRP:HA	1:A:399:CYS:SG	2.55	0.47
1:A:336:ALA:HB3	1:A:337:PRO:HD3	1.97	0.46
1:A:192:CYS:HB3	1:A:241:LEU:HD12	1.98	0.45
1:A:74:ASN:N	6:A:1039:HOH:O	2.51	0.44
1:A:10:ASP:OD1	1:A:12:SER:OG	2.28	0.43
1:A:264:HIS:NE2	4:A:903:PEP:O1	2.51	0.43
1:A:369:TYR:CE1	1:A:377:LEU:HD11	2.53	0.43
1:A:265:MET:HG2	1:A:283:ALA:HB2	2.00	0.43
1:A:243:LYS:NZ	1:A:311:ASP:OD2	2.52	0.43
1:A:270:ILE:HG22	1:A:278:LYS:O	2.18	0.43
1:A:591[A]:GLU:OE2	6:A:1007:HOH:O	2.21	0.42
1:A:446:GLU:OE2	1:A:510:LYS:HE3	2.20	0.42
1:A:88:ILE:HG22	1:A:90:SER:OG	2.20	0.42
1:A:279:TYR:HB2	1:A:427:PRO:O	2.19	0.42
4:A:903:PEP:C2	6:A:1022:HOH:O	2.67	0.42
1:A:219:ILE:HD12	1:A:219:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:ND2	1:A:414:PRO:HG2	2.36	0.41
1:A:340:SER:HB2	1:A:374:ASP:HB3	2.03	0.41
1:A:69:LEU:HD12	1:A:75:CYS:HB3	2.02	0.41
1:A:149[B]:LEU:HD21	1:A:175:ARG:HB3	2.02	0.41
1:A:300:LEU:HD11	1:A:535:ARG:HG2	2.02	0.41
1:A:217:THR:HA	1:A:231:PHE:O	2.21	0.40
1:A:296:MET:HE1	1:A:537:LEU:CD1	2.52	0.40
1:A:244:LYS:NZ	4:A:903:PEP:O1	2.47	0.40
1:A:81:ASP:C	1:A:81:ASP:OD1	2.64	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)
6:A:1018:HOH:O	6:A:1381:HOH:O[1_455]	1.90	0.30
1:A:276:LYS:HE3	6:A:1015:HOH:O[1_455]	1.38	0.22
6:A:1145:HOH:O	6:A:1356:HOH:O[2_555]	2.13	0.07

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	609/624 (98%)	589 (97%)	20 (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	505/520 (97%)	502 (99%)	3 (1%)	78	76

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	LYS
1	A	306	GLU
1	A	571	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	ASN
1	A	344	ASN
1	A	388	ASN
1	A	621	GLN

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDP	A	902	5	29,30,30	1.10	4 (13%)	45,47,47	1.81	9 (20%)
2	CO2	A	901	-	2,2,2	1.08	0	1,1,1	0.50	0
4	PEP	A	903	5	9,9,9	2.06	2 (22%)	11,13,13	1.52	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GDP	A	902	5	-	0/16/32/32	0/3/3/3
4	PEP	A	903	5	-	6/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	PEP	C2-C1	3.92	1.53	1.49
4	A	903	PEP	P-O2	3.84	1.66	1.59
3	A	902	GDP	C5-C4	2.82	1.46	1.38
3	A	902	GDP	C6-N1	-2.49	1.34	1.38
3	A	902	GDP	C4-N9	-2.08	1.32	1.38
3	A	902	GDP	C5-N7	-2.01	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	GDP	C5-C4-N3	-5.80	119.16	128.39
3	A	902	GDP	C2-N3-C4	4.70	120.39	112.30
3	A	902	GDP	N9-C4-N3	3.97	133.89	125.95
4	A	903	PEP	O2'-C1-C2	3.16	119.30	113.91
3	A	902	GDP	C6-C5-N7	3.04	135.82	130.29
3	A	902	GDP	O6-C6-C5	-2.54	119.83	126.53
3	A	902	GDP	C4-C5-N7	-2.49	106.72	110.67
3	A	902	GDP	C2-N1-C6	-2.35	120.85	125.11
3	A	902	GDP	O3B-PB-O2B	2.35	116.60	107.80
3	A	902	GDP	N2-C2-N3	-2.07	115.64	119.67

There are no chirality outliers.

All (6) torsion outliers are listed below:

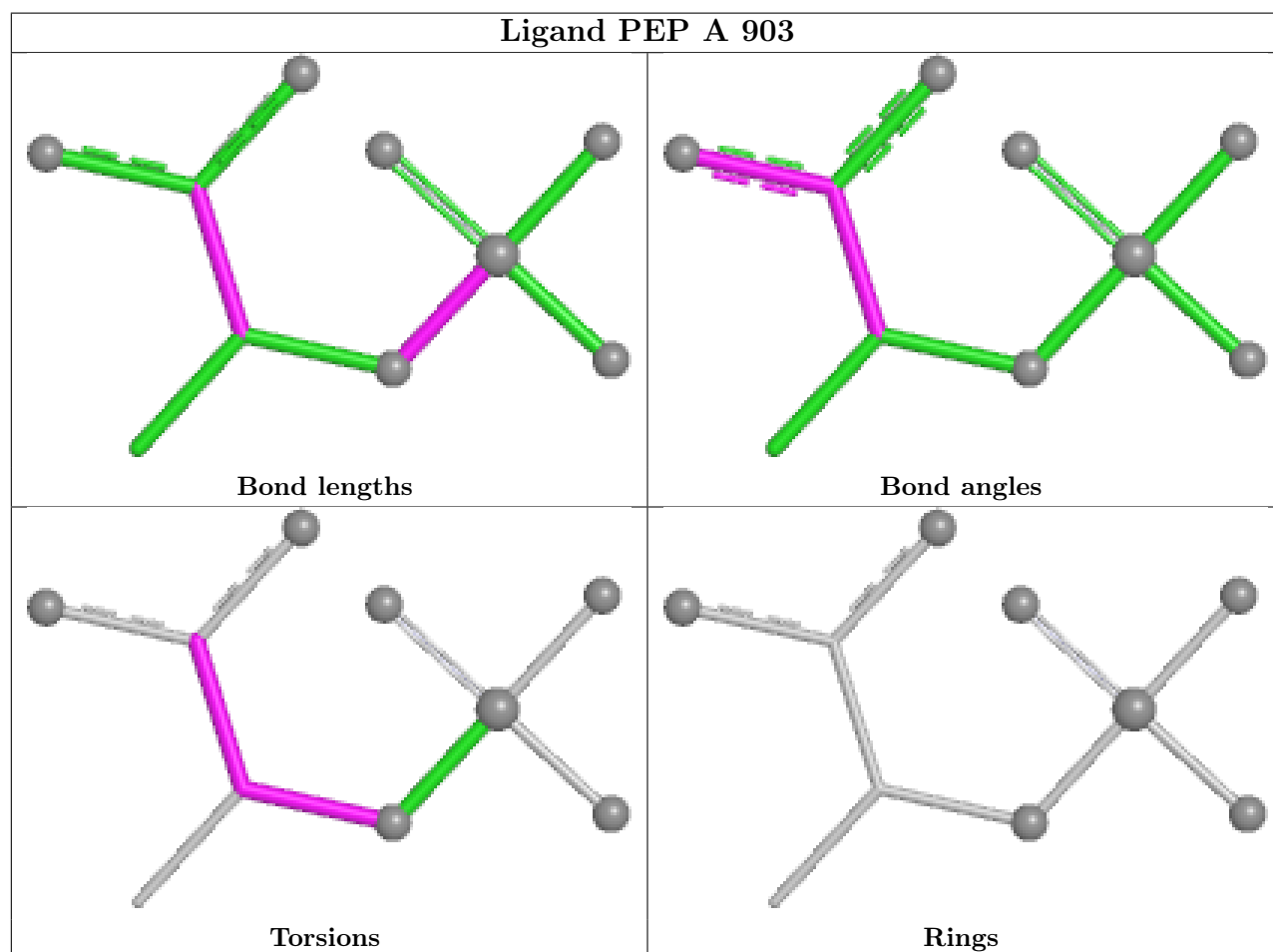
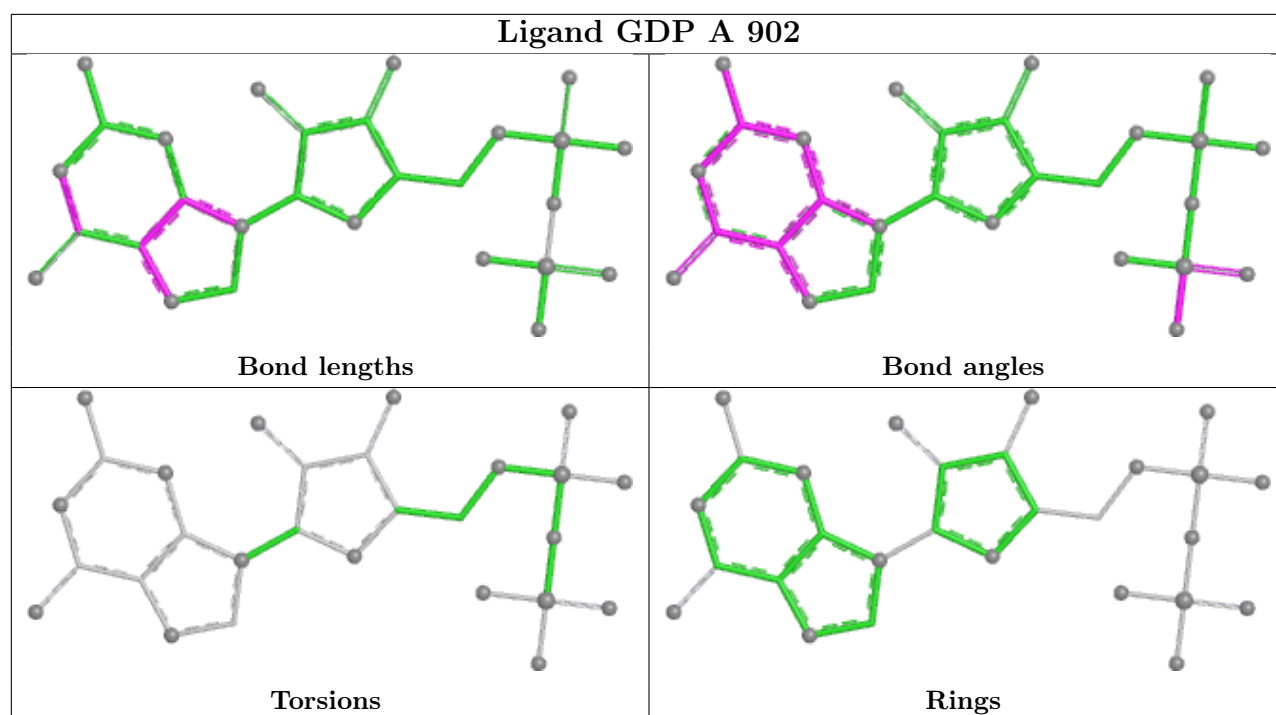
Mol	Chain	Res	Type	Atoms
4	A	903	PEP	O1-C1-C2-C3
4	A	903	PEP	O1-C1-C2-O2
4	A	903	PEP	O2'-C1-C2-C3
4	A	903	PEP	O2'-C1-C2-O2
4	A	903	PEP	C1-C2-O2-P
4	A	903	PEP	C3-C2-O2-P

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	GDP	1	0
4	A	903	PEP	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	70:LYS	C	71:LYS	N	1.08

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	601/624 (96%)	0.28	30 (4%) 34 44	12, 43, 82, 112	9 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	303	TRP	4.1
1	A	381	VAL	3.8
1	A	380	GLY	3.5
1	A	275	GLY	2.8
1	A	376	PRO	2.8
1	A	273	PRO	2.7
1	A	379	PRO	2.7
1	A	272	ASN	2.7
1	A	150	GLY	2.7
1	A	393	PRO	2.7
1	A	504	PRO	2.6
1	A	569	LEU	2.6
1	A	571	ASP	2.6
1	A	392	ARG	2.5
1	A	109	GLY	2.4
1	A	300	LEU	2.4
1	A	377	LEU	2.4
1	A	525	PHE	2.3
1	A	391	TRP	2.2
1	A	578	PHE	2.2
1	A	374	ASP	2.2
1	A	383	ILE	2.2
1	A	399	CYS	2.2
1	A	71	LYS	2.2
1	A	473	LYS	2.2
1	A	415	ILE	2.1
1	A	382	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	276	LYS	2.1
1	A	108	SER	2.0
1	A	343	THR	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](#)

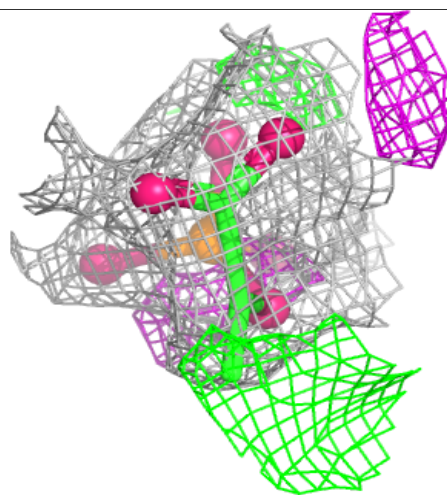
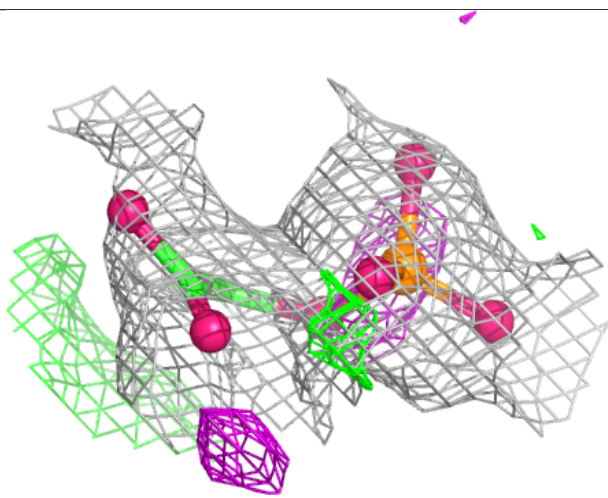
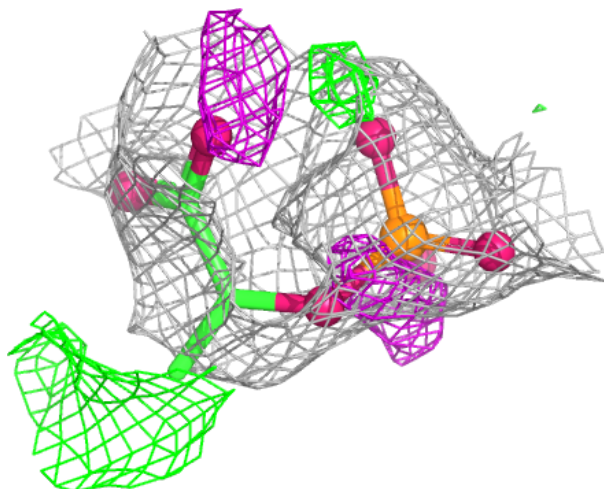
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CO2	A	901	3/3	0.81	0.17	50,50,55,59	0
5	MN	A	905	1/1	0.81	0.12	108,108,108,108	0
4	PEP	A	903	10/10	0.87	0.14	27,59,63,66	0
3	GDP	A	902	28/28	0.93	0.09	39,47,64,74	0
5	MN	A	907	1/1	0.94	0.24	72,72,72,72	0
5	MN	A	906	1/1	0.98	0.06	33,33,33,33	0
5	MN	A	904	1/1	0.99	0.03	43,43,43,43	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.

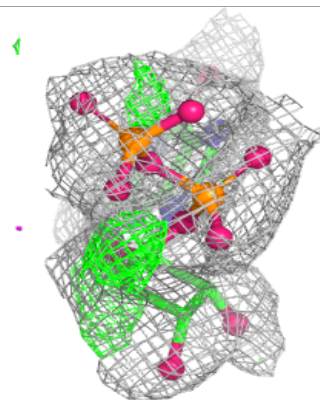
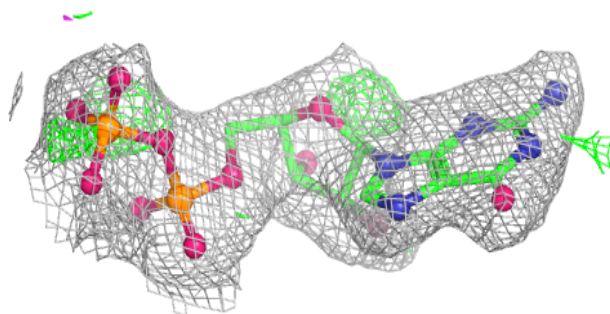
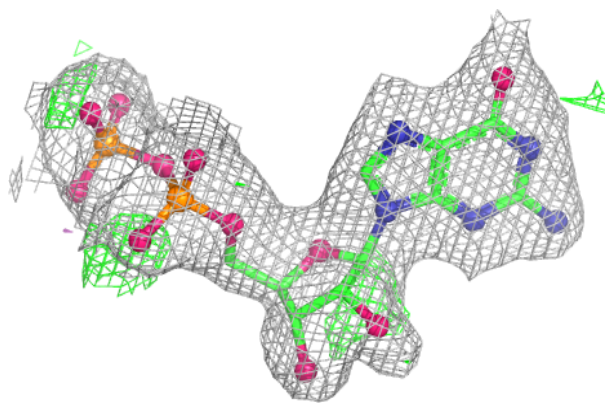
Electron density around PEP A 903:

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



Electron density around GDP A 902:

$2mF_o-DF_c$ (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.