



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:56 AM UTC

PDB ID : 4BXC / pdb_00004bxc
Title : Resolving the activation site of positive regulators in plant phosphoenolpyruvate carboxylase
Authors : Schlieper, D.; Foerster, K.; Paulus, J.K.; Groth, G.
Deposited on : 2013-07-10
Resolution : 2.86 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

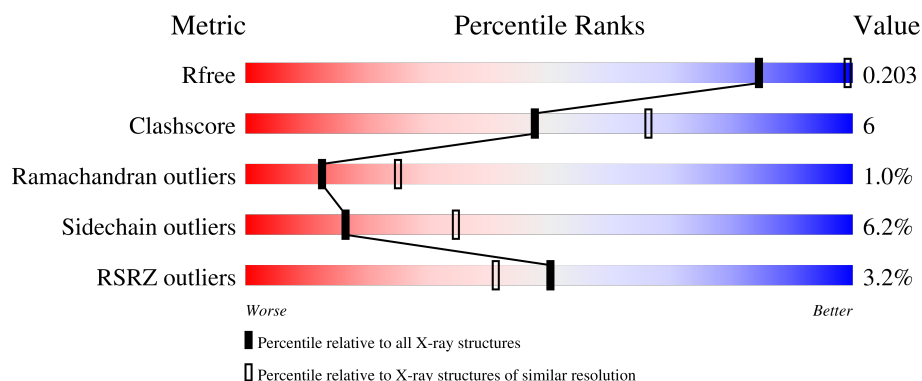
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	990	3% 77% 15% • 6%
1	B	990	3% 78% 14% • 6%

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
3	SO4	A	1968	-	-	X	-
3	SO4	B	1968	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14917 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 C4 PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	929	Total	C	N	O	S	0	0	0
			7425	4711	1290	1390	34			
1	B	929	Total	C	N	O	S	0	0	0
			7421	4710	1285	1392	34			

There are 48 discrepancies between the modelled and reference sequences:

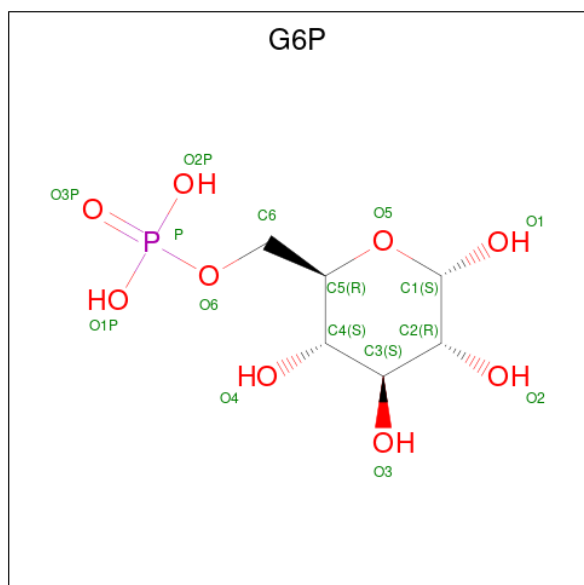
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P30694
A	-22	GLY	-	expression tag	UNP P30694
A	-21	HIS	-	expression tag	UNP P30694
A	-20	HIS	-	expression tag	UNP P30694
A	-19	HIS	-	expression tag	UNP P30694
A	-18	HIS	-	expression tag	UNP P30694
A	-17	HIS	-	expression tag	UNP P30694
A	-16	HIS	-	expression tag	UNP P30694
A	-15	HIS	-	expression tag	UNP P30694
A	-14	HIS	-	expression tag	UNP P30694
A	-13	HIS	-	expression tag	UNP P30694
A	-12	HIS	-	expression tag	UNP P30694
A	-11	SER	-	expression tag	UNP P30694
A	-10	SER	-	expression tag	UNP P30694
A	-9	GLY	-	expression tag	UNP P30694
A	-8	HIS	-	expression tag	UNP P30694
A	-7	GLU	-	expression tag	UNP P30694
A	-6	ASN	-	expression tag	UNP P30694
A	-5	LEU	-	expression tag	UNP P30694
A	-4	TYR	-	expression tag	UNP P30694
A	-3	PHE	-	expression tag	UNP P30694
A	-2	GLN	-	expression tag	UNP P30694
A	-1	GLY	-	expression tag	UNP P30694
A	0	HIS	-	expression tag	UNP P30694
B	-23	MET	-	expression tag	UNP P30694

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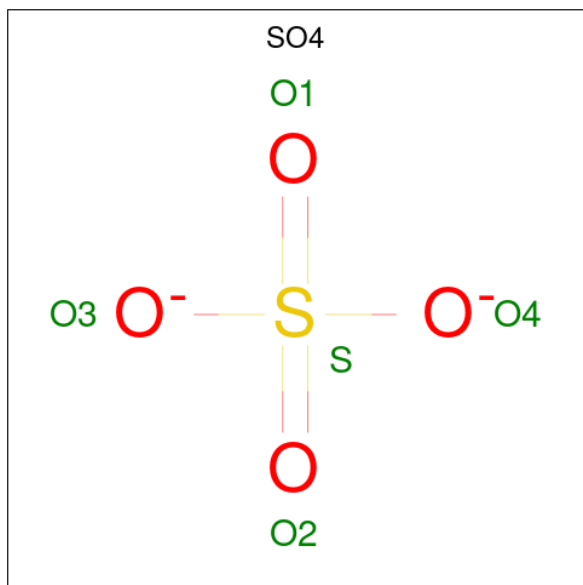
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	GLY	-	expression tag	UNP P30694
B	-21	HIS	-	expression tag	UNP P30694
B	-20	HIS	-	expression tag	UNP P30694
B	-19	HIS	-	expression tag	UNP P30694
B	-18	HIS	-	expression tag	UNP P30694
B	-17	HIS	-	expression tag	UNP P30694
B	-16	HIS	-	expression tag	UNP P30694
B	-15	HIS	-	expression tag	UNP P30694
B	-14	HIS	-	expression tag	UNP P30694
B	-13	HIS	-	expression tag	UNP P30694
B	-12	HIS	-	expression tag	UNP P30694
B	-11	SER	-	expression tag	UNP P30694
B	-10	SER	-	expression tag	UNP P30694
B	-9	GLY	-	expression tag	UNP P30694
B	-8	HIS	-	expression tag	UNP P30694
B	-7	GLU	-	expression tag	UNP P30694
B	-6	ASN	-	expression tag	UNP P30694
B	-5	LEU	-	expression tag	UNP P30694
B	-4	TYR	-	expression tag	UNP P30694
B	-3	PHE	-	expression tag	UNP P30694
B	-2	GLN	-	expression tag	UNP P30694
B	-1	GLY	-	expression tag	UNP P30694
B	0	HIS	-	expression tag	UNP P30694

- Molecule 2 is 6-O-phosphono-alpha-D-glucopyranose (CCD ID: G6P) (formula: C₆H₁₃O₉P).



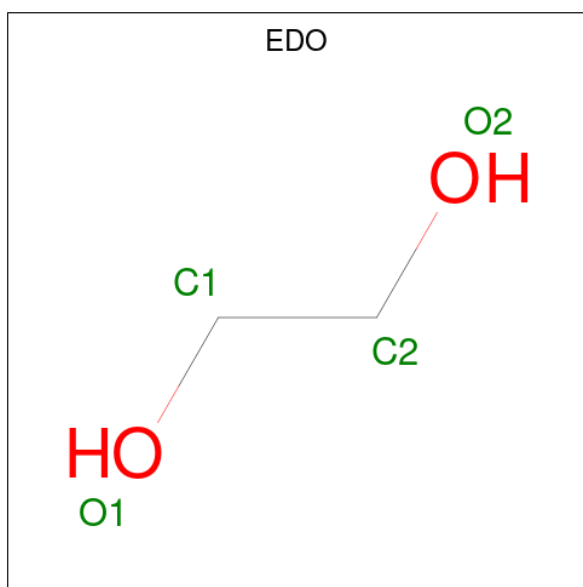
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



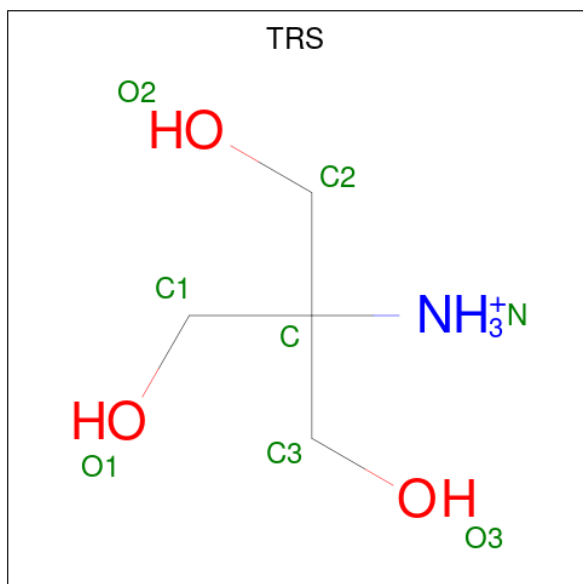
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).

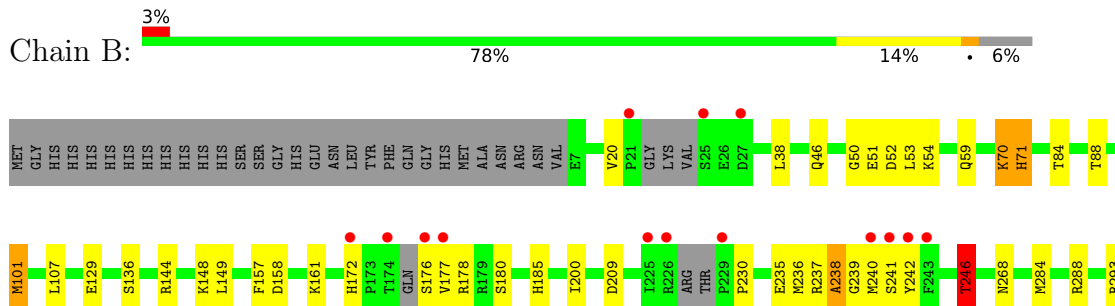


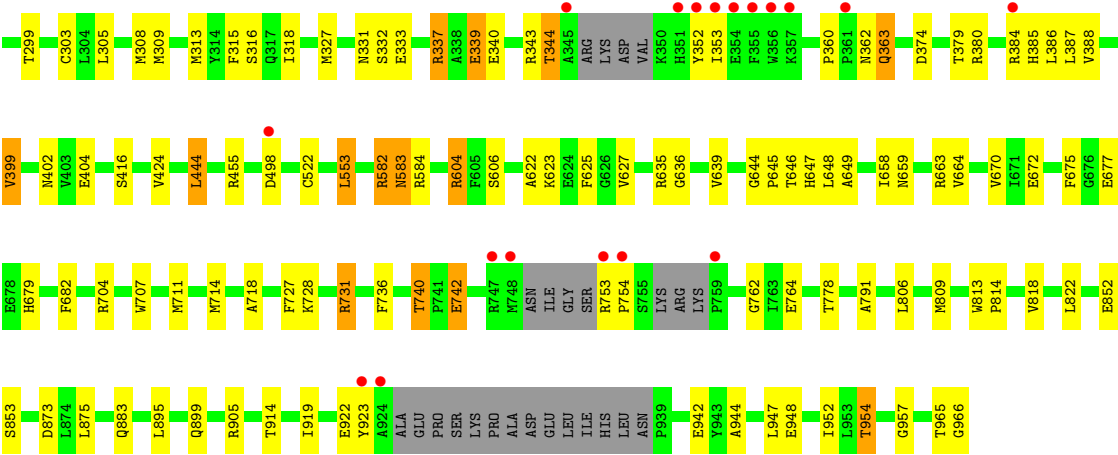
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	B	1	Total 1	O 1	0	0

- Molecule 1: C4 PHOSPHOENOLPYRUVATE CARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	164.41Å 121.23Å 132.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.68 – 2.86 50.68 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.68-2.86) 99.7 (50.68-2.86)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.184 , 0.221 (Not available) , 0.203	Depositor DCC
R_{free} test set	1254 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.7	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	0.95	EDS
Total number of atoms	14917	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: G6P, EDO, TRS, SO4

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	0.95	1/7578 (0.0%)	1.04	7/10246 (0.1%)
1	B	0.89	0/7576	1.02	6/10248 (0.1%)
All	All	0.92	1/15154 (0.0%)	1.03	13/20494 (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	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	747	ARG	CA-C	5.64	1.59	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	782	LEU	CA-C-N	-5.82	113.68	119.56
1	A	782	LEU	C-N-CA	-5.82	113.68	119.56
1	B	246	THR	N-CA-C	5.73	120.80	113.18
1	B	852	GLU	CA-CB-CG	5.59	125.28	114.10
1	B	875	LEU	N-CA-C	5.52	119.31	112.24
1	A	7	GLU	N-CA-C	5.35	118.93	108.18
1	A	952	ILE	CB-CA-C	-5.32	105.16	111.97
1	B	762	GLY	N-CA-C	-5.30	105.91	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	ILE	N-CA-C	-5.23	105.61	110.53
1	A	246	THR	N-CA-C	5.18	120.08	113.18
1	B	363	GLN	CA-C-N	5.10	124.41	118.85
1	B	363	GLN	C-N-CA	5.10	124.41	118.85
1	A	781	HIS	N-CA-C	5.08	119.05	112.86

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	ILE	Peptide
1	B	344	THR	Peptide
1	B	353	ILE	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	7425	0	7350	81	0
1	B	7421	0	7330	85	0
2	A	16	0	11	3	0
2	B	16	0	11	2	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	8	0	12	0	0
6	A	12	0	0	1	0
6	B	1	0	0	0	0
All	All	14917	0	14726	167	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (167) 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:806:LEU:HA	1:A:809:MET:HE3	1.55	0.89
1:A:246:THR:HG21	1:A:675:PHE:O	1.72	0.88
1:B:246:THR:HG21	1:B:675:PHE:O	1.74	0.87
1:B:178:ARG:NH2	3:B:1968:SO4:O4	2.08	0.86
1:B:806:LEU:HA	1:B:809:MET:HE3	1.58	0.85
1:B:308:MET:SD	1:B:384:ARG:HD3	2.19	0.82
1:A:308:MET:SD	1:A:384:ARG:HD3	2.20	0.82
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.47	0.80
1:B:241:SER:OG	1:B:242:TYR:N	2.11	0.77
1:A:337:ARG:HG3	1:A:337:ARG:HH11	1.49	0.76
1:B:635:ARG:HG2	2:B:1967:G6P:H3	1.68	0.76
1:A:241:SER:OG	1:A:242:TYR:N	2.10	0.75
1:A:84:THR:O	1:A:905:ARG:NH2	2.23	0.72
1:B:84:THR:O	1:B:905:ARG:NH2	2.23	0.70
1:B:753:ARG:NH2	2:B:1967:G6P:O2P	2.28	0.67
1:B:157:PHE:CE2	1:B:161:LYS:HE3	2.31	0.65
1:A:677:GLU:OE2	1:A:679:HIS:HD2	1.79	0.65
1:A:178:ARG:NH2	3:A:1968:SO4:O2	2.30	0.63
1:A:157:PHE:CE2	1:A:161:LYS:HE3	2.33	0.62
1:B:236:MET:HA	1:B:284:MET:HE3	1.83	0.60
1:B:20:VAL:HG11	1:B:883:GLN:HG3	1.84	0.60
1:B:240:MET:HE2	1:B:309:MET:HB2	1.84	0.59
1:B:59:GLN:HA	1:B:59:GLN:OE1	2.02	0.59
1:A:236:MET:HA	1:A:284:MET:HE3	1.84	0.58
1:A:240:MET:HE2	1:A:309:MET:HB2	1.86	0.57
1:A:360:PRO:HD2	1:A:363:GLN:HE21	1.69	0.57
1:B:360:PRO:HD2	1:B:363:GLN:HE21	1.69	0.57
1:A:20:VAL:HG11	1:A:883:GLN:HG3	1.86	0.56
1:B:604:ARG:NH2	1:B:636:GLY:O	2.37	0.56
1:B:315:PHE:O	1:B:318:ILE:HG22	2.05	0.56
1:A:315:PHE:O	1:A:318:ILE:HG22	2.06	0.56
1:B:129:GLU:O	1:B:647:HIS:HB3	2.07	0.55
1:A:604:ARG:NH2	1:A:636:GLY:O	2.39	0.55
1:A:129:GLU:O	1:A:647:HIS:HB3	2.08	0.54
1:A:899:GLN:HE21	1:A:954:THR:CG2	2.20	0.54
1:B:899:GLN:HE21	1:B:954:THR:CG2	2.19	0.54
1:A:59:GLN:HA	1:A:59:GLN:OE1	2.08	0.53
1:A:822:LEU:C	1:A:822:LEU:HD23	2.34	0.53
1:B:553:LEU:N	1:B:553:LEU:HD23	2.23	0.53
1:A:136:SER:OG	1:A:144:ARG:NH2	2.41	0.53
1:A:20:VAL:HG13	1:A:20:VAL:O	2.07	0.53
1:B:822:LEU:C	1:B:822:LEU:HD23	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD11	1:B:101:MET:HE3	1.92	0.52
1:B:20:VAL:O	1:B:20:VAL:HG13	2.09	0.52
1:A:70:LYS:O	1:A:71:HIS:HB2	2.10	0.52
1:B:582:ARG:NH1	1:B:625:PHE:O	2.44	0.51
1:A:582:ARG:NH1	1:A:625:PHE:O	2.43	0.51
1:B:70:LYS:O	1:B:71:HIS:HB2	2.10	0.51
1:A:553:LEU:HD23	1:A:553:LEU:N	2.26	0.51
1:A:38:LEU:HD11	1:A:101:MET:HE3	1.93	0.50
1:B:136:SER:OG	1:B:144:ARG:NH2	2.41	0.50
1:B:172:HIS:HB3	1:B:176:SER:HB3	1.93	0.49
1:B:644:GLY:O	1:B:647:HIS:N	2.46	0.49
1:B:385:HIS:O	1:B:386:LEU:C	2.55	0.49
1:A:331:ASN:ND2	1:A:416:SER:HA	2.28	0.48
1:B:379:THR:HA	1:B:399:VAL:HG22	1.96	0.48
1:A:352:TYR:OH	1:A:374:ASP:OD1	2.32	0.48
1:A:644:GLY:O	1:A:647:HIS:N	2.47	0.48
1:A:711:MET:HE3	1:A:813:TRP:HZ3	1.77	0.48
1:B:331:ASN:ND2	1:B:416:SER:HA	2.29	0.48
1:B:553:LEU:HD23	1:B:553:LEU:H	1.79	0.48
1:A:379:THR:HA	1:A:399:VAL:HG22	1.96	0.47
1:B:806:LEU:HA	1:B:809:MET:CE	2.39	0.47
1:B:235:GLU:O	1:B:238:ALA:HB3	2.15	0.47
1:B:923:TYR:CD1	1:B:923:TYR:N	2.81	0.47
1:A:385:HIS:O	1:A:386:LEU:C	2.55	0.47
1:A:748:MET:CB	1:A:752:SER:N	2.77	0.47
1:A:172:HIS:HB3	1:A:176:SER:HB3	1.97	0.47
1:B:240:MET:HG3	1:B:309:MET:SD	2.55	0.47
1:A:740:THR:HG22	1:A:742:GLU:HB3	1.97	0.46
1:B:740:THR:HG22	1:B:742:GLU:HB3	1.98	0.46
1:A:714:MET:HB3	1:A:791:ALA:HB1	1.98	0.46
1:A:889:ASP:O	1:A:890:PRO:C	2.58	0.46
1:B:379:THR:CA	1:B:399:VAL:HG22	2.46	0.46
1:A:736:PHE:O	1:A:740:THR:HB	2.16	0.46
1:A:965:THR:OG1	1:A:966:GLY:N	2.49	0.46
1:B:942:GLU:OE1	1:B:948:GLU:HG2	2.16	0.46
1:A:379:THR:CA	1:A:399:VAL:HG22	2.46	0.46
1:B:727:PHE:CE1	1:B:764:GLU:HG3	2.51	0.46
1:B:965:THR:OG1	1:B:966:GLY:N	2.49	0.46
1:B:806:LEU:HD23	1:B:809:MET:HE3	1.98	0.45
1:B:736:PHE:O	1:B:740:THR:HB	2.17	0.45
1:A:235:GLU:O	1:A:238:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:LEU:HD23	1:A:809:MET:HE3	1.98	0.45
1:B:38:LEU:CD1	1:B:101:MET:HE3	2.47	0.45
1:A:339:GLU:O	1:A:340:GLU:C	2.60	0.45
1:A:718:ALA:HB2	1:A:791:ALA:HB2	1.99	0.45
1:B:53:LEU:O	1:B:54:LYS:C	2.60	0.45
1:B:714:MET:HB3	1:B:791:ALA:HB1	1.98	0.44
1:B:242:TYR:OH	1:B:672:GLU:OE1	2.33	0.44
1:A:704:ARG:HD3	1:A:707:TRP:CZ2	2.52	0.44
1:B:704:ARG:HD3	1:B:707:TRP:CZ2	2.51	0.44
1:B:337:ARG:HH11	1:B:337:ARG:CG	2.24	0.44
1:A:240:MET:HG3	1:A:309:MET:SD	2.58	0.44
1:B:352:TYR:OH	1:B:374:ASP:OD1	2.35	0.44
1:B:711:MET:HE3	1:B:813:TRP:HZ3	1.80	0.44
1:A:53:LEU:O	1:A:54:LYS:C	2.59	0.44
1:B:682:PHE:C	1:B:682:PHE:CD1	2.95	0.44
1:B:180:SER:N	3:B:1968:SO4:O2	2.38	0.44
1:A:236:MET:C	1:A:238:ALA:N	2.76	0.43
1:A:242:TYR:OH	1:A:672:GLU:OE1	2.35	0.43
1:A:283:TRP:CZ3	2:A:1967:G6P:H4	2.53	0.43
1:A:553:LEU:HD23	1:A:553:LEU:H	1.81	0.43
1:B:622:ALA:HB1	1:B:627:VAL:O	2.18	0.43
1:B:658:ILE:O	1:B:659:ASN:C	2.60	0.43
1:A:899:GLN:HB2	1:A:954:THR:CG2	2.49	0.43
1:B:242:TYR:OH	1:B:672:GLU:HA	2.19	0.43
1:A:658:ILE:O	1:A:659:ASN:C	2.60	0.43
1:B:303:CYS:SG	1:B:522:CYS:HB3	2.58	0.43
1:B:899:GLN:HB2	1:B:954:THR:HG23	2.00	0.43
1:A:622:ALA:HB1	1:A:627:VAL:O	2.19	0.43
1:A:241:SER:HG	1:A:242:TYR:H	1.58	0.43
1:B:899:GLN:HE21	1:B:954:THR:HG22	1.83	0.43
1:B:309:MET:O	1:B:313:MET:HG3	2.18	0.43
1:B:332:SER:O	1:B:333:GLU:C	2.61	0.43
1:B:813:TRP:O	1:B:814:PRO:C	2.61	0.43
1:A:166:GLU:CD	1:A:663:ARG:HH11	2.26	0.43
1:A:635:ARG:HD3	2:A:1967:G6P:H5	2.01	0.43
1:A:745:PHE:CD2	1:A:773:PHE:CE1	3.07	0.43
1:B:731:ARG:HG2	1:B:731:ARG:HH11	1.84	0.43
1:B:644:GLY:O	1:B:645:PRO:C	2.59	0.42
1:A:644:GLY:N	1:A:645:PRO:CD	2.82	0.42
1:A:899:GLN:HB2	1:A:954:THR:HG23	2.00	0.42
1:B:899:GLN:HB2	1:B:954:THR:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TYR:OH	1:A:672:GLU:HA	2.19	0.42
1:A:110:GLU:OE1	1:A:189:ARG:NH1	2.51	0.42
1:A:332:SER:O	1:A:333:GLU:C	2.61	0.42
1:A:866:LEU:O	1:A:867:LYS:C	2.63	0.42
1:B:241:SER:HG	1:B:242:TYR:H	1.63	0.42
1:A:166:GLU:OE2	1:A:281:SER:OG	2.32	0.42
1:B:718:ALA:HB2	1:B:791:ALA:HB2	2.00	0.42
1:B:736:PHE:CE1	1:B:740:THR:HG21	2.55	0.42
1:B:50:GLY:O	1:B:51:GLU:C	2.62	0.42
1:A:769:ILE:HB	1:A:770:PRO:HD3	2.02	0.41
1:A:50:GLY:O	1:A:51:GLU:C	2.63	0.41
1:A:180:SER:HB3	3:A:1968:SO4:O1	2.20	0.41
1:B:172:HIS:HB3	1:B:176:SER:CB	2.50	0.41
1:B:339:GLU:O	1:B:340:GLU:C	2.62	0.41
1:A:682:PHE:CD1	1:A:682:PHE:C	2.98	0.41
1:A:707:TRP:O	1:A:708:ARG:C	2.63	0.41
1:A:38:LEU:CD1	1:A:101:MET:HE3	2.50	0.41
1:A:309:MET:O	1:A:313:MET:HG3	2.20	0.41
2:A:1967:G6P:O5	2:A:1967:G6P:P	2.78	0.41
1:A:776:THR:O	1:A:777:GLN:C	2.60	0.41
1:B:948:GLU:O	1:B:952:ILE:HG12	2.20	0.41
1:A:80:GLY:O	1:A:84:THR:HG22	2.20	0.41
1:A:482:GLU:HG2	6:A:2006:HOH:O	2.20	0.41
1:A:899:GLN:HE21	1:A:954:THR:HG22	1.84	0.41
1:B:236:MET:C	1:B:238:ALA:N	2.77	0.41
1:B:583:ASN:ND2	1:B:583:ASN:C	2.79	0.41
1:B:944:ALA:CB	1:B:947:LEU:HD12	2.50	0.41
1:B:52:ASP:HB3	1:B:919:ILE:HG23	2.03	0.41
1:B:288:ARG:NH2	1:B:299:THR:OG1	2.41	0.41
1:B:895:LEU:HD13	1:B:957:GLY:HA3	2.03	0.41
1:B:648:LEU:O	1:B:649:ALA:C	2.64	0.40
1:B:107:LEU:HD21	1:B:185:HIS:HB3	2.04	0.40
1:B:644:GLY:N	1:B:645:PRO:CD	2.85	0.40
1:A:256:ARG:O	1:A:259:ASP:HB2	2.21	0.40
1:A:806:LEU:HA	1:A:809:MET:CE	2.37	0.40
1:A:948:GLU:O	1:A:952:ILE:HG12	2.20	0.40
1:B:46:GLN:HE21	1:B:54:LYS:HE3	1.86	0.40
1:B:305:LEU:HG	1:B:387:LEU:HD21	2.03	0.40
1:B:677:GLU:OE1	1:B:679:HIS:N	2.54	0.40
1:A:455:ARG:HA	1:A:455:ARG:HD3	1.87	0.40
1:A:325:MET:HE1	1:A:417:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:THR:CG2	1:A:742:GLU:H	2.35	0.40
1:B:455:ARG:HA	1:B:455:ARG:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	913/990 (92%)	862 (94%)	42 (5%)	9 (1%)	12	25
1	B	913/990 (92%)	867 (95%)	37 (4%)	9 (1%)	12	25
All	All	1826/1980 (92%)	1729 (95%)	79 (4%)	18 (1%)	12	25

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	PRO
1	B	230	PRO
1	A	71	HIS
1	A	237	ARG
1	A	239	GLY
1	B	71	HIS
1	B	237	ARG
1	B	239	GLY
1	B	344	THR
1	A	362	ASN
1	A	444	LEU
1	B	444	LEU
1	A	238	ALA
1	A	241	SER
1	B	238	ALA
1	B	362	ASN

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Mol	Chain	Res	Type
1	B	754	PRO
1	A	754	PRO

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	800/866 (92%)	749 (94%)	51 (6%)	16	33
1	B	799/866 (92%)	751 (94%)	48 (6%)	17	36
All	All	1599/1732 (92%)	1500 (94%)	99 (6%)	16	34

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	70	LYS
1	A	88	THR
1	A	101	MET
1	A	148	LYS
1	A	149	LEU
1	A	158	ASP
1	A	177	VAL
1	A	200	ILE
1	A	209	ASP
1	A	244	HIS
1	A	246	THR
1	A	268	ASN
1	A	293	ARG
1	A	298	VAL
1	A	316	SER
1	A	327	MET
1	A	337	ARG
1	A	339	GLU
1	A	343	ARG
1	A	380	ARG

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Mol	Chain	Res	Type
1	A	388	VAL
1	A	399	VAL
1	A	402	ASN
1	A	404	GLU
1	A	424	VAL
1	A	444	LEU
1	A	553	LEU
1	A	582	ARG
1	A	583	ASN
1	A	584	ARG
1	A	604	ARG
1	A	606	SER
1	A	623	LYS
1	A	639	VAL
1	A	646	THR
1	A	652	SER
1	A	663	ARG
1	A	664	VAL
1	A	670	VAL
1	A	728	LYS
1	A	731	ARG
1	A	740	THR
1	A	742	GLU
1	A	760	SER
1	A	778	THR
1	A	818	VAL
1	A	853	SER
1	A	873	ASP
1	A	914	THR
1	A	954	THR
1	B	70	LYS
1	B	88	THR
1	B	101	MET
1	B	148	LYS
1	B	149	LEU
1	B	158	ASP
1	B	177	VAL
1	B	200	ILE
1	B	209	ASP
1	B	246	THR
1	B	268	ASN
1	B	293	ARG

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Mol	Chain	Res	Type
1	B	316	SER
1	B	327	MET
1	B	337	ARG
1	B	339	GLU
1	B	343	ARG
1	B	380	ARG
1	B	388	VAL
1	B	399	VAL
1	B	402	ASN
1	B	404	GLU
1	B	424	VAL
1	B	444	LEU
1	B	498	ASP
1	B	553	LEU
1	B	582	ARG
1	B	583	ASN
1	B	584	ARG
1	B	604	ARG
1	B	606	SER
1	B	623	LYS
1	B	639	VAL
1	B	646	THR
1	B	663	ARG
1	B	664	VAL
1	B	670	VAL
1	B	728	LYS
1	B	731	ARG
1	B	740	THR
1	B	742	GLU
1	B	778	THR
1	B	818	VAL
1	B	853	SER
1	B	873	ASP
1	B	914	THR
1	B	922	GLU
1	B	954	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	46	GLN

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Mol	Chain	Res	Type
1	A	172	HIS
1	A	213	HIS
1	A	244	HIS
1	A	268	ASN
1	A	363	GLN
1	A	653	GLN
1	A	679	HIS
1	A	794	HIS
1	A	802	ASN
1	A	838	ASN
1	A	883	GLN
1	A	899	GLN
1	A	910	ASN
1	A	963	GLN
1	B	15	GLN
1	B	46	GLN
1	B	71	HIS
1	B	172	HIS
1	B	213	HIS
1	B	244	HIS
1	B	268	ASN
1	B	363	GLN
1	B	583	ASN
1	B	653	GLN
1	B	794	HIS
1	B	802	ASN
1	B	838	ASN
1	B	883	GLN
1	B	899	GLN
1	B	910	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	TRS	A	1970	-	7,7,7	0.91	0	9,9,9	0.95	1 (11%)
2	G6P	A	1967	-	16,16,16	1.61	4 (25%)	23,24,24	2.48	8 (34%)
2	G6P	B	1967	-	16,16,16	1.11	1 (6%)	23,24,24	1.79	7 (30%)
4	EDO	A	1969	-	3,3,3	0.68	0	2,2,2	0.21	0
4	EDO	B	1969	-	3,3,3	0.72	0	2,2,2	0.27	0
3	SO4	B	1968	-	4,4,4	0.51	0	6,6,6	0.95	0
3	SO4	A	1968	-	4,4,4	0.42	0	6,6,6	0.63	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
5	TRS	A	1970	-	-	7/9/9/9	-
2	G6P	A	1967	-	-	1/6/26/26	0/1/1/1
2	G6P	B	1967	-	-	3/6/26/26	0/1/1/1
4	EDO	A	1969	-	-	1/1/1/1	-
4	EDO	B	1969	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1967	G6P	O3-C3	3.57	1.51	1.43
2	B	1967	G6P	O1-C1	2.71	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1967	G6P	C3-C2	2.65	1.59	1.52
2	A	1967	G6P	C4-C3	2.61	1.59	1.52
2	A	1967	G6P	O1-C1	2.29	1.46	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1967	G6P	C1-C2-C3	5.86	122.31	110.36
2	A	1967	G6P	C1-O5-C5	5.04	123.40	113.65
2	A	1967	G6P	O2-C2-C1	-4.95	97.82	109.25
2	A	1967	G6P	O5-C5-C4	4.90	118.54	109.70
2	B	1967	G6P	C1-O5-C5	3.67	120.75	113.65
2	B	1967	G6P	C1-C2-C3	3.54	117.57	110.36
2	B	1967	G6P	O2-C2-C1	-2.99	102.34	109.25
2	B	1967	G6P	O5-C5-C4	2.59	114.36	109.70
2	B	1967	G6P	O2P-P-O6	-2.25	100.80	106.67
2	A	1967	G6P	O4-C4-C3	2.24	115.67	110.38
2	A	1967	G6P	C3-C4-C5	2.16	114.16	110.23
2	A	1967	G6P	O2-C2-C3	2.16	115.47	110.38
2	A	1967	G6P	O1-C1-C2	2.12	115.13	108.98
2	B	1967	G6P	O5-C1-C2	-2.08	106.65	110.30
2	B	1967	G6P	O1-C1-O5	2.03	116.45	110.41
5	A	1970	TRS	C1-C-N	-2.02	103.02	108.17

There are no chirality outliers.

All (13) torsion outliers are listed below:

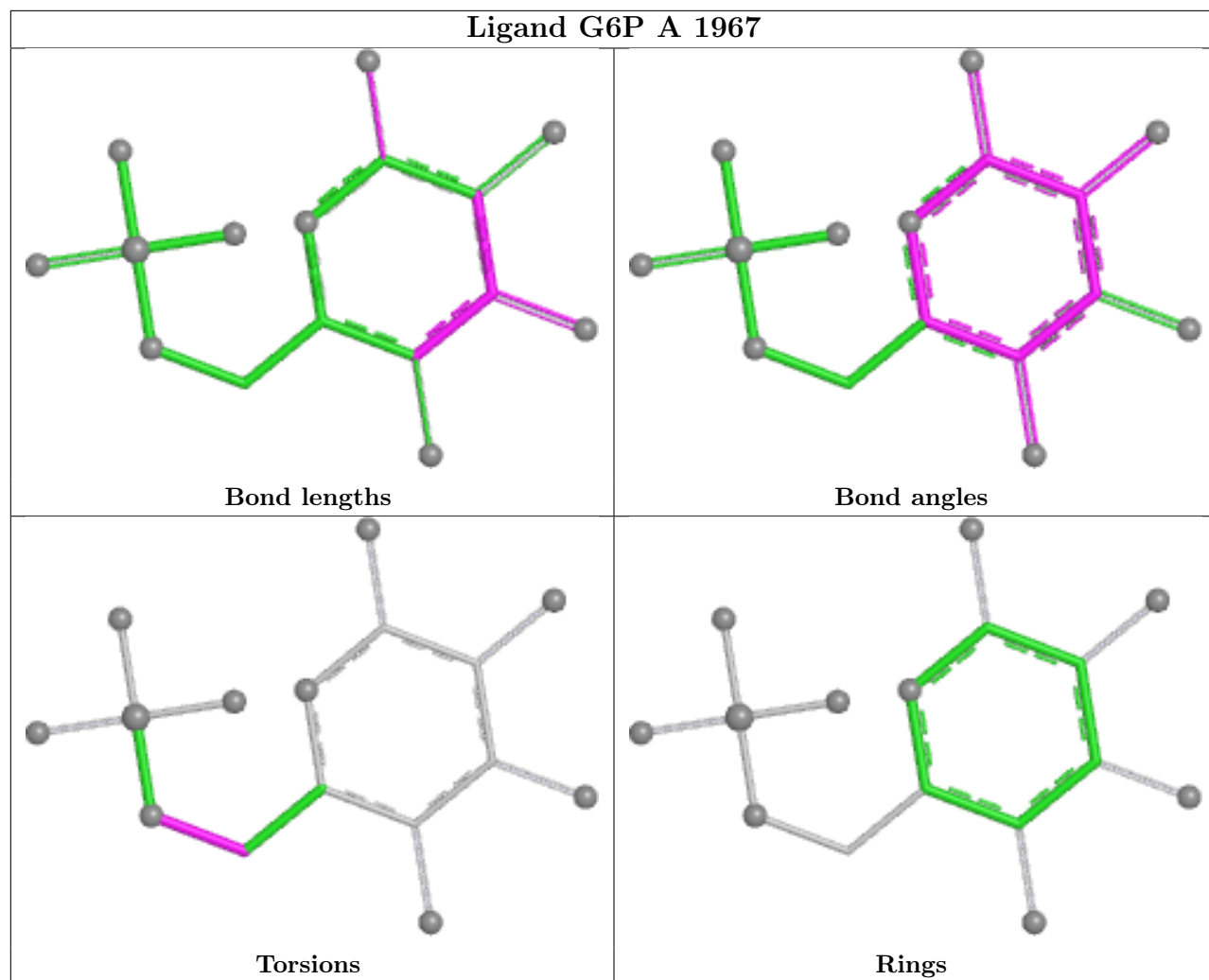
Mol	Chain	Res	Type	Atoms
2	A	1967	G6P	C5-C6-O6-P
2	B	1967	G6P	C4-C5-C6-O6
2	B	1967	G6P	O5-C5-C6-O6
5	A	1970	TRS	N-C-C1-O1
5	A	1970	TRS	N-C-C3-O3
5	A	1970	TRS	C3-C-C1-O1
5	A	1970	TRS	C2-C-C3-O3
2	B	1967	G6P	C5-C6-O6-P
5	A	1970	TRS	C1-C-C2-O2
5	A	1970	TRS	C1-C-C3-O3
5	A	1970	TRS	C3-C-C2-O2
4	A	1969	EDO	O1-C1-C2-O2
4	B	1969	EDO	O1-C1-C2-O2

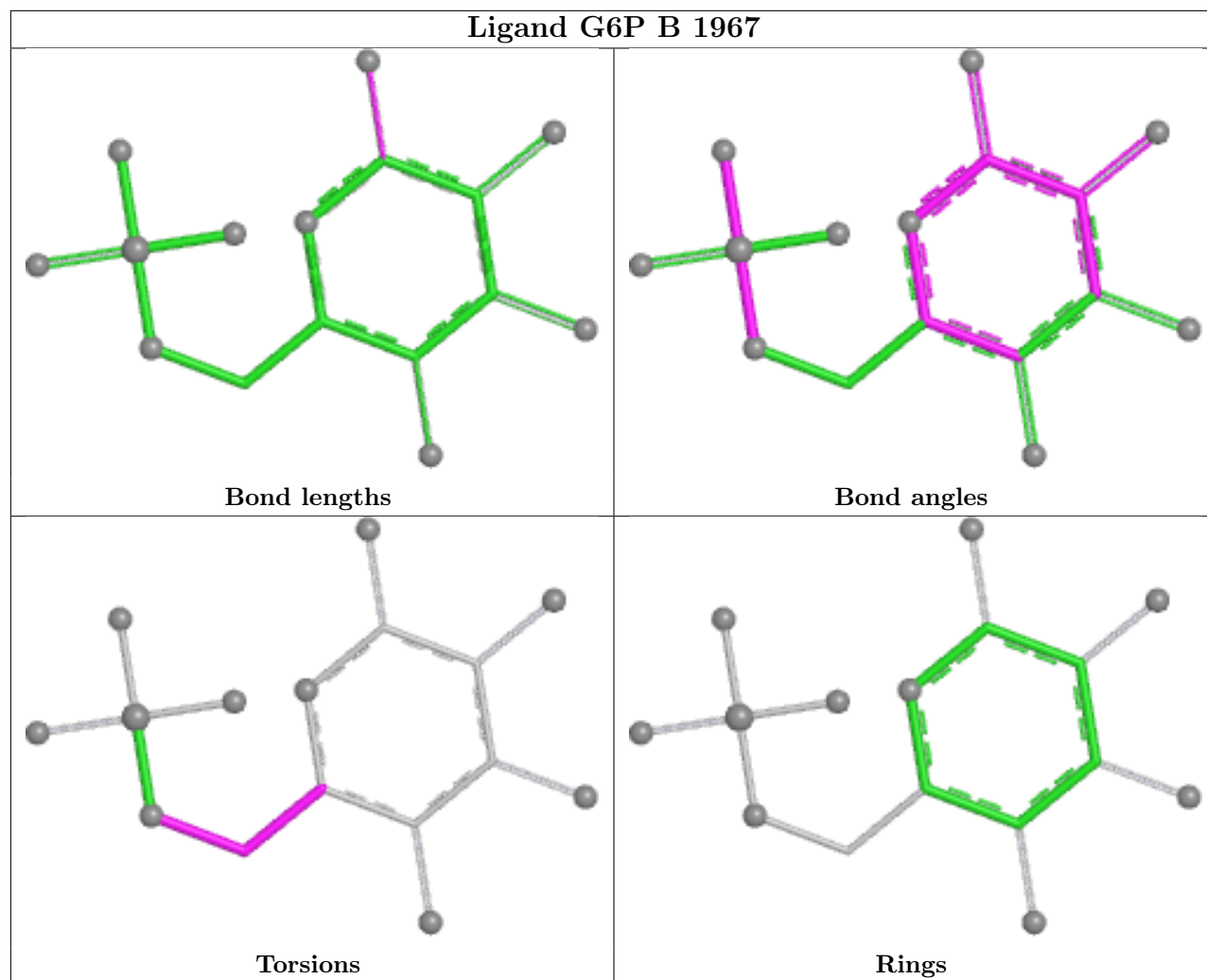
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1967	G6P	3	0
2	B	1967	G6P	2	0
3	B	1968	SO4	2	0
3	A	1968	SO4	2	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	929/990 (93%)	-0.27	28 (3%)	52 44	36, 60, 113, 172	0
1	B	929/990 (93%)	-0.12	32 (3%)	48 38	43, 71, 125, 170	0
All	All	1858/1980 (93%)	-0.20	60 (3%)	50 41	36, 66, 119, 172	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	ARG	4.9
1	B	924	ALA	4.6
1	A	351	HIS	4.5
1	B	748	MET	4.3
1	A	226	ARG	4.2
1	B	351	HIS	4.2
1	A	229	PRO	4.1
1	B	229	PRO	4.0
1	A	6	VAL	3.7
1	A	243	PHE	3.7
1	A	353	ILE	3.7
1	B	225	ILE	3.7
1	B	754	PRO	3.6
1	A	199	ASP	3.5
1	B	177	VAL	3.4
1	A	240	MET	3.3
1	A	752	SER	3.3
1	A	754	PRO	3.3
1	A	355	PHE	3.3
1	B	345	ALA	3.3
1	A	225	ILE	3.2
1	B	353	ILE	3.2
1	A	944	ALA	3.2
1	A	383	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	22	GLY	3.0
1	A	357	LYS	3.0
1	A	356	TRP	3.0
1	B	759	PRO	2.9
1	A	176	SER	2.8
1	B	243	PHE	2.7
1	B	361	PRO	2.7
1	B	356	TRP	2.7
1	A	242	TYR	2.7
1	B	355	PHE	2.6
1	B	352	TYR	2.6
1	A	354	GLU	2.5
1	A	352	TYR	2.5
1	A	179	ARG	2.5
1	B	357	LYS	2.5
1	B	498	ASP	2.4
1	B	354	GLU	2.4
1	B	923	TYR	2.4
1	A	358	ARG	2.4
1	B	172	HIS	2.3
1	A	346	ARG	2.3
1	A	923	TYR	2.3
1	B	176	SER	2.3
1	B	25	SER	2.2
1	A	759	PRO	2.1
1	B	174	THR	2.1
1	B	241	SER	2.1
1	B	242	TYR	2.1
1	B	21	PRO	2.1
1	B	747	ARG	2.1
1	A	25	SER	2.1
1	B	753	ARG	2.1
1	A	177	VAL	2.0
1	B	384	ARG	2.0
1	B	27	ASP	2.0
1	B	240	MET	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

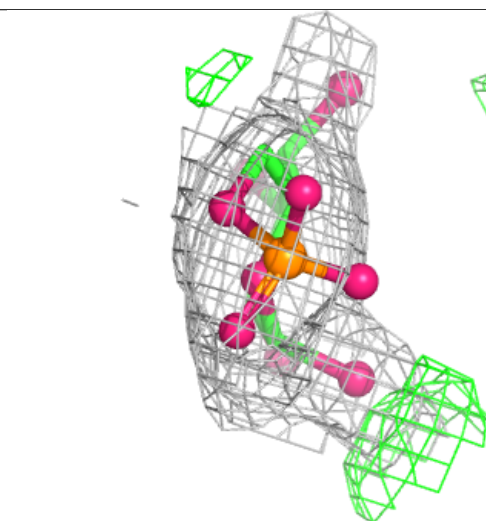
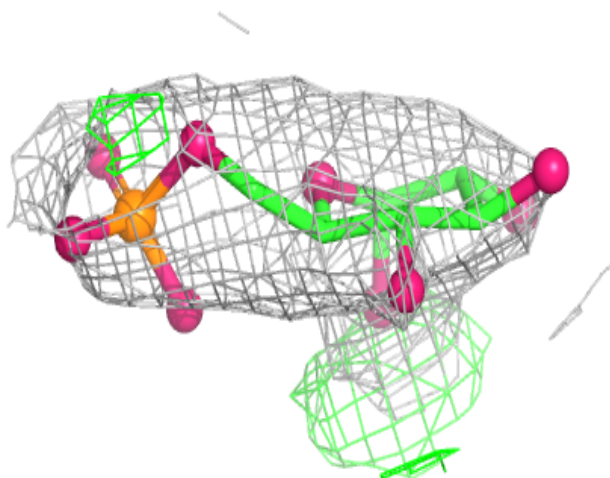
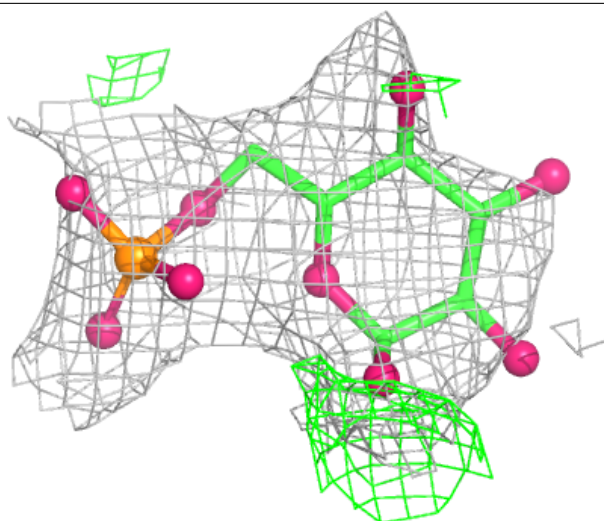
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	EDO	A	1969	4/4	0.70	0.27	63,74,77,79	0
2	G6P	B	1967	16/16	0.75	0.18	98,106,157,158	0
2	G6P	A	1967	16/16	0.75	0.16	58,95,126,134	0
4	EDO	B	1969	4/4	0.87	0.25	74,74,77,82	0
5	TRS	A	1970	8/8	0.91	0.12	64,79,84,86	0
3	SO4	B	1968	5/5	0.92	0.10	69,76,97,97	0
3	SO4	A	1968	5/5	0.93	0.11	72,87,93,102	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.

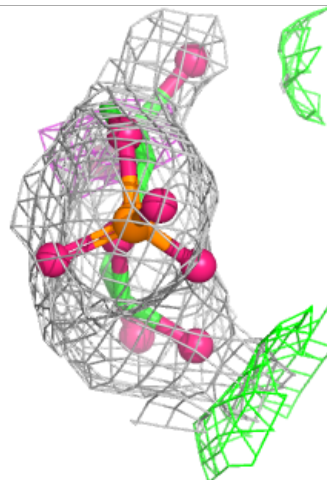
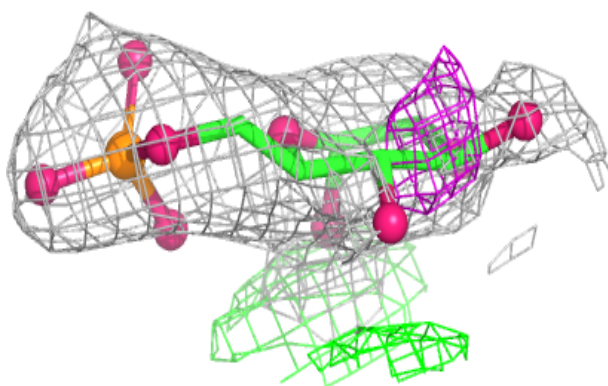
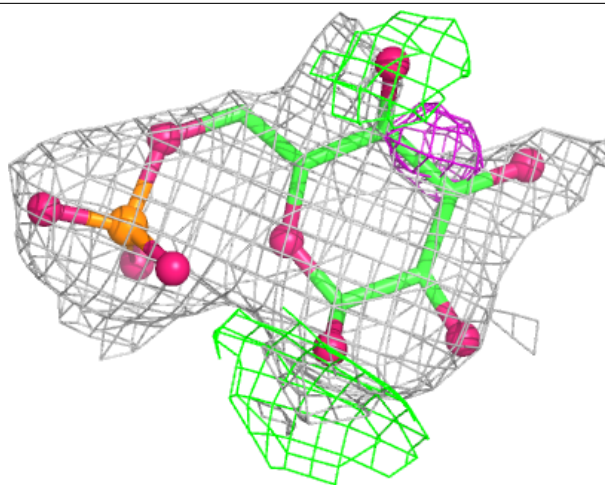
Electron density around G6P B 1967:

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



Electron density around G6P A 1967:

$2mF_o-DF_c$ (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.