Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 03:27 am GMT

PDB ID	:	1OFA
Title	:	Crystal structure of the tyrosine-regulated 3-deoxy-d-arabino-heptuloso nate-7-phosphate synthase from saccharomyces cerevisiae in complex with phosphoenolpyruvate and cobalt(ii)
Authors	:	Koenig, V.; Pfeil, A.; Heinrich, G.; Braus, G.H.; Schneider, T.R.
Deposited on	:	2003-04-09
Resolution	:	2.02 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:

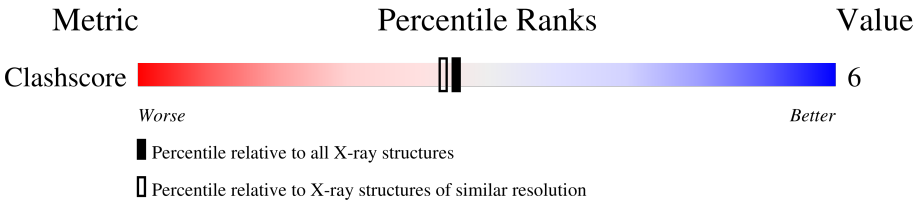
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.02 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))
Clashscore	141614	11643 (2.04-2.00)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	370	76% 14% • 7%
1	B	370	75% 15% • 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5481 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.

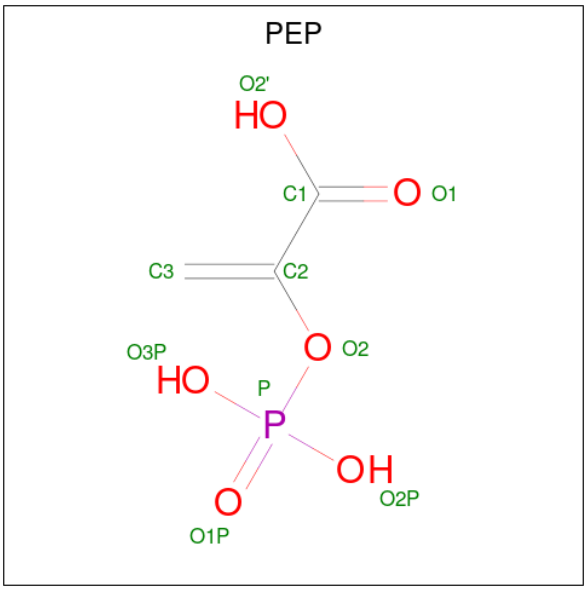
- Molecule 1 is a protein called PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2592	1615	467	500	10			
1	B	338	Total	C	N	O	S	0	0	0
			2560	1593	462	495	10			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

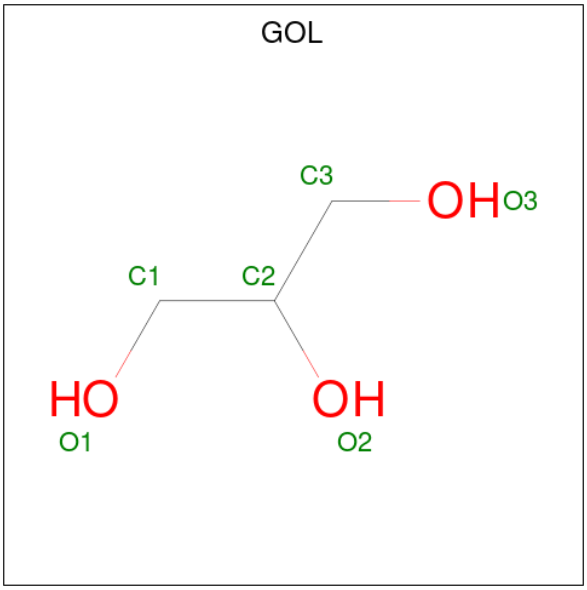
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Co	0	0
			1	1		
2	B	1	Total	Co	0	0
			1	1		

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	145	Total O 145 145	0	0
5	B	144	Total O 144 144	0	0

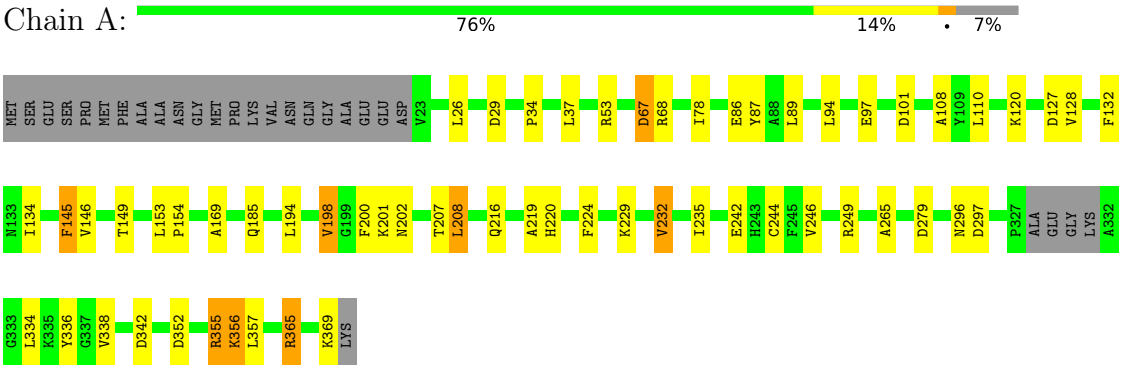
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS failed to run properly.

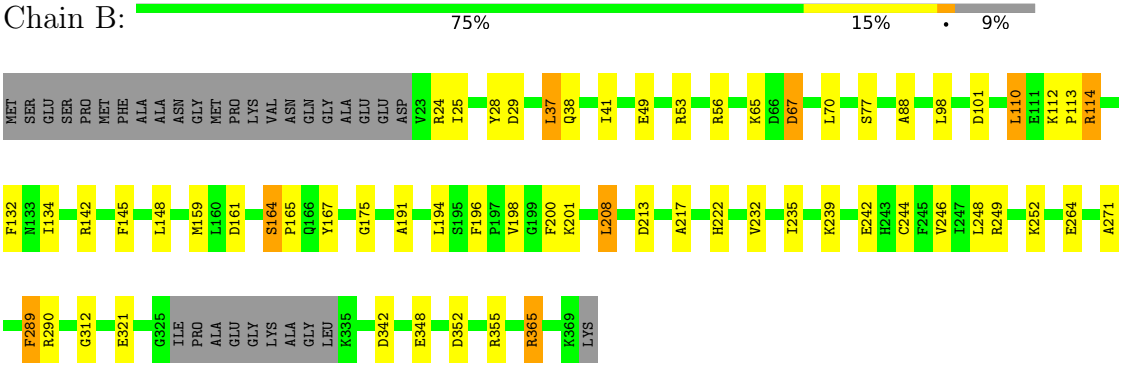
• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain A:



• Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.21Å 50.61Å 64.98Å 90.00° 106.33° 90.00°	Depositor
Resolution (Å)	17.57 – 2.02	Depositor
% Data completeness (in resolution range)	97.1 (17.57-2.02)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.155 , 0.204	Depositor
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.090	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h-2*l,-k,l	Xtriage
Total number of atoms	5481	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, PEP, CO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.35	16/2630 (0.6%)	1.22	22/3560 (0.6%)
1	B	1.40	13/2597 (0.5%)	1.25	22/3514 (0.6%)
All	All	1.37	29/5227 (0.6%)	1.24	44/7074 (0.6%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	SER	CB-OG	-10.53	1.28	1.42
1	B	132	PHE	CE1-CZ	10.27	1.56	1.37
1	A	169	ALA	CA-CB	8.86	1.71	1.52
1	A	356	LYS	CE-NZ	7.60	1.68	1.49
1	B	348	GLU	CD-OE2	7.43	1.33	1.25
1	A	132	PHE	CE1-CZ	7.22	1.51	1.37
1	B	200	PHE	CE2-CZ	7.01	1.50	1.37
1	A	208	LEU	CG-CD1	6.76	1.76	1.51
1	A	200	PHE	CE1-CZ	6.55	1.49	1.37
1	A	87	TYR	CD2-CE2	6.42	1.49	1.39
1	B	167	TYR	CD1-CE1	6.22	1.48	1.39
1	A	246	VAL	CB-CG1	6.17	1.65	1.52
1	A	198	VAL	CB-CG1	6.11	1.65	1.52
1	B	246	VAL	CB-CG2	5.98	1.65	1.52
1	A	356	LYS	CD-CE	5.89	1.66	1.51
1	B	191	ALA	CA-CB	5.85	1.64	1.52
1	A	146	VAL	CA-CB	5.72	1.66	1.54
1	A	338	VAL	CB-CG2	5.69	1.64	1.52
1	B	196	PHE	CE1-CZ	5.67	1.48	1.37
1	A	242	GLU	CD-OE2	5.66	1.31	1.25
1	B	289	PHE	CE1-CZ	5.63	1.48	1.37
1	B	242	GLU	CG-CD	5.51	1.60	1.51
1	A	224	PHE	CE2-CZ	5.48	1.47	1.37
1	B	271	ALA	CA-CB	5.33	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	LYS	CE-NZ	5.26	1.62	1.49
1	A	145	PHE	CE1-CZ	5.25	1.47	1.37
1	A	219	ALA	CA-CB	5.23	1.63	1.52
1	A	232	VAL	CB-CG2	-5.07	1.42	1.52
1	B	264	GLU	CD-OE2	5.07	1.31	1.25

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	LEU	CB-CG-CD2	-14.02	87.17	111.00
1	A	365	ARG	NE-CZ-NH2	-11.97	114.32	120.30
1	A	365	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	B	29	ASP	CB-CG-OD2	10.35	127.61	118.30
1	A	208	LEU	CB-CG-CD1	9.87	127.79	111.00
1	B	365	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	B	114	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	A	29	ASP	CB-CG-OD2	8.86	126.28	118.30
1	A	342	ASP	CB-CG-OD2	8.37	125.83	118.30
1	B	365	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	A	53	ARG	NE-CZ-NH1	-7.63	116.49	120.30
1	A	352	ASP	CB-CG-OD2	7.57	125.11	118.30
1	B	53	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	65	LYS	CD-CE-NZ	7.09	128.00	111.70
1	B	110	LEU	CB-CG-CD2	-6.85	99.36	111.00
1	A	297	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	67	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	53	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	290	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	B	164	SER	N-CA-CB	-6.46	100.81	110.50
1	A	94	LEU	CB-CG-CD2	6.11	121.38	111.00
1	A	357	LEU	CB-CG-CD2	6.03	121.25	111.00
1	B	37	LEU	CB-CG-CD2	5.99	121.18	111.00
1	B	37	LEU	CA-CB-CG	5.98	129.05	115.30
1	A	37	LEU	CB-CG-CD2	5.95	121.12	111.00
1	A	53	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	68	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	127	ASP	CB-CG-OD1	5.86	123.57	118.30
1	B	114	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	279	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	194	LEU	CB-CG-CD2	-5.56	101.54	111.00
1	B	248	LEU	CA-CB-CG	-5.51	102.63	115.30
1	B	98	LEU	CB-CG-CD1	-5.35	101.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	352	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	149	THR	OG1-CB-CG2	-5.28	97.86	110.00
1	A	89	LEU	CB-CG-CD1	5.26	119.94	111.00
1	A	355	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	356	LYS	CD-CE-NZ	5.17	123.59	111.70
1	A	334	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	334	LEU	CB-CG-CD1	5.12	119.70	111.00
1	B	342	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	213	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	355	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	67	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2592	0	2612	42	0
1	B	2560	0	2575	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
4	A	6	0	8	0	0
4	B	12	0	16	1	0
5	A	145	0	0	0	1
5	B	144	0	0	1	1
All	All	5481	0	5215	67	1

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 (67) 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:208:LEU:CD1	1:A:208:LEU:CG	1.76	1.59
1:A:356:LYS:NZ	1:A:356:LYS:CE	1.68	1.52
1:A:232:VAL:HG12	1:B:232:VAL:HG12	1.19	1.15
1:A:97:GLU:OE1	1:A:355:ARG:NH1	1.95	0.98
1:A:78:ILE:HD11	1:A:108:ALA:HA	1.41	0.98
1:B:110:LEU:HD21	1:B:145:PHE:CZ	2.01	0.96
1:A:232:VAL:CG1	1:B:232:VAL:HG12	1.97	0.94
1:A:232:VAL:HG12	1:B:232:VAL:CG1	1.97	0.93
1:A:208:LEU:CD1	1:A:208:LEU:HG	1.97	0.93
1:A:120:LYS:NZ	1:B:222:HIS:HD2	1.77	0.81
1:A:78:ILE:CD1	1:A:108:ALA:HA	2.12	0.79
1:A:207:THR:HG21	1:B:252:LYS:HZ3	1.49	0.76
1:B:164:SER:HB3	1:B:165:PRO:HD3	1.74	0.70
1:B:164:SER:CB	1:B:165:PRO:HD3	2.23	0.69
1:A:207:THR:HG21	1:B:252:LYS:NZ	2.09	0.68
1:A:120:LYS:HZ3	1:B:222:HIS:HD2	1.39	0.68
1:B:164:SER:HB3	1:B:165:PRO:CD	2.27	0.64
1:B:217:ALA:O	1:B:222:HIS:HE1	1.83	0.61
1:B:37:LEU:HD22	1:B:41:ILE:HD12	1.82	0.61
1:A:369:LYS:CB	1:A:369:LYS:NZ	2.64	0.60
1:A:120:LYS:HZ3	1:B:222:HIS:CD2	2.19	0.60
1:A:369:LYS:NZ	1:A:369:LYS:HB2	2.19	0.58
1:A:369:LYS:HB2	1:A:369:LYS:HZ2	1.70	0.57
1:B:49:GLU:OE1	1:B:56:ARG:NH2	2.38	0.56
1:A:185:GLN:NE2	1:B:114:ARG:H	2.03	0.56
1:B:164:SER:CB	1:B:165:PRO:CD	2.85	0.54
1:A:110:LEU:HD22	1:A:145:PHE:CZ	2.43	0.54
1:A:208:LEU:CD1	1:A:208:LEU:CD2	2.76	0.54
1:B:110:LEU:HD21	1:B:145:PHE:HZ	1.69	0.54
1:A:101:ASP:OD1	1:A:365:ARG:NH2	2.41	0.53
1:A:235:ILE:HG23	1:B:134:ILE:HD12	1.90	0.53
1:A:67:ASP:OD2	1:A:365:ARG:HD3	2.09	0.53
1:A:86:GLU:OE2	1:A:336:TYR:OH	2.18	0.53
1:A:208:LEU:HD21	1:A:265:ALA:HB2	1.91	0.52
1:A:78:ILE:CD1	1:A:108:ALA:CA	2.87	0.52
1:A:201:LYS:HD2	1:A:249:ARG:HG2	1.91	0.52
1:A:369:LYS:CB	1:A:369:LYS:HZ3	2.23	0.52
1:B:208:LEU:N	1:B:208:LEU:HD23	2.21	0.51
1:B:201:LYS:HD2	1:B:249:ARG:HG2	1.91	0.51
1:B:110:LEU:CD2	1:B:145:PHE:CZ	2.87	0.50
1:B:161:ASP:HB3	1:B:164:SER:HB2	1.95	0.48
1:A:34:PRO:HD2	1:A:229:LYS:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:SER:HB3	1:B:112:LYS:HD3	1.95	0.48
1:A:296:ASN:HD22	1:A:356:LYS:NZ	2.12	0.47
1:A:198:VAL:O	1:A:244:CYS:HA	2.15	0.47
1:A:120:LYS:NZ	1:B:222:HIS:CD2	2.68	0.46
1:B:67:ASP:OD1	1:B:365:ARG:HD3	2.15	0.46
1:B:289:PHE:HZ	1:B:321:GLU:OE1	1.99	0.46
1:B:198:VAL:O	1:B:244:CYS:HA	2.16	0.46
1:B:113:PRO:O	4:B:603:GOL:C1	2.64	0.45
1:A:26:LEU:HD12	1:B:239:LYS:HB2	1.98	0.45
1:A:128:VAL:O	1:A:128:VAL:HG23	2.17	0.45
1:A:194:LEU:O	1:B:24:ARG:HD2	2.18	0.44
1:A:120:LYS:HZ1	1:B:222:HIS:HD2	1.63	0.44
1:A:185:GLN:HE22	1:B:114:ARG:H	1.63	0.44
1:B:101:ASP:OD1	1:B:365:ARG:NH2	2.50	0.43
1:A:134:ILE:HD12	1:B:235:ILE:HG23	2.01	0.42
1:B:38:GLN:HG2	1:B:142:ARG:CZ	2.50	0.42
1:B:88:ALA:HB2	1:B:148:LEU:HD22	2.00	0.42
1:B:175:GLY:O	1:B:198:VAL:HA	2.20	0.42
1:A:216:GLN:O	1:A:220:HIS:HD2	2.03	0.42
1:B:25:ILE:HG21	1:B:28:TYR:CZ	2.55	0.42
1:B:70:LEU:O	1:B:312:GLY:HA2	2.19	0.42
1:A:110:LEU:CD2	1:A:145:PHE:CZ	3.03	0.41
1:B:159:MET:HA	5:B:2036:HOH:O	2.20	0.41
1:A:202:ASN:HB2	1:A:207:THR:O	2.21	0.40
1:A:153:LEU:HA	1:A:154:PRO:HD3	1.98	0.40

All (1) 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)
5:A:2108:HOH:O	5:B:2047:HOH:O[1_565]	2.03	0.17

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	PEP	B	508	-	9,9,9	2.91	4 (44%)	11,13,13	1.52	3 (27%)
4	GOL	B	603	-	5,5,5	0.80	0	5,5,5	1.72	2 (40%)
3	PEP	A	508	-	9,9,9	2.91	4 (44%)	11,13,13	1.52	3 (27%)
4	GOL	A	601	-	5,5,5	0.61	0	5,5,5	0.84	0
4	GOL	B	601	-	5,5,5	0.57	0	5,5,5	0.98	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
3	PEP	B	508	-	-	0/9/9/9	-
4	GOL	B	603	-	-	2/4/4/4	-
3	PEP	A	508	-	-	0/9/9/9	-
4	GOL	A	601	-	-	0/4/4/4	-
4	GOL	B	601	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	PEP	P-O2	-6.00	1.50	1.59
3	B	508	PEP	P-O2	-6.00	1.50	1.59
3	B	508	PEP	C2-C1	3.47	1.52	1.49
3	A	508	PEP	C2-C1	3.45	1.52	1.49
3	B	508	PEP	P-O1P	-3.07	1.40	1.50
3	A	508	PEP	P-O1P	-3.06	1.40	1.50
3	A	508	PEP	O2'-C1	-2.72	1.22	1.30
3	B	508	PEP	O2'-C1	-2.69	1.22	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	603	GOL	O2-C2-C3	2.72	121.12	109.12
3	A	508	PEP	O3P-P-O2	-2.63	97.24	105.25
3	B	508	PEP	O3P-P-O2	-2.62	97.26	105.25
3	A	508	PEP	O2P-P-O2	2.23	112.06	105.25
3	B	508	PEP	O2P-P-O2	2.22	112.02	105.25
4	B	603	GOL	C3-C2-C1	-2.21	103.10	111.70
3	A	508	PEP	O2'-C1-C2	2.04	117.39	113.91
3	B	508	PEP	O2'-C1-C2	2.03	117.37	113.91

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	GOL	C1-C2-C3-O3
4	B	603	GOL	O2-C2-C3-O3
4	B	601	GOL	C1-C2-C3-O3
4	B	601	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	GOL	1	0

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.