Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:19 PM 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

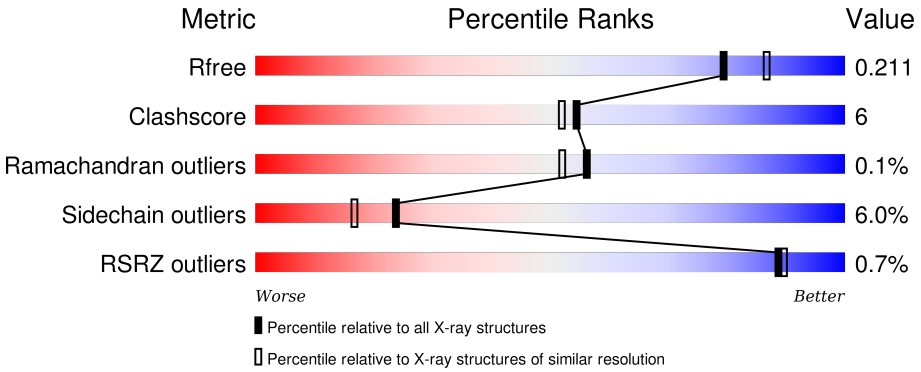
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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))
R_{free}	91344	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	370	% 74% 14% 5% • 7%
1	B	370	% 73% 16% •• 9%

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	GOL	B	603	-	-	-	X

2 Entry composition

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.

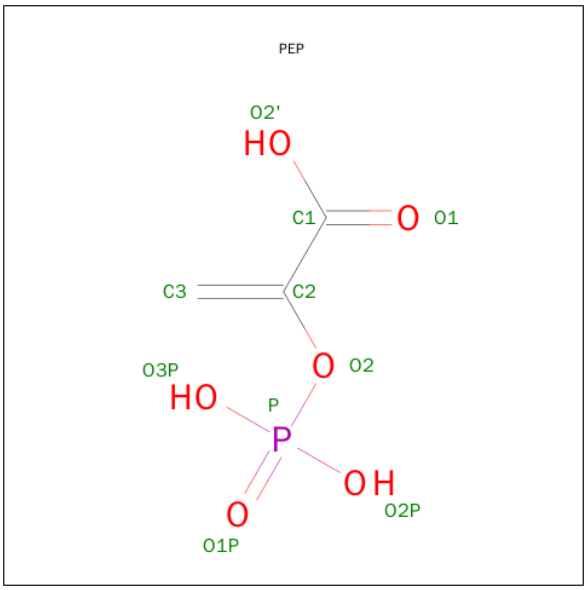
- Molecule 1 is a protein called PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE.

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).

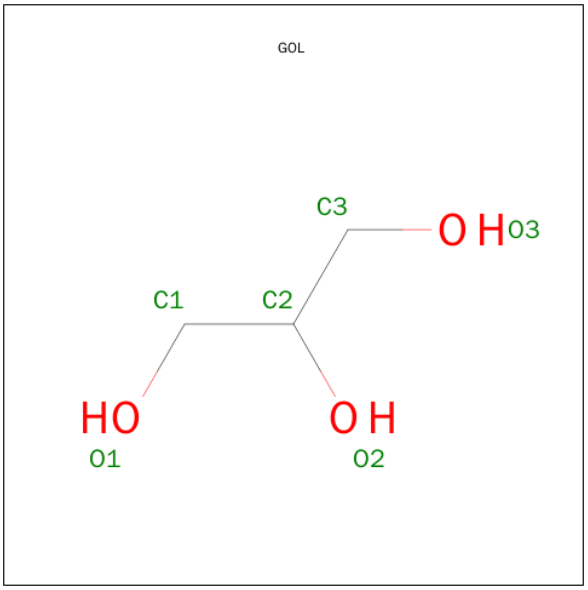
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Co	0	0
			1	1		
2	A	1	Total	Co	0	0
			1	1		

- 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.

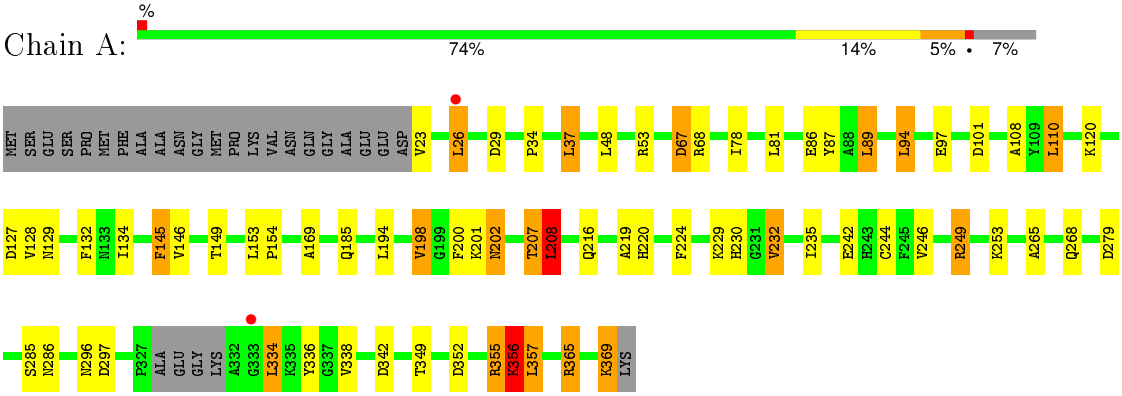
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	145	Total O 145 145	0	0
5	B	144	Total O 144 144	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

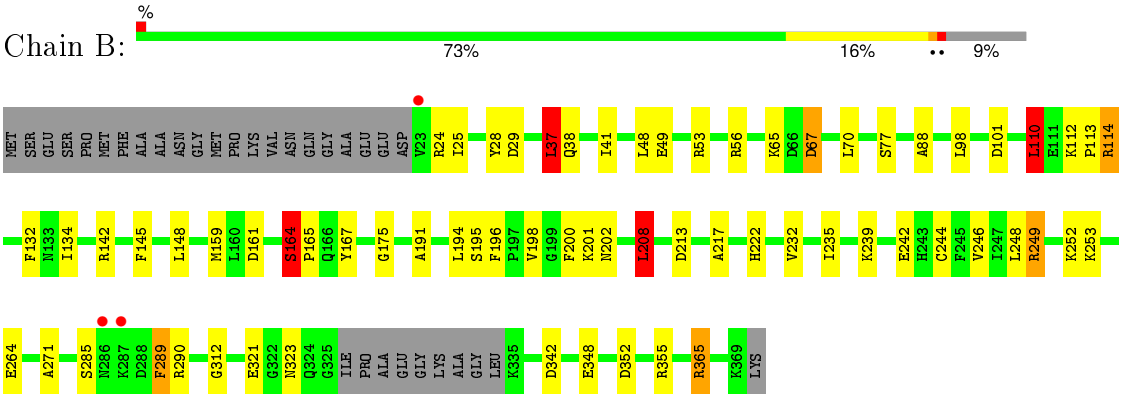
- Molecule 1: PHOSPHO-2-DEHYDRO-3-DEOXYHEPTONATE ALDOLASE

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

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 17.57 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.1 (17.57-2.02) 97.1 (17.57-2.02)	Depositor EDS
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 0.162 , 0.211	Depositor DCC
R_{free} test set	1971 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 48.3	EDS
Estimated twinning fraction	0.016 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 39374 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.96	EDS
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, 0.375 respectively for untwinned datasets, and 0.333, 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, CO, PEP

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:CG	1:A:208:LEU:CD1	1.76	1.59
1:A:356:LYS:CE	1:A:356:LYS:NZ	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:HG	1:A:208:LEU:CD1	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:NZ	1:A:369:LYS:CB	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:HZ2	1:A:369:LYS:HB2	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:235:ILE:HG23	1:B:134:ILE:HD12	1.90	0.53
1:A:101:ASP:OD1	1:A:365:ARG:NH2	2.41	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:369:LYS:HZ3	1:A:369:LYS:CB	2.23	0.52
1:A:201:LYS:HD2	1:A:249:ARG:HG2	1.91	0.52
1:B:208:LEU:HD23	1:B:208:LEU:N	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:HG23	1:A:128:VAL:O	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:70:LEU:O	1:B:312:GLY:HA2	2.19	0.42
1:B:25:ILE:HG21	1:B:28:TYR:CZ	2.55	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)

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	339/370 (92%)	328 (97%)	11 (3%)	0	100 100
1	B	334/370 (90%)	323 (97%)	10 (3%)	1 (0%)	46 40
All	All	673/740 (91%)	651 (97%)	21 (3%)	1 (0%)	56 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	SER

5.3.2 Protein sidechains (i)

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	278/298 (93%)	255 (92%)	23 (8%)	14 8
1	B	275/298 (92%)	265 (96%)	10 (4%)	42 38
All	All	553/596 (93%)	520 (94%)	33 (6%)	24 17

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	26	LEU
1	A	37	LEU
1	A	48	LEU
1	A	81	LEU
1	A	89	LEU
1	A	94	LEU
1	A	110	LEU
1	A	129	ASN
1	A	202	ASN
1	A	207	THR
1	A	208	LEU

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Mol	Chain	Res	Type
1	A	230	HIS
1	A	249	ARG
1	A	253	LYS
1	A	268	GLN
1	A	285	SER
1	A	286	ASN
1	A	334	LEU
1	A	349	THR
1	A	356	LYS
1	A	357	LEU
1	A	369	LYS
1	B	37	LEU
1	B	48	LEU
1	B	110	LEU
1	B	164	SER
1	B	202	ASN
1	B	208	LEU
1	B	249	ARG
1	B	253	LYS
1	B	285	SER
1	B	323	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	185	GLN
1	A	216	GLN
1	A	220	HIS
1	A	296	ASN
1	B	38	GLN
1	B	85	GLN
1	B	139	GLN
1	B	143	GLN
1	B	150	ASN
1	B	222	HIS
1	B	323	ASN
1	B	324	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 carbohydrates 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	A	508	-	5,9,9	2.10	1 (20%)	8,13,13	1.50	2 (25%)
4	GOL	A	601	-	5,5,5	0.56	0	5,5,5	0.86	0
3	PEP	B	508	-	5,9,9	2.09	1 (20%)	8,13,13	1.50	2 (25%)
4	GOL	B	601	-	5,5,5	0.52	0	5,5,5	0.93	0
4	GOL	B	603	-	5,5,5	0.76	0	5,5,5	1.67	2 (40%)

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	A	508	-	-	0/5/9/9	0/0/0/0
4	GOL	A	601	-	-	0/4/4/4	0/0/0/0
3	PEP	B	508	-	-	0/5/9/9	0/0/0/0
4	GOL	B	601	-	-	0/4/4/4	0/0/0/0
4	GOL	B	603	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	508	PEP	P-O1P	-3.20	1.40	1.51
3	A	508	PEP	P-O1P	-3.19	1.40	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	508	PEP	O3P-P-O2	-2.45	97.24	105.25
3	B	508	PEP	O3P-P-O2	-2.45	97.26	105.25
4	B	603	GOL	C3-C2-C1	-2.05	103.10	111.12
3	B	508	PEP	O2P-P-O2	2.07	112.02	105.25
3	A	508	PEP	O2P-P-O2	2.08	112.06	105.25
4	B	603	GOL	O2-C2-C3	2.72	121.12	108.65

There are no chirality outliers.

There are no torsion outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	343/370 (92%)	-0.38	2 (0%)	90	91	18, 25, 38, 52	0
1	B	338/370 (91%)	-0.45	3 (0%)	85	86	17, 24, 36, 48	0
All	All	681/740 (92%)	-0.41	5 (0%)	89	89	17, 25, 37, 52	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	LYS	3.9
1	A	26	LEU	3.4
1	A	333	GLY	3.1
1	B	23	VAL	3.0
1	B	286	ASN	2.4

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	B	603	6/6	0.87	0.14	2.17	36,42,44,44	0
4	GOL	A	601	6/6	0.92	0.12	1.62	28,30,36,36	0
3	PEP	B	508	10/10	0.97	0.10	0.52	21,24,30,32	0
4	GOL	B	601	6/6	0.98	0.11	0.25	23,28,29,29	0
3	PEP	A	508	10/10	0.97	0.09	-0.25	21,24,30,32	0
2	CO	B	400	1/1	0.99	0.03	-3.56	27,27,27,27	0
2	CO	A	400	1/1	0.99	0.02	-4.75	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.