



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:21 PM GMT

PDB ID : 1ONE  
Title : YEAST ENOLASE COMPLEXED WITH AN EQUILIBRIUM MIXTURE  
OF 2'-PHOSPHOGLYCEATE AND PHOSPHOENOLPYRUVATE  
Authors : Larsen, T.M.; Wedekind, J.E.; Rayment, I.; Reed, G.H.  
Deposited on : 1995-12-05  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

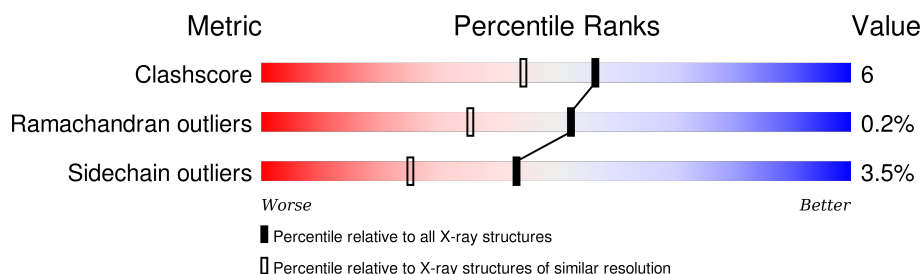
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	436	 78% 19% •
1	B	436	 77% 20% •

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7572 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.

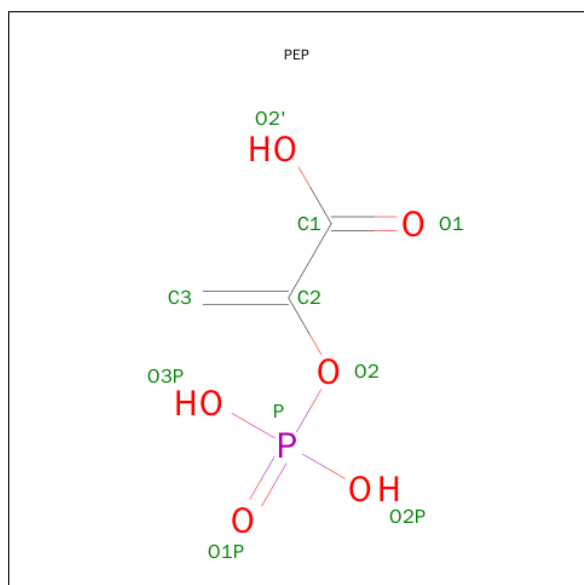
- Molecule 1 is a protein called ENOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3292	2079	570	637	6			
1	B	436	Total	C	N	O	S	0	0	0
			3292	2079	570	637	6			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP, 2PG) (formula:  $C_3H_5O_6P$ ,  $C_3H_7O_7P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	O	P	0	0
			21	6	13	2		
3	B	2	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 4 is water.

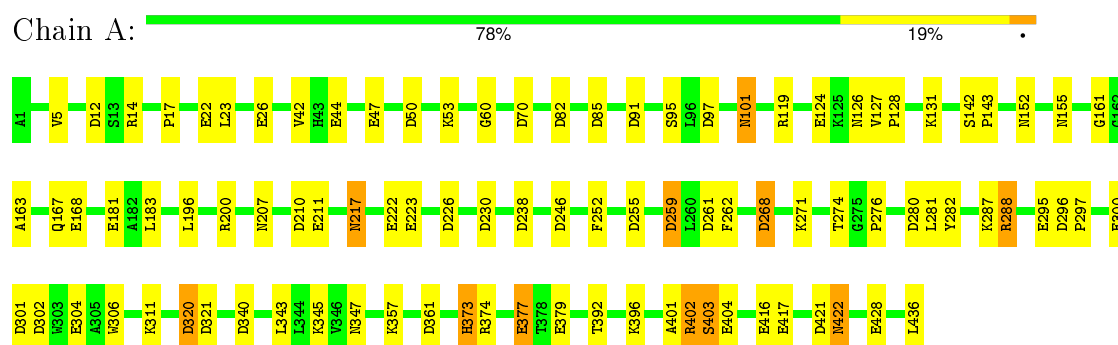
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	473	Total	O	0	0
			473	473		
4	B	469	Total	O	0	0
			469	469		

### 3 Residue-property plots

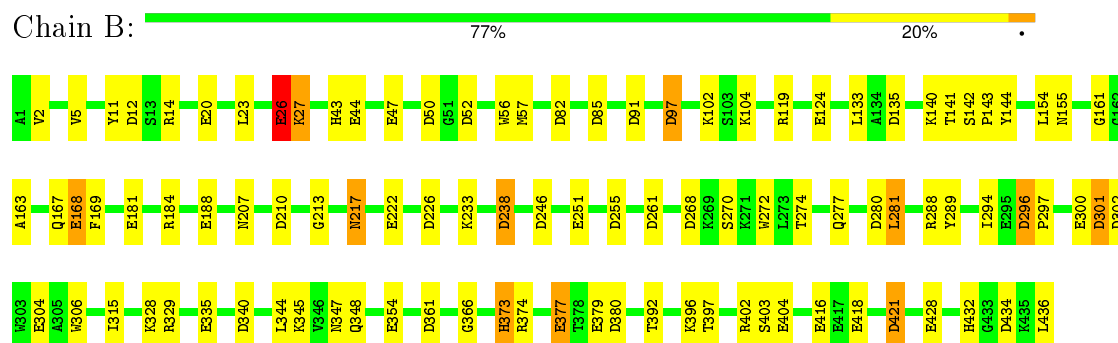
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: ENOLASE



#### • Molecule 1: ENOLASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.90 Å   73.20 Å   93.90 Å 90.00°   93.30°   90.00°	Depositor
Resolution (Å)	60.00 – 1.80	Depositor
% Data completeness (in resolution range)	92.0 (60.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PEP, 2PG

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	1.16	16/3352 (0.5%)	1.28	48/4534 (1.1%)
1	B	1.12	19/3352 (0.6%)	1.34	53/4534 (1.2%)
All	All	1.14	35/6704 (0.5%)	1.31	101/9068 (1.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLU	CD-OE2	9.41	1.35	1.25
1	A	377	GLU	CD-OE2	9.31	1.35	1.25
1	B	428	GLU	CD-OE1	7.68	1.34	1.25
1	B	124	GLU	CD-OE2	7.09	1.33	1.25
1	B	300	GLU	CD-OE2	6.88	1.33	1.25
1	A	181	GLU	CD-OE1	-6.87	1.18	1.25
1	A	44	GLU	CD-OE2	6.87	1.33	1.25
1	A	416	GLU	CD-OE2	6.74	1.33	1.25
1	B	47	GLU	CD-OE1	6.73	1.33	1.25
1	B	222	GLU	CD-OE2	6.59	1.32	1.25
1	B	26	GLU	CB-CG	6.39	1.64	1.52
1	B	251	GLU	CD-OE2	6.22	1.32	1.25
1	A	26	GLU	CD-OE1	6.14	1.32	1.25
1	A	417	GLU	CD-OE1	-6.08	1.19	1.25
1	B	335	GLU	CD-OE1	5.98	1.32	1.25
1	B	181	GLU	CD-OE2	5.92	1.32	1.25
1	A	300	GLU	CD-OE2	5.92	1.32	1.25
1	A	47	GLU	CD-OE1	5.92	1.32	1.25
1	A	222	GLU	CD-OE2	5.91	1.32	1.25
1	B	188	GLU	CD-OE2	5.85	1.32	1.25
1	A	124	GLU	CD-OE2	5.84	1.32	1.25
1	A	304	GLU	CD-OE2	5.84	1.32	1.25
1	B	418	GLU	CD-OE2	5.81	1.32	1.25
1	B	354	GLU	CD-OE2	5.80	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	GLU	CD-OE1	5.64	1.31	1.25
1	A	428	GLU	CD-OE2	5.64	1.31	1.25
1	B	304	GLU	CD-OE2	5.48	1.31	1.25
1	B	377	GLU	CD-OE2	5.43	1.31	1.25
1	B	379	GLU	CD-OE2	5.37	1.31	1.25
1	A	295	GLU	CD-OE2	5.33	1.31	1.25
1	B	416	GLU	CD-OE2	5.29	1.31	1.25
1	B	26	GLU	CD-OE1	5.10	1.31	1.25
1	B	168	GLU	CD-OE2	5.10	1.31	1.25
1	B	20	GLU	CD-OE1	-5.07	1.20	1.25
1	A	22	GLU	CD-OE1	-5.00	1.20	1.25

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ARG	NE-CZ-NH2	-22.48	109.06	120.30
1	B	14	ARG	NE-CZ-NH1	13.07	126.84	120.30
1	B	97	ASP	CB-CG-OD1	8.36	125.82	118.30
1	B	301	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	12	ASP	CB-CG-OD2	-8.03	111.08	118.30
1	A	200	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	A	50	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	B	12	ASP	CB-CG-OD1	7.85	125.37	118.30
1	A	119	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	50	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	226	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	B	97	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	A	12	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	301	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	B	52	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	246	ASP	CB-CG-OD1	7.47	125.03	118.30
1	B	82	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	361	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	246	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	340	ASP	CB-CG-OD1	7.24	124.82	118.30
1	A	340	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	340	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	B	135	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	A	302	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	321	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	B	340	ASP	CB-CG-OD2	-6.93	112.07	118.30
1	A	226	ASP	CB-CG-OD1	6.90	124.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	85	ASP	CB-CG-OD1	6.85	124.47	118.30
1	B	12	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	B	361	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	82	ASP	CB-CG-OD1	6.72	124.35	118.30
1	B	91	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	B	52	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	268	ASP	CB-CG-OD1	-6.71	112.26	118.30
1	A	320	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	246	ASP	N-CA-CB	6.70	122.65	110.60
1	A	280	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	85	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	85	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	A	238	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	A	301	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	B	296	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	255	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	380	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	421	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	A	246	ASP	N-CA-CB	6.37	122.07	110.60
1	A	97	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	A	14	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	302	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	A	97	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	280	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	B	119	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	B	82	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	50	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	226	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	91	ASP	CB-CG-OD1	6.08	123.77	118.30
1	B	329	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	14	ARG	CB-CA-C	-6.02	98.36	110.40
1	A	91	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	210	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	B	434	ASP	CB-CG-OD2	5.95	123.66	118.30
1	A	301	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	259	ASP	CB-CG-OD1	5.93	123.63	118.30
1	B	255	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	210	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	268	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	119	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	261	ASP	CB-CG-OD2	-5.76	113.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	261	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	A	259	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	288	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	210	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	280	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	261	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	230	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	255	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	50	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	421	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	135	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	396	LYS	N-CA-CB	5.46	120.43	110.60
1	B	27	LYS	C-N-CA	-5.39	110.98	122.30
1	B	434	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	B	226	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	302	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	70	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	238	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	B	421	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	403	SER	N-CA-CB	5.26	118.39	110.50
1	A	246	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	268	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	282	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	B	380	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	302	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	A	255	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	14	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	184	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	230	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	321	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	361	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3292	0	3300	40	0
1	B	3292	0	3300	48	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	21	0	5	1	0
3	B	21	0	5	2	0
4	A	473	0	0	3	1
4	B	469	0	0	3	0
All	All	7572	0	6610	81	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 (81) 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:128:PRO:HD2	1:A:131:LYS:HE2	1.47	0.93
1:A:127:VAL:HB	1:A:131:LYS:HE3	1.50	0.93
1:A:161:GLY:H	1:B:207:ASN:HD21	1.32	0.75
1:A:422:ASN:N	1:A:422:ASN:HD22	1.88	0.72
1:A:207:ASN:HD21	1:B:161:GLY:H	1.36	0.72
1:A:128:PRO:HD2	1:A:131:LYS:CE	2.18	0.71
1:B:274:THR:N	1:B:277:GLN:OE1	2.23	0.71
1:A:127:VAL:CB	1:A:131:LYS:HE3	2.23	0.67
1:A:42:VAL:HG11	4:A:1555:HOH:O	2.01	0.61
1:A:167:GLN:HG2	1:A:168:GLU:HG3	1.83	0.60
1:A:101:ASN:H	1:A:101:ASN:HD22	1.49	0.60
1:B:233:LYS:HG3	1:B:238:ASP:OD2	2.02	0.59
1:B:5:VAL:HG22	1:B:23:LEU:CD2	2.34	0.58
1:A:127:VAL:HB	1:A:131:LYS:CE	2.30	0.58
1:A:422:ASN:ND2	1:A:422:ASN:N	2.52	0.57
1:A:101:ASN:HD22	1:A:101:ASN:N	2.02	0.57
1:A:404:GLU:HB3	1:B:403:SER:HB2	1.87	0.56
1:B:5:VAL:HG22	1:B:23:LEU:HD21	1.88	0.55
1:A:127:VAL:CG1	1:A:131:LYS:HE3	2.37	0.55
1:B:97:ASP:O	1:B:104:LYS:HE3	2.07	0.55
1:A:373:HIS:CD2	1:A:373:HIS:H	2.24	0.55
1:B:140:LYS:HE3	1:B:142:SER:O	2.07	0.55
1:B:288:ARG:HD3	1:B:289:TYR:CE2	2.42	0.54
1:B:294:ILE:HG13	1:B:315:ILE:HD11	1.91	0.53
1:B:167:GLN:HG2	1:B:168:GLU:HG3	1.90	0.52
1:A:296:ASP:OD2	1:A:320:ASP:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ALA:H	1:B:217:ASN:ND2	2.08	0.51
1:B:97:ASP:OD2	1:B:102:LYS:HA	2.10	0.51
1:B:2:VAL:HG13	1:B:23:LEU:HD22	1.93	0.51
1:B:2:VAL:CG1	1:B:23:LEU:HD22	2.41	0.51
1:B:43:HIS:HE1	1:B:301:ASP:OD2	1.93	0.51
1:B:274:THR:HG23	1:B:277:GLN:OE1	2.11	0.50
1:B:328:LYS:HE3	4:B:1459:HOH:O	2.11	0.50
1:A:95:SER:HB2	4:A:1779:HOH:O	2.13	0.49
1:A:183:LEU:HD23	1:B:11:TYR:CE1	2.48	0.49
1:B:288:ARG:HD3	1:B:289:TYR:CZ	2.48	0.48
1:A:287:LYS:NZ	4:A:1177:HOH:O	2.46	0.48
1:B:281:LEU:O	1:B:281:LEU:HD22	2.14	0.48
1:B:373:HIS:CD2	1:B:373:HIS:H	2.30	0.48
1:B:142:SER:HA	1:B:143:PRO:HA	1.60	0.47
1:B:43:HIS:HD2	4:B:1754:HOH:O	1.97	0.47
1:A:403:SER:HB2	1:B:404:GLU:HB3	1.96	0.47
1:A:101:ASN:H	1:A:101:ASN:ND2	2.13	0.46
1:A:373:HIS:CD2	1:A:373:HIS:N	2.84	0.46
1:B:297:PRO:HD2	1:B:306:TRP:CH2	2.51	0.46
1:A:274:THR:HB	1:A:276:PRO:HD2	1.97	0.46
1:B:141:THR:HB	1:B:144:TYR:CE2	2.51	0.46
1:A:404:GLU:HB3	1:B:403:SER:CB	2.46	0.45
1:B:345:LYS:HZ1	3:B:440:PEP:C1	2.29	0.45
1:B:26:GLU:H	1:B:26:GLU:HG3	1.23	0.45
1:A:345:LYS:HZ3	3:A:441:2PG:H2	1.82	0.45
1:B:2:VAL:HG11	1:B:23:LEU:CD2	2.47	0.45
1:B:154:LEU:HB3	1:B:169:PHE:HB2	2.00	0.44
1:A:343:LEU:HD21	1:A:396:LYS:HE2	2.00	0.44
1:B:238:ASP:HB2	4:B:1576:HOH:O	2.18	0.44
1:B:373:HIS:CG	1:B:397:THR:HA	2.52	0.44
1:A:403:SER:CB	1:B:404:GLU:HB3	2.48	0.44
1:A:142:SER:HA	1:A:143:PRO:HA	1.67	0.43
1:A:155:ASN:ND2	1:A:211:GLU:H	2.15	0.43
1:B:366:GLY:O	1:B:432:HIS:HE1	2.01	0.43
1:B:56:TRP:C	1:B:57:MET:HG2	2.37	0.43
1:B:374:ARG:O	1:B:377:GLU:HG2	2.18	0.43
1:B:272:TRP:CD1	1:B:272:TRP:N	2.84	0.43
1:A:401:ALA:O	1:A:402:ARG:HB2	2.18	0.42
1:B:345:LYS:HZ1	3:B:441:2PG:C1	2.29	0.42
1:A:374:ARG:O	1:A:377:GLU:HG2	2.19	0.42
1:A:268:ASP:HB3	1:A:271:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:C	1:A:281:LEU:HD23	2.40	0.42
1:B:2:VAL:CG1	1:B:23:LEU:CD2	2.97	0.42
1:A:259:ASP:O	1:A:262:PHE:HB3	2.20	0.42
1:A:163:ALA:H	1:A:217:ASN:ND2	2.17	0.42
1:A:297:PRO:HD2	1:A:306:TRP:CH2	2.55	0.42
1:A:252:PHE:HB3	1:A:262:PHE:CD1	2.55	0.41
1:B:133:LEU:HA	1:B:133:LEU:HD23	1.86	0.41
1:A:5:VAL:HG22	1:A:23:LEU:HG	2.02	0.41
1:A:17:PRO:HG2	1:A:60:GLY:HA2	2.03	0.41
1:B:344:LEU:HD23	1:B:344:LEU:C	2.41	0.41
1:B:44:GLU:CD	1:B:348:GLN:HG2	2.41	0.40
1:B:373:HIS:CD2	1:B:373:HIS:N	2.89	0.40
1:B:296:ASP:HA	1:B:306:TRP:CH2	2.57	0.40
1:B:155:ASN:ND2	1:B:213:GLY:H	2.19	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)
4:A:1526:HOH:O	4:A:1526:HOH:O[2_555]	0.80	1.40

## 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	434/436 (100%)	424 (98%)	9 (2%)	1 (0%)	52	35
1	B	434/436 (100%)	426 (98%)	7 (2%)	1 (0%)	52	35
All	All	868/872 (100%)	850 (98%)	16 (2%)	2 (0%)	52	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	402	ARG
1	A	402	ARG

### 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	344/344 (100%)	330 (96%)	14 (4%)	37	19
1	B	344/344 (100%)	334 (97%)	10 (3%)	50	34
All	All	688/688 (100%)	664 (96%)	24 (4%)	43	25

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	101	ASN
1	A	126	ASN
1	A	152	ASN
1	A	196	LEU
1	A	217	ASN
1	A	288	ARG
1	A	311	LYS
1	A	347	ASN
1	A	357	LYS
1	A	373	HIS
1	A	392	THR
1	A	422	ASN
1	A	436	LEU
1	B	26	GLU
1	B	27	LYS
1	B	217	ASN
1	B	270	SER
1	B	281	LEU
1	B	347	ASN
1	B	373	HIS
1	B	392	THR

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Mol	Chain	Res	Type
1	B	421	ASP
1	B	436	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	101	ASN
1	A	152	ASN
1	A	155	ASN
1	A	207	ASN
1	A	217	ASN
1	A	422	ASN
1	B	43	HIS
1	B	80	ASN
1	B	126	ASN
1	B	152	ASN
1	B	155	ASN
1	B	207	ASN
1	B	217	ASN
1	B	283	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	440	3,2	5,9,9	1.23	0	8,13,13	2.53	3 (37%)
3	2PG	A	441	3,2	6,10,10	1.88	2 (33%)	5,14,14	1.09	0
3	PEP	B	440	3,2	5,9,9	1.23	0	8,13,13	2.53	3 (37%)
3	2PG	B	441	3,2	6,10,10	1.88	2 (33%)	5,14,14	1.10	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	A	440	3,2	-	0/5/9/9	0/0/0/0
3	2PG	A	441	3,2	-	0/7/11/11	0/0/0/0
3	PEP	B	440	3,2	-	0/5/9/9	0/0/0/0
3	2PG	B	441	3,2	-	0/7/11/11	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	441	2PG	P-O1P	2.73	1.68	1.60
3	B	441	2PG	P-O1P	2.73	1.68	1.60
3	A	441	2PG	C3-C2	3.28	1.59	1.52
3	B	441	2PG	C3-C2	3.30	1.59	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	440	PEP	O2-C2-C3	-4.32	115.99	124.73
3	B	440	PEP	O2-C2-C3	-4.31	116.01	124.73
3	B	440	PEP	O3P-P-O2P	2.44	116.66	107.38
3	A	440	PEP	O3P-P-O2P	2.44	116.68	107.38
3	A	440	PEP	C1-C2-C3	4.79	129.46	120.97
3	B	440	PEP	C1-C2-C3	4.81	129.49	120.97



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	441	2PG	1	0
3	B	440	PEP	1	0
3	B	441	2PG	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 was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.