



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2022 – 10:07 AM JST

PDB ID : 6LNK  
Title : Candida albicans Fructose-1,6-bisphosphate aldolase  
Authors : Huang, Y.; Cao, H.; Ren, Y.; Wan, J.  
Deposited on : 2019-12-30  
Resolution : 2.64 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.26

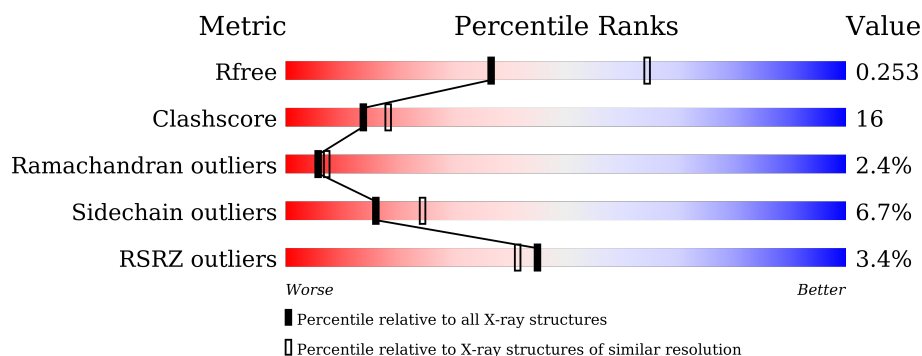
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.64 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))
$R_{free}$	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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  $\geq 3$ , 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	365	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>22%</div> <div>• • 8%</div> </div> </div>
1	B	365	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>6%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5240 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 Fructose-bisphosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2584	1651	433	491	9			
1	B	337	Total	C	N	O	S	0	0	0
			2588	1652	434	493	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	HIS	-	expression tag	UNP Q9URB4
A	360	HIS	-	expression tag	UNP Q9URB4
A	361	HIS	-	expression tag	UNP Q9URB4
A	362	HIS	-	expression tag	UNP Q9URB4
A	363	HIS	-	expression tag	UNP Q9URB4
A	364	HIS	-	expression tag	UNP Q9URB4
B	359	HIS	-	expression tag	UNP Q9URB4
B	360	HIS	-	expression tag	UNP Q9URB4
B	361	HIS	-	expression tag	UNP Q9URB4
B	362	HIS	-	expression tag	UNP Q9URB4
B	363	HIS	-	expression tag	UNP Q9URB4
B	364	HIS	-	expression tag	UNP Q9URB4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

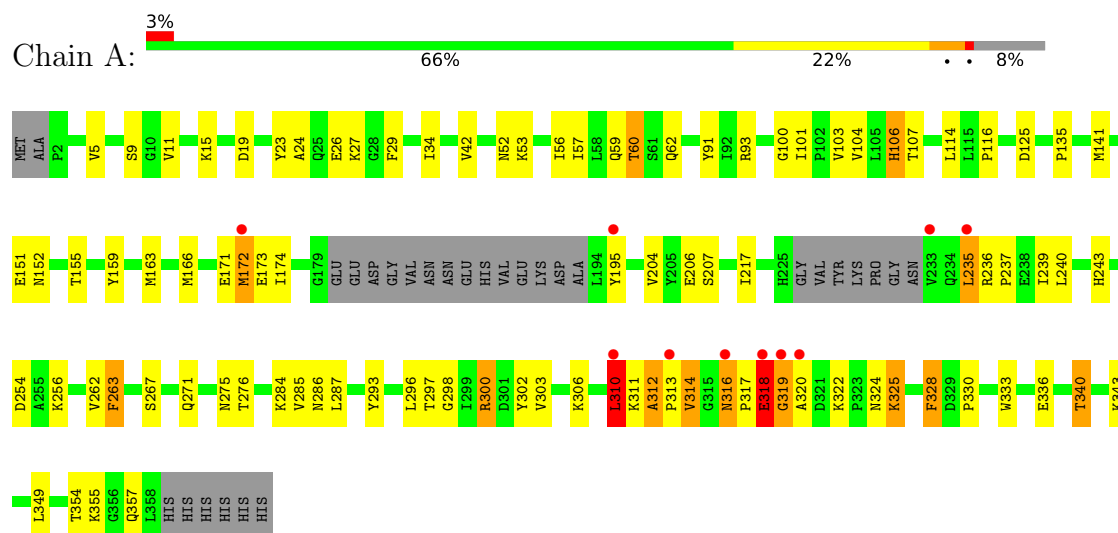
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	32	Total	O	0	0
			32	32		

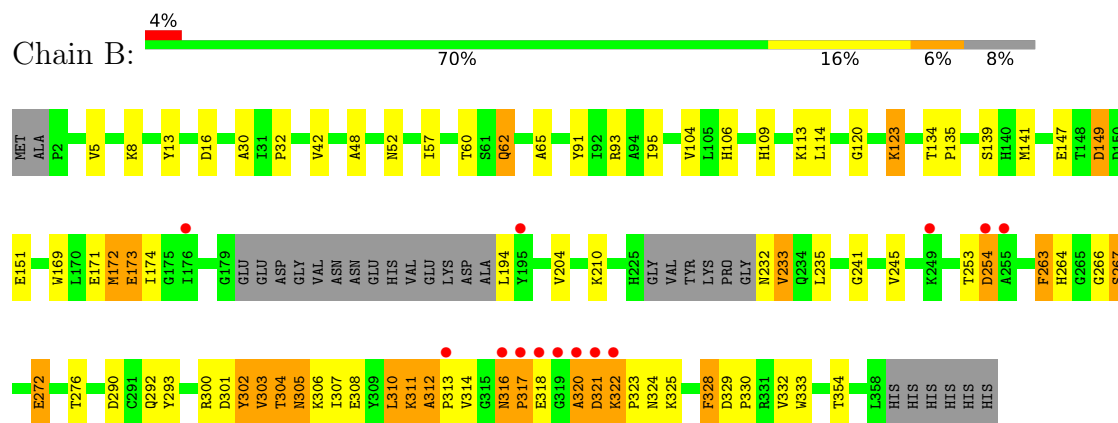
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Fructose-bisphosphate aldolase



#### • Molecule 1: Fructose-bisphosphate aldolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	160.47Å 56.76Å 82.39Å 90.00° 95.85° 90.00°	Depositor
Resolution (Å)	39.91 – 2.64 39.91 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.91-2.64) 99.7 (39.91-2.64)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.198 , 0.259 0.203 , 0.253	Depositor DCC
$R_{free}$ test set	1098 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO

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	1.15	4/2642 (0.2%)	0.77	3/3577 (0.1%)
1	B	0.76	1/2646 (0.0%)	0.69	2/3584 (0.1%)
All	All	0.97	5/5288 (0.1%)	0.73	5/7161 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	PRO	C-N	5.78	1.47	1.34
1	A	293	TYR	CE1-CZ	-5.43	1.31	1.38
1	B	173	GLU	CD-OE1	-5.36	1.19	1.25
1	A	173	GLU	CD-OE1	-5.30	1.19	1.25
1	A	195	TYR	CE1-CZ	-5.03	1.32	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	311	LYS	N-CA-C	5.79	126.62	111.00
1	A	310	LEU	CA-CB-CG	-5.59	102.45	115.30
1	B	320	ALA	N-CA-C	-5.46	96.27	111.00
1	A	319	GLY	N-CA-C	5.19	126.06	113.10
1	A	106	HIS	N-CA-CB	-5.01	101.59	110.60

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	2584	0	2551	102	0
1	B	2588	0	2546	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	6	1	0
3	B	4	0	6	0	0
4	A	26	0	0	1	0
4	B	32	0	0	0	0
All	All	5240	0	5109	163	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 16.

All (163) 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:B:316:ASN:CB	1:B:317:PRO:HD3	1.58	1.30
1:B:316:ASN:HB3	1:B:317:PRO:CD	1.50	1.30
1:A:316:ASN:HB3	1:A:317:PRO:CD	1.65	1.21
1:A:316:ASN:CB	1:A:317:PRO:HD2	1.72	1.19
1:A:316:ASN:CB	1:A:317:PRO:CD	2.21	1.18
1:B:312:ALA:H	1:B:313:PRO:HD2	1.12	1.07
1:A:316:ASN:CG	1:A:317:PRO:HD3	1.78	1.02
1:A:300:ARG:HG2	1:A:300:ARG:HH11	1.20	1.01
1:A:318:GLU:HB2	1:A:322:LYS:HG2	1.37	1.01
1:A:235:LEU:HD23	1:A:237:PRO:HD3	1.44	1.00
1:A:312:ALA:H	1:A:313:PRO:HD2	1.26	0.98
1:A:316:ASN:ND2	1:A:317:PRO:HD3	1.81	0.93
1:B:303:VAL:HG23	1:B:304:THR:H	1.37	0.90
1:A:316:ASN:HB3	1:A:317:PRO:HD2	0.91	0.90
1:A:316:ASN:CG	1:A:317:PRO:CD	2.40	0.88
1:A:336:GLU:O	1:A:340:THR:HG22	1.74	0.87
1:B:312:ALA:N	1:B:313:PRO:HD2	1.88	0.85
1:A:325:LYS:N	1:A:325:LYS:HD3	1.92	0.84
1:A:316:ASN:ND2	1:A:317:PRO:CD	2.42	0.83
1:B:300:ARG:HG2	1:B:300:ARG:HH11	1.43	0.83
1:A:317:PRO:HB2	1:A:322:LYS:HE3	1.64	0.80
1:A:172:MET:CE	1:A:204:VAL:HG11	2.12	0.79
1:A:318:GLU:HB2	1:A:322:LYS:CG	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PRO:HB2	1:A:322:LYS:CE	2.15	0.77
1:B:317:PRO:HB2	1:B:322:LYS:HG3	1.67	0.77
1:A:52:ASN:HB3	1:A:355:LYS:HG3	1.66	0.76
1:B:312:ALA:H	1:B:313:PRO:CD	1.98	0.74
1:A:300:ARG:HG2	1:A:300:ARG:NH1	1.97	0.72
1:B:149:ASP:HB3	1:B:174:ILE:HD11	1.71	0.72
1:B:172:MET:HE2	1:B:204:VAL:HG11	1.71	0.71
1:B:300:ARG:HG2	1:B:300:ARG:NH1	2.02	0.71
1:B:139:SER:HB3	1:B:169:TRP:HB3	1.75	0.68
1:A:236:ARG:HB3	1:A:239:ILE:HG13	1.76	0.67
1:A:172:MET:HE2	1:A:204:VAL:HG11	1.77	0.67
1:A:306:LYS:O	1:A:306:LYS:HG3	1.97	0.65
1:A:15:LYS:NZ	1:A:19:ASP:OD1	2.30	0.64
1:B:172:MET:CE	1:B:204:VAL:HG11	2.29	0.63
1:A:172:MET:HE1	1:A:204:VAL:HG11	1.80	0.63
1:A:325:LYS:HD3	1:A:325:LYS:H	1.63	0.63
1:B:312:ALA:N	1:B:313:PRO:CD	2.58	0.63
1:B:314:VAL:O	1:B:314:VAL:HG13	1.99	0.63
1:A:318:GLU:CB	1:A:322:LYS:HG2	2.22	0.62
1:A:312:ALA:N	1:A:313:PRO:HD2	2.06	0.62
1:B:62:GLN:HG3	1:B:114:LEU:HD13	1.80	0.62
1:A:303:VAL:HG22	1:A:303:VAL:O	2.00	0.61
1:B:316:ASN:HB3	1:B:317:PRO:HD3	0.69	0.61
1:B:32:PRO:HD3	1:B:354:THR:HG21	1.83	0.61
1:B:303:VAL:HG23	1:B:304:THR:N	2.12	0.60
1:A:9:SER:OG	1:A:100:GLY:HA2	2.01	0.60
1:A:317:PRO:CB	1:A:322:LYS:HE3	2.31	0.60
1:A:318:GLU:OE2	1:A:322:LYS:HE2	2.01	0.60
1:B:329:ASP:HB3	1:B:332:VAL:HG23	1.83	0.60
1:B:314:VAL:HG13	1:B:317:PRO:HD2	1.83	0.59
1:A:276:THR:HG22	4:A:519:HOH:O	2.03	0.58
1:A:125:ASP:HB3	1:A:166:MET:HE1	1.84	0.58
1:A:318:GLU:O	1:A:320:ALA:N	2.36	0.58
1:A:330:PRO:HD2	1:B:292:GLN:HG2	1.85	0.58
1:A:271:GLN:HG3	1:A:275:ASN:HD21	1.68	0.57
1:A:263:PHE:HB3	1:A:285:VAL:HG22	1.86	0.57
1:A:349:LEU:HD23	1:A:354:THR:HG23	1.87	0.57
1:B:303:VAL:O	1:B:305:ASN:N	2.37	0.56
1:A:312:ALA:H	1:A:313:PRO:CD	2.08	0.56
1:A:135:PRO:HB3	1:A:166:MET:HE1	1.89	0.55
1:A:59:GLN:HA	1:A:106:HIS:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:TYR:CE1	1:A:27:LYS:HG3	2.43	0.54
1:A:271:GLN:O	1:A:275:ASN:ND2	2.41	0.54
1:A:286:ASN:O	1:A:287:LEU:HD23	2.08	0.53
1:A:23:TYR:CZ	1:A:27:LYS:HG3	2.44	0.53
1:B:253:THR:OG1	1:B:254:ASP:N	2.41	0.53
1:A:317:PRO:CG	1:A:322:LYS:HE3	2.39	0.53
1:A:330:PRO:HA	1:A:333:TRP:CE2	2.43	0.53
1:A:298:GLY:H	1:A:340:THR:HG21	1.74	0.53
1:A:300:ARG:HH11	1:A:300:ARG:CG	2.07	0.53
1:B:310:LEU:O	1:B:324:ASN:ND2	2.42	0.53
1:B:8:LYS:NZ	1:B:16:ASP:OD2	2.41	0.52
1:A:159:TYR:HB3	1:A:163:MET:HE2	1.92	0.52
1:A:318:GLU:H	1:A:318:GLU:CD	2.12	0.52
1:A:317:PRO:HB2	1:A:322:LYS:HE2	1.88	0.52
1:B:300:ARG:HH11	1:B:300:ARG:CG	2.13	0.52
1:B:120:GLY:O	1:B:123:LYS:HG3	2.10	0.51
1:A:235:LEU:HD23	1:A:237:PRO:CD	2.30	0.51
1:B:263:PHE:CE2	1:B:266:GLY:HA3	2.45	0.51
1:A:325:LYS:HD2	1:A:328:PHE:CZ	2.46	0.51
1:A:317:PRO:HG2	1:A:322:LYS:HE3	1.93	0.51
1:A:314:VAL:HG12	1:A:317:PRO:O	2.12	0.50
1:A:151:GLU:O	1:A:155:THR:HG23	2.12	0.49
1:A:256:LYS:O	1:A:256:LYS:HD3	2.12	0.49
1:A:330:PRO:CD	1:B:292:GLN:HG2	2.43	0.49
1:A:328:PHE:CD1	1:A:328:PHE:C	2.86	0.49
1:A:349:LEU:HD23	1:A:354:THR:CG2	2.43	0.48
1:A:135:PRO:HB3	1:A:166:MET:CE	2.44	0.48
1:B:134:THR:HG22	1:B:135:PRO:O	2.13	0.48
1:B:267:SER:HB2	1:B:290:ASP:OD2	2.14	0.48
1:A:11:VAL:HA	1:A:103:VAL:O	2.13	0.48
1:B:60:THR:CG2	1:B:65:ALA:HB2	2.44	0.47
1:A:57:ILE:HG12	1:A:104:VAL:HB	1.97	0.47
1:A:314:VAL:HG13	1:A:316:ASN:H	1.78	0.47
1:B:241:GLY:O	1:B:245:VAL:HG12	2.14	0.47
1:A:34:ILE:HD13	1:A:56:ILE:HD11	1.97	0.47
1:A:316:ASN:HD22	1:A:317:PRO:CD	2.24	0.47
1:A:172:MET:CE	1:A:217:ILE:HG12	2.45	0.47
1:A:314:VAL:HG23	1:A:324:ASN:HD21	1.80	0.47
1:A:300:ARG:NH1	1:A:300:ARG:CG	2.72	0.47
1:B:316:ASN:CG	1:B:317:PRO:HD3	2.31	0.47
1:B:5:VAL:HG22	1:B:16:ASP:OD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ARG:O	1:B:303:VAL:HG13	2.14	0.46
1:B:139:SER:CB	1:B:169:TRP:HB3	2.44	0.46
1:B:301:ASP:C	1:B:303:VAL:H	2.18	0.46
1:B:312:ALA:HB3	1:B:313:PRO:HD3	1.96	0.46
1:B:106:HIS:ND1	1:B:139:SER:OG	2.34	0.46
1:B:173:GLU:OE2	1:B:264:HIS:CE1	2.67	0.46
1:A:314:VAL:HG13	1:A:316:ASN:N	2.31	0.46
1:B:314:VAL:CG1	1:B:317:PRO:HD2	2.45	0.46
1:B:60:THR:HG21	1:B:65:ALA:HB2	1.97	0.46
1:B:308:GLU:HG3	1:B:314:VAL:HG23	1.97	0.46
1:A:141:MET:HG3	1:A:171:GLU:HG2	1.97	0.46
1:A:316:ASN:ND2	1:A:317:PRO:HD2	2.26	0.45
1:B:91:TYR:O	1:B:95:ILE:HG22	2.16	0.45
1:B:322:LYS:HA	1:B:323:PRO:HD3	1.82	0.45
1:A:57:ILE:CD1	1:A:284:LYS:HG3	2.47	0.45
1:B:42:VAL:CG2	1:B:91:TYR:HE2	2.29	0.45
1:B:272:GLU:O	1:B:276:THR:HG23	2.17	0.45
1:B:303:VAL:O	1:B:306:LYS:N	2.50	0.45
1:A:311:LYS:HG3	1:B:293:TYR:CE2	2.51	0.45
1:A:60:THR:HG22	1:A:107:THR:HG22	1.99	0.44
1:A:152:ASN:ND2	1:A:174:ILE:HD12	2.32	0.44
1:A:262:VAL:HG13	1:A:284:LYS:HD3	1.98	0.44
1:A:24:ALA:HA	1:A:29:PHE:CE1	2.53	0.43
1:B:147:GLU:HB3	1:B:151:GLU:OE1	2.18	0.43
1:A:303:VAL:O	1:A:303:VAL:HG13	2.18	0.43
1:A:328:PHE:C	1:A:328:PHE:HD1	2.21	0.43
1:B:141:MET:HE2	1:B:171:GLU:OE2	2.19	0.43
1:A:240:LEU:HA	1:A:243:HIS:CD2	2.53	0.43
1:A:91:TYR:HB2	1:B:91:TYR:HB2	2.01	0.43
1:A:318:GLU:CD	1:A:318:GLU:N	2.71	0.43
1:B:48:ALA:O	1:B:52:ASN:ND2	2.51	0.43
1:A:29:PHE:CE1	1:A:357:GLN:HG2	2.53	0.43
1:A:310:LEU:HD13	1:A:310:LEU:HA	1.46	0.43
1:A:318:GLU:HB2	1:A:322:LYS:CD	2.48	0.42
1:A:325:LYS:HA	1:A:328:PHE:CZ	2.55	0.42
1:A:9:SER:HA	1:A:101:ILE:O	2.19	0.42
1:B:307:ILE:HD13	1:B:307:ILE:HA	1.98	0.42
1:A:62:GLN:HG3	1:A:114:LEU:HD13	2.02	0.42
1:A:296:LEU:HD22	1:B:328:PHE:HB2	2.01	0.41
1:A:5:VAL:HG21	1:A:19:ASP:HB2	2.00	0.41
1:A:24:ALA:HB1	1:A:29:PHE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLY:O	1:B:123:LYS:HE3	2.21	0.41
1:A:56:ILE:HG13	1:A:57:ILE:N	2.36	0.41
1:B:13:TYR:OH	1:B:93:ARG:HD2	2.20	0.41
1:B:310:LEU:HD13	1:B:310:LEU:HA	1.67	0.41
1:A:57:ILE:HD13	1:A:284:LYS:HG3	2.03	0.41
1:B:42:VAL:HG22	1:B:91:TYR:HE2	1.86	0.41
1:A:297:THR:HG22	1:A:300:ARG:NH2	2.35	0.41
1:A:42:VAL:CG2	1:A:91:TYR:HE2	2.33	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.69	0.41
1:B:232:ASN:HB3	1:B:233:VAL:H	1.63	0.41
1:A:262:VAL:HG13	1:A:284:LYS:HB3	2.02	0.41
1:A:325:LYS:HD2	1:A:328:PHE:HZ	1.86	0.41
1:B:30:ALA:O	1:B:354:THR:HB	2.21	0.41
1:B:57:ILE:HG12	1:B:104:VAL:HB	2.03	0.40
1:A:254:ASP:N	1:A:254:ASP:OD2	2.55	0.40
1:A:93:ARG:HD3	3:A:402:EDO:O2	2.21	0.40
1:B:330:PRO:HA	1:B:333:TRP:CE2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/365 (90%)	306 (93%)	18 (6%)	6 (2%)	8	11
1	B	331/365 (91%)	310 (94%)	11 (3%)	10 (3%)	4	5
All	All	661/730 (90%)	616 (93%)	29 (4%)	16 (2%)	6	7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ASN

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Mol	Chain	Res	Type
1	A	319	GLY
1	B	304	THR
1	B	311	LYS
1	B	312	ALA
1	B	316	ASN
1	B	317	PRO
1	A	302	TYR
1	B	303	VAL
1	A	267	SER
1	B	109	HIS
1	A	312	ALA
1	A	318	GLU
1	B	320	ALA
1	B	321	ASP
1	B	302	TYR

### 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	270/295 (92%)	254 (94%)	16 (6%)	19	30
1	B	270/295 (92%)	250 (93%)	20 (7%)	13	21
All	All	540/590 (92%)	504 (93%)	36 (7%)	16	24

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	53	LYS
1	A	60	THR
1	A	172	MET
1	A	206	GLU
1	A	207	SER
1	A	235	LEU
1	A	263	PHE

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Mol	Chain	Res	Type
1	A	300	ARG
1	A	310	LEU
1	A	314	VAL
1	A	318	GLU
1	A	325	LYS
1	A	328	PHE
1	A	340	THR
1	A	343	LYS
1	B	62	GLN
1	B	113	LYS
1	B	123	LYS
1	B	149	ASP
1	B	172	MET
1	B	210	LYS
1	B	233	VAL
1	B	235	LEU
1	B	254	ASP
1	B	263	PHE
1	B	267	SER
1	B	272	GLU
1	B	302	TYR
1	B	305	ASN
1	B	310	LEU
1	B	318	GLU
1	B	321	ASP
1	B	322	LYS
1	B	325	LYS
1	B	328	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	271	GLN
1	A	275	ASN
1	A	316	ASN
1	A	324	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	EDO	A	402	-	3,3,3	0.47	0	2,2,2	0.52	0
3	EDO	B	402	-	3,3,3	0.53	0	2,2,2	0.41	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	EDO	A	402	-	-	0/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	EDO	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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	336/365 (92%)	0.10	10 (2%) 50 46	34, 57, 83, 100	0
1	B	337/365 (92%)	0.12	13 (3%) 39 36	38, 59, 83, 106	0
All	All	673/730 (92%)	0.11	23 (3%) 45 41	34, 58, 83, 106	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	321	ASP	4.9
1	A	313	PRO	4.6
1	B	322	LYS	4.2
1	B	317	PRO	4.0
1	B	313	PRO	4.0
1	B	316	ASN	3.9
1	A	320	ALA	3.8
1	A	318	GLU	3.5
1	B	319	GLY	3.3
1	B	318	GLU	3.2
1	A	319	GLY	3.2
1	B	254	ASP	3.2
1	A	316	ASN	3.2
1	B	320	ALA	3.2
1	A	172	MET	3.0
1	A	233	VAL	2.7
1	A	235	LEU	2.7
1	B	249	LYS	2.5
1	A	195	TYR	2.2
1	B	195	TYR	2.1
1	B	255	ALA	2.1
1	A	310	LEU	2.1
1	B	176	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> 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
3	EDO	A	402	4/4	0.94	0.18	45,47,48,50	0
3	EDO	B	402	4/4	0.95	0.20	45,46,47,47	0
2	ZN	A	401	1/1	0.97	0.08	69,69,69,69	0
2	ZN	B	401	1/1	0.99	0.11	63,63,63,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.