



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 PM UTC

PDB ID : 6LNK / pdb_00006lnk
Title : Candida albicans Fructose-1,6-bisphosphate aldolase
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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

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
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

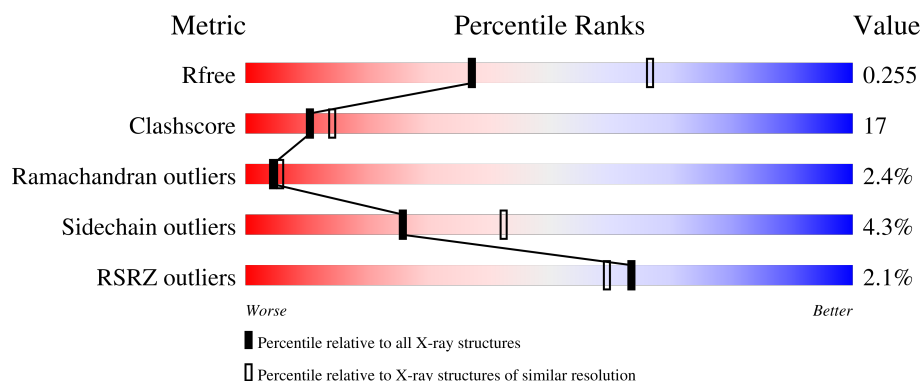
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (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 ≥ 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	2% 58% 27% 7% 8%
1	B	365	% 66% 22% •• 8%

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 (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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		

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.

Chain A:

2% 58% 27% 7% 8%

MET ALA P2 V5 S9 G10 V11 K15 D19 Y23 A24 K27 G28 F29 I34 V42 A49 R50 D51 N52 K53 A54 I56 I57 Q59 T60 S61 Q62 A65 S81 I82 S85 Y91 I92 R93 G100 I101 F102 V103 I104 A105 H106 T107 D108

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.198 , 0.259 0.206 , 0.255	Depositor DCC
R_{free} test set	1098 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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: EDO, ZN

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	1.57	51/2642 (1.9%)	0.96	10/3577 (0.3%)
1	B	0.94	10/2646 (0.4%)	0.83	19/3584 (0.5%)
All	All	1.29	61/5288 (1.2%)	0.90	29/7161 (0.4%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	PRO	C-N	10.24	1.47	1.33
1	A	82	ILE	C-O	-9.11	1.14	1.24
1	A	115	LEU	C-O	-7.59	1.17	1.24
1	A	65	ALA	C-O	-7.36	1.15	1.24
1	A	174	ILE	N-CA	-7.25	1.37	1.46
1	A	284	LYS	C-O	-6.82	1.16	1.23
1	A	171	GLU	C-N	6.59	1.43	1.33
1	B	35	ASN	C-O	-6.58	1.15	1.23
1	B	117	TRP	C-O	-6.52	1.16	1.24
1	A	117	TRP	C-O	-6.51	1.16	1.24
1	A	54	ALA	C-O	-6.50	1.17	1.24
1	A	217	ILE	C-O	-6.48	1.17	1.24
1	A	85	SER	C-O	-6.37	1.16	1.24
1	A	170	LEU	C-O	-6.37	1.16	1.24
1	A	49	ALA	C-O	-6.36	1.16	1.24
1	A	152	ASN	C-O	-6.20	1.17	1.24
1	B	287	LEU	C-O	-6.16	1.17	1.24
1	A	107	THR	C-O	-6.05	1.16	1.23
1	A	262	VAL	C-O	-6.00	1.17	1.24
1	A	141	MET	C-O	-6.00	1.16	1.24
1	A	205	TYR	C-O	-5.90	1.17	1.24
1	A	140	HIS	C-O	-5.83	1.16	1.23
1	A	81	SER	C-O	-5.82	1.16	1.24
1	A	174	ILE	C-O	-5.79	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	ALA	C-O	-5.78	1.17	1.24
1	A	325	LYS	C-O	-5.73	1.17	1.24
1	A	246	TYR	C-O	-5.71	1.17	1.24
1	A	106	HIS	C-O	-5.71	1.16	1.23
1	A	304	THR	N-CA	-5.68	1.38	1.46
1	A	60	THR	C-O	-5.66	1.17	1.24
1	B	313	PRO	C-O	-5.64	1.19	1.24
1	A	302	TYR	C-O	-5.58	1.17	1.24
1	A	114	LEU	C-O	-5.55	1.16	1.24
1	A	207	SER	C-O	-5.53	1.17	1.24
1	A	121	MET	C-O	-5.53	1.17	1.24
1	B	289	THR	C-O	-5.52	1.17	1.24
1	B	243	HIS	C-O	-5.49	1.17	1.24
1	A	142	LEU	C-O	-5.47	1.17	1.24
1	A	342	SER	C-O	-5.45	1.17	1.24
1	A	264	HIS	C-O	-5.45	1.17	1.23
1	A	201	VAL	C-O	-5.42	1.17	1.24
1	A	341	MET	C-O	-5.41	1.17	1.24
1	A	249	LYS	C-O	-5.34	1.18	1.24
1	B	308	GLU	C-O	-5.33	1.17	1.24
1	A	207	SER	CA-C	-5.31	1.45	1.52
1	A	309	TYR	C-O	-5.29	1.17	1.24
1	A	348	ALA	C-O	-5.28	1.18	1.24
1	A	297	THR	C-O	-5.28	1.18	1.24
1	A	250	GLN	CA-C	-5.26	1.46	1.52
1	A	120	GLY	C-O	-5.25	1.17	1.23
1	A	153	ILE	C-O	-5.25	1.17	1.24
1	A	350	ASP	CA-C	-5.25	1.46	1.52
1	A	111	ALA	C-O	-5.24	1.17	1.23
1	A	108	ASP	C-O	-5.18	1.17	1.23
1	B	286	ASN	C-O	-5.18	1.17	1.23
1	A	144	LEU	C-O	-5.16	1.15	1.23
1	B	288	ASP	C-O	-5.11	1.17	1.24
1	A	116	PRO	C-O	-5.09	1.17	1.24
1	A	216	SER	C-O	-5.09	1.17	1.23
1	A	51	ASP	C-O	-5.05	1.17	1.24
1	B	322	LYS	C-O	-5.02	1.17	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	THR	N-CA-C	-9.39	101.95	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	LYS	N-CA-C	8.59	120.26	111.07
1	A	100	GLY	N-CA-C	7.48	124.40	113.48
1	B	311	LYS	N-CA-C	7.43	126.62	110.80
1	B	149	ASP	N-CA-C	7.38	121.38	112.38
1	B	324	ASN	N-CA-C	7.18	122.93	113.30
1	B	320	ALA	N-CA-C	-6.82	96.27	110.80
1	A	290	ASP	N-CA-C	-6.71	103.58	111.03
1	A	54	ALA	N-CA-C	6.58	115.88	108.25
1	B	322	LYS	CA-C-N	6.53	128.00	119.84
1	B	322	LYS	C-N-CA	6.53	128.00	119.84
1	B	289	THR	N-CA-C	6.47	119.16	111.71
1	A	156	CYS	N-CA-C	-6.28	104.35	111.14
1	B	224	VAL	N-CA-C	6.03	117.52	109.37
1	A	303	VAL	CB-CA-C	-5.98	105.31	112.19
1	B	314	VAL	N-CA-C	5.93	116.40	107.80
1	B	197	SER	CA-C-N	5.88	127.19	119.84
1	B	197	SER	C-N-CA	5.88	127.19	119.84
1	A	106	HIS	N-CA-CB	-5.81	101.59	111.69
1	A	302	TYR	N-CA-C	-5.80	98.44	110.80
1	B	233	VAL	CB-CA-C	-5.62	103.94	110.91
1	B	312	ALA	CA-C-N	5.47	127.90	120.79
1	B	312	ALA	C-N-CA	5.47	127.90	120.79
1	B	324	ASN	CB-CA-C	-5.45	100.95	110.17
1	A	319	GLY	N-CA-C	5.44	126.06	113.18
1	B	150	ASP	N-CA-C	-5.22	106.76	113.23
1	B	108	ASP	CA-C-N	5.07	131.22	121.54
1	B	108	ASP	C-N-CA	5.07	131.22	121.54
1	B	319	GLY	N-CA-C	5.04	125.12	113.18

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	2584	0	2551	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2588	0	2546	72	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	173	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 17.

All (173) 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	1.07
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:B:172:MET:HE2	1:B:204:VAL:HG11	1.47	0.96
1:A:172:MET:HE2	1:A:204:VAL:HG11	1.47	0.96
1:A:316:ASN:CG	1:A:317:PRO:CD	2.40	0.94
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: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:125:ASP:HB3	1:A:166:MET:HE1	1.64	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:135:PRO:HB3	1:A:166:MET:HE2	1.67	0.76
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:129:PHE:HB2	1:A:166:MET:HE3	1.68	0.73
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:A:163:MET:HE1	1:A:170:LEU:HD13	1.72	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: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: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:B:291:CYS:HB3	1:B:341:MET:HE3	1.81	0.62
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:172:MET:HE1	1:B:217:ILE:HG23	1.85	0.59
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: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:B:172:MET:CE	1:B:204:VAL:HG11	2.29	0.57
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:A:318:GLU:H	1:A:318:GLU:CD	2.12	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:TYR:HB3	1:B:163:MET:HE3	1.88	0.55
1:A:59:GLN:HA	1:A:106:HIS:O	2.07	0.54
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:328:PHE:CD1	1:A:328:PHE:C	2.86	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: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:A:172:MET:HE2	1:A:204:VAL:CG1	2.30	0.52
1:B:120:GLY:O	1:B:123:LYS:HG3	2.10	0.51
1:B:316:ASN:CG	1:B:317:PRO:HD3	2.31	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:B:301:ASP:C	1:B:303:VAL:H	2.18	0.51
1:A:325:LYS:HD2	1:A:328:PHE:CZ	2.46	0.51
1:B:163:MET:HE1	1:B:170:LEU:HD13	1.93	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:349:LEU:HD23	1:A:354:THR:CG2	2.43	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:A:318:GLU:CD	1:A:318:GLU:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:PHE:C	1:A:328:PHE:HD1	2.21	0.47
1:A:300:ARG:NH1	1:A:300:ARG:CG	2.72	0.47
1:B:5:VAL:HG22	1:B:16:ASP:OD1	2.14	0.46
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: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:135:PRO:HB3	1:A:166:MET:CE	2.44	0.46
1:A:141:MET:HG3	1:A:171:GLU:HG2	1.97	0.46
1:A:129:PHE:CB	1:A:166:MET:HE3	2.44	0.45
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:B:8:LYS:NZ	1:B:16:ASP:OD2	2.41	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:B:141:MET:HE2	1:B:171:GLU:OE2	2.17	0.44
1:A:24:ALA:HA	1:A:29:PHE:CE1	2.53	0.43
1:B:328:PHE:C	1:B:328:PHE:CD1	2.96	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: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:172:MET:HE3	1:A:172:MET:HB3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ASN:CG	1:A:317:PRO:HD2	2.25	0.42
1:B:307:ILE:HD13	1:B:307:ILE:HA	1.98	0.42
1:A:159:TYR:HB3	1:A:163:MET:HE2	2.01	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
1:B:172:MET:HE3	1:B:172:MET:HB3	1.73	0.41
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: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 [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	330/365 (90%)	306 (93%)	18 (6%)	6 (2%)	6 9

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

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
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 ⓘ

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%)	255 (94%)	15 (6%)	19	31
1	B	270/295 (92%)	262 (97%)	8 (3%)	36	56
All	All	540/590 (92%)	517 (96%)	23 (4%)	26	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	60	THR
1	A	174	ILE
1	A	206	GLU
1	A	207	SER
1	A	300	ARG
1	A	306	LYS
1	A	310	LEU
1	A	311	LYS
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	149	ASP
1	B	233	VAL
1	B	289	THR
1	B	308	GLU
1	B	310	LEU
1	B	318	GLU
1	B	321	ASP
1	B	322	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	HIS
1	A	243	HIS
1	A	271	GLN
1	A	275	ASN
1	A	324	ASN
1	B	214	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 oligosaccharides 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	B	402	-	3,3,3	0.50	0	2,2,2	0.45	0
3	EDO	A	402	-	3,3,3	0.45	0	2,2,2	0.55	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	B	402	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	336/365 (92%)	-0.03	9 (2%) 56 51	34, 57, 83, 100	0
1	B	337/365 (92%)	0.05	5 (1%) 72 69	38, 59, 83, 106	0
All	All	673/730 (92%)	0.01	14 (2%) 63 59	34, 58, 83, 106	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	VAL	3.9
1	A	310	LEU	3.7
1	A	312	ALA	3.3
1	A	316	ASN	3.2
1	A	313	PRO	3.1
1	A	172	MET	2.8
1	A	320	ALA	2.8
1	B	179	GLY	2.4
1	B	320	ALA	2.2
1	B	313	PRO	2.2
1	A	315	GLY	2.2
1	B	310	LEU	2.1
1	B	309	TYR	2.0
1	A	266	GLY	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 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
3	EDO	B	402	4/4	0.92	0.11	45,46,47,47	0
3	EDO	A	402	4/4	0.93	0.08	45,47,48,50	0
2	ZN	A	401	1/1	0.97	0.06	69,69,69,69	0
2	ZN	B	401	1/1	1.00	0.01	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.