



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 PM UTC

PDB ID : 1XYA / pdb_00001xya
Title : X-RAY CRYSTALLOGRAPHIC STRUCTURES OF D-XYLOSE ISOMERASE-SUBSTRATE COMPLEXES POSITION THE SUBSTRATE AND PROVIDE EVIDENCE FOR METAL MOVEMENT DURING CATALYSIS
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Deposited on : 1994-01-03
Resolution : 1.81 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

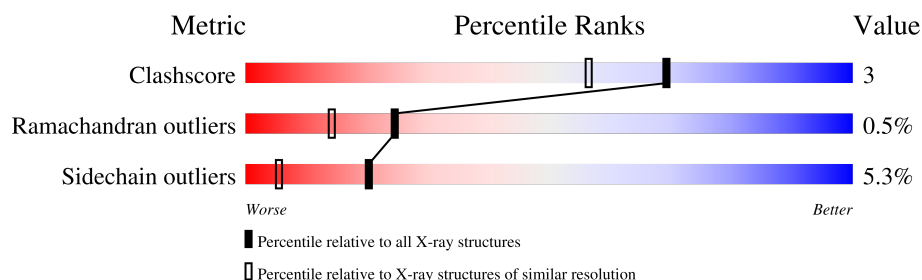
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	
1	B	386	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6550 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.

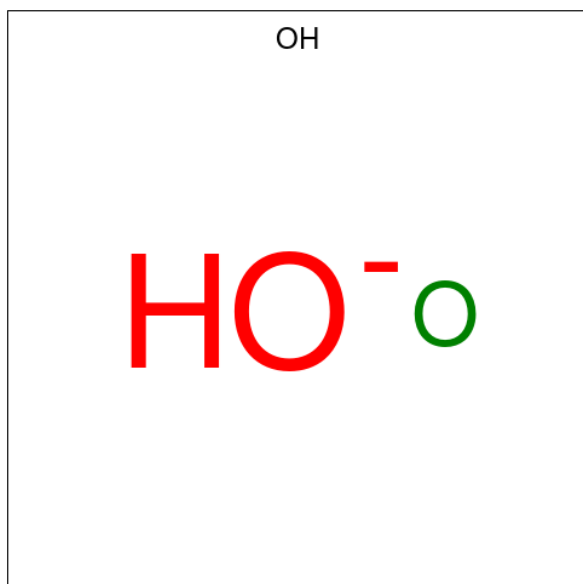
- Molecule 1 is a protein called XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3024	1904	540	572	8			
1	B	386	Total	C	N	O	S	0	0	0
			3024	1904	540	572	8			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total 235	O 235	0	0
4	B	261	Total 261	O 261	0	0

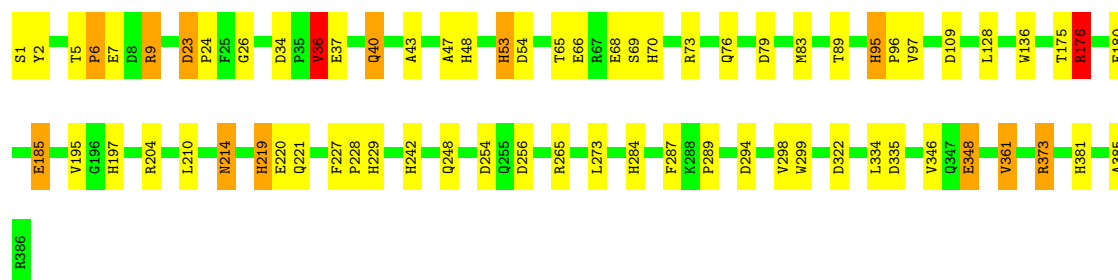
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

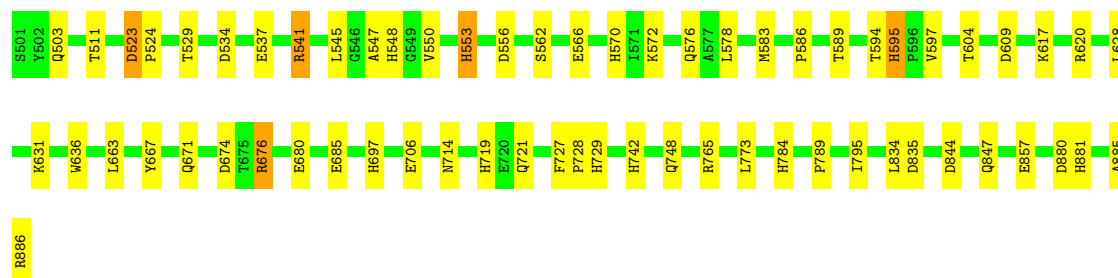
• Molecule 1: XYLOSE ISOMERASE

Chain A: 



• Molecule 1: XYLOSE ISOMERASE

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.60Å 99.34Å 94.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.81	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.81)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.161 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6550	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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: MG, OH

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	1.03	15/3096 (0.5%)	1.55	36/4197 (0.9%)
1	B	1.02	14/3096 (0.5%)	1.53	22/4197 (0.5%)
All	All	1.03	29/6192 (0.5%)	1.54	58/8394 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	HIS	CD2-NE2	-7.43	1.29	1.37
1	B	595	HIS	CD2-NE2	-7.09	1.30	1.37
1	A	95	HIS	CD2-NE2	-7.03	1.30	1.37
1	B	570	HIS	CD2-NE2	-6.73	1.30	1.37
1	B	553	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	70	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	197	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	284	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	881	HIS	CD2-NE2	-6.43	1.30	1.37
1	B	742	HIS	CD2-NE2	-6.27	1.30	1.37
1	B	719	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	697	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	242	HIS	CD2-NE2	-6.10	1.31	1.37
1	B	548	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	229	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	53	HIS	CD2-NE2	-5.72	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	729	HIS	CD2-NE2	-5.59	1.31	1.37
1	B	784	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	219	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	381	HIS	CD2-NE2	-5.49	1.31	1.37
1	B	729	HIS	CG-ND1	-5.46	1.32	1.38
1	B	719	HIS	CG-ND1	-5.44	1.32	1.38
1	A	219	HIS	CG-ND1	-5.41	1.32	1.38
1	A	284	HIS	CG-ND1	-5.41	1.32	1.38
1	B	604	THR	CA-CB	5.34	1.60	1.53
1	A	95	HIS	CG-ND1	-5.28	1.32	1.38
1	A	229	HIS	CG-ND1	-5.12	1.32	1.38
1	B	548	HIS	CG-ND1	-5.11	1.32	1.38
1	A	36	VAL	CA-CB	5.05	1.60	1.54

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ASP	CA-CB-CG	9.42	122.02	112.60
1	B	609	ASP	CA-CB-CG	8.31	120.91	112.60
1	B	523	ASP	CA-CB-CG	7.92	120.52	112.60
1	B	534	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	23	ASP	CA-CB-CG	7.71	120.31	112.60
1	A	335	ASP	CA-CB-CG	7.33	119.93	112.60
1	B	674	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	881	HIS	CB-CG-CD2	-6.95	122.16	131.20
1	B	835	ASP	CA-CB-CG	6.83	119.43	112.60
1	B	765	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	A	70	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	109	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	9	ARG	CA-CB-CG	6.51	127.11	114.10
1	A	294	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	322	ASP	CA-CB-CG	6.28	118.88	112.60
1	A	66	GLU	N-CA-CB	6.26	119.98	110.28
1	A	175	THR	N-CA-C	6.24	118.35	110.24
1	A	175	THR	N-CA-CB	-6.13	100.11	109.92
1	B	885	ALA	CA-C-N	6.06	132.60	121.70
1	B	885	ALA	C-N-CA	6.06	132.60	121.70
1	A	66	GLU	CB-CA-C	-6.05	99.05	110.67
1	A	5	THR	CA-C-N	5.98	127.31	119.84
1	A	5	THR	C-N-CA	5.98	127.31	119.84
1	A	34	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	53	HIS	N-CA-C	-5.97	100.82	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	A	346	VAL	N-CA-C	5.89	116.63	110.62
1	A	373	ARG	O-C-N	-5.86	115.91	122.12
1	B	789	PRO	CA-C-N	5.82	125.83	119.90
1	B	789	PRO	C-N-CA	5.82	125.83	119.90
1	B	556	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	385	ALA	CA-C-N	5.72	131.99	121.70
1	A	385	ALA	C-N-CA	5.72	131.99	121.70
1	B	548	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	B	844	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	595	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	B	570	HIS	CB-CG-CD2	-5.46	124.10	131.20
1	A	176	ARG	CD-NE-CZ	5.42	131.99	124.40
1	B	553	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	A	53	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	B	795	ILE	O-C-N	-5.36	116.46	121.87
1	A	299	TRP	CG-CD2-CE3	5.32	139.22	133.90
1	A	214	ASN	CA-C-N	5.27	125.17	119.85
1	A	214	ASN	C-N-CA	5.27	125.17	119.85
1	A	348	GLU	CB-CG-CD	5.27	121.56	112.60
1	B	881	HIS	CB-CG-ND1	5.21	130.51	122.70
1	A	373	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	48	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	322	ASP	CA-C-N	5.15	125.19	119.32
1	A	322	ASP	C-N-CA	5.15	125.19	119.32
1	B	636	TRP	CG-CD2-CE3	5.14	139.04	133.90
1	B	742	HIS	CB-CG-CD2	-5.13	124.53	131.20
1	B	617	LYS	CG-CD-CE	5.13	123.09	111.30
1	A	54	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	242	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	A	40	GLN	CB-CA-C	-5.08	102.91	110.88
1	A	361	VAL	N-CA-CB	-5.06	102.99	110.58
1	A	381	HIS	CA-CB-CG	-5.03	108.77	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	373	ARG	Mainchain

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	3024	0	2909	25	0
1	B	3024	0	2906	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	235	0	0	5	0
4	B	261	0	0	1	0
All	All	6550	0	5815	41	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 3.

All (41) 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:136:TRP:CD1	4:A:1423:HOH:O	2.20	0.93
1:A:176:ARG:HH11	1:A:176:ARG:HB2	1.52	0.74
1:A:136:TRP:NE1	4:A:1423:HOH:O	2.17	0.72
1:A:219:HIS:HE1	4:A:1423:HOH:O	1.72	0.70
1:B:537:GLU:HB2	1:B:541:ARG:NH2	2.07	0.69
1:B:595:HIS:HD2	1:B:597:VAL:H	1.42	0.67
1:A:95:HIS:HD2	1:A:97:VAL:H	1.45	0.62
1:B:680:GLU:HG3	1:B:714:ASN:O	2.02	0.60
1:B:523:ASP:HB2	1:B:524:PRO:HD2	1.85	0.58
1:B:583:MET:HA	1:B:583:MET:HE2	1.84	0.58
1:B:550:VAL:HG13	4:B:1365:HOH:O	2.04	0.56
1:A:24:PRO:HD3	1:B:524:PRO:HD3	1.89	0.55
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.73	0.53
1:B:547:ALA:O	1:B:583:MET:HE1	2.09	0.53
1:A:180:GLU:HG3	1:A:214:ASN:O	2.09	0.53
1:A:219:HIS:CE1	4:A:1423:HOH:O	2.53	0.53
1:A:96:PRO:HB3	1:B:529:THR:HG22	1.91	0.52
1:A:256:ASP:HB3	1:A:287:PHE:HA	1.93	0.51
1:B:721:GLN:HE21	1:B:748:GLN:HB3	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.91	0.51
1:A:43:ALA:N	1:A:83:MET:HE2	2.25	0.50
1:B:595:HIS:CD2	1:B:597:VAL:H	2.26	0.49
1:B:880:ASP:HB3	1:B:886:ARG:HG2	1.93	0.49
1:A:289:PRO:HG2	1:A:298:VAL:HG13	1.96	0.47
1:A:95:HIS:CD2	1:A:97:VAL:H	2.29	0.47
1:B:676:ARG:HB3	1:B:676:ARG:HH11	1.79	0.47
1:B:727:PHE:HB3	1:B:728:PRO:HD3	1.96	0.47
1:A:36:VAL:O	1:A:40:GLN:HG2	2.15	0.46
1:B:511:THR:HG21	1:B:586:PRO:HG2	1.96	0.46
1:B:562:SER:HB3	1:B:566:GLU:HB2	1.98	0.45
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.52	0.45
1:B:667:TYR:O	1:B:671:GLN:HG2	2.17	0.45
1:A:185:GLU:OE1	1:A:254:ASP:HB3	2.17	0.44
1:A:265:ARG:HG3	4:A:1064:HOH:O	2.17	0.44
1:B:553:HIS:CD2	1:B:589:THR:HG23	2.54	0.43
1:A:73:ARG:O	1:A:76:GLN:HB3	2.19	0.43
1:A:26:GLY:HA2	1:B:594:THR:HA	2.00	0.42
1:A:69:SER:O	1:A:73:ARG:HG3	2.19	0.42
1:A:227:PHE:HB3	1:A:228:PRO:HD3	2.01	0.41
1:A:47:ALA:HB3	1:A:83:MET:HE1	2.03	0.41
1:A:195:VAL:HG23	1:A:220:GLU:CD	2.46	0.41

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	384/386 (100%)	371 (97%)	10 (3%)	3 (1%)	16	6
1	B	384/386 (100%)	368 (96%)	15 (4%)	1 (0%)	36	26
All	All	768/772 (100%)	739 (96%)	25 (3%)	4 (0%)	24	14

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	685	GLU
1	A	2	TYR
1	A	6	PRO

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	302/302 (100%)	286 (95%)	16 (5%)	20	5
1	B	302/302 (100%)	286 (95%)	16 (5%)	20	5
All	All	604/604 (100%)	572 (95%)	32 (5%)	20	5

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	6	PRO
1	A	7	GLU
1	A	9	ARG
1	A	36	VAL
1	A	37	GLU
1	A	65	THR
1	A	68	GLU
1	A	128	LEU
1	A	176	ARG
1	A	204	ARG
1	A	210	LEU
1	A	273	LEU
1	A	334	LEU
1	A	348	GLU
1	A	361	VAL
1	B	503	GLN
1	B	541	ARG
1	B	545	LEU

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Mol	Chain	Res	Type
1	B	572	LYS
1	B	576	GLN
1	B	578	LEU
1	B	620	ARG
1	B	628	LEU
1	B	631	LYS
1	B	663	LEU
1	B	676	ARG
1	B	706	GLU
1	B	773	LEU
1	B	834	LEU
1	B	847	GLN
1	B	857	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	221	GLN
1	A	308	ASN
1	A	326	GLN
1	B	548	HIS
1	B	595	HIS
1	B	721	GLN
1	B	808	ASN
1	B	847	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.