



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:58 pm BST

PDB ID : 1XYL
Title : THE ROLE OF THE DIVALENT METAL ION IN SUGAR BINDING,
RING OPENING, AND ISOMERIZATION BY D-XYLOSE ISOMERASE:
REPLACEMENT OF A CATALYTIC METAL BY AN AMINO-ACID
Authors : Allen, K.N.; Lavie, A.; Petsko, G.A.; Ringe, D.
Deposited on : 1993-12-07
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

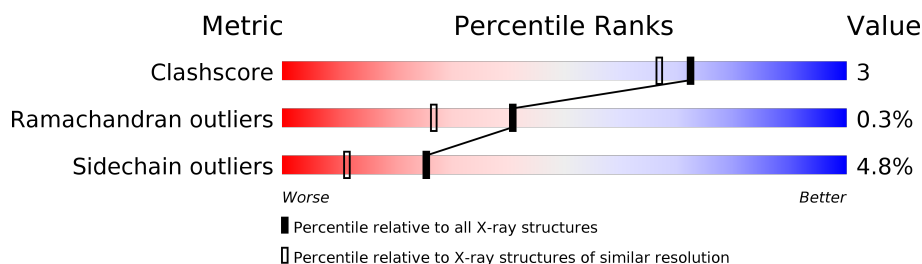
1 Overall quality at a glance

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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 ≥ 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

There are 4 unique types of molecules in this entry. The entry contains 8826 atoms, of which 2298 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	H	N	O	S	0	0	0
			3696	1905	672	541	570	8			
1	B	386	Total	C	H	N	O	S	0	0	0
			3696	1905	672	541	570	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	LYS	GLU	CONFLICT	UNP P15587
B	680	LYS	GLU	CONFLICT	UNP P15587

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

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

- Molecule 3 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

- Molecule 4 is water.

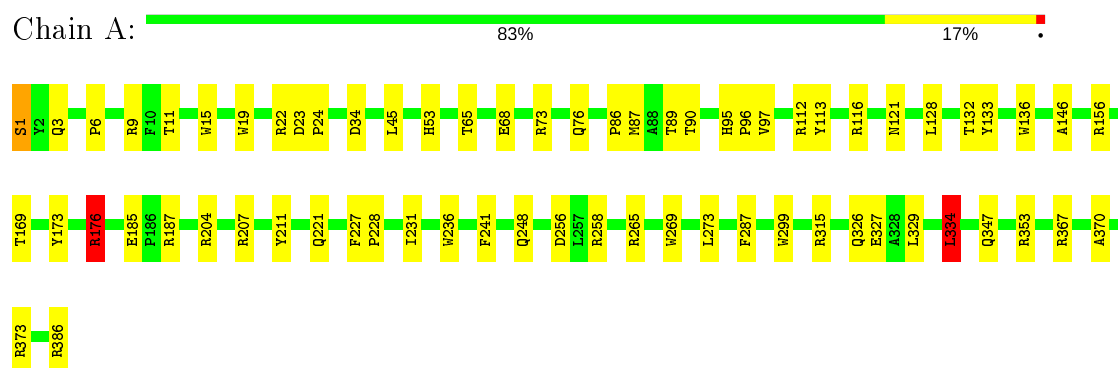
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	238	Total	H	O	0	0
			714	476	238		
4	B	238	Total	H	O	0	0
			714	476	238		

3 Residue-property plots [i](#)

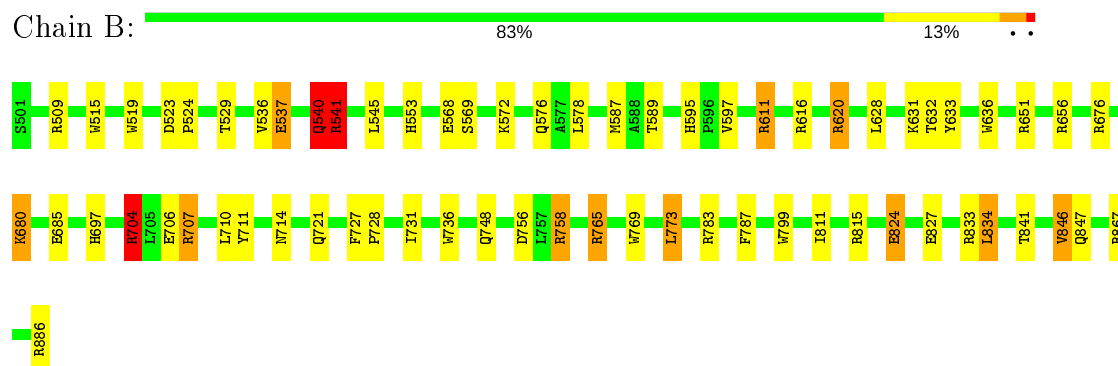
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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



• Molecule 1: XYLOSE ISOMERASE



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	87.72Å 99.49Å 94.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8826	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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, 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	0.81	0/3096	1.48	50/4196 (1.2%)
1	B	0.80	0/3096	1.46	47/4196 (1.1%)
All	All	0.81	0/6192	1.47	97/8392 (1.2%)

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	B	0	1

There are no bond length outliers.

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ARG	NE-CZ-NH2	-15.07	112.77	120.30
1	B	765	ARG	NE-CZ-NH1	14.74	127.67	120.30
1	A	265	ARG	NE-CZ-NH1	13.83	127.21	120.30
1	B	765	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	A	176	ARG	NE-CZ-NH1	11.33	125.96	120.30
1	B	616	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	758	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	B	707	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	A	258	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	B	704	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	A	9	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	211	TYR	CB-CG-CD1	-8.19	116.09	121.00
1	A	299	TRP	CD1-CG-CD2	8.06	112.75	106.30
1	B	651	ARG	NE-CZ-NH2	-8.01	116.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	846	VAL	CG1-CB-CG2	-7.90	98.27	110.90
1	A	136	TRP	CD1-CG-CD2	7.84	112.57	106.30
1	B	656	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	334	LEU	CA-CB-CG	-7.74	97.51	115.30
1	A	15	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	B	867	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	258	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	616	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	541	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	A	19	TRP	CD1-CG-CD2	7.43	112.25	106.30
1	A	136	TRP	CE2-CD2-CG	-7.38	101.40	107.30
1	A	15	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	A	299	TRP	CE2-CD2-CG	-7.27	101.48	107.30
1	B	509	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	769	TRP	CD1-CG-CD2	7.14	112.01	106.30
1	B	736	TRP	CD1-CG-CD2	7.11	111.99	106.30
1	B	834	LEU	CA-CB-CG	-7.05	99.09	115.30
1	A	236	TRP	CD1-CG-CD2	7.02	111.92	106.30
1	B	515	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	B	636	TRP	CD1-CG-CD2	6.96	111.87	106.30
1	B	515	TRP	CD1-CG-CD2	6.90	111.82	106.30
1	B	519	TRP	CD1-CG-CD2	6.88	111.80	106.30
1	B	758	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	B	509	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	19	TRP	CE2-CD2-CG	-6.71	101.93	107.30
1	A	112	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	711	TYR	CB-CG-CD1	-6.58	117.06	121.00
1	A	373	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	736	TRP	CE2-CD2-CG	-6.50	102.10	107.30
1	B	636	TRP	CE2-CD2-CG	-6.47	102.13	107.30
1	B	886	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	112	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	236	TRP	CE2-CD2-CG	-6.34	102.23	107.30
1	A	176	ARG	CG-CD-NE	6.28	124.99	111.80
1	B	867	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	833	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	116	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	676	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	15	TRP	CG-CD2-CE3	6.17	139.46	133.90
1	A	176	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	176	ARG	CD-NE-CZ	6.14	132.20	123.60
1	B	799	TRP	CD1-CG-CD2	6.05	111.14	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	519	TRP	CE2-CD2-CG	-5.99	102.51	107.30
1	A	76	GLN	CA-CB-CG	5.98	126.55	113.40
1	B	541	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	68	GLU	CA-CB-CG	5.92	126.42	113.40
1	A	353	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	34	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	769	TRP	CE2-CD2-CG	-5.82	102.64	107.30
1	A	299	TRP	CB-CG-CD1	-5.78	119.49	127.00
1	A	299	TRP	CG-CD1-NE1	-5.68	104.42	110.10
1	A	299	TRP	CG-CD2-CE3	5.68	139.02	133.90
1	B	799	TRP	CE2-CD2-CG	-5.67	102.76	107.30
1	B	620	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	204	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	136	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	B	769	TRP	CG-CD1-NE1	-5.56	104.54	110.10
1	A	386	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	783	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	187	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	269	TRP	CD1-CG-CD2	5.54	110.73	106.30
1	A	156	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	116	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	569	SER	N-CA-CB	-5.44	102.34	110.50
1	B	824	GLU	CA-CB-CG	-5.40	101.52	113.40
1	A	73	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	773	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	113	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	B	515	TRP	CG-CD2-CE3	5.34	138.71	133.90
1	A	236	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	B	537	GLU	CA-CB-CG	5.28	125.01	113.40
1	B	537	GLU	N-CA-CB	-5.27	101.11	110.60
1	A	156	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	173	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	A	207	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	19	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	A	367	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	B	515	TRP	CB-CG-CD1	-5.11	120.36	127.00
1	B	736	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	B	611	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	1	SER	CA-C-N	5.05	128.31	117.20
1	B	540	GLN	CB-CA-C	-5.04	100.33	110.40
1	A	15	TRP	CG-CD1-NE1	-5.02	105.08	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	633	TYR	Sidechain

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	672	2916	20	2
1	B	3024	672	2913	22	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	1	0	0	0
3	B	1	1	0	0	0
4	A	238	476	0	3	2
4	B	238	476	0	3	3
All	All	6528	2298	5829	40	6

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 (40) 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:537:GLU:HG3	1:B:541:ARG:NH1	2.01	0.76
1:B:595:HIS:HD2	1:B:597:VAL:H	1.37	0.70
1:B:537:GLU:HG3	1:B:541:ARG:HH12	1.56	0.68
1:B:523:ASP:HB2	1:B:524:PRO:HD2	1.75	0.68
1:A:326:GLN:HG3	4:A:1017:HOH:O	1.95	0.67
1:B:765:ARG:HG3	4:B:1248:HOH:O	2.01	0.60
1:A:95:HIS:HD2	1:A:97:VAL:H	1.50	0.60
1:B:680:LYS:HG2	1:B:714:ASN:O	2.02	0.59
1:A:176:ARG:HH11	1:A:176:ARG:HB2	1.69	0.57
1:A:24:PRO:HD3	1:B:524:PRO:HB3	1.89	0.54
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.44	0.53
1:B:595:HIS:CD2	1:B:597:VAL:H	2.23	0.52
1:B:721:GLN:HE21	1:B:748:GLN:HB3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PHE:HB3	1:A:228:PRO:HD3	1.92	0.51
1:B:827:GLU:HG3	4:B:1401:HOH:O	2.12	0.50
1:A:176:ARG:HD2	1:A:241:PHE:CE2	2.48	0.49
1:B:704:ARG:HH11	1:B:704:ARG:HB3	1.78	0.49
1:B:756:ASP:HB3	1:B:787:PHE:HA	1.95	0.49
1:B:536:VAL:O	1:B:540:GLN:HG2	2.12	0.48
1:A:227:PHE:CZ	1:A:231:ILE:HD11	2.49	0.47
1:A:347:GLN:HB2	4:A:1458:HOH:O	2.14	0.46
1:B:553:HIS:CD2	1:B:589:THR:HG23	2.51	0.46
1:B:727:PHE:CZ	1:B:731:ILE:HD11	2.51	0.45
1:A:329:LEU:HD23	1:A:334:LEU:HD13	1.97	0.45
1:A:95:HIS:CD2	1:A:97:VAL:H	2.31	0.45
1:A:87:MET:HA	1:A:132:THR:O	2.18	0.43
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.84	0.43
1:B:727:PHE:HB3	1:B:728:PRO:HD3	2.00	0.43
1:A:256:ASP:HB3	1:A:287:PHE:HA	2.01	0.43
1:A:327:GLU:HG3	4:A:1029:HOH:O	2.18	0.43
1:A:11:THR:HG21	1:A:86:PRO:HG2	2.01	0.42
1:A:121:ASN:HB3	1:A:133:TYR:OH	2.19	0.42
1:B:587:MET:HA	1:B:632:THR:O	2.19	0.42
1:A:23:ASP:HB2	1:A:24:PRO:HD2	2.00	0.42
1:B:706:GLU:HG3	1:B:707:ARG:HG3	2.02	0.41
1:A:315:ARG:HA	1:A:315:ARG:HD3	1.82	0.41
1:B:811:ILE:O	1:B:815:ARG:HG2	2.21	0.41
1:B:824:GLU:HG2	4:B:1223:HOH:O	2.21	0.40
1:B:540:GLN:HG2	1:B:540:GLN:H	1.78	0.40
1:A:96:PRO:HB3	1:B:529:THR:HG22	2.04	0.40

All (6) 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)
1:B:697:HIS:HE2	4:B:1142:HOH:H1[2_555]	1.00	0.60
4:B:1419:HOH:H1	4:B:1421:HOH:H1[2_555]	1.15	0.45
1:A:146:ALA:H	4:A:1063:HOH:H1[2_555]	1.15	0.45
1:B:611:ARG:HE	1:B:841:THR:HG1[2_555]	1.15	0.45
1:A:370:ALA:H	4:B:1073:HOH:H1[2_555]	1.21	0.39
1:B:758:ARG:H	4:A:1095:HOH:H2[2_555]	1.28	0.32

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	384/386 (100%)	370 (96%)	13 (3%)	1 (0%)	41	27
1	B	384/386 (100%)	371 (97%)	12 (3%)	1 (0%)	41	27
All	All	768/772 (100%)	741 (96%)	25 (3%)	2 (0%)	41	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	685	GLU

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%)	290 (96%)	12 (4%)	31	16
1	B	302/302 (100%)	285 (94%)	17 (6%)	21	8
All	All	604/604 (100%)	575 (95%)	29 (5%)	25	11

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	3	GLN
1	A	6	PRO
1	A	22	ARG

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Mol	Chain	Res	Type
1	A	45	LEU
1	A	65	THR
1	A	90	THR
1	A	128	LEU
1	A	169	THR
1	A	176	ARG
1	A	273	LEU
1	A	334	LEU
1	B	540	GLN
1	B	541	ARG
1	B	545	LEU
1	B	568	GLU
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	680	LYS
1	B	704	ARG
1	B	710	LEU
1	B	773	LEU
1	B	834	LEU
1	B	846	VAL
1	B	847	GLN

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	95	HIS
1	A	221	GLN
1	A	308	ASN
1	A	326	GLN
1	B	595	HIS
1	B	721	GLN
1	B	808	ASN
1	B	839	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are modelled with single atom and 2 are monoatomic - 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 [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 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.