Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:38 PM GMT

PDB ID	:	1XYA
Title	:	X-RAY CRYSTALLOGRAPHIC STRUCTURES OF D-XYLOSE ISOMERASE-SUBSTRATE COMPLEXES POSITION THE SUBSTRATE AND PROVIDE EVIDENCE FOR METAL MOVEMENT DURING CATALYSIS
Authors	:	Lavie, A.; Allen, K.N.; Petsko, G.A.; Ringe, D.
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

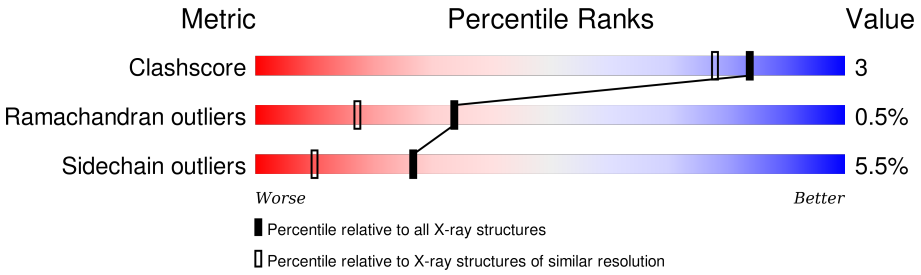
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)

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. 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 <=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	386	82% 15% •
1	B	386	83% 16% •

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.

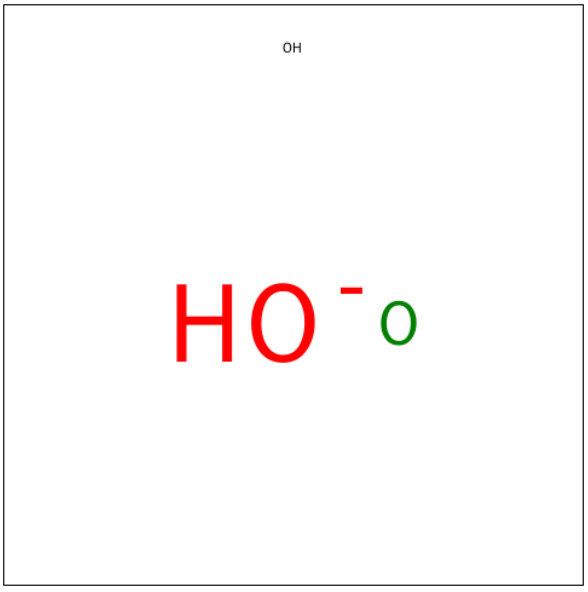
- Molecule 1 is a protein called XYLOSE ISOMERASE.

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



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

- Molecule 4 is water.

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

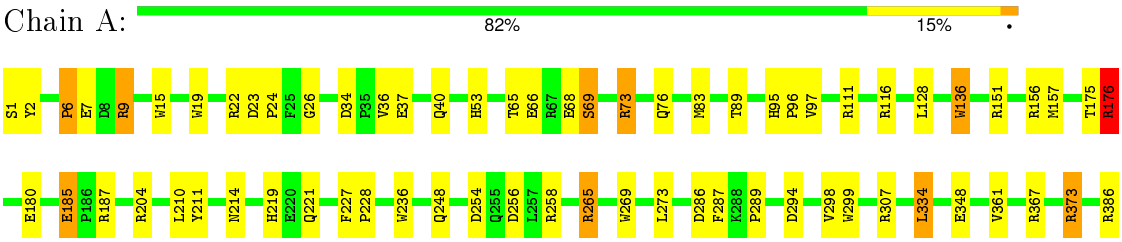
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 (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.

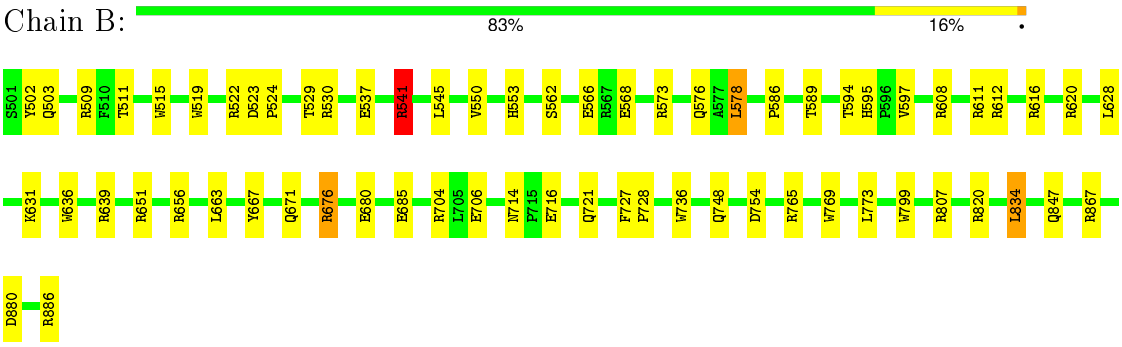
- Molecule 1: XYLOSE ISOMERASE

Chain A:



- Molecule 1: XYLOSE ISOMERASE

Chain B:



4 Data and refinement statistics (i)

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

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	1.42	52/4197 (1.2%)
1	B	0.80	1/3096 (0.0%)	1.41	44/4197 (1.0%)
All	All	0.81	1/6192 (0.0%)	1.42	96/8394 (1.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	716	GLU	CD-OE1	-5.11	1.20	1.25

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	765	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	A	176	ARG	NE-CZ-NH1	14.25	127.42	120.30
1	B	765	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	367	ARG	NE-CZ-NH2	-10.90	114.85	120.30
1	B	867	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	A	187	ARG	NE-CZ-NH1	10.10	125.35	120.30
1	A	367	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	B	820	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	156	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	799	TRP	CD1-CG-CD2	8.16	112.83	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	TRP	CD1-CG-CD2	7.99	112.69	106.30
1	B	651	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	A	15	TRP	CD1-CG-CD2	7.88	112.61	106.30
1	B	769	TRP	CD1-CG-CD2	7.64	112.42	106.30
1	A	269	TRP	CD1-CG-CD2	7.62	112.40	106.30
1	B	616	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	15	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	A	136	TRP	CD1-CG-CD2	7.58	112.36	106.30
1	A	19	TRP	CD1-CG-CD2	7.48	112.28	106.30
1	A	265	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	236	TRP	CD1-CG-CD2	7.43	112.25	106.30
1	A	299	TRP	CE2-CD2-CG	-7.39	101.39	107.30
1	B	515	TRP	CD1-CG-CD2	7.37	112.19	106.30
1	B	515	TRP	CE2-CD2-CG	-7.30	101.46	107.30
1	B	656	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	B	616	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	799	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	B	541	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	834	LEU	CA-CB-CG	-7.17	98.82	115.30
1	A	373	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	334	LEU	CA-CB-CG	-7.06	99.06	115.30
1	A	236	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	A	269	TRP	CE2-CD2-CG	-6.89	101.78	107.30
1	B	519	TRP	CD1-CG-CD2	6.89	111.81	106.30
1	A	176	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	736	TRP	CE2-CD2-CG	-6.81	101.85	107.30
1	B	736	TRP	CD1-CG-CD2	6.72	111.68	106.30
1	A	111	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	136	TRP	CE2-CD2-CG	-6.61	102.01	107.30
1	A	19	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	B	769	TRP	CE2-CD2-CG	-6.54	102.06	107.30
1	A	386	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	636	TRP	CD1-CG-CD2	6.54	111.53	106.30
1	B	636	TRP	CE2-CD2-CG	-6.53	102.08	107.30
1	B	573	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	265	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	258	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	530	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	639	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	9	ARG	CA-CB-CG	6.23	127.11	113.40
1	B	522	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	612	ARG	NE-CZ-NH1	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	608	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	156	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	522	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	176	ARG	CD-NE-CZ	5.99	131.99	123.60
1	A	386	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	807	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	73	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	299	TRP	CG-CD2-CE3	5.91	139.22	133.90
1	B	519	TRP	CE2-CD2-CG	-5.89	102.58	107.30
1	A	286	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	211	TYR	CB-CG-CD1	-5.85	117.49	121.00
1	A	34	ASP	CB-CG-OD1	5.80	123.53	118.30
1	B	799	TRP	CG-CD1-NE1	-5.80	104.30	110.10
1	B	799	TRP	CB-CG-CD1	-5.80	119.46	127.00
1	A	307	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	636	TRP	CG-CD2-CE3	5.71	139.04	133.90
1	A	83	MET	CG-SD-CE	5.68	109.29	100.20
1	A	66	GLU	CB-CA-C	-5.68	99.05	110.40
1	A	236	TRP	CG-CD1-NE1	-5.67	104.43	110.10
1	A	299	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A	116	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	820	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	299	TRP	CB-CG-CD1	-5.54	119.79	127.00
1	B	736	TRP	CG-CD2-CE3	5.52	138.87	133.90
1	B	608	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	769	TRP	CG-CD1-NE1	-5.44	104.66	110.10
1	A	236	TRP	CG-CD2-CE3	5.42	138.78	133.90
1	A	175	THR	N-CA-CB	-5.37	100.11	110.30
1	A	15	TRP	CB-CG-CD1	-5.33	120.06	127.00
1	B	502	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	578	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	19	TRP	CG-CD1-NE1	-5.28	104.82	110.10
1	B	754	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	19	TRP	CG-CD2-CE3	5.23	138.60	133.90
1	A	66	GLU	N-CA-CB	5.21	119.98	110.60
1	B	611	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	509	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	136	TRP	CG-CD1-NE1	-5.14	104.96	110.10
1	A	15	TRP	CG-CD2-CE3	5.10	138.49	133.90
1	A	294	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	157	MET	CG-SD-CE	-5.05	92.13	100.20
1	B	611	ARG	NE-CZ-NH1	5.04	122.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	573	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	151	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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 (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	3024	0	2909	22	0
1	B	3024	0	2906	17	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	36	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 (36) 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:HB2	1:A:176:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.91	0.51
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:HH11	1:B:676:ARG:HB3	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

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%)	24 8
1	B	384/386 (100%)	368 (96%)	15 (4%)	1 (0%)	46 29
All	All	768/772 (100%)	739 (96%)	25 (3%)	4 (0%)	34 17

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 (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	302/302 (100%)	285 (94%)	17 (6%)	26 10
1	B	302/302 (100%)	286 (95%)	16 (5%)	28 11
All	All	604/604 (100%)	571 (94%)	33 (6%)	27 10

All (33) 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	22	ARG
1	A	37	GLU
1	A	65	THR
1	A	68	GLU
1	A	69	SER

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Mol	Chain	Res	Type
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
1	B	568	GLU
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	704	ARG
1	B	706	GLU
1	B	773	LEU
1	B	834	LEU
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	76	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	847	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are modelled with single atom and 4 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

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 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.