



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 2, 2016 – 12:03 AM GMT

PDB ID : 9XIA  
Title : X-RAY ANALYSIS OF D-XYLOSE ISOMERASE AT 1.9 ANGSTROMS:  
NATIVE ENZYME IN COMPLEX WITH SUBSTRATE AND WITH A  
MECHANISM-DESIGNED INACTIVATOR  
Authors : Carrell, H.L.; Glusker, J.P.  
Deposited on : 1990-10-11  
Resolution : 1.90 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

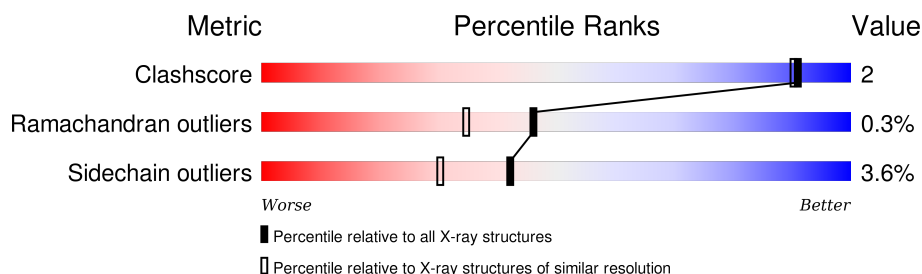
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	 73% 22% •

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3360 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.

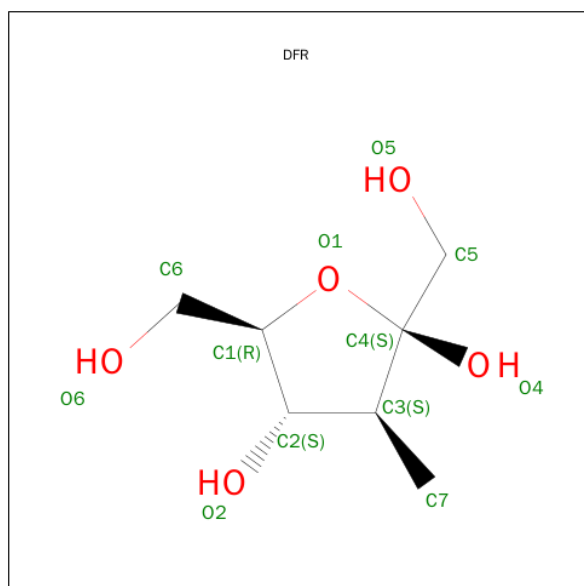
- Molecule 1 is a protein called XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3047	1915	548	575	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLN	ARG	SEE REMARK 999	UNP P24300

- Molecule 2 is SUGAR (3-DEOXY-3-METHYL-D-FRUCTOSE) (three-letter code: DFR) (formula:  $C_7H_{14}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	7	5		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mn 2	0	0

- Molecule 4 is water.

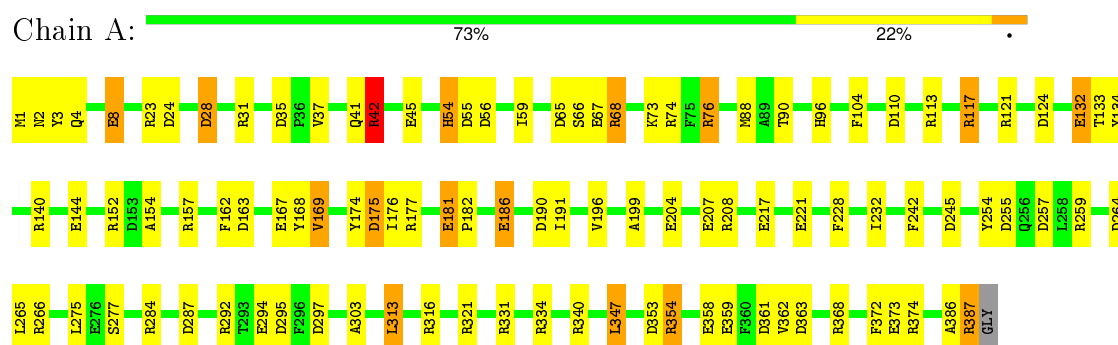
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	299	Total 299	O 299	0	0

### 3 Residue-property plots

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



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.80 Å   100.00 Å   103.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	8.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.141 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	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: MN, DFR

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	1.40	7/3119 (0.2%)	2.33	132/4222 (3.1%)

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	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	217	GLU	CD-OE1	-10.43	1.14	1.25
1	A	217	GLU	CD-OE2	-8.05	1.16	1.25
1	A	340	ARG	CZ-NH1	6.32	1.41	1.33
1	A	162	PHE	CE2-CZ	5.97	1.48	1.37
1	A	186	GLU	CD-OE2	-5.83	1.19	1.25
1	A	294	GLU	CD-OE1	-5.44	1.19	1.25
1	A	181	GLU	CG-CD	-5.16	1.44	1.51

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	NE-CZ-NH2	27.85	134.22	120.30
1	A	76	ARG	NE-CZ-NH2	-23.61	108.49	120.30
1	A	68	ARG	NE-CZ-NH2	22.47	131.53	120.30
1	A	266	ARG	NE-CZ-NH2	-22.38	109.11	120.30
1	A	74	ARG	NE-CZ-NH2	-21.76	109.42	120.30
1	A	340	ARG	NE-CZ-NH1	-18.76	110.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ARG	NE-CZ-NH2	-16.67	111.97	120.30
1	A	208	ARG	NE-CZ-NH2	-16.59	112.00	120.30
1	A	368	ARG	NE-CZ-NH1	16.41	128.50	120.30
1	A	259	ARG	NE-CZ-NH2	15.06	127.83	120.30
1	A	152	ARG	NE-CZ-NH2	-14.89	112.85	120.30
1	A	157	ARG	NE-CZ-NH1	14.43	127.51	120.30
1	A	316	ARG	NE-CZ-NH1	13.96	127.28	120.30
1	A	152	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	A	259	ARG	NE-CZ-NH1	-13.10	113.75	120.30
1	A	316	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	A	74	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	A	113	ARG	NE-CZ-NH2	-12.73	113.94	120.30
1	A	124	ASP	CB-CG-OD1	12.34	129.41	118.30
1	A	266	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	386	ALA	C-N-CA	11.75	151.06	121.70
1	A	42	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	A	354	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	A	56	ASP	CB-CG-OD1	11.22	128.40	118.30
1	A	68	ARG	NH1-CZ-NH2	-11.16	107.12	119.40
1	A	28	ASP	CB-CG-OD1	11.14	128.33	118.30
1	A	245	ASP	CB-CG-OD2	11.11	128.30	118.30
1	A	28	ASP	CB-CG-OD2	-10.70	108.67	118.30
1	A	208	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	A	31	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	A	354	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	A	292	ARG	NE-CZ-NH1	10.35	125.48	120.30
1	A	340	ARG	CD-NE-CZ	10.12	137.77	123.60
1	A	117	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	A	297	ASP	CB-CG-OD1	9.59	126.93	118.30
1	A	35	ASP	CB-CG-OD1	-9.48	109.77	118.30
1	A	117	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	A	68	ARG	CA-CB-CG	9.39	134.05	113.40
1	A	368	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	A	255	ASP	CB-CG-OD2	9.18	126.56	118.30
1	A	292	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	181	GLU	CB-CG-CD	8.79	137.93	114.20
1	A	353	ASP	CB-CG-OD1	-8.52	110.63	118.30
1	A	113	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	76	ARG	NH1-CZ-NH2	8.16	128.38	119.40
1	A	287	ASP	CB-CG-OD1	8.09	125.58	118.30
1	A	24	ASP	CB-CA-C	8.04	126.48	110.40
1	A	190	ASP	CB-CG-OD1	-7.92	111.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	LEU	CB-CG-CD1	7.83	124.32	111.00
1	A	168	TYR	CB-CG-CD1	-7.80	116.32	121.00
1	A	2	ASN	CB-CA-C	7.79	125.99	110.40
1	A	175	ASP	CB-CG-OD1	-7.74	111.34	118.30
1	A	257	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	277	SER	CB-CA-C	7.71	124.75	110.10
1	A	144	GLU	OE1-CD-OE2	-7.59	114.19	123.30
1	A	124	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	284	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	347	LEU	CB-CG-CD2	7.30	123.41	111.00
1	A	242	PHE	CB-CG-CD2	-7.15	115.80	120.80
1	A	42	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	295	ASP	CB-CG-OD2	7.03	124.63	118.30
1	A	316	ARG	CD-NE-CZ	-7.00	113.80	123.60
1	A	168	TYR	CB-CG-CD2	7.00	125.20	121.00
1	A	67	GLU	CG-CD-OE2	-6.98	104.34	118.30
1	A	3	TYR	CB-CG-CD1	6.95	125.17	121.00
1	A	35	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	3	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	A	3	TYR	N-CA-CB	-6.82	98.33	110.60
1	A	163	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	110	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	121	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	334	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	A	292	ARG	CD-NE-CZ	6.61	132.85	123.60
1	A	361	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	A	104	PHE	CB-CG-CD2	-6.58	116.19	120.80
1	A	35	ASP	N-CA-CB	-6.58	98.75	110.60
1	A	176	ILE	O-C-N	6.54	133.16	122.70
1	A	207	GLU	CG-CD-OE1	6.38	131.07	118.30
1	A	255	ASP	OD1-CG-OD2	-6.35	111.23	123.30
1	A	196	VAL	CA-CB-CG2	-6.33	101.40	110.90
1	A	254	TYR	CB-CG-CD1	-6.28	117.23	121.00
1	A	132	GLU	N-CA-CB	-6.26	99.34	110.60
1	A	374	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	196	VAL	CG1-CB-CG2	-5.95	101.39	110.90
1	A	55	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	265	LEU	CB-CG-CD2	-5.88	101.00	111.00
1	A	275	LEU	CB-CG-CD1	-5.87	101.02	111.00
1	A	358	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	A	363	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	277	SER	O-C-N	-5.83	113.38	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ASP	OD1-CG-OD2	-5.82	112.23	123.30
1	A	207	GLU	CG-CD-OE2	-5.82	106.66	118.30
1	A	373	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	362	VAL	CA-CB-CG2	5.78	119.57	110.90
1	A	132	GLU	CA-CB-CG	5.75	126.06	113.40
1	A	2	ASN	N-CA-CB	5.74	120.94	110.60
1	A	134	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	A	76	ARG	CG-CD-NE	-5.68	99.87	111.80
1	A	175	ASP	CA-CB-CG	-5.67	100.93	113.40
1	A	347	LEU	CA-CB-CG	5.65	128.30	115.30
1	A	140	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	A	177	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	76	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	8	GLU	CA-CB-CG	5.63	125.79	113.40
1	A	73	LYS	CB-CA-C	5.62	121.64	110.40
1	A	144	GLU	CG-CD-OE1	5.62	129.53	118.30
1	A	264	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	54	HIS	CB-CA-C	-5.61	99.17	110.40
1	A	331	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	A	175	ASP	OD1-CG-OD2	5.58	133.91	123.30
1	A	204	GLU	CG-CD-OE1	5.58	129.46	118.30
1	A	373	GLU	CG-CD-OE1	5.53	129.35	118.30
1	A	169	VAL	CA-CB-CG1	5.49	119.13	110.90
1	A	45	GLU	CG-CD-OE2	-5.46	107.39	118.30
1	A	372	PHE	CB-CG-CD2	-5.45	116.99	120.80
1	A	154	ALA	CB-CA-C	5.37	118.16	110.10
1	A	242	PHE	CB-CG-CD1	5.35	124.54	120.80
1	A	90	THR	N-CA-CB	-5.32	100.19	110.30
1	A	134	TYR	CA-CB-CG	-5.31	103.31	113.40
1	A	303	ALA	O-C-N	-5.29	114.24	122.70
1	A	362	VAL	O-C-N	5.26	131.11	122.70
1	A	199	ALA	CB-CA-C	5.25	117.97	110.10
1	A	96	HIS	CA-CB-CG	-5.24	104.70	113.60
1	A	121	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	23	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	221	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	A	387	ARG	N-CA-CB	5.12	119.82	110.60
1	A	65	ASP	CB-CA-C	5.12	120.64	110.40
1	A	191	ILE	CA-CB-CG1	5.10	120.69	111.00
1	A	174	TYR	CA-CB-CG	5.08	123.06	113.40
1	A	331	ARG	CG-CD-NE	-5.06	101.17	111.80
1	A	167	GLU	CG-CD-OE2	-5.00	108.30	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	42	ARG	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	3047	0	2917	12	1
2	A	12	0	14	5	0
3	A	2	0	0	0	0
4	A	299	0	0	1	1
All	All	3360	0	2931	12	1

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 2.

All (12) 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:54:HIS:NE2	2:A:389:DFR:H72	1.22	1.45
1:A:54:HIS:CE1	2:A:389:DFR:H72	1.73	1.21
1:A:54:HIS:NE2	2:A:389:DFR:H73	1.69	1.06
1:A:387:ARG:NH1	4:A:672:HOH:O	2.10	0.83
1:A:59:ILE:HG21	1:A:68:ARG:HG2	1.88	0.55
1:A:354:ARG:HB3	1:A:359:GLU:HG3	1.90	0.53
1:A:54:HIS:CE1	2:A:389:DFR:C7	2.58	0.47
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.50	0.46
1:A:37:VAL:O	1:A:41:GLN:HG3	2.16	0.45
1:A:54:HIS:CD2	2:A:389:DFR:H73	2.47	0.42
1:A:181:GLU:HA	1:A:182:PRO:HD3	1.87	0.42
1:A:88:MET:HA	1:A:133:THR:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASP:OD2	4:A:595:HOH:O[3_656]	1.82	0.38

## 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	385/388 (99%)	375 (97%)	9 (2%)	1 (0%)	46 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU

### 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	304/304 (100%)	293 (96%)	11 (4%)	42 30

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	GLN
1	A	8	GLU

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Mol	Chain	Res	Type
1	A	42	ARG
1	A	66	SER
1	A	76	ARG
1	A	132	GLU
1	A	169	VAL
1	A	175	ASP
1	A	313	LEU
1	A	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	GLN
1	A	185	ASN

### 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
2	DFR	A	389	1,3	11,12,12	1.30	1 (9%)	9,18,18	3.77	6 (66%)

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
2	DFR	A	389	1,3	-	0/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	389	DFR	O1-C4	-2.53	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	DFR	O5-C5-C4	-6.96	97.86	111.39
2	A	389	DFR	C5-C4-C3	-5.78	96.77	114.68
2	A	389	DFR	C6-C1-C2	-4.42	104.62	115.08
2	A	389	DFR	O6-C6-C1	-2.54	102.93	111.33
2	A	389	DFR	C7-C3-C4	2.00	119.36	114.81
2	A	389	DFR	O4-C4-O1	3.45	116.48	109.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	389	DFR	5	0

## 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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.