



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:04 AM UTC

PDB ID : 9XIA / pdb_00009xia
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

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)	:	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

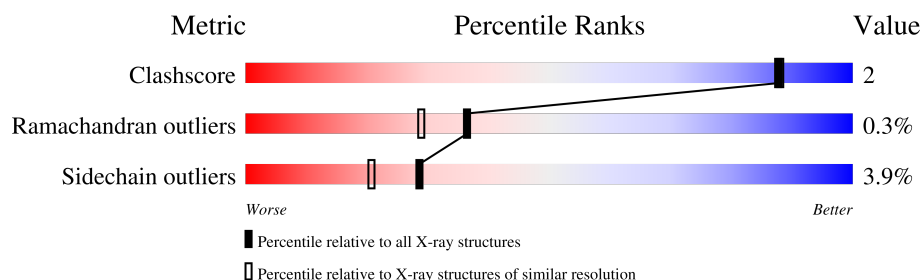
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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	388	 65% 31% ..

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.

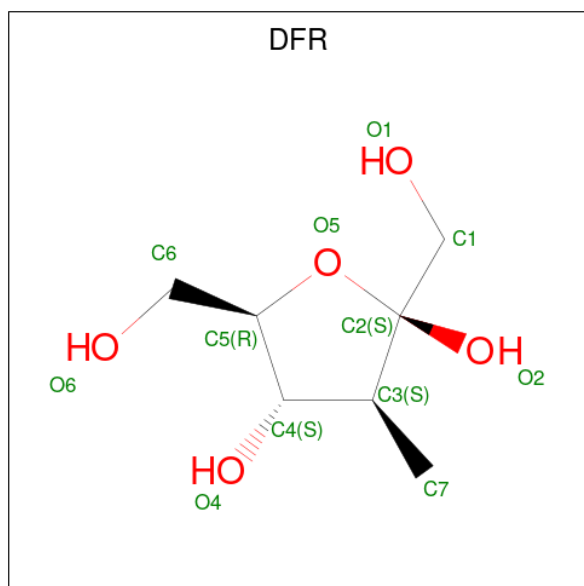
- Molecule 1 is a protein called XYLOSE ISOMERASE.

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

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 3-deoxy-3-methyl-beta-D-fructofuranose (CCD ID: DFR) (formula: C₇H₁₄O₅).



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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

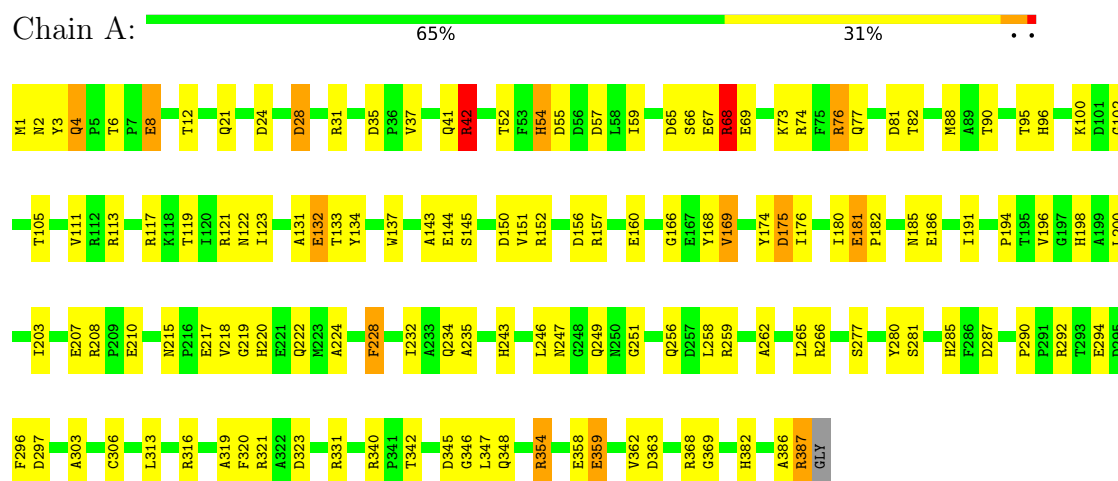
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	299	Total 299	O 299	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.80Å 100.00Å 103.00Å 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 ²)	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: DFR, MN

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	1.77	26/3119 (0.8%)	2.33	151/4222 (3.6%)

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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	THR	CA-CB	7.91	1.66	1.54
1	A	228	PHE	N-CA	7.79	1.53	1.46
1	A	218	VAL	CA-CB	7.57	1.62	1.54
1	A	382	HIS	N-CA	7.56	1.55	1.46
1	A	196	VAL	CA-CB	7.03	1.63	1.54
1	A	105	THR	N-CA	6.22	1.53	1.46
1	A	340	ARG	CZ-NH1	6.08	1.41	1.32
1	A	247	ASN	N-CA	6.03	1.54	1.46
1	A	234	GLN	C-O	5.99	1.31	1.24
1	A	217	GLU	CD-OE1	-5.88	1.14	1.25
1	A	111	VAL	N-CA	5.66	1.53	1.46
1	A	316	ARG	CD-NE	5.64	1.54	1.46
1	A	196	VAL	N-CA	5.59	1.53	1.46
1	A	194	PRO	CA-CB	5.51	1.62	1.53
1	A	102	GLY	C-O	5.48	1.28	1.23
1	A	219	GLY	N-CA	5.42	1.52	1.45
1	A	31	ARG	CD-NE	5.40	1.53	1.46
1	A	131	ALA	N-CA	5.32	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	ASP	N-CA	5.31	1.52	1.46
1	A	296	PHE	C-N	-5.25	1.27	1.33
1	A	346	GLY	CA-C	-5.22	1.47	1.52
1	A	249	GLN	N-CA	5.20	1.52	1.46
1	A	200	LEU	CA-CB	5.17	1.61	1.53
1	A	156	ASP	N-CA	5.10	1.52	1.46
1	A	320	PHE	C-O	5.03	1.29	1.24
1	A	143	ALA	CA-CB	5.00	1.61	1.53

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	NE-CZ-NH2	16.70	134.22	119.20
1	A	386	ALA	CA-C-N	16.31	151.06	121.70
1	A	386	ALA	C-N-CA	16.31	151.06	121.70
1	A	181	GLU	CB-CG-CD	14.90	137.93	112.60
1	A	68	ARG	NE-CZ-NH2	13.70	131.53	119.20
1	A	76	ARG	NE-CZ-NH2	-11.89	108.49	119.20
1	A	175	ASP	CA-CB-CG	-11.67	100.93	112.60
1	A	266	ARG	NE-CZ-NH2	-11.21	109.11	119.20
1	A	74	ARG	NE-CZ-NH2	-10.87	109.42	119.20
1	A	340	ARG	NE-CZ-NH1	-10.58	110.92	121.50
1	A	68	ARG	CA-CB-CG	9.98	134.05	114.10
1	A	259	ARG	NE-CZ-NH2	9.59	127.83	119.20
1	A	340	ARG	CD-NE-CZ	9.55	137.77	124.40
1	A	362	VAL	O-C-N	9.53	131.11	121.87
1	A	362	VAL	CA-C-O	-9.52	111.05	120.95
1	A	68	ARG	NH1-CZ-NH2	-9.37	107.12	119.30
1	A	96	HIS	CA-CB-CG	-9.10	104.70	113.80
1	A	176	ILE	O-C-N	8.68	133.16	123.09
1	A	55	ASP	CA-CB-CG	8.60	121.20	112.60
1	A	69	GLU	CB-CG-CD	8.45	126.97	112.60
1	A	2	ASN	CB-CA-C	8.42	125.99	109.66
1	A	24	ASP	CB-CA-C	8.28	126.48	110.17
1	A	362	VAL	N-CA-CB	8.21	121.70	110.54
1	A	3	TYR	N-CA-CB	-8.18	98.33	111.58
1	A	382	HIS	CA-CB-CG	-8.11	105.69	113.80
1	A	331	ARG	NE-CZ-NH2	-8.04	111.97	119.20
1	A	208	ARG	NE-CZ-NH2	-7.99	112.00	119.20
1	A	259	ARG	NE-CZ-NH1	-7.75	113.75	121.50
1	A	132	GLU	N-CA-CB	-7.61	99.34	110.53
1	A	316	ARG	CD-NE-CZ	-7.57	113.80	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	386	ALA	N-CA-C	-7.49	102.37	112.26
1	A	285	HIS	CA-C-O	-7.46	112.11	120.54
1	A	198	HIS	CA-C-O	-7.45	112.66	120.55
1	A	303	ALA	O-C-N	-7.43	114.24	122.12
1	A	345	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	21	GLN	OE1-CD-NE2	7.37	129.97	122.60
1	A	277	SER	CB-CA-C	7.33	124.75	110.67
1	A	90	THR	N-CA-CB	-7.32	100.19	111.46
1	A	277	SER	O-C-N	-7.23	113.38	122.27
1	A	176	ILE	CA-C-O	-7.23	113.17	120.90
1	A	4	GLN	OE1-CD-NE2	-7.21	115.39	122.60
1	A	137	TRP	CA-C-O	-7.16	112.80	120.46
1	A	152	ARG	NE-CZ-NH2	-7.05	112.85	119.20
1	A	151	VAL	N-CA-C	7.04	117.80	110.62
1	A	368	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	A	76	ARG	NH1-CZ-NH2	6.98	128.38	119.30
1	A	35	ASP	N-CA-CB	-6.91	98.75	110.01
1	A	150	ASP	N-CA-C	-6.91	97.98	108.96
1	A	256	GLN	CB-CG-CD	-6.88	100.91	112.60
1	A	210	GLU	CB-CG-CD	6.84	124.23	112.60
1	A	358	GLU	CA-C-O	-6.83	113.59	120.90
1	A	73	LYS	CB-CA-C	6.77	121.64	110.81
1	A	160	GLU	O-C-N	-6.75	114.96	122.12
1	A	168	TYR	O-C-N	-6.72	115.14	122.07
1	A	235	ALA	N-CA-C	-6.71	104.05	111.36
1	A	207	GLU	CA-C-O	-6.64	113.52	120.55
1	A	203	ILE	O-C-N	6.63	128.38	121.89
1	A	194	PRO	N-CA-C	6.55	122.04	113.86
1	A	235	ALA	CA-C-O	-6.53	113.50	120.42
1	A	28	ASP	CA-CB-CG	-6.48	106.12	112.60
1	A	208	ARG	N-CA-CB	-6.46	101.71	111.21
1	A	54	HIS	CA-CB-CG	-6.39	107.41	113.80
1	A	215	ASN	CA-CB-CG	-6.36	106.24	112.60
1	A	68	ARG	N-CA-CB	6.35	119.48	109.82
1	A	160	GLU	CA-C-N	6.33	128.67	120.44
1	A	160	GLU	C-N-CA	6.33	128.67	120.44
1	A	294	GLU	N-CA-C	6.27	120.14	110.42
1	A	359	GLU	CB-CG-CD	6.26	123.25	112.60
1	A	262	ALA	N-CA-C	-6.25	102.47	110.53
1	A	67	GLU	CG-CD-OE2	-6.11	104.34	118.40
1	A	54	HIS	CB-CA-C	-6.11	99.17	109.50
1	A	342	THR	O-C-N	6.09	129.09	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ILE	CA-CB-CG1	6.05	120.69	110.40
1	A	144	GLU	N-CA-C	-6.05	105.86	113.72
1	A	292	ARG	CD-NE-CZ	6.04	132.85	124.40
1	A	157	ARG	NE-CZ-NH1	6.01	127.51	121.50
1	A	2	ASN	N-CA-CB	6.01	120.94	111.20
1	A	290	PRO	N-CA-C	-6.00	103.38	110.70
1	A	246	LEU	O-C-N	6.00	130.05	123.27
1	A	132	GLU	CA-CB-CG	5.98	126.06	114.10
1	A	316	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	A	150	ASP	CA-CB-CG	-5.98	106.62	112.60
1	A	95	THR	N-CA-C	5.95	118.66	111.40
1	A	169	VAL	N-CA-CB	-5.94	103.60	110.55
1	A	134	TYR	CA-CB-CG	-5.88	103.31	113.90
1	A	113	ARG	NE-CZ-NH2	-5.85	113.94	119.20
1	A	100	LYS	CA-C-O	-5.85	113.65	120.20
1	A	8	GLU	CA-CB-CG	5.84	125.79	114.10
1	A	166	GLY	N-CA-C	-5.83	105.56	113.37
1	A	277	SER	CA-CB-OG	-5.82	99.46	111.10
1	A	185	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	316	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	A	369	GLY	O-C-N	-5.76	115.44	122.76
1	A	296	PHE	CA-C-O	-5.76	114.45	120.55
1	A	8	GLU	CB-CG-CD	5.71	122.32	112.60
1	A	152	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	A	265	LEU	CA-C-O	-5.69	114.52	120.55
1	A	73	LYS	O-C-N	-5.67	116.20	122.09
1	A	54	HIS	N-CA-C	-5.67	101.05	110.17
1	A	196	VAL	CA-C-O	-5.60	115.23	121.05
1	A	76	ARG	CG-CD-NE	-5.51	99.87	112.00
1	A	207	GLU	CG-CD-OE1	5.51	131.07	118.40
1	A	297	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	387	ARG	N-CA-CB	5.48	119.82	110.50
1	A	208	ARG	CD-NE-CZ	-5.44	116.78	124.40
1	A	220	HIS	CA-C-O	-5.44	115.09	120.70
1	A	280	TYR	CA-C-N	-5.43	113.96	122.49
1	A	280	TYR	C-N-CA	-5.43	113.96	122.49
1	A	152	ARG	CA-C-O	-5.43	114.80	120.55
1	A	77	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	A	362	VAL	CA-CB-CG2	5.40	119.57	110.40
1	A	57	ASP	N-CA-C	-5.38	105.45	112.23
1	A	102	GLY	O-C-N	5.35	128.43	123.35
1	A	287	ASP	CA-CB-CG	-5.33	107.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLN	CG-CD-NE2	5.33	124.39	116.40
1	A	169	VAL	CB-CA-C	5.31	118.77	111.97
1	A	319	ALA	N-CA-C	-5.30	105.50	111.28
1	A	123	ILE	O-C-N	5.30	127.11	121.91
1	A	196	VAL	CA-CB-CG2	-5.29	101.40	110.40
1	A	74	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	A	121	ARG	O-C-N	-5.27	116.53	122.12
1	A	363	ASP	CA-C-O	-5.26	114.98	120.55
1	A	65	ASP	CB-CA-C	5.25	120.64	110.46
1	A	296	PHE	N-CA-CB	5.25	117.83	110.12
1	A	222	GLN	OE1-CD-NE2	-5.25	117.36	122.60
1	A	122	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	119	THR	O-C-N	5.19	127.42	122.07
1	A	168	TYR	CA-C-O	5.18	126.26	120.82
1	A	258	LEU	N-CA-C	-5.18	103.56	110.55
1	A	42	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	A	354	ARG	N-CA-CB	5.14	118.92	110.39
1	A	169	VAL	CA-CB-CG1	5.14	119.13	110.40
1	A	180	ILE	CA-CB-CG1	-5.12	101.70	110.40
1	A	316	ARG	CA-C-O	-5.12	115.12	120.55
1	A	12	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	207	GLU	CG-CD-OE2	-5.10	106.66	118.40
1	A	224	ALA	N-CA-C	-5.09	106.31	112.88
1	A	348	GLN	CB-CA-C	5.09	119.25	110.79
1	A	174	TYR	CA-CB-CG	5.09	123.06	113.90
1	A	52	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	251	GLY	O-C-N	-5.09	118.08	122.91
1	A	323	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	6	THR	O-C-N	5.08	125.51	121.55
1	A	81	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	243	HIS	O-C-N	5.06	128.58	123.26
1	A	234	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	219	GLY	CA-C-O	-5.03	114.97	120.40
1	A	145	SER	CA-C-N	5.03	125.56	119.98
1	A	145	SER	C-N-CA	5.03	125.56	119.98
1	A	281	SER	CA-CB-OG	-5.01	101.08	111.10
1	A	306	CYS	O-C-N	5.01	127.23	122.07

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	11	1
2	A	12	0	11	4	0
3	A	2	0	0	0	0
4	A	299	0	0	1	1
All	All	3360	0	2928	11	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 (11) 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:CE1	2:A:389:DFR:H71	1.62	1.34
1:A:54:HIS:NE2	2:A:389:DFR:H71	0.94	1.25
1:A:387:ARG:NH1	4:A:672:HOH:O	2.10	0.83
1:A:54:HIS:NE2	2:A:389:DFR:H72	2.02	0.64
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	0.51
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: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 symmetry 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%)	36 29

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%)	292 (96%)	12 (4%)	28 21

All (12) 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
1	A	42	ARG
1	A	66	SER

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Mol	Chain	Res	Type
1	A	68	ARG
1	A	76	ARG
1	A	132	GLU
1	A	169	VAL
1	A	175	ASP
1	A	313	LEU
1	A	347	LEU

Sometimes 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	234	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	3,1	12,12,12	1.28	1 (8%)	12,18,18	3.39	7 (58%)

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	3,1	-	1/5/24/24	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	O5-C2	-2.68	1.39	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	DFR	O1-C1-C2	-6.24	97.86	111.67
2	A	389	DFR	O5-C2-C3	-6.24	96.69	103.99
2	A	389	DFR	C6-C5-C4	-4.44	104.62	115.10
2	A	389	DFR	O2-C2-O5	3.73	116.48	109.33
2	A	389	DFR	C7-C3-C2	2.77	119.36	114.91
2	A	389	DFR	O6-C6-C5	-2.47	102.93	111.33
2	A	389	DFR	C7-C3-C4	2.41	119.86	114.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	DFR	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	389	DFR	4	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

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.