



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:33 PM BST

PDB ID : 1XIE
Title : MODES OF BINDING SUBSTRATES AND THEIR ANALOGUES TO THE
ENZYME D-XYLOSE ISOMERASE
Authors : Carrell, H.L.; Glusker, J.P.
Deposited on : 1994-03-07
Resolution : 1.70 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.13.1

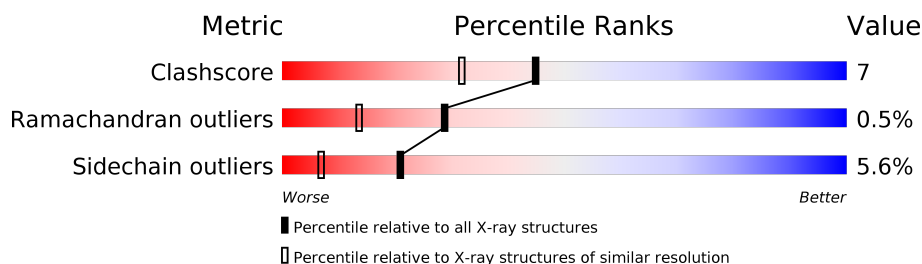
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)

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	388	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3437 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.

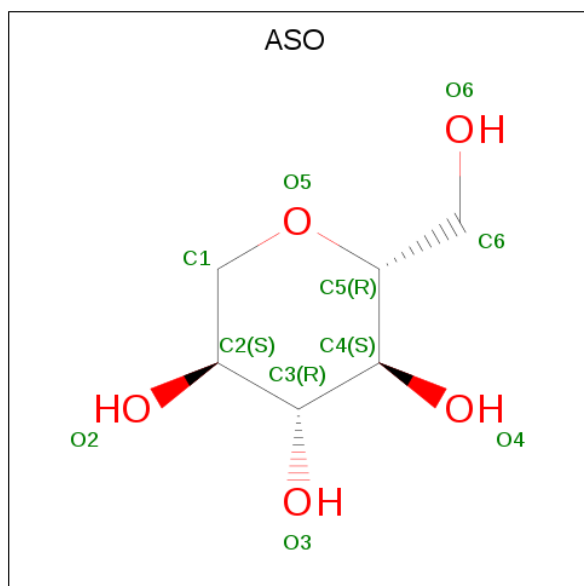
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	1	0
			3048	1915	549	575	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	GLN	ARG	conflict	UNP P24300

- Molecule 2 is 1,5-anhydro-D-glucitol (three-letter code: ASO) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	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.

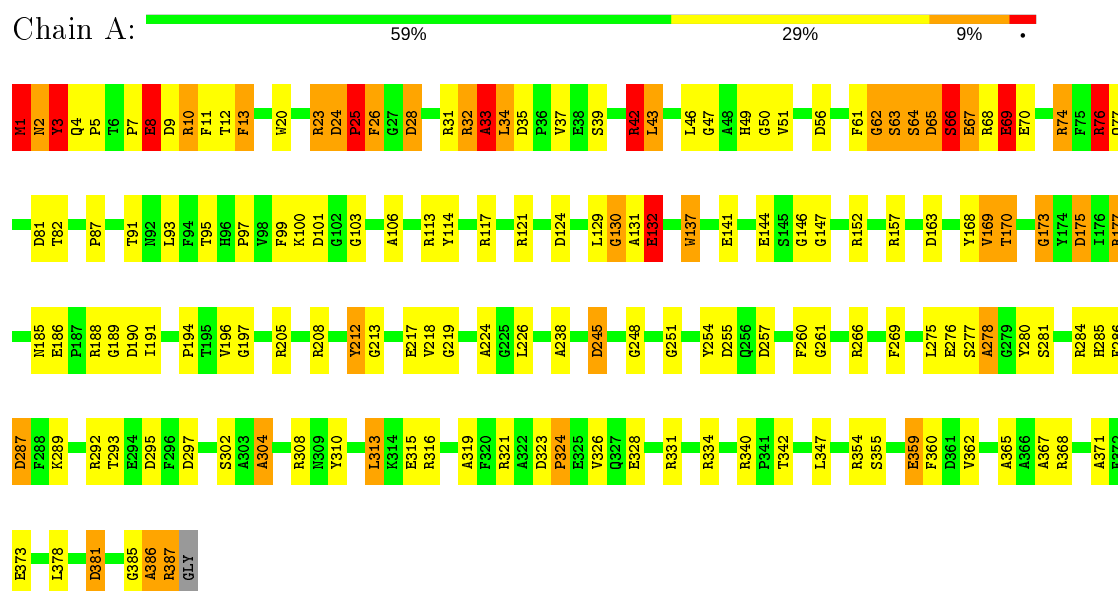
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	376	Total 376	O 376	0	0

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: D-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	93.50Å 99.56Å 102.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.162 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3437	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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, ASO

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	1.57	59/3126 (1.9%)	2.18	121/4231 (2.9%)

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	1	35

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	ASN	C-N	24.95	1.91	1.34
1	A	1	MET	C-N	23.52	1.88	1.34
1	A	3	TYR	C-N	-15.64	0.98	1.34
1	A	141	GLU	C-N	12.23	1.55	1.33
1	A	278	ALA	C-N	11.48	1.53	1.33
1	A	8	GLU	C-N	11.22	1.59	1.34
1	A	212	TYR	C-N	11.11	1.53	1.33
1	A	175	ASP	C-N	-10.51	1.09	1.34
1	A	254	TYR	C-N	10.20	1.57	1.34
1	A	304	ALA	C-N	9.96	1.50	1.33
1	A	63	SER	C-N	9.67	1.56	1.34
1	A	25	PRO	C-N	9.43	1.55	1.34
1	A	297	ASP	C-N	8.81	1.49	1.33
1	A	28	ASP	C-N	8.73	1.54	1.34
1	A	328	GLU	C-N	8.63	1.53	1.34
1	A	191	ILE	C-N	8.31	1.53	1.34
1	A	269	PHE	C-N	8.06	1.52	1.34
1	A	61	PHE	C-N	-8.02	1.18	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	319	ALA	C-N	7.88	1.52	1.34
1	A	238	ALA	C-N	-7.85	1.19	1.33
1	A	302	SER	C-N	7.51	1.51	1.34
1	A	24	ASP	C-N	7.50	1.48	1.34
1	A	255	ASP	C-N	7.47	1.51	1.34
1	A	114	TYR	C-N	7.43	1.51	1.34
1	A	95	THR	C-N	-7.20	1.17	1.34
1	A	82	THR	C-N	7.19	1.46	1.33
1	A	205	ARG	C-N	6.99	1.50	1.34
1	A	49	HIS	C-N	6.90	1.45	1.33
1	A	281	SER	C-N	6.85	1.45	1.33
1	A	146	GLY	C-N	6.72	1.45	1.33
1	A	129	LEU	C-N	6.37	1.44	1.33
1	A	132	GLU	C-N	6.27	1.48	1.34
1	A	93	LEU	C-N	6.17	1.48	1.34
1	A	33	ALA	C-N	6.11	1.48	1.34
1	A	385	GLY	C-N	6.09	1.48	1.34
1	A	100	LYS	C-N	6.09	1.48	1.34
1	A	378	LEU	C-N	6.08	1.48	1.34
1	A	99	PHE	C-N	6.06	1.48	1.34
1	A	324	PRO	C-N	6.04	1.48	1.34
1	A	65	ASP	C-N	5.93	1.47	1.34
1	A	101	ASP	C-N	5.87	1.43	1.33
1	A	130	GLY	C-N	5.83	1.47	1.34
1	A	77	GLN	C-N	5.66	1.47	1.34
1	A	367	ALA	C-N	5.50	1.46	1.34
1	A	121	ARG	C-N	5.41	1.46	1.34
1	A	365	ALA	C-N	5.40	1.46	1.34
1	A	218	VAL	C-N	5.38	1.42	1.33
1	A	124	ASP	C-N	5.38	1.46	1.34
1	A	47	GLY	C-N	-5.25	1.22	1.34
1	A	11	PHE	C-N	5.25	1.46	1.34
1	A	217	GLU	C-N	5.23	1.46	1.34
1	A	308	ARG	C-N	5.20	1.46	1.34
1	A	226	LEU	C-N	5.16	1.46	1.34
1	A	67	GLU	C-N	-5.14	1.22	1.34
1	A	321	ARG	C-N	5.11	1.45	1.34
1	A	334	ARG	C-N	5.09	1.45	1.34
1	A	197	GLY	C-N	5.08	1.45	1.34
1	A	113	ARG	C-N	5.06	1.45	1.34
1	A	217	GLU	CD-OE1	-5.02	1.20	1.25

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	32.44	169.01	123.60
1	A	1	MET	O-C-N	23.88	160.91	122.70
1	A	1	MET	CA-C-N	-20.35	72.42	117.20
1	A	76	ARG	NE-CZ-NH2	-14.55	113.02	120.30
1	A	334	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	A	386	ALA	C-N-CA	13.64	155.81	121.70
1	A	31	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	A	331	ARG	NE-CZ-NH2	-12.52	114.04	120.30
1	A	368	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	A	10	ARG	CD-NE-CZ	12.21	140.70	123.60
1	A	2	ASN	CA-C-N	-12.10	90.59	117.20
1	A	31	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	A	386	ALA	O-C-N	-11.38	104.49	122.70
1	A	292	ARG	NE-CZ-NH2	-11.17	114.71	120.30
1	A	340	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	A	56	ASP	CB-CG-OD1	9.95	127.25	118.30
1	A	334	ARG	NE-CZ-NH1	9.91	125.25	120.30
1	A	10	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	69	GLU	O-C-N	-9.29	107.83	122.70
1	A	3	TYR	C-N-CA	9.10	144.46	121.70
1	A	177	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	A	245	ASP	CB-CG-OD1	8.71	126.14	118.30
1	A	2	ASN	O-C-N	-8.63	108.89	122.70
1	A	266	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	A	65	ASP	O-C-N	-8.49	109.11	122.70
1	A	157	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	A	3	TYR	O-C-N	-8.36	109.33	122.70
1	A	8	GLU	O-C-N	-8.31	109.40	122.70
1	A	308	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	A	5	PRO	O-C-N	8.07	135.62	122.70
1	A	66	SER	O-C-N	-7.96	109.96	122.70
1	A	7	PRO	O-C-N	-7.93	110.00	122.70
1	A	173	GLY	O-C-N	-7.84	110.15	122.70
1	A	373	GLU	OE1-CD-OE2	-7.84	113.89	123.30
1	A	101	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	74	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	254	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	A	326	VAL	O-C-N	-7.30	111.01	122.70
1	A	340	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	175	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	316	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	A	208	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	124	ASP	CB-CG-OD1	7.06	124.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	GLY	O-C-N	7.01	133.92	122.70
1	A	284	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	188	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	A	42	ARG	CD-NE-CZ	6.97	133.36	123.60
1	A	331	ARG	NH1-CZ-NH2	6.94	127.04	119.40
1	A	321	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	23	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	46	LEU	C-N-CA	-6.81	108.00	122.30
1	A	163	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	64	SER	O-C-N	-6.74	111.92	122.70
1	A	188	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	69	GLU	C-N-CA	6.68	138.41	121.70
1	A	117	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	266	ARG	CD-NE-CZ	6.60	132.84	123.60
1	A	63	SER	C-N-CA	-6.49	105.48	121.70
1	A	213	GLY	O-C-N	6.42	132.97	122.70
1	A	313	LEU	CB-CG-CD1	6.39	121.87	111.00
1	A	287	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	378	LEU	CA-C-O	6.36	133.45	120.10
1	A	26	PHE	O-C-N	-6.35	112.41	123.20
1	A	137	TRP	C-N-CA	-6.34	108.98	122.30
1	A	319	ALA	N-CA-CB	-6.32	101.25	110.10
1	A	293	THR	CA-CB-CG2	-6.31	103.56	112.40
1	A	76	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	A	371	ALA	O-C-N	-6.30	112.62	122.70
1	A	321	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	188	ARG	NH1-CZ-NH2	-6.25	112.53	119.40
1	A	308	ARG	NH1-CZ-NH2	6.17	126.19	119.40
1	A	23	ARG	CD-NE-CZ	6.16	132.22	123.60
1	A	212	TYR	CB-CG-CD1	-6.15	117.31	121.00
1	A	280	TYR	C-N-CA	-6.12	106.41	121.70
1	A	295	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	49	HIS	O-C-N	-6.05	112.92	123.20
1	A	25	PRO	O-C-N	-6.04	113.03	122.70
1	A	81	ASP	O-C-N	-6.02	113.07	122.70
1	A	355	SER	O-C-N	6.01	132.31	122.70
1	A	342	THR	O-C-N	5.98	132.27	122.70
1	A	319	ALA	O-C-N	-5.96	113.16	122.70
1	A	35	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	168	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	A	190	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	23	ARG	O-C-N	-5.72	113.54	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	GLU	O-C-N	-5.72	113.54	122.70
1	A	189	GLY	CA-C-N	-5.71	104.64	117.20
1	A	74	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	101	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	28	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	170	THR	O-C-N	-5.64	113.67	122.70
1	A	334	ARG	O-C-N	-5.62	113.70	122.70
1	A	5	PRO	CA-C-N	-5.61	104.87	117.20
1	A	208	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	245	ASP	O-C-N	5.58	131.62	122.70
1	A	169	VAL	O-C-N	-5.55	113.81	122.70
1	A	13	PHE	C-N-CA	-5.54	110.66	122.30
1	A	35	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	144	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	A	260	PHE	C-N-CA	5.49	133.84	122.30
1	A	308	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	32	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	32	ARG	C-N-CA	5.43	135.27	121.70
1	A	147	GLY	O-C-N	-5.38	114.09	122.70
1	A	34	LEU	O-C-N	5.37	131.30	122.70
1	A	163	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	131	ALA	N-CA-CB	-5.23	102.78	110.10
1	A	24	ASP	CB-CA-C	5.12	120.64	110.40
1	A	316	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	A	106	ALA	CB-CA-C	-5.09	102.47	110.10
1	A	51	VAL	O-C-N	-5.07	114.59	122.70
1	A	287	ASP	OD1-CG-OD2	-5.07	113.67	123.30
1	A	168	TYR	O-C-N	-5.06	114.61	122.70
1	A	146	GLY	O-C-N	-5.04	114.62	123.20
1	A	8	GLU	CA-CB-CG	5.04	124.48	113.40
1	A	275	LEU	O-C-N	5.02	130.74	122.70
1	A	12	THR	O-C-N	5.02	130.73	122.70
1	A	26	PHE	CA-C-N	5.02	126.23	116.20
1	A	224	ALA	CB-CA-C	5.01	117.62	110.10
1	A	310	TYR	CB-CG-CD1	5.01	124.01	121.00
1	A	323	ASP	CB-CG-OD1	5.01	122.81	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	37	VAL	CA

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	GLY	Mainchain
1	A	13	PHE	Mainchain
1	A	132	GLU	Mainchain
1	A	170	THR	Mainchain
1	A	173	GLY	Mainchain
1	A	177	ARG	Mainchain
1	A	194	PRO	Mainchain
1	A	196	VAL	Mainchain
1	A	219	GLY	Mainchain
1	A	23	ARG	Mainchain
1	A	248	GLY	Mainchain
1	A	25	PRO	Mainchain
1	A	257	ASP	Mainchain
1	A	261	GLY	Mainchain
1	A	276	GLU	Mainchain
1	A	277	SER	Mainchain
1	A	278	ALA	Mainchain
1	A	286	PHE	Mainchain
1	A	287	ASP	Mainchain
1	A	3	TYR	Mainchain
1	A	304	ALA	Mainchain
1	A	324	PRO	Mainchain
1	A	33	ALA	Mainchain
1	A	359	GLU	Mainchain
1	A	381	ASP	Mainchain
1	A	386	ALA	Mainchain,Peptide
1	A	62	GLY	Mainchain
1	A	64	SER	Mainchain
1	A	65	ASP	Mainchain
1	A	66	SER	Mainchain
1	A	67	GLU	Mainchain
1	A	69	GLU	Mainchain
1	A	8	GLU	Mainchain
1	A	87	PRO	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	3048	0	2906	38	1
2	A	11	0	11	2	0
3	A	2	0	0	0	0
4	A	376	0	0	10	2
All	All	3437	0	2917	39	2

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 7.

All (39) 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:1:MET:C	1:A:2:ASN:N	1.88	1.26
1:A:2:ASN:C	1:A:3:TYR:N	1.91	1.24
1:A:1:MET:CA	1:A:2:ASN:N	2.03	1.20
1:A:1:MET:HA	1:A:2:ASN:N	1.89	0.87
1:A:2:ASN:CA	1:A:3:TYR:N	2.45	0.80
1:A:381:ASP:HB3	1:A:387:ARG:HG3	1.70	0.74
1:A:387:ARG:NH1	4:A:684:HOH:O	2.22	0.71
1:A:1:MET:N	1:A:2:ASN:N	2.40	0.70
1:A:152:ARG:HB3	4:A:726:HOH:O	1.93	0.68
1:A:212:TYR:HB3	4:A:739:HOH:O	1.93	0.68
1:A:68:ARG:NH2	4:A:557:HOH:O	2.31	0.57
1:A:20:TRP:CE2	1:A:289:LYS:HE2	2.39	0.56
1:A:2:ASN:HA	1:A:3:TYR:N	2.20	0.56
1:A:25:PRO:HG2	1:A:26:PHE:CD2	2.41	0.56
1:A:1:MET:C	1:A:2:ASN:CA	2.73	0.55
1:A:1:MET:H2	1:A:2:ASN:N	2.04	0.54
1:A:39:SER:O	1:A:43:LEU:HB2	2.09	0.53
1:A:360:PHE:CD2	1:A:362:VAL:HG12	2.44	0.51
1:A:10:ARG:NH1	4:A:741:HOH:O	2.38	0.51
1:A:354:ARG:NH2	1:A:359:GLU:OE2	2.42	0.50
1:A:251:GLY:HA3	4:A:713:HOH:O	2.12	0.50
1:A:76:ARG:HD3	4:A:770:HOH:O	2.11	0.50
2:A:389:ASO:H62	4:A:585:HOH:O	2.10	0.50
1:A:42:ARG:HA	1:A:42:ARG:HE	1.78	0.49
1:A:25:PRO:HG2	1:A:26:PHE:CE2	2.47	0.48
1:A:354:ARG:HB3	1:A:359:GLU:HG3	1.96	0.48
1:A:32:ARG:NH1	1:A:33:ALA:O	2.46	0.48
1:A:381:ASP:CB	1:A:387:ARG:HG3	2.42	0.48
1:A:70:GLU:O	1:A:74:ARG:HG3	2.14	0.47
1:A:34:LEU:HD13	1:A:39:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLY:N	4:A:665:HOH:O	2.48	0.46
1:A:130:GLY:HA2	4:A:756:HOH:O	2.16	0.46
1:A:245:ASP:OD1	1:A:285:HIS:HD2	2.00	0.45
1:A:9:ASP:O	1:A:10:ARG:HB2	2.17	0.43
1:A:24:ASP:HB2	1:A:25:PRO:CD	2.48	0.43
1:A:69:GLU:O	1:A:69:GLU:HG3	2.19	0.43
1:A:137:TRP:CE3	2:A:389:ASO:H2	2.54	0.42
1:A:354:ARG:NE	1:A:359:GLU:OE2	2.52	0.41
1:A:20:TRP:NE1	1:A:289:LYS:HE2	2.36	0.41

All (2) 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)
4:A:492:HOH:O	4:A:594:HOH:O[6_554]	2.12	0.08
1:A:28:ASP:OD2	4:A:599:HOH:O[3_656]	2.19	0.01

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	386/388 (100%)	368 (95%)	16 (4%)	2 (0%)	29 13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER
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	303/304 (100%)	286 (94%)	17 (6%)	21 7

All (17) 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	37	VAL
1	A	42	ARG
1	A	43	LEU
1	A	66	SER
1	A	76	ARG
1	A	91	THR
1	A	97	PRO
1	A	132	GLU
1	A	169	VAL
1	A	175	ASP
1	A	185	ASN
1	A	313	LEU
1	A	347	LEU
1	A	387	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	285	HIS

5.3.3 RNA [i](#)

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 monosaccharides 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	ASO	A	389	3	11,11,11	0.67	0	15,15,15	3.79	5 (33%)

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	ASO	A	389	3	-	2/2/19/19	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	389	ASO	O5-C5-C6	-13.10	86.67	107.20
2	A	389	ASO	C1-O5-C5	3.71	117.22	112.19
2	A	389	ASO	C3-C4-C5	2.89	115.39	110.24
2	A	389	ASO	O4-C4-C3	2.88	117.00	110.35
2	A	389	ASO	O3-C3-C4	-2.17	105.33	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	389	ASO	O5-C5-C6-O6
2	A	389	ASO	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	389	ASO	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2:ASN	C	3:TYR	N	1.91
1	A	1:MET	C	2:ASN	N	1.88
1	A	61:PHE	C	62:GLY	N	1.18
1	A	238:ALA	C	239:GLY	N	1.18
1	A	95:THR	C	96:HIS	N	1.17
1	A	175:ASP	C	176:ILE	N	1.09
1	A	3:TYR	C	4:GLN	N	0.98

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.