



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:49 AM UTC

PDB ID : 1XIE / pdb_00001xie
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 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

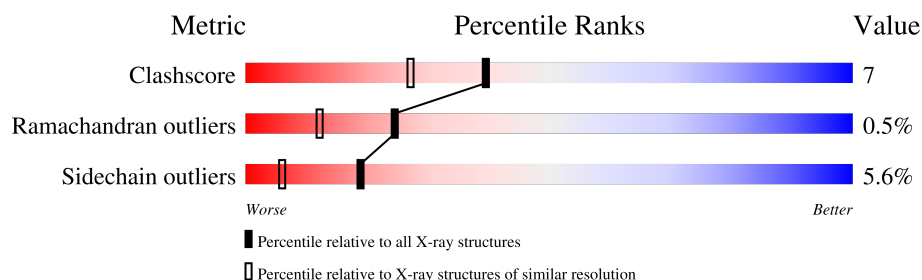
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (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 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	

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.

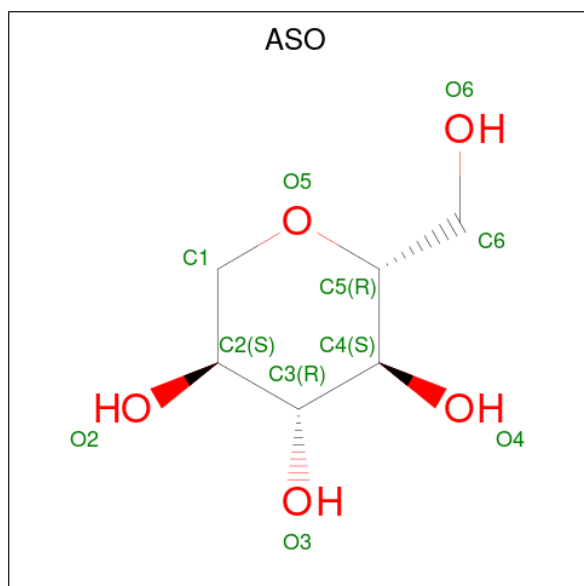
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

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 (CCD ID: 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 (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

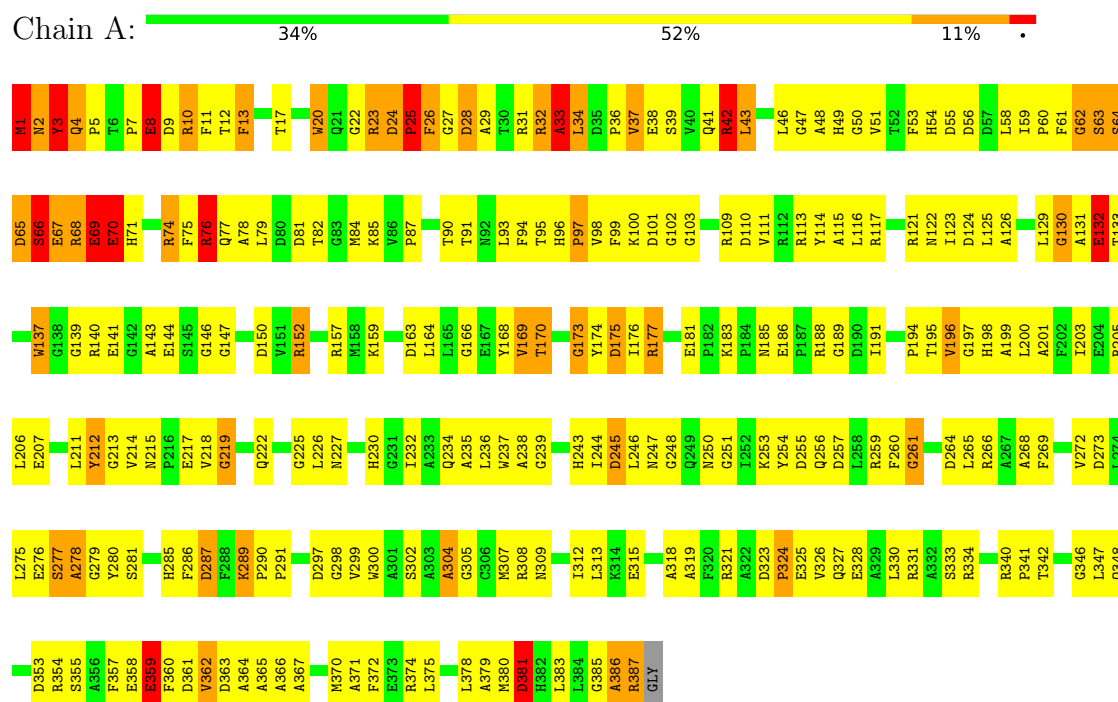
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	376	Total 376	O 376	0	0

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: ASO, 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	2.49	142/3126 (4.5%)	2.63	262/4231 (6.2%)

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	A	1	35

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	C-N	43.66	1.88	1.33
1	A	2	ASN	C-N	41.25	1.91	1.33
1	A	141	GLU	C-N	19.76	1.55	1.33
1	A	8	GLU	C-N	18.82	1.59	1.33
1	A	63	SER	C-N	18.27	1.56	1.33
1	A	175	ASP	C-N	-17.49	1.09	1.33
1	A	3	TYR	C-N	-17.14	0.98	1.33
1	A	254	TYR	C-N	16.87	1.57	1.33
1	A	278	ALA	C-N	15.93	1.53	1.33
1	A	28	ASP	C-N	15.79	1.54	1.33
1	A	25	PRO	C-N	15.72	1.55	1.33
1	A	328	GLU	C-N	15.35	1.53	1.33
1	A	191	ILE	C-N	15.05	1.53	1.33
1	A	24	ASP	C-N	14.68	1.48	1.34
1	A	319	ALA	C-N	14.40	1.52	1.33
1	A	212	TYR	C-N	13.39	1.53	1.33
1	A	114	TYR	C-N	13.13	1.51	1.33
1	A	302	SER	C-N	12.79	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	PHE	C-N	12.56	1.52	1.33
1	A	255	ASP	C-N	12.14	1.51	1.33
1	A	205	ARG	C-N	12.09	1.50	1.33
1	A	304	ALA	C-N	12.04	1.50	1.33
1	A	238	ALA	C-N	-11.84	1.19	1.33
1	A	297	ASP	C-N	11.40	1.49	1.33
1	A	95	THR	C-N	-10.95	1.17	1.33
1	A	49	HIS	C-N	10.71	1.45	1.33
1	A	130	GLY	C-N	10.70	1.47	1.33
1	A	61	PHE	C-N	-10.66	1.18	1.33
1	A	99	PHE	C-N	10.46	1.48	1.34
1	A	17	THR	C-N	10.44	1.45	1.34
1	A	93	LEU	C-N	10.39	1.48	1.33
1	A	378	LEU	C-N	10.37	1.48	1.33
1	A	65	ASP	C-N	10.31	1.47	1.33
1	A	385	GLY	C-N	10.26	1.48	1.33
1	A	124	ASP	C-N	10.22	1.46	1.33
1	A	324	PRO	C-N	10.12	1.48	1.34
1	A	33	ALA	C-N	10.10	1.48	1.33
1	A	100	LYS	C-N	10.07	1.48	1.33
1	A	77	GLN	C-N	10.02	1.47	1.33
1	A	67	GLU	C-N	-9.72	1.22	1.33
1	A	367	ALA	C-N	9.63	1.46	1.33
1	A	132	GLU	C-N	9.63	1.48	1.33
1	A	365	ALA	C-N	9.32	1.46	1.34
1	A	217	GLU	C-N	9.15	1.46	1.33
1	A	129	LEU	C-N	8.98	1.44	1.33
1	A	47	GLY	C-N	-8.94	1.22	1.33
1	A	82	THR	C-N	8.89	1.46	1.33
1	A	308	ARG	C-N	8.89	1.46	1.33
1	A	78	ALA	C-N	8.84	1.45	1.33
1	A	74	ARG	C-N	8.76	1.45	1.33
1	A	152	ARG	C-N	8.76	1.45	1.33
1	A	226	LEU	C-N	8.67	1.46	1.33
1	A	113	ARG	C-N	8.64	1.45	1.33
1	A	121	ARG	C-N	8.64	1.46	1.33
1	A	334	ARG	C-N	8.55	1.45	1.34
1	A	79	LEU	C-N	8.54	1.45	1.33
1	A	197	GLY	C-N	8.53	1.45	1.34
1	A	307	MET	C-N	8.52	1.44	1.33
1	A	261	GLY	C-N	8.36	1.44	1.33
1	A	11	PHE	C-N	8.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	ILE	C-N	8.31	1.45	1.33
1	A	62	GLY	C-N	8.17	1.45	1.33
1	A	225	GLY	C-N	8.16	1.44	1.33
1	A	321	ARG	C-N	8.08	1.45	1.33
1	A	146	GLY	C-N	7.98	1.45	1.33
1	A	281	SER	C-N	7.98	1.45	1.33
1	A	256	GLN	C-N	7.96	1.44	1.33
1	A	110	ASP	C-N	-7.95	1.23	1.33
1	A	125	LEU	C-N	7.93	1.43	1.33
1	A	123	ILE	C-N	7.90	1.44	1.33
1	A	7	PRO	C-N	7.85	1.44	1.34
1	A	346	GLY	C-N	7.79	1.44	1.33
1	A	117	ARG	C-N	7.77	1.43	1.33
1	A	144	GLU	C-N	7.73	1.43	1.33
1	A	27	GLY	C-N	-7.72	1.23	1.33
1	A	363	ASP	C-N	7.45	1.44	1.33
1	A	218	VAL	C-N	7.34	1.42	1.33
1	A	246	LEU	C-N	7.23	1.43	1.33
1	A	279	GLY	C-N	7.23	1.43	1.33
1	A	37	VAL	C-N	-7.16	1.25	1.33
1	A	131	ALA	C-N	-7.08	1.24	1.33
1	A	143	ALA	C-N	7.03	1.44	1.33
1	A	157	ARG	C-N	-7.00	1.24	1.33
1	A	362	VAL	C-N	-6.99	1.24	1.33
1	A	189	GLY	C-N	6.99	1.43	1.33
1	A	234	GLN	C-N	6.96	1.42	1.33
1	A	101	ASP	C-N	6.95	1.43	1.33
1	A	264	ASP	C-N	-6.88	1.24	1.33
1	A	98	VAL	C-N	6.87	1.44	1.33
1	A	22	GLY	C-N	-6.65	1.24	1.33
1	A	36	PRO	C-N	6.64	1.42	1.33
1	A	94	PHE	C-N	6.62	1.42	1.33
1	A	236	LEU	C-N	-6.61	1.25	1.34
1	A	20	TRP	C-N	6.59	1.43	1.33
1	A	109	ARG	C-N	6.55	1.43	1.34
1	A	222	GLN	C-N	6.40	1.42	1.33
1	A	230	HIS	C-N	-6.36	1.25	1.33
1	A	41	GLN	C-N	6.33	1.42	1.33
1	A	173	GLY	C-N	-6.25	1.24	1.33
1	A	56	ASP	C-N	6.21	1.43	1.33
1	A	122	ASN	C-N	6.12	1.41	1.33
1	A	330	LEU	C-N	6.10	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	GLU	C-N	6.10	1.41	1.33
1	A	359	GLU	C-N	6.08	1.42	1.33
1	A	331	ARG	C-N	-6.07	1.25	1.34
1	A	361	ASP	C-N	6.06	1.41	1.33
1	A	201	ALA	C-N	6.06	1.41	1.33
1	A	244	ILE	C-N	6.03	1.41	1.33
1	A	386	ALA	C-N	6.01	1.41	1.33
1	A	371	ALA	C-N	5.96	1.42	1.33
1	A	312	ILE	C-N	5.96	1.42	1.34
1	A	181	GLU	C-N	5.92	1.40	1.33
1	A	348	GLN	C-N	5.90	1.41	1.33
1	A	126	ALA	C-N	5.82	1.41	1.33
1	A	341	PRO	C-N	5.82	1.41	1.33
1	A	200	LEU	C-N	5.82	1.41	1.33
1	A	195	THR	C-N	5.77	1.41	1.33
1	A	265	LEU	C-N	5.76	1.41	1.33
1	A	85	LYS	C-N	5.75	1.39	1.33
1	A	176	ILE	C-N	-5.72	1.25	1.33
1	A	211	LEU	C-N	5.68	1.41	1.33
1	A	245	ASP	C-N	-5.68	1.25	1.33
1	A	58	LEU	C-N	-5.63	1.27	1.33
1	A	53	PHE	C-N	5.63	1.41	1.33
1	A	116	LEU	C-N	5.53	1.41	1.33
1	A	353	ASP	C-N	-5.52	1.26	1.34
1	A	12	THR	C-N	5.52	1.41	1.33
1	A	96	HIS	C-N	5.47	1.41	1.33
1	A	97	PRO	C-N	5.45	1.40	1.34
1	A	219	GLY	C-N	5.36	1.41	1.33
1	A	237	TRP	C-N	5.31	1.41	1.33
1	A	379	ALA	C-N	5.30	1.40	1.33
1	A	166	GLY	C-N	5.27	1.40	1.33
1	A	102	GLY	C-N	5.25	1.41	1.33
1	A	102	GLY	C-O	5.25	1.28	1.23
1	A	115	ALA	C-N	5.20	1.41	1.33
1	A	298	GLY	C-N	5.19	1.40	1.33
1	A	305	GLY	C-N	5.17	1.40	1.33
1	A	60	PRO	C-N	-5.16	1.26	1.33
1	A	133	THR	C-N	5.16	1.41	1.33
1	A	358	GLU	C-N	5.14	1.42	1.34
1	A	277	SER	C-N	-5.03	1.26	1.33

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ARG	CD-NE-CZ	31.87	169.01	124.40
1	A	1	MET	O-C-N	23.69	160.91	123.00
1	A	386	ALA	CA-C-N	18.95	155.81	121.70
1	A	386	ALA	C-N-CA	18.95	155.81	121.70
1	A	69	GLU	O-C-N	-13.83	107.83	122.07
1	A	386	ALA	O-C-N	-13.61	104.49	122.59
1	A	2	ASN	O-C-N	-12.78	108.89	123.33
1	A	378	LEU	CA-C-O	12.17	133.45	120.55
1	A	10	ARG	CD-NE-CZ	11.64	140.70	124.40
1	A	173	GLY	O-C-N	-11.35	110.15	122.41
1	A	37	VAL	N-CA-C	10.87	121.78	110.36
1	A	69	GLU	CA-C-N	10.83	138.41	121.19
1	A	69	GLU	C-N-CA	10.83	138.41	121.19
1	A	326	VAL	O-C-N	-10.47	111.01	121.90
1	A	8	GLU	O-C-N	-10.46	109.40	122.27
1	A	24	ASP	O-C-N	-10.31	113.72	121.14
1	A	63	SER	CA-C-N	-10.29	105.48	121.74
1	A	63	SER	C-N-CA	-10.29	105.48	121.74
1	A	5	PRO	O-C-N	10.21	135.62	123.06
1	A	13	PHE	CA-C-N	-10.18	110.66	121.45
1	A	13	PHE	C-N-CA	-10.18	110.66	121.45
1	A	3	TYR	O-C-N	-9.97	109.33	122.59
1	A	32	ARG	CA-C-N	9.63	135.27	121.50
1	A	32	ARG	C-N-CA	9.63	135.27	121.50
1	A	280	TYR	CA-C-N	-9.42	106.41	122.14
1	A	280	TYR	C-N-CA	-9.42	106.41	122.14
1	A	3	TYR	CA-C-N	9.29	144.46	121.80
1	A	3	TYR	C-N-CA	9.29	144.46	121.80
1	A	7	PRO	O-C-N	-9.13	110.00	122.24
1	A	65	ASP	O-C-N	-9.12	109.11	122.43
1	A	59	ILE	CA-C-N	8.90	129.46	119.93
1	A	59	ILE	C-N-CA	8.90	129.46	119.93
1	A	50	GLY	O-C-N	8.89	133.92	123.61
1	A	46	LEU	CA-C-N	-8.89	108.00	122.40
1	A	46	LEU	C-N-CA	-8.89	108.00	122.40
1	A	342	THR	O-C-N	8.88	132.27	122.15
1	A	66	SER	O-C-N	-8.73	109.96	122.36
1	A	269	PHE	N-CA-C	-8.71	101.73	111.14
1	A	49	HIS	CA-C-O	8.48	128.82	119.24
1	A	169	VAL	O-C-N	-8.31	113.81	121.87
1	A	315	GLU	O-C-N	-8.28	113.54	122.07
1	A	275	LEU	O-C-N	8.13	130.74	122.12
1	A	90	THR	O-C-N	-8.06	114.80	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	SER	O-C-N	-7.96	111.92	121.79
1	A	213	GLY	O-C-N	7.90	132.97	122.70
1	A	23	ARG	O-C-N	-7.71	113.54	123.02
1	A	24	ASP	CB-CA-C	7.64	120.64	109.48
1	A	243	HIS	CA-C-O	-7.64	113.05	121.23
1	A	51	VAL	O-C-N	-7.64	114.59	123.00
1	A	62	GLY	O-C-N	-7.63	114.71	122.65
1	A	26	PHE	O-C-N	-7.55	112.41	122.22
1	A	357	PHE	CA-C-N	7.52	130.69	120.38
1	A	357	PHE	C-N-CA	7.52	130.69	120.38
1	A	319	ALA	O-C-N	-7.41	113.16	122.27
1	A	50	GLY	CA-C-N	-7.34	112.35	122.92
1	A	50	GLY	C-N-CA	-7.34	112.35	122.92
1	A	68	ARG	CA-C-N	-7.34	110.89	120.44
1	A	68	ARG	C-N-CA	-7.34	110.89	120.44
1	A	319	ALA	CA-C-O	7.31	128.38	119.97
1	A	4	GLN	O-C-N	-7.30	112.93	121.32
1	A	168	TYR	O-C-N	-7.25	114.61	122.07
1	A	207	GLU	CA-C-N	-7.20	113.74	123.46
1	A	207	GLU	C-N-CA	-7.20	113.74	123.46
1	A	269	PHE	CA-C-O	7.19	128.10	120.70
1	A	355	SER	O-C-N	7.14	132.31	122.46
1	A	207	GLU	CA-C-O	-7.07	113.05	120.55
1	A	49	HIS	O-C-N	-7.05	112.92	122.36
1	A	34	LEU	O-C-N	7.02	131.30	123.16
1	A	183	LYS	CA-C-O	-7.00	112.08	119.50
1	A	245	ASP	O-C-N	6.99	131.62	123.30
1	A	81	ASP	O-C-N	-6.99	113.07	122.43
1	A	1	MET	CA-C-N	-6.95	109.55	121.85
1	A	1	MET	C-N-CA	-6.95	109.55	121.85
1	A	272	VAL	CA-C-O	-6.93	113.74	120.95
1	A	327	GLN	CA-C-O	-6.89	113.25	120.55
1	A	76	ARG	NE-CZ-NH2	-6.86	113.02	119.20
1	A	371	ALA	CA-C-O	6.86	129.32	120.81
1	A	207	GLU	O-C-N	6.83	129.36	122.12
1	A	325	GLU	O-C-N	6.83	130.67	122.27
1	A	38	GLU	O-C-N	6.79	130.41	122.20
1	A	367	ALA	CA-C-N	-6.79	111.45	120.95
1	A	367	ALA	C-N-CA	-6.79	111.45	120.95
1	A	189	GLY	O-C-N	6.71	128.63	122.19
1	A	191	ILE	CA-C-O	6.64	128.28	120.72
1	A	147	GLY	O-C-N	-6.63	114.09	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	VAL	N-CA-CB	-6.58	101.59	110.54
1	A	319	ALA	N-CA-C	-6.54	104.23	111.82
1	A	375	LEU	O-C-N	-6.54	115.19	122.12
1	A	374	ARG	O-C-N	-6.50	114.73	122.15
1	A	375	LEU	CA-C-O	6.47	127.41	120.55
1	A	334	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	A	146	GLY	O-C-N	-6.42	114.62	122.71
1	A	170	THR	O-C-N	-6.42	113.67	122.46
1	A	42	ARG	CD-NE-CZ	6.40	133.36	124.40
1	A	111	VAL	O-C-N	6.40	128.42	121.83
1	A	37	VAL	N-CA-CB	6.38	117.59	110.51
1	A	71	HIS	O-C-N	6.37	128.71	122.09
1	A	269	PHE	CA-C-N	-6.35	110.03	121.14
1	A	269	PHE	C-N-CA	-6.35	110.03	121.14
1	A	24	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	93	LEU	N-CA-CB	-6.35	102.03	111.43
1	A	326	VAL	N-CA-C	-6.35	104.56	110.53
1	A	28	ASP	CA-C-O	6.35	129.23	121.99
1	A	137	TRP	CA-C-N	-6.34	108.98	121.41
1	A	137	TRP	C-N-CA	-6.34	108.98	121.41
1	A	260	PHE	CA-C-N	6.34	133.84	121.41
1	A	260	PHE	C-N-CA	6.34	133.84	121.41
1	A	4	GLN	CA-C-O	6.33	128.84	120.16
1	A	374	ARG	CA-C-O	6.33	127.13	120.42
1	A	287	ASP	CA-C-O	-6.33	114.98	122.13
1	A	67	GLU	CA-C-N	6.28	131.18	121.19
1	A	67	GLU	C-N-CA	6.28	131.18	121.19
1	A	302	SER	CA-C-O	6.27	127.41	120.82
1	A	5	PRO	CA-C-N	-6.25	114.96	123.96
1	A	5	PRO	C-N-CA	-6.25	114.96	123.96
1	A	358	GLU	N-CA-C	-6.22	103.81	111.33
1	A	42	ARG	CA-C-O	6.19	126.98	120.42
1	A	191	ILE	O-C-N	-6.18	116.84	123.14
1	A	227	ASN	OD1-CG-ND2	6.17	128.77	122.60
1	A	159	LYS	CA-C-O	6.16	127.08	120.55
1	A	177	ARG	NE-CZ-NH2	6.15	124.74	119.20
1	A	11	PHE	O-C-N	-6.14	115.85	123.04
1	A	157	ARG	CA-C-O	-6.14	114.04	120.55
1	A	131	ALA	CA-C-O	-6.14	114.87	121.56
1	A	235	ALA	CA-C-O	-6.12	114.39	120.82
1	A	12	THR	O-C-N	6.09	130.73	123.24
1	A	110	ASP	O-C-N	6.09	129.76	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ARG	CD-NE-CZ	6.03	132.84	124.40
1	A	175	ASP	CA-CB-CG	-6.02	106.58	112.60
1	A	71	HIS	CA-C-N	-6.01	112.99	120.56
1	A	71	HIS	C-N-CA	-6.01	112.99	120.56
1	A	366	ALA	CA-C-O	-6.01	113.31	120.10
1	A	33	ALA	CA-C-N	-5.99	113.23	122.09
1	A	33	ALA	C-N-CA	-5.99	113.23	122.09
1	A	253[1]	LYS	CA-C-O	-5.99	114.72	120.94
1	A	253[2]	LYS	CA-C-O	-5.99	114.72	120.94
1	A	370	MET	CA-C-O	-5.98	112.06	119.18
1	A	169	VAL	CA-C-O	5.97	127.16	120.95
1	A	133	THR	CA-C-N	-5.96	114.37	123.07
1	A	133	THR	C-N-CA	-5.96	114.37	123.07
1	A	331	ARG	NH1-CZ-NH2	5.95	127.04	119.30
1	A	31	ARG	NE-CZ-NH2	-5.94	113.86	119.20
1	A	307	MET	N-CA-C	5.93	117.75	111.28
1	A	67	GLU	O-C-N	-5.92	115.70	122.09
1	A	75	PHE	CA-C-O	5.91	127.02	120.82
1	A	141	GLU	CA-C-O	5.89	126.89	120.58
1	A	324	PRO	O-C-N	-5.88	115.48	122.24
1	A	273	ASP	CA-C-O	5.87	127.18	120.90
1	A	319	ALA	N-CA-CB	-5.83	101.25	110.28
1	A	364	ALA	CA-C-O	5.82	126.59	120.42
1	A	289	LYS	CA-C-N	-5.81	114.39	120.38
1	A	289	LYS	C-N-CA	-5.81	114.39	120.38
1	A	206	LEU	CA-C-N	-5.79	112.52	120.28
1	A	206	LEU	C-N-CA	-5.79	112.52	120.28
1	A	323	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	150	ASP	CA-C-O	-5.78	113.79	120.49
1	A	372	PHE	CA-C-O	-5.75	114.32	120.42
1	A	362	VAL	N-CA-C	5.75	116.53	110.72
1	A	141	GLU	CA-C-N	-5.74	112.00	121.12
1	A	141	GLU	C-N-CA	-5.74	112.00	121.12
1	A	331	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	A	174	TYR	O-C-N	5.72	129.79	123.16
1	A	300	TRP	CA-C-N	5.70	127.85	120.44
1	A	300	TRP	C-N-CA	5.70	127.85	120.44
1	A	268	ALA	CA-C-O	-5.68	113.69	120.10
1	A	250	ASN	OD1-CG-ND2	5.67	128.28	122.60
1	A	60	PRO	O-C-N	5.67	129.77	122.85
1	A	163	ASP	O-C-N	-5.67	116.11	122.12
1	A	309	ASN	OD1-CG-ND2	5.65	128.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LEU	CA-C-N	-5.62	114.50	122.94
1	A	211	LEU	C-N-CA	-5.62	114.50	122.94
1	A	65	ASP	CA-C-N	5.61	132.13	122.09
1	A	65	ASP	C-N-CA	5.61	132.13	122.09
1	A	379	ALA	N-CA-C	5.60	117.46	111.36
1	A	23	ARG	CD-NE-CZ	5.59	132.22	124.40
1	A	234	GLN	CB-CG-CD	5.58	122.08	112.60
1	A	159	LYS	O-C-N	-5.57	116.21	122.12
1	A	244	ILE	CB-CA-C	5.57	119.71	110.30
1	A	37	VAL	CB-CA-C	5.56	119.00	111.88
1	A	130	GLY	CA-C-N	-5.55	112.22	120.94
1	A	130	GLY	C-N-CA	-5.55	112.22	120.94
1	A	140	ARG	O-C-N	-5.55	115.64	122.25
1	A	273	ASP	CA-CB-CG	-5.55	107.05	112.60
1	A	331	ARG	O-C-N	5.55	129.09	122.27
1	A	371	ALA	O-C-N	-5.54	112.62	122.21
1	A	132	GLU	N-CA-CB	-5.54	102.38	110.47
1	A	199	ALA	CA-C-N	5.54	127.71	120.28
1	A	199	ALA	C-N-CA	5.54	127.71	120.28
1	A	215	ASN	N-CA-CB	-5.54	103.06	111.21
1	A	41	GLN	CB-CG-CD	5.53	122.00	112.60
1	A	189	GLY	CA-C-O	5.53	126.44	120.75
1	A	247	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	7	PRO	CA-C-N	5.51	128.69	120.31
1	A	7	PRO	C-N-CA	5.51	128.69	120.31
1	A	232	ILE	CA-C-N	5.50	127.97	120.54
1	A	232	ILE	C-N-CA	5.50	127.97	120.54
1	A	164	LEU	CA-C-O	-5.49	113.66	119.97
1	A	24	ASP	N-CA-CB	5.47	117.70	109.82
1	A	25	PRO	O-C-N	-5.47	113.03	122.17
1	A	380	MET	CA-C-O	-5.47	115.08	120.82
1	A	48	ALA	O-C-N	-5.45	116.38	122.75
1	A	198	HIS	CA-CB-CG	-5.44	108.36	113.80
1	A	185	ASN	OD1-CG-ND2	5.42	128.03	122.60
1	A	217	GLU	O-C-N	5.42	129.88	123.27
1	A	76	ARG	NH1-CZ-NH2	5.42	126.34	119.30
1	A	331	ARG	CA-C-O	-5.41	113.75	119.97
1	A	82	THR	N-CA-C	-5.41	107.04	113.97
1	A	139	GLY	N-CA-C	-5.40	108.24	115.32
1	A	312	ILE	O-C-N	-5.38	116.64	121.91
1	A	304	ALA	CA-C-N	-5.37	113.43	120.14
1	A	304	ALA	C-N-CA	-5.37	113.43	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ASP	O-C-N	-5.36	115.67	122.27
1	A	318	ALA	O-C-N	-5.34	116.45	122.12
1	A	268	ALA	CA-C-N	5.34	127.70	120.44
1	A	268	ALA	C-N-CA	5.34	127.70	120.44
1	A	237	TRP	O-C-N	-5.32	116.00	122.22
1	A	378	LEU	N-CA-C	5.32	117.08	111.28
1	A	239	GLY	O-C-N	-5.31	116.67	122.41
1	A	205	ARG	CA-C-N	-5.31	110.09	121.45
1	A	205	ARG	C-N-CA	-5.31	110.09	121.45
1	A	308	ARG	NH1-CZ-NH2	5.30	126.19	119.30
1	A	196	VAL	CA-C-O	-5.29	115.77	121.27
1	A	275	LEU	CA-C-N	-5.29	111.69	120.68
1	A	275	LEU	C-N-CA	-5.29	111.69	120.68
1	A	374	ARG	CA-C-N	5.28	127.36	120.28
1	A	374	ARG	C-N-CA	5.28	127.36	120.28
1	A	326	VAL	CA-C-O	5.28	126.91	121.05
1	A	308	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	A	84	MET	O-C-N	5.26	129.07	122.86
1	A	200	LEU	CA-C-O	5.25	126.12	120.55
1	A	308	ARG	CA-C-O	5.24	126.32	120.82
1	A	101	ASP	CA-C-N	-5.23	114.18	122.65
1	A	101	ASP	C-N-CA	-5.23	114.18	122.65
1	A	359	GLU	CA-C-N	-5.23	115.25	122.30
1	A	359	GLU	C-N-CA	-5.23	115.25	122.30
1	A	302	SER	O-C-N	-5.21	116.70	122.07
1	A	188	ARG	NH1-CZ-NH2	-5.21	112.53	119.30
1	A	383	LEU	CA-C-O	-5.21	114.21	120.10
1	A	29	ALA	CA-C-O	-5.20	115.89	121.56
1	A	8	GLU	CA-CB-CG	5.19	124.48	114.10
1	A	333	SER	CA-C-O	5.18	125.55	119.28
1	A	68	ARG	O-C-N	5.17	128.46	122.20
1	A	225	GLY	N-CA-C	-5.17	106.94	114.90
1	A	123	ILE	CA-C-N	-5.16	113.37	120.28
1	A	123	ILE	C-N-CA	-5.16	113.37	120.28
1	A	299	VAL	O-C-N	5.16	127.53	121.96
1	A	281	SER	CA-C-N	-5.15	113.78	121.87
1	A	281	SER	C-N-CA	-5.15	113.78	121.87
1	A	131	ALA	N-CA-CB	-5.13	102.78	110.17
1	A	34	LEU	CA-C-O	-5.11	115.04	120.92
1	A	188	ARG	NE-CZ-NH2	5.10	123.79	119.20
1	A	213	GLY	CA-C-N	-5.09	114.16	122.57
1	A	213	GLY	C-N-CA	-5.09	114.16	122.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	GLY	CA-C-O	5.09	126.04	119.68
1	A	214	VAL	CA-C-O	-5.08	115.76	121.75
1	A	27	GLY	CA-C-O	-5.05	116.52	121.06
1	A	12	THR	CA-C-N	-5.04	114.77	122.62
1	A	12	THR	C-N-CA	-5.04	114.77	122.62
1	A	259	ARG	CA-C-O	5.03	127.40	121.87
1	A	348	GLN	N-CA-C	5.03	116.76	111.28
1	A	299	VAL	CA-C-N	-5.01	112.35	120.72
1	A	299	VAL	C-N-CA	-5.01	112.35	120.72

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

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Mol	Chain	Res	Type	Group
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	2911	39	1
2	A	11	0	11	2	0
3	A	2	0	0	0	0
4	A	376	0	0	9	2
All	All	3437	0	2922	40	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 (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:A:1:MET:C	1:A:2:ASN:N	1.88	1.31
1:A:2:ASN:C	1:A:3:TYR:N	1.91	1.28
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:TYR:HB3	4:A:739:HOH:O	1.93	0.68
1:A:1:MET:C	1:A:2:ASN:CA	2.73	0.61
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: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:76:ARG:HD3	4:A:770:HOH:O	2.11	0.50
1:A:251:GLY:HA3	4:A:713:HOH:O	2.12	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
1:A:1:MET:H2	1:A:2:ASN:N	2.11	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:54:HIS:O	1:A:55:ASP:C	2.62	0.41
1:A:20:TRP:NE1	1:A:289:LYS:HE2	2.36	0.41
1:A:290:PRO:O	1:A:291:PRO:C	2.63	0.40

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

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	386/388 (100%)	368 (95%)	16 (4%)	2 (0%)	24 12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	SER
1	A	186	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	303/304 (100%)	286 (94%)	17 (6%)	19 6

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	70	GLU
1	A	76	ARG

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Mol	Chain	Res	Type
1	A	91	THR
1	A	97	PRO
1	A	132	GLU
1	A	169	VAL
1	A	175	ASP
1	A	313	LEU
1	A	347	LEU
1	A	387	ARG

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	41	GLN
1	A	285	HIS
1	A	348	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 oligosaccharides 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	ASO	A	389	3	11,11,11	0.64	0	15,15,15	3.26	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	-10.79	86.67	107.66
2	A	389	ASO	C1-O5-C5	3.75	117.22	112.19
2	A	389	ASO	C3-C4-C5	2.84	115.39	110.23
2	A	389	ASO	O4-C4-C3	2.81	117.00	110.38
2	A	389	ASO	O3-C3-C4	-2.14	105.33	110.38

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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.