



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:49 AM UTC

PDB ID : 1XLG / pdb_00001xlg
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT
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Deposited on : 1991-10-09
Resolution : 2.50 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

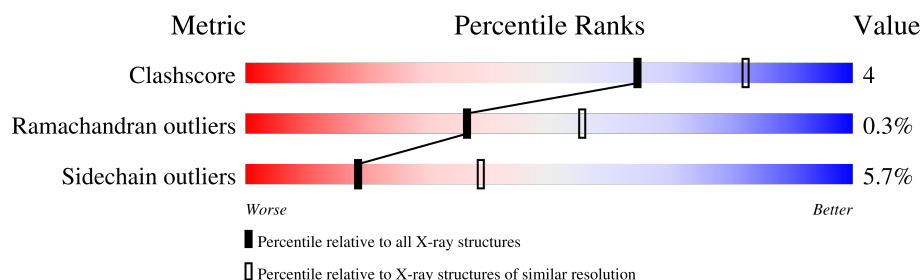
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	394	
1	B	394	

2 Entry composition [i](#)

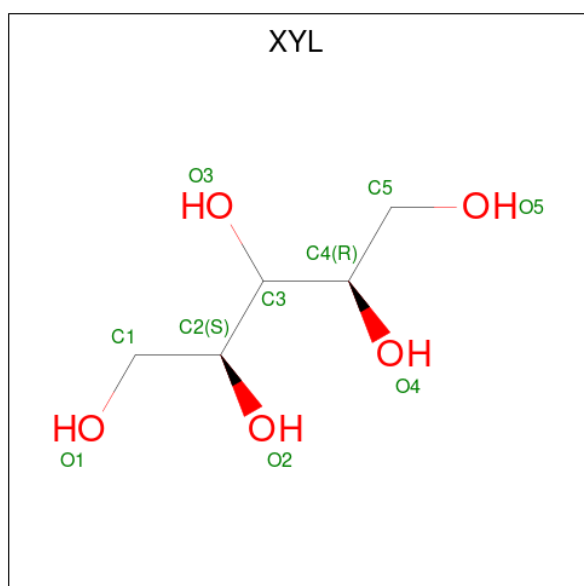
There are 5 unique types of molecules in this entry. The entry contains 6614 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	393	Total	C	N	O	S	0	0	0
			3027	1919	520	579	9			
1	B	393	Total	C	N	O	S	0	0	0
			3027	1919	520	579	9			

- Molecule 2 is Xylitol (CCD ID: XYL) (formula: C₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is ALUMINUM ION (CCD ID: AL) (formula: Al).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Al 1	0	0
4	B	1	Total 1	Al 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	266	Total 266	O 266	0	0
5	B	270	Total 270	O 270	0	0

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.80 Å 105.80 Å 153.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6614	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AL, MG, XYL

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	1.35	4/3101 (0.1%)	2.62	263/4204 (6.3%)
1	B	1.40	10/3101 (0.3%)	2.61	266/4204 (6.3%)
All	All	1.37	14/6202 (0.2%)	2.61	529/8408 (6.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	105	SER	C-O	8.36	1.33	1.23
1	A	102	GLY	CA-C	7.71	1.56	1.51
1	B	219	HIS	CG-ND1	5.71	1.44	1.38
1	B	5	THR	CB-OG1	5.54	1.52	1.43
1	B	217	THR	CA-CB	5.52	1.62	1.53
1	A	95	HIS	CA-CB	5.45	1.61	1.53
1	B	276	ASN	C-O	5.34	1.31	1.24
1	B	347	THR	CA-CB	5.32	1.61	1.53
1	B	20	THR	C-O	5.18	1.30	1.24
1	B	228	THR	C-O	5.17	1.30	1.24
1	B	104	THR	CA-CB	5.15	1.60	1.53
1	B	81	THR	CA-CB	5.15	1.61	1.53
1	A	217	THR	CA-CB	5.13	1.61	1.53
1	A	101	GLY	N-CA	5.09	1.49	1.45

All (529) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLU	CB-CG-CD	19.98	146.56	112.60
1	A	358	MET	CA-C-N	15.69	141.36	120.65
1	A	358	MET	C-N-CA	15.69	141.36	120.65
1	B	9	HIS	CA-CB-CG	13.27	127.07	113.80
1	A	6	PRO	CA-C-N	12.96	142.37	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	PRO	C-N-CA	12.96	142.37	120.72
1	B	174	ASN	OD1-CG-ND2	12.14	134.74	122.60
1	A	103	PHE	CA-CB-CG	11.90	125.70	113.80
1	B	217	THR	CA-C-N	11.88	133.17	119.98
1	B	217	THR	C-N-CA	11.88	133.17	119.98
1	B	319	LYS	CA-C-N	11.43	135.29	120.44
1	B	319	LYS	C-N-CA	11.43	135.29	120.44
1	B	187	ARG	NE-CZ-NH2	-11.31	109.02	119.20
1	A	71	LEU	CA-C-N	10.51	131.61	119.94
1	A	71	LEU	C-N-CA	10.51	131.61	119.94
1	B	208	GLY	CA-C-N	10.33	134.12	120.28
1	B	208	GLY	C-N-CA	10.33	134.12	120.28
1	A	244	ASP	CA-CB-CG	10.05	122.65	112.60
1	B	20	THR	N-CA-CB	-9.75	95.15	110.46
1	A	137	GLY	CA-C-N	9.61	132.15	120.14
1	A	137	GLY	C-N-CA	9.61	132.15	120.14
1	B	219	HIS	CB-CG-ND1	-9.45	108.53	122.70
1	A	31	LYS	CA-C-O	-9.35	111.02	121.87
1	B	206	GLU	CA-CB-CG	9.29	132.68	114.10
1	A	360	ASP	CA-C-N	9.13	133.43	120.28
1	A	360	ASP	C-N-CA	9.13	133.43	120.28
1	A	84	LYS	CA-C-N	9.12	139.01	122.13
1	A	84	LYS	C-N-CA	9.12	139.01	122.13
1	B	266	SER	CA-C-N	9.12	132.29	120.44
1	B	266	SER	C-N-CA	9.12	132.29	120.44
1	A	267	ALA	CA-C-N	9.11	133.45	120.79
1	A	267	ALA	C-N-CA	9.11	133.45	120.79
1	A	56	ASP	CA-C-N	9.08	134.34	121.71
1	A	56	ASP	C-N-CA	9.08	134.34	121.71
1	B	330	GLU	CA-CB-CG	9.04	132.18	114.10
1	B	332	GLN	CA-C-N	9.02	133.10	120.29
1	B	332	GLN	C-N-CA	9.02	133.10	120.29
1	B	40	HIS	CA-CB-CG	-8.95	104.85	113.80
1	B	37	GLU	CA-C-N	8.89	131.99	120.44
1	B	37	GLU	C-N-CA	8.89	131.99	120.44
1	B	56	ASP	N-CA-C	-8.78	100.89	111.69
1	A	174	ASN	CA-C-N	8.73	137.38	122.37
1	A	174	ASN	C-N-CA	8.73	137.38	122.37
1	B	6	PRO	CA-C-N	8.69	134.51	120.60
1	B	6	PRO	C-N-CA	8.69	134.51	120.60
1	A	372	ALA	O-C-N	-8.67	112.93	122.12
1	B	121	ASN	CA-CB-CG	-8.61	103.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	GLU	CA-C-O	8.47	128.04	118.97
1	A	102	GLY	N-CA-C	-8.45	102.52	110.21
1	B	199	LEU	CA-C-N	8.43	131.90	120.44
1	B	199	LEU	C-N-CA	8.43	131.90	120.44
1	B	308	ALA	CA-C-N	8.41	131.37	120.44
1	B	308	ALA	C-N-CA	8.41	131.37	120.44
1	A	254	ASP	CA-CB-CG	8.40	121.00	112.60
1	A	375	ARG	NE-CZ-NH2	-8.36	111.67	119.20
1	A	149	ASP	N-CA-C	-8.36	93.91	108.20
1	B	174	ASN	CA-CB-CG	-8.33	104.27	112.60
1	A	6	PRO	O-C-N	-8.28	111.46	122.64
1	B	300	GLY	O-C-N	-8.28	115.69	122.81
1	A	193	PRO	N-CA-C	8.19	125.33	114.27
1	A	111	ARG	CA-CB-CG	8.19	130.48	114.10
1	A	286	THR	CA-CB-OG1	-8.16	97.37	109.60
1	B	219	HIS	CB-CG-CD2	8.14	141.78	131.20
1	A	221	GLN	CA-C-N	8.02	134.12	120.72
1	A	221	GLN	C-N-CA	8.02	134.12	120.72
1	A	359	ASN	CA-CB-CG	7.92	120.52	112.60
1	B	231	ILE	CA-C-N	7.90	130.71	120.44
1	B	231	ILE	C-N-CA	7.90	130.71	120.44
1	A	266	SER	CA-C-N	7.87	131.17	120.54
1	A	266	SER	C-N-CA	7.87	131.17	120.54
1	B	163	THR	CA-C-O	-7.83	112.60	120.82
1	B	20	THR	CB-CA-C	7.79	124.67	109.72
1	B	221	GLN	CA-C-N	7.77	133.69	120.72
1	B	221	GLN	C-N-CA	7.77	133.69	120.72
1	A	357	LEU	CA-C-O	-7.75	112.20	120.42
1	A	290	HIS	CA-CB-CG	7.75	121.55	113.80
1	B	336	LYS	CB-CA-C	7.71	124.81	110.70
1	A	222	MET	CA-C-N	7.70	134.43	122.49
1	A	222	MET	C-N-CA	7.70	134.43	122.49
1	B	106	ASN	CA-C-N	7.70	132.89	121.72
1	B	106	ASN	C-N-CA	7.70	132.89	121.72
1	A	273	LEU	CA-C-O	-7.62	112.82	120.82
1	B	203	GLU	CA-C-N	7.56	135.01	122.54
1	B	203	GLU	C-N-CA	7.56	135.01	122.54
1	A	381	ARG	CA-C-O	-7.55	112.89	120.82
1	B	286	THR	N-CA-CB	-7.55	99.21	110.61
1	B	346	THR	CA-CB-OG1	-7.54	98.30	109.60
1	A	320	GLU	CA-CB-CG	7.52	129.13	114.10
1	B	149	ASP	N-CA-C	-7.51	95.36	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	ASP	CA-CB-CG	7.50	120.10	112.60
1	B	335	MET	CA-C-O	7.49	128.49	120.55
1	A	302	ASP	CA-C-N	7.47	128.28	119.98
1	A	302	ASP	C-N-CA	7.47	128.28	119.98
1	B	214	ASN	OD1-CG-ND2	-7.47	115.12	122.60
1	B	365	ALA	CA-C-O	-7.44	112.94	120.90
1	A	12	PHE	CA-C-N	-7.40	111.14	121.13
1	A	12	PHE	C-N-CA	-7.40	111.14	121.13
1	A	95	HIS	CA-C-N	7.40	128.06	119.47
1	A	95	HIS	C-N-CA	7.40	128.06	119.47
1	B	310	ALA	O-C-N	-7.40	114.28	122.12
1	A	174	ASN	N-CA-CB	-7.37	102.10	110.35
1	A	352	GLU	N-CA-C	-7.35	96.34	108.76
1	B	297	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	A	169	LYS	CA-C-N	7.33	129.97	120.44
1	A	169	LYS	C-N-CA	7.33	129.97	120.44
1	A	379	PHE	CA-CB-CG	7.25	121.05	113.80
1	A	217	THR	CA-C-N	7.24	128.02	119.98
1	A	217	THR	C-N-CA	7.24	128.02	119.98
1	A	372	ALA	CA-C-O	7.24	128.22	120.55
1	B	56	ASP	N-CA-CB	7.24	120.98	110.20
1	A	320	GLU	CA-C-N	7.22	129.96	120.28
1	A	320	GLU	C-N-CA	7.22	129.96	120.28
1	B	235	LEU	CA-C-O	7.22	128.40	120.82
1	A	167	TYR	CA-C-O	-7.21	113.25	120.82
1	A	371	ALA	CA-C-N	7.20	129.93	120.28
1	A	371	ALA	C-N-CA	7.20	129.93	120.28
1	B	372	ALA	O-C-N	-7.19	114.49	122.12
1	A	43	ALA	O-C-N	-7.19	114.66	122.07
1	B	187	ARG	NE-CZ-NH1	7.19	128.69	121.50
1	A	190	ILE	CA-C-O	-7.18	112.53	120.72
1	B	361	SER	CA-C-N	7.17	130.61	120.28
1	B	361	SER	C-N-CA	7.17	130.61	120.28
1	B	5	THR	CA-CB-CG2	7.14	122.64	110.50
1	A	26	GLY	O-C-N	7.13	130.40	123.76
1	B	249	ARG	CA-C-O	-7.10	112.78	121.58
1	B	20	THR	CA-CB-CG2	7.09	122.55	110.50
1	B	7	ALA	CA-C-N	7.02	132.44	120.72
1	B	7	ALA	C-N-CA	7.02	132.44	120.72
1	A	300	GLY	CA-C-O	-7.01	115.27	122.28
1	B	194	THR	CA-CB-OG1	-7.01	99.09	109.60
1	A	279	PRO	O-C-N	-7.01	113.69	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	324	ALA	CA-C-N	7.00	129.54	120.44
1	B	324	ALA	C-N-CA	7.00	129.54	120.44
1	B	23	ASP	CB-CA-C	6.99	123.94	110.17
1	B	197	HIS	CA-C-N	6.99	127.69	119.94
1	B	197	HIS	C-N-CA	6.99	127.69	119.94
1	A	23	ASP	CA-CB-CG	6.97	119.57	112.60
1	B	207	HIS	CA-C-N	6.93	128.80	120.14
1	B	207	HIS	C-N-CA	6.93	128.80	120.14
1	B	131	GLU	CA-C-O	6.92	126.75	119.14
1	B	214	ASN	CB-CG-ND2	6.92	126.78	116.40
1	B	334	ALA	CA-C-N	6.91	129.54	120.28
1	B	334	ALA	C-N-CA	6.91	129.54	120.28
1	A	203	GLU	CA-C-N	6.90	133.18	122.49
1	A	203	GLU	C-N-CA	6.90	133.18	122.49
1	B	237	ALA	CA-C-N	6.89	132.40	122.35
1	B	237	ALA	C-N-CA	6.89	132.40	122.35
1	A	103	PHE	CA-C-O	-6.88	113.26	120.55
1	A	174	ASN	CA-CB-CG	6.88	119.48	112.60
1	A	65	ALA	CA-C-O	-6.86	113.62	120.82
1	A	194	THR	CA-CB-CG2	6.86	122.16	110.50
1	A	190	ILE	O-C-N	6.86	130.13	123.14
1	A	334	ALA	CA-C-N	6.84	129.45	120.28
1	A	334	ALA	C-N-CA	6.84	129.45	120.28
1	A	33	LEU	CA-C-O	-6.84	112.98	120.43
1	A	289	ARG	CA-CB-CG	6.82	127.74	114.10
1	B	19	TRP	N-CA-CB	6.82	120.22	109.71
1	A	333	GLU	CA-CB-CG	6.82	127.74	114.10
1	A	223	ALA	CA-C-N	6.79	133.03	120.87
1	A	223	ALA	C-N-CA	6.79	133.03	120.87
1	B	194	THR	CA-CB-CG2	6.78	122.03	110.50
1	A	370	GLU	CA-C-O	-6.77	112.18	119.97
1	B	168	ILE	CA-C-N	6.76	129.23	120.44
1	B	168	ILE	C-N-CA	6.76	129.23	120.44
1	A	54	ASP	CA-C-O	-6.76	113.67	120.90
1	A	343	LEU	CA-C-N	6.75	132.36	120.74
1	A	343	LEU	C-N-CA	6.75	132.36	120.74
1	B	180	GLU	CA-C-O	6.73	126.69	120.09
1	B	203	GLU	O-C-N	-6.73	113.18	122.46
1	A	250	GLY	N-CA-C	6.71	122.86	112.45
1	A	298	THR	CA-C-N	6.69	131.99	122.09
1	A	298	THR	C-N-CA	6.69	131.99	122.09
1	A	342	GLU	CG-CD-OE2	-6.67	103.07	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LYS	CA-C-N	6.66	129.08	120.56
1	A	117	LYS	C-N-CA	6.66	129.08	120.56
1	B	241	PHE	CA-CB-CG	6.66	120.46	113.80
1	B	384	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	A	25	PHE	CA-CB-CG	-6.64	107.16	113.80
1	B	234	ALA	CA-C-N	6.64	129.07	120.44
1	B	234	ALA	C-N-CA	6.64	129.07	120.44
1	A	336	LYS	CA-C-N	6.63	129.49	120.54
1	A	336	LYS	C-N-CA	6.63	129.49	120.54
1	A	109	SER	N-CA-C	-6.63	103.98	111.14
1	B	127	GLU	CA-CB-CG	6.62	127.33	114.10
1	B	280	ASN	OD1-CG-ND2	-6.61	115.99	122.60
1	A	352	GLU	CA-C-O	-6.60	112.99	120.32
1	A	156	ARG	NE-CZ-NH2	-6.59	113.27	119.20
1	A	96	PRO	O-C-N	-6.59	114.20	122.17
1	A	215	PRO	CA-C-O	-6.58	113.64	121.67
1	B	43	ALA	CA-C-N	6.58	129.76	120.28
1	B	43	ALA	C-N-CA	6.58	129.76	120.28
1	A	335	MET	CA-C-N	6.58	129.38	120.44
1	A	335	MET	C-N-CA	6.58	129.38	120.44
1	B	103	PHE	N-CA-C	6.57	120.16	111.75
1	B	164	ALA	CA-C-N	6.56	129.37	120.44
1	B	164	ALA	C-N-CA	6.56	129.37	120.44
1	B	360	ASP	CA-CB-CG	6.56	119.16	112.60
1	A	120	HIS	CA-CB-CG	-6.55	107.25	113.80
1	A	285	TYR	CA-C-N	-6.51	112.34	122.37
1	A	285	TYR	C-N-CA	-6.51	112.34	122.37
1	A	297	ARG	CA-C-N	6.51	130.21	120.31
1	A	297	ARG	C-N-CA	6.51	130.21	120.31
1	A	14	LEU	O-C-N	-6.50	114.61	122.22
1	B	246	ASN	CA-CB-CG	6.50	119.10	112.60
1	A	84	LYS	O-C-N	-6.49	115.31	122.84
1	B	37	GLU	CB-CG-CD	6.49	123.63	112.60
1	A	19	TRP	CA-C-O	6.46	128.13	120.70
1	B	305	TRP	CB-CA-C	6.45	121.82	110.85
1	B	153	ALA	CA-C-N	6.44	129.43	120.29
1	B	153	ALA	C-N-CA	6.44	129.43	120.29
1	A	66	GLU	CB-CG-CD	6.43	123.53	112.60
1	B	130	ALA	CA-C-O	-6.42	114.09	121.47
1	B	305	TRP	O-C-N	-6.42	114.83	122.15
1	A	288	PRO	CA-C-O	-6.41	113.86	121.67
1	B	158	ARG	NE-CZ-NH2	-6.41	113.44	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	261	HIS	CA-C-N	6.40	133.95	121.41
1	B	261	HIS	C-N-CA	6.40	133.95	121.41
1	B	378	ALA	CA-C-N	6.38	130.01	120.31
1	B	378	ALA	C-N-CA	6.38	130.01	120.31
1	B	382	LEU	CA-C-O	-6.37	113.79	120.55
1	A	270	THR	CA-CB-CG2	6.36	121.32	110.50
1	A	233	GLN	OE1-CD-NE2	-6.35	116.25	122.60
1	A	94	SER	CA-C-O	-6.35	113.19	120.24
1	B	303	GLY	CA-C-N	6.34	128.54	120.56
1	B	303	GLY	C-N-CA	6.34	128.54	120.56
1	B	120	HIS	CA-C-N	6.32	129.38	120.28
1	B	120	HIS	C-N-CA	6.32	129.38	120.28
1	B	253	TYR	CA-C-N	-6.31	112.48	121.50
1	B	253	TYR	C-N-CA	-6.31	112.48	121.50
1	A	199	LEU	CA-C-N	6.30	128.63	120.44
1	A	199	LEU	C-N-CA	6.30	128.63	120.44
1	A	98	PHE	CA-C-N	6.29	129.34	120.28
1	A	98	PHE	C-N-CA	6.29	129.34	120.28
1	A	12	PHE	CA-C-O	-6.29	113.43	120.66
1	B	389	HIS	CA-CB-CG	-6.28	107.52	113.80
1	A	208	GLY	O-C-N	-6.26	115.58	122.84
1	B	330	GLU	CA-C-N	6.24	128.55	120.56
1	B	330	GLU	C-N-CA	6.24	128.55	120.56
1	A	163	THR	CA-C-O	-6.23	113.94	120.55
1	B	68	GLU	CB-CG-CD	6.22	123.18	112.60
1	A	64	GLU	CA-C-N	6.22	128.52	120.44
1	A	64	GLU	C-N-CA	6.22	128.52	120.44
1	B	207	HIS	CA-CB-CG	-6.20	107.60	113.80
1	A	329	PRO	CA-C-N	6.20	128.58	120.28
1	A	329	PRO	C-N-CA	6.20	128.58	120.28
1	A	297	ARG	O-C-N	-6.19	113.92	122.46
1	B	391	LEU	CA-C-N	6.16	133.48	121.41
1	B	391	LEU	C-N-CA	6.16	133.48	121.41
1	B	250	GLY	N-CA-C	6.16	119.78	112.33
1	B	80	ASP	CA-C-N	6.15	133.10	122.09
1	B	80	ASP	C-N-CA	6.15	133.10	122.09
1	A	106	ASN	N-CA-C	-6.15	104.66	111.36
1	B	178	ALA	O-C-N	-6.14	116.08	123.27
1	A	51	THR	CA-CB-CG2	6.14	120.94	110.50
1	A	156	ARG	NE-CZ-NH1	6.12	127.61	121.50
1	A	356	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	53	HIS	N-CA-CB	6.12	120.61	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASP	N-CA-CB	6.11	119.83	109.87
1	B	178	ALA	CB-CA-C	6.11	119.92	110.14
1	B	286	THR	CA-CB-CG2	6.11	120.89	110.50
1	B	279	PRO	CA-C-N	6.11	132.62	122.54
1	B	279	PRO	C-N-CA	6.11	132.62	122.54
1	A	19	TRP	CA-C-N	6.10	133.48	121.58
1	A	19	TRP	C-N-CA	6.10	133.48	121.58
1	A	20	THR	N-CA-CB	-6.09	100.18	110.41
1	B	254	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	185	GLU	CG-CD-OE1	-6.07	104.43	118.40
1	A	35	PRO	CA-C-N	6.07	128.33	120.56
1	A	35	PRO	C-N-CA	6.07	128.33	120.56
1	A	164	ALA	CA-C-N	6.07	128.91	120.29
1	A	164	ALA	C-N-CA	6.07	128.91	120.29
1	A	328	ASP	CA-C-N	6.07	126.24	119.32
1	A	328	ASP	C-N-CA	6.07	126.24	119.32
1	B	286	THR	CB-CA-C	6.04	120.37	110.17
1	B	274	LEU	O-C-N	6.01	128.59	122.09
1	A	305	TRP	CA-C-N	6.00	128.24	120.44
1	A	305	TRP	C-N-CA	6.00	128.24	120.44
1	A	187	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	B	115	LEU	CA-C-N	5.99	128.79	120.29
1	B	115	LEU	C-N-CA	5.99	128.79	120.29
1	A	75	ASN	CA-C-N	5.98	128.55	120.65
1	A	75	ASN	C-N-CA	5.98	128.55	120.65
1	B	383	ASN	CA-CB-CG	-5.98	106.62	112.60
1	A	276	ASN	OD1-CG-ND2	-5.97	116.62	122.60
1	B	127	GLU	O-C-N	-5.97	115.79	122.12
1	B	190	ILE	CA-C-O	-5.96	113.91	121.48
1	B	54	ASP	O-C-N	-5.96	115.25	122.11
1	B	68	GLU	CA-C-N	5.96	128.18	120.44
1	B	68	GLU	C-N-CA	5.96	128.18	120.44
1	B	342	GLU	CG-CD-OE2	-5.95	104.72	118.40
1	A	53	HIS	N-CA-CB	5.93	120.30	110.52
1	B	213	LEU	N-CA-CB	-5.93	101.60	111.20
1	A	156	ARG	CA-C-N	5.92	128.22	120.28
1	A	156	ARG	C-N-CA	5.92	128.22	120.28
1	A	165	ALA	CA-C-N	5.92	126.55	119.98
1	A	165	ALA	C-N-CA	5.92	126.55	119.98
1	A	121	ASN	CA-C-N	5.91	128.82	120.42
1	A	121	ASN	C-N-CA	5.91	128.82	120.42
1	A	320	GLU	CG-CD-OE2	5.90	131.97	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	VAL	CA-C-O	-5.88	115.15	121.27
1	B	12	PHE	CA-C-N	-5.88	115.21	121.45
1	B	12	PHE	C-N-CA	-5.88	115.21	121.45
1	B	270	THR	N-CA-C	-5.88	104.79	111.14
1	B	106	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	352	GLU	N-CA-CB	5.87	120.95	110.80
1	B	73	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	131	GLU	CA-C-O	5.85	126.02	119.41
1	B	336	LYS	N-CA-C	-5.85	104.50	111.69
1	A	236	TRP	CA-C-O	-5.83	114.37	120.55
1	B	188	GLY	O-C-N	-5.83	116.53	122.19
1	A	329	PRO	O-C-N	-5.83	115.54	122.24
1	A	56	ASP	CA-CB-CG	5.83	118.42	112.60
1	B	122	ILE	CA-C-N	5.81	128.34	120.44
1	B	122	ILE	C-N-CA	5.81	128.34	120.44
1	B	119	LEU	CB-CA-C	5.81	120.00	110.88
1	A	20	THR	CB-CA-C	5.80	121.49	109.95
1	B	359	ASN	CA-CB-CG	5.80	118.40	112.60
1	A	237	ALA	CA-C-N	5.80	130.40	122.34
1	A	237	ALA	C-N-CA	5.80	130.40	122.34
1	B	238	GLU	CG-CD-OE1	5.79	131.71	118.40
1	B	137	GLY	CA-C-N	5.77	127.36	120.14
1	B	137	GLY	C-N-CA	5.77	127.36	120.14
1	A	252	LYS	CA-C-O	-5.77	114.94	120.94
1	A	59	PRO	CB-CA-C	5.77	118.77	111.39
1	B	103	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	89	THR	O-C-N	-5.74	115.72	122.96
1	B	393	SER	CB-CA-C	5.74	119.02	109.38
1	A	206	GLU	N-CA-CB	5.72	118.37	110.07
1	B	252	LYS	CA-C-O	-5.72	115.00	120.94
1	A	136	TRP	N-CA-CB	5.71	120.11	110.46
1	B	379	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	305	TRP	CA-C-N	5.70	127.85	120.44
1	B	305	TRP	C-N-CA	5.70	127.85	120.44
1	A	308	ALA	CA-C-N	5.70	127.84	120.44
1	A	308	ALA	C-N-CA	5.70	127.84	120.44
1	A	101	GLY	O-C-N	5.69	129.17	123.48
1	B	75	ASN	CA-C-N	5.69	127.84	120.44
1	B	75	ASN	C-N-CA	5.69	127.84	120.44
1	B	307	SER	CA-C-N	5.69	127.84	120.44
1	B	307	SER	C-N-CA	5.69	127.84	120.44
1	A	107	ASP	CA-C-N	5.69	128.37	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASP	C-N-CA	5.69	128.37	120.29
1	B	74	PHE	CA-C-O	-5.68	114.85	120.82
1	A	44	GLU	CA-CB-CG	5.68	125.45	114.10
1	A	75	ASN	CA-CB-CG	5.67	118.27	112.60
1	B	370	GLU	CA-C-O	-5.67	114.41	120.42
1	B	162	ASP	CA-CB-CG	5.66	118.26	112.60
1	A	223	ALA	CA-C-O	5.64	126.04	119.32
1	B	190	ILE	O-C-N	5.64	129.12	122.69
1	A	185	GLU	O-C-N	-5.64	114.83	121.32
1	B	385	LEU	CB-CA-C	5.64	120.43	110.85
1	B	203	GLU	CG-CD-OE2	5.63	131.36	118.40
1	B	381	ARG	CA-C-N	5.63	127.83	120.28
1	B	381	ARG	C-N-CA	5.63	127.83	120.28
1	A	323	LEU	N-CA-C	-5.63	104.77	111.69
1	B	181	PRO	CB-CA-C	5.62	118.34	110.98
1	A	26	GLY	CA-C-O	-5.61	115.51	121.29
1	A	26	GLY	N-CA-C	5.60	119.25	110.91
1	A	383	ASN	CA-CB-CG	-5.60	107.00	112.60
1	B	358	MET	O-C-N	5.59	128.06	122.08
1	A	281	GLY	CA-C-O	-5.59	117.76	122.29
1	A	372	ALA	CA-C-N	5.58	131.37	120.99
1	A	372	ALA	C-N-CA	5.58	131.37	120.99
1	A	285	TYR	N-CA-CB	5.58	118.96	109.87
1	A	127	GLU	N-CA-CB	5.57	118.30	110.12
1	B	294	LYS	CB-CA-C	-5.56	102.76	110.16
1	B	111	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	A	231	ILE	CA-C-O	-5.56	114.47	120.47
1	B	57	LEU	N-CA-CB	-5.56	100.99	110.33
1	B	384	GLN	CA-C-N	5.56	128.18	120.29
1	B	384	GLN	C-N-CA	5.56	128.18	120.29
1	A	111	ARG	CA-C-N	5.55	128.18	120.29
1	A	111	ARG	C-N-CA	5.55	128.18	120.29
1	B	367	PHE	CA-C-O	-5.55	114.36	120.69
1	A	73	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	213	LEU	CA-C-N	5.55	128.95	122.85
1	A	213	LEU	C-N-CA	5.55	128.95	122.85
1	B	186	PRO	N-CA-C	5.55	126.52	112.10
1	A	28	ALA	CA-C-O	-5.54	115.05	121.15
1	B	306	ASP	CA-C-N	5.54	127.71	120.28
1	B	306	ASP	C-N-CA	5.54	127.71	120.28
1	B	272	ASP	O-C-N	-5.54	116.36	122.07
1	B	328	ASP	CA-C-N	5.54	125.20	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	328	ASP	C-N-CA	5.54	125.20	119.05
1	A	387	ILE	O-C-N	-5.54	116.50	121.87
1	A	229	HIS	CA-C-N	5.54	126.09	120.00
1	A	229	HIS	C-N-CA	5.54	126.09	120.00
1	A	272	ASP	CB-CA-C	5.52	119.55	110.88
1	B	312	MET	O-C-N	-5.52	115.86	122.15
1	B	121	ASN	CA-C-N	5.52	128.02	120.46
1	B	121	ASN	C-N-CA	5.52	128.02	120.46
1	B	120	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	228	THR	N-CA-CB	5.51	118.00	110.01
1	A	73	ASP	CA-C-O	-5.50	115.04	120.82
1	B	36	VAL	CB-CA-C	5.50	119.81	112.22
1	B	381	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	B	34	ASP	CA-C-N	5.49	125.31	119.28
1	B	34	ASP	C-N-CA	5.49	125.31	119.28
1	B	208	GLY	O-C-N	-5.48	116.43	122.24
1	A	389	HIS	N-CA-CB	5.48	118.27	110.16
1	B	361	SER	CA-C-O	-5.47	114.72	120.63
1	A	58	ILE	N-CA-C	5.47	112.97	107.55
1	A	59	PRO	CA-C-N	5.47	127.56	120.44
1	A	59	PRO	C-N-CA	5.47	127.56	120.44
1	A	163	THR	CA-C-N	5.46	127.60	120.28
1	A	163	THR	C-N-CA	5.46	127.60	120.28
1	B	267	ALA	CA-C-O	-5.46	115.08	120.82
1	B	174	ASN	CB-CG-ND2	-5.46	108.22	116.40
1	B	388	GLU	CA-C-O	-5.44	114.78	120.55
1	B	267	ALA	O-C-N	5.44	127.67	122.07
1	A	301	TYR	N-CA-C	5.43	117.96	111.71
1	B	340	VAL	N-CA-CB	5.42	116.89	110.55
1	B	32	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	297	ARG	CA-C-N	5.41	128.54	120.31
1	B	297	ARG	C-N-CA	5.41	128.54	120.31
1	A	177	ILE	O-C-N	5.40	129.09	122.83
1	B	384	GLN	O-C-N	-5.40	116.40	122.12
1	A	159	GLU	CA-CB-CG	5.40	124.89	114.10
1	A	18	GLY	CA-C-O	-5.39	113.14	119.50
1	A	39	VAL	CA-CB-CG2	5.38	119.55	110.40
1	A	279	PRO	CA-C-N	5.38	131.25	122.65
1	A	279	PRO	C-N-CA	5.38	131.25	122.65
1	B	267	ALA	N-CA-C	-5.38	105.32	111.07
1	A	172	GLY	CA-C-N	5.36	128.48	120.87
1	A	172	GLY	C-N-CA	5.36	128.48	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	N-CA-C	-5.35	97.79	107.75
1	B	64	GLU	CA-C-N	5.35	127.72	120.44
1	B	64	GLU	C-N-CA	5.35	127.72	120.44
1	A	189	ASP	CA-C-O	-5.35	113.70	120.28
1	A	324	ALA	CA-C-N	5.35	128.22	120.79
1	A	324	ALA	C-N-CA	5.35	128.22	120.79
1	B	31	LYS	CB-CA-C	5.34	120.38	109.76
1	B	146	GLY	CA-C-N	5.32	128.40	120.31
1	B	146	GLY	C-N-CA	5.32	128.40	120.31
1	B	233	GLN	N-CA-CB	5.31	117.93	110.12
1	A	388	GLU	CA-C-N	5.31	127.83	120.29
1	A	388	GLU	C-N-CA	5.31	127.83	120.29
1	B	12	PHE	N-CA-CB	5.30	121.02	111.37
1	A	235	LEU	CA-C-O	5.29	126.38	120.82
1	A	130	ALA	CA-C-O	-5.29	115.94	121.55
1	B	373	ALA	N-CA-C	5.29	119.48	113.19
1	B	112	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	B	290	HIS	CA-C-O	5.28	126.50	120.54
1	B	358	MET	N-CA-CB	5.28	117.84	109.82
1	A	207	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	9	HIS	CA-C-N	5.27	129.84	121.99
1	B	9	HIS	C-N-CA	5.27	129.84	121.99
1	A	149	ASP	N-CA-CB	5.27	119.06	110.37
1	B	188	GLY	CA-C-N	5.26	131.17	122.33
1	B	188	GLY	C-N-CA	5.26	131.17	122.33
1	A	310	ALA	CA-C-O	-5.26	115.27	120.90
1	A	48	TYR	N-CA-C	-5.26	106.99	113.41
1	B	394	ARG	NH1-CZ-NH2	5.26	126.14	119.30
1	B	294	LYS	CA-C-O	-5.25	114.94	119.72
1	A	313	SER	N-CA-CB	5.25	117.62	110.01
1	A	152	ALA	CA-C-O	-5.24	113.94	119.97
1	A	163	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	93	PHE	N-CA-C	5.23	121.34	114.75
1	A	38	ALA	CA-C-N	5.23	127.35	120.60
1	A	38	ALA	C-N-CA	5.23	127.35	120.60
1	B	227	PHE	CA-C-O	-5.23	115.00	120.55
1	B	286	THR	CA-CB-OG1	-5.22	101.77	109.60
1	B	96	PRO	O-C-N	-5.22	115.25	122.24
1	B	374	GLU	CA-C-N	5.21	129.55	121.26
1	B	374	GLU	C-N-CA	5.21	129.55	121.26
1	A	235	LEU	CA-C-N	5.21	127.26	120.28
1	A	235	LEU	C-N-CA	5.21	127.26	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	GLU	CB-CA-C	-5.20	101.00	110.63
1	A	16	THR	CB-CA-C	5.19	120.75	110.42
1	B	138	GLY	N-CA-C	5.19	120.04	113.24
1	B	300	GLY	CA-C-N	5.19	127.75	120.28
1	B	300	GLY	C-N-CA	5.19	127.75	120.28
1	B	201	PHE	CB-CA-C	-5.18	102.52	110.81
1	A	390	LEU	CA-C-N	5.18	131.69	121.58
1	A	390	LEU	C-N-CA	5.18	131.69	121.58
1	A	351	GLY	CA-C-N	5.17	130.71	122.74
1	A	351	GLY	C-N-CA	5.17	130.71	122.74
1	B	200	ALA	O-C-N	5.17	127.67	122.09
1	A	223	ALA	O-C-N	-5.16	116.00	122.24
1	B	163	THR	CA-CB-OG1	-5.15	101.87	109.60
1	B	213	LEU	CA-C-N	5.15	128.51	122.85
1	B	213	LEU	C-N-CA	5.15	128.51	122.85
1	B	48	TYR	N-CA-CB	-5.14	102.96	110.47
1	B	143	GLU	O-C-N	-5.14	116.26	122.48
1	B	334	ALA	O-C-N	-5.14	116.78	122.07
1	B	330	GLU	CG-CD-OE1	-5.13	106.59	118.40
1	B	188	GLY	N-CA-C	-5.13	106.20	112.77
1	A	206	GLU	N-CA-C	-5.13	105.60	111.14
1	B	229	HIS	CA-C-N	5.13	125.63	119.94
1	B	229	HIS	C-N-CA	5.13	125.63	119.94
1	B	170	ASP	CA-C-O	-5.12	114.32	120.10
1	B	259	PHE	CA-C-O	-5.11	115.09	120.92
1	B	57	LEU	CB-CA-C	5.10	118.76	110.24
1	B	320	GLU	CB-CG-CD	-5.10	103.93	112.60
1	B	31	LYS	CA-C-O	-5.10	115.80	121.81
1	B	294	LYS	CA-C-N	5.09	125.25	119.90
1	B	294	LYS	C-N-CA	5.09	125.25	119.90
1	B	235	LEU	O-C-N	-5.09	116.83	122.07
1	A	239	LYS	CA-CB-CG	5.08	124.27	114.10
1	B	209	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	21	GLY	N-CA-C	5.08	122.43	115.27
1	A	292	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	7	ALA	O-C-N	-5.07	115.80	122.39
1	A	105	SER	N-CA-C	-5.07	103.46	110.35
1	B	96	PRO	CA-C-N	5.07	128.47	120.47
1	B	96	PRO	C-N-CA	5.07	128.47	120.47
1	A	13	GLY	N-CA-C	-5.06	104.97	113.02
1	A	201	PHE	CA-CB-CG	5.06	118.86	113.80
1	B	5	THR	CA-C-N	5.06	126.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	THR	C-N-CA	5.06	126.16	119.84
1	A	344	GLY	CA-C-O	-5.05	113.69	119.65
1	A	286	THR	N-CA-C	5.04	120.05	112.94
1	B	60	PHE	CA-CB-CG	5.04	118.84	113.80
1	A	94	SER	N-CA-C	5.03	117.88	111.69
1	A	53	HIS	N-CA-C	-5.03	101.52	109.76
1	B	150	LEU	CA-C-O	-5.03	114.42	120.10
1	B	9	HIS	CG-CD2-NE2	5.03	112.23	107.20
1	B	249	ARG	O-C-N	-5.03	117.31	122.64
1	A	387	ILE	CA-C-N	5.02	127.01	120.28
1	A	387	ILE	C-N-CA	5.02	127.01	120.28
1	A	276	ASN	CA-C-O	-5.02	113.40	119.27
1	A	290	HIS	CA-C-O	-5.02	115.23	120.80
1	A	175	LEU	CB-CA-C	-5.01	99.20	109.38
1	A	394	ARG	CD-NE-CZ	5.01	131.42	124.40
1	A	127	GLU	CA-CB-CG	5.01	124.11	114.10
1	A	203	GLU	CG-CD-OE2	5.01	129.92	118.40
1	B	131	GLU	CB-CG-CD	5.01	121.11	112.60
1	A	66	GLU	CA-C-N	5.00	126.94	120.44
1	A	66	GLU	C-N-CA	5.00	126.94	120.44

There are no chirality outliers.

There are no planarity outliers.

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	3027	0	2882	24	0
1	B	3027	0	2882	26	0
2	A	10	0	11	0	0
2	B	10	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	266	0	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	270	0	0	1	0
All	All	6614	0	5785	46	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 4.

All (46) 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:B:275:GLU:HG3	1:B:319:LYS:HG3	1.63	0.81
1:A:95:HIS:HD2	1:A:97:VAL:H	1.35	0.75
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.73	0.70
1:B:95:HIS:HD2	1:B:97:VAL:H	1.40	0.67
1:A:235:LEU:HD12	1:A:273:LEU:HD21	1.77	0.66
1:B:235:LEU:HD12	1:B:273:LEU:HD21	1.79	0.65
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.79	0.63
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.80	0.63
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.70	0.56
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.88	0.56
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.72	0.54
1:A:95:HIS:CD2	1:A:97:VAL:H	2.23	0.54
1:A:296:SER:H	1:B:380:ILE:HD11	1.74	0.53
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.73	0.52
1:A:124:LEU:HA	1:A:127:GLU:HG3	1.93	0.51
1:B:55:ASN:HA	1:B:58:ILE:O	2.13	0.48
1:B:158:ARG:HD2	5:B:737(B):HOH:O	2.12	0.48
1:B:202:ILE:HD11	1:B:213:LEU:HD23	1.96	0.48
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.79	0.47
1:A:380:ILE:HD11	1:B:296:SER:HB2	1.96	0.47
1:B:249:ARG:O	1:B:252:LYS:HE3	2.13	0.47
1:A:20:THR:HG23	1:A:28:ALA:CB	2.44	0.47
1:A:75:ASN:ND2	5:A:568(A):HOH:O	2.48	0.46
1:A:296:SER:N	1:B:380:ILE:HD11	2.30	0.46
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.46
1:A:307:SER:HB3	1:B:380:ILE:HG21	1.98	0.45
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.41	0.45
1:A:222:MET:SD	1:A:254:ASP:HB3	2.56	0.45
1:B:243:ILE:O	1:B:290:HIS:HB3	2.17	0.45
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.99	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CD2	2.52	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.83	0.43
1:A:58:ILE:HD11	1:A:71:LEU:HD21	2.01	0.43
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.80	0.42
1:B:95:HIS:CD2	1:B:97:VAL:H	2.29	0.42
1:A:120:HIS:O	1:A:123:ASP:HB2	2.20	0.42
1:A:217:THR:HA	1:A:227:PHE:CD1	2.55	0.41
1:A:8:ASP:O	1:A:9:HIS:HB2	2.20	0.41
1:A:59:PRO:HG2	5:A:564(A):HOH:O	2.19	0.41
1:B:79:LYS:O	1:B:80:ASP:C	2.64	0.41
1:A:23:ASP:HB2	1:A:24:PRO:CD	2.50	0.41
1:A:243:ILE:O	1:A:290:HIS:HB3	2.21	0.41
1:B:216:GLU:HA	1:B:244:ASP:O	2.21	0.41
1:A:20:THR:HG23	1:A:28:ALA:HB1	2.02	0.40
1:B:185:GLU:HA	1:B:186:PRO:HA	1.78	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)
5:A:477(A):HOH:O	5:A:630(A):HOH:O[4_555]	2.10	0.10
5:A:473(A):HOH:O	5:A:596(A):HOH:O[4_555]	2.11	0.09

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	391/394 (99%)	376 (96%)	14 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	376 (96%)	14 (4%)	1 (0%)	36	55
All	All	782/788 (99%)	752 (96%)	28 (4%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	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	305/310 (98%)	292 (96%)	13 (4%)	26	51
1	B	305/310 (98%)	283 (93%)	22 (7%)	13	28
All	All	610/620 (98%)	575 (94%)	35 (6%)	18	39

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	94	SER
1	A	127	GLU
1	A	149	ASP
1	A	184	ASN
1	A	185	GLU
1	A	286	THR
1	A	309	LYS
1	A	330	GLU
1	A	359	ASN
1	A	363	SER
1	A	370	GLU
1	B	5	THR
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	69	LYS
1	B	90	THR
1	B	94	SER
1	B	131	GLU
1	B	149	ASP

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Mol	Chain	Res	Type
1	B	174	ASN
1	B	185	GLU
1	B	213	LEU
1	B	235	LEU
1	B	286	THR
1	B	320	GLU
1	B	330	GLU
1	B	333	GLU
1	B	357	LEU
1	B	359	ASN
1	B	370	GLU
1	B	391	LEU
1	B	393	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	174	ASN
1	A	184	ASN
1	A	221	GLN
1	A	233	GLN
1	A	383	ASN
1	A	384	GLN
1	B	95	HIS
1	B	184	ASN
1	B	221	GLN
1	B	359	ASN
1	B	384	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	XYL	B	400	3,4	9,9,9	0.86	1 (11%)	11,11,11	1.92	2 (18%)
2	XYL	A	400	3,4	9,9,9	0.89	0	11,11,11	1.97	4 (36%)

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	XYL	B	400	3,4	-	0/12/12/12	-
2	XYL	A	400	3,4	-	0/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	XYL	C4-C3	-2.33	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	XYL	C4-C3-C2	4.26	120.67	113.57
2	A	400	XYL	C4-C3-C2	3.87	120.01	113.57
2	A	400	XYL	O2-C2-C3	3.18	116.69	109.25
2	B	400	XYL	O1-C1-C2	2.83	117.10	111.16
2	A	400	XYL	O2-C2-C1	-2.39	103.59	109.03
2	A	400	XYL	C1-C2-C3	-2.20	107.69	112.17

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 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.