



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:32 AM UTC

PDB ID : 1XLD / pdb_00001xld
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT
Authors : Collyer, C.A.; Henrick, K.; Blow, D.M.
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

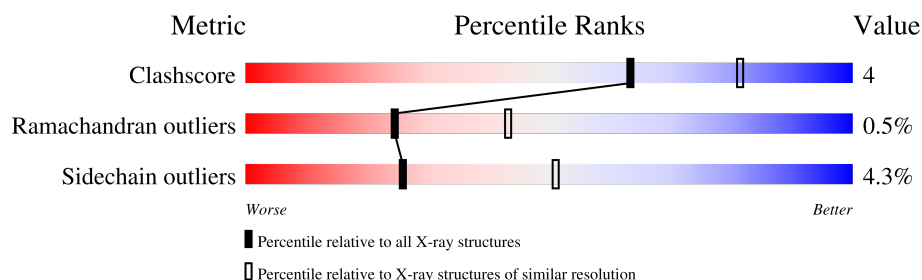
1 Overall quality at a glance

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](#)

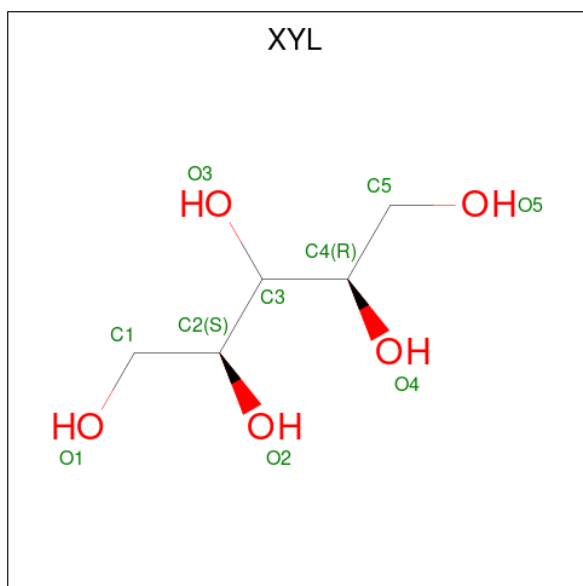
There are 4 unique types of molecules in this entry. The entry contains 6578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

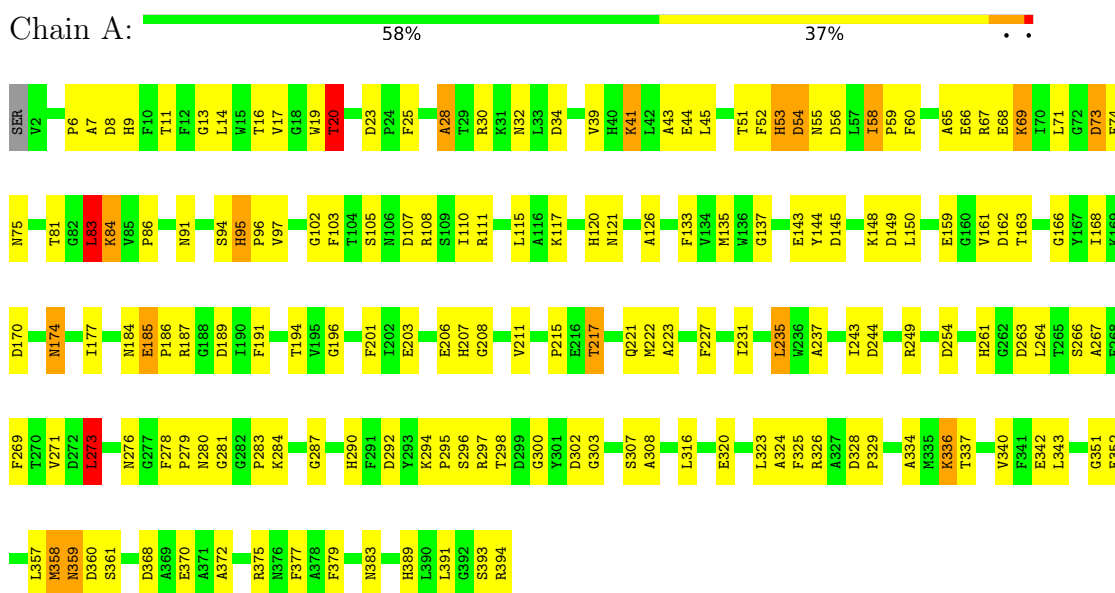
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	247	Total 247	O 247	0	0
4	B	253	Total 253	O 253	0	0

3 Residue-property plots

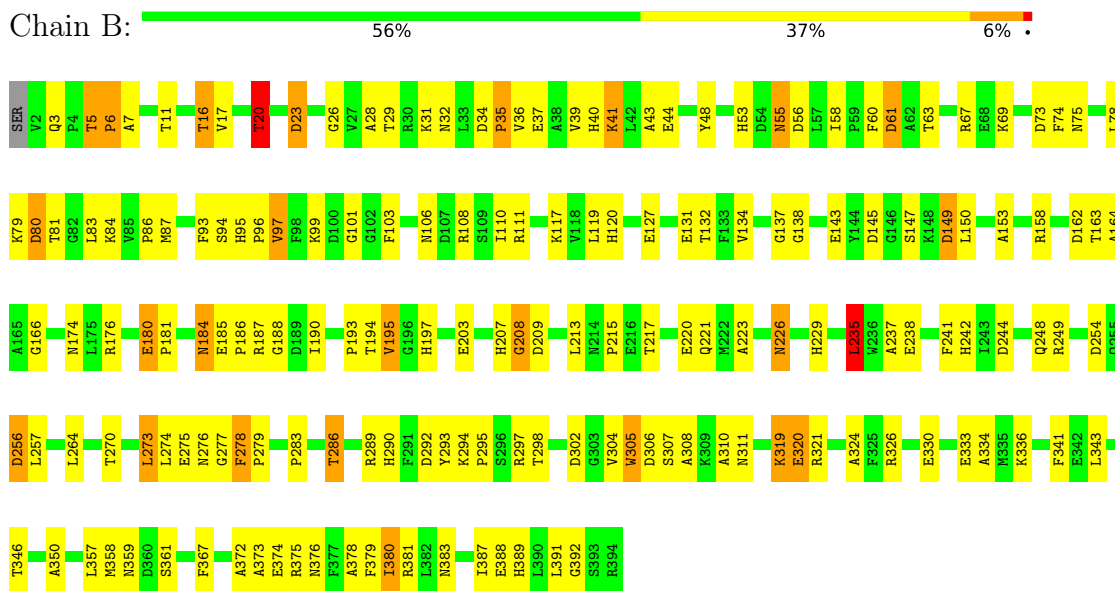
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



• 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	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.60 Å 105.60 Å 153.50 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}	0.148 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6578	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: XYL, 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	1.34	2/3101 (0.1%)	2.65	244/4204 (5.8%)
1	B	1.34	9/3101 (0.3%)	2.52	225/4204 (5.4%)
All	All	1.34	11/6202 (0.2%)	2.59	469/8408 (5.6%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	THR	CA-CB	6.17	1.63	1.53
1	B	277	GLY	N-CA	5.69	1.54	1.45
1	B	20	THR	N-CA	5.54	1.53	1.46
1	B	350	ALA	N-CA	5.49	1.53	1.46
1	A	264	LEU	C-O	5.42	1.30	1.24
1	B	286	THR	CA-CB	5.27	1.60	1.53
1	B	298	THR	CA-CB	5.09	1.61	1.53
1	A	103	PHE	C-O	5.08	1.30	1.24
1	B	23	ASP	N-CA	5.07	1.53	1.46
1	B	193	PRO	C-O	5.06	1.30	1.24
1	B	373	ALA	C-O	5.03	1.30	1.24

All (469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ASN	CA-CB-CG	28.51	141.11	112.60
1	A	394	ARG	CD-NE-CZ	26.47	161.46	124.40
1	A	67	ARG	CD-NE-CZ	15.83	146.57	124.40
1	A	244	ASP	CA-CB-CG	13.64	126.24	112.60
1	A	6	PRO	CA-C-N	13.57	143.38	120.72
1	A	6	PRO	C-N-CA	13.57	143.38	120.72
1	A	137	GLY	CA-C-N	13.13	134.56	119.98
1	A	137	GLY	C-N-CA	13.13	134.56	119.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	GLU	CA-CB-CG	11.95	137.99	114.10
1	B	60	PHE	CA-C-N	11.20	139.73	120.58
1	B	60	PHE	C-N-CA	11.20	139.73	120.58
1	B	381	ARG	NE-CZ-NH2	-10.85	109.43	119.20
1	A	372	ALA	O-C-N	-10.68	110.80	122.12
1	A	394	ARG	NE-CZ-NH1	10.64	132.14	121.50
1	A	103	PHE	CA-CB-CG	10.60	124.40	113.80
1	B	73	ASP	CA-CB-CG	10.20	122.80	112.60
1	B	217	THR	CA-C-N	10.19	131.44	120.03
1	B	217	THR	C-N-CA	10.19	131.44	120.03
1	A	342	GLU	N-CA-CB	10.19	125.91	110.22
1	B	32	ASN	CA-CB-CG	-9.92	102.68	112.60
1	B	20	THR	N-CA-CB	-9.84	94.48	110.42
1	B	237	ALA	CA-C-N	9.47	135.50	122.34
1	B	237	ALA	C-N-CA	9.47	135.50	122.34
1	A	65	ALA	N-CA-C	-9.46	100.66	110.97
1	B	164	ALA	CA-C-N	9.45	133.29	120.44
1	B	164	ALA	C-N-CA	9.45	133.29	120.44
1	B	372	ALA	O-C-N	-9.41	112.14	122.12
1	A	105	SER	CA-C-N	9.31	134.46	120.31
1	A	105	SER	C-N-CA	9.31	134.46	120.31
1	A	7	ALA	CA-C-N	9.19	133.34	120.29
1	A	7	ALA	C-N-CA	9.19	133.34	120.29
1	B	392	GLY	CA-C-N	9.18	136.28	120.68
1	B	392	GLY	C-N-CA	9.18	136.28	120.68
1	A	54	ASP	CA-CB-CG	9.15	121.75	112.60
1	B	379	PHE	CA-CB-CG	9.11	122.91	113.80
1	B	346	THR	CA-CB-OG1	-9.09	95.97	109.60
1	B	127	GLU	CA-CB-CG	8.95	131.99	114.10
1	A	28	ALA	CA-C-O	-8.93	111.32	121.15
1	A	149	ASP	N-CA-CB	8.93	125.11	110.37
1	B	343	LEU	CA-C-N	8.74	131.32	120.22
1	B	343	LEU	C-N-CA	8.74	131.32	120.22
1	B	319	LYS	CA-C-N	8.74	131.80	120.44
1	B	319	LYS	C-N-CA	8.74	131.80	120.44
1	B	143	GLU	CA-C-O	8.71	129.25	119.41
1	B	308	ALA	CA-C-N	8.53	131.53	120.44
1	B	308	ALA	C-N-CA	8.53	131.53	120.44
1	B	389	HIS	CA-CB-CG	-8.52	105.28	113.80
1	B	101	GLY	O-C-N	8.51	131.43	123.35
1	A	58	ILE	CA-C-O	8.50	125.41	119.20
1	A	297	ARG	CA-C-N	8.47	133.18	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ARG	C-N-CA	8.47	133.18	120.31
1	B	174	ASN	CA-C-N	8.45	136.22	122.29
1	B	174	ASN	C-N-CA	8.45	136.22	122.29
1	B	187	ARG	NE-CZ-NH2	-8.44	111.60	119.20
1	A	379	PHE	CA-CB-CG	8.41	122.21	113.80
1	A	149	ASP	N-CA-C	-8.33	93.96	108.20
1	A	389	HIS	CA-CB-CG	-8.30	105.50	113.80
1	B	302	ASP	CA-C-N	8.29	129.12	120.00
1	B	302	ASP	C-N-CA	8.29	129.12	120.00
1	B	93	PHE	CA-C-O	-8.26	108.70	120.51
1	B	20	THR	CB-CA-C	8.22	125.72	110.11
1	B	286	THR	N-CA-CB	-8.20	97.67	111.20
1	B	241	PHE	CA-CB-CG	8.19	121.99	113.80
1	A	329	PRO	CA-C-N	8.17	131.06	120.44
1	A	329	PRO	C-N-CA	8.17	131.06	120.44
1	B	180	GLU	CA-C-O	8.16	127.29	119.62
1	A	261	HIS	CA-C-N	8.08	137.25	121.41
1	A	261	HIS	C-N-CA	8.08	137.25	121.41
1	A	308	ALA	CA-C-N	8.05	131.07	120.28
1	A	308	ALA	C-N-CA	8.05	131.07	120.28
1	B	298	THR	CA-C-N	8.02	136.27	122.64
1	B	298	THR	C-N-CA	8.02	136.27	122.64
1	B	6	PRO	CA-C-N	8.00	131.80	120.28
1	B	6	PRO	C-N-CA	8.00	131.80	120.28
1	A	51	THR	CA-CB-CG2	7.95	124.02	110.50
1	B	137	GLY	CA-C-N	7.95	130.07	120.14
1	B	137	GLY	C-N-CA	7.95	130.07	120.14
1	A	6	PRO	O-C-N	-7.94	111.92	122.64
1	A	334	ALA	CA-C-N	7.89	130.85	120.28
1	A	334	ALA	C-N-CA	7.89	130.85	120.28
1	A	352	GLU	CA-C-O	-7.87	111.86	120.36
1	A	187	ARG	NE-CZ-NH2	-7.85	112.13	119.20
1	B	56	ASP	N-CA-CB	7.84	121.76	110.16
1	B	359	ASN	CA-CB-CG	-7.83	104.77	112.60
1	B	244	ASP	CA-CB-CG	7.81	120.41	112.60
1	A	222	MET	CA-C-N	7.75	134.50	122.49
1	A	222	MET	C-N-CA	7.75	134.50	122.49
1	A	143	GLU	CA-C-O	7.73	128.14	119.41
1	A	120	HIS	CA-CB-CG	-7.72	106.08	113.80
1	B	75	ASN	CA-CB-CG	-7.69	104.91	112.60
1	B	56	ASP	N-CA-C	-7.65	103.02	111.36
1	A	328	ASP	CA-C-O	7.64	127.06	119.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	LEU	CA-C-N	7.64	128.42	119.94
1	A	71	LEU	C-N-CA	7.64	128.42	119.94
1	B	75	ASN	OD1-CG-ND2	7.62	130.22	122.60
1	B	149	ASP	N-CA-C	-7.58	95.23	108.20
1	B	37	GLU	CB-CG-CD	7.58	125.48	112.60
1	B	103	PHE	CA-CB-CG	7.56	121.36	113.80
1	A	303	GLY	O-C-N	-7.56	114.94	122.19
1	B	361	SER	CA-C-N	7.51	131.73	120.31
1	B	361	SER	C-N-CA	7.51	131.73	120.31
1	B	248	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	A	203	GLU	CA-C-N	7.42	135.09	122.26
1	A	203	GLU	C-N-CA	7.42	135.09	122.26
1	A	372	ALA	CA-C-N	7.41	134.78	120.99
1	A	372	ALA	C-N-CA	7.41	134.78	120.99
1	A	237	ALA	CA-C-N	7.40	132.63	122.34
1	A	237	ALA	C-N-CA	7.40	132.63	122.34
1	A	352	GLU	N-CA-C	-7.36	96.90	108.90
1	B	383	ASN	CA-C-N	7.36	130.47	120.38
1	B	383	ASN	C-N-CA	7.36	130.47	120.38
1	B	150	LEU	CA-C-O	-7.36	112.75	120.55
1	A	375	ARG	NE-CZ-NH2	-7.34	112.60	119.20
1	B	7	ALA	CA-C-N	7.32	132.94	120.72
1	B	7	ALA	C-N-CA	7.32	132.94	120.72
1	B	120	HIS	CA-C-N	7.28	130.76	120.28
1	B	120	HIS	C-N-CA	7.28	130.76	120.28
1	B	111	ARG	CA-C-N	7.25	129.86	120.44
1	B	111	ARG	C-N-CA	7.25	129.86	120.44
1	A	94	SER	N-CA-C	7.24	120.23	111.40
1	A	368	ASP	CA-C-N	7.24	129.98	120.28
1	A	368	ASP	C-N-CA	7.24	129.98	120.28
1	A	145	ASP	CA-C-O	-7.21	111.95	120.10
1	A	377	PHE	CA-C-O	-7.19	111.70	119.97
1	A	20	THR	N-CA-CB	-7.18	98.70	110.40
1	A	52	PHE	O-C-N	7.16	130.78	123.26
1	A	115	LEU	CB-CA-C	7.15	122.66	110.79
1	B	23	ASP	CB-CA-C	7.15	124.26	110.17
1	B	238	GLU	CA-CB-CG	-7.12	99.87	114.10
1	A	32	ASN	CA-CB-CG	-7.12	105.48	112.60
1	A	107	ASP	CA-CB-CG	7.08	119.68	112.60
1	B	207	HIS	CA-C-N	7.08	129.05	120.13
1	B	207	HIS	C-N-CA	7.08	129.05	120.13
1	A	117	LYS	CA-C-N	7.07	129.61	120.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	LYS	C-N-CA	7.07	129.61	120.56
1	A	276	ASN	CA-C-O	-7.07	110.06	119.11
1	A	370	GLU	CA-C-O	-7.06	112.93	120.42
1	B	256	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	213	LEU	CA-C-N	7.04	130.59	122.85
1	B	213	LEU	C-N-CA	7.04	130.59	122.85
1	B	311	ASN	CA-C-N	7.04	130.28	120.29
1	B	311	ASN	C-N-CA	7.04	130.28	120.29
1	A	196	GLY	CA-C-N	7.03	129.70	120.28
1	A	196	GLY	C-N-CA	7.03	129.70	120.28
1	A	59	PRO	CB-CA-C	7.00	120.35	111.39
1	B	367	PHE	CA-C-N	-7.00	113.13	122.85
1	B	367	PHE	C-N-CA	-7.00	113.13	122.85
1	A	56	ASP	CA-C-N	6.95	131.38	121.71
1	A	56	ASP	C-N-CA	6.95	131.38	121.71
1	B	203	GLU	CA-C-N	6.94	133.99	122.54
1	B	203	GLU	C-N-CA	6.94	133.99	122.54
1	B	40	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	357	LEU	CA-C-O	-6.85	113.64	120.70
1	A	94	SER	CA-C-O	-6.81	113.26	120.55
1	A	23	ASP	CB-CA-C	6.79	123.54	110.17
1	B	334	ALA	CA-C-N	6.78	129.37	120.28
1	B	334	ALA	C-N-CA	6.78	129.37	120.28
1	B	264	LEU	N-CA-C	6.76	118.31	111.07
1	A	174	ASN	CA-C-N	6.73	133.94	122.37
1	A	174	ASN	C-N-CA	6.73	133.94	122.37
1	B	207	HIS	CA-CB-CG	-6.72	107.08	113.80
1	A	19	TRP	CA-C-N	6.72	132.90	121.14
1	A	19	TRP	C-N-CA	6.72	132.90	121.14
1	B	84	LYS	N-CA-C	-6.70	100.87	110.59
1	B	235	LEU	CA-C-O	6.70	127.85	120.82
1	A	13	GLY	N-CA-C	-6.69	102.38	113.02
1	A	342	GLU	CB-CA-C	-6.68	98.28	110.63
1	B	36	VAL	CA-C-N	6.65	129.74	120.29
1	B	36	VAL	C-N-CA	6.65	129.74	120.29
1	B	44	GLU	CG-CD-OE1	-6.64	103.12	118.40
1	A	269	PHE	CA-C-O	-6.63	112.34	119.97
1	B	48	TYR	N-CA-CB	-6.63	100.78	110.47
1	A	324	ALA	CA-C-N	6.59	129.35	120.65
1	A	324	ALA	C-N-CA	6.59	129.35	120.65
1	A	217	THR	CA-C-N	6.58	128.36	120.14
1	A	217	THR	C-N-CA	6.58	128.36	120.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	81	THR	N-CA-C	6.58	121.39	113.23
1	B	283	PRO	CB-CA-C	6.58	119.57	110.95
1	B	75	ASN	CA-C-N	6.56	128.97	120.44
1	B	75	ASN	C-N-CA	6.56	128.97	120.44
1	A	389	HIS	CA-C-N	6.55	129.36	120.38
1	A	389	HIS	C-N-CA	6.55	129.36	120.38
1	B	96	PRO	CA-C-N	6.54	130.80	120.47
1	B	96	PRO	C-N-CA	6.54	130.80	120.47
1	A	263	ASP	CA-CB-CG	6.51	119.11	112.60
1	A	25	PHE	CA-CB-CG	-6.50	107.30	113.80
1	A	143	GLU	CA-C-N	6.50	132.69	122.94
1	A	143	GLU	C-N-CA	6.50	132.69	122.94
1	A	44	GLU	O-C-N	-6.48	115.25	122.12
1	B	188	GLY	CA-C-N	6.48	131.91	122.77
1	B	188	GLY	C-N-CA	6.48	131.91	122.77
1	A	105	SER	N-CA-C	-6.46	101.57	110.35
1	A	168	ILE	CA-C-N	6.45	129.16	120.65
1	A	168	ILE	C-N-CA	6.45	129.16	120.65
1	B	145	ASP	CA-C-O	-6.45	112.55	119.97
1	A	74	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	215	PRO	CA-C-O	-6.41	113.85	121.67
1	A	144	TYR	CA-C-O	6.40	127.61	120.70
1	B	106	ASN	CA-C-N	6.39	130.44	121.24
1	B	106	ASN	C-N-CA	6.39	130.44	121.24
1	B	43	ALA	CA-C-O	-6.39	113.78	120.55
1	A	187	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	A	53	HIS	N-CA-CB	6.37	121.04	110.52
1	A	276	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	A	208	GLY	O-C-N	-6.37	115.48	122.68
1	B	391	LEU	CA-C-N	6.36	133.40	120.80
1	B	391	LEU	C-N-CA	6.36	133.40	120.80
1	A	269	PHE	CA-C-N	6.36	129.09	120.44
1	A	269	PHE	C-N-CA	6.36	129.09	120.44
1	B	359	ASN	CB-CA-C	6.36	121.68	110.37
1	A	300	GLY	CA-C-O	-6.34	115.94	122.28
1	A	280	ASN	OD1-CG-ND2	-6.33	116.28	122.60
1	A	120	HIS	O-C-N	-6.31	115.52	122.09
1	B	5	THR	CA-CB-CG2	6.31	121.22	110.50
1	B	311	ASN	OD1-CG-ND2	6.30	128.91	122.60
1	B	333	GLU	CA-CB-CG	6.29	126.69	114.10
1	A	221	GLN	CA-C-N	6.28	131.21	120.72
1	A	221	GLN	C-N-CA	6.28	131.21	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ALA	CA-C-O	-6.28	114.41	121.00
1	A	394	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	A	302	ASP	CA-C-N	6.27	126.94	119.98
1	A	302	ASP	C-N-CA	6.27	126.94	119.98
1	B	208	GLY	CA-C-N	6.27	128.97	120.38
1	B	208	GLY	C-N-CA	6.27	128.97	120.38
1	B	380	ILE	N-CA-CB	6.26	117.88	110.55
1	A	206	GLU	N-CA-CB	6.23	119.04	110.01
1	A	361	SER	N-CA-C	6.22	118.07	111.28
1	B	32	ASN	OD1-CG-ND2	6.22	128.82	122.60
1	A	359	ASN	CB-CG-ND2	6.21	125.72	116.40
1	B	274	LEU	O-C-N	6.18	129.20	122.15
1	B	117	LYS	CA-C-N	6.17	128.46	120.56
1	B	117	LYS	C-N-CA	6.17	128.46	120.56
1	B	34	ASP	CA-C-N	6.17	125.90	119.05
1	B	34	ASP	C-N-CA	6.17	125.90	119.05
1	B	341	PHE	N-CA-C	-6.16	104.12	111.69
1	A	91	ASN	CB-CG-ND2	-6.15	107.17	116.40
1	A	235	LEU	CA-C-N	6.15	128.52	120.28
1	A	235	LEU	C-N-CA	6.15	128.52	120.28
1	A	133	PHE	CA-C-O	6.14	126.85	120.40
1	A	360	ASP	CA-C-N	6.13	128.50	120.28
1	A	360	ASP	C-N-CA	6.13	128.50	120.28
1	A	34	ASP	O-C-N	6.12	127.40	121.28
1	B	36	VAL	CB-CA-C	6.12	120.67	112.22
1	A	283	PRO	CB-CA-C	6.11	119.00	111.12
1	B	184	ASN	OD1-CG-ND2	-6.09	116.50	122.60
1	A	95	HIS	CA-C-N	6.08	125.97	119.28
1	A	95	HIS	C-N-CA	6.08	125.97	119.28
1	A	211	VAL	CA-CB-CG2	6.05	120.68	110.40
1	B	120	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	243	ILE	CA-C-O	-6.04	114.97	121.19
1	B	324	ALA	CA-C-N	6.02	128.27	120.44
1	B	324	ALA	C-N-CA	6.02	128.27	120.44
1	B	138	GLY	CA-C-O	-6.01	113.90	120.40
1	B	209	ASP	CA-C-O	-6.01	114.13	120.63
1	B	53	HIS	N-CA-CB	5.99	120.41	110.52
1	B	194	THR	CA-CB-CG2	5.98	120.67	110.50
1	B	94	SER	N-CA-C	5.98	119.04	111.69
1	B	383	ASN	O-C-N	-5.98	115.79	122.12
1	B	221	GLN	CA-C-N	5.96	130.68	120.72
1	B	221	GLN	C-N-CA	5.96	130.68	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASP	O-C-N	5.96	128.21	122.07
1	B	108	ARG	CD-NE-CZ	5.95	132.73	124.40
1	B	101	GLY	CA-C-O	-5.95	116.84	122.13
1	A	108	ARG	CD-NE-CZ	5.94	132.72	124.40
1	A	19	TRP	CA-C-O	5.93	127.46	120.58
1	A	383	ASN	CA-CB-CG	-5.93	106.67	112.60
1	A	60	PHE	CA-CB-CG	5.93	119.73	113.80
1	B	376	ASN	CB-CG-ND2	5.93	125.29	116.40
1	A	297	ARG	NE-CZ-NH2	-5.92	113.88	119.20
1	A	266	SER	CA-C-N	5.91	128.12	120.44
1	A	266	SER	C-N-CA	5.91	128.12	120.44
1	B	298	THR	O-C-N	-5.90	115.32	122.22
1	B	163	THR	CA-CB-OG1	-5.89	100.77	109.60
1	A	287	GLY	CA-C-O	5.88	129.93	121.52
1	B	286	THR	OG1-CB-CG2	5.88	121.06	109.30
1	A	358	MET	CA-C-N	5.87	130.66	120.68
1	A	358	MET	C-N-CA	5.87	130.66	120.68
1	A	292	ASP	CA-C-O	-5.87	113.89	121.11
1	B	249	ARG	O-C-N	-5.86	115.81	122.84
1	A	281	GLY	CA-C-O	-5.86	117.18	122.57
1	A	84	LYS	CA-CB-CG	5.85	125.80	114.10
1	A	14	LEU	CA-C-O	5.82	126.67	119.97
1	B	97	VAL	CA-CB-CG1	5.82	120.29	110.40
1	B	56	ASP	O-C-N	5.82	128.78	122.15
1	A	163	THR	CA-C-N	5.80	128.53	120.29
1	A	163	THR	C-N-CA	5.80	128.53	120.29
1	A	162	ASP	CA-C-O	-5.80	114.28	120.42
1	A	39	VAL	CA-C-N	5.79	128.32	120.44
1	A	39	VAL	C-N-CA	5.79	128.32	120.44
1	A	249	ARG	NE-CZ-NH1	5.79	127.29	121.50
1	A	271	VAL	O-C-N	-5.79	116.24	121.91
1	A	16	THR	CA-CB-OG1	-5.78	100.92	109.60
1	A	14	LEU	CA-C-N	5.77	130.36	120.72
1	A	14	LEU	C-N-CA	5.77	130.36	120.72
1	A	298	THR	CA-C-N	5.76	130.62	122.09
1	A	298	THR	C-N-CA	5.76	130.62	122.09
1	A	170	ASP	CA-C-O	-5.76	114.41	120.63
1	A	235	LEU	CA-C-O	5.75	126.86	120.82
1	B	242	HIS	N-CA-C	-5.75	100.62	108.38
1	B	372	ALA	CB-CA-C	5.75	120.33	110.79
1	B	388	GLU	CA-C-N	5.75	127.98	120.28
1	B	388	GLU	C-N-CA	5.75	127.98	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	HIS	CA-C-N	5.74	128.54	120.28
1	A	120	HIS	C-N-CA	5.74	128.54	120.28
1	A	56	ASP	N-CA-CB	5.73	118.64	110.16
1	A	352	GLU	N-CA-CB	5.72	120.29	110.68
1	B	310	ALA	O-C-N	-5.72	116.06	122.12
1	B	297	ARG	CA-C-N	5.71	128.50	120.28
1	B	297	ARG	C-N-CA	5.71	128.50	120.28
1	A	66	GLU	O-C-N	-5.71	116.16	122.09
1	A	189	ASP	CA-C-O	-5.70	113.27	120.28
1	A	279	PRO	CA-C-N	5.70	131.49	122.60
1	A	279	PRO	C-N-CA	5.70	131.49	122.60
1	B	278	PHE	N-CA-C	5.70	117.25	110.07
1	A	359	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	A	370	GLU	CB-CG-CD	5.68	122.26	112.60
1	B	74	PHE	CA-C-O	-5.68	114.85	120.82
1	A	320	GLU	CA-CB-CG	5.67	125.44	114.10
1	A	308	ALA	CA-C-O	5.64	126.75	120.82
1	A	194	THR	CA-CB-CG2	5.64	120.09	110.50
1	B	31	LYS	CA-C-O	-5.64	115.41	121.56
1	A	83	LEU	CB-CA-C	5.64	119.08	109.72
1	B	257	LEU	O-C-N	5.61	129.69	122.23
1	B	26	GLY	N-CA-C	5.59	119.84	110.56
1	B	53	HIS	CA-CB-CG	5.58	119.38	113.80
1	A	343	LEU	CA-C-N	5.58	130.33	120.74
1	A	343	LEU	C-N-CA	5.58	130.33	120.74
1	B	330	GLU	CG-CD-OE1	-5.57	105.60	118.40
1	B	81	THR	CA-C-O	-5.56	112.76	119.27
1	B	190	ILE	CA-C-O	-5.54	114.40	120.72
1	B	302	ASP	CA-C-O	-5.54	113.60	119.97
1	B	20	THR	CA-CB-CG2	5.54	119.91	110.50
1	A	96	PRO	N-CA-CB	5.53	109.36	103.39
1	A	108	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	B	35	PRO	N-CA-CB	5.53	109.42	103.33
1	B	336	LYS	N-CA-C	-5.53	105.17	111.14
1	B	305	TRP	O-C-N	-5.53	115.75	122.22
1	A	391	LEU	CA-C-N	5.51	132.21	121.41
1	A	391	LEU	C-N-CA	5.51	132.21	121.41
1	B	320	GLU	CA-C-N	5.51	127.66	120.28
1	B	320	GLU	C-N-CA	5.51	127.66	120.28
1	B	166	GLY	N-CA-C	-5.50	106.12	112.73
1	A	267	ALA	CA-C-N	5.50	127.97	120.54
1	A	267	ALA	C-N-CA	5.50	127.97	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ALA	CA-C-N	5.50	128.10	120.29
1	B	153	ALA	C-N-CA	5.50	128.10	120.29
1	B	147	SER	CA-C-N	5.50	131.20	122.62
1	B	147	SER	C-N-CA	5.50	131.20	122.62
1	B	34	ASP	CB-CA-C	5.50	118.05	109.42
1	B	73	ASP	N-CA-CB	5.49	117.97	110.01
1	B	306	ASP	CA-CB-CG	5.49	118.09	112.60
1	A	163	THR	CA-CB-OG1	-5.49	101.37	109.60
1	B	176	ARG	CB-CG-CD	5.47	123.87	111.30
1	A	121	ASN	CA-C-N	5.46	128.17	120.42
1	A	121	ASN	C-N-CA	5.46	128.17	120.42
1	B	195	VAL	CA-C-N	5.46	126.16	119.99
1	B	195	VAL	C-N-CA	5.46	126.16	119.99
1	A	203	GLU	CB-CG-CD	5.45	121.87	112.60
1	B	330	GLU	CG-CD-OE2	5.44	130.91	118.40
1	A	166	GLY	N-CA-C	-5.44	106.19	112.50
1	B	378	ALA	CA-C-N	5.44	128.57	120.31
1	B	378	ALA	C-N-CA	5.44	128.57	120.31
1	A	316	LEU	CB-CA-C	5.43	119.81	110.79
1	A	20	THR	CB-CA-C	5.42	121.31	109.99
1	B	389	HIS	N-CA-CB	5.40	118.06	110.12
1	B	223	ALA	O-C-N	-5.40	115.86	122.34
1	B	274	LEU	CA-C-O	-5.39	114.70	120.42
1	A	231	ILE	CA-C-N	5.39	127.50	120.28
1	A	231	ILE	C-N-CA	5.39	127.50	120.28
1	B	278	PHE	CA-C-N	5.38	125.45	119.32
1	B	278	PHE	C-N-CA	5.38	125.45	119.32
1	B	55	ASN	CA-C-N	5.38	127.93	120.29
1	B	55	ASN	C-N-CA	5.38	127.93	120.29
1	A	102	GLY	N-CA-C	-5.37	100.45	113.18
1	A	351	GLY	CA-C-N	5.37	130.57	122.99
1	A	351	GLY	C-N-CA	5.37	130.57	122.99
1	B	16	THR	OG1-CB-CG2	5.37	120.04	109.30
1	A	30	ARG	O-C-N	5.36	130.16	123.19
1	B	187	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	A	326	ARG	NE-CZ-NH2	-5.35	114.38	119.20
1	A	297	ARG	N-CA-C	5.35	119.43	113.01
1	B	80	ASP	CA-C-N	5.35	131.07	121.66
1	B	80	ASP	C-N-CA	5.35	131.07	121.66
1	A	207	HIS	CA-C-N	5.33	130.28	120.79
1	A	207	HIS	C-N-CA	5.33	130.28	120.79
1	A	159	GLU	CA-C-N	5.32	125.84	119.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	GLU	C-N-CA	5.32	125.84	119.94
1	A	110	ILE	O-C-N	-5.31	116.70	121.91
1	A	280	ASN	CA-CB-CG	5.30	117.91	112.60
1	B	321	ARG	CA-C-N	5.30	128.36	120.31
1	B	321	ARG	C-N-CA	5.30	128.36	120.31
1	A	96	PRO	CA-C-N	5.29	127.99	120.53
1	A	96	PRO	C-N-CA	5.29	127.99	120.53
1	B	215	PRO	CA-C-O	-5.28	115.43	121.56
1	A	53	HIS	CB-CA-C	-5.28	100.61	109.48
1	B	276	ASN	CA-C-N	-5.27	111.21	121.01
1	B	276	ASN	C-N-CA	-5.27	111.21	121.01
1	B	119	LEU	CA-C-N	5.27	127.34	120.28
1	B	119	LEU	C-N-CA	5.27	127.34	120.28
1	B	99	LYS	CA-C-O	-5.26	114.15	120.10
1	A	17	VAL	CA-C-O	5.25	126.14	120.47
1	A	254	ASP	CB-CA-C	5.24	118.64	110.67
1	A	66	GLU	CA-C-N	5.24	127.30	120.28
1	A	66	GLU	C-N-CA	5.24	127.30	120.28
1	A	223	ALA	CA-C-O	5.24	125.56	119.32
1	B	197	HIS	CA-CB-CG	-5.24	108.56	113.80
1	B	292	ASP	CA-C-O	-5.24	116.21	122.13
1	A	111	ARG	CA-C-N	5.23	127.24	120.44
1	A	111	ARG	C-N-CA	5.23	127.24	120.44
1	B	29	THR	N-CA-C	-5.22	105.78	113.61
1	B	254	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	226	ASN	CA-CB-CG	-5.21	107.39	112.60
1	B	69	LYS	CA-C-N	5.20	127.31	120.60
1	B	69	LYS	C-N-CA	5.20	127.31	120.60
1	B	289	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	67	ARG	NE-CZ-NH1	5.20	126.69	121.50
1	A	297	ARG	CD-NE-CZ	5.20	131.67	124.40
1	B	134	VAL	CA-CB-CG1	5.20	119.23	110.40
1	A	278	PHE	CA-C-N	5.19	125.49	119.47
1	A	278	PHE	C-N-CA	5.19	125.49	119.47
1	A	59	PRO	CA-C-N	5.19	127.18	120.44
1	A	59	PRO	C-N-CA	5.19	127.18	120.44
1	A	336	LYS	CA-C-N	5.18	127.48	120.38
1	A	336	LYS	C-N-CA	5.18	127.48	120.38
1	A	96	PRO	O-C-N	-5.18	115.54	122.22
1	B	174	ASN	CB-CA-C	5.18	120.11	112.03
1	A	294	LYS	CB-CA-C	-5.17	103.28	110.16
1	B	387	ILE	N-CA-CB	5.17	117.56	110.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	203	GLU	CG-CD-OE2	5.16	130.27	118.40
1	B	44	GLU	N-CA-CB	5.16	117.70	110.12
1	B	307	SER	CA-C-N	5.15	127.14	120.44
1	B	307	SER	C-N-CA	5.15	127.14	120.44
1	B	63	THR	CA-CB-OG1	-5.15	101.88	109.60
1	A	325	PHE	CA-CB-CG	5.14	118.94	113.80
1	B	138	GLY	O-C-N	5.14	127.69	122.24
1	B	119	LEU	CB-CA-C	5.14	118.95	110.88
1	B	213	LEU	CA-CB-CG	5.14	134.28	116.30
1	B	376	ASN	CA-C-O	-5.14	115.08	120.58
1	A	75	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	292	ASP	O-C-N	5.13	129.00	122.84
1	B	304	VAL	CA-C-O	-5.13	115.80	121.29
1	A	81	THR	CA-CB-OG1	-5.13	101.91	109.60
1	A	207	HIS	O-C-N	-5.12	115.77	122.59
1	B	270	THR	N-CA-C	-5.12	105.61	111.14
1	A	84	LYS	CB-CA-C	5.12	118.80	109.83
1	A	107	ASP	CA-C-N	5.12	127.14	120.28
1	A	107	ASP	C-N-CA	5.12	127.14	120.28
1	A	359	ASN	CA-C-O	-5.12	113.75	119.79
1	B	186	PRO	N-CA-C	5.12	125.41	112.10
1	A	372	ALA	CA-C-O	5.12	126.16	120.63
1	A	126	ALA	O-C-N	-5.09	116.83	122.07
1	A	20	THR	CA-CB-CG2	5.09	119.15	110.50
1	A	273	LEU	CA-C-O	-5.09	115.16	120.55
1	B	326	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	A	323	LEU	N-CA-C	-5.08	105.45	111.69
1	B	44	GLU	CG-CD-OE2	5.07	130.06	118.40
1	B	78	LEU	N-CA-C	-5.07	105.65	111.07
1	A	290	HIS	CA-CB-CG	5.06	118.86	113.80
1	A	340	VAL	CA-C-O	-5.05	115.69	120.95
1	A	320	GLU	CG-CD-OE2	5.05	130.02	118.40
1	B	290	HIS	CA-CB-CG	5.05	118.85	113.80
1	A	201	PHE	CA-CB-CG	5.05	118.85	113.80
1	B	110	ILE	CB-CG1-CD1	5.05	124.40	113.80
1	A	393	SER	CA-C-N	5.04	130.78	121.70
1	A	393	SER	C-N-CA	5.04	130.78	121.70
1	B	61	ASP	CA-C-O	-5.04	114.64	120.24
1	B	67	ARG	CG-CD-NE	5.04	123.09	112.00
1	A	337	THR	CB-CA-C	-5.03	102.12	110.68
1	B	242	HIS	CA-CB-CG	5.03	118.83	113.80

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	25	0
2	A	10	0	10	0	0
2	B	10	0	10	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	247	0	0	2	0
4	B	253	0	0	1	0
All	All	6578	0	5784	47	0

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 (47) 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:95:HIS:HD2	1:A:97:VAL:H	1.31	0.79
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.78	0.66
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.77	0.65
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.79	0.63
1:B:95:HIS:HD2	1:B:97:VAL:H	1.47	0.63
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.82	0.62
1:A:135:MET:HE2	1:A:177:ILE:HG21	1.82	0.60
1:A:95:HIS:CD2	1:A:97:VAL:H	2.19	0.57
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.87	0.56
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.71	0.56
1:A:135:MET:HE1	1:A:161:VAL:HG22	1.86	0.56
1:B:235:LEU:HD12	1:B:273:LEU:HD11	1.89	0.55
1:B:55:ASN:HA	1:B:58:ILE:O	2.08	0.54
1:A:20:THR:HG23	1:A:28:ALA:CB	2.38	0.53
1:A:84:LYS:HB2	4:A:734(A):HOH:O	2.09	0.53
1:B:20:THR:HG23	1:B:28:ALA:CB	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLY:HA3	4:B:602(B):HOH:O	2.11	0.50
1:A:135:MET:CE	1:A:161:VAL:HG22	2.42	0.49
1:A:84:LYS:HD2	4:A:431(A):HOH:O	2.13	0.49
1:A:8:ASP:O	1:A:9:HIS:HB2	2.13	0.48
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.94	0.48
1:A:55:ASN:HA	1:A:58:ILE:O	2.15	0.47
1:A:217:THR:HA	1:A:227:PHE:CD1	2.50	0.47
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.74	0.47
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.16	0.46
1:A:307:SER:HB3	1:B:380:ILE:HG21	1.98	0.45
1:B:256:ASP:HB3	1:B:293:TYR:HA	1.98	0.45
1:A:135:MET:HE2	1:A:177:ILE:CG2	2.47	0.45
1:A:53:HIS:O	1:A:54:ASP:C	2.60	0.45
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.99	0.44
1:B:41:LYS:HG2	1:B:305:TRP:CD2	2.52	0.44
1:B:158:ARG:O	1:B:162:ASP:HB2	2.17	0.44
1:B:79:LYS:O	1:B:80:ASP:C	2.61	0.43
1:B:87:MET:HA	1:B:132:THR:O	2.18	0.43
1:B:35:PRO:O	1:B:39:VAL:HG23	2.19	0.43
1:A:307:SER:CB	1:B:380:ILE:HG21	2.50	0.42
1:B:374:GLU:O	1:B:375:ARG:C	2.61	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.98	0.42
1:A:295:PRO:O	1:A:296:SER:C	2.61	0.42
1:B:358:MET:HE2	1:B:358:MET:HB3	2.00	0.41
1:A:185:GLU:HA	1:A:186:PRO:HA	1.93	0.41
1:B:226:ASN:HB3	1:B:229:HIS:HB2	2.02	0.41
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.91	0.41
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.45	0.41
1:B:16:THR:OG1	1:B:17:VAL:N	2.54	0.41
1:A:235:LEU:HD12	1:A:273:LEU:HD11	2.03	0.40
1:A:41:LYS:O	1:A:45:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

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%)	368 (94%)	22 (6%)	1 (0%)	36	55
1	B	391/394 (99%)	375 (96%)	13 (3%)	3 (1%)	16	31
All	All	782/788 (99%)	743 (95%)	35 (4%)	4 (0%)	24	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU
1	B	3	GLN
1	B	23	ASP

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%)	292 (96%)	13 (4%)	26	51
All	All	610/620 (98%)	584 (96%)	26 (4%)	26	51

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	68	GLU
1	A	69	LYS
1	A	83	LEU
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	273	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	284	LYS
1	A	336	LYS
1	A	358	MET
1	A	359	ASN
1	B	5	THR
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	61	ASP
1	B	131	GLU
1	B	149	ASP
1	B	184	ASN
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	320	GLU
1	B	357	LEU

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	9	HIS
1	A	32	ASN
1	A	95	HIS
1	A	120	HIS
1	A	184	ASN
1	A	221	GLN
1	A	383	ASN
1	A	384	GLN
1	B	32	ASN
1	B	75	ASN
1	B	95	HIS
1	B	221	GLN
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 [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 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	A	400	3	9,9,9	0.60	0	11,11,11	2.05	2 (18%)
2	XYL	B	400	3	9,9,9	0.70	0	11,11,11	1.34	1 (9%)

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	A	400	3	-	1/12/12/12	-
2	XYL	B	400	3	-	0/12/12/12	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	XYL	C4-C3-C2	-4.91	105.40	113.57
2	A	400	XYL	O3-C3-C2	3.43	116.73	108.93
2	B	400	XYL	C5-C4-C3	-3.01	106.04	112.17

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	XYL	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

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.