



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:05 AM UTC

PDB ID : 1XLH / pdb_00001xlh
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
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

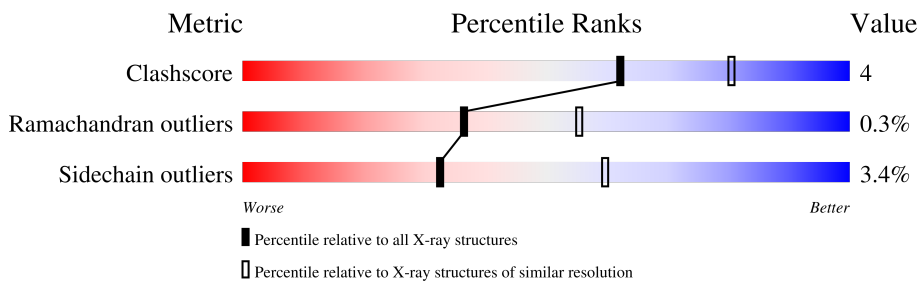
1 Overall quality at a glance

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

There are 3 unique types of molecules in this entry. The entry contains 6602 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 ALUMINUM ION (CCD ID: AL) (formula: Al).

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

- Molecule 3 is water.

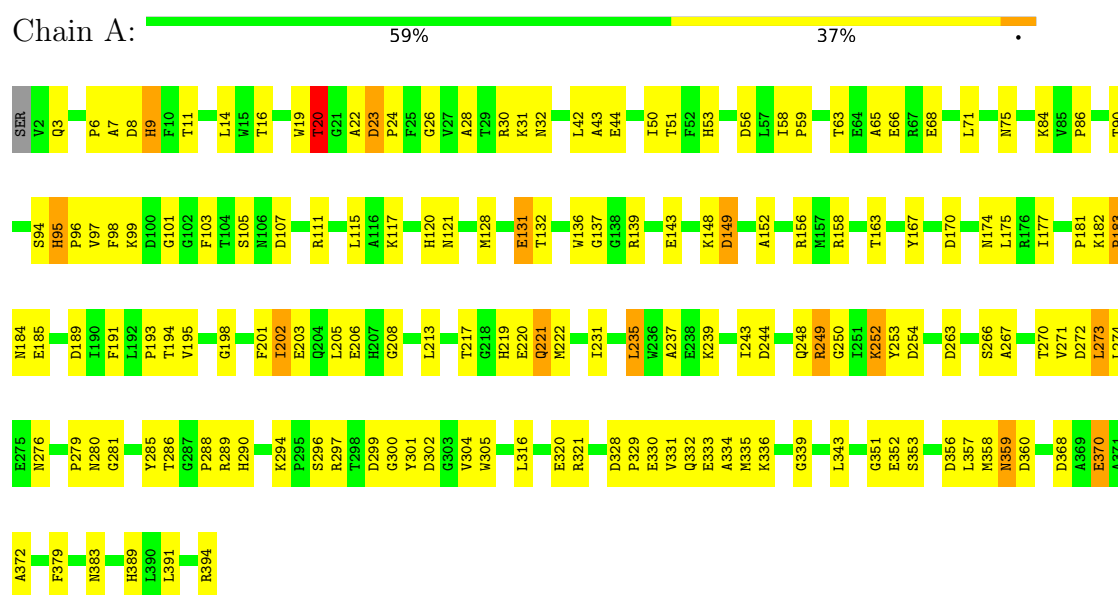
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	270	Total	O	0	0
			270	270		
3	B	276	Total	O	0	0
			276	276		

3 Residue-property plots

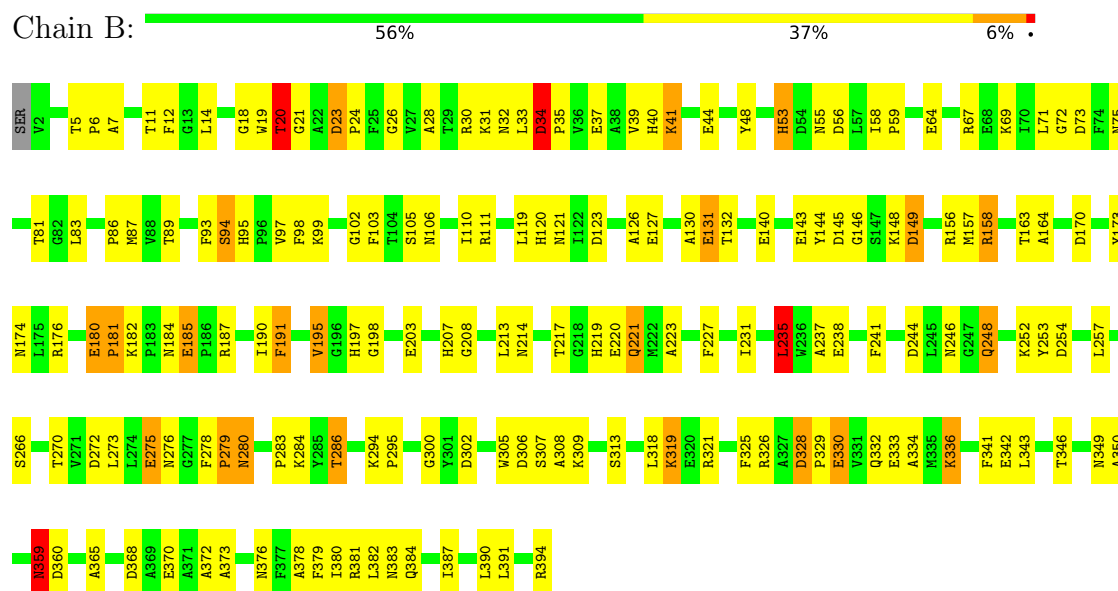
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	105.80Å 105.80Å 153.50Å 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}	0.154 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6602	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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:
AL

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	1.31	8/3101 (0.3%)	2.62	235/4204 (5.6%)
1	B	1.34	7/3101 (0.2%)	2.52	227/4204 (5.4%)
All	All	1.33	15/6202 (0.2%)	2.57	462/8408 (5.5%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	252	LYS	C-O	9.21	1.32	1.24
1	B	254	ASP	CA-CB	-8.28	1.41	1.53
1	B	102	GLY	CA-C	8.16	1.56	1.51
1	A	252	LYS	C-O	6.28	1.30	1.24
1	A	254	ASP	CA-CB	-6.07	1.44	1.53
1	A	9	HIS	ND1-CE1	6.07	1.38	1.32
1	B	373	ALA	C-O	5.64	1.31	1.24
1	A	272	ASP	C-O	5.38	1.30	1.24
1	B	105	SER	C-O	5.37	1.30	1.23
1	A	19	TRP	C-N	-5.31	1.25	1.33
1	B	217	THR	CA-CB	5.31	1.62	1.53
1	B	276	ASN	C-O	5.22	1.30	1.24
1	A	286	THR	CA-CB	5.20	1.61	1.53
1	A	289	ARG	CD-NE	-5.10	1.39	1.46
1	A	339	GLY	C-O	5.09	1.30	1.23

All (462) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	ASN	CA-CB-CG	28.62	141.22	112.60
1	B	254	ASP	CA-CB-CG	26.32	138.92	112.60
1	A	394	ARG	CD-NE-CZ	25.84	160.57	124.40
1	A	254	ASP	CA-CB-CG	20.81	133.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ARG	CD-NE-CZ	13.46	143.25	124.40
1	A	6	PRO	CA-C-N	13.46	143.19	120.72
1	A	6	PRO	C-N-CA	13.46	143.19	120.72
1	A	131	GLU	CB-CG-CD	13.09	134.85	112.60
1	B	187	ARG	NE-CZ-NH2	-11.39	108.95	119.20
1	A	44	GLU	CA-CB-CG	11.23	136.56	114.10
1	B	158	ARG	NE-CZ-NH2	-10.90	109.39	119.20
1	A	358	MET	CA-C-N	10.56	134.17	120.44
1	A	358	MET	C-N-CA	10.56	134.17	120.44
1	A	103	PHE	CA-CB-CG	10.41	124.21	113.80
1	B	359	ASN	CA-CB-CG	10.13	122.73	112.60
1	A	19	TRP	CA-C-N	10.08	138.78	121.14
1	A	19	TRP	C-N-CA	10.08	138.78	121.14
1	B	174	ASN	OD1-CG-ND2	9.97	132.57	122.60
1	B	394	ARG	NE-CZ-NH2	-9.94	110.26	119.20
1	B	32	ASN	CA-CB-CG	-9.92	102.68	112.60
1	B	302	ASP	CA-C-N	9.67	130.71	119.98
1	B	302	ASP	C-N-CA	9.67	130.71	119.98
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	A	143	GLU	CA-C-O	9.55	130.20	119.41
1	A	6	PRO	O-C-N	-9.23	110.17	122.64
1	B	208	GLY	CA-C-N	9.13	132.89	120.38
1	B	208	GLY	C-N-CA	9.13	132.89	120.38
1	A	59	PRO	CA-C-N	9.12	132.30	120.44
1	A	59	PRO	C-N-CA	9.12	132.30	120.44
1	A	379	PHE	CA-CB-CG	9.07	122.87	113.80
1	B	174	ASN	CA-CB-CG	-9.04	103.56	112.60
1	A	94	SER	N-CA-C	9.03	120.90	111.14
1	A	32	ASN	CA-CB-CG	-8.98	103.62	112.60
1	A	266	SER	CA-C-N	8.97	132.65	120.54
1	A	266	SER	C-N-CA	8.97	132.65	120.54
1	B	102	GLY	O-C-N	8.93	126.85	121.85
1	B	219	HIS	CB-CG-CD2	8.86	142.72	131.20
1	B	20	THR	N-CA-CB	-8.86	95.53	110.41
1	B	379	PHE	CA-CB-CG	8.81	122.61	113.80
1	A	244	ASP	CA-CB-CG	8.76	121.36	112.60
1	A	302	ASP	CA-C-N	8.75	129.88	119.99
1	A	302	ASP	C-N-CA	8.75	129.88	119.99
1	B	381	ARG	NE-CZ-NH2	-8.64	111.42	119.20
1	B	44	GLU	CA-CB-CG	8.62	131.35	114.10
1	A	221	GLN	CA-C-N	8.62	134.39	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLN	C-N-CA	8.62	134.39	120.60
1	A	297	ARG	CA-C-N	8.57	133.34	120.31
1	A	297	ARG	C-N-CA	8.57	133.34	120.31
1	A	107	ASP	CA-CB-CG	8.57	121.17	112.60
1	B	131	GLU	CA-CB-CG	8.54	131.17	114.10
1	A	66	GLU	CB-CG-CD	8.47	127.01	112.60
1	B	217	THR	CA-C-N	8.41	130.65	120.14
1	B	217	THR	C-N-CA	8.41	130.65	120.14
1	B	286	THR	N-CA-CB	-8.37	97.17	110.98
1	B	64	GLU	CA-C-N	8.34	131.97	120.63
1	B	64	GLU	C-N-CA	8.34	131.97	120.63
1	A	320	GLU	CB-CG-CD	8.30	126.71	112.60
1	B	203	GLU	CA-C-N	8.29	136.22	122.54
1	B	203	GLU	C-N-CA	8.29	136.22	122.54
1	A	286	THR	CA-CB-OG1	-8.15	97.37	109.60
1	B	149	ASP	N-CA-C	-8.14	95.30	108.41
1	B	319	LYS	CA-C-N	8.11	131.35	120.65
1	B	319	LYS	C-N-CA	8.11	131.35	120.65
1	A	23	ASP	CA-CB-CG	8.07	120.67	112.60
1	B	73	ASP	CA-CB-CG	8.05	120.65	112.60
1	A	263	ASP	CA-CB-CG	7.98	120.58	112.60
1	B	164	ALA	CA-C-N	7.96	131.26	120.44
1	B	164	ALA	C-N-CA	7.96	131.26	120.44
1	A	103	PHE	CA-C-O	-7.89	112.18	120.55
1	A	320	GLU	CA-C-N	7.88	130.69	120.44
1	A	320	GLU	C-N-CA	7.88	130.69	120.44
1	A	372	ALA	O-C-N	-7.84	113.81	122.12
1	B	102	GLY	N-CA-C	-7.84	103.08	110.21
1	B	334	ALA	CA-C-N	7.81	131.08	120.38
1	B	334	ALA	C-N-CA	7.81	131.08	120.38
1	A	222	MET	CA-C-N	7.80	134.58	122.49
1	A	222	MET	C-N-CA	7.80	134.58	122.49
1	B	372	ALA	O-C-N	-7.79	113.86	122.12
1	B	40	HIS	CA-CB-CG	-7.76	106.04	113.80
1	A	149	ASP	N-CA-C	-7.74	94.97	108.20
1	B	20	THR	CB-CA-C	7.74	125.35	109.95
1	B	12	PHE	CA-CB-CG	7.73	121.53	113.80
1	B	346	THR	CA-CB-OG1	-7.72	98.02	109.60
1	A	267	ALA	CA-C-N	7.71	130.46	120.44
1	A	267	ALA	C-N-CA	7.71	130.46	120.44
1	A	332	GLN	CA-C-N	7.65	130.84	120.44
1	A	332	GLN	C-N-CA	7.65	130.84	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	ARG	NE-CZ-NH1	7.62	129.12	121.50
1	B	7	ALA	CA-C-N	7.57	131.82	120.31
1	B	7	ALA	C-N-CA	7.57	131.82	120.31
1	A	51	THR	CA-CB-CG2	7.57	123.36	110.50
1	A	343	LEU	CA-C-N	7.55	134.23	120.79
1	A	343	LEU	C-N-CA	7.55	134.23	120.79
1	A	217	THR	CA-C-N	7.55	128.36	119.98
1	A	217	THR	C-N-CA	7.55	128.36	119.98
1	A	206	GLU	N-CA-CB	7.44	120.86	110.07
1	B	23	ASP	CB-CA-C	7.40	124.75	110.17
1	A	333	GLU	CA-CB-CG	7.39	128.88	114.10
1	B	308	ALA	CA-C-N	7.38	130.04	120.44
1	B	308	ALA	C-N-CA	7.38	130.04	120.44
1	A	273	LEU	CA-C-O	-7.38	113.07	120.82
1	B	390	LEU	O-C-N	-7.38	114.30	122.12
1	A	301	TYR	CA-C-O	-7.25	111.90	120.10
1	A	31	LYS	CA-C-O	-7.25	113.25	121.81
1	B	94	SER	N-CA-C	7.25	120.60	111.69
1	A	301	TYR	N-CA-C	7.22	120.01	111.71
1	A	370	GLU	CA-C-O	-7.20	111.70	119.97
1	A	285	TYR	CA-C-N	-7.17	111.33	122.37
1	A	285	TYR	C-N-CA	-7.17	111.33	122.37
1	B	241	PHE	CA-CB-CG	7.15	120.95	113.80
1	A	276	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	B	56	ASP	N-CA-CB	7.12	120.81	110.20
1	A	320	GLU	CA-CB-CG	7.11	128.32	114.10
1	A	167	TYR	CA-C-O	-7.10	113.37	120.82
1	B	34	ASP	CA-C-N	7.07	127.06	119.28
1	B	34	ASP	C-N-CA	7.07	127.06	119.28
1	B	181	PRO	CB-CA-C	7.05	120.80	110.85
1	A	181	PRO	CB-CA-C	7.02	120.67	110.63
1	B	103	PHE	CA-CB-CG	7.01	120.81	113.80
1	B	309	LYS	CA-C-O	7.00	128.18	120.82
1	A	235	LEU	CA-C-O	6.98	128.15	120.82
1	B	275	GLU	CA-C-N	6.96	133.91	121.66
1	B	275	GLU	C-N-CA	6.96	133.91	121.66
1	B	106	ASN	CA-C-N	6.95	131.25	121.24
1	B	106	ASN	C-N-CA	6.95	131.25	121.24
1	A	254	ASP	N-CA-CB	6.95	120.72	109.95
1	B	330	GLU	CA-CB-CG	6.95	127.99	114.10
1	B	127	GLU	CA-CB-CG	6.92	127.93	114.10
1	B	309	LYS	CA-C-N	6.90	129.41	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	LYS	C-N-CA	6.90	129.41	120.44
1	B	360	ASP	CA-C-N	6.87	129.79	120.38
1	B	360	ASP	C-N-CA	6.87	129.79	120.38
1	A	279	PRO	O-C-N	-6.86	114.35	122.24
1	B	231	ILE	CA-C-N	6.85	129.35	120.44
1	B	231	ILE	C-N-CA	6.85	129.35	120.44
1	A	174	ASN	CA-C-N	6.83	134.11	122.37
1	A	174	ASN	C-N-CA	6.83	134.11	122.37
1	A	383	ASN	CA-CB-CG	-6.82	105.78	112.60
1	A	394	ARG	NE-CZ-NH1	6.81	128.31	121.50
1	A	300	GLY	CA-C-O	-6.80	112.98	122.36
1	A	332	GLN	CB-CG-CD	6.79	124.15	112.60
1	A	117	LYS	CG-CD-CE	6.76	126.85	111.30
1	A	193	PRO	N-CA-C	6.76	122.31	113.86
1	A	360	ASP	CA-C-N	6.76	130.01	120.28
1	A	360	ASP	C-N-CA	6.76	130.01	120.28
1	B	219	HIS	CB-CG-ND1	-6.75	112.57	122.70
1	A	297	ARG	CD-NE-CZ	6.75	133.85	124.40
1	B	56	ASP	N-CA-C	-6.74	103.40	111.69
1	B	130	ALA	CA-C-O	-6.73	113.37	121.05
1	B	146	GLY	CA-C-N	6.73	130.54	120.31
1	B	146	GLY	C-N-CA	6.73	130.54	120.31
1	B	207	HIS	CA-C-N	6.72	128.59	120.13
1	B	207	HIS	C-N-CA	6.72	128.59	120.13
1	A	208	GLY	O-C-N	-6.71	115.05	122.84
1	B	20	THR	CA-CB-CG2	6.70	121.89	110.50
1	B	332	GLN	CA-C-N	6.70	129.80	120.29
1	B	332	GLN	C-N-CA	6.70	129.80	120.29
1	B	376	ASN	CA-C-O	-6.69	113.42	120.58
1	A	71	LEU	CA-C-N	6.68	127.35	120.00
1	A	71	LEU	C-N-CA	6.68	127.35	120.00
1	B	221	GLN	CA-C-N	6.67	131.86	120.72
1	B	221	GLN	C-N-CA	6.67	131.86	120.72
1	A	143	GLU	CA-C-N	6.67	132.94	122.94
1	A	143	GLU	C-N-CA	6.67	132.94	122.94
1	A	289	ARG	CA-CB-CG	6.64	127.39	114.10
1	B	30	ARG	NE-CZ-NH1	6.64	128.14	121.50
1	B	383	ASN	CA-C-N	6.58	129.10	120.28
1	B	383	ASN	C-N-CA	6.58	129.10	120.28
1	A	290	HIS	CA-CB-CG	6.57	120.37	113.80
1	A	357	LEU	CA-C-O	-6.56	113.47	120.42
1	A	276	ASN	CA-C-O	-6.55	111.61	119.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ALA	CA-C-O	-6.54	113.95	120.82
1	B	384	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	B	343	LEU	CA-C-N	6.53	132.41	120.79
1	B	343	LEU	C-N-CA	6.53	132.41	120.79
1	B	372	ALA	CB-CA-C	6.52	121.61	110.79
1	A	286	THR	OG1-CB-CG2	6.50	122.30	109.30
1	B	5	THR	CA-CB-CG2	6.49	121.53	110.50
1	A	202	ILE	CA-C-N	6.46	133.01	120.99
1	A	202	ILE	C-N-CA	6.46	133.01	120.99
1	B	53	HIS	N-CA-CB	6.45	121.16	110.52
1	A	270	THR	CA-CB-CG2	6.44	121.45	110.50
1	B	198	GLY	CA-C-N	6.41	128.87	120.28
1	B	198	GLY	C-N-CA	6.41	128.87	120.28
1	A	288	PRO	O-C-N	6.40	130.94	123.06
1	B	246	ASN	CA-C-N	6.40	126.54	121.61
1	B	246	ASN	C-N-CA	6.40	126.54	121.61
1	A	66	GLU	CA-C-N	6.38	128.74	120.44
1	A	66	GLU	C-N-CA	6.38	128.74	120.44
1	A	189	ASP	CA-C-O	-6.38	113.24	120.32
1	B	203	GLU	CG-CD-OE2	6.35	133.01	118.40
1	A	351	GLY	CA-C-N	6.34	132.50	122.74
1	A	351	GLY	C-N-CA	6.34	132.50	122.74
1	B	208	GLY	O-C-N	-6.32	115.68	122.19
1	B	294	LYS	CB-CA-C	-6.31	101.76	110.16
1	B	383	ASN	OD1-CG-ND2	6.31	128.91	122.60
1	B	37	GLU	CA-C-N	6.31	129.06	120.54
1	B	37	GLU	C-N-CA	6.31	129.06	120.54
1	A	163	THR	N-CA-CB	6.30	119.15	110.01
1	A	206	GLU	CA-C-O	-6.30	114.21	120.70
1	A	111	ARG	CA-C-N	6.30	128.72	120.28
1	A	111	ARG	C-N-CA	6.30	128.72	120.28
1	A	156	ARG	CA-C-N	6.29	128.61	120.44
1	A	156	ARG	C-N-CA	6.29	128.61	120.44
1	B	266	SER	CA-C-N	6.29	128.61	120.44
1	B	266	SER	C-N-CA	6.29	128.61	120.44
1	B	34	ASP	CB-CA-C	6.28	119.28	109.42
1	A	95	HIS	CA-C-N	6.28	127.69	119.84
1	A	95	HIS	C-N-CA	6.28	127.69	119.84
1	A	56	ASP	N-CA-C	-6.27	104.52	111.36
1	A	94	SER	CA-C-O	-6.27	114.24	120.70
1	A	243	ILE	O-C-N	6.26	129.88	123.00
1	B	93	PHE	CA-C-O	-6.23	111.37	118.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASN	CA-CB-CG	-6.20	106.40	112.60
1	A	368	ASP	CA-C-N	6.19	128.58	120.28
1	A	368	ASP	C-N-CA	6.19	128.58	120.28
1	A	352	GLU	N-CA-C	-6.17	98.33	108.76
1	B	280	ASN	OD1-CG-ND2	-6.17	116.43	122.60
1	A	328	ASP	CA-C-O	6.15	125.58	119.49
1	A	121	ASN	CA-C-N	6.14	128.87	120.46
1	A	121	ASN	C-N-CA	6.14	128.87	120.46
1	B	131	GLU	CA-C-O	6.14	126.34	119.41
1	A	372	ALA	CA-C-O	6.13	127.05	120.55
1	A	334	ALA	CA-C-N	6.12	128.48	120.28
1	A	334	ALA	C-N-CA	6.12	128.48	120.28
1	A	352	GLU	CA-C-O	-6.12	113.53	120.32
1	A	30	ARG	NE-CZ-NH2	-6.12	113.70	119.20
1	A	177	ILE	O-C-N	6.12	129.41	122.93
1	A	56	ASP	CA-C-N	6.11	130.05	120.89
1	A	56	ASP	C-N-CA	6.11	130.05	120.89
1	A	297	ARG	CG-CD-NE	6.10	125.41	112.00
1	A	201	PHE	CA-CB-CG	6.08	119.88	113.80
1	B	185	GLU	CB-CG-CD	6.08	122.94	112.60
1	B	14	LEU	CA-C-N	6.07	130.86	120.72
1	B	14	LEU	C-N-CA	6.07	130.86	120.72
1	A	117	LYS	CA-C-N	6.07	128.33	120.56
1	A	117	LYS	C-N-CA	6.07	128.33	120.56
1	B	391	LEU	CA-C-N	6.07	133.30	121.41
1	B	391	LEU	C-N-CA	6.07	133.30	121.41
1	A	208	GLY	CA-C-O	6.06	126.89	119.01
1	A	391	LEU	CA-C-N	6.01	133.18	121.41
1	A	391	LEU	C-N-CA	6.01	133.18	121.41
1	B	19	TRP	N-CA-CB	6.00	118.95	109.71
1	B	131	GLU	CG-CD-OE2	6.00	132.20	118.40
1	B	6	PRO	CA-C-N	5.98	130.71	120.72
1	B	6	PRO	C-N-CA	5.98	130.71	120.72
1	A	304	VAL	CA-C-O	-5.97	115.20	121.41
1	B	180	GLU	CA-C-O	5.97	125.23	119.62
1	A	19	TRP	CA-C-O	5.96	127.55	120.70
1	B	174	ASN	CB-CG-ND2	-5.96	107.47	116.40
1	A	149	ASP	N-CA-CB	5.95	120.18	110.37
1	B	382	LEU	CA-C-O	-5.95	114.24	120.55
1	A	249	ARG	CD-NE-CZ	5.95	132.72	124.40
1	A	389	HIS	N-CA-CB	5.93	118.68	110.07
1	B	176	ARG	CB-CG-CD	5.93	124.94	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	ASP	O-C-N	5.92	129.97	123.04
1	A	202	ILE	O-C-N	-5.92	116.09	121.89
1	A	56	ASP	N-CA-CB	5.91	118.91	110.16
1	B	99	LYS	CA-C-O	-5.90	113.43	120.10
1	B	173	TYR	N-CA-C	-5.90	101.75	110.48
1	B	156	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	A	84	LYS	CA-C-N	5.88	133.02	122.13
1	A	84	LYS	C-N-CA	5.88	133.02	122.13
1	A	98	PHE	CA-C-N	5.88	128.75	120.28
1	A	98	PHE	C-N-CA	5.88	128.75	120.28
1	B	126	ALA	CA-C-N	5.87	128.43	120.38
1	B	126	ALA	C-N-CA	5.87	128.43	120.38
1	A	84	LYS	O-C-N	-5.87	116.03	122.84
1	A	20	THR	CA-CB-OG1	-5.87	100.80	109.60
1	A	68	GLU	CA-C-N	5.86	128.39	120.65
1	A	68	GLU	C-N-CA	5.86	128.39	120.65
1	A	22	ALA	CB-CA-C	5.85	119.41	109.53
1	A	120	HIS	CA-CB-CG	-5.82	107.98	113.80
1	A	90	THR	CA-C-O	-5.82	114.41	120.70
1	A	203	GLU	CG-CD-OE2	5.82	131.78	118.40
1	B	284	LYS	CA-C-N	5.82	130.50	122.77
1	B	284	LYS	C-N-CA	5.82	130.50	122.77
1	B	187	ARG	NE-CZ-NH1	5.81	127.31	121.50
1	B	394	ARG	NH1-CZ-NH2	5.80	126.84	119.30
1	A	16	THR	CA-CB-OG1	-5.80	100.91	109.60
1	A	20	THR	CA-CB-CG2	5.79	120.34	110.50
1	B	330	GLU	CG-CD-OE1	-5.77	105.14	118.40
1	A	20	THR	N-CA-CB	-5.76	101.01	110.40
1	A	328	ASP	CA-C-N	5.76	125.89	119.32
1	A	328	ASP	C-N-CA	5.76	125.89	119.32
1	B	143	GLU	CA-C-O	5.76	125.92	119.41
1	B	286	THR	CB-CA-C	5.76	120.55	110.64
1	B	295	PRO	CA-C-N	5.76	129.02	120.90
1	B	295	PRO	C-N-CA	5.76	129.02	120.90
1	A	316	LEU	CB-CA-C	5.75	120.34	110.79
1	B	163	THR	CA-C-O	-5.74	114.80	120.82
1	B	111	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	B	48	TYR	N-CA-CB	-5.71	102.14	110.47
1	A	286	THR	N-CA-C	5.70	120.98	112.94
1	B	214	ASN	CB-CG-ND2	5.69	124.94	116.40
1	A	237	ALA	CA-C-N	5.69	130.82	122.63
1	A	237	ALA	C-N-CA	5.69	130.82	122.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	235	LEU	CA-C-O	5.68	126.78	120.82
1	A	220	GLU	CA-C-O	-5.67	114.53	120.55
1	A	194	THR	CA-CB-CG2	5.67	120.14	110.50
1	B	120	HIS	CA-C-N	5.67	128.44	120.28
1	B	120	HIS	C-N-CA	5.67	128.44	120.28
1	A	329	PRO	CA-C-N	5.64	127.84	120.28
1	A	329	PRO	C-N-CA	5.64	127.84	120.28
1	B	19	TRP	CA-C-O	5.64	127.12	120.58
1	B	33	LEU	CA-C-O	-5.63	114.29	120.43
1	B	72	GLY	CA-C-O	-5.62	114.93	121.00
1	B	368	ASP	CA-C-N	5.62	127.82	120.28
1	B	368	ASP	C-N-CA	5.62	127.82	120.28
1	B	98	PHE	CA-C-N	5.61	128.36	120.28
1	B	98	PHE	C-N-CA	5.61	128.36	120.28
1	A	152	ALA	CA-C-O	-5.59	113.54	119.97
1	A	105	SER	N-CA-C	-5.59	102.75	110.35
1	B	26	GLY	N-CA-C	5.59	119.84	110.56
1	B	174	ASN	N-CA-CB	-5.59	103.71	110.53
1	A	58	ILE	O-C-N	5.59	124.89	121.37
1	B	7	ALA	O-C-N	-5.57	114.96	122.43
1	A	372	ALA	CA-C-N	5.55	131.32	120.99
1	A	372	ALA	C-N-CA	5.55	131.32	120.99
1	A	58	ILE	N-CA-C	5.54	113.04	107.55
1	B	190	ILE	CA-C-O	-5.54	114.44	121.48
1	A	96	PRO	CA-C-N	5.53	129.37	120.30
1	A	96	PRO	C-N-CA	5.53	129.37	120.30
1	B	174	ASN	CA-C-N	5.53	131.41	122.29
1	B	174	ASN	C-N-CA	5.53	131.41	122.29
1	B	336	LYS	N-CA-C	-5.51	105.18	111.14
1	A	96	PRO	O-C-N	-5.51	115.20	122.64
1	B	219	HIS	CA-CB-CG	-5.49	108.31	113.80
1	B	111	ARG	NE-CZ-NH2	-5.48	114.27	119.20
1	B	328	ASP	CA-C-N	5.48	125.31	119.28
1	B	328	ASP	C-N-CA	5.48	125.31	119.28
1	A	321	ARG	CA-CB-CG	-5.47	103.16	114.10
1	B	342	GLU	CG-CD-OE2	-5.46	105.83	118.40
1	A	9	HIS	N-CA-C	5.46	119.25	112.58
1	B	18	GLY	CA-C-N	5.46	129.11	121.24
1	B	18	GLY	C-N-CA	5.46	129.11	121.24
1	B	270	THR	CA-C-N	5.45	127.42	120.56
1	B	270	THR	C-N-CA	5.45	127.42	120.56
1	A	131	GLU	CA-C-O	5.44	126.64	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	PHE	N-CA-C	5.44	117.97	111.71
1	B	67	ARG	CG-CD-NE	5.42	123.92	112.00
1	B	350	ALA	CA-C-O	-5.42	115.05	120.96
1	B	244	ASP	N-CA-CB	5.42	119.05	110.55
1	A	280	ASN	CA-C-O	-5.41	112.88	119.43
1	B	365	ALA	CA-C-O	-5.41	115.11	120.90
1	B	59	PRO	CA-C-N	5.40	127.51	120.28
1	B	59	PRO	C-N-CA	5.40	127.51	120.28
1	B	283	PRO	CB-CA-C	5.40	118.08	111.12
1	B	67	ARG	CA-C-N	5.39	127.50	120.28
1	B	67	ARG	C-N-CA	5.39	127.50	120.28
1	A	75	ASN	CA-C-N	5.39	128.28	120.79
1	A	75	ASN	C-N-CA	5.39	128.28	120.79
1	A	359	ASN	CA-C-O	-5.39	115.16	120.82
1	A	170	ASP	CA-C-O	-5.38	114.82	120.63
1	B	326	ARG	CA-C-N	5.38	128.48	120.31
1	B	326	ARG	C-N-CA	5.38	128.48	120.31
1	B	21	GLY	N-CA-C	5.38	123.49	115.64
1	B	254	ASP	CB-CA-C	5.36	119.08	110.29
1	B	71	LEU	CA-C-N	5.36	125.89	119.94
1	B	71	LEU	C-N-CA	5.36	125.89	119.94
1	B	156	ARG	O-C-N	-5.36	116.44	122.12
1	A	274	LEU	CA-C-N	5.36	129.65	120.71
1	A	274	LEU	C-N-CA	5.36	129.65	120.71
1	A	19	TRP	N-CA-CB	5.35	117.96	109.51
1	A	286	THR	N-CA-CB	-5.34	102.16	110.98
1	B	321	ARG	CA-CB-CG	-5.33	103.43	114.10
1	B	270	THR	N-CA-C	-5.33	105.16	110.97
1	B	313	SER	CA-C-N	5.32	127.73	120.54
1	B	313	SER	C-N-CA	5.32	127.73	120.54
1	A	128	MET	CA-C-N	5.32	129.53	120.91
1	A	128	MET	C-N-CA	5.32	129.53	120.91
1	B	279	PRO	CA-C-N	5.32	131.31	122.54
1	B	279	PRO	C-N-CA	5.32	131.31	122.54
1	B	191	PHE	CA-CB-CG	5.30	119.10	113.80
1	B	318	LEU	CA-C-N	5.30	127.70	120.54
1	B	318	LEU	C-N-CA	5.30	127.70	120.54
1	A	59	PRO	CB-CA-C	5.30	118.17	111.39
1	B	126	ALA	CB-CA-C	5.30	119.12	110.96
1	B	300	GLY	CA-C-N	5.30	127.91	120.28
1	B	300	GLY	C-N-CA	5.30	127.91	120.28
1	B	349	ASN	CB-CG-ND2	5.29	124.33	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	383	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	B	170	ASP	CA-C-O	-5.28	114.95	120.55
1	A	9	HIS	ND1-CE1-NE2	5.28	113.68	108.40
1	A	53	HIS	N-CA-CB	5.27	119.23	110.63
1	B	144	TYR	CA-C-O	5.27	126.39	120.70
1	A	336	LYS	CA-C-N	5.26	127.65	120.54
1	A	336	LYS	C-N-CA	5.26	127.65	120.54
1	A	253	TYR	CA-C-N	-5.26	113.98	121.50
1	A	253	TYR	C-N-CA	-5.26	113.98	121.50
1	B	306	ASP	CA-CB-CG	5.25	117.86	112.60
1	A	63	THR	N-CA-C	-5.25	103.76	110.53
1	A	281	GLY	CA-C-O	-5.25	118.04	122.29
1	A	271	VAL	O-C-N	-5.25	116.78	121.87
1	A	136	TRP	CA-C-O	-5.23	114.86	120.46
1	A	14	LEU	O-C-N	-5.22	116.11	122.22
1	A	352	GLU	N-CA-CB	5.22	119.83	110.80
1	B	81	THR	CA-CB-OG1	-5.22	101.77	109.60
1	B	272	ASP	O-C-N	-5.20	116.71	122.07
1	A	183	PRO	N-CA-C	5.20	120.37	113.40
1	B	195	VAL	CA-C-N	5.19	125.70	119.94
1	B	195	VAL	C-N-CA	5.19	125.70	119.94
1	A	14	LEU	CA-C-N	5.18	129.38	120.72
1	A	14	LEU	C-N-CA	5.18	129.38	120.72
1	B	378	ALA	CA-C-N	5.18	128.18	120.31
1	B	378	ALA	C-N-CA	5.18	128.18	120.31
1	A	96	PRO	CB-CA-C	-5.17	103.03	111.56
1	B	223	ALA	CA-C-N	5.17	131.03	120.80
1	B	223	ALA	C-N-CA	5.17	131.03	120.80
1	B	110	ILE	CB-CG1-CD1	5.17	124.65	113.80
1	A	370	GLU	CG-CD-OE1	-5.16	106.52	118.40
1	A	26	GLY	O-C-N	5.16	128.56	123.76
1	A	99	LYS	CA-C-O	-5.15	114.28	120.10
1	A	299	ASP	CA-C-O	5.15	126.84	120.92
1	A	305	TRP	CA-C-N	5.14	127.13	120.44
1	A	305	TRP	C-N-CA	5.14	127.13	120.44
1	B	123	ASP	N-CA-C	-5.14	105.57	111.07
1	B	257	LEU	O-C-N	5.14	128.97	122.65
1	B	280	ASN	CA-C-O	-5.14	113.34	119.35
1	A	294	LYS	CA-C-O	-5.14	115.05	119.72
1	B	248	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	231	ILE	CA-C-O	-5.13	114.93	120.47
1	B	75	ASN	CA-C-N	5.13	127.11	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASN	C-N-CA	5.13	127.11	120.44
1	A	115	LEU	CA-C-N	5.12	127.10	120.44
1	A	115	LEU	C-N-CA	5.12	127.10	120.44
1	A	219	HIS	CB-CG-CD2	5.12	137.86	131.20
1	B	387	ILE	N-CA-CB	5.12	117.50	110.54
1	A	7	ALA	CA-C-N	5.12	129.38	120.68
1	A	7	ALA	C-N-CA	5.12	129.38	120.68
1	A	43	ALA	O-C-N	-5.11	116.80	122.07
1	B	280	ASN	N-CA-C	-5.11	106.73	113.17
1	A	297	ARG	O-C-N	-5.11	115.41	122.46
1	A	198	GLY	CA-C-N	5.11	127.12	120.28
1	A	198	GLY	C-N-CA	5.11	127.12	120.28
1	B	307	SER	O-C-N	-5.10	116.81	122.07
1	A	235	LEU	CA-C-N	5.10	127.43	120.54
1	A	235	LEU	C-N-CA	5.10	127.43	120.54
1	A	289	ARG	N-CA-C	-5.09	97.60	107.62
1	A	195	VAL	CA-C-O	-5.08	115.98	121.27
1	A	272	ASP	CB-CA-C	5.08	118.85	110.88
1	A	279	PRO	CA-C-N	5.08	131.29	122.56
1	A	279	PRO	C-N-CA	5.08	131.29	122.56
1	B	119	LEU	CB-CA-C	5.08	118.85	110.88
1	B	56	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	31	LYS	CA-C-O	-5.07	115.83	121.81
1	B	106	ASN	N-CA-CB	5.06	118.02	110.22
1	B	203	GLU	O-C-N	-5.05	115.49	122.46
1	A	3	GLN	O-C-N	5.05	126.94	121.23
1	A	175	LEU	O-C-N	5.05	129.44	123.33
1	B	325	PHE	CA-CB-CG	5.04	118.84	113.80
1	B	145	ASP	CA-C-O	-5.03	114.18	119.97
1	A	250	GLY	N-CA-C	5.02	120.24	112.45
1	B	253	TYR	CA-C-N	-5.02	114.44	121.72
1	B	253	TYR	C-N-CA	-5.02	114.44	121.72
1	B	197	HIS	CA-C-N	5.02	125.51	119.94
1	B	197	HIS	C-N-CA	5.02	125.51	119.94
1	B	227	PHE	CA-C-N	5.01	127.41	120.29
1	B	227	PHE	C-N-CA	5.01	127.41	120.29
1	A	120	HIS	CA-C-N	5.01	127.49	120.28
1	A	120	HIS	C-N-CA	5.01	127.49	120.28

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	22	0
1	B	3027	0	2882	28	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	270	0	0	0	1
3	B	276	0	0	1	1
All	All	6602	0	5764	48	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 (48) 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	1.37	0.70
1:B:95:HIS:HD2	1:B:97:VAL:H	1.40	0.68
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.74	0.68
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.76	0.68
1:B:235:LEU:HD12	1:B:273:LEU:HD21	1.79	0.65
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.84	0.59
1:A:235:LEU:HD12	1:A:273:LEU:HD21	1.84	0.58
1:B:140:GLU:HG3	1:B:157:MET:HE1	1.84	0.57
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.88	0.55
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.73	0.53
1:B:182:LYS:HE2	1:B:184:ASN:O	2.09	0.53
1:A:296:SER:H	1:B:380:ILE:HD11	1.75	0.52
1:A:202:ILE:HG21	1:A:239:LYS:HE3	1.92	0.51
1:A:182:LYS:HE2	1:A:184:ASN:O	2.11	0.51
1:A:20:THR:HG23	1:A:28:ALA:CB	2.43	0.49
1:B:148:LYS:HG3	1:B:191:PHE:HZ	1.77	0.49
1:B:158:ARG:HD2	3:B:469(B):HOH:O	2.13	0.48
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.96	0.47
1:A:131:GLU:HG3	1:A:132:THR:N	2.28	0.47
1:A:182:LYS:HG3	1:A:183:PRO:HD2	1.95	0.46
1:B:359:ASN:C	1:B:359:ASN:HD22	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:THR:HG23	1:B:28:ALA:CB	2.45	0.46
1:A:23:ASP:HB2	1:A:24:PRO:CD	2.46	0.46
1:A:42:LEU:HD12	1:A:50:ILE:HD12	1.99	0.45
1:B:35:PRO:O	1:B:39:VAL:HG23	2.15	0.45
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.81	0.45
1:A:296:SER:N	1:B:380:ILE:HD11	2.32	0.45
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.82	0.45
1:A:101:GLY:HA2	1:A:139:ARG:HB2	1.99	0.45
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.98	0.44
1:A:95:HIS:CD2	1:A:97:VAL:H	2.27	0.44
1:A:353:SER:H	1:A:356:ASP:HB2	1.82	0.44
1:A:8:ASP:O	1:A:9:HIS:HB2	2.18	0.43
1:B:280:ASN:OD1	1:B:341:PHE:HA	2.18	0.43
1:B:41:LYS:HG2	1:B:305:TRP:CE2	2.54	0.42
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.90	0.42
1:A:158:ARG:HG3	1:A:205:LEU:HD23	2.01	0.41
1:B:180:GLU:HA	1:B:181:PRO:HD3	1.77	0.41
1:B:53:HIS:CD2	1:B:89:THR:HG23	2.55	0.41
1:A:331:VAL:O	1:A:335:MET:HG3	2.21	0.41
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.45	0.41
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.86	0.41
1:A:20:THR:HG23	1:A:28:ALA:HB2	2.01	0.41
1:B:34:ASP:HA	1:B:35:PRO:HD3	1.81	0.41
1:B:55:ASN:HA	1:B:58:ILE:O	2.21	0.41
1:B:237:ALA:O	1:B:238:GLU:HB2	2.21	0.40
1:B:87:MET:HA	1:B:132:THR:O	2.22	0.40
1:A:249:ARG:O	1:A:252:LYS:HE3	2.21	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)
3:B:573(B):HOH:O	3:B:614(B):HOH:O[4_555]	2.01	0.19
3:A:473(A):HOH:O	3:A:597(A):HOH:O[4_555]	2.18	0.02

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%)	375 (96%)	15 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	376 (96%)	14 (4%)	1 (0%)	36	55
All	All	782/788 (99%)	751 (96%)	29 (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%)	299 (98%)	6 (2%)	48	75
1	B	305/310 (98%)	290 (95%)	15 (5%)	22	45
All	All	610/620 (98%)	589 (97%)	21 (3%)	32	60

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	149	ASP
1	A	213	LEU
1	A	330	GLU

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Mol	Chain	Res	Type
1	A	359	ASN
1	A	370	GLU
1	B	20	THR
1	B	34	ASP
1	B	41	LYS
1	B	69	LYS
1	B	94	SER
1	B	131	GLU
1	B	149	ASP
1	B	213	LEU
1	B	235	LEU
1	B	286	THR
1	B	330	GLU
1	B	333	GLU
1	B	336	LYS
1	B	359	ASN
1	B	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	383	ASN
1	A	384	GLN
1	B	9	HIS
1	B	95	HIS
1	B	120	HIS
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 [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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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.