



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:19 PM UTC

PDB ID : 4XIA / pdb_00004xia
Title : STRUCTURES OF D-XYLOSE ISOMERASE FROM ARTHROBACTER STRAIN B3728 CONTAINING THE INHIBITORS XYLITOL AND D-SORBITOL AT 2.5 ANGSTROMS AND 2.3 ANGSTROMS RESOLUTION, RESPECTIVELY
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Deposited on : 1989-07-05
Resolution : 2.30 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

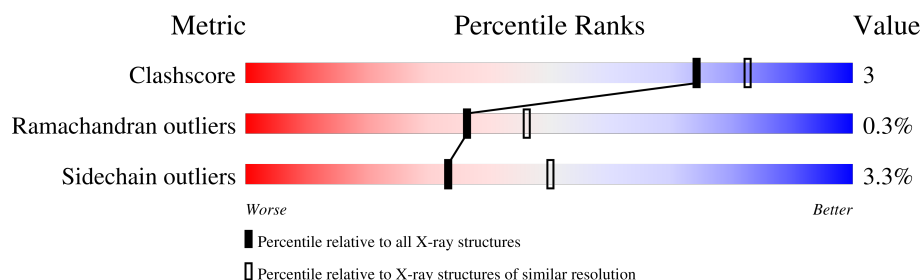
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	393	 64% 30% 6% •
1	B	393	 61% 34% 5% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6618 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.

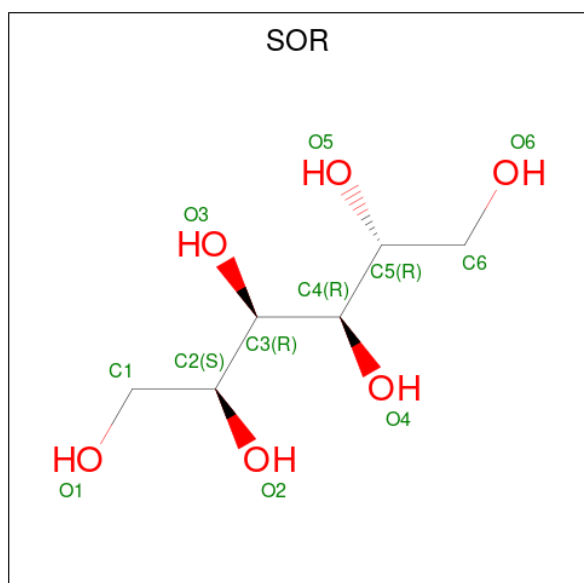
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	LYS	conflict	UNP P12070
A	64	ALA	GLU	conflict	UNP P12070
A	79	ALA	LYS	conflict	UNP P12070
B	31	ALA	LYS	conflict	UNP P12070
B	64	ALA	GLU	conflict	UNP P12070
B	79	ALA	LYS	conflict	UNP P12070

- Molecule 2 is sorbitol (CCD ID: SOR) (formula: C₆H₁₄O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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

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

- Molecule 4 is water.

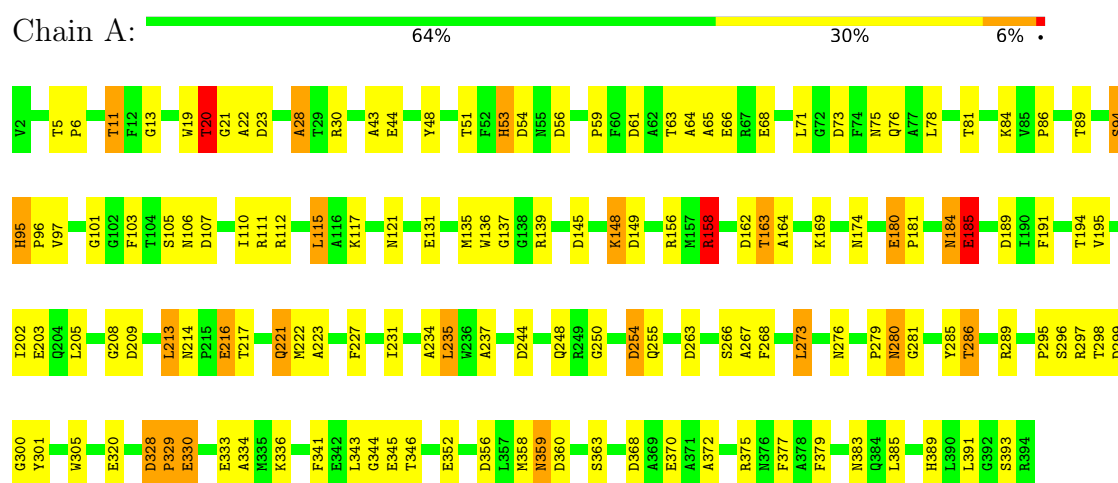
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	268	Total	O	0	0
			268	268		
4	B	270	Total	O	0	0
			270	270		

3 Residue-property plots

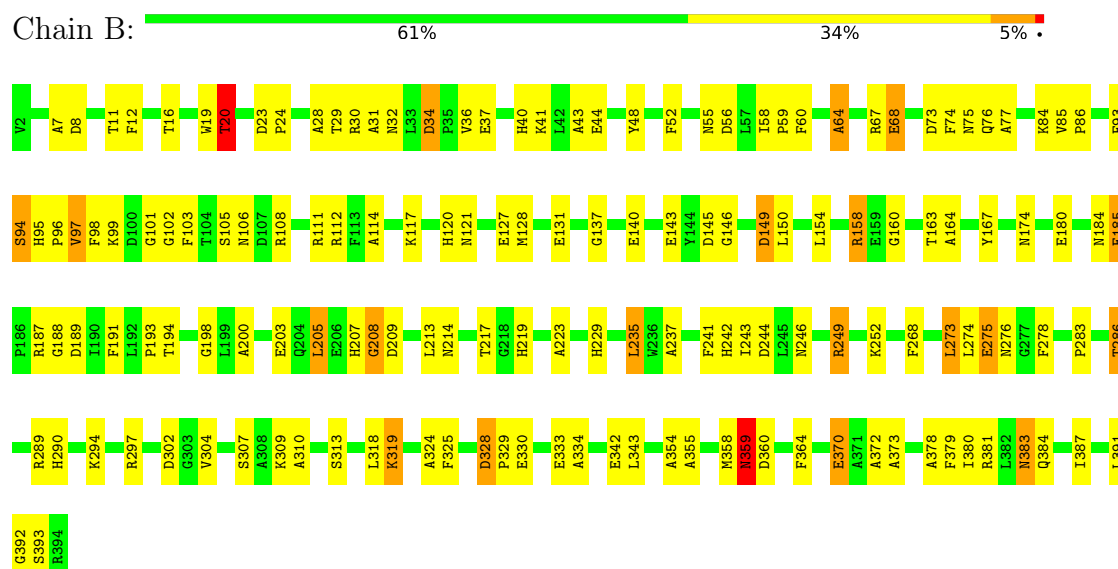
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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	105.80 Å 105.80 Å 153.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.147 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6618	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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: MG, SOR

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	1.39	4/3101 (0.1%)	2.57	235/4204 (5.6%)
1	B	1.41	10/3101 (0.3%)	2.50	215/4204 (5.1%)
All	All	1.40	14/6202 (0.2%)	2.54	450/8408 (5.4%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	158	ARG	CD-NE	-9.10	1.33	1.46
1	A	158	ARG	CD-NE	-8.66	1.34	1.46
1	B	101	GLY	C-N	-6.56	1.27	1.33
1	B	358	MET	C-N	-5.96	1.24	1.33
1	A	289	ARG	CD-NE	-5.77	1.38	1.46
1	B	268	PHE	C-O	5.75	1.30	1.24
1	A	286	THR	CA-CB	5.61	1.62	1.53
1	B	219	HIS	CG-ND1	5.45	1.44	1.38
1	B	146	GLY	N-CA	5.34	1.51	1.45
1	B	373	ALA	C-O	5.31	1.30	1.24
1	B	20	THR	C-O	5.23	1.30	1.24
1	B	217	THR	CA-CB	5.18	1.61	1.53
1	B	187	ARG	NE-CZ	5.13	1.38	1.33
1	A	95	HIS	CA-CB	5.05	1.60	1.53

All (450) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	CD-NE-CZ	31.08	167.91	124.40
1	B	358	MET	CA-C-N	18.75	158.14	121.58
1	B	358	MET	C-N-CA	18.75	158.14	121.58
1	B	359	ASN	CA-CB-CG	18.04	130.64	112.60
1	A	289	ARG	CD-NE-CZ	17.76	149.27	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	MET	CA-C-N	15.23	143.45	120.31
1	A	358	MET	C-N-CA	15.23	143.45	120.31
1	B	289	ARG	CD-NE-CZ	12.26	141.56	124.40
1	A	131	GLU	CB-CG-CD	12.01	133.02	112.60
1	A	359	ASN	CA-CB-CG	11.87	124.47	112.60
1	B	158	ARG	CD-NE-CZ	11.76	140.86	124.40
1	A	6	PRO	CA-C-N	11.29	139.57	120.72
1	A	6	PRO	C-N-CA	11.29	139.57	120.72
1	B	73	ASP	CA-CB-CG	11.21	123.81	112.60
1	A	112	ARG	NE-CZ-NH2	10.91	129.02	119.20
1	B	302	ASP	CA-C-N	10.86	132.04	119.98
1	B	302	ASP	C-N-CA	10.86	132.04	119.98
1	B	32	ASN	CA-CB-CG	-10.73	101.87	112.60
1	B	158	ARG	NE-CZ-NH2	-10.63	109.64	119.20
1	B	20	THR	N-CA-CB	-10.47	92.82	110.41
1	A	103	PHE	CA-CB-CG	9.89	123.69	113.80
1	B	112	ARG	CD-NE-CZ	9.88	138.23	124.40
1	A	372	ALA	O-C-N	-9.71	111.83	122.12
1	B	30	ARG	NE-CZ-NH2	9.68	127.91	119.20
1	B	102	GLY	N-CA-C	-9.52	101.55	110.21
1	A	320	GLU	CB-CG-CD	9.43	128.63	112.60
1	B	319	LYS	CA-C-N	9.26	132.87	120.65
1	B	319	LYS	C-N-CA	9.26	132.87	120.65
1	B	208	GLY	CA-C-N	9.22	133.56	120.28
1	B	208	GLY	C-N-CA	9.22	133.56	120.28
1	A	320	GLU	CA-CB-CG	8.86	131.82	114.10
1	B	214	ASN	CB-CG-ND2	8.84	129.65	116.40
1	B	20	THR	CB-CA-C	8.58	127.03	109.95
1	A	111	ARG	CA-C-N	8.58	132.11	120.44
1	A	111	ARG	C-N-CA	8.58	132.11	120.44
1	B	217	THR	CA-C-N	8.53	130.80	120.14
1	B	217	THR	C-N-CA	8.53	130.80	120.14
1	B	131	GLU	CB-CG-CD	8.50	127.05	112.60
1	B	286	THR	N-CA-CB	-8.47	97.01	110.98
1	A	235	LEU	CA-C-O	8.46	129.70	120.82
1	B	158	ARG	CG-CD-NE	8.36	130.38	112.00
1	B	297	ARG	NE-CZ-NH2	8.30	126.67	119.20
1	A	28	ALA	CA-C-O	-8.29	112.03	121.15
1	A	286	THR	CA-CB-OG1	-8.27	97.19	109.60
1	A	334	ALA	CA-C-N	8.21	131.28	120.28
1	A	334	ALA	C-N-CA	8.21	131.28	120.28
1	A	20	THR	N-CA-CB	-8.19	97.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ASP	N-CA-C	-8.19	95.23	108.41
1	A	298	THR	CA-C-N	8.11	134.10	122.09
1	A	298	THR	C-N-CA	8.11	134.10	122.09
1	B	143	GLU	CA-C-O	7.98	128.43	119.41
1	B	37	GLU	CB-CG-CD	7.96	126.13	112.60
1	B	203	GLU	CA-C-N	7.94	134.80	122.49
1	B	203	GLU	C-N-CA	7.94	134.80	122.49
1	B	333	GLU	CB-CG-CD	7.92	126.06	112.60
1	A	73	ASP	CA-CB-CG	7.90	120.50	112.60
1	B	207	HIS	CA-CB-CG	-7.88	105.92	113.80
1	A	56	ASP	N-CA-CB	7.88	121.82	110.16
1	B	149	ASP	N-CA-C	-7.87	95.74	108.41
1	A	112	ARG	CD-NE-CZ	7.84	135.37	124.40
1	A	137	GLY	CA-C-N	7.75	129.83	120.14
1	A	137	GLY	C-N-CA	7.75	129.83	120.14
1	B	379	PHE	CA-CB-CG	7.75	121.55	113.80
1	B	137	GLY	CA-C-N	7.71	129.78	120.14
1	B	137	GLY	C-N-CA	7.71	129.78	120.14
1	B	381	ARG	NE-CZ-NH2	-7.71	112.27	119.20
1	B	103	PHE	CA-CB-CG	7.67	121.47	113.80
1	A	235	LEU	CA-C-N	7.65	130.53	120.28
1	A	235	LEU	C-N-CA	7.65	130.53	120.28
1	A	273	LEU	CA-C-O	-7.65	112.79	120.82
1	B	23	ASP	CB-CA-C	7.62	125.18	110.17
1	B	108	ARG	NE-CZ-NH1	7.62	129.12	121.50
1	B	108	ARG	CD-NE-CZ	7.61	135.06	124.40
1	B	75	ASN	CA-C-N	7.58	130.75	120.44
1	B	75	ASN	C-N-CA	7.58	130.75	120.44
1	A	393	SER	CA-C-N	7.56	135.30	121.70
1	A	393	SER	C-N-CA	7.56	135.30	121.70
1	B	127	GLU	CA-CB-CG	7.55	129.21	114.10
1	A	297	ARG	CA-C-N	7.49	131.70	120.31
1	A	297	ARG	C-N-CA	7.49	131.70	120.31
1	A	375	ARG	NE-CZ-NH2	-7.49	112.46	119.20
1	B	96	PRO	CA-C-N	7.47	132.27	120.47
1	B	96	PRO	C-N-CA	7.47	132.27	120.47
1	A	352	GLU	CA-C-O	-7.44	112.36	120.24
1	A	174	ASN	N-CA-CB	-7.41	102.05	110.35
1	A	285	TYR	CA-C-N	-7.36	110.80	122.29
1	A	285	TYR	C-N-CA	-7.36	110.80	122.29
1	A	360	ASP	CA-C-N	7.33	130.11	120.28
1	A	360	ASP	C-N-CA	7.33	130.11	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	GLU	N-CA-C	-7.31	96.34	108.34
1	B	19	TRP	CA-C-O	7.31	129.06	120.58
1	A	174	ASN	CA-C-N	7.31	134.94	122.37
1	A	174	ASN	C-N-CA	7.31	134.94	122.37
1	A	6	PRO	O-C-N	-7.29	112.47	122.24
1	A	194	THR	CA-CB-CG2	7.29	122.89	110.50
1	A	107	ASP	CA-C-O	7.27	128.92	120.49
1	B	98	PHE	O-C-N	-7.25	113.08	122.37
1	A	377	PHE	CA-C-N	7.25	132.65	122.36
1	A	377	PHE	C-N-CA	7.25	132.65	122.36
1	A	121	ASN	CA-C-N	7.17	130.61	120.42
1	A	121	ASN	C-N-CA	7.17	130.61	120.42
1	B	163	THR	CA-C-O	-7.16	113.33	120.70
1	A	101	GLY	O-C-N	7.15	130.14	123.35
1	A	267	ALA	CA-C-N	7.07	130.62	120.79
1	A	267	ALA	C-N-CA	7.07	130.62	120.79
1	A	59	PRO	CB-CA-C	7.04	120.40	111.39
1	B	163	THR	CA-CB-OG1	-7.03	99.05	109.60
1	B	164	ALA	CA-C-N	7.03	130.27	120.29
1	B	164	ALA	C-N-CA	7.03	130.27	120.29
1	B	121	ASN	CA-CB-CG	-7.03	105.57	112.60
1	B	205	LEU	O-C-N	7.01	130.84	122.85
1	A	208	GLY	CA-C-O	7.00	127.49	119.09
1	B	48	TYR	N-CA-CB	-7.00	100.25	110.47
1	A	320	GLU	CG-CD-OE1	6.98	134.45	118.40
1	B	145	ASP	CA-C-O	-6.97	111.95	119.97
1	A	75	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	B	198	GLY	CA-C-N	6.94	129.58	120.28
1	B	198	GLY	C-N-CA	6.94	129.58	120.28
1	A	44	GLU	N-CA-CB	6.94	120.90	110.22
1	B	380	ILE	N-CA-CB	6.91	118.64	110.55
1	A	43	ALA	O-C-N	-6.91	114.80	122.12
1	A	158	ARG	CG-CD-NE	6.89	127.15	112.00
1	B	324	ALA	CA-C-N	6.85	129.79	120.54
1	B	324	ALA	C-N-CA	6.85	129.79	120.54
1	A	64	ALA	CA-C-N	6.85	129.34	120.44
1	A	64	ALA	C-N-CA	6.85	129.34	120.44
1	B	106	ASN	CA-C-N	6.83	131.07	121.24
1	B	106	ASN	C-N-CA	6.83	131.07	121.24
1	A	343	LEU	CA-C-N	6.81	132.91	120.79
1	A	343	LEU	C-N-CA	6.81	132.91	120.79
1	B	334	ALA	CA-C-N	6.80	129.40	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ALA	C-N-CA	6.80	129.40	120.28
1	B	241	PHE	CA-CB-CG	6.80	120.60	113.80
1	A	96	PRO	O-C-N	-6.79	113.96	122.17
1	A	235	LEU	O-C-N	-6.78	115.09	122.07
1	A	391	LEU	CA-C-N	6.78	133.47	120.66
1	A	391	LEU	C-N-CA	6.78	133.47	120.66
1	A	276	ASN	CA-C-O	-6.77	111.35	119.27
1	A	5	THR	CA-C-N	6.75	126.44	119.56
1	A	5	THR	C-N-CA	6.75	126.44	119.56
1	B	244	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	370	GLU	CA-C-O	-6.74	113.27	120.42
1	B	31	ALA	CA-C-O	-6.74	113.72	121.47
1	A	268	PHE	O-C-N	-6.74	114.87	122.08
1	B	180	GLU	CA-C-O	6.73	125.94	119.62
1	B	154	LEU	CB-CA-C	6.72	122.27	110.85
1	B	207	HIS	CA-C-N	6.71	128.59	120.13
1	B	207	HIS	C-N-CA	6.71	128.59	120.13
1	B	342	GLU	CB-CG-CD	6.70	123.99	112.60
1	A	185	GLU	CG-CD-OE1	6.70	133.80	118.40
1	A	180	GLU	CA-C-O	6.68	125.90	119.62
1	B	391	LEU	CA-C-N	6.68	133.29	120.66
1	B	391	LEU	C-N-CA	6.68	133.29	120.66
1	A	370	GLU	CA-C-O	-6.68	113.34	120.42
1	B	229	HIS	CA-C-N	6.67	127.34	119.94
1	B	229	HIS	C-N-CA	6.67	127.34	119.94
1	A	56	ASP	N-CA-C	-6.66	104.10	111.36
1	B	7	ALA	CA-C-N	6.66	131.85	120.72
1	B	7	ALA	C-N-CA	6.66	131.85	120.72
1	A	328	ASP	CA-C-O	6.65	126.08	119.49
1	B	121	ASN	CA-C-N	6.65	129.86	120.42
1	B	121	ASN	C-N-CA	6.65	129.86	120.42
1	B	187	ARG	NE-CZ-NH2	-6.65	113.22	119.20
1	B	274	LEU	CA-C-O	-6.63	113.39	120.42
1	B	74	PHE	CA-C-O	-6.62	113.87	120.82
1	B	208	GLY	N-CA-C	6.61	122.06	113.27
1	B	381	ARG	CA-C-N	6.61	129.03	120.44
1	B	381	ARG	C-N-CA	6.61	129.03	120.44
1	A	263	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	189	ASP	CA-C-O	-6.60	112.17	120.28
1	B	359	ASN	N-CA-CB	-6.58	99.35	110.41
1	A	105	SER	N-CA-C	-6.57	101.42	110.35
1	B	12	PHE	CA-CB-CG	6.54	120.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	PRO	CA-C-N	6.53	129.03	120.28
1	B	59	PRO	C-N-CA	6.53	129.03	120.28
1	A	333	GLU	CA-CB-CG	6.51	127.12	114.10
1	A	216	GLU	CA-C-N	6.50	129.32	120.54
1	A	216	GLU	C-N-CA	6.50	129.32	120.54
1	B	209	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	167	TYR	CA-C-O	-6.48	114.02	120.70
1	A	65	ALA	N-CA-C	-6.48	104.14	111.07
1	B	93	PHE	CA-C-O	-6.41	111.34	120.51
1	B	34	ASP	CA-C-N	6.41	126.03	119.56
1	B	34	ASP	C-N-CA	6.41	126.03	119.56
1	A	149	ASP	N-CA-CB	6.40	120.39	110.21
1	A	202	ILE	CA-C-N	6.38	130.81	120.60
1	A	202	ILE	C-N-CA	6.38	130.81	120.60
1	A	20	THR	CB-CA-C	6.37	123.31	109.99
1	B	372	ALA	O-C-N	-6.37	115.37	122.12
1	A	329	PRO	CA-C-N	6.33	128.67	120.44
1	A	329	PRO	C-N-CA	6.33	128.67	120.44
1	A	279	PRO	O-C-N	-6.33	114.96	122.24
1	A	84	LYS	CA-C-N	6.32	133.83	122.13
1	A	84	LYS	C-N-CA	6.32	133.83	122.13
1	A	51	THR	CA-CB-CG2	6.32	121.25	110.50
1	A	44	GLU	CA-CB-CG	6.32	126.74	114.10
1	A	63	THR	CA-C-N	6.32	128.74	120.28
1	A	63	THR	C-N-CA	6.32	128.74	120.28
1	B	150	LEU	CA-C-O	-6.31	112.97	120.10
1	B	174	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	95	HIS	CG-CD2-NE2	6.27	113.47	107.20
1	B	60	PHE	CA-CB-CG	6.27	120.07	113.80
1	B	44	GLU	CG-CD-OE2	-6.25	104.02	118.40
1	B	189	ASP	CA-C-O	-6.25	113.62	120.24
1	B	187	ARG	NE-CZ-NH1	6.24	127.74	121.50
1	B	96	PRO	O-C-N	-6.23	114.63	122.17
1	A	53	HIS	CB-CA-C	-6.23	99.26	109.53
1	A	297	ARG	CD-NE-CZ	6.21	133.10	124.40
1	A	389	HIS	CA-C-O	-6.21	114.31	120.70
1	A	281	GLY	CA-C-O	-6.21	116.86	122.57
1	A	112	ARG	NH1-CZ-NH2	-6.20	111.24	119.30
1	B	20	THR	CA-CB-CG2	6.20	121.04	110.50
1	A	163	THR	CA-CB-OG1	-6.20	100.31	109.60
1	A	145	ASP	CA-C-O	-6.19	112.85	119.97
1	A	266	SER	CA-C-O	-6.18	114.33	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ARG	CB-CG-CD	6.18	125.51	111.30
1	B	249	ARG	O-C-N	-6.17	115.58	122.55
1	B	158	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	A	372	ALA	CA-C-O	6.14	127.06	120.55
1	A	71	LEU	CA-C-N	6.12	126.61	119.94
1	A	71	LEU	C-N-CA	6.12	126.61	119.94
1	A	222	MET	CA-C-N	6.12	131.97	122.49
1	A	222	MET	C-N-CA	6.12	131.97	122.49
1	B	310	ALA	O-C-N	-6.11	115.64	122.12
1	A	344	GLY	CA-C-O	-6.10	112.30	119.50
1	B	318	LEU	CA-C-O	-6.10	113.95	120.42
1	A	66	GLU	O-C-N	-6.08	115.76	122.09
1	A	330	GLU	N-CA-CB	6.07	118.81	110.01
1	A	250	GLY	N-CA-C	6.05	119.45	111.70
1	B	160	GLY	CA-C-O	-6.05	114.46	121.00
1	A	110	ILE	O-C-N	-6.05	116.00	121.87
1	A	209	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	278	PHE	CA-C-N	6.04	126.20	119.32
1	B	278	PHE	C-N-CA	6.04	126.20	119.32
1	B	242	HIS	CA-C-O	-6.03	114.99	121.38
1	A	95	HIS	CA-C-N	6.02	126.45	119.47
1	A	95	HIS	C-N-CA	6.02	126.45	119.47
1	A	148	LYS	N-CA-C	6.02	119.01	109.50
1	A	389	HIS	N-CA-CB	6.02	118.79	110.07
1	A	389	HIS	CA-CB-CG	-5.98	107.82	113.80
1	B	43	ALA	CA-C-O	-5.98	114.21	120.55
1	B	120	HIS	CA-C-N	5.96	128.86	120.28
1	B	120	HIS	C-N-CA	5.96	128.86	120.28
1	B	219	HIS	CB-CG-CD2	5.95	138.94	131.20
1	B	76	GLN	N-CA-CB	5.95	118.69	110.07
1	B	56	ASP	N-CA-C	-5.94	104.89	111.36
1	B	343	LEU	CA-C-N	5.93	131.35	120.79
1	B	343	LEU	C-N-CA	5.93	131.35	120.79
1	B	384	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	255	GLN	OE1-CD-NE2	5.92	128.52	122.60
1	B	29	THR	CA-CB-OG1	-5.91	100.74	109.60
1	A	286	THR	N-CA-C	5.91	122.47	113.61
1	A	96	PRO	CA-C-N	5.90	130.30	120.62
1	A	96	PRO	C-N-CA	5.90	130.30	120.62
1	A	107	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	383	ASN	CA-CB-CG	-5.90	106.70	112.60
1	A	94	SER	N-CA-C	5.90	118.94	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ASN	CA-CB-CG	5.89	118.49	112.60
1	B	97	VAL	CA-CB-CG1	5.86	120.36	110.40
1	A	53	HIS	CA-C-O	-5.86	114.19	120.92
1	A	56	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	359	ASN	CA-C-O	-5.84	113.26	119.97
1	B	34	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	290	HIS	CA-C-O	5.80	126.75	120.43
1	A	263	ASP	CA-C-N	5.80	128.32	120.44
1	A	263	ASP	C-N-CA	5.80	128.32	120.44
1	B	328	ASP	CA-C-O	5.79	125.19	119.51
1	B	99	LYS	CA-C-O	-5.78	112.49	119.49
1	A	195	VAL	CA-C-O	-5.78	115.26	121.27
1	B	37	GLU	CA-C-N	5.78	127.95	120.44
1	B	37	GLU	C-N-CA	5.78	127.95	120.44
1	A	19	TRP	N-CA-CB	5.77	118.62	109.51
1	B	309	LYS	CA-C-N	5.76	128.00	120.28
1	B	309	LYS	C-N-CA	5.76	128.00	120.28
1	A	273	LEU	CD1-CG-CD2	-5.76	98.12	110.80
1	B	64	ALA	N-CA-CB	5.76	118.59	110.12
1	B	193	PRO	O-C-N	-5.75	114.50	122.27
1	B	203	GLU	CG-CD-OE1	5.75	131.63	118.40
1	B	276	ASN	CB-CG-ND2	5.75	125.03	116.40
1	A	286	THR	N-CA-CB	-5.74	102.24	110.80
1	A	156	ARG	CA-CB-CG	5.73	125.55	114.10
1	A	363	SER	N-CA-C	5.71	119.43	112.23
1	B	330	GLU	CA-CB-CG	5.71	125.52	114.10
1	B	223	ALA	O-C-N	-5.69	115.23	122.34
1	A	19	TRP	CA-C-O	5.68	127.24	120.70
1	B	364	PHE	CA-CB-CG	-5.67	108.13	113.80
1	A	163	THR	CA-CB-CG2	5.67	120.13	110.50
1	B	188	GLY	CA-C-N	5.66	130.75	122.77
1	B	188	GLY	C-N-CA	5.66	130.75	122.77
1	A	111	ARG	NE-CZ-NH1	5.66	127.16	121.50
1	A	163	THR	CA-C-N	5.66	127.86	120.28
1	A	163	THR	C-N-CA	5.66	127.86	120.28
1	B	108	ARG	NE-CZ-NH2	-5.65	114.11	119.20
1	A	280	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	B	223	ALA	CA-C-N	5.65	130.98	120.87
1	B	223	ALA	C-N-CA	5.65	130.98	120.87
1	A	53	HIS	N-CA-CB	5.64	119.37	110.23
1	B	184	ASN	O-C-N	5.64	129.19	123.26
1	B	84	LYS	N-CA-C	-5.64	102.41	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	GLY	CA-C-O	-5.63	116.39	122.47
1	B	8	ASP	CA-C-N	5.63	130.13	122.19
1	B	8	ASP	C-N-CA	5.63	130.13	122.19
1	A	286	THR	OG1-CB-CG2	5.62	120.55	109.30
1	A	385	LEU	CA-C-O	-5.62	114.92	120.82
1	B	237	ALA	CA-C-N	5.62	130.15	122.34
1	B	237	ALA	C-N-CA	5.62	130.15	122.34
1	B	392	GLY	CA-C-O	-5.62	113.29	120.03
1	A	115	LEU	CA-C-N	5.61	127.73	120.44
1	A	115	LEU	C-N-CA	5.61	127.73	120.44
1	A	360	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	40	HIS	CA-CB-CG	-5.58	108.22	113.80
1	A	213	LEU	N-CA-C	5.57	118.78	110.14
1	B	333	GLU	O-C-N	-5.57	115.81	122.15
1	A	107	ASP	O-C-N	-5.56	116.18	123.02
1	B	77	ALA	O-C-N	-5.56	116.22	122.12
1	A	280	ASN	CA-C-O	-5.56	113.06	119.56
1	B	360	ASP	CA-C-N	5.55	128.28	120.28
1	B	360	ASP	C-N-CA	5.55	128.28	120.28
1	B	105	SER	CA-C-O	-5.54	115.06	121.15
1	B	150	LEU	CA-C-N	5.54	128.16	120.29
1	B	150	LEU	C-N-CA	5.54	128.16	120.29
1	B	194	THR	CA-CB-CG2	5.53	119.90	110.50
1	B	137	GLY	O-C-N	-5.53	115.52	122.70
1	A	356	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	208	GLY	CA-C-O	5.49	126.05	120.45
1	A	164	ALA	CA-C-N	5.49	128.08	120.29
1	A	164	ALA	C-N-CA	5.49	128.08	120.29
1	B	383	ASN	CA-CB-CG	-5.49	107.11	112.60
1	B	219	HIS	CB-CG-ND1	-5.48	114.48	122.70
1	B	286	THR	CB-CA-C	5.48	120.07	110.64
1	A	346	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	336	LYS	CA-C-O	-5.48	115.06	120.70
1	B	325	PHE	CA-CB-CG	5.48	119.28	113.80
1	A	276	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	B	114	ALA	CA-C-N	5.46	127.59	120.28
1	B	114	ALA	C-N-CA	5.46	127.59	120.28
1	A	21	GLY	N-CA-C	5.45	122.85	115.00
1	B	174	ASN	CA-CB-CG	-5.45	107.15	112.60
1	A	169	LYS	CA-C-N	5.45	127.52	120.44
1	A	169	LYS	C-N-CA	5.45	127.52	120.44
1	A	352	GLU	N-CA-CB	5.44	119.31	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	LEU	CA-C-O	-5.44	114.65	120.42
1	A	372	ALA	CA-C-N	5.43	131.09	120.99
1	A	372	ALA	C-N-CA	5.43	131.09	120.99
1	B	191	PHE	CA-C-O	-5.43	115.64	121.56
1	B	378	ALA	CA-C-N	5.43	128.56	120.31
1	B	378	ALA	C-N-CA	5.43	128.56	120.31
1	A	280	ASN	N-CA-C	-5.42	106.25	112.92
1	B	111	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	B	294	LYS	CB-CA-C	-5.41	102.96	110.16
1	A	368	ASP	CA-C-N	5.41	127.53	120.28
1	A	368	ASP	C-N-CA	5.41	127.53	120.28
1	B	328	ASP	CA-C-N	5.41	125.06	119.05
1	B	328	ASP	C-N-CA	5.41	125.06	119.05
1	B	307	SER	O-C-N	-5.40	116.39	122.12
1	B	342	GLU	O-C-N	-5.40	115.90	122.22
1	A	117	LYS	CA-C-N	5.40	127.47	120.56
1	A	117	LYS	C-N-CA	5.40	127.47	120.56
1	B	274	LEU	O-C-N	5.40	128.30	122.15
1	A	48	TYR	N-CA-C	-5.38	106.39	113.12
1	A	78	LEU	O-C-N	5.38	127.61	122.07
1	A	223	ALA	CA-C-O	5.37	125.70	119.32
1	A	135	MET	CA-C-O	5.36	126.04	120.30
1	A	30	ARG	CA-C-O	-5.36	114.84	121.11
1	A	81	THR	CA-CB-OG1	-5.36	101.56	109.60
1	A	305	TRP	O-C-N	-5.36	116.04	122.15
1	B	140	GLU	CB-CG-CD	5.35	121.69	112.60
1	A	221	GLN	CA-C-N	5.35	129.65	120.72
1	A	221	GLN	C-N-CA	5.35	129.65	120.72
1	B	359	ASN	CB-CA-C	5.34	120.58	109.95
1	B	101	GLY	O-C-N	5.34	128.82	123.48
1	B	243	ILE	CA-C-O	-5.33	115.71	121.19
1	A	352	GLU	CG-CD-OE1	5.32	130.63	118.40
1	B	275	GLU	CA-C-N	5.31	131.01	121.66
1	B	275	GLU	C-N-CA	5.31	131.01	121.66
1	A	237	ALA	CA-C-N	5.30	130.27	122.63
1	A	237	ALA	C-N-CA	5.30	130.27	122.63
1	B	67	ARG	CA-C-O	-5.30	115.25	120.82
1	A	203	GLU	CA-C-N	5.29	131.41	122.26
1	A	203	GLU	C-N-CA	5.29	131.41	122.26
1	B	131	GLU	CA-C-O	5.29	124.96	119.14
1	A	254	ASP	N-CA-CB	5.28	118.26	109.60
1	A	43	ALA	CB-CA-C	5.27	119.54	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	352	GLU	CB-CG-CD	5.27	121.55	112.60
1	A	13	GLY	N-CA-C	-5.27	104.65	113.02
1	B	16	THR	CA-CB-OG1	-5.26	101.72	109.60
1	B	68	GLU	CB-CA-C	-5.26	102.40	110.81
1	B	30	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	301	TYR	N-CA-CB	5.24	118.30	110.22
1	A	59	PRO	O-C-N	-5.24	116.34	122.99
1	B	85	VAL	N-CA-CB	5.23	118.53	111.21
1	B	246	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	117	LYS	CG-CD-CE	5.22	123.32	111.30
1	B	313	SER	CA-C-N	5.22	127.59	120.54
1	B	313	SER	C-N-CA	5.22	127.59	120.54
1	A	11	THR	O-C-N	-5.22	116.40	123.19
1	B	64	ALA	CA-C-N	5.22	128.05	120.79
1	B	64	ALA	C-N-CA	5.22	128.05	120.79
1	A	234	ALA	CA-C-N	5.22	127.22	120.44
1	A	234	ALA	C-N-CA	5.22	127.22	120.44
1	A	328	ASP	CA-C-N	5.21	124.83	119.05
1	A	328	ASP	C-N-CA	5.21	124.83	119.05
1	B	304	VAL	CA-C-O	-5.21	115.72	121.29
1	B	354	ALA	N-CA-C	-5.21	105.50	111.07
1	B	60	PHE	CA-C-O	-5.20	115.04	120.55
1	A	185	GLU	O-C-N	-5.19	115.35	121.32
1	A	393	SER	CA-C-O	5.19	124.76	119.05
1	A	68	GLU	CA-C-N	5.18	127.49	120.65
1	A	68	GLU	C-N-CA	5.18	127.49	120.65
1	B	393	SER	N-CA-C	-5.18	107.09	113.41
1	B	242	HIS	N-CA-C	-5.18	101.04	108.60
1	A	286	THR	CA-C-O	-5.17	113.08	119.18
1	A	139	ARG	NH1-CZ-NH2	-5.17	112.58	119.30
1	B	94	SER	N-CA-C	5.17	118.05	111.69
1	A	30	ARG	CD-NE-CZ	5.17	131.63	124.40
1	A	299	ASP	CA-C-O	5.16	126.85	120.92
1	B	117	LYS	CA-C-N	5.14	127.04	120.56
1	B	117	LYS	C-N-CA	5.14	127.04	120.56
1	A	266	SER	CA-C-N	5.14	127.48	120.54
1	A	266	SER	C-N-CA	5.14	127.48	120.54
1	A	305	TRP	CB-CA-C	5.14	119.58	110.85
1	A	76	GLN	OE1-CD-NE2	-5.13	117.47	122.60
1	A	345	GLU	CB-CG-CD	5.12	121.31	112.60
1	B	36	VAL	CB-CA-C	5.12	119.28	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	PRO	CB-CA-C	5.11	117.94	110.63
1	B	24	PRO	O-C-N	-5.11	115.39	122.24
1	B	208	GLY	O-C-N	-5.11	116.93	122.19
1	B	98	PHE	CA-C-N	5.11	128.77	120.60
1	B	98	PHE	C-N-CA	5.11	128.77	120.60
1	A	174	ASN	O-C-N	-5.09	116.16	122.83
1	A	320	GLU	CB-CA-C	5.08	118.86	110.88
1	A	23	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	375	ARG	CB-CA-C	-5.08	102.22	109.84
1	A	61	ASP	CA-C-N	5.08	127.98	120.82
1	A	61	ASP	C-N-CA	5.08	127.98	120.82
1	A	250	GLY	CA-C-O	-5.07	117.24	122.26
1	A	95	HIS	O-C-N	-5.05	116.10	121.30
1	A	162	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	101	GLY	CA-C-O	-5.04	118.69	122.37
1	A	231	ILE	CA-C-N	5.03	127.44	120.29
1	A	231	ILE	C-N-CA	5.03	127.44	120.29
1	A	22	ALA	N-CA-CB	-5.03	102.46	110.06
1	A	136	TRP	CA-C-O	-5.03	114.24	120.57
1	B	286	THR	OG1-CB-CG2	5.03	119.36	109.30
1	A	30	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	A	356	ASP	CA-C-N	5.02	127.27	120.44
1	A	356	ASP	C-N-CA	5.02	127.27	120.44
1	B	200	ALA	CA-C-N	5.01	127.31	120.54
1	B	200	ALA	C-N-CA	5.01	127.31	120.54

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	2891	19	0
1	B	3027	0	2890	18	0
2	A	12	0	12	0	0
2	B	12	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	268	0	0	0	0
4	B	270	0	0	2	0
All	All	6618	0	5804	37	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 3.

All (37) 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	1.30	0.77
1:B:95:HIS:HD2	1:B:97:VAL:H	1.36	0.74
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.73	0.70
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.72	0.70
1:A:235:LEU:HD12	1:A:273:LEU:HD21	1.77	0.66
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.87	0.56
1:A:95:HIS:CD2	1:A:97:VAL:H	2.19	0.56
1:B:20:THR:HG23	1:B:28:ALA:CB	2.37	0.54
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.52
1:B:158:ARG:HG3	1:B:205:LEU:HD23	1.91	0.52
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.74	0.51
1:A:20:THR:HG23	1:A:28:ALA:CB	2.40	0.51
1:B:208:GLY:HA3	4:B:602:HOH:O	2.12	0.49
1:A:184:ASN:HD22	1:A:185:GLU:HB2	1.78	0.49
1:B:249:ARG:O	1:B:252:LYS:HE3	2.15	0.47
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.81	0.46
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.97	0.45
1:A:216:GLU:HB2	1:A:244:ASP:HB2	1.97	0.45
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.74	0.45
1:B:64:ALA:O	1:B:68:GLU:HG2	2.16	0.45
1:B:158:ARG:HD2	4:B:489:HOH:O	2.16	0.45
1:B:355:ALA:O	1:B:359:ASN:HB3	2.16	0.45
1:B:235:LEU:HD22	1:B:283:PRO:HB2	1.99	0.45
1:B:235:LEU:HD12	1:B:273:LEU:HD21	1.99	0.44
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.85	0.44
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.51	0.44
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.98	0.43
1:B:383:ASN:O	1:B:387:ILE:HG12	2.19	0.43
1:B:52:PHE:CZ	1:B:128:MET:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:HG3	1:A:214:ASN:O	2.20	0.42
1:B:55:ASN:HA	1:B:58:ILE:O	2.19	0.42
1:A:53:HIS:O	1:A:54:ASP:C	2.63	0.42
1:A:217:THR:HA	1:A:227:PHE:CD2	2.56	0.41
1:B:95:HIS:CD2	1:B:97:VAL:H	2.26	0.41
1:A:115:LEU:HD21	1:A:163:THR:HG21	2.03	0.41
1:A:295:PRO:O	1:A:296:SER:C	2.62	0.41
1:A:280:ASN:OD1	1:A:341:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/393 (100%)	377 (96%)	13 (3%)	1 (0%)	36	46
1	B	391/393 (100%)	379 (97%)	11 (3%)	1 (0%)	36	46
All	All	782/786 (100%)	756 (97%)	24 (3%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	B	185	GLU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	305/306 (100%)	296 (97%)	9 (3%)	36	53
1	B	305/306 (100%)	294 (96%)	11 (4%)	31	47
All	All	610/612 (100%)	590 (97%)	20 (3%)	33	50

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	94	SER
1	A	158	ARG
1	A	184	ASN
1	A	213	LEU
1	A	254	ASP
1	A	286	THR
1	A	330	GLU
1	A	359	ASN
1	B	20	THR
1	B	34	ASP
1	B	41	LYS
1	B	94	SER
1	B	149	ASP
1	B	185	GLU
1	B	213	LEU
1	B	235	LEU
1	B	286	THR
1	B	359	ASN
1	B	370	GLU

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	95	HIS
1	A	174	ASN
1	A	184	ASN
1	A	221	GLN
1	A	383	ASN
1	A	384	GLN
1	B	32	ASN
1	B	95	HIS

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Mol	Chain	Res	Type
1	B	120	HIS
1	B	184	ASN
1	B	221	GLN
1	B	359	ASN
1	B	384	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	SOR	A	400	3	11,11,11	1.85	2 (18%)	14,14,14	3.10	7 (50%)
2	SOR	B	400	3	11,11,11	2.03	2 (18%)	14,14,14	3.71	10 (71%)

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	SOR	A	400	3	-	2/16/16/16	-
2	SOR	B	400	3	-	2/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	SOR	O3-C3	4.86	1.55	1.43
2	A	400	SOR	O3-C3	4.24	1.53	1.43
2	B	400	SOR	O5-C5	-3.67	1.35	1.43
2	A	400	SOR	C4-C3	3.35	1.59	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	SOR	C2-C3-C4	-9.02	98.63	112.48
2	B	400	SOR	C2-C3-C4	-6.63	102.30	112.48
2	B	400	SOR	C5-C4-C3	-6.17	103.00	112.48
2	B	400	SOR	O3-C3-C4	4.43	119.82	109.46
2	B	400	SOR	C6-C5-C4	-4.20	103.62	112.17
2	A	400	SOR	C5-C4-C3	-4.06	106.25	112.48
2	B	400	SOR	O2-C2-C3	3.94	118.47	109.25
2	B	400	SOR	O6-C6-C5	-3.61	103.58	111.16
2	B	400	SOR	O4-C4-C5	-3.52	100.92	108.93
2	B	400	SOR	O5-C5-C6	-3.25	101.64	109.03
2	B	400	SOR	O3-C3-C2	2.95	115.64	108.93
2	A	400	SOR	O2-C2-C3	2.91	116.05	109.25
2	A	400	SOR	O3-C3-C2	2.52	114.66	108.93
2	B	400	SOR	O2-C2-C1	-2.35	103.67	109.03
2	A	400	SOR	O3-C3-C4	2.34	114.92	109.46
2	A	400	SOR	O2-C2-C1	-2.29	103.82	109.03
2	A	400	SOR	O5-C5-C4	-2.24	104.01	109.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	SOR	C4-C5-C6-O6
2	B	400	SOR	O5-C5-C6-O6
2	B	400	SOR	C4-C5-C6-O6
2	A	400	SOR	O5-C5-C6-O6

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.