



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:00 PM UTC

PDB ID : 1DIE / pdb_00001die
Title : OBSERVATIONS OF REACTION INTERMEDIATES AND THE MECHANISM OF ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE
Authors : Collyer, C.A.; Viehmann, H.; Goldberg, J.D.; Blow, D.M.
Deposited on : 1992-06-04
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

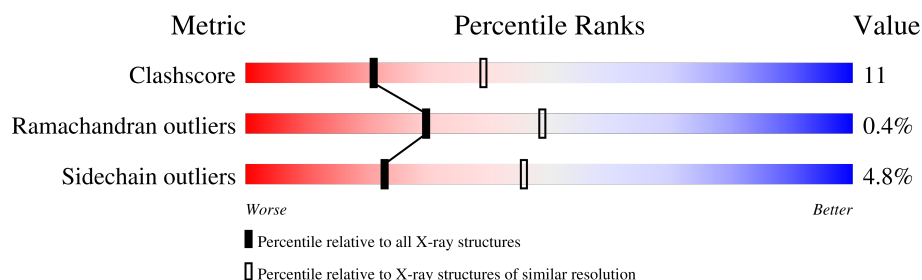
1 Overall quality at a glance

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 6659 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.

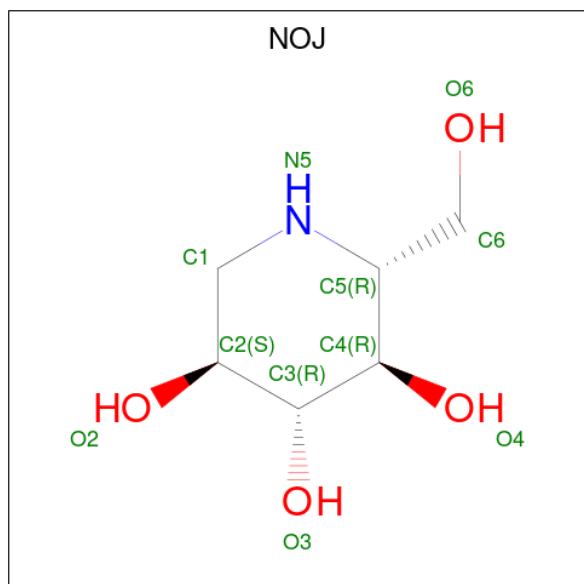
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3026	1919	521	577	9			
1	B	393	Total	C	N	O	S	0	0	0
			3026	1919	521	577	9			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is 1-DEOXYNOJIRIMYCIN (CCD ID: NOJ) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	1	4		
3	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 4 is water.

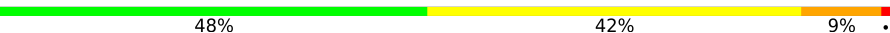
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	291	Total	O	0	0
			291	291		
4	B	290	Total	O	0	0
			290	290		

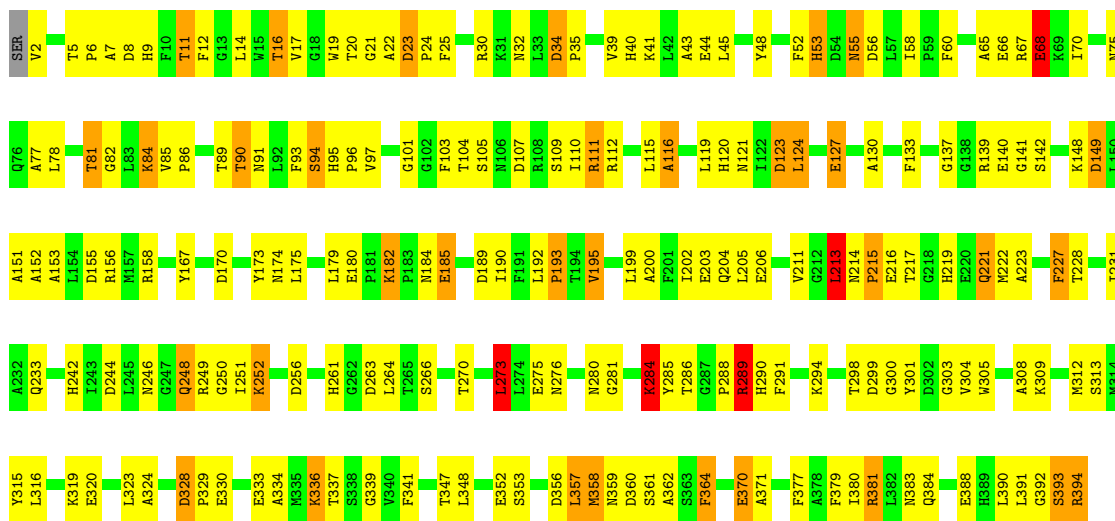
3 Residue-property plots

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.

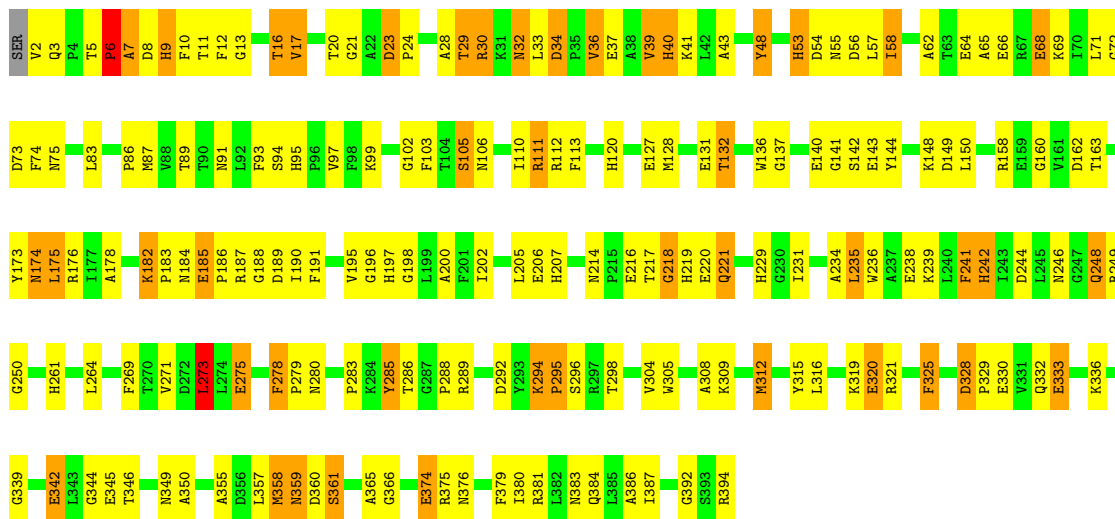
• Molecule 1: D-XYLOSE ISOMERASE

Chain A: 



• Molecule 1: D-XYLOSE ISOMERASE

Chain B: 



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 153.40 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}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6659	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: NOJ, MG

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	1.46	6/3100 (0.2%)	2.51	223/4201 (5.3%)
1	B	1.46	6/3100 (0.2%)	2.42	187/4201 (4.5%)
All	All	1.46	12/6200 (0.2%)	2.46	410/8402 (4.9%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	GLY	N-CA	7.04	1.51	1.45
1	B	231	ILE	N-CA	6.42	1.54	1.46
1	A	305	TRP	N-CA	6.22	1.54	1.46
1	B	3	GLN	CA-C	5.64	1.59	1.52
1	A	115	LEU	N-CA	5.55	1.53	1.46
1	B	316	LEU	C-O	5.51	1.30	1.24
1	B	217	THR	CA-CB	5.30	1.62	1.53
1	A	341	PHE	N-CA	5.25	1.52	1.46
1	A	339	GLY	C-O	5.24	1.30	1.24
1	B	198	GLY	C-O	5.16	1.30	1.23
1	A	286	THR	CA-CB	5.13	1.61	1.53
1	B	295	PRO	C-N	-5.08	1.26	1.33

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	ASN	CA-CB-CG	18.57	131.17	112.60
1	A	379	PHE	CA-CB-CG	14.46	128.26	113.80
1	B	289	ARG	CD-NE-CZ	12.42	141.79	124.40
1	B	34	ASP	CA-CB-CG	11.95	124.55	112.60
1	B	68	GLU	CB-CG-CD	11.36	131.91	112.60
1	B	127	GLU	CA-CB-CG	11.23	136.55	114.10
1	A	244	ASP	CA-CB-CG	11.08	123.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	GLU	CB-CG-CD	10.96	131.23	112.60
1	A	276	ASN	CA-C-O	-10.43	106.55	119.38
1	A	281	GLY	CA-C-O	-10.21	114.02	122.29
1	B	394	ARG	CD-NE-CZ	10.11	138.56	124.40
1	B	94	SER	N-CA-C	10.01	123.61	111.40
1	A	356	ASP	CA-CB-CG	9.93	122.53	112.60
1	B	217	THR	CA-C-N	9.85	131.07	120.03
1	B	217	THR	C-N-CA	9.85	131.07	120.03
1	A	175	LEU	O-C-N	9.78	135.20	123.27
1	A	111	ARG	NE-CZ-NH2	-9.68	110.49	119.20
1	B	381	ARG	NE-CZ-NH2	-9.50	110.65	119.20
1	B	68	GLU	CA-CB-CG	9.41	132.93	114.10
1	A	21	GLY	N-CA-C	9.41	128.54	115.27
1	A	133	PHE	CA-C-O	9.38	130.50	120.46
1	B	32	ASN	CA-CB-CG	-9.35	103.25	112.60
1	B	249	ARG	CD-NE-CZ	9.29	137.41	124.40
1	A	141	GLY	CA-C-O	-9.29	114.50	120.91
1	B	375	ARG	NE-CZ-NH2	-9.26	110.87	119.20
1	B	379	PHE	CA-CB-CG	9.07	122.87	113.80
1	A	107	ASP	CA-CB-CG	9.06	121.66	112.60
1	B	33	LEU	CA-C-O	-9.05	110.52	120.38
1	A	170	ASP	CA-C-O	-9.01	111.26	120.90
1	B	346	THR	CA-CB-OG1	-8.71	96.54	109.60
1	B	56	ASP	N-CA-C	-8.66	101.03	111.69
1	B	238	GLU	CB-CG-CD	8.63	127.27	112.60
1	A	68	GLU	CB-CG-CD	8.55	127.14	112.60
1	A	93	PHE	CA-C-O	-8.47	108.40	120.51
1	A	127	GLU	CA-CB-CG	8.45	130.99	114.10
1	A	227	PHE	CA-C-O	-8.44	111.60	120.55
1	A	215	PRO	CA-C-O	-8.35	111.49	121.67
1	A	40	HIS	CA-C-O	-8.33	112.12	120.70
1	A	142	SER	CA-C-O	-8.30	112.58	121.38
1	B	120	HIS	CA-CB-CG	-8.27	105.53	113.80
1	B	12	PHE	CA-CB-CG	8.26	122.06	113.80
1	B	40	HIS	CA-CB-CG	-8.25	105.55	113.80
1	A	263	ASP	CA-C-N	8.18	131.56	120.44
1	A	263	ASP	C-N-CA	8.18	131.56	120.44
1	A	137	GLY	CA-C-N	8.03	130.18	120.14
1	A	137	GLY	C-N-CA	8.03	130.18	120.14
1	A	120	HIS	CA-CB-CG	-7.96	105.84	113.80
1	A	189	ASP	CA-C-O	-7.82	110.66	120.28
1	A	227	PHE	CA-CB-CG	7.77	121.57	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	ARG	NE-CZ-NH2	-7.77	112.21	119.20
1	B	190	ILE	CA-C-O	-7.75	111.64	121.48
1	A	167	TYR	CA-C-O	-7.66	112.77	120.82
1	A	228	THR	O-C-N	-7.66	114.19	122.07
1	B	392	GLY	CA-C-N	7.62	135.54	121.52
1	B	392	GLY	C-N-CA	7.62	135.54	121.52
1	B	248	GLN	OE1-CD-NE2	-7.62	114.98	122.60
1	B	200	ALA	O-C-N	7.61	129.91	122.07
1	B	56	ASP	CA-CB-CG	7.59	120.19	112.60
1	B	178	ALA	O-C-N	-7.57	114.49	123.27
1	B	241	PHE	CA-CB-CG	7.52	121.32	113.80
1	A	105	SER	CA-C-N	7.50	131.70	120.31
1	A	105	SER	C-N-CA	7.50	131.70	120.31
1	B	344	GLY	CA-C-N	7.44	132.67	122.19
1	B	344	GLY	C-N-CA	7.44	132.67	122.19
1	A	149	ASP	N-CA-C	-7.43	96.44	108.41
1	B	75	ASN	CA-CB-CG	-7.42	105.18	112.60
1	B	91	ASN	OD1-CG-ND2	-7.42	115.19	122.60
1	A	124	LEU	CA-C-O	-7.40	113.23	121.00
1	A	360	ASP	CA-C-N	7.39	130.50	120.38
1	A	360	ASP	C-N-CA	7.39	130.50	120.38
1	A	158	ARG	CD-NE-CZ	7.37	134.72	124.40
1	B	250	GLY	CA-C-O	7.37	128.34	122.52
1	B	275	GLU	CA-C-O	-7.37	112.67	120.55
1	B	207	HIS	CA-CB-CG	-7.36	106.44	113.80
1	A	7	ALA	CA-C-N	7.35	133.17	120.68
1	A	7	ALA	C-N-CA	7.35	133.17	120.68
1	A	381	ARG	CA-C-O	-7.32	113.14	120.82
1	A	334	ALA	CA-C-N	7.29	129.91	120.44
1	A	334	ALA	C-N-CA	7.29	129.91	120.44
1	A	328	ASP	CA-C-O	7.27	126.64	119.51
1	B	16	THR	CA-CB-OG1	-7.25	98.72	109.60
1	A	56	ASP	CA-C-N	7.25	133.66	122.42
1	A	56	ASP	C-N-CA	7.25	133.66	122.42
1	A	370	GLU	CA-C-O	-7.24	111.64	119.97
1	B	93	PHE	CA-C-O	-7.23	110.17	120.51
1	A	246	ASN	OD1-CG-ND2	-7.19	115.41	122.60
1	B	110	ILE	CB-CG1-CD1	7.19	128.89	113.80
1	B	286	THR	CA-CB-OG1	-7.18	98.83	109.60
1	B	187	ARG	CD-NE-CZ	7.17	134.44	124.40
1	A	377	PHE	CA-C-O	-7.16	110.57	119.38
1	A	388	GLU	CA-C-O	-7.16	112.96	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ASP	CB-CA-C	7.16	124.27	110.17
1	B	246	ASN	OD1-CG-ND2	-7.15	115.45	122.60
1	A	352	GLU	CA-C-O	-7.13	112.61	120.38
1	B	30	ARG	CD-NE-CZ	6.99	134.19	124.40
1	A	223	ALA	CA-C-N	6.92	133.26	120.87
1	A	223	ALA	C-N-CA	6.92	133.26	120.87
1	B	380	ILE	N-CA-CB	6.92	118.47	110.65
1	A	263	ASP	CA-CB-CG	6.91	119.51	112.60
1	B	283	PRO	CB-CA-C	6.90	120.02	111.12
1	A	107	ASP	CA-C-O	6.87	128.13	120.43
1	A	320	GLU	CA-CB-CG	6.85	127.80	114.10
1	A	7	ALA	CA-C-O	6.83	127.76	119.49
1	A	90	THR	CA-CB-OG1	-6.83	99.35	109.60
1	A	394	ARG	CD-NE-CZ	6.83	133.96	124.40
1	A	324	ALA	CA-C-N	6.81	130.25	120.79
1	A	324	ALA	C-N-CA	6.81	130.25	120.79
1	A	139	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	B	29	THR	CA-CB-OG1	-6.80	99.40	109.60
1	B	72	GLY	CA-C-O	-6.79	113.30	120.90
1	B	375	ARG	NH1-CZ-NH2	6.79	128.13	119.30
1	A	148	LYS	N-CA-C	6.76	119.70	109.23
1	A	357	LEU	CA-C-O	-6.75	113.75	120.70
1	A	304	VAL	CA-C-O	-6.74	114.03	121.17
1	A	111	ARG	NE-CZ-NH1	6.72	128.22	121.50
1	B	221	GLN	CA-C-O	-6.70	112.26	119.97
1	A	116	ALA	O-C-N	6.70	129.33	122.09
1	B	48	TYR	N-CA-CB	-6.70	100.28	110.33
1	A	357	LEU	O-C-N	6.69	129.31	122.09
1	B	112	ARG	NE-CZ-NH2	6.67	125.21	119.20
1	A	312	MET	CA-C-O	-6.66	113.49	120.55
1	A	44	GLU	CA-CB-CG	6.64	127.37	114.10
1	A	252	LYS	CB-CG-CD	6.64	126.56	111.30
1	A	290	HIS	CA-CB-CG	6.63	120.43	113.80
1	A	193	PRO	N-CA-C	6.62	122.13	113.86
1	B	294	LYS	O-C-N	6.62	127.73	121.38
1	A	43	ALA	CB-CA-C	6.60	121.32	110.90
1	B	191	PHE	CA-C-O	-6.58	113.90	121.47
1	A	289	ARG	NE-CZ-NH1	6.54	128.04	121.50
1	A	330	GLU	CB-CG-CD	-6.54	101.47	112.60
1	A	140	GLU	CB-CG-CD	6.52	123.68	112.60
1	A	56	ASP	N-CA-CB	6.50	119.78	110.16
1	A	152	ALA	CA-C-O	-6.50	113.53	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ALA	CA-C-O	6.49	127.85	120.90
1	A	65	ALA	CB-CA-C	6.49	121.07	110.88
1	A	333	GLU	CA-CB-CG	6.48	127.06	114.10
1	B	285	TYR	CA-C-N	-6.47	112.25	122.79
1	B	285	TYR	C-N-CA	-6.47	112.25	122.79
1	A	39	VAL	CA-C-N	6.47	129.24	120.44
1	A	39	VAL	C-N-CA	6.47	129.24	120.44
1	A	288	PRO	O-C-N	6.46	131.00	123.06
1	A	360	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	115	LEU	CB-CA-C	6.43	123.02	110.67
1	A	195	VAL	N-CA-C	-6.42	103.61	110.36
1	A	359	ASN	CA-C-O	-6.42	111.51	119.28
1	B	136	TRP	CA-C-O	-6.42	113.66	120.40
1	A	353	SER	O-C-N	6.42	130.52	122.43
1	B	103	PHE	CA-CB-CG	6.41	120.21	113.80
1	A	133	PHE	O-C-N	-6.41	115.06	123.13
1	B	13	GLY	CA-C-O	6.39	126.81	121.18
1	B	383	ASN	OD1-CG-ND2	6.39	128.99	122.60
1	A	280	ASN	CA-C-O	-6.38	111.72	119.32
1	B	345	GLU	CA-CB-CG	6.38	126.87	114.10
1	B	103	PHE	CA-C-O	-6.37	112.90	120.10
1	A	303	GLY	CA-C-O	6.33	127.27	120.75
1	A	66	GLU	CG-CD-OE2	6.33	132.95	118.40
1	A	91	ASN	O-C-N	6.32	130.64	122.87
1	A	43	ALA	O-C-N	-6.31	115.28	122.09
1	B	113	PHE	CA-C-O	-6.31	114.20	120.70
1	A	358	MET	CA-C-N	-6.30	110.97	122.38
1	A	358	MET	C-N-CA	-6.30	110.97	122.38
1	A	298	THR	CA-C-N	6.25	131.34	122.09
1	A	298	THR	C-N-CA	6.25	131.34	122.09
1	A	337	THR	CB-CA-C	-6.24	100.83	110.81
1	B	34	ASP	CA-C-N	6.23	125.79	119.19
1	B	34	ASP	C-N-CA	6.23	125.79	119.19
1	A	81	THR	CA-C-O	-6.23	112.31	118.97
1	A	390	LEU	CA-C-O	-6.22	113.96	120.55
1	B	249	ARG	NE-CZ-NH1	6.20	127.69	121.50
1	B	106	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	278	PHE	CA-C-N	6.18	126.36	119.32
1	B	278	PHE	C-N-CA	6.18	126.36	119.32
1	B	175	LEU	O-C-N	6.17	130.43	123.27
1	B	7	ALA	N-CA-CB	6.17	119.88	110.44
1	A	199	LEU	CA-C-N	6.16	128.85	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LEU	C-N-CA	6.16	128.85	120.54
1	B	174	ASN	N-CA-CB	6.14	119.51	110.49
1	A	228	THR	CA-C-N	6.13	128.50	120.28
1	A	228	THR	C-N-CA	6.13	128.50	120.28
1	B	142	SER	CA-C-O	-6.11	114.91	121.38
1	B	358	MET	O-C-N	6.10	128.59	122.12
1	A	156	ARG	CB-CG-CD	6.10	125.33	111.30
1	A	352	GLU	N-CA-C	-6.09	99.26	109.07
1	B	149	ASP	N-CA-C	-6.08	98.62	108.41
1	B	269	PHE	CA-C-N	6.07	128.70	120.44
1	B	269	PHE	C-N-CA	6.07	128.70	120.44
1	B	387	ILE	CB-CA-C	6.07	119.74	111.97
1	B	219	HIS	CB-CG-CD2	6.06	139.08	131.20
1	A	53	HIS	N-CA-CB	6.05	120.51	110.52
1	A	270	THR	O-C-N	6.04	128.62	122.09
1	A	264	LEU	CA-C-O	-6.04	114.48	120.70
1	B	349	ASN	N-CA-C	-6.03	102.41	110.55
1	B	345	GLU	CB-CG-CD	6.02	122.83	112.60
1	A	273	LEU	CA-C-O	-6.00	114.52	120.82
1	A	383	ASN	CA-CB-CG	-6.00	106.60	112.60
1	A	358	MET	O-C-N	5.99	128.47	122.12
1	A	52	PHE	O-C-N	5.99	129.55	123.26
1	B	339	GLY	CA-C-O	-5.97	112.19	119.06
1	B	229	HIS	N-CA-CB	5.96	119.52	110.28
1	A	352	GLU	CB-CG-CD	5.95	122.72	112.60
1	B	34	ASP	CB-CG-OD1	5.95	132.09	118.40
1	A	133	PHE	CA-CB-CG	-5.95	107.86	113.80
1	A	101	GLY	O-C-N	5.93	130.27	123.21
1	B	73	ASP	O-C-N	5.93	128.41	122.12
1	B	40	HIS	CA-C-O	-5.93	114.59	120.82
1	B	41	LYS	CA-C-O	-5.92	113.41	120.10
1	A	256	ASP	CB-CG-OD1	5.92	132.02	118.40
1	A	103	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	347	THR	CA-CB-OG1	-5.91	100.74	109.60
1	B	357	LEU	O-C-N	5.90	128.38	122.12
1	A	16	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	381	ARG	NE-CZ-NH1	5.90	127.40	121.50
1	B	280	ASN	N-CA-C	-5.89	105.67	112.92
1	B	360	ASP	CB-CG-OD2	5.88	131.93	118.40
1	A	105	SER	N-CA-C	-5.88	102.35	110.35
1	A	170	ASP	N-CA-CB	5.88	118.70	109.94
1	A	291	PHE	CA-C-O	5.88	126.75	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	GLU	CB-CG-CD	5.88	122.59	112.60
1	A	370	GLU	CB-CG-CD	5.87	122.58	112.60
1	B	132	THR	CA-CB-OG1	-5.87	100.80	109.60
1	B	244	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	197	HIS	N-CA-CB	5.85	118.72	110.12
1	A	383	ASN	N-CA-CB	5.85	118.49	110.01
1	A	381	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	A	203	GLU	CG-CD-OE2	5.84	131.84	118.40
1	B	316	LEU	CA-C-O	-5.83	114.24	120.42
1	A	233	GLN	N-CA-CB	5.83	118.78	110.16
1	B	358	MET	N-CA-CB	5.82	118.67	110.12
1	A	242	HIS	O-C-N	-5.82	117.70	123.46
1	A	336	LYS	CA-C-N	5.82	128.39	120.54
1	A	336	LYS	C-N-CA	5.82	128.39	120.54
1	B	387	ILE	CA-C-O	-5.82	115.00	121.17
1	A	204	GLN	CA-C-O	5.81	125.45	119.05
1	A	213	LEU	N-CA-C	5.81	119.15	110.14
1	A	174	ASN	CB-CA-C	5.80	120.65	112.07
1	A	34	ASP	O-C-N	5.80	127.08	121.28
1	B	53	HIS	CA-CB-CG	5.79	119.59	113.80
1	B	188	GLY	N-CA-C	-5.79	105.62	113.37
1	B	359	ASN	N-CA-CB	-5.78	101.06	110.42
1	B	294	LYS	CB-CG-CD	-5.76	98.05	111.30
1	B	280	ASN	CB-CG-ND2	5.76	125.04	116.40
1	A	84	LYS	CA-C-N	5.75	132.78	122.13
1	A	84	LYS	C-N-CA	5.75	132.78	122.13
1	A	213	LEU	CA-C-N	5.75	130.11	123.15
1	A	213	LEU	C-N-CA	5.75	130.11	123.15
1	B	72	GLY	O-C-N	5.75	127.71	122.19
1	B	374	GLU	CA-CB-CG	5.74	125.58	114.10
1	A	361	SER	N-CA-C	5.74	118.27	111.33
1	A	299	ASP	CA-CB-CG	-5.70	106.90	112.60
1	A	101	GLY	N-CA-C	-5.70	106.23	112.04
1	A	121	ASN	CA-C-N	5.69	128.50	120.42
1	A	121	ASN	C-N-CA	5.69	128.50	120.42
1	A	22	ALA	CB-CA-C	5.69	119.11	109.84
1	B	206	GLU	CA-CB-CG	5.67	125.45	114.10
1	B	56	ASP	O-C-N	5.66	129.58	122.23
1	A	109	SER	CB-CA-C	5.65	119.75	110.88
1	A	313	SER	O-C-N	5.64	128.10	122.12
1	A	91	ASN	CA-C-O	-5.64	114.75	120.84
1	A	316	LEU	CB-CA-C	5.63	119.72	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	GLY	O-C-N	5.63	130.02	122.70
1	B	143	GLU	N-CA-C	-5.62	106.78	113.97
1	A	392	GLY	CA-C-N	5.60	131.61	121.92
1	A	392	GLY	C-N-CA	5.60	131.61	121.92
1	B	333	GLU	CB-CG-CD	5.59	122.11	112.60
1	A	358	MET	CA-C-O	-5.59	114.63	120.55
1	A	285	TYR	CA-C-O	-5.57	114.33	120.69
1	B	242	HIS	N-CA-C	-5.57	100.86	108.38
1	B	316	LEU	CB-CA-C	5.56	120.31	110.85
1	B	312	MET	CB-CA-C	5.56	120.30	110.85
1	A	323	LEU	N-CA-C	-5.56	104.62	111.40
1	B	173	TYR	N-CA-C	-5.56	102.26	110.48
1	B	308	ALA	CA-C-N	5.56	127.67	120.44
1	B	308	ALA	C-N-CA	5.56	127.67	120.44
1	B	264	LEU	N-CA-C	5.55	117.01	111.07
1	A	23	ASP	CB-CA-C	5.55	121.10	110.17
1	B	298	THR	CA-C-N	5.53	132.04	122.64
1	B	298	THR	C-N-CA	5.53	132.04	122.64
1	B	376	ASN	CA-C-O	-5.53	115.17	120.92
1	B	264	LEU	CA-C-O	-5.53	115.02	120.82
1	A	362	ALA	O-C-N	5.51	129.05	122.27
1	B	160	GLY	CA-C-O	-5.51	114.72	120.90
1	A	104	THR	CA-CB-OG1	-5.51	101.33	109.60
1	A	250	GLY	N-CA-C	5.50	119.88	112.17
1	B	148	LYS	N-CA-C	5.50	117.75	109.23
1	B	234	ALA	CA-C-N	5.48	127.89	120.44
1	B	234	ALA	C-N-CA	5.48	127.89	120.44
1	A	149	ASP	CA-CB-CG	5.47	118.07	112.60
1	B	39	VAL	O-C-N	5.47	127.17	121.87
1	A	65	ALA	CA-C-O	-5.46	115.09	120.82
1	B	320	GLU	N-CA-CB	5.45	118.23	110.16
1	B	221	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	A	139	ARG	NH1-CZ-NH2	-5.44	112.23	119.30
1	B	2	VAL	CA-C-N	5.44	129.43	122.64
1	B	2	VAL	C-N-CA	5.44	129.43	122.64
1	B	132	THR	O-C-N	5.43	130.29	123.23
1	A	60	PHE	O-C-N	5.43	127.66	122.07
1	B	162	ASP	CA-C-O	-5.43	113.73	119.97
1	B	219	HIS	CA-CB-CG	-5.43	108.37	113.80
1	A	370	GLU	O-C-N	5.43	128.94	122.27
1	A	248	GLN	CA-C-N	-5.42	115.52	122.79
1	A	248	GLN	C-N-CA	-5.42	115.52	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	THR	CB-CA-C	5.42	120.18	109.66
1	B	383	ASN	CA-C-N	5.42	127.81	120.38
1	B	383	ASN	C-N-CA	5.42	127.81	120.38
1	A	78	LEU	O-C-N	5.41	127.86	122.12
1	A	371	ALA	CA-C-O	-5.40	114.25	120.24
1	B	144	TYR	CB-CG-CD1	-5.40	112.70	120.80
1	B	273	LEU	CA-CB-CG	5.40	135.20	116.30
1	A	300	GLY	N-CA-C	-5.39	104.32	112.41
1	B	111	ARG	CA-C-N	5.39	127.51	120.28
1	B	111	ARG	C-N-CA	5.39	127.51	120.28
1	A	393	SER	N-CA-CB	-5.37	102.63	110.53
1	A	112	ARG	O-C-N	5.37	127.89	122.09
1	A	44	GLU	N-CA-CB	5.37	118.49	110.22
1	A	25	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	350	ALA	O-C-N	5.36	129.49	123.06
1	B	69	LYS	CB-CG-CD	5.36	123.63	111.30
1	A	284	LYS	CA-C-O	-5.36	115.06	121.11
1	B	304	VAL	N-CA-C	-5.35	105.50	110.53
1	A	330	GLU	CG-CD-OE2	-5.35	106.09	118.40
1	A	182	LYS	CD-CE-NZ	5.35	129.02	111.90
1	A	179	LEU	CB-CA-C	5.34	118.34	109.53
1	B	21	GLY	N-CA-C	5.34	123.43	115.64
1	A	174	ASN	O-C-N	-5.33	115.84	122.83
1	B	72	GLY	N-CA-C	-5.33	106.04	112.49
1	A	394	ARG	CA-C-O	-5.33	111.74	120.80
1	A	151	ALA	N-CA-C	-5.33	105.14	111.69
1	A	94	SER	CA-C-O	-5.32	113.38	119.60
1	A	127	GLU	CA-C-O	-5.32	114.89	120.63
1	B	196	GLY	CA-C-N	5.31	127.40	120.28
1	B	196	GLY	C-N-CA	5.31	127.40	120.28
1	B	305	TRP	CB-CA-C	5.31	120.87	110.67
1	B	62	ALA	CA-C-O	5.31	127.18	121.55
1	A	316	LEU	CA-C-O	-5.31	115.25	120.82
1	A	12	PHE	O-C-N	5.30	129.42	123.27
1	B	218	GLY	CA-C-O	5.29	125.98	120.80
1	A	280	ASN	N-CA-C	-5.28	106.23	113.30
1	A	249	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	359	ASN	N-CA-CB	5.27	118.50	110.44
1	A	213	LEU	CD1-CG-CD2	-5.26	99.22	110.80
1	A	170	ASP	O-C-N	5.26	127.56	122.09
1	A	361	SER	O-C-N	5.26	127.69	122.12
1	B	9	HIS	CB-CA-C	5.25	119.18	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ILE	CA-C-O	-5.25	115.81	121.27
1	A	353	SER	CA-C-O	-5.25	115.06	121.88
1	B	102	GLY	N-CA-C	-5.24	100.76	113.18
1	B	32	ASN	CA-C-O	-5.24	116.11	121.87
1	B	8	ASP	CA-C-N	5.23	129.56	122.19
1	B	8	ASP	C-N-CA	5.23	129.56	122.19
1	A	153	ALA	CA-C-O	-5.21	115.02	120.55
1	A	221	GLN	CA-C-N	5.21	129.41	120.72
1	A	221	GLN	C-N-CA	5.21	129.41	120.72
1	A	55	ASN	CA-C-N	5.21	127.68	120.29
1	A	55	ASN	C-N-CA	5.21	127.68	120.29
1	B	56	ASP	N-CA-CB	5.21	117.95	110.20
1	A	123	ASP	N-CA-C	-5.20	105.50	111.07
1	A	394	ARG	CA-CB-CG	5.20	124.50	114.10
1	B	36	VAL	CB-CA-C	5.19	119.39	112.22
1	A	219	HIS	CA-C-O	-5.19	115.37	120.82
1	A	393	SER	O-C-N	5.17	129.42	122.49
1	B	328	ASP	CA-C-N	5.17	124.97	119.28
1	B	328	ASP	C-N-CA	5.17	124.97	119.28
1	A	211	VAL	CB-CA-C	5.16	118.26	110.63
1	B	182	LYS	O-C-N	5.16	127.25	121.32
1	B	103	PHE	O-C-N	5.15	128.25	122.22
1	B	342	GLU	CG-CD-OE2	-5.15	106.56	118.40
1	B	325	PHE	CA-CB-CG	5.15	118.95	113.80
1	B	58	ILE	O-C-N	5.13	125.47	121.46
1	B	69	LYS	CA-CB-CG	5.13	124.37	114.10
1	B	392	GLY	O-C-N	-5.13	117.90	122.57
1	A	216	GLU	O-C-N	-5.13	117.20	123.30
1	B	28	ALA	CA-C-O	-5.12	115.91	121.44
1	B	105	SER	CA-C-O	-5.12	115.56	121.19
1	B	191	PHE	O-C-N	5.12	128.75	122.96
1	B	74	PHE	CA-C-O	-5.11	115.46	120.82
1	B	330	GLU	CG-CD-OE1	-5.11	106.65	118.40
1	B	30	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	A	111	ARG	CA-C-O	5.10	126.14	120.63
1	A	82	GLY	CA-C-O	-5.10	113.54	119.10
1	A	119	LEU	CB-CA-C	5.09	118.88	110.88
1	A	109	SER	N-CA-C	-5.09	105.62	111.07
1	B	163	THR	CA-CB-OG1	-5.09	101.96	109.60
1	B	246	ASN	CA-C-N	5.09	125.11	121.65
1	B	246	ASN	C-N-CA	5.09	125.11	121.65
1	B	40	HIS	N-CA-C	-5.08	105.63	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	191	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	127	GLU	CA-C-N	5.08	130.44	120.99
1	A	127	GLU	C-N-CA	5.08	130.44	120.99
1	A	53	HIS	CB-CG-CD2	5.08	137.80	131.20
1	B	206	GLU	N-CA-C	-5.08	105.45	111.69
1	A	308	ALA	CA-C-O	5.07	126.15	120.82
1	A	155	ASP	N-CA-C	-5.06	105.67	111.14
1	A	206	GLU	N-CA-C	-5.06	105.66	111.07
1	B	271	VAL	CA-C-O	-5.06	115.69	120.95
1	A	352	GLU	CG-CD-OE2	5.06	130.03	118.40
1	B	216	GLU	CG-CD-OE1	5.05	130.02	118.40
1	B	57	LEU	N-CA-CB	-5.05	101.23	110.27
1	A	249	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	B	16	THR	OG1-CB-CG2	5.04	119.39	109.30
1	B	273	LEU	CA-C-O	-5.04	114.18	119.97
1	A	9	HIS	CA-CB-CG	-5.03	108.77	113.80
1	B	332	GLN	CB-CA-C	5.02	119.13	110.79
1	B	150	LEU	CA-C-O	-5.02	115.23	120.55
1	A	81	THR	CA-CB-OG1	-5.02	102.08	109.60
1	B	248	GLN	CA-C-O	-5.02	114.11	120.28
1	A	364	PHE	CA-C-N	5.01	128.34	120.82
1	A	364	PHE	C-N-CA	5.01	128.34	120.82
1	A	149	ASP	CB-CG-OD1	5.01	129.92	118.40
1	A	206	GLU	N-CA-CB	5.01	117.27	110.01
1	A	266	SER	CB-CA-C	5.01	119.10	110.79

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	3026	0	2888	61	1
1	B	3026	0	2888	73	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	11	0	12	2	0
3	B	11	0	12	1	0
4	A	291	0	0	20	4
4	B	290	0	0	19	3
All	All	6659	0	5800	131	5

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 11.

All (131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:GLU:HG2	4:B:402:HOH:O	1.25	1.33
1:A:5:THR:HB	4:A:563:HOH:O	1.38	1.20
1:B:374:GLU:CG	4:B:402:HOH:O	1.85	1.00
1:A:364:PHE:HB2	4:A:628:HOH:O	1.69	0.92
1:A:95:HIS:HD2	1:A:97:VAL:H	1.33	0.77
1:B:95:HIS:HD2	1:B:97:VAL:H	1.31	0.76
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.12	0.75
1:B:342:GLU:OE1	4:B:622:HOH:O	2.04	0.74
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.69	0.73
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.69	0.73
1:B:40:HIS:HE1	4:B:585:HOH:O	1.72	0.72
1:A:294:LYS:NZ	4:A:691:HOH:O	2.24	0.71
1:B:6:PRO:O	1:B:9:HIS:HD2	1.74	0.70
1:A:394:ARG:HD3	4:A:618:HOH:O	1.90	0.70
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.58	0.69
1:A:32:ASN:ND2	4:A:568:HOH:O	2.26	0.69
1:A:68:GLU:HG3	4:A:580:HOH:O	1.95	0.66
1:B:65:ALA:HA	1:B:68:GLU:HG3	1.78	0.66
1:A:20:THR:HG22	4:A:564:HOH:O	1.95	0.66
1:B:16:THR:OG1	1:B:17:VAL:N	2.29	0.64
1:B:292:ASP:OD2	3:B:400:NOJ:H3	1.96	0.64
1:B:9:HIS:HB2	4:B:580:HOH:O	1.96	0.63
1:B:24:PRO:HA	4:B:582:HOH:O	1.98	0.63
1:B:176:ARG:HB3	1:B:241:PHE:CE2	2.34	0.63
1:B:333:GLU:CG	4:B:662:HOH:O	2.47	0.63
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.80	0.63
1:B:374:GLU:HG3	4:B:402:HOH:O	1.75	0.62
1:B:6:PRO:O	1:B:9:HIS:CD2	2.53	0.62
1:B:333:GLU:HG3	4:B:662:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ASP:HB2	1:A:24:PRO:HD2	1.82	0.60
1:A:95:HIS:CD2	1:A:97:VAL:H	2.15	0.60
1:B:361:SER:OG	1:B:365:ALA:HB3	2.02	0.59
1:A:202:ILE:O	1:A:205:LEU:HB2	2.04	0.58
1:A:68:GLU:OE1	4:A:585:HOH:O	2.17	0.58
1:A:301:TYR:HD2	4:A:527:HOH:O	1.86	0.58
1:A:252:LYS:HE3	4:B:406:HOH:O	2.03	0.58
1:A:217:THR:HA	1:A:227:PHE:CD1	2.39	0.57
1:A:284:LYS:HE3	4:A:520:HOH:O	2.04	0.57
1:A:75:ASN:ND2	4:A:587:HOH:O	2.35	0.57
1:B:64:GLU:CB	4:B:652:HOH:O	2.52	0.57
1:B:87:MET:HA	1:B:132:THR:O	2.06	0.56
1:B:55:ASN:HA	1:B:58:ILE:O	2.07	0.55
1:B:221:GLN:HE21	1:B:248:GLN:HB3	1.70	0.55
1:B:319:LYS:HD3	4:B:546:HOH:O	2.05	0.55
1:B:333:GLU:CB	4:B:662:HOH:O	2.54	0.55
1:B:40:HIS:CE1	4:B:585:HOH:O	2.52	0.55
1:B:235:LEU:HD12	1:B:273:LEU:HD11	1.89	0.54
1:A:252:LYS:CE	4:B:406:HOH:O	2.54	0.54
1:B:361:SER:O	1:B:366:GLY:N	2.32	0.54
1:A:68:GLU:CG	4:A:580:HOH:O	2.54	0.54
1:A:123:ASP:OD1	1:A:173:TYR:OH	2.22	0.54
1:B:5:THR:O	1:B:7:ALA:N	2.41	0.53
1:A:273:LEU:HD23	4:A:521:HOH:O	2.08	0.53
1:B:333:GLU:HB2	4:B:662:HOH:O	2.09	0.53
1:B:95:HIS:CD2	1:B:97:VAL:HG12	2.44	0.53
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.91	0.52
1:A:89:THR:HG21	3:A:400:NOJ:H62	1.92	0.51
1:B:285:TYR:OH	1:B:288:PRO:O	2.26	0.51
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.92	0.51
1:A:11:THR:HG21	1:A:86:PRO:HG2	1.93	0.50
1:B:34:ASP:OD1	1:B:36:VAL:HB	2.11	0.50
1:A:55:ASN:HA	1:A:58:ILE:O	2.11	0.50
1:A:6:PRO:HD2	4:A:563:HOH:O	2.11	0.50
1:B:105:SER:O	1:B:111:ARG:HD3	2.10	0.50
1:B:182:LYS:HE2	1:B:184:ASN:O	2.11	0.50
1:A:20:THR:HB	1:A:30:ARG:O	2.11	0.50
1:B:43:ALA:HA	1:B:83:LEU:HD21	1.92	0.50
1:A:222:MET:O	1:A:251:ILE:HG23	2.12	0.49
1:B:66:GLU:HA	4:B:589:HOH:O	2.12	0.49
1:A:19:TRP:CE3	1:A:294:LYS:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:CZ	1:A:84:LYS:HG3	2.48	0.49
1:A:380:ILE:HD11	1:B:296:SER:HB2	1.95	0.49
1:A:217:THR:O	1:A:221:GLN:HG3	2.13	0.48
1:A:182:LYS:HD3	1:A:185:GLU:O	2.13	0.48
1:B:141:GLY:HA3	1:B:189:ASP:O	2.14	0.48
1:A:16:THR:OG1	1:A:17:VAL:N	2.46	0.47
1:B:6:PRO:O	1:B:48:TYR:CD1	2.66	0.47
1:B:95:HIS:CD2	1:B:97:VAL:H	2.21	0.47
1:B:53:HIS:CD2	1:B:89:THR:HG23	2.49	0.47
1:B:355:ALA:O	1:B:359:ASN:HB3	2.14	0.47
1:A:328:ASP:OD2	4:A:618:HOH:O	2.20	0.47
1:A:124:LEU:HA	1:A:127:GLU:HG3	1.97	0.47
1:A:14:LEU:HD11	4:A:570:HOH:O	2.14	0.47
1:B:71:LEU:HD22	1:B:128:MET:CE	2.44	0.47
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.85	0.46
1:A:289:ARG:HD2	4:A:403:HOH:O	2.14	0.46
1:B:315:TYR:O	1:B:319:LYS:HB2	2.16	0.46
1:B:20:THR:HB	1:B:30:ARG:O	2.16	0.46
1:B:53:HIS:HA	1:B:89:THR:O	2.15	0.46
1:A:110:ILE:O	1:A:111:ARG:C	2.58	0.46
1:A:85:VAL:O	1:A:130:ALA:HA	2.16	0.46
1:A:348:LEU:HD23	1:A:357:LEU:HD22	1.97	0.46
1:B:294:LYS:HA	1:B:295:PRO:HD3	1.78	0.45
1:A:329:PRO:HG3	4:A:664:HOH:O	2.16	0.45
1:B:10:PHE:CD2	1:B:312:MET:HG2	2.52	0.45
1:A:381:ARG:HG3	4:A:634:HOH:O	2.16	0.45
1:B:137:GLY:CA	1:B:140:GLU:HG2	2.47	0.45
1:A:58:ILE:HD13	1:A:67:ARG:HG3	1.99	0.45
1:B:158:ARG:HG3	1:B:205:LEU:HD23	1.98	0.45
1:B:9:HIS:CB	4:B:580:HOH:O	2.62	0.44
1:B:131:GLU:O	1:B:175:LEU:HA	2.18	0.44
1:A:95:HIS:CD2	1:A:96:PRO:HD2	2.53	0.44
1:B:176:ARG:HB3	1:B:241:PHE:HE2	1.80	0.44
1:A:5:THR:O	1:A:8:ASP:HB2	2.17	0.44
1:B:202:ILE:HG21	1:B:239:LYS:HE3	1.99	0.44
1:A:77:ALA:O	1:A:81:THR:HG23	2.18	0.44
1:B:176:ARG:HB2	4:B:471:HOH:O	2.18	0.43
1:A:34:ASP:HA	1:A:35:PRO:HD3	1.87	0.43
1:A:192:LEU:N	1:A:193:PRO:CD	2.81	0.43
1:A:261:HIS:NE2	1:B:384:GLN:NE2	2.65	0.43
1:A:384:GLN:NE2	1:B:261:HIS:NE2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:HG3	1:A:214:ASN:O	2.18	0.43
1:B:235:LEU:O	1:B:236:TRP:C	2.62	0.43
1:A:289:ARG:HG2	1:A:315:TYR:CE2	2.54	0.42
1:B:328:ASP:HA	1:B:329:PRO:HD2	1.76	0.42
1:A:53:HIS:NE2	3:A:400:NOJ:N5	2.68	0.41
1:B:71:LEU:CD2	1:B:128:MET:CE	2.98	0.41
1:A:53:HIS:CD2	1:A:89:THR:HG23	2.54	0.41
1:A:289:ARG:CD	4:A:403:HOH:O	2.68	0.41
1:A:215:PRO:HG2	1:A:231:ILE:HG22	2.02	0.41
1:B:20:THR:O	1:B:29:THR:N	2.48	0.41
1:B:218:GLY:HA2	1:B:248:GLN:HB2	2.02	0.41
1:A:182:LYS:O	1:A:190:ILE:HB	2.21	0.41
1:A:41:LYS:O	1:A:45:LEU:HG	2.21	0.40
1:A:202:ILE:CD1	1:A:213:LEU:HD23	2.51	0.40
1:B:23:ASP:CB	1:B:24:PRO:HD2	2.48	0.40
1:B:185:GLU:HA	1:B:186:PRO:HA	1.85	0.40
1:B:325:PHE:CZ	1:B:386:ALA:HB2	2.56	0.40
1:B:53:HIS:O	1:B:54:ASP:C	2.63	0.40
1:B:182:LYS:HG2	1:B:183:PRO:HD2	2.03	0.40
1:B:214:ASN:OD1	1:B:242:HIS:ND1	2.45	0.40

All (5) 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)
1:A:116:ALA:CB	4:A:628:HOH:O[4_555]	1.44	0.76
4:B:529:HOH:O	4:B:609:HOH:O[4_555]	2.03	0.17
4:A:472:HOH:O	4:A:600:HOH:O[4_555]	2.05	0.15
4:A:552:HOH:O	4:B:679:HOH:O[4_555]	2.18	0.02
4:A:566:HOH:O	4:B:435:HOH:O[4_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/394 (99%)	375 (96%)	15 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	378 (97%)	11 (3%)	2 (0%)	24	43
All	All	782/788 (99%)	753 (96%)	26 (3%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	PRO
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%)	288 (94%)	17 (6%)	19	39
1	B	305/310 (98%)	293 (96%)	12 (4%)	28	55
All	All	610/620 (98%)	581 (95%)	29 (5%)	23	46

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	68	GLU
1	A	90	THR
1	A	94	SER
1	A	149	ASP
1	A	184	ASN
1	A	195	VAL
1	A	213	LEU
1	A	273	LEU
1	A	284	LYS
1	A	289	ARG

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Mol	Chain	Res	Type
1	A	309	LYS
1	A	336	LYS
1	A	358	MET
1	A	370	GLU
1	A	391	LEU
1	A	393	SER
1	B	6	PRO
1	B	17	VAL
1	B	32	ASN
1	B	99	LYS
1	B	174	ASN
1	B	235	LEU
1	B	273	LEU
1	B	309	LYS
1	B	320	GLU
1	B	336	LYS
1	B	358	MET
1	B	361	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	40	HIS
1	A	95	HIS
1	A	221	GLN
1	A	384	GLN
1	B	9	HIS
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 ⓘ

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	$\# Z > 2$
3	NOJ	B	400	2	11,11,11	4.05	3 (27%)	13,15,15	1.83	5 (38%)
3	NOJ	A	400	2	11,11,11	4.21	4 (36%)	13,15,15	2.29	7 (53%)

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
3	NOJ	B	400	2	-	2/2/19/19	0/1/1/1
3	NOJ	A	400	2	-	2/2/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	400	NOJ	C5-N5	-10.20	1.33	1.47
3	B	400	NOJ	C5-N5	-9.69	1.33	1.47
3	A	400	NOJ	C1-N5	-8.61	1.35	1.47
3	B	400	NOJ	C1-N5	-8.15	1.36	1.47
3	A	400	NOJ	O6-C6	2.83	1.54	1.42
3	B	400	NOJ	C1-C2	2.68	1.54	1.52
3	A	400	NOJ	C1-C2	2.06	1.54	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	NOJ	C1-N5-C5	4.33	119.22	109.71
3	B	400	NOJ	O2-C2-C3	3.30	116.99	110.15
3	A	400	NOJ	C2-C3-C4	-3.03	105.53	110.86
3	A	400	NOJ	O6-C6-C5	-2.79	104.33	111.10
3	B	400	NOJ	C4-C5-N5	2.65	114.47	109.12
3	B	400	NOJ	C2-C3-C4	-2.60	106.28	110.86
3	B	400	NOJ	O6-C6-C5	-2.38	105.33	111.10
3	A	400	NOJ	O2-C2-C1	2.27	114.05	109.65
3	A	400	NOJ	C4-C5-N5	2.06	113.27	109.12
3	B	400	NOJ	C1-N5-C5	2.05	114.21	109.71
3	A	400	NOJ	O4-C4-C5	-2.04	105.17	109.40
3	A	400	NOJ	O2-C2-C3	2.01	114.32	110.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	NOJ	C4-C5-C6-O6
3	A	400	NOJ	N5-C5-C6-O6
3	B	400	NOJ	C4-C5-C6-O6
3	B	400	NOJ	N5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	NOJ	1	0
3	A	400	NOJ	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.