



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:34 AM UTC

PDB ID : 1XLL / pdb_00001xll
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

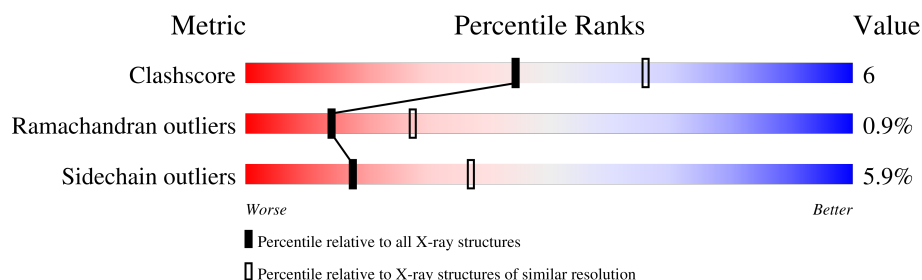
1 Overall quality at a glance

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 6583 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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

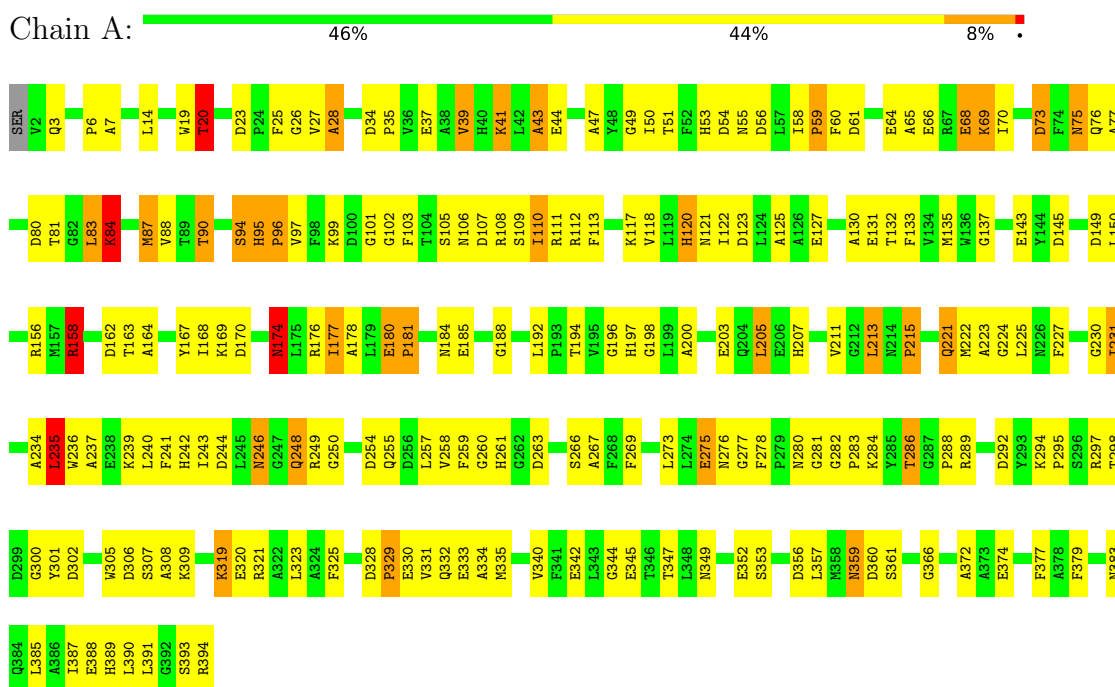
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	257	Total	O	0	0
			257	257		
3	B	268	Total	O	0	0
			268	268		

3 Residue-property plots

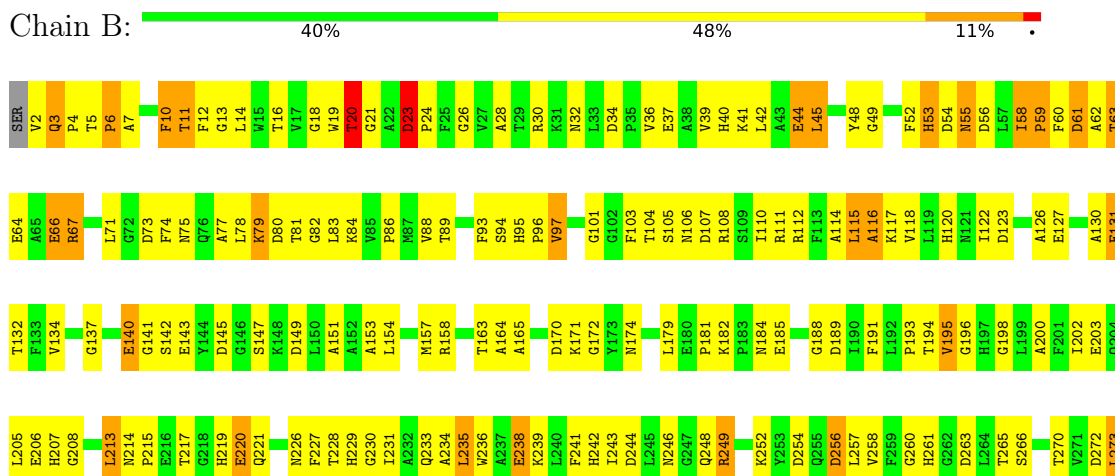
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

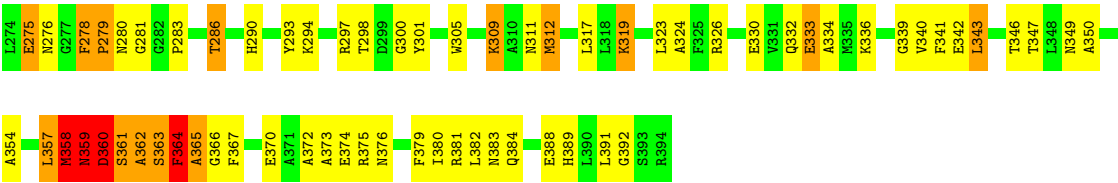
Note EDS was not executed.

• 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 154.10 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}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6583	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: ZN

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	1.54	15/3101 (0.5%)	2.87	334/4204 (7.9%)
1	B	1.63	32/3101 (1.0%)	3.03	353/4204 (8.4%)
All	All	1.59	47/6202 (0.8%)	2.95	687/8408 (8.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	361	SER	C-N	-8.54	1.21	1.33
1	A	282	GLY	N-CA	7.38	1.54	1.44
1	B	362	ALA	N-CA	-7.34	1.36	1.46
1	B	193	PRO	C-O	6.96	1.33	1.24
1	B	361	SER	CA-CB	-6.92	1.36	1.53
1	B	81	THR	CA-CB	6.61	1.63	1.54
1	B	258	VAL	N-CA	6.17	1.54	1.46
1	B	263	ASP	C-O	6.07	1.31	1.23
1	A	105	SER	C-O	6.04	1.31	1.23
1	B	239	LYS	CA-C	-6.00	1.45	1.52
1	A	281	GLY	N-CA	5.91	1.51	1.45
1	B	231	ILE	N-CA	5.82	1.53	1.46
1	B	59	PRO	CA-C	-5.81	1.46	1.52
1	A	289	ARG	CD-NE	-5.77	1.38	1.46
1	B	49	GLY	C-O	5.73	1.29	1.23
1	A	300	GLY	N-CA	5.73	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	ILE	CA-CB	5.71	1.60	1.54
1	B	265	THR	C-O	5.58	1.30	1.24
1	B	140	GLU	C-O	5.56	1.30	1.23
1	B	230	GLY	N-CA	5.50	1.52	1.45
1	B	349	ASN	N-CA	5.46	1.53	1.45
1	B	361	SER	CB-OG	5.45	1.53	1.42
1	B	53	HIS	C-O	5.38	1.30	1.23
1	B	227	PHE	C-O	5.35	1.30	1.24
1	B	340	VAL	C-O	5.34	1.30	1.24
1	B	126	ALA	C-O	5.29	1.30	1.24
1	A	158	ARG	CD-NE	-5.28	1.38	1.46
1	B	270	THR	C-O	5.27	1.30	1.24
1	A	263	ASP	C-O	5.22	1.30	1.24
1	B	242	HIS	C-O	5.22	1.29	1.23
1	B	20	THR	CB-OG1	5.22	1.52	1.43
1	A	110	ILE	C-O	5.21	1.30	1.24
1	B	182	LYS	C-O	5.21	1.30	1.24
1	B	298	THR	CA-CB	5.20	1.62	1.53
1	A	197	HIS	CG-CD2	5.18	1.41	1.35
1	B	153	ALA	C-O	5.17	1.30	1.24
1	B	179	LEU	C-O	5.15	1.30	1.23
1	A	267	ALA	C-O	5.14	1.29	1.24
1	B	359	ASN	N-CA	-5.13	1.39	1.46
1	A	273	LEU	C-O	5.12	1.30	1.24
1	B	88	VAL	N-CA	5.11	1.51	1.46
1	B	228	THR	C-O	5.10	1.30	1.24
1	B	122	ILE	C-O	5.08	1.29	1.24
1	B	373	ALA	C-O	5.08	1.30	1.24
1	A	90	THR	CA-CB	5.07	1.62	1.53
1	A	101	GLY	N-CA	5.04	1.49	1.45
1	A	200	ALA	C-O	5.02	1.29	1.24

All (687) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	SER	CA-C-N	28.57	176.11	121.54
1	B	361	SER	C-N-CA	28.57	176.11	121.54
1	B	358	MET	CA-C-N	27.50	174.06	121.54
1	B	358	MET	C-N-CA	27.50	174.06	121.54
1	A	112	ARG	CD-NE-CZ	25.88	160.63	124.40
1	B	359	ASN	CA-C-N	17.59	155.13	121.54
1	B	359	ASN	C-N-CA	17.59	155.13	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	361	SER	N-CA-CB	16.25	140.87	110.82
1	B	358	MET	CA-C-O	15.94	143.31	120.51
1	A	394	ARG	CD-NE-CZ	15.83	146.56	124.40
1	A	359	ASN	CA-CB-CG	15.24	127.84	112.60
1	B	361	SER	CB-CA-C	-14.60	89.57	111.77
1	B	357	LEU	O-C-N	-14.21	103.70	122.59
1	A	289	ARG	CD-NE-CZ	14.15	144.21	124.40
1	B	360	ASP	CA-C-O	-14.02	100.47	120.51
1	A	6	PRO	CA-C-N	13.81	142.70	120.60
1	A	6	PRO	C-N-CA	13.81	142.70	120.60
1	B	392	GLY	CA-C-N	13.57	138.09	120.44
1	B	392	GLY	C-N-CA	13.57	138.09	120.44
1	A	244	ASP	CA-CB-CG	12.85	125.45	112.60
1	B	73	ASP	CA-CB-CG	12.65	125.25	112.60
1	B	343	LEU	CA-C-N	12.44	135.68	120.14
1	B	343	LEU	C-N-CA	12.44	135.68	120.14
1	B	357	LEU	CA-C-N	12.25	144.95	121.54
1	B	357	LEU	C-N-CA	12.25	144.95	121.54
1	A	107	ASP	CA-CB-CG	12.12	124.72	112.60
1	B	360	ASP	O-C-N	-12.03	106.59	122.59
1	B	254	ASP	CA-CB-CG	11.99	124.59	112.60
1	A	329	PRO	CA-C-N	11.31	135.14	120.44
1	A	329	PRO	C-N-CA	11.31	135.14	120.44
1	B	137	GLY	CA-C-N	11.28	134.23	120.14
1	B	137	GLY	C-N-CA	11.28	134.23	120.14
1	A	255	GLN	CA-C-O	11.13	132.17	120.70
1	B	32	ASN	CA-CB-CG	-11.12	101.48	112.60
1	B	112	ARG	CD-NE-CZ	11.02	139.82	124.40
1	B	358	MET	N-CA-CB	10.95	128.99	110.49
1	B	362	ALA	CA-C-O	-10.91	104.91	120.51
1	B	364	PHE	O-C-N	-10.74	108.30	122.59
1	A	158	ARG	CD-NE-CZ	10.74	139.43	124.40
1	B	44	GLU	CA-CB-CG	10.70	135.51	114.10
1	A	65	ALA	N-CA-C	-10.29	99.61	111.03
1	B	358	MET	O-C-N	-10.26	108.95	122.59
1	A	281	GLY	CA-C-O	-10.08	115.28	122.23
1	B	379	PHE	CA-CB-CG	10.07	123.87	113.80
1	B	217	THR	CA-C-N	9.94	131.01	119.98
1	B	217	THR	C-N-CA	9.94	131.01	119.98
1	B	37	GLU	CB-CG-CD	9.91	129.45	112.60
1	A	14	LEU	CA-C-O	9.80	131.24	119.97
1	A	387	ILE	CA-C-N	9.76	133.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	ILE	C-N-CA	9.76	133.36	120.28
1	B	219	HIS	CA-C-O	-9.76	110.65	120.70
1	B	359	ASN	CA-CB-CG	-9.67	102.93	112.60
1	A	379	PHE	CA-CB-CG	9.63	123.43	113.80
1	A	393	SER	CA-C-N	9.53	138.86	121.70
1	A	393	SER	C-N-CA	9.53	138.86	121.70
1	B	281	GLY	CA-C-O	-9.51	114.46	121.88
1	B	238	GLU	CB-CG-CD	9.45	128.66	112.60
1	A	94	SER	CA-C-O	-9.44	109.76	120.24
1	A	334	ALA	CA-C-N	9.33	132.78	120.28
1	A	334	ALA	C-N-CA	9.33	132.78	120.28
1	B	249	ARG	O-C-N	-9.30	112.78	122.64
1	B	279	PRO	O-C-N	-9.20	111.66	122.24
1	A	127	GLU	N-CA-CB	9.18	123.74	110.16
1	A	308	ALA	CA-C-O	9.12	130.39	120.82
1	B	242	HIS	CA-CB-CG	9.08	122.88	113.80
1	B	75	ASN	CA-CB-CG	-9.05	103.55	112.60
1	A	222	MET	CA-C-N	9.03	136.48	122.49
1	A	222	MET	C-N-CA	9.03	136.48	122.49
1	A	333	GLU	CA-CB-CG	9.01	132.12	114.10
1	B	82	GLY	CA-C-O	-8.96	109.03	119.06
1	A	105	SER	CA-C-N	8.94	132.99	120.29
1	A	105	SER	C-N-CA	8.94	132.99	120.29
1	A	342	GLU	CA-CB-CG	8.91	131.92	114.10
1	A	356	ASP	CA-CB-CG	8.89	121.49	112.60
1	A	149	ASP	N-CA-CB	8.86	125.01	110.39
1	A	162	ASP	CA-CB-CG	8.84	121.44	112.60
1	B	319	LYS	CA-C-N	8.78	131.85	120.44
1	B	319	LYS	C-N-CA	8.78	131.85	120.44
1	B	248	GLN	OE1-CD-NE2	-8.72	113.88	122.60
1	B	20	THR	N-CA-CB	-8.67	95.85	110.41
1	B	342	GLU	CG-CD-OE2	-8.65	98.52	118.40
1	B	208	GLY	CA-C-N	8.64	132.22	120.38
1	B	208	GLY	C-N-CA	8.64	132.22	120.38
1	B	207	HIS	CA-C-N	8.62	129.68	120.03
1	B	207	HIS	C-N-CA	8.62	129.68	120.03
1	B	79	LYS	O-C-N	-8.62	113.07	122.03
1	A	349	ASN	OD1-CG-ND2	-8.61	113.99	122.60
1	B	359	ASN	CB-CA-C	8.58	127.50	110.42
1	B	108	ARG	NE-CZ-NH1	8.52	130.02	121.50
1	A	7	ALA	CA-C-N	8.52	135.16	120.68
1	A	7	ALA	C-N-CA	8.52	135.16	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	381	ARG	NE-CZ-NH2	-8.49	111.55	119.20
1	B	334	ALA	CA-C-N	8.46	131.44	120.44
1	B	334	ALA	C-N-CA	8.46	131.44	120.44
1	B	362	ALA	N-CA-C	-8.44	92.81	110.80
1	B	382	LEU	CA-C-O	-8.43	111.96	120.82
1	A	356	ASP	CA-C-N	8.41	131.87	120.44
1	A	356	ASP	C-N-CA	8.41	131.87	120.44
1	B	67	ARG	CG-CD-NE	8.41	130.49	112.00
1	A	68	GLU	CA-CB-CG	-8.40	97.30	114.10
1	A	200	ALA	CA-C-O	8.38	129.62	120.82
1	B	60	PHE	CA-C-N	8.35	136.36	121.66
1	B	60	PHE	C-N-CA	8.35	136.36	121.66
1	A	6	PRO	O-C-N	-8.35	111.37	122.64
1	A	342	GLU	N-CA-CB	8.34	123.07	110.22
1	A	103	PHE	CA-CB-CG	8.33	122.13	113.80
1	A	125	ALA	CA-C-O	8.32	129.80	120.90
1	B	20	THR	CB-CA-C	8.27	126.41	109.95
1	B	20	THR	CA-CB-CG2	8.26	124.54	110.50
1	A	112	ARG	NE-CZ-NH1	8.23	129.74	121.50
1	B	384	GLN	CA-C-N	8.23	131.98	120.29
1	B	384	GLN	C-N-CA	8.23	131.98	120.29
1	B	26	GLY	N-CA-C	8.18	124.14	110.56
1	B	241	PHE	CA-CB-CG	8.18	121.98	113.80
1	A	215	PRO	CA-C-O	-8.14	111.92	121.86
1	B	111	ARG	CA-C-N	8.14	131.02	120.44
1	B	111	ARG	C-N-CA	8.14	131.02	120.44
1	B	324	ALA	CA-C-N	8.13	131.50	120.44
1	B	324	ALA	C-N-CA	8.13	131.50	120.44
1	A	137	GLY	CA-C-N	8.13	134.72	120.74
1	A	137	GLY	C-N-CA	8.13	134.72	120.74
1	A	84	LYS	CA-CB-CG	8.12	130.34	114.10
1	A	235	LEU	O-C-N	-8.10	113.73	122.07
1	B	108	ARG	CD-NE-CZ	8.09	135.72	124.40
1	A	359	ASN	CA-C-O	-8.08	110.25	119.79
1	A	342	GLU	CB-CA-C	-8.07	95.69	110.63
1	A	181	PRO	O-C-N	8.04	133.25	123.13
1	B	151	ALA	O-C-N	-8.02	113.43	122.09
1	A	107	ASP	CA-C-O	8.01	129.87	120.58
1	A	243	ILE	CA-C-O	-8.00	112.34	120.90
1	A	84	LYS	CG-CD-CE	7.98	129.65	111.30
1	A	145	ASP	CA-C-O	-7.95	110.82	119.97
1	A	320	GLU	CA-CB-CG	7.92	129.93	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	ALA	CA-C-O	-7.91	112.51	120.82
1	A	84	LYS	N-CA-CB	-7.90	97.81	110.46
1	A	280	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	B	200	ALA	CA-C-N	7.90	131.21	120.54
1	B	200	ALA	C-N-CA	7.90	131.21	120.54
1	B	172	GLY	O-C-N	7.86	129.72	122.57
1	B	53	HIS	CA-CB-CG	7.86	121.66	113.80
1	B	372	ALA	O-C-N	-7.86	113.79	122.12
1	B	279	PRO	CA-C-N	7.84	135.47	122.54
1	B	279	PRO	C-N-CA	7.84	135.47	122.54
1	A	77	ALA	CA-C-N	7.82	130.61	120.44
1	A	77	ALA	C-N-CA	7.82	130.61	120.44
1	B	79	LYS	CA-C-O	7.81	129.20	121.00
1	B	298	THR	CA-C-N	7.80	134.27	122.65
1	B	298	THR	C-N-CA	7.80	134.27	122.65
1	A	28	ALA	CA-C-O	-7.80	113.28	121.55
1	B	246	ASN	OD1-CG-ND2	-7.79	114.81	122.60
1	A	131	GLU	CB-CG-CD	7.76	125.79	112.60
1	A	127	GLU	CA-CB-CG	7.75	129.59	114.10
1	B	297	ARG	NE-CZ-NH2	7.72	126.15	119.20
1	A	167	TYR	O-C-N	-7.72	113.94	122.12
1	B	141	GLY	CA-C-O	-7.71	115.59	120.91
1	B	363	SER	CB-CA-C	7.70	123.05	109.65
1	A	321	ARG	CA-C-N	7.69	130.58	120.28
1	A	321	ARG	C-N-CA	7.69	130.58	120.28
1	A	143	GLU	CA-C-O	7.68	128.09	119.41
1	B	363	SER	N-CA-C	7.67	122.81	113.38
1	B	214	ASN	CB-CG-ND2	7.63	127.85	116.40
1	B	164	ALA	CA-C-N	7.61	130.33	120.44
1	B	164	ALA	C-N-CA	7.61	130.33	120.44
1	B	110	ILE	CB-CG1-CD1	7.59	129.75	113.80
1	A	73	ASP	CA-CB-CG	7.59	120.19	112.60
1	B	357	LEU	N-CA-C	-7.58	94.64	110.80
1	A	101	GLY	O-C-N	7.57	131.05	123.48
1	A	249	ARG	NE-CZ-NH1	7.57	129.07	121.50
1	A	248	GLN	OE1-CD-NE2	-7.57	115.03	122.60
1	A	53	HIS	N-CA-CB	7.54	122.92	110.63
1	B	7	ALA	CA-C-O	-7.54	109.25	119.05
1	B	61	ASP	CA-CB-CG	7.52	120.12	112.60
1	A	221	GLN	CA-C-N	7.48	133.22	120.72
1	A	221	GLN	C-N-CA	7.48	133.22	120.72
1	A	110	ILE	O-C-N	-7.47	114.47	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ASN	CA-C-O	-7.46	112.60	120.58
1	B	388	GLU	O-C-N	-7.44	113.11	122.27
1	A	176	ARG	CA-C-N	7.43	131.95	122.37
1	A	176	ARG	C-N-CA	7.43	131.95	122.37
1	A	332	GLN	OE1-CD-NE2	-7.43	115.17	122.60
1	B	360	ASP	CA-C-N	-7.41	111.81	123.23
1	B	360	ASP	C-N-CA	-7.41	111.81	123.23
1	B	221	GLN	CA-C-N	7.41	133.09	120.72
1	B	221	GLN	C-N-CA	7.41	133.09	120.72
1	B	78	LEU	N-CA-C	-7.40	103.15	111.07
1	A	258	VAL	CA-C-O	-7.38	113.24	121.36
1	B	350	ALA	N-CA-CB	7.38	121.38	109.28
1	A	263	ASP	CA-CB-CG	7.38	119.98	112.60
1	A	235	LEU	CA-C-N	7.37	130.16	120.28
1	A	235	LEU	C-N-CA	7.37	130.16	120.28
1	B	2	VAL	CA-CB-CG2	7.37	122.92	110.40
1	A	120	HIS	CA-C-N	7.36	130.88	120.28
1	A	120	HIS	C-N-CA	7.36	130.88	120.28
1	B	117	LYS	CA-C-N	7.36	129.97	120.56
1	B	117	LYS	C-N-CA	7.36	129.97	120.56
1	B	311	ASN	CA-C-N	7.34	129.99	120.44
1	B	311	ASN	C-N-CA	7.34	129.99	120.44
1	A	391	LEU	CA-C-N	7.33	135.77	121.41
1	A	391	LEU	C-N-CA	7.33	135.77	121.41
1	B	388	GLU	CA-C-N	7.32	130.40	120.44
1	B	388	GLU	C-N-CA	7.32	130.40	120.44
1	A	192	LEU	CA-C-N	7.32	126.95	119.56
1	A	192	LEU	C-N-CA	7.32	126.95	119.56
1	B	233	GLN	OE1-CD-NE2	-7.32	115.28	122.60
1	B	364	PHE	CA-CB-CG	-7.31	106.49	113.80
1	B	317	LEU	CA-C-O	-7.30	112.81	120.55
1	B	358	MET	CA-CB-CG	-7.30	99.50	114.10
1	B	286	THR	N-CA-CB	-7.30	98.94	110.98
1	A	325	PHE	CA-CB-CG	7.29	121.09	113.80
1	A	23	ASP	CB-CA-C	7.21	124.38	110.17
1	B	244	ASP	N-CA-CB	7.21	121.86	110.55
1	A	305	TRP	CA-C-N	7.19	130.14	120.65
1	A	305	TRP	C-N-CA	7.19	130.14	120.65
1	A	194	THR	CA-CB-CG2	7.19	122.72	110.50
1	B	143	GLU	CA-C-O	7.18	127.52	119.41
1	A	388	GLU	CA-C-O	-7.18	112.94	120.55
1	B	174	ASN	CA-C-N	7.15	134.67	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ASN	C-N-CA	7.15	134.67	122.37
1	A	213	LEU	CA-C-N	7.14	130.31	122.74
1	A	213	LEU	C-N-CA	7.14	130.31	122.74
1	B	300	GLY	O-C-N	-7.14	116.67	122.81
1	B	379	PHE	CA-C-N	7.14	129.70	120.56
1	B	379	PHE	C-N-CA	7.14	129.70	120.56
1	B	154	LEU	CB-CA-C	7.13	122.97	110.85
1	B	294	LYS	CB-CA-C	-7.13	100.39	109.65
1	A	320	GLU	CB-CG-CD	7.08	124.64	112.60
1	B	34	ASP	CA-C-N	7.08	126.91	119.05
1	B	34	ASP	C-N-CA	7.08	126.91	119.05
1	B	149	ASP	N-CA-C	-7.08	96.09	108.20
1	B	54	ASP	CA-CB-CG	7.07	119.67	112.60
1	B	18	GLY	CA-C-N	7.04	132.65	121.66
1	B	18	GLY	C-N-CA	7.04	132.65	121.66
1	A	259	PHE	CA-C-O	7.04	128.94	120.92
1	A	377	PHE	CA-C-O	-7.03	112.16	120.10
1	B	206	GLU	CA-CB-CG	7.00	128.09	114.10
1	A	149	ASP	N-CA-C	-6.98	94.76	107.75
1	B	234	ALA	N-CA-C	-6.97	103.61	111.14
1	B	96	PRO	CA-C-N	6.97	131.48	120.47
1	B	96	PRO	C-N-CA	6.97	131.48	120.47
1	B	364	PHE	CA-C-O	6.96	130.46	120.51
1	B	23	ASP	CB-CA-C	6.93	123.83	110.17
1	B	361	SER	CA-C-O	6.93	134.07	120.69
1	B	103	PHE	CA-CB-CG	6.93	120.73	113.80
1	A	352	GLU	N-CA-C	-6.93	97.60	108.90
1	A	94	SER	N-CA-C	6.92	120.21	111.69
1	B	106	ASN	CA-C-N	6.91	131.20	121.24
1	B	106	ASN	C-N-CA	6.91	131.20	121.24
1	B	317	LEU	O-C-N	6.91	129.45	122.12
1	A	96	PRO	CA-C-N	6.88	130.23	120.53
1	A	96	PRO	C-N-CA	6.88	130.23	120.53
1	B	363	SER	O-C-N	-6.87	113.42	122.42
1	A	47	ALA	CA-C-O	6.86	128.82	121.55
1	A	301	TYR	N-CA-C	6.86	119.60	111.71
1	A	333	GLU	CA-C-N	6.86	129.47	120.28
1	A	333	GLU	C-N-CA	6.86	129.47	120.28
1	A	53	HIS	CB-CA-C	-6.84	97.93	109.50
1	A	352	GLU	CA-C-O	-6.84	112.97	120.36
1	B	19	TRP	N-CA-CB	6.84	120.82	109.60
1	B	254	ASP	CB-CA-C	6.84	121.06	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ALA	O-C-N	-6.82	114.38	122.15
1	A	387	ILE	O-C-N	-6.81	115.23	121.91
1	B	32	ASN	OD1-CG-ND2	6.79	129.39	122.60
1	A	275	GLU	CA-C-O	-6.79	113.67	120.80
1	B	333	GLU	OE1-CD-OE2	6.77	139.16	122.90
1	B	172	GLY	CA-C-O	-6.76	111.91	120.03
1	B	163	THR	CA-CB-OG1	-6.76	99.46	109.60
1	A	280	ASN	CB-CG-ND2	6.74	126.52	116.40
1	A	120	HIS	O-C-N	-6.74	115.08	122.09
1	A	239	LYS	CA-CB-CG	6.74	127.58	114.10
1	A	389	HIS	CA-C-O	-6.74	113.27	120.42
1	B	389	HIS	CA-CB-CG	-6.73	107.07	113.80
1	B	120	HIS	CA-CB-CG	-6.73	107.07	113.80
1	A	353	SER	O-C-N	6.73	130.75	122.14
1	A	66	GLU	CA-C-N	6.72	129.18	120.44
1	A	66	GLU	C-N-CA	6.72	129.18	120.44
1	A	96	PRO	O-C-N	-6.72	114.04	122.17
1	A	56	ASP	N-CA-C	-6.70	104.06	111.36
1	A	170	ASP	CA-C-O	-6.69	113.40	120.63
1	B	189	ASP	CA-C-O	-6.68	113.16	120.24
1	A	162	ASP	CA-C-O	-6.68	112.29	119.97
1	A	255	GLN	O-C-N	-6.67	114.89	122.09
1	B	380	ILE	N-CA-CB	6.65	119.09	110.57
1	B	12	PHE	CA-C-O	-6.65	112.62	120.60
1	A	20	THR	N-CA-CB	-6.64	99.25	110.41
1	A	56	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	27	VAL	CA-CB-CG2	6.63	121.67	110.40
1	B	367	PHE	CA-C-N	-6.61	113.66	122.85
1	B	367	PHE	C-N-CA	-6.61	113.66	122.85
1	A	360	ASP	CA-C-N	6.57	129.09	120.28
1	A	360	ASP	C-N-CA	6.57	129.09	120.28
1	A	230	GLY	O-C-N	-6.57	115.88	122.18
1	B	53	HIS	N-CA-CB	6.57	121.35	110.52
1	A	390	LEU	CA-C-N	6.56	134.25	122.38
1	A	390	LEU	C-N-CA	6.56	134.25	122.38
1	A	163	THR	CA-C-N	6.55	129.06	120.28
1	A	163	THR	C-N-CA	6.55	129.06	120.28
1	A	223	ALA	CA-C-O	6.55	127.11	119.32
1	B	359	ASN	CA-C-O	-6.54	111.16	120.51
1	B	213	LEU	CA-C-N	6.52	130.02	122.85
1	B	213	LEU	C-N-CA	6.52	130.02	122.85
1	A	297	ARG	CG-CD-NE	6.51	126.33	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	ILE	CA-C-O	-6.51	113.60	120.57
1	A	231	ILE	CA-C-N	6.51	129.53	120.29
1	A	231	ILE	C-N-CA	6.51	129.53	120.29
1	B	213	LEU	CA-CB-CG	6.51	139.09	116.30
1	B	118	VAL	O-C-N	6.51	128.67	121.90
1	A	70	ILE	CA-C-O	-6.47	114.54	121.27
1	A	75	ASN	OD1-CG-ND2	-6.47	116.13	122.60
1	A	224	GLY	CA-C-O	-6.46	111.83	119.72
1	A	215	PRO	O-C-N	6.46	131.27	123.13
1	B	55	ASN	CA-C-N	6.46	129.46	120.29
1	B	55	ASN	C-N-CA	6.46	129.46	120.29
1	B	130	ALA	CA-C-O	-6.45	114.09	121.19
1	A	234	ALA	CA-C-N	6.45	128.82	120.44
1	A	234	ALA	C-N-CA	6.45	128.82	120.44
1	B	108	ARG	NE-CZ-NH2	-6.45	113.40	119.20
1	A	54	ASP	CA-CB-CG	6.44	119.04	112.60
1	A	266	SER	CA-C-O	-6.44	114.06	120.82
1	A	76	GLN	CA-C-N	6.42	129.21	120.54
1	A	76	GLN	C-N-CA	6.42	129.21	120.54
1	A	361	SER	CA-C-O	6.42	127.36	120.55
1	A	323	LEU	CA-C-O	-6.40	113.13	120.24
1	B	275	GLU	CA-C-O	-6.40	113.70	120.55
1	B	364	PHE	CA-C-N	6.40	129.18	120.54
1	B	364	PHE	C-N-CA	6.40	129.18	120.54
1	B	196	GLY	CA-C-N	6.40	128.76	120.44
1	B	196	GLY	C-N-CA	6.40	128.76	120.44
1	A	54	ASP	CA-C-O	-6.39	113.54	121.02
1	B	48	TYR	N-CA-CB	-6.38	101.16	110.47
1	B	309	LYS	O-C-N	6.36	129.40	122.15
1	A	51	THR	CA-CB-CG2	6.35	121.30	110.50
1	B	248	GLN	CA-C-N	-6.35	113.47	123.12
1	B	248	GLN	C-N-CA	-6.35	113.47	123.12
1	A	20	THR	CB-CA-C	6.35	122.58	109.95
1	A	249	ARG	CD-NE-CZ	6.33	133.26	124.40
1	B	384	GLN	OE1-CD-NE2	-6.32	116.28	122.60
1	B	127	GLU	CA-CB-CG	6.32	126.74	114.10
1	B	354	ALA	N-CA-C	-6.32	104.31	111.07
1	B	280	ASN	CA-C-O	-6.31	111.97	119.35
1	A	361	SER	CA-C-N	6.30	129.24	120.29
1	A	361	SER	C-N-CA	6.30	129.24	120.29
1	A	167	TYR	CA-C-N	6.29	129.08	120.46
1	A	167	TYR	C-N-CA	6.29	129.08	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	THR	CA-C-O	-6.28	114.23	120.70
1	A	95	HIS	CA-C-N	6.28	126.76	119.47
1	A	95	HIS	C-N-CA	6.28	126.76	119.47
1	A	174	ASN	CB-CA-C	-6.28	102.70	112.12
1	B	188	GLY	CA-C-N	6.28	131.62	122.77
1	B	188	GLY	C-N-CA	6.28	131.62	122.77
1	A	34	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	213	LEU	CD1-CG-CD2	-6.26	97.04	110.80
1	A	188	GLY	CA-C-O	-6.25	114.31	120.75
1	B	21	GLY	N-CA-C	6.23	124.74	115.64
1	B	206	GLU	N-CA-C	-6.23	103.80	111.40
1	A	260	GLY	CA-C-O	6.22	126.04	119.07
1	A	330	GLU	O-C-N	6.22	128.48	122.07
1	B	84	LYS	N-CA-C	-6.22	101.58	110.59
1	B	283	PRO	CB-CA-C	6.21	119.09	110.95
1	B	191	PHE	CA-CB-CG	6.21	120.01	113.80
1	B	198	GLY	CA-C-N	6.20	128.50	120.44
1	B	198	GLY	C-N-CA	6.20	128.50	120.44
1	A	278	PHE	CA-C-N	6.20	127.59	119.84
1	A	278	PHE	C-N-CA	6.20	127.59	119.84
1	B	5	THR	CA-C-N	6.19	127.58	119.84
1	B	5	THR	C-N-CA	6.19	127.58	119.84
1	A	345	GLU	CB-CG-CD	6.19	123.12	112.60
1	A	121	ASN	CA-C-N	6.16	128.90	120.46
1	A	121	ASN	C-N-CA	6.16	128.90	120.46
1	B	359	ASN	N-CA-C	6.14	123.89	110.80
1	B	332	GLN	CA-C-N	6.14	129.01	120.29
1	B	332	GLN	C-N-CA	6.14	129.01	120.29
1	A	306	ASP	CA-C-N	6.13	128.78	120.38
1	A	306	ASP	C-N-CA	6.13	128.78	120.38
1	A	207	HIS	O-C-N	-6.13	114.44	122.59
1	A	121	ASN	O-C-N	-6.12	115.06	122.22
1	A	81	THR	CA-CB-OG1	-6.12	100.42	109.60
1	B	227	PHE	CA-C-O	-6.12	114.40	120.82
1	A	320	GLU	CG-CD-OE2	6.10	132.43	118.40
1	B	323	LEU	N-CA-CB	6.10	119.28	110.20
1	A	178	ALA	CA-C-O	-6.08	113.80	120.30
1	B	75	ASN	OD1-CG-ND2	6.07	128.67	122.60
1	B	376	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	B	37	GLU	CA-C-N	6.07	128.66	120.65
1	B	37	GLU	C-N-CA	6.07	128.66	120.65
1	B	181	PRO	CB-CA-C	6.07	118.93	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ILE	O-C-N	6.05	130.11	123.09
1	A	84	LYS	O-C-N	-6.05	116.17	122.94
1	B	107	ASP	O-C-N	-6.05	115.34	122.96
1	A	14	LEU	CA-C-N	6.04	130.81	120.72
1	A	14	LEU	C-N-CA	6.04	130.81	120.72
1	A	66	GLU	O-C-N	-6.04	115.17	122.11
1	B	342	GLU	OE1-CD-OE2	6.02	137.36	122.90
1	A	26	GLY	N-CA-C	6.01	121.97	111.14
1	A	108	ARG	NE-CZ-NH1	6.01	127.52	121.50
1	B	55	ASN	OD1-CG-ND2	-6.01	116.59	122.60
1	A	295	PRO	CA-C-O	-6.00	114.81	121.23
1	B	220	GLU	O-C-N	-6.00	115.20	122.22
1	B	346	THR	CA-CB-OG1	-5.99	100.62	109.60
1	A	361	SER	N-CA-C	5.98	117.80	111.28
1	B	333	GLU	CA-C-N	5.97	128.21	120.44
1	B	333	GLU	C-N-CA	5.97	128.21	120.44
1	A	227	PHE	CA-C-N	5.97	128.28	120.28
1	A	227	PHE	C-N-CA	5.97	128.28	120.28
1	B	205	LEU	O-C-N	5.96	129.64	122.85
1	B	260	GLY	O-C-N	-5.96	115.92	122.65
1	A	297	ARG	CA-C-N	5.95	129.35	120.31
1	A	297	ARG	C-N-CA	5.95	129.35	120.31
1	A	149	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	203	GLU	CB-CG-CD	5.94	122.70	112.60
1	B	235	LEU	CA-C-N	5.93	128.51	120.38
1	B	235	LEU	C-N-CA	5.93	128.51	120.38
1	B	14	LEU	CA-C-N	5.91	131.49	121.14
1	B	14	LEU	C-N-CA	5.91	131.49	121.14
1	A	283	PRO	CB-CA-C	5.91	118.74	111.12
1	A	246	ASN	O-C-N	5.90	129.60	122.75
1	B	171	LYS	CA-C-O	5.90	126.85	119.12
1	B	93	PHE	CA-C-O	-5.90	112.08	120.51
1	B	147	SER	CA-C-N	5.89	131.81	122.62
1	B	147	SER	C-N-CA	5.89	131.81	122.62
1	A	302	ASP	CA-C-N	5.89	126.51	119.98
1	A	302	ASP	C-N-CA	5.89	126.51	119.98
1	A	389	HIS	N-CA-CB	5.89	118.87	110.16
1	A	75	ASN	CA-C-N	5.88	128.42	120.65
1	A	75	ASN	C-N-CA	5.88	128.42	120.65
1	B	334	ALA	N-CA-C	-5.88	104.78	111.07
1	B	257	LEU	O-C-N	5.87	130.04	122.23
1	A	297	ARG	CA-CB-CG	5.87	125.84	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ALA	CA-C-N	5.86	130.48	122.34
1	A	237	ALA	C-N-CA	5.86	130.48	122.34
1	A	309	LYS	CA-CB-CG	5.85	125.80	114.10
1	A	118	VAL	CA-CB-CG1	5.82	120.29	110.40
1	A	3	GLN	CB-CA-C	5.81	121.62	110.17
1	B	127	GLU	CG-CD-OE2	5.81	131.76	118.40
1	A	349	ASN	CB-CG-ND2	5.80	125.11	116.40
1	B	391	LEU	CA-C-N	5.80	132.96	121.53
1	B	391	LEU	C-N-CA	5.80	132.96	121.53
1	B	103	PHE	CA-C-O	-5.80	113.71	120.20
1	B	361	SER	O-C-N	-5.78	113.69	122.93
1	B	290	HIS	CA-CB-CG	5.78	119.58	113.80
1	B	381	ARG	NE-CZ-NH1	5.76	127.26	121.50
1	B	151	ALA	CA-C-O	5.76	126.64	120.70
1	B	40	HIS	CA-C-O	-5.75	114.78	120.82
1	A	180	GLU	CA-C-O	5.74	125.01	119.62
1	A	298	THR	CA-C-N	5.73	130.57	122.09
1	A	298	THR	C-N-CA	5.73	130.57	122.09
1	B	347	THR	CA-CB-OG1	-5.72	101.02	109.60
1	B	330	GLU	CA-C-N	5.71	128.53	120.42
1	B	330	GLU	C-N-CA	5.71	128.53	120.42
1	B	381	ARG	CA-C-N	5.71	127.86	120.44
1	B	381	ARG	C-N-CA	5.71	127.86	120.44
1	A	176	ARG	NH1-CZ-NH2	-5.71	111.88	119.30
1	B	64	GLU	N-CA-CB	5.70	118.27	110.01
1	A	164	ALA	CA-C-N	5.70	128.38	120.29
1	A	164	ALA	C-N-CA	5.70	128.38	120.29
1	A	112	ARG	NH1-CZ-NH2	-5.69	111.90	119.30
1	B	347	THR	CA-CB-CG2	5.69	120.17	110.50
1	B	97	VAL	CA-CB-CG1	5.68	120.05	110.40
1	B	145	ASP	CA-C-O	-5.68	112.39	119.38
1	A	297	ARG	O-C-N	-5.68	114.63	122.46
1	A	205	LEU	CA-C-O	5.64	127.47	121.05
1	B	278	PHE	N-CA-C	5.64	118.09	110.31
1	A	254	ASP	CA-C-N	5.63	128.10	120.44
1	A	254	ASP	C-N-CA	5.63	128.10	120.44
1	A	37	GLU	CA-C-N	5.63	127.76	120.44
1	A	37	GLU	C-N-CA	5.63	127.76	120.44
1	A	41	LYS	CA-C-N	5.63	128.29	120.29
1	A	41	LYS	C-N-CA	5.63	128.29	120.29
1	A	34	ASP	OD1-CG-OD2	-5.62	109.41	122.90
1	A	39	VAL	CA-C-N	5.62	128.08	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	VAL	C-N-CA	5.62	128.08	120.44
1	A	84	LYS	CB-CA-C	5.62	119.66	109.83
1	A	276	ASN	CA-C-O	-5.60	111.94	119.11
1	A	289	ARG	N-CA-CB	5.60	119.64	110.39
1	B	23	ASP	OD1-CG-OD2	-5.60	109.45	122.90
1	A	53	HIS	N-CA-C	-5.60	101.16	110.17
1	B	333	GLU	N-CA-CB	-5.60	101.88	110.16
1	B	361	SER	N-CA-C	5.59	120.28	107.48
1	B	340	VAL	CB-CA-C	5.59	119.93	112.22
1	A	25	PHE	CA-C-N	5.58	130.44	121.17
1	A	25	PHE	C-N-CA	5.58	130.44	121.17
1	A	283	PRO	CA-C-N	5.58	131.33	122.62
1	A	283	PRO	C-N-CA	5.58	131.33	122.62
1	B	360	ASP	N-CA-CB	5.58	119.92	110.49
1	A	198	GLY	CA-C-O	5.58	127.02	121.00
1	A	156	ARG	CD-NE-CZ	5.58	132.21	124.40
1	A	14	LEU	O-C-N	-5.57	115.42	122.27
1	B	244	ASP	CA-CB-CG	5.57	118.17	112.60
1	B	350	ALA	CA-C-O	-5.57	114.79	120.80
1	A	235	LEU	CD1-CG-CD2	-5.56	98.56	110.80
1	B	311	ASN	CA-C-O	5.54	126.64	120.82
1	B	143	GLU	CA-C-N	5.54	130.96	122.93
1	B	143	GLU	C-N-CA	5.54	130.96	122.93
1	A	211	VAL	CA-CB-CG2	5.53	119.81	110.40
1	A	319	LYS	CA-C-N	5.53	127.63	120.44
1	A	319	LYS	C-N-CA	5.53	127.63	120.44
1	B	115	LEU	CB-CA-C	5.53	119.56	110.88
1	A	249	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	A	280	ASN	CA-C-O	-5.52	113.10	119.56
1	B	384	GLN	CB-CG-CD	5.51	121.98	112.60
1	B	272	ASP	CA-C-O	-5.50	115.01	120.90
1	B	116	ALA	CA-C-N	5.50	127.65	120.28
1	B	116	ALA	C-N-CA	5.50	127.65	120.28
1	A	34	ASP	CA-C-N	5.50	125.16	119.05
1	A	34	ASP	C-N-CA	5.50	125.16	119.05
1	B	257	LEU	CA-C-N	-5.50	112.72	120.75
1	B	257	LEU	C-N-CA	-5.50	112.72	120.75
1	A	176	ARG	NE-CZ-NH2	5.50	124.15	119.20
1	A	391	LEU	O-C-N	-5.50	114.79	122.37
1	B	140	GLU	CB-CG-CD	5.50	121.94	112.60
1	B	195	VAL	CA-C-O	-5.50	115.34	121.17
1	B	365	ALA	N-CA-C	5.50	117.70	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	ASN	CA-C-N	5.50	127.64	120.28
1	B	383	ASN	C-N-CA	5.50	127.64	120.28
1	B	14	LEU	N-CA-CB	-5.49	101.76	110.22
1	B	362	ALA	CB-CA-C	5.49	121.35	110.42
1	A	109	SER	CA-C-N	5.49	127.68	120.60
1	A	109	SER	C-N-CA	5.49	127.68	120.60
1	B	16	THR	CB-CA-C	5.49	119.92	110.86
1	B	74	PHE	CA-C-O	-5.48	115.24	121.00
1	A	203	GLU	CA-C-N	5.48	131.74	122.26
1	A	203	GLU	C-N-CA	5.48	131.74	122.26
1	B	11	THR	CB-CA-C	5.47	119.38	109.37
1	B	107	ASP	CA-C-O	5.46	126.92	120.58
1	B	383	ASN	O-C-N	-5.46	115.92	122.15
1	A	332	GLN	CA-C-N	5.46	128.04	120.29
1	A	332	GLN	C-N-CA	5.46	128.04	120.29
1	A	49	GLY	O-C-N	5.46	129.07	123.29
1	A	332	GLN	CB-CG-CD	5.45	121.87	112.60
1	A	340	VAL	N-CA-C	-5.45	105.06	110.62
1	B	354	ALA	N-CA-CB	5.45	117.91	110.01
1	A	269	PHE	CA-C-O	-5.44	113.71	119.97
1	B	383	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	156	ARG	CA-C-N	5.44	127.83	120.65
1	A	156	ARG	C-N-CA	5.44	127.83	120.65
1	A	43	ALA	O-C-N	-5.44	116.47	122.07
1	B	248	GLN	CB-CA-C	5.44	119.04	109.80
1	B	341	PHE	N-CA-C	-5.43	105.01	111.69
1	B	207	HIS	CA-C-O	5.43	129.55	120.65
1	A	292	ASP	O-C-N	5.42	129.35	122.84
1	B	266	SER	CA-C-N	5.42	127.48	120.44
1	B	266	SER	C-N-CA	5.42	127.48	120.44
1	B	236	TRP	CA-CB-CG	5.42	123.89	113.60
1	B	379	PHE	CB-CA-C	5.41	121.06	110.67
1	A	292	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	19	TRP	CB-CA-C	-5.41	102.45	110.67
1	B	132	THR	O-C-N	5.41	130.26	123.23
1	A	26	GLY	O-C-N	-5.40	118.53	123.56
1	A	349	ASN	N-CA-C	-5.39	102.54	110.52
1	A	122	ILE	CA-C-N	5.38	127.76	120.65
1	A	122	ILE	C-N-CA	5.38	127.76	120.65
1	A	102	GLY	N-CA-C	-5.38	100.43	113.18
1	A	248	GLN	CA-C-N	-5.38	115.58	122.79
1	A	248	GLN	C-N-CA	-5.38	115.58	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ILE	O-C-N	5.38	125.87	120.92
1	B	194	THR	CA-C-O	5.38	127.82	121.58
1	B	359	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	B	16	THR	OG1-CB-CG2	5.37	120.03	109.30
1	A	286	THR	CA-C-O	-5.36	113.16	119.05
1	B	326	ARG	CA-C-N	5.35	129.65	120.72
1	B	326	ARG	C-N-CA	5.35	129.65	120.72
1	B	52	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	225	LEU	N-CA-CB	-5.35	102.29	110.42
1	B	11	THR	O-C-N	-5.34	116.43	123.16
1	A	99	LYS	CA-C-O	-5.34	114.07	120.10
1	A	236	TRP	O-C-N	-5.33	116.47	122.12
1	B	45	LEU	CA-C-N	5.33	129.98	122.63
1	B	45	LEU	C-N-CA	5.33	129.98	122.63
1	A	393	SER	N-CA-C	-5.32	106.17	113.30
1	A	292	ASP	CA-C-O	-5.32	114.57	121.11
1	A	169	LYS	N-CA-C	-5.32	105.18	110.97
1	B	36	VAL	CA-C-N	5.31	127.39	120.28
1	B	36	VAL	C-N-CA	5.31	127.39	120.28
1	B	77	ALA	CA-C-O	5.29	126.16	120.55
1	B	389	HIS	N-CA-C	-5.29	105.42	111.14
1	A	174	ASN	OD1-CG-ND2	5.29	127.89	122.60
1	A	23	ASP	CB-CG-OD1	5.29	130.56	118.40
1	B	30	ARG	CG-CD-NE	5.29	123.63	112.00
1	B	123	ASP	CA-C-O	-5.28	115.28	120.82
1	A	130	ALA	CA-C-N	5.28	131.22	121.52
1	A	130	ALA	C-N-CA	5.28	131.22	121.52
1	B	142	SER	O-C-N	5.28	128.80	123.26
1	B	165	ALA	CA-C-O	5.27	126.35	120.82
1	B	286	THR	CB-CA-C	5.27	119.70	110.64
1	A	109	SER	CB-CA-C	5.27	119.80	110.85
1	B	246	ASN	CA-C-O	-5.26	115.47	120.94
1	B	153	ALA	CA-C-O	-5.26	114.97	120.55
1	B	256	ASP	CB-CG-OD1	5.26	130.50	118.40
1	B	305	TRP	CA-C-N	5.26	127.60	120.44
1	B	305	TRP	C-N-CA	5.26	127.60	120.44
1	B	214	ASN	OD1-CG-ND2	-5.25	117.34	122.60
1	A	168	ILE	CA-C-O	5.25	126.41	120.95
1	A	374	GLU	CA-C-O	-5.24	112.81	119.31
1	B	301	TYR	CA-C-N	5.24	128.27	120.31
1	B	301	TYR	C-N-CA	5.24	128.27	120.31
1	A	385	LEU	CA-C-O	-5.23	115.33	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	B	58	ILE	CB-CA-C	-5.22	105.17	111.18
1	B	286	THR	OG1-CB-CG2	5.22	119.75	109.30
1	B	134	VAL	CA-CB-CG1	5.22	119.27	110.40
1	B	158	ARG	O-C-N	5.22	127.65	122.12
1	A	263	ASP	CA-C-N	5.22	127.54	120.65
1	A	263	ASP	C-N-CA	5.22	127.54	120.65
1	B	67	ARG	CB-CA-C	5.22	119.21	110.92
1	B	114	ALA	O-C-N	-5.21	116.70	122.07
1	B	132	THR	CA-C-O	-5.21	115.07	120.70
1	B	7	ALA	CA-C-N	5.20	127.77	120.28
1	B	7	ALA	C-N-CA	5.20	127.77	120.28
1	A	149	ASP	CA-C-N	5.20	127.77	120.28
1	A	149	ASP	C-N-CA	5.20	127.77	120.28
1	B	10	PHE	CA-CB-CG	5.20	119.00	113.80
1	B	297	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	B	363	SER	N-CA-CB	-5.19	102.80	110.53
1	A	88	VAL	O-C-N	5.19	128.81	123.05
1	B	96	PRO	O-C-N	-5.18	115.64	122.64
1	B	107	ASP	N-CA-CB	-5.18	101.73	109.71
1	A	80	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	63	THR	CA-CB-OG1	-5.18	101.84	109.60
1	B	379	PHE	O-C-N	-5.18	115.90	122.27
1	A	366	GLY	O-C-N	5.17	129.43	122.70
1	A	353	SER	CA-C-O	-5.17	115.04	121.55
1	B	333	GLU	CG-CD-OE2	-5.17	106.52	118.40
1	A	357	LEU	O-C-N	5.16	127.66	122.09
1	A	117	LYS	CA-C-N	5.16	127.16	120.56
1	A	117	LYS	C-N-CA	5.16	127.16	120.56
1	A	250	GLY	N-CA-C	5.16	118.30	111.70
1	A	64	GLU	N-CA-C	5.15	117.80	111.82
1	A	60	PHE	CA-C-N	5.14	131.68	122.38
1	A	60	PHE	C-N-CA	5.14	131.68	122.38
1	B	215	PRO	CA-C-O	-5.14	115.60	121.56
1	A	101	GLY	CA-C-O	-5.14	118.62	122.37
1	A	347	THR	CA-CB-OG1	-5.14	101.90	109.60
1	A	307	SER	CA-C-N	5.13	127.11	120.44
1	A	307	SER	C-N-CA	5.13	127.11	120.44
1	B	339	GLY	CA-C-O	-5.13	112.77	119.44
1	B	6	PRO	CA-CB-CG	-5.12	94.76	104.50
1	A	259	PHE	O-C-N	-5.12	116.60	122.95
1	B	233	GLN	CB-CG-CD	5.12	121.31	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	TYR	CA-C-O	-5.12	115.12	120.55
1	A	177	ILE	CA-C-N	-5.12	115.78	123.00
1	A	177	ILE	C-N-CA	-5.12	115.78	123.00
1	A	221	GLN	O-C-N	-5.10	115.59	122.43
1	A	61	ASP	CA-C-N	5.09	128.00	120.82
1	A	61	ASP	C-N-CA	5.09	128.00	120.82
1	A	261	HIS	CA-C-N	5.09	131.39	121.41
1	A	261	HIS	C-N-CA	5.09	131.39	121.41
1	A	302	ASP	N-CA-C	-5.09	105.73	111.28
1	B	56	ASP	N-CA-CB	5.09	117.69	110.16
1	A	241	PHE	CB-CG-CD1	5.08	129.34	120.70
1	B	333	GLU	CB-CG-CD	-5.08	103.96	112.60
1	B	230	GLY	CA-C-O	-5.08	115.21	120.90
1	B	336	LYS	CA-C-N	5.08	127.39	120.54
1	B	336	LYS	C-N-CA	5.08	127.39	120.54
1	B	101	GLY	O-C-N	5.07	128.17	123.35
1	B	273	LEU	CA-CB-CG	5.07	134.06	116.30
1	A	223	ALA	CA-C-N	5.07	129.94	120.87
1	A	223	ALA	C-N-CA	5.07	129.94	120.87
1	B	312	MET	N-CA-CB	-5.07	102.67	110.01
1	B	261	HIS	CA-CB-CG	5.06	118.86	113.80
1	B	60	PHE	O-C-N	-5.06	116.30	122.22
1	B	213	LEU	N-CA-CB	-5.06	103.00	111.20
1	B	13	GLY	CA-C-N	5.05	127.56	120.28
1	B	13	GLY	C-N-CA	5.05	127.56	120.28
1	A	344	GLY	CA-C-O	-5.05	112.44	119.01
1	A	113	PHE	CB-CG-CD2	-5.05	112.12	120.70
1	A	158	ARG	CB-CG-CD	5.05	122.91	111.30
1	A	106	ASN	N-CA-C	-5.04	105.86	111.36
1	A	87	MET	CA-C-N	5.04	129.97	122.71
1	A	87	MET	C-N-CA	5.04	129.97	122.71
1	B	244	ASP	CA-C-O	-5.04	114.78	120.32
1	B	330	GLU	CA-C-O	-5.03	114.18	119.97
1	A	278	PHE	CA-C-O	5.03	124.42	120.19
1	B	170	ASP	CA-C-O	-5.03	115.52	120.90
1	B	278	PHE	CA-C-N	5.03	125.05	119.32
1	B	278	PHE	C-N-CA	5.03	125.05	119.32
1	A	14	LEU	N-CA-CB	-5.02	102.49	110.28
1	A	196	GLY	CA-C-N	5.02	127.01	120.28
1	A	196	GLY	C-N-CA	5.02	127.01	120.28
1	A	243	ILE	O-C-N	5.01	128.91	123.09
1	A	59	PRO	CA-C-N	5.01	126.95	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	PRO	C-N-CA	5.01	126.95	120.44
1	B	142	SER	CA-C-O	-5.01	116.07	121.38
1	B	203	GLU	CA-C-N	5.01	130.25	122.49
1	B	203	GLU	C-N-CA	5.01	130.25	122.49
1	A	56	ASP	CA-C-N	5.01	130.97	121.81
1	A	56	ASP	C-N-CA	5.01	130.97	121.81
1	A	383	ASN	CA-CB-CG	-5.00	107.59	112.60
1	B	298	THR	CA-C-O	5.00	125.53	119.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	359	ASN	Mainchain
1	B	362	ALA	Mainchain
1	B	364	PHE	Mainchain

5.2 Too-close contacts [i](#)

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	33	1
1	B	3027	0	2879	38	12
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	257	0	0	4	0
3	B	268	0	0	3	5
All	All	6583	0	5761	71	12

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 6.

All (71) 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:357:LEU:HG	1:B:359:ASN:HA	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLU:HG3	1:B:319:LYS:HG3	1.67	0.75
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.76	0.68
1:B:95:HIS:HD2	1:B:97:VAL:H	1.41	0.66
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.81	0.63
1:B:361:SER:HB3	1:B:366:GLY:H	1.62	0.63
1:A:158:ARG:HG3	1:A:205:LEU:HD23	1.79	0.63
1:A:95:HIS:HD2	1:A:97:VAL:H	1.48	0.61
1:A:215:PRO:HG2	1:A:231:ILE:HG22	1.85	0.58
1:B:361:SER:CB	1:B:366:GLY:H	2.17	0.58
1:B:131:GLU:HG3	3:B:649(B):HOH:O	2.04	0.58
1:A:84:LYS:HB2	3:A:660(A):HOH:O	2.03	0.57
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.90	0.54
1:A:20:THR:HG23	1:A:28:ALA:CB	2.38	0.54
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.91	0.53
1:A:277:GLY:HA3	1:A:284:LYS:HD3	1.91	0.52
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.90	0.52
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.76	0.51
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.11	0.50
1:B:361:SER:HB2	1:B:365:ALA:N	2.27	0.50
1:B:361:SER:CB	1:B:364:PHE:H	2.25	0.50
1:B:364:PHE:HB3	3:B:539(B):HOH:O	2.11	0.49
1:A:242:HIS:CD2	1:A:288:PRO:HG2	2.48	0.48
1:B:45:LEU:HD22	1:B:309:LYS:CD	2.43	0.48
1:B:53:HIS:HA	1:B:89:THR:O	2.12	0.48
1:B:357:LEU:O	1:B:360:ASP:N	2.45	0.48
1:A:135:MET:HE3	1:A:177:ILE:HG21	1.95	0.48
1:A:235:LEU:HG	1:A:240:LEU:HD23	1.96	0.47
1:B:140:GLU:HG3	1:B:157:MET:HE1	1.96	0.47
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.75	0.46
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.15	0.46
1:A:246:ASN:HB2	1:A:257:LEU:O	2.16	0.46
1:A:55:ASN:HA	1:A:58:ILE:O	2.16	0.46
1:A:87:MET:HA	1:A:132:THR:O	2.16	0.45
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.98	0.45
1:B:226:ASN:HB3	1:B:229:HIS:HB2	1.98	0.45
1:A:158:ARG:HB3	3:A:459(A):HOH:O	2.17	0.45
1:B:23:ASP:HB2	1:B:24:PRO:HD2	1.99	0.45
1:B:67:ARG:HG3	1:B:71:LEU:HD12	1.99	0.45
1:B:10:PHE:CD2	1:B:312:MET:HG2	2.51	0.45
1:B:79:LYS:O	1:B:80:ASP:C	2.59	0.44
1:B:62:ALA:HA	1:B:66:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:PRO:O	1:A:39:VAL:HG23	2.17	0.44
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.42	0.44
1:A:75:ASN:ND2	3:A:561(A):HOH:O	2.50	0.44
1:A:120:HIS:O	1:A:123:ASP:HB2	2.17	0.44
1:B:278:PHE:HA	1:B:279:PRO:HD3	1.88	0.44
1:B:249:ARG:O	1:B:252:LYS:HE3	2.18	0.43
1:B:357:LEU:HD23	1:B:359:ASN:ND2	2.32	0.43
1:A:95:HIS:CD2	1:A:97:VAL:H	2.33	0.43
1:A:19:TRP:CE3	1:A:294:LYS:HB3	2.53	0.43
1:A:20:THR:HG23	1:A:28:ALA:HB2	2.00	0.43
1:A:20:THR:HB	3:A:546(A):HOH:O	2.17	0.43
1:A:331:VAL:O	1:A:335:MET:HG3	2.19	0.43
1:A:133:PHE:O	1:A:177:ILE:HA	2.19	0.43
1:B:238:GLU:HG3	3:B:647(B):HOH:O	2.19	0.42
1:B:360:ASP:O	1:B:363:SER:N	2.52	0.42
1:A:110:ILE:O	1:A:111:ARG:C	2.62	0.42
1:B:256:ASP:HB3	1:B:293:TYR:HA	2.02	0.42
1:A:58:ILE:HA	1:A:59:PRO:HD3	1.81	0.42
1:B:309:LYS:HE2	1:B:312:MET:HE3	2.02	0.42
1:A:231:ILE:O	1:A:235:LEU:HB2	2.21	0.41
1:B:63:THR:H	1:B:66:GLU:CD	2.28	0.41
1:B:3:GLN:HA	1:B:4:PRO:HD2	1.95	0.41
1:B:374:GLU:O	1:B:375:ARG:C	2.62	0.41
1:B:42:LEU:HD23	1:B:42:LEU:HA	1.96	0.41
1:A:174:ASN:HD22	1:A:174:ASN:N	2.19	0.41
1:B:61:ASP:O	1:B:62:ALA:C	2.63	0.40
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.78	0.40
1:B:11:THR:HG21	1:B:86:PRO:HG2	2.02	0.40
1:B:55:ASN:HA	1:B:58:ILE:O	2.22	0.40

All (12) 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:B:105:SER:N	3:B:592(B):HOH:O[4_555]	1.17	1.03
1:B:116:ALA:N	1:B:359:ASN:OD1[4_555]	1.20	1.00
1:B:116:ALA:CB	1:B:359:ASN:CB[4_555]	1.30	0.90
1:B:116:ALA:CA	1:B:359:ASN:OD1[4_555]	1.35	0.85
1:B:104:THR:C	3:B:592(B):HOH:O[4_555]	1.38	0.82
1:B:105:SER:CA	3:B:592(B):HOH:O[4_555]	1.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ALA:CA	1:B:359:ASN:CG[4_555]	1.76	0.44
1:B:115:LEU:C	1:B:359:ASN:OD1[4_555]	1.86	0.34
1:B:104:THR:O	3:B:592(B):HOH:O[4_555]	1.92	0.28
1:B:116:ALA:CA	1:B:359:ASN:CB[4_555]	2.01	0.19
1:B:343:LEU:CD2	3:B:438(B):HOH:O[4_555]	2.11	0.09
1:A:69:LYS:NZ	1:B:276:ASN:O[6_665]	2.14	0.06

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	391/394 (99%)	374 (96%)	16 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	366 (94%)	19 (5%)	6 (2%)	8	16
All	All	782/788 (99%)	740 (95%)	35 (4%)	7 (1%)	14	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	MET
1	B	359	ASN
1	B	360	ASP
1	A	185	GLU
1	B	185	GLU
1	B	3	GLN
1	B	23	ASP

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	305/310 (98%)	286 (94%)	19 (6%)	16	34
1	B	305/310 (98%)	288 (94%)	17 (6%)	19	39
All	All	610/620 (98%)	574 (94%)	36 (6%)	18	37

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	41	LYS
1	A	44	GLU
1	A	50	ILE
1	A	68	GLU
1	A	69	LYS
1	A	83	LEU
1	A	84	LYS
1	A	90	THR
1	A	94	SER
1	A	96	PRO
1	A	150	LEU
1	A	158	ARG
1	A	174	ASN
1	A	184	ASN
1	A	213	LEU
1	A	235	LEU
1	A	286	THR
1	A	359	ASN
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	44	GLU
1	B	59	PRO
1	B	66	GLU
1	B	94	SER
1	B	131	GLU
1	B	184	ASN
1	B	213	LEU
1	B	235	LEU
1	B	273	LEU
1	B	286	THR
1	B	333	GLU

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Mol	Chain	Res	Type
1	B	358	MET
1	B	360	ASP
1	B	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	95	HIS
1	A	174	ASN
1	A	184	ASN
1	A	214	ASN
1	A	221	GLN
1	A	383	ASN
1	A	384	GLN
1	B	32	ASN
1	B	75	ASN
1	B	95	HIS
1	B	221	GLN
1	B	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, 4 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.