



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:13 AM UTC

PDB ID : 1XLF / pdb_00001xlf
Title : MECHANISM FOR ALDOSE-KETOSE INTERCONVERSION BY D-XYLOSE ISOMERASE INVOLVING RING OPENING FOLLOWED BY A 1,2-HYDRIDE SHIFT
Authors : Collyer, C.A.; Henrick, K.; Blow, D.M.
Deposited on : 1991-10-09
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

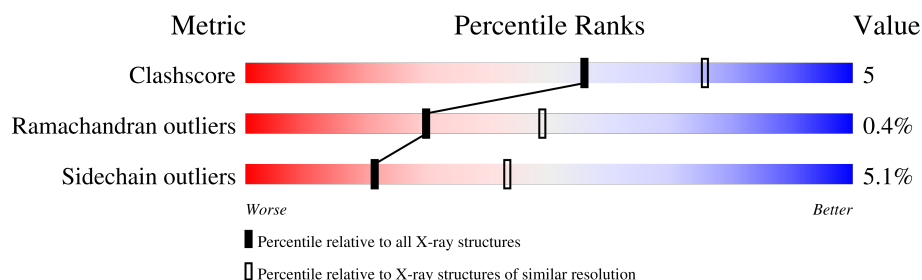
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	394	
1	B	394	

2 Entry composition [i](#)

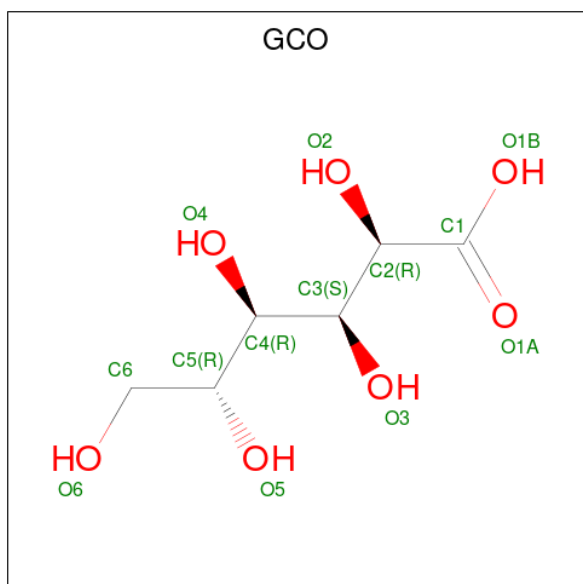
There are 4 unique types of molecules in this entry. The entry contains 6599 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-gluconic acid (CCD ID: GCO) (formula: $C_6H_{12}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total 253	O 253	0	0
4	B	262	Total 262	O 262	0	0

A310	N311	M312	S313		L318	K319	E320		L323	A324		P329	E330	V331	Q332	E333	A334		E342	L343		T346	T347		A350		L357	M358	N359	D360	S361	A362		F367		E370	A371	A372		N376		F379	I380	R381	L382	N383	Q384	L385	A386	I387	E388	H389	L390	L391	G392	S393	R394
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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	106.00Å 106.00Å 153.80Å 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}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6599	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: GCO, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.50	12/3101 (0.4%)	2.76	289/4204 (6.9%)
1	B	1.51	11/3101 (0.4%)	2.66	289/4204 (6.9%)
All	All	1.50	23/6202 (0.4%)	2.71	578/8408 (6.9%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	PHE	C-O	6.71	1.31	1.24
1	A	107	ASP	CA-CB	-6.05	1.44	1.53
1	B	61	ASP	N-CA	-5.88	1.38	1.46
1	B	265	THR	C-O	5.88	1.30	1.24
1	A	282	GLY	N-CA	5.79	1.52	1.44
1	A	57	LEU	N-CA	-5.77	1.40	1.47
1	B	239	LYS	CA-C	-5.55	1.45	1.52
1	A	394	ARG	NE-CZ	-5.51	1.26	1.33
1	B	270	THR	C-O	5.46	1.30	1.24
1	B	149	ASP	CA-CB	-5.45	1.46	1.53
1	A	168	ILE	CA-CB	5.44	1.60	1.54
1	B	152	ALA	C-O	5.43	1.30	1.24
1	B	144	TYR	CA-C	-5.43	1.46	1.52
1	A	154	LEU	C-O	5.40	1.30	1.24
1	A	343	LEU	C-O	5.38	1.30	1.24
1	A	50	ILE	C-O	5.36	1.29	1.24
1	B	298	THR	CA-CB	5.27	1.62	1.53
1	B	277	GLY	N-CA	5.18	1.52	1.45
1	A	81	THR	CA-CB	5.18	1.61	1.53
1	B	254	ASP	N-CA	5.16	1.52	1.46
1	A	174	ASN	CA-CB	-5.13	1.46	1.52
1	A	187	ARG	NE-CZ	5.10	1.38	1.33
1	A	197	HIS	C-O	5.00	1.29	1.24

All (578) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	CD-NE-CZ	33.24	170.94	124.40
1	A	6	PRO	CA-C-N	17.18	145.02	120.28
1	A	6	PRO	C-N-CA	17.18	145.02	120.28
1	A	174	ASN	CA-CB-CG	15.65	128.25	112.60
1	B	60	PHE	CA-C-N	15.34	148.66	121.66
1	B	60	PHE	C-N-CA	15.34	148.66	121.66
1	A	174	ASN	OD1-CG-ND2	13.88	136.48	122.60
1	A	244	ASP	CA-CB-CG	12.56	125.16	112.60
1	A	107	ASP	CA-CB-CG	12.52	125.11	112.60
1	A	103	PHE	CA-CB-CG	12.10	125.90	113.80
1	B	32	ASN	CA-CB-CG	-12.09	100.51	112.60
1	A	281	GLY	CA-C-O	-11.20	114.51	122.23
1	B	254	ASP	CA-CB-CG	11.06	123.66	112.60
1	B	379	PHE	CA-CB-CG	11.06	124.86	113.80
1	B	238	GLU	CB-CG-CD	11.01	131.32	112.60
1	A	137	GLY	CA-C-N	10.77	133.60	120.14
1	A	137	GLY	C-N-CA	10.77	133.60	120.14
1	B	319	LYS	CA-C-N	10.37	133.92	120.44
1	B	319	LYS	C-N-CA	10.37	133.92	120.44
1	B	127	GLU	CA-CB-CG	10.35	134.81	114.10
1	A	19	TRP	CA-C-O	10.28	132.53	120.70
1	B	61	ASP	CA-CB-CG	-9.95	102.65	112.60
1	A	117	LYS	CA-C-N	9.87	133.19	120.56
1	A	117	LYS	C-N-CA	9.87	133.19	120.56
1	A	65	ALA	N-CA-C	-9.69	100.70	111.07
1	A	297	ARG	CA-C-N	9.61	134.92	120.31
1	A	297	ARG	C-N-CA	9.61	134.92	120.31
1	A	359	ASN	CA-CB-CG	9.53	122.13	112.60
1	B	249	ARG	O-C-N	-9.52	112.55	122.64
1	B	207	HIS	CA-C-N	9.52	132.12	120.13
1	B	207	HIS	C-N-CA	9.52	132.12	120.13
1	A	107	ASP	CA-C-O	9.47	131.48	120.49
1	A	162	ASP	CA-CB-CG	9.42	122.02	112.60
1	A	215	PRO	O-C-N	9.39	134.61	123.06
1	B	188	GLY	CA-C-N	9.32	136.19	122.39
1	B	188	GLY	C-N-CA	9.32	136.19	122.39
1	B	20	THR	N-CA-CB	-9.32	94.75	110.41
1	B	246	ASN	OD1-CG-ND2	-9.26	113.34	122.60
1	A	215	PRO	CA-C-O	-9.21	110.43	121.67
1	A	112	ARG	CB-CG-CD	9.08	132.18	111.30
1	A	105	SER	CA-C-N	9.03	133.11	120.29
1	A	105	SER	C-N-CA	9.03	133.11	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	PHE	CA-C-O	-8.96	111.47	120.70
1	A	71	LEU	CA-C-N	8.91	129.81	120.00
1	A	71	LEU	C-N-CA	8.91	129.81	120.00
1	B	79	LYS	O-C-N	-8.85	112.83	122.03
1	B	174	ASN	CA-C-N	8.79	136.33	122.62
1	B	174	ASN	C-N-CA	8.79	136.33	122.62
1	A	393	SER	CA-C-N	8.71	137.37	121.70
1	A	393	SER	C-N-CA	8.71	137.37	121.70
1	B	37	GLU	CA-C-N	8.68	131.72	120.44
1	B	37	GLU	C-N-CA	8.68	131.72	120.44
1	B	272	ASP	O-C-N	-8.65	113.09	122.09
1	A	66	GLU	O-C-N	-8.63	113.12	122.09
1	A	6	PRO	O-C-N	-8.61	111.02	122.64
1	A	7	ALA	CA-C-N	8.59	132.49	120.29
1	A	7	ALA	C-N-CA	8.59	132.49	120.29
1	A	342	GLU	N-CA-CB	8.59	123.45	110.22
1	A	158	ARG	CD-NE-CZ	8.58	136.41	124.40
1	B	115	LEU	CB-CA-C	8.54	124.30	110.88
1	B	391	LEU	CA-C-N	8.46	136.01	120.87
1	B	391	LEU	C-N-CA	8.46	136.01	120.87
1	B	206	GLU	CA-CB-CG	8.33	130.77	114.10
1	A	149	ASP	N-CA-C	-8.29	94.03	108.20
1	A	121	ASN	CA-C-N	8.26	132.15	120.42
1	A	121	ASN	C-N-CA	8.26	132.15	120.42
1	B	108	ARG	CD-NE-CZ	8.25	135.95	124.40
1	B	241	PHE	CA-CB-CG	8.18	121.98	113.80
1	B	20	THR	CB-CA-C	8.10	126.08	109.95
1	A	358	MET	CA-C-N	8.10	132.62	120.31
1	A	358	MET	C-N-CA	8.10	132.62	120.31
1	B	208	GLY	CA-C-N	8.09	131.93	120.28
1	B	208	GLY	C-N-CA	8.09	131.93	120.28
1	A	342	GLU	CA-CB-CG	8.08	130.26	114.10
1	B	372	ALA	O-C-N	-8.00	112.86	122.22
1	A	388	GLU	CA-C-O	-7.96	112.11	120.55
1	B	324	ALA	CA-C-N	7.94	130.76	120.44
1	B	324	ALA	C-N-CA	7.94	130.76	120.44
1	A	145	ASP	CA-C-O	-7.92	109.64	119.38
1	B	32	ASN	OD1-CG-ND2	7.92	130.52	122.60
1	A	298	THR	CA-C-N	7.91	133.79	122.09
1	A	298	THR	C-N-CA	7.91	133.79	122.09
1	A	14	LEU	CA-C-O	7.89	128.91	120.55
1	B	137	GLY	CA-C-N	7.86	129.97	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	GLY	C-N-CA	7.86	129.97	120.14
1	A	320	GLU	CA-CB-CG	7.83	129.76	114.10
1	B	203	GLU	CA-C-N	7.81	134.60	122.49
1	B	203	GLU	C-N-CA	7.81	134.60	122.49
1	B	53	HIS	CA-CB-CG	7.73	121.53	113.80
1	B	56	ASP	N-CA-CB	7.67	121.50	110.16
1	B	279	PRO	O-C-N	-7.66	113.43	122.24
1	B	180	GLU	CA-C-O	7.65	126.63	119.59
1	A	263	ASP	CA-CB-CG	7.64	120.24	112.60
1	B	56	ASP	N-CA-C	-7.64	103.04	111.36
1	B	248	GLN	OE1-CD-NE2	-7.61	114.99	122.60
1	B	23	ASP	CB-CA-C	7.59	125.12	110.17
1	B	296	SER	CA-C-O	7.58	129.22	120.96
1	B	162	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	20	THR	N-CA-CB	-7.54	97.74	110.41
1	A	161	VAL	CA-C-O	-7.53	113.12	120.95
1	B	37	GLU	CB-CG-CD	7.53	125.40	112.60
1	A	243	ILE	CA-C-O	-7.53	113.44	121.19
1	B	310	ALA	O-C-N	-7.52	114.14	122.12
1	A	206	GLU	N-CA-CB	7.52	120.91	110.01
1	A	320	GLU	CB-CG-CD	7.49	125.33	112.60
1	A	334	ALA	CA-C-N	7.48	130.91	120.29
1	A	334	ALA	C-N-CA	7.48	130.91	120.29
1	A	14	LEU	O-C-N	-7.47	114.20	122.12
1	B	106	ASN	CA-C-N	7.47	131.99	121.24
1	B	106	ASN	C-N-CA	7.47	131.99	121.24
1	A	149	ASP	N-CA-CB	7.46	122.68	110.37
1	B	103	PHE	CA-CB-CG	7.46	121.26	113.80
1	B	388	GLU	O-C-N	-7.43	113.13	122.27
1	B	44	GLU	CG-CD-OE1	-7.40	101.38	118.40
1	B	2	VAL	CA-C-N	7.39	139.82	121.80
1	B	2	VAL	C-N-CA	7.39	139.82	121.80
1	B	69	LYS	CA-CB-CG	7.38	128.87	114.10
1	A	84	LYS	CA-CB-CG	7.36	128.81	114.10
1	B	68	GLU	CB-CA-C	7.35	123.35	110.85
1	B	217	THR	CA-C-N	7.30	128.08	119.98
1	B	217	THR	C-N-CA	7.30	128.08	119.98
1	A	133	PHE	CA-C-O	7.29	128.05	120.40
1	B	389	HIS	CA-CB-CG	-7.26	106.54	113.80
1	B	93	PHE	CA-C-O	-7.26	110.19	118.47
1	A	266	SER	CA-C-O	-7.25	113.20	120.82
1	B	294	LYS	CB-CA-C	-7.25	100.51	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	PHE	CA-C-N	7.25	129.87	120.44
1	A	227	PHE	C-N-CA	7.25	129.87	120.44
1	B	358	MET	CA-C-N	7.24	135.70	121.58
1	B	358	MET	C-N-CA	7.24	135.70	121.58
1	A	352	GLU	N-CA-C	-7.23	97.11	108.90
1	B	383	ASN	O-C-N	-7.20	113.94	122.15
1	A	213	LEU	CD1-CG-CD2	-7.17	95.04	110.80
1	A	51	THR	CA-CB-CG2	7.15	122.66	110.50
1	A	222	MET	CA-C-N	7.15	133.76	122.60
1	A	222	MET	C-N-CA	7.15	133.76	122.60
1	B	164	ALA	CA-C-N	7.15	130.16	120.44
1	B	164	ALA	C-N-CA	7.15	130.16	120.44
1	B	268	PHE	CA-C-N	7.14	131.17	120.31
1	B	268	PHE	C-N-CA	7.14	131.17	120.31
1	A	333	GLU	CA-CB-CG	7.12	128.34	114.10
1	A	360	ASP	CA-C-N	7.10	130.51	120.28
1	A	360	ASP	C-N-CA	7.10	130.51	120.28
1	B	233	GLN	CB-CG-CD	7.10	124.67	112.60
1	B	388	GLU	CA-C-N	7.10	130.37	120.29
1	B	388	GLU	C-N-CA	7.10	130.37	120.29
1	A	194	THR	CA-C-N	7.09	129.74	120.60
1	A	194	THR	C-N-CA	7.09	129.74	120.60
1	A	329	PRO	CA-C-N	7.06	129.62	120.44
1	A	329	PRO	C-N-CA	7.06	129.62	120.44
1	B	159	GLU	CA-CB-CG	7.04	128.18	114.10
1	B	40	HIS	CA-CB-CG	-7.01	106.79	113.80
1	A	342	GLU	CB-CA-C	-7.00	97.67	110.63
1	A	23	ASP	CB-CA-C	7.00	123.95	110.17
1	B	75	ASN	CA-C-N	6.98	129.93	120.44
1	B	75	ASN	C-N-CA	6.98	129.93	120.44
1	A	328	ASP	CA-C-O	6.97	126.39	119.49
1	B	55	ASN	CA-C-N	6.95	130.16	120.29
1	B	55	ASN	C-N-CA	6.95	130.16	120.29
1	B	214	ASN	CB-CG-ND2	6.95	126.82	116.40
1	B	376	ASN	CA-C-O	-6.94	113.15	120.58
1	B	119	LEU	CB-CA-C	6.91	121.73	110.88
1	A	193	PRO	N-CA-C	6.90	122.49	113.86
1	B	193	PRO	O-C-N	-6.89	112.96	122.27
1	B	60	PHE	O-C-N	-6.89	114.35	122.20
1	A	273	LEU	CA-C-O	-6.87	113.62	120.70
1	B	53	HIS	N-CA-CB	6.87	121.86	110.52
1	A	370	GLU	CA-C-O	-6.84	113.16	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	GLU	CA-CB-CG	6.84	127.78	114.10
1	B	280	ASN	CA-C-O	-6.83	111.36	119.35
1	A	120	HIS	CA-CB-CG	-6.81	106.99	113.80
1	B	134	VAL	CA-CB-CG1	6.80	121.96	110.40
1	B	76	GLN	CA-C-N	6.74	129.31	120.28
1	B	76	GLN	C-N-CA	6.74	129.31	120.28
1	A	67	ARG	CA-C-O	6.74	127.89	120.82
1	B	143	GLU	CA-C-O	6.74	127.03	119.41
1	A	65	ALA	CA-C-O	-6.73	113.75	120.82
1	A	336	LYS	CA-C-O	-6.73	113.77	120.70
1	A	36	VAL	O-C-N	6.73	128.50	121.91
1	A	131	GLU	N-CA-C	-6.73	105.20	113.41
1	A	352	GLU	CA-C-O	-6.72	113.10	120.36
1	B	30	ARG	CA-C-N	6.72	131.49	120.94
1	B	30	ARG	C-N-CA	6.72	131.49	120.94
1	A	127	GLU	N-CA-CB	6.71	119.99	110.12
1	A	297	ARG	N-CA-C	6.70	120.91	112.87
1	B	346	THR	CA-CB-OG1	-6.69	99.57	109.60
1	B	48	TYR	N-CA-CB	-6.67	100.73	110.47
1	B	149	ASP	N-CA-C	-6.67	97.68	108.41
1	A	297	ARG	O-C-N	-6.66	113.57	122.43
1	A	56	ASP	N-CA-CB	6.66	120.01	110.16
1	B	154	LEU	CB-CA-C	6.64	122.15	110.85
1	B	213	LEU	CA-CB-CG	6.64	139.54	116.30
1	B	12	PHE	CA-C-O	-6.64	112.63	120.60
1	A	216	GLU	CG-CD-OE1	6.61	133.61	118.40
1	B	149	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	302	ASP	CA-C-N	6.58	127.29	119.98
1	A	302	ASP	C-N-CA	6.58	127.29	119.98
1	A	91	ASN	CB-CG-ND2	-6.58	106.53	116.40
1	B	221	GLN	OE1-CD-NE2	-6.56	116.04	122.60
1	A	269	PHE	CA-C-O	-6.53	112.46	119.97
1	A	107	ASP	O-C-N	-6.50	115.02	123.02
1	A	263	ASP	CA-C-N	6.48	129.26	120.44
1	A	263	ASP	C-N-CA	6.48	129.26	120.44
1	B	278	PHE	CA-C-N	6.47	126.69	119.32
1	B	278	PHE	C-N-CA	6.47	126.69	119.32
1	B	357	LEU	CA-C-O	-6.46	113.70	120.55
1	A	196	GLY	CA-C-N	6.46	128.94	120.28
1	A	196	GLY	C-N-CA	6.46	128.94	120.28
1	B	311	ASN	CA-C-N	6.45	129.44	120.29
1	B	311	ASN	C-N-CA	6.45	129.44	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	GLY	CA-C-N	6.43	128.90	120.28
1	B	196	GLY	C-N-CA	6.43	128.90	120.28
1	A	53	HIS	N-CA-CB	6.42	121.12	110.52
1	B	329	PRO	CB-CA-C	6.42	121.48	112.11
1	A	33	LEU	CA-C-O	-6.42	113.24	120.43
1	B	308	ALA	CA-C-N	6.42	129.40	120.29
1	B	308	ALA	C-N-CA	6.42	129.40	120.29
1	A	27	VAL	CA-CB-CG2	6.41	121.30	110.40
1	B	381	ARG	NE-CZ-NH2	-6.41	113.44	119.20
1	B	286	THR	N-CA-CB	-6.40	100.86	111.49
1	A	391	LEU	CA-C-N	6.40	133.95	121.41
1	A	391	LEU	C-N-CA	6.40	133.95	121.41
1	B	40	HIS	CA-C-O	-6.39	114.28	121.00
1	B	342	GLU	CG-CD-OE2	-6.39	103.70	118.40
1	A	115	LEU	CB-CA-C	6.39	121.40	110.79
1	A	286	THR	CA-C-O	-6.37	111.96	119.48
1	A	292	ASP	CA-CB-CG	6.37	118.97	112.60
1	B	26	GLY	N-CA-C	6.36	121.11	110.56
1	A	127	GLU	CB-CA-C	-6.33	100.28	110.79
1	B	313	SER	CA-C-N	6.31	129.06	120.54
1	B	313	SER	C-N-CA	6.31	129.06	120.54
1	B	347	THR	CA-CB-OG1	-6.31	100.13	109.60
1	B	302	ASP	CA-C-N	6.31	126.94	120.00
1	B	302	ASP	C-N-CA	6.31	126.94	120.00
1	A	356	ASP	CA-C-N	6.30	129.01	120.44
1	A	356	ASP	C-N-CA	6.30	129.01	120.44
1	B	371	ALA	CA-C-O	-6.30	113.74	120.42
1	A	68	GLU	OE1-CD-OE2	6.30	138.01	122.90
1	B	73	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	56	ASP	CA-C-N	6.29	130.45	121.71
1	A	56	ASP	C-N-CA	6.29	130.45	121.71
1	A	211	VAL	CA-CB-CG2	6.27	121.06	110.40
1	A	139	ARG	NE-CZ-NH2	6.25	124.83	119.20
1	B	392	GLY	CA-C-N	6.25	133.03	121.52
1	B	392	GLY	C-N-CA	6.25	133.03	121.52
1	B	333	GLU	CA-C-N	6.25	128.56	120.44
1	B	333	GLU	C-N-CA	6.25	128.56	120.44
1	A	385	LEU	CA-C-O	-6.23	114.28	120.82
1	A	276	ASN	CA-C-O	-6.22	111.15	119.11
1	A	368	ASP	CA-C-N	6.21	128.61	120.28
1	A	368	ASP	C-N-CA	6.21	128.61	120.28
1	A	249	ARG	CD-NE-CZ	6.21	133.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	GLY	O-C-N	-6.21	116.23	122.19
1	B	79	LYS	CA-C-O	6.20	127.51	121.00
1	A	297	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	A	150	LEU	CA-C-O	-6.17	112.87	119.97
1	B	67	ARG	CG-CD-NE	6.16	125.54	112.00
1	A	346	THR	CA-CB-OG1	-6.15	100.37	109.60
1	B	186	PRO	N-CA-C	6.15	128.09	112.10
1	B	99	LYS	CA-C-O	-6.15	111.82	119.38
1	A	389	HIS	CA-C-O	-6.14	114.38	120.70
1	A	91	ASN	CB-CG-OD1	6.13	133.06	120.80
1	B	223	ALA	O-C-N	-6.12	114.69	122.34
1	A	96	PRO	O-C-N	-6.12	114.77	122.17
1	A	379	PHE	CA-CB-CG	6.11	119.91	113.80
1	A	58	ILE	CA-C-O	6.11	123.89	119.25
1	B	205	LEU	O-C-N	6.11	129.78	122.94
1	A	377	PHE	CA-C-O	-6.09	111.89	119.38
1	B	330	GLU	CA-C-O	-6.09	113.97	120.42
1	A	266	SER	CA-C-N	6.08	128.43	120.28
1	A	266	SER	C-N-CA	6.08	128.43	120.28
1	B	75	ASN	N-CA-C	6.08	118.70	111.71
1	B	261	HIS	CA-C-N	6.08	133.32	121.41
1	B	261	HIS	C-N-CA	6.08	133.32	121.41
1	A	166	GLY	N-CA-C	-6.07	105.46	112.50
1	A	202	ILE	CA-C-O	-6.06	114.97	121.27
1	B	270	THR	N-CA-C	-6.05	104.60	111.14
1	B	168	ILE	CA-C-O	6.05	127.57	121.27
1	B	290	HIS	CA-CB-CG	6.05	119.85	113.80
1	B	203	GLU	CG-CD-OE2	6.05	132.32	118.40
1	B	334	ALA	N-CA-C	-6.05	104.60	111.07
1	A	194	THR	CA-CB-CG2	6.04	120.78	110.50
1	B	107	ASP	CA-C-O	6.04	127.58	120.58
1	B	261	HIS	CA-CB-CG	6.03	119.83	113.80
1	A	14	LEU	CA-C-N	6.02	130.78	120.72
1	A	14	LEU	C-N-CA	6.02	130.78	120.72
1	A	215	PRO	N-CA-CB	6.01	108.92	103.33
1	A	357	LEU	CA-C-O	-6.01	114.51	120.70
1	B	101	GLY	O-C-N	6.01	129.06	123.35
1	B	8	ASP	CA-C-N	6.00	130.64	122.19
1	B	8	ASP	C-N-CA	6.00	130.64	122.19
1	A	221	GLN	CA-C-N	5.98	130.71	120.72
1	A	221	GLN	C-N-CA	5.98	130.71	120.72
1	B	298	THR	CA-C-N	5.98	132.80	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	298	THR	C-N-CA	5.98	132.80	122.64
1	B	194	THR	CA-CB-CG2	5.98	120.66	110.50
1	A	170	ASP	CA-C-O	-5.97	114.22	120.55
1	A	200	ALA	CA-C-O	5.96	127.08	120.82
1	B	138	GLY	CA-C-O	-5.95	113.97	120.40
1	B	208	GLY	O-C-N	-5.95	116.06	122.19
1	B	44	GLU	CB-CG-CD	-5.95	102.49	112.60
1	A	235	LEU	CA-C-O	5.95	127.06	120.82
1	A	359	ASN	CA-C-O	-5.95	113.13	119.97
1	B	244	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	109	SER	CB-CA-C	5.93	120.93	110.85
1	B	278	PHE	CA-C-O	-5.93	114.68	120.19
1	B	56	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	207	HIS	O-C-N	-5.92	114.71	122.59
1	A	325	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	368	ASP	OD1-CG-OD2	-5.91	108.72	122.90
1	B	387	ILE	CB-CG1-CD1	5.91	126.20	113.80
1	A	127	GLU	CA-CB-CG	5.90	125.89	114.10
1	B	297	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	A	32	ASN	CA-CB-CG	-5.89	106.71	112.60
1	B	61	ASP	N-CA-C	5.88	120.52	113.23
1	B	271	VAL	CA-C-O	-5.88	114.83	120.95
1	B	279	PRO	CA-C-N	5.88	132.24	122.54
1	B	279	PRO	C-N-CA	5.88	132.24	122.54
1	A	180	GLU	CA-C-O	5.86	125.13	119.62
1	B	36	VAL	CA-C-N	5.86	128.13	120.28
1	B	36	VAL	C-N-CA	5.86	128.13	120.28
1	B	216	GLU	CG-CD-OE2	-5.86	104.92	118.40
1	B	156	ARG	CA-C-O	-5.85	114.22	120.42
1	B	214	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	B	78	LEU	N-CA-C	-5.85	104.81	111.07
1	B	361	SER	CA-C-N	5.85	130.48	120.72
1	B	361	SER	C-N-CA	5.85	130.48	120.72
1	A	95	HIS	CA-C-N	5.84	126.24	119.47
1	A	95	HIS	C-N-CA	5.84	126.24	119.47
1	A	301	TYR	N-CA-C	5.84	118.42	111.71
1	A	43	ALA	O-C-N	-5.84	116.06	122.07
1	A	276	ASN	CB-CG-ND2	5.83	125.15	116.40
1	B	197	HIS	CA-CB-CG	-5.83	107.97	113.80
1	B	29	THR	CA-CB-OG1	-5.81	100.88	109.60
1	B	304	VAL	CB-CA-C	5.81	119.08	111.81
1	A	189	ASP	CA-C-O	-5.81	113.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ARG	CA-C-N	5.79	128.51	120.29
1	A	111	ARG	C-N-CA	5.79	128.51	120.29
1	B	194	THR	CA-CB-OG1	-5.79	100.92	109.60
1	A	127	GLU	CA-C-O	-5.78	114.43	120.55
1	B	20	THR	CA-CB-CG2	5.77	120.30	110.50
1	B	125	ALA	CA-C-N	5.76	127.93	120.44
1	B	125	ALA	C-N-CA	5.76	127.93	120.44
1	B	298	THR	O-C-N	-5.73	114.75	122.43
1	B	163	THR	CA-C-O	-5.73	114.80	120.70
1	B	44	GLU	CG-CD-OE2	5.73	131.58	118.40
1	A	174	ASN	CB-CA-C	-5.73	103.53	112.12
1	B	360	ASP	CB-CA-C	5.72	120.33	110.77
1	A	276	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	B	304	VAL	N-CA-C	-5.72	104.75	110.30
1	A	259	PHE	CA-C-O	5.71	127.43	120.92
1	A	214	ASN	OD1-CG-ND2	-5.70	116.90	122.60
1	A	8	ASP	CB-CG-OD2	5.70	131.51	118.40
1	A	121	ASN	O-C-N	-5.70	115.55	122.22
1	A	267	ALA	CA-C-N	5.69	128.70	120.79
1	A	267	ALA	C-N-CA	5.69	128.70	120.79
1	B	278	PHE	N-CA-CB	-5.68	100.73	110.11
1	B	391	LEU	O-C-N	-5.68	113.98	122.39
1	A	5	THR	O-C-N	-5.68	116.91	121.80
1	B	102	GLY	CA-C-N	5.68	128.67	120.38
1	B	102	GLY	C-N-CA	5.68	128.67	120.38
1	A	75	ASN	CA-C-N	5.68	128.14	120.65
1	A	75	ASN	C-N-CA	5.68	128.14	120.65
1	A	287	GLY	CA-C-O	5.67	129.63	121.52
1	B	187	ARG	NE-CZ-NH2	-5.67	114.09	119.20
1	A	228	THR	CA-C-O	-5.66	114.88	120.82
1	B	53	HIS	N-CA-C	-5.66	100.48	109.76
1	A	73	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	200	ALA	CA-C-N	5.65	128.17	120.54
1	B	200	ALA	C-N-CA	5.65	128.17	120.54
1	B	386	ALA	N-CA-CB	5.65	118.20	110.01
1	A	164	ALA	CA-C-N	5.64	128.31	120.29
1	A	164	ALA	C-N-CA	5.64	128.31	120.29
1	B	143	GLU	N-CA-C	-5.64	106.52	113.41
1	B	343	LEU	CA-C-N	5.64	130.83	120.79
1	B	343	LEU	C-N-CA	5.64	130.83	120.79
1	A	53	HIS	CA-CB-CG	5.64	119.44	113.80
1	A	19	TRP	O-C-N	-5.62	115.54	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	VAL	CB-CA-C	5.62	119.97	112.22
1	A	125	ALA	CA-C-N	5.61	127.74	120.44
1	A	125	ALA	C-N-CA	5.61	127.74	120.44
1	A	389	HIS	CA-CB-CG	-5.61	108.19	113.80
1	B	3	GLN	N-CA-CB	5.60	120.34	110.37
1	B	283	PRO	CB-CA-C	5.60	118.28	110.95
1	B	174	ASN	CB-CA-C	5.59	120.35	112.07
1	A	344	GLY	CA-C-O	-5.59	112.90	119.50
1	B	5	THR	CA-CB-CG2	5.58	119.99	110.50
1	A	203	GLU	CA-C-N	5.57	131.13	122.49
1	A	203	GLU	C-N-CA	5.57	131.13	122.49
1	A	133	PHE	O-C-N	-5.57	115.77	123.12
1	B	84	LYS	N-CA-C	-5.57	102.51	110.59
1	A	216	GLU	CA-C-N	5.57	128.53	120.79
1	A	216	GLU	C-N-CA	5.57	128.53	120.79
1	A	239	LYS	CA-CB-CG	5.56	125.22	114.10
1	B	127	GLU	O-C-N	-5.56	116.23	122.12
1	B	309	LYS	CA-C-N	5.56	127.73	120.28
1	B	309	LYS	C-N-CA	5.56	127.73	120.28
1	B	384	GLN	CB-CG-CD	5.56	122.05	112.60
1	B	323	LEU	N-CA-C	-5.56	105.30	111.36
1	A	241	PHE	CA-CB-CG	5.55	119.35	113.80
1	A	308	ALA	CA-C-N	5.55	127.99	120.44
1	A	308	ALA	C-N-CA	5.55	127.99	120.44
1	B	21	GLY	N-CA-C	5.54	123.08	115.27
1	B	184	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	B	367	PHE	CA-C-N	-5.53	113.49	122.34
1	B	367	PHE	C-N-CA	-5.53	113.49	122.34
1	B	150	LEU	CA-C-O	-5.53	114.69	120.55
1	A	213	LEU	CA-C-N	5.53	128.60	122.74
1	A	213	LEU	C-N-CA	5.53	128.60	122.74
1	A	377	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	342	GLU	OE1-CD-OE2	5.52	136.15	122.90
1	A	11	THR	CB-CA-C	5.51	120.19	109.33
1	B	394	ARG	CG-CD-NE	-5.51	99.88	112.00
1	A	389	HIS	CA-C-N	5.50	127.66	120.28
1	A	389	HIS	C-N-CA	5.50	127.66	120.28
1	B	206	GLU	N-CA-C	-5.50	104.80	112.45
1	A	364	PHE	CA-C-N	5.50	129.06	120.82
1	A	364	PHE	C-N-CA	5.50	129.06	120.82
1	A	235	LEU	CA-C-N	5.49	127.64	120.28
1	A	235	LEU	C-N-CA	5.49	127.64	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	SER	O-C-N	-5.49	116.06	122.81
1	B	202	ILE	CA-C-O	-5.49	115.24	120.95
1	A	229	HIS	CA-C-N	5.49	126.03	119.94
1	A	229	HIS	C-N-CA	5.49	126.03	119.94
1	B	268	PHE	O-C-N	-5.48	116.39	122.09
1	A	68	GLU	CB-CG-CD	-5.48	103.29	112.60
1	B	332	GLN	CG-CD-NE2	5.47	124.61	116.40
1	A	76	GLN	N-CA-CB	5.47	117.90	109.91
1	A	208	GLY	CA-C-O	5.47	125.95	119.50
1	B	323	LEU	N-CA-CB	5.46	118.25	110.16
1	B	362	ALA	CA-C-O	-5.46	112.66	119.38
1	A	84	LYS	CB-CG-CD	5.46	123.86	111.30
1	A	294	LYS	CB-CA-C	-5.46	101.83	110.02
1	B	295	PRO	CA-C-O	-5.46	114.81	121.03
1	A	144	TYR	CA-C-O	5.45	126.58	120.70
1	A	360	ASP	CA-CB-CG	5.45	118.05	112.60
1	A	320	GLU	CA-C-N	5.44	127.52	120.44
1	A	320	GLU	C-N-CA	5.44	127.52	120.44
1	B	209	ASP	CA-C-O	-5.44	113.95	120.10
1	A	187	ARG	NE-CZ-NH2	-5.44	114.31	119.20
1	B	350	ALA	N-CA-CB	5.43	117.89	109.48
1	B	77	ALA	CA-C-N	5.42	127.49	120.44
1	B	77	ALA	C-N-CA	5.42	127.49	120.44
1	B	207	HIS	CA-CB-CG	-5.42	108.38	113.80
1	B	216	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	101	GLY	O-C-N	5.40	129.64	123.21
1	B	174	ASN	N-CA-CB	-5.40	104.30	110.35
1	A	290	HIS	CA-CB-CG	5.40	119.20	113.80
1	A	320	GLU	CB-CA-C	5.40	119.36	110.88
1	A	113	PHE	CA-C-O	5.40	126.49	120.82
1	B	118	VAL	O-C-N	5.39	127.19	121.91
1	B	30	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	B	155	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	275	GLU	CA-C-O	-5.38	115.15	120.80
1	A	81	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	56	ASP	N-CA-C	-5.37	105.51	111.36
1	B	102	GLY	N-CA-C	-5.36	100.47	113.18
1	A	20	THR	CB-CA-C	5.36	120.62	109.95
1	B	74	PHE	O-C-N	5.35	127.86	122.09
1	A	343	LEU	CA-C-N	5.34	130.30	120.79
1	A	343	LEU	C-N-CA	5.34	130.30	120.79
1	B	153	ALA	CA-C-N	5.34	127.88	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	153	ALA	C-N-CA	5.34	127.88	120.29
1	A	22	ALA	CB-CA-C	5.34	118.78	109.65
1	B	223	ALA	CA-C-O	5.34	125.60	119.35
1	B	23	ASP	CA-C-O	5.34	127.47	120.16
1	A	96	PRO	CA-C-N	5.33	128.04	120.53
1	A	96	PRO	C-N-CA	5.33	128.04	120.53
1	B	16	THR	CA-CB-OG1	-5.32	101.62	109.60
1	B	30	ARG	NE-CZ-NH1	5.32	126.82	121.50
1	B	174	ASN	O-C-N	-5.32	115.87	122.83
1	B	140	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	237	ALA	CA-C-N	5.31	129.72	122.34
1	A	237	ALA	C-N-CA	5.31	129.72	122.34
1	B	3	GLN	CA-C-O	5.30	127.42	120.16
1	B	18	GLY	CA-C-N	5.29	129.91	121.66
1	B	18	GLY	C-N-CA	5.29	129.91	121.66
1	B	34	ASP	CA-C-N	5.29	124.79	119.19
1	B	34	ASP	C-N-CA	5.29	124.79	119.19
1	B	37	GLU	O-C-N	-5.27	116.54	122.12
1	A	316	LEU	CB-CA-C	5.27	119.53	110.79
1	A	249	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	B	278	PHE	N-CA-C	5.26	117.58	110.31
1	B	82	GLY	CA-C-O	-5.26	113.17	119.06
1	B	393	SER	CA-C-O	-5.26	113.45	119.60
1	B	111	ARG	CA-C-N	5.26	127.76	120.29
1	B	111	ARG	C-N-CA	5.26	127.76	120.29
1	B	75	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	235	LEU	CA-C-N	5.25	127.57	120.38
1	B	235	LEU	C-N-CA	5.25	127.57	120.38
1	A	105	SER	N-CA-C	-5.25	103.21	110.35
1	A	209	ASP	CA-C-O	-5.25	114.17	120.10
1	A	110	ILE	O-C-N	-5.24	116.79	121.87
1	A	196	GLY	O-C-N	-5.23	116.95	122.13
1	B	19	TRP	N-CA-CB	5.23	118.18	109.60
1	B	203	GLU	O-C-N	-5.22	114.06	122.41
1	B	393	SER	CB-CA-C	5.22	120.16	109.67
1	B	73	ASP	CB-CA-C	-5.21	102.13	110.79
1	B	90	THR	CA-C-O	-5.21	115.18	120.71
1	B	6	PRO	CA-C-O	-5.21	111.11	120.60
1	A	270	THR	N-CA-C	-5.21	105.51	111.14
1	B	187	ARG	CD-NE-CZ	-5.20	117.12	124.40
1	A	336	LYS	CA-C-N	5.20	127.50	120.38
1	A	336	LYS	C-N-CA	5.20	127.50	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	PRO	CA-C-N	5.20	127.20	120.44
1	A	59	PRO	C-N-CA	5.20	127.20	120.44
1	B	32	ASN	CA-C-O	-5.20	115.43	121.15
1	B	37	GLU	CA-C-O	5.19	126.05	120.55
1	B	243	ILE	O-C-N	5.19	128.71	123.00
1	B	43	ALA	CA-C-O	-5.18	115.05	120.55
1	A	44	GLU	CA-C-O	-5.17	114.25	120.10
1	A	294	LYS	CA-C-O	5.17	124.83	119.86
1	B	148	LYS	N-CA-C	5.17	117.24	109.23
1	B	242	HIS	N-CA-C	-5.17	101.41	108.38
1	B	5	THR	CB-CA-C	-5.16	101.45	109.55
1	A	201	PHE	CA-C-N	5.16	127.26	120.60
1	A	201	PHE	C-N-CA	5.16	127.26	120.60
1	B	304	VAL	CA-C-O	-5.16	115.77	121.29
1	A	174	ASN	CA-C-N	5.16	131.24	122.37
1	A	174	ASN	C-N-CA	5.16	131.24	122.37
1	B	68	GLU	CB-CG-CD	5.15	121.36	112.60
1	A	175	LEU	CA-C-N	5.15	130.66	122.94
1	A	175	LEU	C-N-CA	5.15	130.66	122.94
1	B	73	ASP	O-C-N	5.14	127.57	122.12
1	B	100	ASP	CA-C-O	5.13	125.54	119.48
1	A	47	ALA	CA-C-O	5.13	126.99	121.55
1	B	81	THR	CA-C-O	-5.13	113.62	119.41
1	A	25	PHE	CA-CB-CG	-5.12	108.68	113.80
1	A	364	PHE	CA-CB-CG	-5.12	108.68	113.80
1	B	117	LYS	CA-C-N	5.12	127.02	120.56
1	B	117	LYS	C-N-CA	5.12	127.02	120.56
1	A	13	GLY	N-CA-C	-5.12	104.88	113.02
1	A	342	GLU	CG-CD-OE2	-5.12	106.62	118.40
1	B	380	ILE	N-CA-CB	5.12	117.12	110.57
1	A	16	THR	OG1-CB-CG2	5.12	119.54	109.30
1	A	79	LYS	N-CA-CB	5.12	117.43	110.01
1	A	227	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	40	HIS	N-CA-C	-5.10	105.63	111.14
1	A	102	GLY	N-CA-C	-5.10	101.09	113.18
1	B	360	ASP	CA-C-O	5.10	126.36	120.60
1	A	274	LEU	CA-C-N	5.10	129.14	120.88
1	A	274	LEU	C-N-CA	5.10	129.14	120.88
1	B	243	ILE	CA-C-O	-5.09	115.94	121.19
1	B	318	LEU	CA-C-N	5.09	127.06	120.44
1	B	318	LEU	C-N-CA	5.09	127.06	120.44
1	A	233	GLN	CB-CG-CD	5.09	121.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLU	N-CA-C	-5.08	105.63	111.07
1	A	230	GLY	O-C-N	-5.08	117.31	122.18
1	A	254	ASP	CB-CA-C	5.07	118.38	110.67
1	B	227	PHE	CA-C-O	-5.07	115.50	120.82
1	A	163	THR	N-CA-CB	5.06	117.56	110.12
1	A	188	GLY	CA-C-O	-5.06	115.54	120.75
1	A	223	ALA	CA-C-N	5.06	129.93	120.87
1	A	223	ALA	C-N-CA	5.06	129.93	120.87
1	A	35	PRO	CA-C-N	5.06	126.93	120.56
1	A	35	PRO	C-N-CA	5.06	126.93	120.56
1	A	67	ARG	CG-CD-NE	-5.06	100.87	112.00
1	A	112	ARG	CG-CD-NE	5.06	123.13	112.00
1	A	112	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	A	99	LYS	CA-C-O	-5.05	113.37	119.49
1	A	268	PHE	CA-C-N	5.05	127.99	120.31
1	A	268	PHE	C-N-CA	5.05	127.99	120.31
1	B	156	ARG	N-CA-CB	5.05	117.64	110.16
1	A	176	ARG	CA-C-N	5.05	128.89	122.37
1	A	176	ARG	C-N-CA	5.05	128.89	122.37
1	A	321	ARG	CA-CB-CG	-5.05	104.00	114.10
1	A	295	PRO	CA-C-O	-5.04	115.98	121.27
1	B	71	LEU	CA-C-N	5.03	125.52	119.94
1	B	71	LEU	C-N-CA	5.03	125.52	119.94
1	A	203	GLU	CG-CD-OE2	5.03	129.97	118.40
1	B	188	GLY	O-C-N	-5.02	117.37	122.19
1	A	305	TRP	CB-CA-C	5.02	120.61	110.38
1	B	116	ALA	CA-C-N	5.02	127.00	120.28
1	B	116	ALA	C-N-CA	5.02	127.00	120.28
1	A	243	ILE	O-C-N	5.01	128.51	123.00
1	A	41	LYS	CA-C-N	5.01	126.95	120.44
1	A	41	LYS	C-N-CA	5.01	126.95	120.44
1	B	244	ASP	CB-CG-OD1	5.00	129.91	118.40

There are no chirality outliers.

There are no planarity outliers.

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	0
1	B	3027	0	2881	23	1
2	A	13	0	10	0	0
2	B	13	0	11	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	253	0	0	6	0
4	B	262	0	0	3	1
All	All	6599	0	5784	56	1

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 5.

All (56) 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:275:GLU:HG3	1:B:319:LYS:HG3	1.63	0.80
1:A:95:HIS:HD2	1:A:97:VAL:H	1.37	0.71
1:A:84:LYS:HB2	4:A:675(A):HOH:O	1.94	0.68
1:B:95:HIS:HD2	1:B:97:VAL:H	1.41	0.67
1:B:20:THR:HG23	1:B:28:ALA:HB1	1.79	0.65
1:A:84:LYS:HD2	4:A:548(A):HOH:O	2.03	0.59
1:B:11:THR:HG21	1:B:86:PRO:HG2	1.85	0.58
1:A:221:GLN:HE21	1:A:248:GLN:HB3	1.68	0.57
1:A:20:THR:HG23	1:A:28:ALA:HB1	1.87	0.56
1:A:84:LYS:HG3	1:A:86:PRO:HG3	1.86	0.56
1:B:20:THR:HG23	1:B:28:ALA:CB	2.35	0.56
1:B:39:VAL:HG13	1:B:83:LEU:HD12	1.87	0.54
1:A:27:VAL:HG21	4:A:960(B):HOH:O	2.07	0.54
1:B:238:GLU:HG3	4:B:1012(B):HOH:O	2.08	0.54
1:A:95:HIS:CD2	1:A:97:VAL:H	2.23	0.53
1:A:20:THR:HG23	1:A:28:ALA:CB	2.39	0.52
1:A:275:GLU:HG3	1:A:319:LYS:HG3	1.90	0.52
1:A:148:LYS:HG3	1:A:191:PHE:HZ	1.75	0.52
1:A:8:ASP:O	1:A:9:HIS:HB2	2.10	0.51
1:B:45:LEU:HD22	1:B:309:LYS:HE3	1.93	0.50
1:B:55:ASN:HA	1:B:58:ILE:O	2.13	0.49
1:B:195:VAL:HG23	1:B:220:GLU:CD	2.37	0.48
1:B:249:ARG:O	1:B:252:LYS:HE3	2.15	0.47
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.80	0.47
1:A:43:ALA:HB2	1:A:83:LEU:HD13	1.98	0.46
1:B:45:LEU:HB3	1:B:309:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:HIS:O	1:A:123:ASP:HB2	2.15	0.46
1:B:35:PRO:O	1:B:39:VAL:HG23	2.16	0.46
1:A:331:VAL:O	1:A:335:MET:HG3	2.16	0.46
1:A:69:LYS:HE2	1:A:73:ASP:OD2	2.16	0.46
1:B:63:THR:HG23	1:B:66:GLU:OE2	2.17	0.45
1:B:131:GLU:HG3	4:B:1014(B):HOH:O	2.16	0.45
1:B:79:LYS:O	1:B:80:ASP:C	2.59	0.45
1:A:55:ASN:HA	1:A:58:ILE:O	2.17	0.45
1:B:60:PHE:HE1	1:B:117:LYS:HE3	1.82	0.45
1:A:180:GLU:HG3	1:A:214:ASN:O	2.18	0.44
1:A:53:HIS:O	1:A:54:ASP:C	2.61	0.44
1:A:20:THR:HB	4:A:695(A):HOH:O	2.17	0.44
1:A:180:GLU:HA	1:A:181:PRO:HD3	1.74	0.44
1:A:181:PRO:HA	4:A:1006(A):HOH:O	2.17	0.44
1:A:11:THR:HG21	1:A:86:PRO:HG2	2.01	0.43
1:B:69:LYS:HE2	4:B:919(B):HOH:O	2.17	0.43
1:A:51:THR:HG21	1:A:87:MET:HE3	2.01	0.42
1:B:41:LYS:HG2	1:B:305:TRP:CE2	2.54	0.42
1:A:87:MET:HA	1:A:132:THR:O	2.19	0.42
1:A:242:HIS:CD2	1:A:288:PRO:HG2	2.54	0.42
1:A:50:ILE:HG12	1:A:51:THR:N	2.35	0.42
1:B:267:ALA:O	1:B:271:VAL:HG23	2.20	0.42
1:B:256:ASP:HB3	1:B:293:TYR:HA	2.02	0.42
1:A:192:LEU:N	1:A:193:PRO:HD3	2.35	0.41
1:A:202:ILE:O	1:A:205:LEU:HB2	2.21	0.41
1:A:301:TYR:HD2	4:A:534(A):HOH:O	2.03	0.41
1:A:16:THR:OG1	1:A:17:VAL:N	2.54	0.41
1:B:2:VAL:HG23	1:B:3:GLN:H	1.84	0.41
1:A:295:PRO:O	1:A:296:SER:C	2.63	0.40
1:B:235:LEU:HD12	1:B:273:LEU:HD11	2.03	0.40

All (1) 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:343:LEU:CD2	4:B:1017(B):HOH:O[4_555]	2.06	0.14

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%)	374 (96%)	16 (4%)	1 (0%)	36	55
1	B	391/394 (99%)	371 (95%)	18 (5%)	2 (0%)	24	43
All	All	782/788 (99%)	745 (95%)	34 (4%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

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

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%)	290 (95%)	15 (5%)	22	45
1	B	305/310 (98%)	289 (95%)	16 (5%)	21	42
All	All	610/620 (98%)	579 (95%)	31 (5%)	21	43

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	20	THR
1	A	41	LYS

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Mol	Chain	Res	Type
1	A	44	GLU
1	A	69	LYS
1	A	90	THR
1	A	112	ARG
1	A	150	LEU
1	A	174	ASN
1	A	184	ASN
1	A	213	LEU
1	A	284	LYS
1	A	320	GLU
1	A	359	ASN
1	A	370	GLU
1	B	6	PRO
1	B	20	THR
1	B	41	LYS
1	B	61	ASP
1	B	90	THR
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	320	GLU
1	B	333	GLU
1	B	357	LEU
1	B	370	GLU
1	B	387	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	95	HIS
1	A	184	ASN
1	A	221	GLN
1	A	359	ASN
1	A	384	GLN
1	B	32	ASN
1	B	40	HIS
1	B	75	ASN
1	B	76	GLN

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Mol	Chain	Res	Type
1	B	95	HIS
1	B	120	HIS
1	B	184	ASN
1	B	221	GLN
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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GCO	A	400	3	12,12,12	0.77	0	15,16,16	0.91	0
2	GCO	B	400	3	12,12,12	1.55	2 (16%)	15,16,16	3.28	8 (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
2	GCO	A	400	3	-	7/18/18/18	-
2	GCO	B	400	3	-	5/18/18/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	GCO	C5-C4	-3.25	1.47	1.53
2	B	400	GCO	O4-C4	2.03	1.48	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	GCO	O5-C5-C6	-7.33	92.36	109.03
2	B	400	GCO	O3-C3-C4	5.15	121.48	109.46
2	B	400	GCO	O1B-C1-C2	3.82	123.92	113.31
2	B	400	GCO	C4-C3-C2	-3.55	107.33	113.62
2	B	400	GCO	C6-C5-C4	3.43	119.17	112.17
2	B	400	GCO	O6-C6-C5	-3.40	104.02	111.16
2	B	400	GCO	O1A-C1-C2	-2.74	114.31	121.62
2	B	400	GCO	O5-C5-C4	2.62	115.38	109.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	GCO	C3-C4-C5-C6
2	A	400	GCO	O4-C4-C5-O5
2	A	400	GCO	C3-C4-C5-O5
2	B	400	GCO	C3-C4-C5-C6
2	A	400	GCO	O4-C4-C5-C6
2	B	400	GCO	C2-C3-C4-C5
2	B	400	GCO	C2-C3-C4-O4
2	B	400	GCO	O3-C3-C4-O4
2	B	400	GCO	O3-C3-C4-C5
2	A	400	GCO	O3-C3-C4-O4
2	A	400	GCO	O3-C3-C4-C5
2	A	400	GCO	C2-C3-C4-O4

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.