



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 PM UTC

PDB ID : 1XIN / pdb_00001xin
Title : PROTEIN ENGINEERING OF XYLOSE (GLUCOSE) ISOMERASE FROM ACTINOPLANES MISSOURIENSIS. 1. CRYSTALLOGRAPHY AND SITE-DIRECTED MUTAGENESIS OF METAL BINDING SITES
Authors : Janin, J.
Deposited on : 1992-04-06
Resolution : 2.40 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

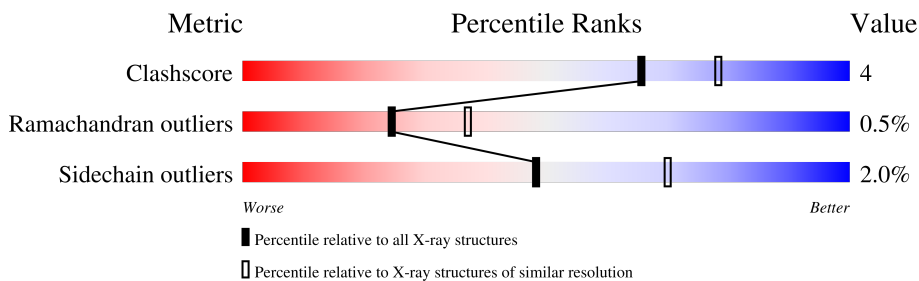
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	393	 71% 25% •
1	B	393	 74% 22% •
1	C	393	 74% 23% •
1	D	393	 70% 26% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13137 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.

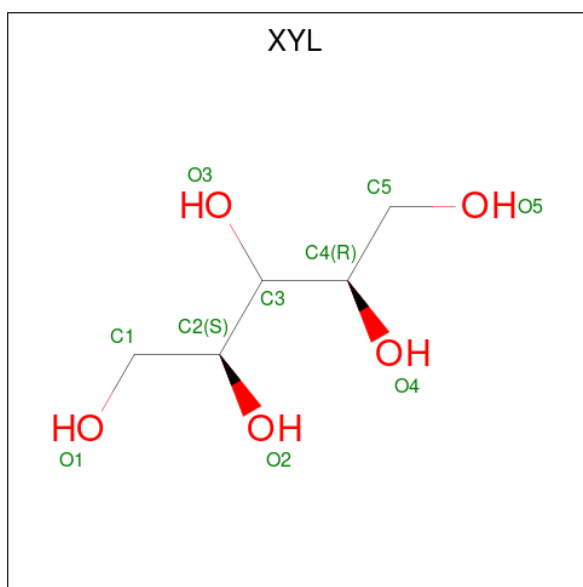
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	B	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	C	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			
1	D	392	Total	C	N	O	S	0	0	0
			3051	1937	531	579	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	ASN	HIS	conflict	UNP P12851
B	220	ASN	HIS	conflict	UNP P12851
C	220	ASN	HIS	conflict	UNP P12851
D	220	ASN	HIS	conflict	UNP P12851

- Molecule 2 is Xylitol (CCD ID: XYL) (formula: C₅H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	220	Total	O	0	0
			220	220		

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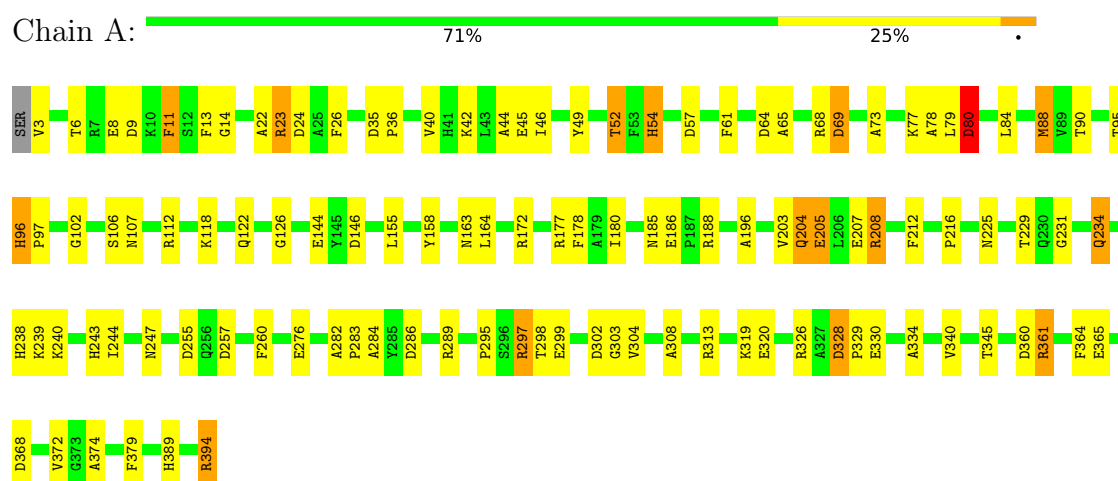
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	217	Total 217	O 217	0	0
4	C	232	Total 232	O 232	0	0
4	D	220	Total 220	O 220	0	0

3 Residue-property plots

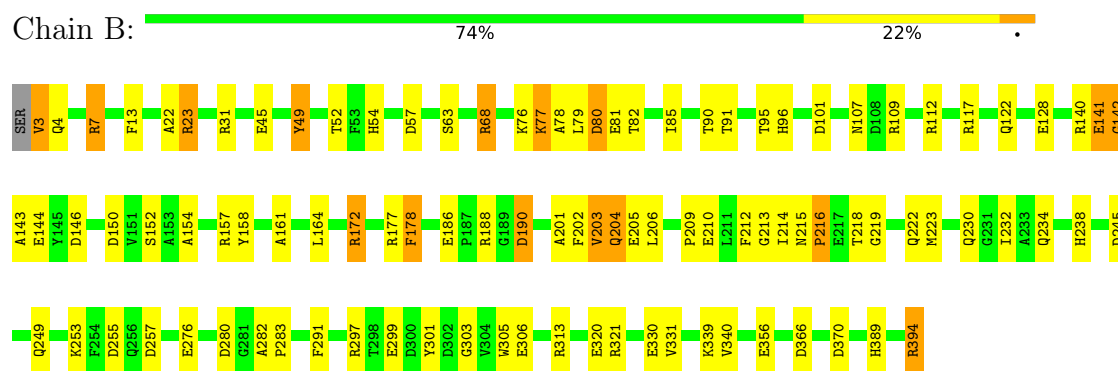
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

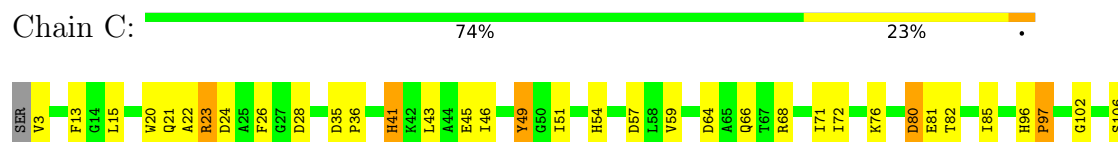
• Molecule 1: D-XYLOSE ISOMERASE

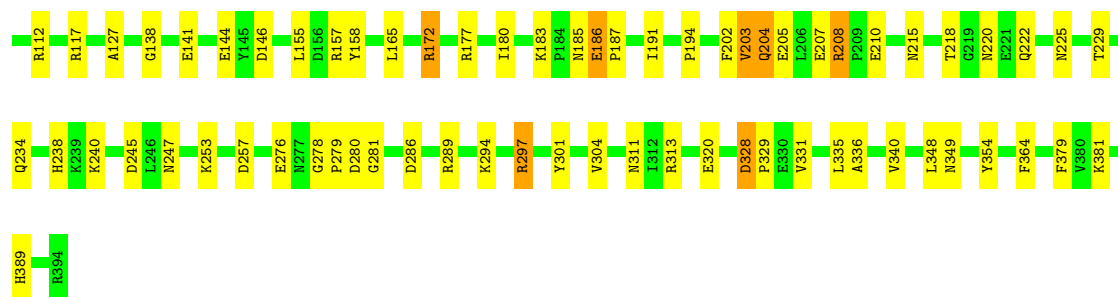


• Molecule 1: D-XYLOSE ISOMERASE



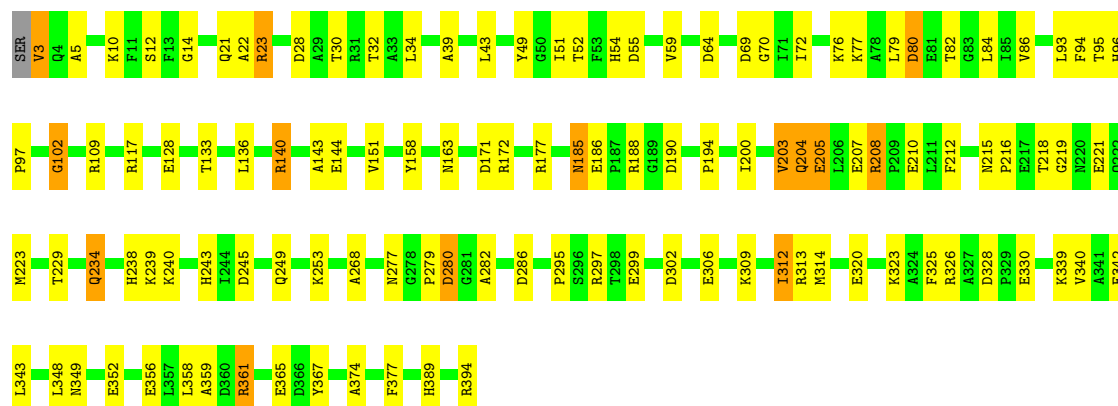
• Molecule 1: D-XYLOSE ISOMERASE





• Molecule 1: D-XYLOSE ISOMERASE

Chain D: 70% 26% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13137	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: MG, XYZ

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	0.99	0/3122	2.06	113/4229 (2.7%)
1	B	0.98	0/3122	2.02	96/4229 (2.3%)
1	C	0.99	0/3122	2.03	103/4229 (2.4%)
1	D	1.01	0/3122	2.11	117/4229 (2.8%)
All	All	1.00	0/12488	2.06	429/16916 (2.5%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	CA-CB-CG	-18.38	94.22	112.60
1	D	204	GLN	OE1-CD-NE2	-15.73	106.87	122.60
1	B	204	GLN	OE1-CD-NE2	-14.16	108.44	122.60
1	A	204	GLN	OE1-CD-NE2	-10.65	111.94	122.60
1	D	172	ARG	CD-NE-CZ	10.39	138.95	124.40
1	C	204	GLN	OE1-CD-NE2	-10.06	112.54	122.60
1	A	286	ASP	CA-CB-CG	-9.79	102.81	112.60
1	D	80	ASP	CA-CB-CG	-9.26	103.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	ASP	CA-CB-CG	-9.18	103.42	112.60
1	B	117	ARG	NE-CZ-NH1	8.92	130.42	121.50
1	B	394	ARG	NE-CZ-NH2	-8.49	111.56	119.20
1	D	328	ASP	CA-CB-CG	8.41	121.01	112.60
1	A	244	ILE	CA-C-O	-8.36	111.95	120.90
1	A	172	ARG	CD-NE-CZ	8.36	136.10	124.40
1	A	320	GLU	CB-CG-CD	8.26	126.63	112.60
1	A	188	ARG	CD-NE-CZ	8.23	135.93	124.40
1	B	245	ASP	CA-CB-CG	8.19	120.79	112.60
1	D	54	HIS	N-CA-C	-8.17	97.32	110.32
1	A	26	PHE	CA-C-O	-8.07	109.95	119.48
1	A	107	ASN	CA-CB-CG	8.06	120.66	112.60
1	C	64	ASP	CA-CB-CG	-8.05	104.55	112.60
1	C	185	ASN	OD1-CG-ND2	-8.03	114.57	122.60
1	C	229	THR	CA-CB-OG1	-8.03	97.55	109.60
1	B	142	GLY	CA-C-O	-7.98	115.41	120.91
1	B	95	THR	N-CA-C	7.90	119.80	111.03
1	B	172	ARG	NE-CZ-NH1	7.89	129.39	121.50
1	C	54	HIS	N-CA-C	-7.66	99.18	110.52
1	D	95	THR	N-CA-C	7.65	119.41	111.14
1	C	24	ASP	CA-CB-CG	7.57	120.17	112.60
1	B	13	PHE	CA-CB-CG	7.53	121.33	113.80
1	C	28	ASP	CA-CB-CG	7.50	120.10	112.60
1	D	286	ASP	CA-C-O	-7.49	110.65	119.48
1	D	313	ARG	NE-CZ-NH2	7.47	125.92	119.20
1	B	394	ARG	N-CA-CB	7.43	123.12	110.50
1	B	150	ASP	CA-CB-CG	-7.41	105.19	112.60
1	D	171	ASP	CA-C-O	-7.37	112.60	120.42
1	D	188	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	D	349	ASN	CA-CB-CG	-7.23	105.37	112.60
1	C	57	ASP	CA-CB-CG	7.21	119.81	112.60
1	A	95	THR	N-CA-C	7.21	118.93	111.14
1	B	117	ARG	NE-CZ-NH2	-7.17	112.74	119.20
1	D	377	PHE	CA-C-O	-7.16	110.98	119.15
1	A	319	LYS	CA-C-O	7.14	128.54	120.90
1	A	79	LEU	CA-C-O	7.10	128.07	120.55
1	B	141	GLU	CB-CG-CD	7.09	124.65	112.60
1	A	394	ARG	NH1-CZ-NH2	7.09	128.51	119.30
1	C	146	ASP	CA-C-O	-7.07	113.06	120.55
1	C	15	LEU	CA-C-O	7.05	128.03	120.55
1	B	82	THR	CA-C-O	-7.00	111.08	119.27
1	C	222	GLN	OE1-CD-NE2	-6.97	115.63	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	HIS	N-CA-CB	6.96	121.76	110.41
1	D	342	GLU	CB-CG-CD	6.94	124.40	112.60
1	D	144	GLU	N-CA-C	-6.93	105.09	113.97
1	D	10	LYS	CB-CA-C	-6.91	102.07	111.89
1	B	161	ALA	CA-C-O	-6.91	113.09	120.42
1	D	204	GLN	CB-CG-CD	6.89	124.31	112.60
1	A	379	PHE	CA-CB-CG	6.88	120.68	113.80
1	C	354	TYR	CA-C-O	-6.86	113.28	120.55
1	D	389	HIS	CA-CB-CG	-6.86	106.94	113.80
1	C	304	VAL	CA-C-O	-6.83	113.93	121.17
1	A	13	PHE	CA-C-O	-6.79	113.19	121.06
1	D	286	ASP	CA-CB-CG	-6.79	105.81	112.60
1	B	80	ASP	CA-CB-CG	-6.78	105.82	112.60
1	D	52	THR	CA-C-O	-6.76	113.74	121.58
1	A	26	PHE	O-C-N	6.75	130.36	122.19
1	C	278	GLY	CA-C-N	6.71	128.23	119.84
1	C	278	GLY	C-N-CA	6.71	128.23	119.84
1	B	257	ASP	CA-C-O	-6.69	113.82	121.65
1	C	191	ILE	CA-CB-CG2	6.68	121.85	110.50
1	B	85	ILE	CA-C-O	-6.67	115.31	121.72
1	C	297	ARG	NE-CZ-NH2	6.67	125.21	119.20
1	D	28	ASP	CA-CB-CG	6.66	119.26	112.60
1	C	340	VAL	CB-CA-C	6.65	120.39	111.88
1	B	157	ARG	NE-CZ-NH1	6.65	128.15	121.50
1	B	172	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	C	389	HIS	CA-CB-CG	-6.64	107.16	113.80
1	D	55	ASP	O-C-N	6.63	128.99	122.09
1	D	239	LYS	CB-CA-C	-6.63	103.33	111.82
1	C	208	ARG	CD-NE-CZ	-6.62	115.14	124.40
1	C	71	ILE	O-C-N	6.62	128.39	121.91
1	D	151	VAL	CA-C-O	6.62	127.83	120.95
1	D	151	VAL	N-CA-C	6.61	117.36	110.62
1	B	68	ARG	NE-CZ-NH1	-6.60	114.90	121.50
1	D	95	THR	O-C-N	6.54	129.15	122.09
1	A	180	ILE	N-CA-CB	6.52	117.63	110.53
1	D	14	GLY	N-CA-C	-6.51	103.25	112.37
1	B	77	LYS	O-C-N	6.51	129.12	122.09
1	C	177	ARG	N-CA-CB	6.49	121.14	110.69
1	C	81	GLU	CB-CG-CD	6.47	123.61	112.60
1	C	247	ASN	OD1-CG-ND2	-6.47	116.12	122.60
1	A	118	LYS	CA-C-N	6.46	128.83	120.56
1	A	118	LYS	C-N-CA	6.46	128.83	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	ASP	CA-CB-CG	-6.46	106.14	112.60
1	C	194	PRO	N-CA-C	6.46	121.93	113.86
1	A	61	PHE	CA-C-O	-6.45	114.50	120.95
1	A	231	GLY	CA-C-N	6.44	129.57	120.42
1	A	231	GLY	C-N-CA	6.44	129.57	120.42
1	A	14	GLY	N-CA-C	-6.43	103.37	112.37
1	B	320	GLU	CB-CG-CD	6.43	123.53	112.60
1	D	79	LEU	CA-C-O	6.42	127.36	120.55
1	C	180	ILE	N-CA-CB	6.42	117.53	110.53
1	B	313	ARG	CA-C-N	6.42	128.79	120.44
1	B	313	ARG	C-N-CA	6.42	128.79	120.44
1	A	57	ASP	CA-CB-CG	6.42	119.02	112.60
1	C	185	ASN	O-C-N	6.41	129.70	123.29
1	D	93	LEU	CA-C-O	-6.41	113.78	121.34
1	D	313	ARG	N-CA-CB	6.41	119.30	110.01
1	B	45	GLU	CB-CG-CD	6.41	123.49	112.60
1	D	64	ASP	N-CA-C	-6.40	102.53	110.41
1	A	229	THR	CA-CB-OG1	-6.40	100.00	109.60
1	A	68	ARG	CD-NE-CZ	6.39	133.34	124.40
1	A	11	PHE	CA-C-O	-6.38	113.42	120.69
1	D	109	ARG	CD-NE-CZ	6.37	133.32	124.40
1	A	394	ARG	CA-CB-CG	6.37	126.83	114.10
1	B	389	HIS	CA-CB-CG	-6.36	107.44	113.80
1	C	313	ARG	CD-NE-CZ	6.36	133.30	124.40
1	D	253	LYS	CA-C-O	-6.36	114.32	121.25
1	C	165	LEU	O-C-N	6.36	128.86	122.12
1	A	244	ILE	O-C-N	6.33	130.44	123.09
1	A	243	HIS	CA-CB-CG	6.33	120.13	113.80
1	D	218	THR	CA-C-O	-6.32	114.11	121.07
1	D	326	ARG	NE-CZ-NH2	6.32	124.89	119.20
1	D	299	GLU	N-CA-C	6.30	120.19	110.42
1	C	331	VAL	N-CA-C	-6.28	104.63	110.53
1	A	204	GLN	CB-CG-CD	6.26	123.24	112.60
1	B	90	THR	CA-CB-OG1	-6.26	100.21	109.60
1	C	328	ASP	CA-CB-CG	6.25	118.85	112.60
1	D	302	ASP	CA-C-O	-6.24	114.27	120.70
1	B	91	THR	CA-C-O	-6.23	113.97	120.70
1	B	213	GLY	O-C-N	6.23	130.80	122.70
1	C	172	ARG	CD-NE-CZ	-6.22	115.69	124.40
1	A	295	PRO	N-CA-C	-6.22	101.40	110.80
1	D	143	ALA	N-CA-CB	-6.21	102.13	111.56
1	C	202	PHE	CA-C-N	6.20	128.96	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	PHE	C-N-CA	6.20	128.96	120.46
1	C	257	ASP	CA-C-O	-6.19	114.41	121.65
1	A	126	GLY	CA-C-N	6.18	128.56	120.28
1	A	126	GLY	C-N-CA	6.18	128.56	120.28
1	A	313	ARG	N-CA-CB	-6.18	101.05	110.01
1	C	13	PHE	CA-C-O	-6.18	113.89	121.06
1	D	243	HIS	CA-C-O	-6.18	114.83	121.38
1	B	54	HIS	N-CA-C	-6.16	100.52	110.32
1	B	178	PHE	O-C-N	6.15	130.62	123.30
1	B	140	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	D	207	GLU	CA-CB-CG	6.13	126.37	114.10
1	A	69	ASP	CA-CB-CG	-6.12	106.48	112.60
1	B	144	GLU	N-CA-C	-6.09	106.39	113.88
1	A	44	ALA	CA-C-O	6.09	127.00	120.55
1	D	21	GLN	CB-CG-CD	-6.09	102.25	112.60
1	C	281	GLY	N-CA-C	-6.08	98.77	113.18
1	D	136	LEU	CA-C-O	-6.08	114.02	120.40
1	A	257	ASP	CA-C-O	-6.07	114.54	121.65
1	A	180	ILE	CB-CA-C	-6.06	103.27	111.15
1	C	117	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	B	331	VAL	N-CA-C	-6.05	104.84	110.53
1	D	216	PRO	CA-C-O	-6.05	114.29	121.67
1	A	276	GLU	N-CA-C	6.04	120.84	112.45
1	C	304	VAL	O-C-N	6.03	127.82	121.91
1	C	379	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	52	THR	CA-C-O	-6.02	114.60	121.58
1	D	374	ALA	CA-C-O	-6.02	112.02	119.18
1	C	138	GLY	CA-C-N	6.00	127.64	120.14
1	C	138	GLY	C-N-CA	6.00	127.64	120.14
1	B	394	ARG	CD-NE-CZ	-5.99	116.01	124.40
1	B	96	HIS	CA-C-O	-5.98	113.95	120.17
1	C	207	GLU	CA-C-O	-5.98	114.54	120.70
1	A	80	ASP	OD1-CG-OD2	5.98	137.24	122.90
1	A	326	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	8	GLU	CA-CB-CG	-5.96	102.19	114.10
1	B	146	ASP	CA-C-O	-5.95	114.25	120.55
1	A	122	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	D	133	THR	CA-CB-OG1	-5.94	100.69	109.60
1	B	77	LYS	CB-CA-C	-5.94	101.51	110.90
1	B	57	ASP	N-CA-C	-5.94	104.39	111.69
1	A	334	ALA	CA-C-O	-5.93	114.13	120.42
1	C	311	ASN	O-C-N	5.92	128.17	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	ARG	CA-C-O	-5.91	113.17	119.97
1	D	239	LYS	O-C-N	5.90	129.33	122.67
1	C	172	ARG	NE-CZ-NH1	5.89	127.39	121.50
1	B	276	GLU	N-CA-C	5.89	120.59	113.41
1	B	31	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	D	245	ASP	CA-CB-CG	5.88	118.48	112.60
1	D	349	ASN	O-C-N	5.88	127.83	121.60
1	C	335	LEU	O-C-N	5.87	128.35	122.12
1	A	364	PHE	CA-C-N	5.87	128.46	120.54
1	A	364	PHE	C-N-CA	5.87	128.46	120.54
1	D	212	PHE	N-CA-C	5.87	118.96	109.40
1	B	57	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	107	ASN	N-CA-C	-5.86	104.89	111.28
1	D	55	ASP	CA-CB-CG	5.86	118.46	112.60
1	D	342	GLU	CG-CD-OE2	5.85	131.87	118.40
1	B	23	ARG	N-CA-C	-5.85	98.99	108.41
1	A	394	ARG	CD-NE-CZ	-5.84	116.22	124.40
1	C	45	GLU	CA-CB-CG	5.82	125.74	114.10
1	B	190	ASP	N-CA-CB	5.79	120.53	110.81
1	D	312	ILE	CA-C-O	-5.78	114.72	120.85
1	A	78	ALA	CA-C-O	-5.77	114.43	120.55
1	A	158	TYR	CA-C-N	5.76	127.93	120.44
1	A	158	TYR	C-N-CA	5.76	127.93	120.44
1	A	216	PRO	CA-C-O	-5.76	114.64	121.67
1	B	291	PHE	CA-C-O	-5.76	114.42	120.58
1	C	23	ARG	N-CA-C	-5.75	99.14	108.41
1	B	79	LEU	CA-C-O	5.75	126.65	120.55
1	B	313	ARG	CB-CA-C	5.75	120.33	110.79
1	A	205	GLU	CG-CD-OE2	5.75	131.62	118.40
1	A	389	HIS	CA-CB-CG	-5.75	108.05	113.80
1	D	314	MET	N-CA-CB	5.75	118.50	109.94
1	D	203	VAL	CA-CB-CG1	5.74	120.16	110.40
1	D	32	THR	CA-CB-OG1	-5.73	101.01	109.60
1	C	41	HIS	CA-CB-CG	-5.71	108.08	113.80
1	D	234	GLN	CA-C-O	-5.71	114.36	120.42
1	D	140	ARG	NH1-CZ-NH2	5.71	126.72	119.30
1	B	177	ARG	CA-C-O	-5.70	114.72	121.16
1	A	374	ALA	CA-C-O	-5.69	112.41	119.18
1	D	203	VAL	CB-CA-C	5.69	119.50	112.04
1	D	358	LEU	CA-C-O	5.69	126.53	120.10
1	C	276	GLU	CG-CD-OE2	5.69	131.48	118.40
1	C	141	GLU	CB-CG-CD	5.67	122.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	240	LYS	CA-C-O	-5.67	112.80	119.48
1	A	54	HIS	CA-C-O	-5.66	114.60	121.28
1	D	86	VAL	O-C-N	5.64	127.53	121.10
1	A	284	ALA	N-CA-C	-5.64	106.23	113.23
1	C	286	ASP	CA-CB-CG	-5.64	106.96	112.60
1	D	10	LYS	O-C-N	5.63	129.53	122.55
1	D	30	THR	O-C-N	5.63	128.84	122.20
1	D	325	PHE	CA-C-O	5.62	126.91	120.90
1	D	194	PRO	N-CA-C	5.61	120.92	113.57
1	C	15	LEU	O-C-N	-5.60	116.18	122.12
1	B	122	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	C	172	ARG	NE-CZ-NH2	-5.60	114.16	119.20
1	C	349	ASN	N-CA-C	-5.60	102.06	110.24
1	D	306	GLU	N-CA-C	-5.60	105.10	111.14
1	C	328	ASP	CB-CA-C	5.59	118.46	109.51
1	A	308	ALA	N-CA-C	-5.59	105.11	111.14
1	C	245	ASP	CA-CB-CG	5.58	118.19	112.60
1	B	63	SER	O-C-N	5.58	129.72	123.19
1	D	320	GLU	CA-CB-CG	5.57	125.24	114.10
1	A	57	ASP	CA-C-O	-5.57	114.06	120.24
1	D	210	GLU	CB-CG-CD	5.56	122.05	112.60
1	A	304	VAL	CA-C-O	-5.55	115.28	121.17
1	C	158	TYR	N-CA-C	-5.55	105.31	111.36
1	A	80	ASP	O-C-N	5.55	127.81	122.03
1	D	140	ARG	NE-CZ-NH2	-5.55	114.20	119.20
1	B	299	GLU	N-CA-C	5.54	119.10	110.17
1	A	57	ASP	N-CA-CB	5.54	118.46	110.20
1	B	202	PHE	CA-C-N	5.54	129.23	120.47
1	B	202	PHE	C-N-CA	5.54	129.23	120.47
1	B	356	GLU	CA-C-O	-5.54	114.54	120.42
1	A	158	TYR	CA-C-O	5.54	126.41	120.70
1	A	172	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	B	158	TYR	N-CA-C	-5.53	105.17	111.14
1	B	305	TRP	CA-CB-CG	-5.53	103.10	113.60
1	B	215	ASN	CA-CB-CG	-5.52	107.08	112.60
1	B	216	PRO	CA-C-O	-5.52	114.93	121.67
1	A	207	GLU	CA-CB-CG	5.52	125.14	114.10
1	C	21	GLN	CA-C-N	5.52	130.41	122.35
1	C	21	GLN	C-N-CA	5.52	130.41	122.35
1	D	171	ASP	O-C-N	5.52	128.44	122.15
1	D	117	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	A	255	ASP	CB-CA-C	5.51	119.05	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	ASP	CA-C-N	5.51	125.95	119.94
1	D	69	ASP	C-N-CA	5.51	125.95	119.94
1	B	201	ALA	CA-C-N	5.49	127.58	120.44
1	B	201	ALA	C-N-CA	5.49	127.58	120.44
1	A	394	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	A	96	HIS	CA-CB-CG	-5.48	108.32	113.80
1	C	240	LYS	CA-C-O	-5.47	113.03	119.48
1	C	127	ALA	CA-C-N	5.47	127.60	120.28
1	C	127	ALA	C-N-CA	5.47	127.60	120.28
1	D	177	ARG	N-CA-C	-5.46	100.50	109.40
1	B	107	ASN	N-CA-CB	5.45	118.13	110.12
1	D	367	TYR	CA-C-O	-5.45	114.48	120.69
1	D	277	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	B	54	HIS	N-CA-CB	5.43	119.26	110.41
1	A	177	ARG	N-CA-C	-5.43	100.55	109.40
1	B	370	ASP	CA-C-O	-5.43	114.80	120.55
1	D	328	ASP	CB-CA-C	5.42	117.19	109.38
1	C	320	GLU	CB-CG-CD	5.42	121.81	112.60
1	C	26	PHE	CA-C-O	-5.42	113.50	119.78
1	A	102	GLY	O-C-N	5.41	128.89	123.48
1	C	210	GLU	CB-CG-CD	5.41	121.79	112.60
1	D	215	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	73	ALA	CA-C-N	5.40	125.94	120.00
1	A	73	ALA	C-N-CA	5.40	125.94	120.00
1	A	188	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	96	HIS	CA-CB-CG	-5.39	108.41	113.80
1	B	204	GLN	CG-CD-OE1	5.39	131.59	120.80
1	B	218	THR	CA-CB-OG1	-5.38	101.52	109.60
1	C	215	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	45	GLU	CA-C-O	-5.36	114.86	120.55
1	B	202	PHE	O-C-N	-5.36	116.55	122.07
1	D	200	ILE	N-CA-CB	5.36	116.82	110.55
1	B	253	LYS	CA-C-O	-5.35	115.38	120.94
1	C	207	GLU	CG-CD-OE1	5.35	130.71	118.40
1	A	340	VAL	O-C-N	5.35	127.06	121.87
1	B	366	ASP	CA-C-O	-5.35	113.64	119.95
1	A	340	VAL	CA-C-O	-5.34	115.39	120.95
1	D	205	GLU	CG-CD-OE2	5.34	130.69	118.40
1	C	301	TYR	CA-C-O	-5.34	114.06	120.10
1	D	185	ASN	CA-C-O	-5.34	115.57	121.28
1	A	155	LEU	CB-CA-C	5.33	119.64	110.79
1	B	109	ARG	N-CA-C	5.33	117.09	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	VAL	CB-CA-C	5.33	118.70	111.88
1	D	133	THR	O-C-N	5.33	129.77	123.27
1	C	66	GLN	N-CA-CB	5.32	117.72	110.01
1	C	82	THR	CA-CB-OG1	-5.32	101.62	109.60
1	D	306	GLU	CB-CA-C	-5.32	102.49	110.90
1	D	163	ASN	O-C-N	5.31	127.75	122.12
1	C	311	ASN	CA-C-O	-5.31	115.25	120.82
1	D	70	GLY	O-C-N	5.31	127.29	122.19
1	A	297	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	D	204	GLN	CG-CD-NE2	5.30	124.36	116.40
1	C	354	TYR	O-C-N	5.30	127.74	122.12
1	A	42	LYS	CB-CG-CD	-5.30	99.12	111.30
1	B	366	ASP	O-C-N	5.29	128.77	122.26
1	A	196	ALA	CA-C-N	5.29	125.81	119.94
1	A	196	ALA	C-N-CA	5.29	125.81	119.94
1	B	188	ARG	CA-C-O	-5.29	115.39	121.47
1	C	203	VAL	N-CA-CB	-5.29	103.35	110.54
1	D	309	LYS	CA-C-O	-5.28	114.95	120.55
1	C	15	LEU	CA-C-N	5.27	131.61	121.18
1	C	15	LEU	C-N-CA	5.27	131.61	121.18
1	D	128	GLU	CA-CB-CG	5.27	124.64	114.10
1	A	260	PHE	CA-CB-CG	-5.27	108.53	113.80
1	D	328	ASP	CA-C-O	5.27	123.22	119.32
1	C	289	ARG	CD-NE-CZ	5.26	131.77	124.40
1	B	210	GLU	CB-CG-CD	5.25	121.53	112.60
1	B	177	ARG	N-CA-C	-5.25	101.61	109.95
1	C	28	ASP	O-C-N	5.25	129.10	122.65
1	D	158	TYR	CA-C-O	5.24	126.33	120.82
1	C	155	LEU	CB-CA-C	5.24	119.49	110.79
1	D	221	GLU	CG-CD-OE1	5.24	130.46	118.40
1	A	24	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	339	LYS	CB-CA-C	-5.23	103.24	111.51
1	D	340	VAL	CB-CA-C	5.23	118.67	111.97
1	B	303	GLY	N-CA-C	-5.23	106.07	112.77
1	A	361	ARG	NE-CZ-NH1	5.22	126.72	121.50
1	C	222	GLN	CG-CD-NE2	5.22	124.23	116.40
1	A	52	THR	CA-CB-OG1	-5.22	101.77	109.60
1	D	93	LEU	O-C-N	5.22	129.00	121.95
1	A	64	ASP	N-CA-C	-5.22	103.99	110.41
1	C	85	ILE	CA-C-O	5.21	126.72	121.72
1	A	243	HIS	CA-C-N	-5.21	114.07	122.25
1	A	243	HIS	C-N-CA	-5.21	114.07	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GLN	CA-C-O	-5.21	115.34	120.70
1	A	225	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	B	218	THR	CA-C-N	5.20	125.75	119.98
1	B	218	THR	C-N-CA	5.20	125.75	119.98
1	C	225	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	C	253	LYS	CA-C-O	-5.20	115.58	121.25
1	C	294	LYS	CB-CA-C	-5.20	102.23	110.02
1	C	180	ILE	CB-CA-C	-5.19	104.40	111.15
1	D	239	LYS	CA-C-O	-5.19	115.22	121.40
1	B	230	GLN	CA-C-O	-5.19	115.05	120.55
1	C	158	TYR	CA-CB-CG	5.19	123.24	113.90
1	B	7	ARG	CA-CB-CG	-5.19	103.73	114.10
1	A	46	ILE	CA-C-O	-5.18	112.81	119.39
1	B	13	PHE	CA-C-O	-5.18	115.05	121.06
1	D	295	PRO	CB-CA-C	5.18	118.17	111.64
1	A	54	HIS	N-CA-C	-5.18	101.83	110.17
1	C	336	ALA	CA-C-O	-5.18	115.37	120.70
1	D	339	LYS	CB-CA-C	-5.17	103.34	111.51
1	C	177	ARG	N-CA-C	-5.17	101.26	109.59
1	A	163	ASN	O-C-N	5.17	127.60	122.12
1	C	218	THR	CA-C-N	5.16	125.71	119.98
1	C	218	THR	C-N-CA	5.16	125.71	119.98
1	C	328	ASP	CA-C-N	5.16	125.20	119.32
1	C	328	ASP	C-N-CA	5.16	125.20	119.32
1	A	208	ARG	CA-CB-CG	5.16	124.42	114.10
1	C	144	GLU	N-CA-CB	5.16	117.83	110.67
1	A	247	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	D	55	ASP	CA-C-O	-5.15	115.39	120.90
1	B	255	ASP	N-CA-CB	-5.15	101.79	110.49
1	A	144	GLU	N-CA-CB	5.14	117.82	110.67
1	D	144	GLU	N-CA-CB	5.13	117.81	110.67
1	D	59	VAL	O-C-N	5.13	125.64	120.92
1	B	78	ALA	CA-C-O	-5.13	115.11	120.55
1	C	102	GLY	CA-C-O	-5.13	118.63	122.37
1	A	345	THR	O-C-N	5.11	126.84	121.42
1	B	112	ARG	CG-CD-NE	5.11	123.25	112.00
1	B	45	GLU	CA-CB-CG	5.11	124.32	114.10
1	D	23	ARG	N-CA-C	-5.11	100.19	108.41
1	B	301	TYR	CA-CB-CG	-5.11	104.71	113.90
1	A	146	ASP	CA-C-O	-5.10	115.15	120.55
1	A	107	ASN	N-CA-C	-5.09	105.92	111.82
1	D	309	LYS	CA-C-N	5.09	127.10	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	LYS	C-N-CA	5.09	127.10	120.28
1	D	268	ALA	N-CA-C	-5.09	105.81	111.36
1	B	112	ARG	NE-CZ-NH1	-5.09	116.41	121.50
1	D	361	ARG	CA-CB-CG	5.08	124.27	114.10
1	C	49	TYR	N-CA-C	-5.08	107.25	113.50
1	C	64	ASP	N-CA-C	-5.08	103.82	110.53
1	A	360	ASP	CA-C-N	5.08	127.59	120.28
1	A	360	ASP	C-N-CA	5.08	127.59	120.28
1	A	42	LYS	CB-CA-C	-5.07	102.37	110.79
1	D	82	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	298	THR	CA-CB-CG2	5.07	119.11	110.50
1	A	68	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	B	143	ALA	N-CA-CB	-5.06	103.06	111.57
1	A	88	MET	CA-C-O	-5.06	115.32	120.99
1	D	94	PHE	O-C-N	5.06	128.25	121.67
1	D	313	ARG	CA-CB-CG	5.06	124.22	114.10
1	B	232	ILE	N-CA-C	-5.06	105.61	110.72
1	D	94	PHE	CA-C-O	-5.06	112.17	118.54
1	B	330	GLU	OE1-CD-OE2	5.05	135.03	122.90
1	D	77	LYS	CA-C-N	5.05	127.01	120.44
1	D	77	LYS	C-N-CA	5.05	127.01	120.44
1	B	370	ASP	O-C-N	5.05	127.47	122.12
1	C	294	LYS	O-C-N	5.05	126.23	121.38
1	D	279	PRO	CA-C-O	5.05	126.79	121.03
1	A	289	ARG	N-CA-C	-5.04	99.12	108.24
1	B	321	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	C	144	GLU	N-CA-C	-5.04	107.52	113.97
1	D	102	GLY	CA-C-O	5.04	127.25	122.26
1	D	12	SER	CA-C-O	-5.04	115.55	121.44
1	D	229	THR	CA-CB-OG1	-5.04	102.05	109.60
1	C	80	ASP	OD1-CG-OD2	5.03	134.97	122.90
1	A	328	ASP	CA-C-N	5.03	124.81	119.28
1	A	328	ASP	C-N-CA	5.03	124.81	119.28
1	A	302	ASP	O-C-N	5.03	127.25	122.07
1	C	97	PRO	O-C-N	5.02	128.25	122.17
1	D	249	GLN	CA-CB-CG	5.02	124.15	114.10
1	A	289	ARG	CA-C-N	5.02	129.27	122.19
1	A	289	ARG	C-N-CA	5.02	129.27	122.19
1	A	286	ASP	CA-C-O	-5.01	113.53	119.05
1	D	190	ASP	N-CA-CB	5.01	119.23	110.81
1	B	204	GLN	CB-CG-CD	5.01	121.11	112.60
1	A	240	LYS	CA-C-O	-5.00	113.58	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	GLU	CG-CD-OE2	-5.00	106.89	118.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	B	172	ARG	Sidechain
1	C	172	ARG	Sidechain
1	D	208	ARG	Sidechain

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	3051	0	2953	27	0
1	B	3051	0	2953	29	0
1	C	3051	0	2953	22	0
1	D	3051	0	2953	23	0
2	A	10	0	12	0	0
2	B	10	0	12	1	0
2	C	10	0	11	1	0
2	D	10	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	220	0	0	1	0
4	B	217	0	0	2	0
4	C	232	0	0	2	0
4	D	220	0	0	4	0
All	All	13137	0	11859	91	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (91) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.65	1.13
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.70	1.08
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.18	0.92
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.19	0.87
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.21	0.84
1:D:3:VAL:HG23	4:D:601:HOH:O	1.76	0.84
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.83
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.67	0.76
1:D:330:GLU:OE1	4:D:613:HOH:O	2.11	0.68
1:B:141:GLU:OE2	4:B:569:HOH:O	2.14	0.65
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.79	0.64
1:A:36:PRO:O	1:A:40:VAL:HG23	1.97	0.63
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.82	0.63
2:B:397:XYL:H12	4:B:593:HOH:O	1.99	0.62
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.82	0.61
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.83	0.61
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.85	0.59
2:C:397:XYL:H12	4:C:609:HOH:O	2.02	0.58
1:A:204:GLN:HG2	4:A:548:HOH:O	2.02	0.58
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.85	0.57
1:C:59:VAL:HG11	1:C:68:ARG:HG3	1.87	0.56
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.89	0.55
1:C:72:ILE:O	1:C:76:LYS:HG3	2.06	0.55
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.87	0.54
1:B:77:LYS:O	1:B:80:ASP:HB2	2.08	0.53
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.10	0.53
1:C:41:HIS:HE1	4:C:522:HOH:O	1.91	0.52
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.91	0.51
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.92	0.51
1:B:3:VAL:HG12	1:B:4:GLN:H	1.76	0.50
1:B:164:LEU:C	1:B:164:LEU:HD23	2.37	0.49
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.78	0.49
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.94	0.49
1:A:6:THR:O	1:A:9:ASP:HB2	2.13	0.49
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.95	0.49
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.95	0.48
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.48	0.48
1:A:65:ALA:O	1:A:69:ASP:HB2	2.13	0.48
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.95	0.48
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.48	0.48
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.94	0.48
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.29	0.47
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.74	0.47
1:C:106:SER:O	1:C:112:ARG:HD3	2.15	0.47
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.96	0.46
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.76	0.46
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.92	0.46
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.50	0.45
1:A:164:LEU:C	1:A:164:LEU:HD23	2.41	0.45
1:A:238:HIS:O	1:A:239:LYS:HB2	2.15	0.45
1:A:368:ASP:O	1:A:372:VAL:HG23	2.17	0.45
1:B:101:ASP:CG	1:B:101:ASP:O	2.58	0.45
1:A:77:LYS:O	1:A:80:ASP:CB	2.65	0.44
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.71	0.44
1:B:219:GLY:O	1:B:223:MET:HG3	2.18	0.44
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.13	0.44
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.89	0.44
1:A:52:THR:HG21	1:A:88:MET:HE3	2.00	0.43
1:A:299:GLU:HB3	1:A:303:GLY:HA3	2.00	0.43
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.54	0.42
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.54	0.42
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.84	0.42
1:A:164:LEU:HD12	1:C:348:LEU:HD11	2.00	0.42
1:B:142:GLY:HA3	1:B:190:ASP:O	2.18	0.42
1:C:186:GLU:HA	1:C:187:PRO:HA	1.91	0.42
1:D:356:GLU:O	1:D:359:ALA:HB3	2.19	0.42
1:B:280:ASP:C	1:B:282:ALA:H	2.27	0.42
1:B:282:ALA:HB1	1:B:283:PRO:HD2	2.01	0.42
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.50	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.89	0.42
1:A:330:GLU:OE1	1:A:394:ARG:NH1	2.52	0.42
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.02	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.41
1:C:59:VAL:HG21	1:C:68:ARG:HG3	2.02	0.41
1:D:22:ALA:HB1	1:D:297:ARG:HG3	2.02	0.41
1:B:152:SER:HB2	4:D:572:HOH:O	2.20	0.41
1:B:206:LEU:O	1:B:209:PRO:HD3	2.19	0.41
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.86	0.41
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.46	0.41
1:D:219:GLY:O	1:D:223:MET:HG3	2.20	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:C:183:LYS:HG3	1:C:220:ASN:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:O	1:D:76:LYS:HG3	2.21	0.41
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.51	0.41
1:D:280:ASP:C	1:D:282:ALA:H	2.28	0.41
1:A:106:SER:O	1:A:112:ARG:HD3	2.21	0.41
1:B:214:ILE:HG13	1:B:216:PRO:HD3	2.03	0.40
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.36	0.40
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.57	0.40
1:D:394:ARG:NH1	4:D:609:HOH:O	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	50
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	50
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	12	20
1	D	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	24	37
All	All	1560/1572 (99%)	1504 (96%)	48 (3%)	8 (0%)	24	37

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO
1	D	186	GLU
1	D	280	ASP

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Mol	Chain	Res	Type
1	C	364	PHE

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	306/310 (99%)	299 (98%)	7 (2%)	44	66
1	B	306/310 (99%)	301 (98%)	5 (2%)	55	76
1	C	306/310 (99%)	301 (98%)	5 (2%)	55	76
1	D	306/310 (99%)	298 (97%)	8 (3%)	40	63
All	All	1224/1240 (99%)	1199 (98%)	25 (2%)	48	70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	185	ASN
1	A	203	VAL
1	A	208	ARG
1	B	3	VAL
1	B	49	TYR
1	B	81	GLU
1	B	203	VAL
1	B	394	ARG
1	C	3	VAL
1	C	46	ILE
1	C	49	TYR
1	C	80	ASP
1	C	203	VAL
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP

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Mol	Chain	Res	Type
1	D	84	LEU
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG
1	D	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	238	HIS
1	A	332	GLN
1	B	204	GLN
1	B	222	GLN
1	B	238	HIS
1	C	41	HIS
1	C	222	GLN
1	C	238	HIS
1	D	41	HIS
1	D	185	ASN
1	D	222	GLN
1	D	238	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	XYL	A	397	3	9,9,9	0.54	0	11,11,11	1.50	2 (18%)
2	XYL	C	397	3	9,9,9	0.55	0	11,11,11	1.81	2 (18%)
2	XYL	D	397	3	9,9,9	0.56	0	11,11,11	1.89	3 (27%)
2	XYL	B	397	3	9,9,9	0.50	0	11,11,11	2.43	4 (36%)

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	XYL	A	397	3	-	1/12/12/12	-
2	XYL	C	397	3	-	0/12/12/12	-
2	XYL	D	397	3	-	2/12/12/12	-
2	XYL	B	397	3	-	2/12/12/12	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XYL	C1-C2-C3	4.98	122.32	112.17
2	B	397	XYL	O4-C4-C3	4.94	120.80	109.25
2	D	397	XYL	C5-C4-C3	4.12	120.56	112.17
2	A	397	XYL	O4-C4-C3	3.85	118.25	109.25
2	C	397	XYL	O4-C4-C3	3.77	118.07	109.25
2	C	397	XYL	C1-C2-C3	3.52	119.34	112.17
2	D	397	XYL	C1-C2-C3	3.24	118.77	112.17
2	B	397	XYL	O2-C2-C3	-2.48	103.44	109.25
2	B	397	XYL	C5-C4-C3	2.34	116.95	112.17
2	A	397	XYL	C1-C2-C3	2.15	116.55	112.17
2	D	397	XYL	O2-C2-C1	-2.02	104.44	109.03

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	397	XYL	O4-C4-C5-O5
2	D	397	XYL	C2-C3-C4-C5
2	A	397	XYL	O4-C4-C5-O5
2	B	397	XYL	O3-C3-C4-C5
2	D	397	XYL	O3-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	397	XYL	1	0
2	B	397	XYL	1	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

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.