



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:44 AM UTC

PDB ID : 5XIM / pdb_00005xim
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 : 1992-03-30
Resolution : 2.60 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

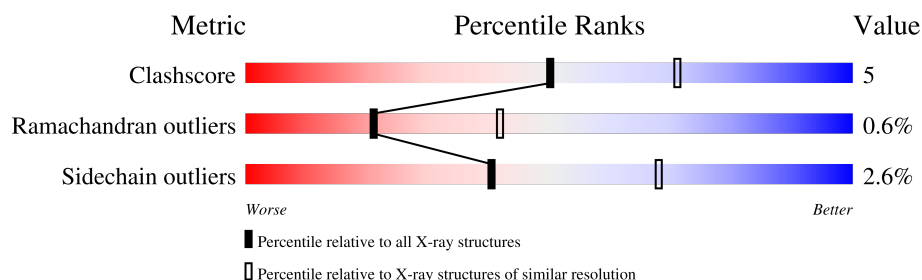
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	67% 27% 6%
1	B	393	67% 29% .
1	C	393	72% 24% .
1	D	393	72% 23% 5%

2 Entry composition [i](#)

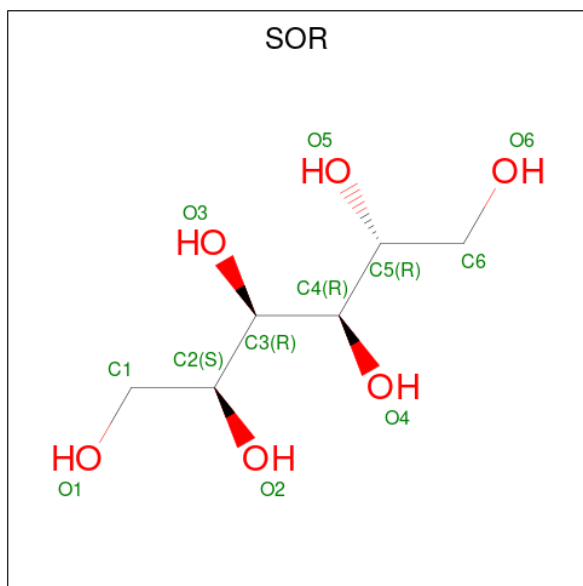
There are 4 unique types of molecules in this entry. The entry contains 13132 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			3053	1939	532	578	4			
1	B	392	Total	C	N	O	S	0	0	0
			3053	1939	532	578	4			
1	C	392	Total	C	N	O	S	0	0	0
			3053	1939	532	578	4			
1	D	392	Total	C	N	O	S	0	0	0
			3053	1939	532	578	4			

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



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

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

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

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

- Molecule 4 is water.

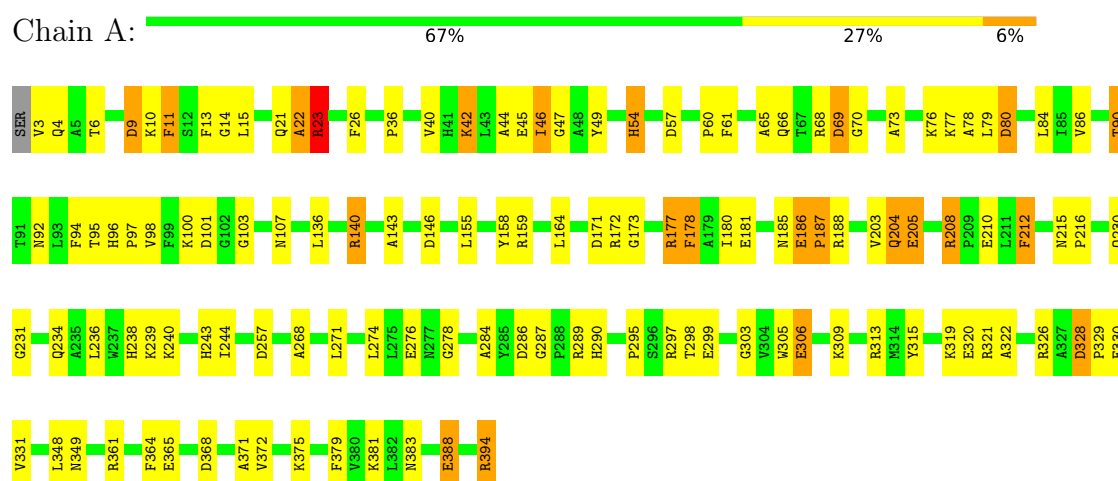
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	218	Total	O	0	0
			218	218		
4	B	206	Total	O	0	0
			206	206		
4	C	234	Total	O	0	0
			234	234		
4	D	210	Total	O	0	0
			210	210		

3 Residue-property plots

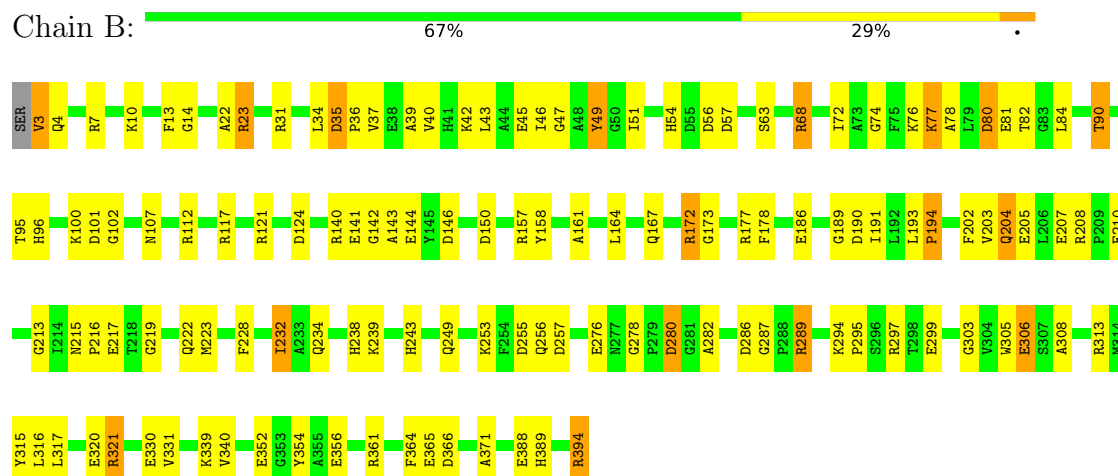
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

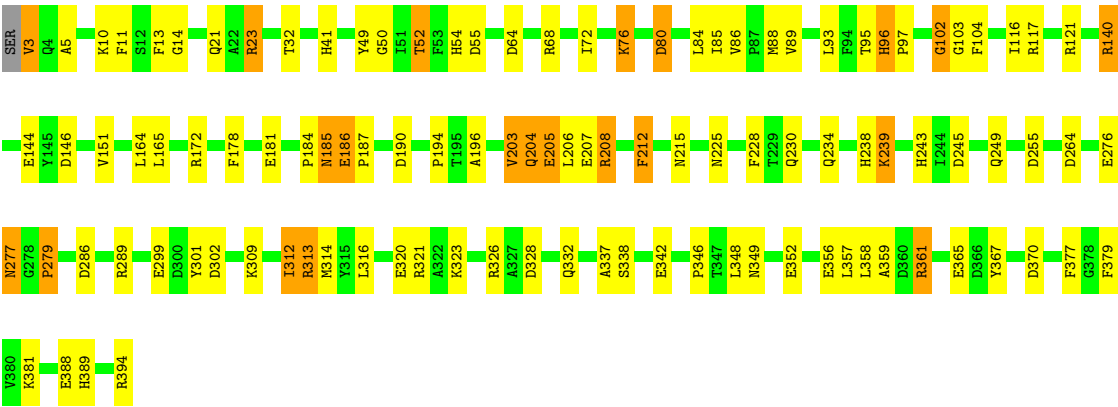


• Molecule 1: D-XYLOSE ISOMERASE





● Molecule 1: D-XYLOSE ISOMERASE



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) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.144 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13132	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: MG, SOR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	1/3125 (0.0%)	2.15	127/4233 (3.0%)
1	B	1.01	0/3125	2.09	110/4233 (2.6%)
1	C	1.01	0/3125	2.07	103/4233 (2.4%)
1	D	1.04	1/3125 (0.0%)	2.10	106/4233 (2.5%)
All	All	1.02	2/12500 (0.0%)	2.10	446/16932 (2.6%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	GLY	N-CA	7.41	1.50	1.45
1	A	103	GLY	CA-C	5.53	1.55	1.51

All (446) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	CA-CB-CG	-16.08	96.52	112.60
1	D	204	GLN	OE1-CD-NE2	-15.54	107.06	122.60
1	B	204	GLN	OE1-CD-NE2	-12.28	110.32	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	ASP	CA-CB-CG	-11.16	101.44	112.60
1	A	107	ASN	CA-CB-CG	11.06	123.66	112.60
1	A	204	GLN	OE1-CD-NE2	-10.92	111.68	122.60
1	A	394	ARG	NH1-CZ-NH2	10.79	133.33	119.30
1	D	172	ARG	CD-NE-CZ	10.08	138.51	124.40
1	B	172	ARG	NE-CZ-NH1	9.83	131.33	121.50
1	D	80	ASP	CA-CB-CG	-9.72	102.88	112.60
1	C	204	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	A	244	ILE	CA-C-O	-9.62	110.61	120.90
1	A	379	PHE	CA-CB-CG	9.53	123.33	113.80
1	D	313	ARG	NE-CZ-NH2	9.36	127.62	119.20
1	C	361	ARG	NE-CZ-NH2	9.33	127.60	119.20
1	B	140	ARG	CD-NE-CZ	9.11	137.15	124.40
1	C	379	PHE	CA-CB-CG	8.97	122.77	113.80
1	B	96	HIS	CA-CB-CG	-8.93	104.88	113.80
1	B	31	ARG	NE-CZ-NH2	8.86	127.17	119.20
1	C	172	ARG	NE-CZ-NH2	-8.79	111.29	119.20
1	B	394	ARG	NE-CZ-NH2	-8.77	111.31	119.20
1	B	80	ASP	CA-CB-CG	-8.62	103.98	112.60
1	B	177	ARG	NE-CZ-NH2	-8.60	111.46	119.20
1	B	389	HIS	CA-CB-CG	-8.59	105.21	113.80
1	C	28	ASP	CA-CB-CG	8.59	121.19	112.60
1	C	172	ARG	NE-CZ-NH1	8.55	130.05	121.50
1	B	172	ARG	NE-CZ-NH2	-8.55	111.51	119.20
1	A	394	ARG	NE-CZ-NH1	-8.48	113.02	121.50
1	C	54	HIS	N-CA-C	-8.46	98.00	110.52
1	D	328	ASP	CA-CB-CG	8.45	121.05	112.60
1	B	394	ARG	N-CA-CB	8.35	124.70	110.50
1	D	286	ASP	CA-CB-CG	-8.26	104.34	112.60
1	B	321	ARG	NE-CZ-NH2	-8.22	111.80	119.20
1	B	95	THR	N-CA-C	8.19	120.12	111.03
1	C	95	THR	N-CA-C	8.13	119.92	111.14
1	A	204	GLN	CB-CG-CD	8.07	126.33	112.60
1	B	102	GLY	CA-C-O	-7.97	116.55	122.37
1	B	117	ARG	NE-CZ-NH1	7.88	129.38	121.50
1	A	394	ARG	CD-NE-CZ	-7.88	113.37	124.40
1	C	134	LEU	CA-C-O	-7.86	111.89	120.30
1	C	340	VAL	CB-CA-C	7.84	121.91	111.88
1	D	207	GLU	CA-CB-CG	7.82	129.75	114.10
1	D	342	GLU	CB-CG-CD	7.81	125.88	112.60
1	C	253	LYS	CA-C-O	-7.81	112.74	121.25
1	A	320	GLU	CB-CG-CD	7.79	125.83	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ARG	NE-CZ-NH1	7.77	129.27	121.50
1	C	170	GLU	CA-C-O	-7.73	112.73	120.70
1	A	394	ARG	CA-CB-CG	7.72	129.54	114.10
1	B	306	GLU	CA-C-O	7.69	128.90	120.82
1	D	54	HIS	N-CA-C	-7.67	97.82	110.17
1	C	208	ARG	CD-NE-CZ	-7.64	113.70	124.40
1	D	55	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	328	ASP	CA-C-O	7.57	126.58	119.24
1	D	144	GLU	N-CA-C	-7.50	104.36	113.97
1	A	216	PRO	CA-C-O	-7.45	112.77	121.86
1	C	349	ASN	OD1-CG-ND2	-7.43	115.17	122.60
1	B	217	GLU	CA-C-O	-7.38	112.88	120.71
1	A	77	LYS	O-C-N	7.34	129.63	122.07
1	A	79	LEU	CA-C-O	7.32	128.38	119.97
1	D	10	LYS	CB-CA-C	-7.29	102.09	111.86
1	D	312	ILE	CA-C-O	-7.21	113.21	120.85
1	A	26	PHE	O-C-N	7.20	130.90	122.19
1	D	321	ARG	NE-CZ-NH2	7.19	125.67	119.20
1	D	349	ASN	CA-CB-CG	-7.18	105.42	112.60
1	A	257	ASP	CA-CB-CG	7.17	119.78	112.60
1	C	389	HIS	CA-CB-CG	-7.17	106.63	113.80
1	A	26	PHE	CA-C-O	-7.14	111.05	119.48
1	B	13	PHE	CA-CB-CG	7.14	120.94	113.80
1	D	389	HIS	CA-CB-CG	-7.12	106.68	113.80
1	A	80	ASP	O-C-N	7.12	129.44	122.03
1	C	80	ASP	CA-CB-CG	-7.10	105.50	112.60
1	C	135	VAL	O-C-N	7.07	130.43	122.93
1	A	95	THR	N-CA-C	7.07	118.87	111.03
1	D	21	GLN	CB-CG-CD	-7.07	100.59	112.60
1	C	23	ARG	CA-C-O	-7.04	113.05	120.58
1	D	302	ASP	CA-C-O	-7.04	113.43	120.82
1	D	181	GLU	CB-CA-C	-7.04	102.36	110.17
1	B	161	ALA	CA-C-O	-7.03	112.97	120.42
1	B	150	ASP	CA-CB-CG	-6.97	105.63	112.60
1	B	331	VAL	N-CA-C	-6.96	103.98	110.53
1	B	243	HIS	CA-CB-CG	6.96	120.76	113.80
1	B	77	LYS	O-C-N	6.95	129.22	122.07
1	B	313	ARG	CA-C-N	6.94	129.46	120.44
1	B	313	ARG	C-N-CA	6.94	129.46	120.44
1	B	316	LEU	CA-C-O	-6.93	113.07	120.42
1	B	371	ALA	CA-C-O	-6.93	113.07	120.42
1	A	287	GLY	O-C-N	6.93	128.70	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH1	6.92	128.42	121.50
1	D	370	ASP	CA-C-O	-6.91	113.23	120.55
1	C	203	VAL	N-CA-CB	-6.90	101.84	110.47
1	A	45	GLU	CA-C-O	-6.86	113.28	120.55
1	C	222	GLN	OE1-CD-NE2	-6.86	115.74	122.60
1	B	57	ASP	N-CA-C	-6.81	103.31	111.69
1	D	93	LEU	CA-C-O	-6.81	113.31	121.34
1	C	146	ASP	CA-C-O	-6.79	113.35	120.55
1	D	203	VAL	CB-CA-C	6.79	120.93	112.04
1	C	383	ASN	OD1-CG-ND2	6.75	129.35	122.60
1	D	117	ARG	NE-CZ-NH2	-6.75	113.13	119.20
1	C	394	ARG	CD-NE-CZ	-6.72	114.99	124.40
1	C	96	HIS	CA-CB-CG	-6.72	107.08	113.80
1	C	394	ARG	NE-CZ-NH1	-6.72	114.78	121.50
1	B	191	ILE	CA-C-O	-6.71	113.06	120.84
1	B	117	ARG	NE-CZ-NH2	-6.71	113.16	119.20
1	D	332	GLN	CA-C-O	6.71	127.66	120.55
1	B	54	HIS	N-CA-C	-6.69	99.40	110.17
1	C	255	ASP	N-CA-CB	-6.68	99.19	110.49
1	B	23	ARG	CD-NE-CZ	6.65	133.71	124.40
1	A	86	VAL	O-C-N	6.64	128.67	121.10
1	C	278	GLY	CA-C-N	6.63	128.13	119.84
1	C	278	GLY	C-N-CA	6.63	128.13	119.84
1	A	306	GLU	CB-CA-C	-6.60	100.52	110.88
1	C	64	ASP	N-CA-C	-6.56	101.69	110.55
1	D	313	ARG	N-CA-CB	6.56	119.52	110.01
1	D	204	GLN	CB-CG-CD	6.55	123.73	112.60
1	C	158	TYR	CA-CB-CG	6.54	125.67	113.90
1	A	23	ARG	CA-C-O	-6.54	113.59	120.58
1	A	244	ILE	O-C-N	6.53	130.66	123.09
1	C	64	ASP	CA-CB-CG	-6.53	106.07	112.60
1	C	41	HIS	CA-C-O	-6.53	113.98	120.70
1	A	372	VAL	CA-C-O	-6.52	113.42	120.47
1	C	159	ARG	NE-CZ-NH1	-6.52	114.98	121.50
1	D	104	PHE	CA-C-O	-6.50	112.75	120.10
1	D	204	GLN	CG-CD-OE1	6.48	133.75	120.80
1	A	155	LEU	CB-CA-C	6.47	121.85	110.85
1	A	394	ARG	N-CA-CB	6.45	121.46	110.50
1	C	117	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	D	239	LYS	CB-CA-C	-6.43	103.24	111.86
1	A	205	GLU	CG-CD-OE2	6.42	133.17	118.40
1	D	302	ASP	CA-CB-CG	-6.42	106.18	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	202	PHE	CA-C-N	6.42	129.58	120.53
1	B	202	PHE	C-N-CA	6.42	129.58	120.53
1	D	140	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	B	54	HIS	N-CA-CB	6.41	121.07	110.63
1	B	90	THR	CA-CB-OG1	-6.41	99.99	109.60
1	B	107	ASN	N-CA-C	-6.40	104.31	111.28
1	A	171	ASP	CA-C-O	-6.39	113.65	120.42
1	B	320	GLU	CB-CG-CD	6.39	123.46	112.60
1	B	286	ASP	CA-C-O	-6.38	111.95	119.48
1	D	190	ASP	CA-C-O	-6.35	112.47	120.28
1	C	207	GLU	CG-CD-OE2	-6.35	103.80	118.40
1	D	194	PRO	N-CA-C	6.34	121.78	113.86
1	D	342	GLU	CG-CD-OE2	6.34	132.97	118.40
1	B	253	LYS	CA-C-O	-6.33	114.41	121.05
1	C	194	PRO	N-CA-C	6.32	121.75	113.86
1	D	357	LEU	O-C-N	6.30	128.56	122.07
1	D	388	GLU	CG-CD-OE1	-6.30	103.90	118.40
1	C	66	GLN	O-C-N	6.30	128.56	122.07
1	A	371	ALA	CA-C-O	-6.30	114.22	120.70
1	C	331	VAL	N-CA-C	-6.29	104.61	110.53
1	C	71	ILE	O-C-N	6.29	127.97	121.87
1	C	172	ARG	CB-CG-CD	-6.29	96.84	111.30
1	B	303	GLY	N-CA-C	-6.28	104.95	113.37
1	B	255	ASP	N-CA-CB	-6.28	99.87	110.49
1	A	78	ALA	CA-C-O	-6.28	113.89	120.55
1	A	90	THR	CA-CB-OG1	-6.28	100.19	109.60
1	B	68	ARG	NE-CZ-NH1	-6.27	115.23	121.50
1	A	14	GLY	N-CA-C	-6.25	101.35	112.54
1	C	208	ARG	NE-CZ-NH1	-6.24	115.26	121.50
1	D	205	GLU	CG-CD-OE2	6.24	132.75	118.40
1	A	158	TYR	CA-C-O	6.24	127.03	120.42
1	B	366	ASP	CA-C-O	-6.23	112.60	119.95
1	D	358	LEU	CA-C-O	6.23	127.14	120.10
1	B	146	ASP	CA-C-O	-6.22	113.96	120.55
1	A	173	GLY	CA-C-O	-6.21	112.58	120.03
1	A	10	LYS	CB-CA-C	-6.20	103.08	111.89
1	B	80	ASP	O-C-N	6.20	128.72	122.08
1	D	52	THR	CA-CB-OG1	-6.20	100.31	109.60
1	D	146	ASP	O-C-N	6.19	128.69	122.12
1	C	225	ASN	OD1-CG-ND2	-6.19	116.41	122.60
1	C	57	ASP	N-CA-CB	6.19	119.42	110.20
1	A	321	ARG	NE-CZ-NH2	-6.17	113.64	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NE-CZ-NH2	-6.17	113.65	119.20
1	A	205	GLU	CB-CG-CD	6.14	123.04	112.60
1	C	328	ASP	CA-C-N	6.14	125.87	119.05
1	C	328	ASP	C-N-CA	6.14	125.87	119.05
1	C	66	GLN	N-CA-C	-6.12	104.52	111.07
1	C	13	PHE	CA-C-O	-6.12	113.96	121.06
1	A	11	PHE	CA-C-O	-6.12	113.71	120.69
1	A	13	PHE	CA-C-O	-6.12	113.95	121.11
1	D	239	LYS	CA-C-O	-6.12	114.49	121.65
1	B	177	ARG	CB-CG-CD	-6.11	97.26	111.30
1	C	6	THR	N-CA-CB	6.10	121.08	111.20
1	D	185	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	D	225	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	46	ILE	CA-C-O	-6.06	111.70	119.39
1	D	96	HIS	CA-CB-CG	-6.06	107.74	113.80
1	D	243	HIS	CA-C-O	-6.05	114.96	121.38
1	D	346	PRO	CA-C-O	-6.05	114.65	121.43
1	B	215	ASN	CA-CB-CG	-6.05	106.55	112.60
1	D	316	LEU	CB-CA-C	6.05	120.37	110.88
1	C	65	ALA	N-CA-C	6.03	117.85	111.28
1	A	100	LYS	CA-C-O	-6.02	113.30	120.10
1	C	138	GLY	CA-C-N	6.02	127.67	120.14
1	C	138	GLY	C-N-CA	6.02	127.67	120.14
1	C	121	ARG	NE-CZ-NH1	6.01	127.51	121.50
1	D	377	PHE	CA-C-O	-6.01	112.03	119.18
1	B	177	ARG	N-CA-C	-6.01	100.40	109.95
1	D	357	LEU	CA-C-O	-6.00	114.52	120.82
1	A	54	HIS	CA-C-O	-5.99	114.21	121.28
1	A	231	GLY	CA-C-N	5.97	128.90	120.42
1	A	231	GLY	C-N-CA	5.97	128.90	120.42
1	C	292	ASP	O-C-N	5.97	128.97	122.64
1	D	230	GLN	CA-C-N	5.97	126.56	120.00
1	D	230	GLN	C-N-CA	5.97	126.56	120.00
1	A	284	ALA	N-CA-C	-5.96	105.84	113.23
1	B	56	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	173	GLY	CA-C-O	-5.95	113.03	119.82
1	B	35	ASP	CB-CA-C	5.95	119.04	109.41
1	A	172	ARG	CD-NE-CZ	5.94	132.72	124.40
1	D	41	HIS	CA-CB-CG	-5.94	107.86	113.80
1	B	68	ARG	CD-NE-CZ	-5.92	116.12	124.40
1	D	144	GLU	N-CA-CB	5.92	118.89	110.67
1	A	69	ASP	O-C-N	5.91	128.38	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	312	ILE	O-C-N	5.91	127.91	121.83
1	A	177	ARG	N-CA-C	-5.90	100.28	109.72
1	D	320	GLU	CA-CB-CG	5.90	125.90	114.10
1	C	370	ASP	O-C-N	5.90	128.37	122.12
1	D	95	THR	N-CA-C	5.89	118.58	111.40
1	B	96	HIS	CA-C-O	-5.87	114.06	120.17
1	A	140	ARG	CD-NE-CZ	5.87	132.62	124.40
1	A	315	TYR	CA-C-O	-5.87	114.66	120.82
1	A	181	GLU	O-C-N	5.86	127.80	121.12
1	D	68	ARG	CD-NE-CZ	-5.84	116.22	124.40
1	B	82	THR	CA-C-O	-5.82	112.46	119.27
1	C	155	LEU	CB-CA-C	5.82	120.74	110.85
1	D	121	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	C	113	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	A	271	LEU	CA-C-O	-5.80	114.72	120.70
1	A	158	TYR	N-CA-C	-5.80	105.04	111.36
1	A	54	HIS	N-CA-C	-5.78	100.86	110.17
1	A	243	HIS	CA-CB-CG	5.78	119.58	113.80
1	B	243	HIS	CA-C-O	-5.78	114.74	121.10
1	B	388	GLU	CG-CD-OE1	-5.78	105.11	118.40
1	C	328	ASP	CB-CA-C	5.77	118.74	109.51
1	B	107	ASN	CB-CG-ND2	5.77	125.05	116.40
1	D	328	ASP	CB-CA-C	5.77	117.68	109.38
1	D	361	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	D	309	LYS	CA-C-O	-5.76	114.44	120.55
1	A	146	ASP	CA-C-O	-5.76	114.44	120.55
1	B	63	SER	N-CA-C	-5.76	100.31	109.76
1	D	313	ARG	CA-CB-CG	5.76	125.62	114.10
1	C	177	ARG	N-CA-CB	5.75	120.84	110.83
1	D	104	PHE	O-C-N	5.75	128.95	122.22
1	A	188	ARG	CA-C-O	-5.75	115.03	121.81
1	C	24	ASP	CA-CB-CG	5.74	118.34	112.60
1	D	146	ASP	CA-C-O	-5.74	114.47	120.55
1	A	240	LYS	CA-C-O	-5.73	113.19	119.95
1	A	326	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	D	328	ASP	CA-C-O	5.72	123.55	119.32
1	A	388	GLU	CA-CB-CG	-5.72	102.66	114.10
1	D	80	ASP	O-C-N	5.71	127.95	122.07
1	A	331	VAL	N-CA-C	-5.71	105.16	110.53
1	A	368	ASP	O-C-N	5.70	128.99	122.55
1	B	63	SER	O-C-N	5.69	129.85	123.19
1	C	275	LEU	CA-C-O	-5.69	114.39	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	HIS	N-CA-CB	5.69	119.90	110.63
1	A	290	HIS	CA-C-O	-5.68	114.12	120.54
1	A	95	THR	O-C-N	5.67	128.15	122.03
1	A	73	ALA	CA-C-N	5.66	126.23	120.00
1	A	73	ALA	C-N-CA	5.66	126.23	120.00
1	B	280	ASP	N-CA-C	-5.66	103.47	111.56
1	C	15	LEU	CA-C-O	5.65	126.54	120.55
1	A	21	GLN	CB-CG-CD	-5.64	103.00	112.60
1	A	278	GLY	N-CA-C	-5.64	105.40	112.23
1	B	305	TRP	CA-CB-CG	-5.64	102.88	113.60
1	D	14	GLY	N-CA-C	-5.63	102.45	112.54
1	D	212	PHE	N-CA-C	5.63	118.58	109.40
1	C	177	ARG	CB-CG-CD	-5.63	98.36	111.30
1	A	42	LYS	CB-CG-CD	-5.61	98.39	111.30
1	D	32	THR	CA-CB-OG1	-5.61	101.18	109.60
1	A	143	ALA	N-CA-CB	-5.61	102.14	111.57
1	B	394	ARG	NH1-CZ-NH2	5.61	126.59	119.30
1	C	72	ILE	O-C-N	5.61	127.31	121.87
1	D	239	LYS	O-C-N	5.61	129.31	122.58
1	A	268	ALA	N-CA-C	-5.61	105.25	111.36
1	A	322	ALA	N-CA-C	-5.61	105.25	111.36
1	D	277	ASN	N-CA-C	-5.60	103.59	110.65
1	C	366	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	171	ASP	CA-CB-CG	5.59	118.19	112.60
1	B	289	ARG	N-CA-C	-5.59	96.72	107.57
1	C	23	ARG	N-CA-C	-5.59	99.41	108.41
1	C	172	ARG	CD-NE-CZ	-5.58	116.58	124.40
1	C	316	LEU	CA-C-O	-5.57	114.64	120.55
1	B	77	LYS	CB-CA-C	-5.57	102.14	110.88
1	B	299	GLU	N-CA-C	5.57	119.13	110.17
1	D	86	VAL	O-C-N	5.56	127.44	121.10
1	A	349	ASN	OD1-CG-ND2	5.55	128.16	122.60
1	A	101	ASP	CA-CB-CG	5.55	118.15	112.60
1	B	158	TYR	N-CA-C	-5.54	105.16	111.14
1	C	171	ASP	CA-CB-CG	-5.54	107.06	112.60
1	A	44	ALA	N-CA-C	-5.53	105.25	111.28
1	A	57	ASP	N-CA-CB	5.53	118.44	110.20
1	B	256	GLN	OE1-CD-NE2	5.53	128.13	122.60
1	C	365	GLU	CA-C-O	-5.53	114.69	120.55
1	B	74	GLY	O-C-N	5.52	127.54	122.19
1	A	107	ASN	N-CA-C	-5.52	105.42	111.82
1	B	330	GLU	OE1-CD-OE2	5.51	136.13	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	281	GLY	CA-C-N	5.51	129.06	120.68
1	C	281	GLY	C-N-CA	5.51	129.06	120.68
1	B	194	PRO	CA-C-O	-5.51	111.28	119.00
1	C	286	ASP	CA-CB-CG	-5.51	107.09	112.60
1	D	264	ASP	CB-CA-C	5.50	120.93	111.68
1	D	367	TYR	O-C-N	5.50	129.50	123.22
1	C	229	THR	CA-CB-OG1	-5.48	101.38	109.60
1	A	276	GLU	N-CA-C	5.48	120.06	112.45
1	C	167	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	C	349	ASN	N-CA-C	-5.46	102.26	110.24
1	C	281	GLY	N-CA-C	-5.46	100.25	113.18
1	B	321	ARG	NH1-CZ-NH2	5.45	126.39	119.30
1	C	82	THR	CA-CB-OG1	-5.45	101.43	109.60
1	D	301	TYR	CB-CA-C	5.45	120.70	110.63
1	D	314	MET	CA-C-O	-5.45	115.07	120.90
1	B	276	GLU	N-CA-C	5.44	119.92	113.12
1	A	178	PHE	O-C-N	5.44	129.71	123.29
1	B	45	GLU	N-CA-C	5.44	117.21	111.28
1	B	80	ASP	CB-CA-C	-5.44	102.27	110.92
1	D	64	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	136	LEU	CA-C-O	-5.44	114.69	120.40
1	B	54	HIS	O-C-N	5.44	129.35	123.10
1	A	22	ALA	N-CA-C	5.43	119.20	111.92
1	B	124	ASP	O-C-N	5.43	127.66	122.07
1	A	328	ASP	CB-CG-OD2	5.42	130.86	118.40
1	B	239	LYS	CA-CB-CG	-5.42	103.27	114.10
1	D	388	GLU	CA-CB-CG	-5.42	103.27	114.10
1	A	313	ARG	N-CA-CB	-5.41	102.17	110.01
1	A	295	PRO	N-CA-C	-5.41	102.64	110.80
1	A	381	LYS	CA-CB-CG	-5.40	103.29	114.10
1	B	315	TYR	CA-C-O	-5.40	115.15	120.82
1	C	292	ASP	CA-C-O	-5.40	114.88	121.58
1	B	213	GLY	O-C-N	5.40	129.72	122.70
1	A	9	ASP	N-CA-C	-5.40	105.43	112.23
1	A	15	LEU	N-CA-CB	-5.39	101.92	110.22
1	D	249	GLN	CA-CB-CG	5.39	124.88	114.10
1	C	282	ALA	O-C-N	5.39	127.46	121.53
1	D	289	ARG	N-CA-C	-5.39	96.52	107.41
1	C	177	ARG	N-CA-C	-5.38	100.62	109.40
1	C	203	VAL	CB-CA-C	5.38	119.09	112.04
1	A	243	HIS	CA-C-N	-5.38	113.80	122.25
1	A	243	HIS	C-N-CA	-5.38	113.80	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	PRO	CA-C-O	-5.38	115.41	121.43
1	A	47	GLY	N-CA-C	5.37	122.74	115.00
1	B	340	VAL	CB-CA-C	5.37	118.84	111.97
1	A	286	ASP	N-CA-C	5.36	120.68	113.72
1	D	337	ALA	CA-C-O	-5.34	114.89	120.55
1	C	215	ASN	CA-CB-CG	-5.34	107.26	112.60
1	D	76	LYS	O-C-N	5.33	128.46	122.22
1	A	95	THR	CA-C-O	-5.33	115.41	120.90
1	A	215	ASN	O-C-N	5.33	126.17	121.37
1	B	207	GLU	CG-CD-OE1	5.33	130.66	118.40
1	B	157	ARG	CA-C-N	5.31	127.67	120.44
1	B	157	ARG	C-N-CA	5.31	127.67	120.44
1	C	135	VAL	CA-C-O	-5.31	114.68	120.84
1	D	243	HIS	CA-CB-CG	5.31	119.11	113.80
1	C	340	VAL	N-CA-CB	-5.30	104.63	110.51
1	B	207	GLU	CG-CD-OE2	-5.29	106.23	118.40
1	A	69	ASP	CA-CB-CG	-5.29	107.31	112.60
1	B	141	GLU	CB-CG-CD	5.28	121.57	112.60
1	B	14	GLY	N-CA-C	-5.27	104.99	112.37
1	C	141	GLU	CB-CG-CD	5.27	121.55	112.60
1	B	339	LYS	O-C-N	5.27	131.32	122.21
1	B	102	GLY	O-C-N	5.26	128.74	123.48
1	B	210	GLU	CA-CB-CG	5.25	124.61	114.10
1	A	180	ILE	CB-CA-C	-5.24	104.34	111.15
1	B	10	LYS	CB-CA-C	-5.24	104.46	112.11
1	C	23	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	D	245	ASP	CA-CB-CG	5.22	117.83	112.60
1	C	81	GLU	CB-CG-CD	5.21	121.46	112.60
1	C	188	ARG	CA-CB-CG	5.21	124.53	114.10
1	D	277	ASN	O-C-N	5.21	130.59	122.67
1	A	66	GLN	N-CA-CB	5.21	117.57	110.01
1	D	151	VAL	N-CA-C	5.21	115.94	110.62
1	B	257	ASP	CA-C-O	-5.20	115.56	121.65
1	C	333	GLU	CA-C-O	-5.20	115.36	120.82
1	C	35	ASP	CA-C-N	5.20	124.82	119.05
1	C	35	ASP	C-N-CA	5.20	124.82	119.05
1	A	159	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	D	89	VAL	CB-CA-C	5.19	118.44	110.55
1	A	375	LYS	CA-C-O	-5.18	115.14	121.05
1	C	143	ALA	O-C-N	5.18	128.47	123.29
1	D	215	ASN	CB-CG-ND2	5.18	124.16	116.40
1	B	23	ARG	N-CA-C	-5.17	100.08	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	23	ARG	N-CA-C	-5.17	100.08	108.41
1	D	206	LEU	CA-C-O	-5.17	115.99	121.94
1	D	302	ASP	O-C-N	5.16	127.38	122.07
1	B	143	ALA	N-CA-CB	-5.16	102.91	111.57
1	B	366	ASP	O-C-N	5.16	128.60	122.26
1	C	112	ARG	CG-CD-NE	5.15	123.32	112.00
1	C	328	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	178	PHE	O-C-N	5.14	129.91	123.23
1	C	134	LEU	O-C-N	5.14	129.23	123.27
1	D	21	GLN	OE1-CD-NE2	5.14	127.74	122.60
1	D	64	ASP	N-CA-C	-5.14	103.75	110.53
1	D	13	PHE	CA-CB-CG	5.13	118.94	113.80
1	B	339	LYS	CB-CA-C	-5.12	103.42	111.51
1	D	388	GLU	CG-CD-OE2	5.12	130.18	118.40
1	B	232	ILE	CA-C-O	-5.12	115.43	120.85
1	D	102	GLY	CA-C-O	5.12	126.11	122.37
1	A	23	ARG	N-CA-C	-5.11	100.18	108.41
1	A	177	ARG	N-CA-CB	5.11	119.81	111.08
1	B	210	GLU	CB-CG-CD	5.11	121.28	112.60
1	B	107	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	D	326	ARG	CA-CB-CG	5.10	124.31	114.10
1	A	177	ARG	CA-CB-CG	5.10	124.30	114.10
1	B	112	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	C	177	ARG	CA-CB-CG	5.10	124.30	114.10
1	D	314	MET	N-CA-CB	5.10	117.53	109.94
1	C	365	GLU	O-C-N	5.09	127.52	122.12
1	A	328	ASP	CA-C-N	5.09	124.88	119.28
1	A	328	ASP	C-N-CA	5.09	124.88	119.28
1	C	391	LEU	O-C-N	5.08	129.91	122.39
1	B	144	GLU	N-CA-C	-5.08	107.64	113.88
1	A	80	ASP	OD1-CG-OD2	5.08	135.08	122.90
1	B	47	GLY	N-CA-C	5.08	122.11	114.95
1	D	279	PRO	CB-CA-C	5.08	117.60	111.46
1	D	165	LEU	CA-C-O	-5.07	115.50	120.82
1	D	299	GLU	N-CA-C	5.07	118.33	110.17
1	A	4	GLN	CA-C-O	5.07	126.48	120.66
1	A	274	LEU	CA-C-O	-5.06	115.51	120.82
1	A	330	GLU	N-CA-CB	5.06	117.65	110.16
1	B	177	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	212	PHE	N-CA-C	5.05	117.64	109.40
1	A	383	ASN	CA-CB-CG	-5.05	107.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	ALA	CA-C-N	5.05	125.55	119.94
1	D	196	ALA	C-N-CA	5.05	125.55	119.94
1	B	189	GLY	N-CA-C	-5.05	106.67	112.73
1	B	295	PRO	N-CA-C	-5.05	103.18	110.80
1	C	158	TYR	N-CA-C	-5.05	105.86	111.36
1	A	319	LYS	CA-C-N	5.04	127.00	120.44
1	A	319	LYS	C-N-CA	5.04	127.00	120.44
1	B	96	HIS	CA-C-N	5.04	125.32	119.47
1	B	96	HIS	C-N-CA	5.04	125.32	119.47
1	D	276	GLU	N-CA-C	5.04	119.50	112.90
1	A	57	ASP	N-CA-C	-5.04	105.50	111.69
1	A	289	ARG	N-CA-C	-5.04	97.24	107.41
1	B	228	PHE	CA-C-O	-5.03	115.71	121.00
1	A	205	GLU	OE1-CD-OE2	-5.03	110.83	122.90
1	C	15	LEU	CA-C-N	5.03	131.38	121.58
1	C	15	LEU	C-N-CA	5.03	131.38	121.58
1	A	70	GLY	O-C-N	5.02	127.00	122.18
1	A	68	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	B	276	GLU	CG-CD-OE1	-5.02	106.86	118.40
1	A	230	GLN	CA-C-N	5.01	125.54	119.98
1	A	230	GLN	C-N-CA	5.01	125.54	119.98
1	D	228	PHE	CA-C-O	-5.01	115.56	120.82
1	C	95	THR	CA-CB-OG1	-5.00	102.09	109.60

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	3053	0	2954	36	0
1	B	3053	0	2954	45	0
1	C	3053	0	2954	31	0
1	D	3053	0	2954	35	0
2	A	12	0	12	0	0
2	B	12	0	12	1	0
2	C	12	0	12	0	0
2	D	12	0	13	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	218	0	0	1	0
4	B	206	0	0	3	0
4	C	234	0	0	1	0
4	D	210	0	0	8	0
All	All	13132	0	11865	128	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 5.

All (128) 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	1.64	1.12
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.75	1.00
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.49	0.94
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.20	0.90
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.20	0.89
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.29	0.80
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.27	0.80
1:A:204:GLN:HG2	4:A:548:HOH:O	1.85	0.76
1:C:59:VAL:HG11	1:C:68:ARG:HG3	1.68	0.75
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.72	0.71
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.74	0.68
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.31	0.66
1:B:294:LYS:HE2	4:B:556:HOH:O	1.96	0.65
1:A:238:HIS:O	1:A:239:LYS:HB2	1.97	0.64
1:D:3:VAL:HB	4:D:591:HOH:O	1.97	0.63
1:B:3:VAL:HG12	1:B:4:GLN:H	1.64	0.61
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.83	0.61
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.83	0.60
1:C:41:HIS:HE1	4:C:522:HOH:O	1.85	0.59
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.86	0.58
1:B:317:LEU:O	1:B:321:ARG:HD2	2.05	0.57
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.40	0.57
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.68	0.57
1:D:186:GLU:OE1	1:D:255:ASP:HB2	2.05	0.56
1:C:228:PHE:CE1	1:C:232:ILE:HD11	2.40	0.55
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.87	0.55
1:D:394:ARG:HD2	4:D:599:HOH:O	2.07	0.55
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.88	0.54
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.42	0.54
1:A:36:PRO:O	1:A:40:VAL:HG23	2.07	0.54
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.12	0.54
1:D:394:ARG:NH1	4:D:599:HOH:O	1.92	0.53
1:D:72:ILE:O	1:D:76:LYS:HG3	2.07	0.53
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.91	0.53
1:D:52:THR:HG21	1:D:88:MET:HE3	1.90	0.53
1:D:3:VAL:HG23	4:D:591:HOH:O	2.09	0.52
1:B:354:TYR:HB3	1:D:164:LEU:HD21	1.92	0.52
1:A:60:PRO:O	1:A:61:PHE:C	2.53	0.51
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.44	0.51
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.93	0.50
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.92	0.50
1:D:356:GLU:O	1:D:359:ALA:HB3	2.11	0.50
1:B:77:LYS:O	1:B:80:ASP:HB2	2.11	0.50
1:C:72:ILE:O	1:C:76:LYS:HG3	2.12	0.50
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.46	0.50
1:D:3:VAL:CB	4:D:591:HOH:O	2.59	0.49
1:A:65:ALA:O	1:A:69:ASP:HB2	2.13	0.48
1:B:287:GLY:O	1:B:289:ARG:NH1	2.39	0.48
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.13	0.48
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.96	0.47
1:B:68:ARG:HH11	1:B:68:ARG:CG	2.24	0.47
1:B:219:GLY:O	1:B:223:MET:HG3	2.14	0.47
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.95	0.47
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.95	0.47
1:A:388:GLU:OE2	1:D:313:ARG:HD3	2.14	0.47
1:B:72:ILE:O	1:B:76:LYS:HG3	2.14	0.47
1:A:96:HIS:ND1	1:A:98:VAL:HG12	2.30	0.47
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.42	0.46
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.98	0.46
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.49	0.46
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.81	0.46
1:D:338:SER:HB3	1:D:379:PHE:CE1	2.51	0.46
1:D:50:GLY:HA2	1:D:85:ILE:O	2.15	0.46
1:A:164:LEU:C	1:A:164:LEU:HD23	2.41	0.46
1:B:36:PRO:O	1:B:40:VAL:HG23	2.15	0.46
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.51	0.46
1:B:352:GLU:HG2	1:B:356:GLU:HB2	1.98	0.45
1:A:186:GLU:HA	1:A:187:PRO:HA	1.78	0.45
1:C:238:HIS:O	1:C:239:LYS:HB2	2.16	0.45
1:D:116:ILE:HD13	1:D:116:ILE:HG21	1.78	0.45
1:A:42:LYS:HA	1:A:42:LYS:HD3	1.70	0.45
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.51	0.45
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.16	0.45
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.71	0.45
1:D:238:HIS:O	1:D:239:LYS:HB2	2.16	0.45
1:A:164:LEU:HD21	1:C:354:TYR:HB3	2.00	0.44
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.52	0.44
1:A:305:TRP:O	1:A:309:LYS:HG3	2.17	0.44
1:A:348:LEU:HD11	1:C:164:LEU:HD12	1.98	0.44
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.17	0.44
1:C:86:VAL:O	1:C:131:ALA:HA	2.18	0.44
1:D:3:VAL:CG2	4:D:591:HOH:O	2.65	0.44
1:A:94:PHE:HA	1:A:140:ARG:HG3	1.99	0.44
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.00	0.44
1:B:101:ASP:CG	1:B:101:ASP:O	2.61	0.44
1:A:204:GLN:CD	1:C:204:GLN:OE1	2.53	0.43
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.32	0.43
1:B:42:LYS:O	1:B:46:ILE:HG23	2.17	0.43
1:B:7:ARG:HD3	4:B:492:HOH:O	2.19	0.43
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.82	0.43
1:D:184:PRO:HD3	4:D:459:HOH:O	2.18	0.43
1:B:121:ARG:HD3	4:B:440:HOH:O	2.17	0.43
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.96	0.43
1:A:6:THR:O	1:A:9:ASP:HB2	2.19	0.42
1:A:348:LEU:HD11	1:C:164:LEU:CD1	2.48	0.42
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.88	0.42
1:D:279:PRO:O	4:D:526:HOH:O	2.22	0.42
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:CG	1:B:68:ARG:NH1	2.81	0.42
1:B:142:GLY:HA3	1:B:190:ASP:O	2.18	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.88	0.42
1:C:101:ASP:O	1:C:101:ASP:CG	2.62	0.42
1:A:23:ARG:CG	1:B:23:ARG:NH1	2.83	0.41
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.50	0.41
1:B:193:LEU:N	1:B:194:PRO:HD3	2.34	0.41
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.90	0.41
1:B:46:ILE:CD1	1:B:308:ALA:HB1	2.50	0.41
1:A:92:ASN:OD1	1:A:92:ASN:C	2.62	0.41
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.82	0.41
1:D:277:ASN:OD1	1:D:323:LYS:HD2	2.21	0.41
1:B:34:LEU:HD21	1:B:39:ALA:HB2	2.03	0.41
1:B:35:ASP:HA	1:B:36:PRO:HD3	1.93	0.41
1:B:90:THR:HG21	2:B:397:SOR:H61	2.02	0.41
1:C:6:THR:OG1	1:C:8:GLU:HB3	2.21	0.41
1:C:15:LEU:HD12	1:C:15:LEU:HA	1.81	0.41
1:D:178:PHE:HB2	1:D:212:PHE:CD1	2.56	0.41
1:D:186:GLU:HA	1:D:187:PRO:HA	1.82	0.41
1:B:232:ILE:HD13	1:B:232:ILE:HA	1.89	0.40
1:A:236:LEU:HD23	1:A:236:LEU:HA	1.92	0.40
1:B:278:GLY:CA	1:B:282:ALA:O	2.69	0.40
1:B:280:ASP:C	1:B:282:ALA:H	2.28	0.40
1:C:319:LYS:O	1:C:323:LYS:HG2	2.22	0.40
1:A:298:THR:HA	1:B:100:LYS:HD2	2.02	0.40
1:B:216:PRO:HG2	1:B:232:ILE:HD11	2.04	0.40
1:B:354:TYR:CD1	1:B:354:TYR:C	3.00	0.40
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.34	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%)	377 (97%)	11 (3%)	2 (0%)	24	46
1	B	390/393 (99%)	376 (96%)	12 (3%)	2 (0%)	24	46
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	12	28
1	D	390/393 (99%)	374 (96%)	15 (4%)	1 (0%)	36	58
All	All	1560/1572 (99%)	1501 (96%)	50 (3%)	9 (1%)	21	42

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	C	279	PRO
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	D	186	GLU
1	A	364	PHE
1	B	364	PHE
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%)	293 (96%)	13 (4%)	26	52
1	B	306/310 (99%)	300 (98%)	6 (2%)	48	74
1	C	306/310 (99%)	300 (98%)	6 (2%)	48	74
1	D	306/310 (99%)	299 (98%)	7 (2%)	44	71
All	All	1224/1240 (99%)	1192 (97%)	32 (3%)	40	68

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	23	ARG

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Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	TYR
1	A	76	LYS
1	A	80	ASP
1	A	84	LEU
1	A	177	ARG
1	A	185	ASN
1	A	187	PRO
1	A	203	VAL
1	A	208	ARG
1	A	394	ARG
1	B	3	VAL
1	B	49	TYR
1	B	81	GLU
1	B	84	LEU
1	B	203	VAL
1	B	394	ARG
1	C	3	VAL
1	C	38	GLU
1	C	80	ASP
1	C	84	LEU
1	C	203	VAL
1	C	279	PRO
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG

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	230	GLN
1	A	234	GLN
1	A	238	HIS
1	B	204	GLN
1	B	222	GLN
1	B	238	HIS
1	B	256	GLN

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Mol	Chain	Res	Type
1	C	41	HIS
1	C	222	GLN
1	C	238	HIS
1	D	167	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	SOR	B	397	3	11,11,11	1.02	1 (9%)	14,14,14	1.69	4 (28%)
2	SOR	D	397	3	11,11,11	1.15	0	14,14,14	1.38	3 (21%)
2	SOR	A	397	3	11,11,11	1.06	0	14,14,14	1.77	5 (35%)
2	SOR	C	397	3	11,11,11	0.94	0	14,14,14	1.77	5 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SOR	B	397	3	-	3/16/16/16	-
2	SOR	D	397	3	-	2/16/16/16	-
2	SOR	A	397	3	-	1/16/16/16	-
2	SOR	C	397	3	-	2/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	397	SOR	C2-C3	2.00	1.56	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	397	SOR	O6-C6-C5	-3.41	103.99	111.16
2	B	397	SOR	C2-C3-C4	-2.83	108.13	112.48
2	A	397	SOR	C2-C3-C4	-2.81	108.17	112.48
2	A	397	SOR	O4-C4-C5	2.77	115.23	108.93
2	D	397	SOR	O6-C6-C5	-2.76	105.36	111.16
2	B	397	SOR	O4-C4-C3	2.74	115.87	109.46
2	C	397	SOR	O5-C5-C6	2.72	115.21	109.03
2	C	397	SOR	C2-C3-C4	-2.63	108.44	112.48
2	B	397	SOR	O6-C6-C5	-2.56	105.78	111.16
2	A	397	SOR	C5-C4-C3	2.50	116.31	112.48
2	A	397	SOR	C6-C5-C4	2.35	116.97	112.17
2	C	397	SOR	C6-C5-C4	-2.34	107.40	112.17
2	B	397	SOR	O4-C4-C5	2.33	114.23	108.93
2	D	397	SOR	O4-C4-C5	2.30	114.17	108.93
2	D	397	SOR	C2-C3-C4	-2.21	109.08	112.48
2	C	397	SOR	O1-C1-C2	-2.11	106.72	111.16
2	A	397	SOR	O6-C6-C5	-2.04	106.88	111.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	397	SOR	O5-C5-C6-O6
2	C	397	SOR	O5-C5-C6-O6
2	B	397	SOR	O4-C4-C5-C6
2	D	397	SOR	C4-C5-C6-O6
2	A	397	SOR	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	397	SOR	O3-C3-C4-C5
2	B	397	SOR	O4-C4-C5-O5
2	C	397	SOR	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	397	SOR	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.