



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:44 AM UTC

PDB ID : 3XIN / pdb_00003xin
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 : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

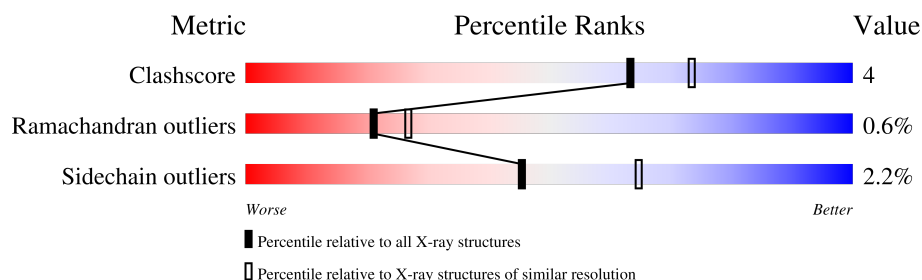
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	76% 20% . .
1	B	393	76% 20% .
1	C	393	77% 20% .
1	D	393	74% 22% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13116 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	533	577	4			
1	B	392	Total	C	N	O	S	0	0	0
			3053	1939	533	577	4			
1	C	392	Total	C	N	O	S	0	0	0
			3053	1939	533	577	4			
1	D	392	Total	C	N	O	S	0	0	0
			3053	1939	533	577	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	GLN	GLU	conflict	UNP P12851
B	181	GLN	GLU	conflict	UNP P12851
C	181	GLN	GLU	conflict	UNP P12851
D	181	GLN	GLU	conflict	UNP P12851

- Molecule 2 is water.

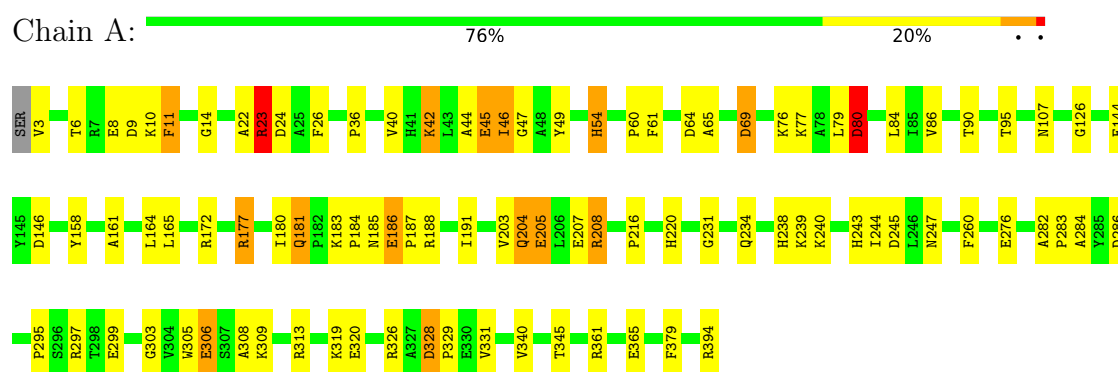
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	229	Total	O	0	0
			229	229		
2	B	221	Total	O	0	0
			221	221		
2	C	238	Total	O	0	0
			238	238		
2	D	216	Total	O	0	0
			216	216		

3 Residue-property plots

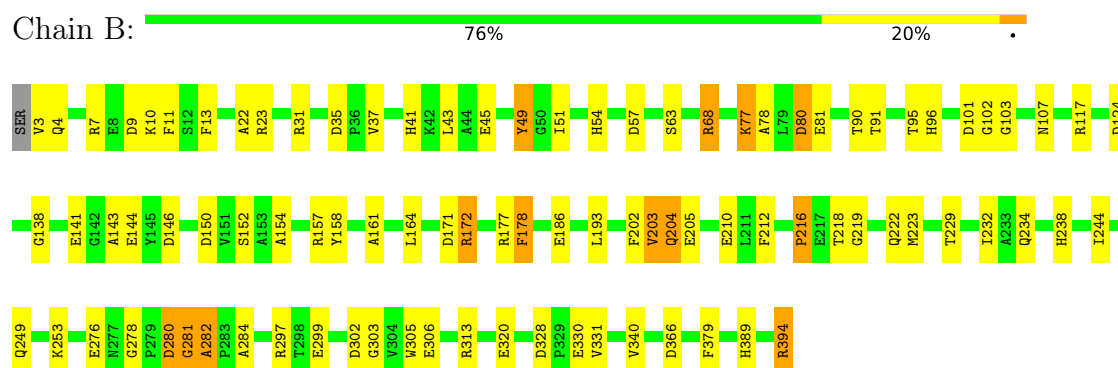
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

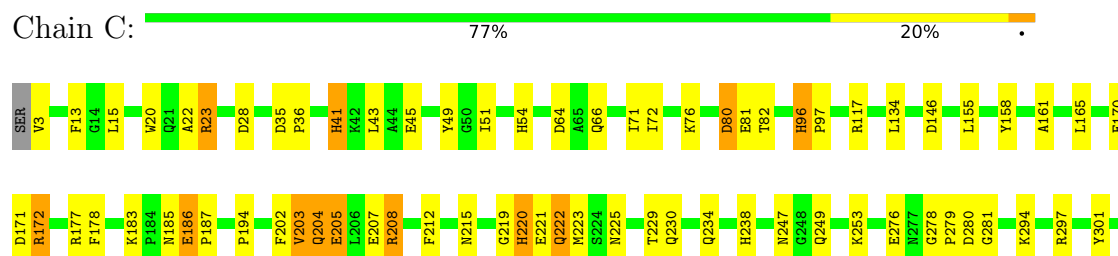
• Molecule 1: D-XYLOSE ISOMERASE



• Molecule 1: D-XYLOSE ISOMERASE

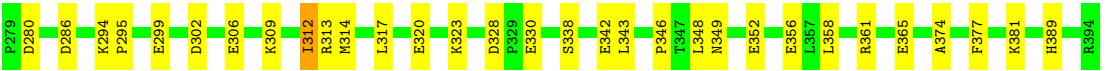
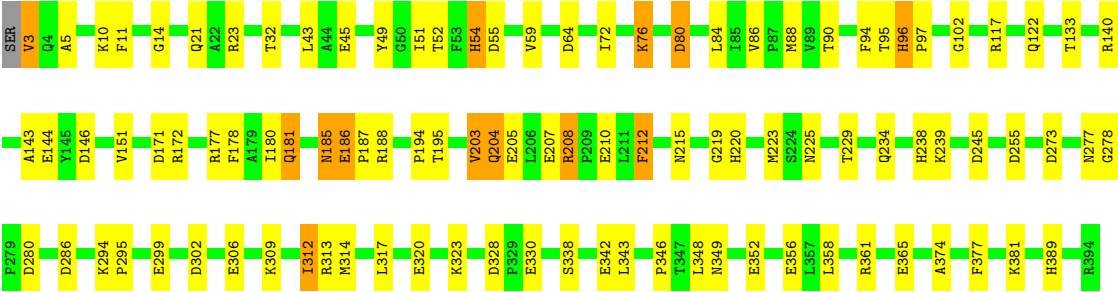


• Molecule 1: D-XYLOSE ISOMERASE





● 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) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.153 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13116	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.96	0/3125	1.95	78/4233 (1.8%)
1	B	0.95	1/3125 (0.0%)	1.92	83/4233 (2.0%)
1	C	0.96	0/3125	1.91	76/4233 (1.8%)
1	D	0.96	0/3125	1.93	74/4233 (1.7%)
All	All	0.96	1/12500 (0.0%)	1.93	311/16932 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	GLY	CA-C	6.66	1.56	1.51

All (311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	CA-CB-CG	-15.13	97.47	112.60
1	B	204	GLN	OE1-CD-NE2	-12.72	109.88	122.60
1	D	204	GLN	OE1-CD-NE2	-12.00	110.60	122.60
1	A	204	GLN	OE1-CD-NE2	-10.69	111.91	122.60
1	A	286	ASP	CA-CB-CG	-10.13	102.47	112.60
1	B	394	ARG	NE-CZ-NH2	-10.10	110.11	119.20
1	C	204	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	379	PHE	CA-CB-CG	9.00	122.80	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ASP	CA-CB-CG	-8.54	104.06	112.60
1	B	172	ARG	NE-CZ-NH1	8.45	129.95	121.50
1	A	244	ILE	CA-C-O	-8.34	111.97	120.90
1	D	313	ARG	NE-CZ-NH2	8.27	126.64	119.20
1	A	394	ARG	NH1-CZ-NH2	8.11	129.85	119.30
1	D	54	HIS	N-CA-C	-8.11	97.42	110.32
1	A	107	ASN	CA-CB-CG	8.10	120.70	112.60
1	D	172	ARG	CD-NE-CZ	7.99	135.59	124.40
1	A	172	ARG	CD-NE-CZ	7.86	135.41	124.40
1	D	80	ASP	CA-CB-CG	-7.83	104.77	112.60
1	A	188	ARG	CD-NE-CZ	7.83	135.36	124.40
1	B	394	ARG	N-CA-CB	7.77	123.70	110.50
1	D	328	ASP	CA-CB-CG	7.76	120.36	112.60
1	D	122	GLN	OE1-CD-NE2	-7.74	114.86	122.60
1	D	328	ASP	CA-C-O	7.73	125.04	119.32
1	C	54	HIS	N-CA-C	-7.69	99.14	110.52
1	C	28	ASP	CA-CB-CG	7.61	120.21	112.60
1	A	26	PHE	CA-C-O	-7.57	110.55	119.48
1	B	13	PHE	CA-CB-CG	7.50	121.30	113.80
1	C	146	ASP	CA-C-O	-7.48	112.62	120.55
1	C	301	TYR	CA-C-O	-7.45	111.69	120.10
1	D	55	ASP	CA-CB-CG	7.38	119.98	112.60
1	C	64	ASP	CA-CB-CG	-7.26	105.33	112.60
1	C	172	ARG	NE-CZ-NH2	-7.24	112.69	119.20
1	C	208	ARG	CD-NE-CZ	-7.16	114.37	124.40
1	D	313	ARG	N-CA-CB	7.09	120.29	110.01
1	B	117	ARG	NE-CZ-NH1	7.00	128.50	121.50
1	B	95	THR	N-CA-C	6.98	119.91	111.40
1	A	172	ARG	NE-CZ-NH1	6.96	128.46	121.50
1	C	45	GLU	CA-CB-CG	6.95	128.01	114.10
1	D	144	GLU	N-CA-C	-6.94	105.08	113.97
1	C	134	LEU	CA-C-O	-6.93	112.69	120.32
1	D	286	ASP	CA-CB-CG	-6.92	105.68	112.60
1	D	10	LYS	CB-CA-C	-6.83	102.19	111.89
1	D	286	ASP	CA-C-O	-6.82	111.44	119.48
1	A	394	ARG	CA-CB-CG	6.73	127.56	114.10
1	C	229	THR	CA-CB-OG1	-6.64	99.63	109.60
1	B	171	ASP	CA-C-O	-6.62	113.41	120.42
1	A	220	HIS	CA-C-O	-6.62	113.87	120.82
1	B	161	ALA	CA-C-O	-6.61	113.41	120.42
1	D	203	VAL	CB-CA-C	6.61	120.70	112.04
1	A	181	GLN	OE1-CD-NE2	-6.61	115.99	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	PHE	CA-C-O	-6.60	113.17	120.69
1	D	181	GLN	OE1-CD-NE2	-6.55	116.05	122.60
1	C	340	VAL	CB-CA-C	6.54	120.26	111.88
1	B	150	ASP	CA-CB-CG	-6.52	106.08	112.60
1	D	171	ASP	CA-C-O	-6.51	113.65	120.55
1	A	95	THR	N-CA-C	6.49	118.14	111.14
1	C	172	ARG	CD-NE-CZ	-6.48	115.33	124.40
1	C	185	ASN	O-C-N	6.48	129.77	123.29
1	D	342	GLU	CG-CD-OE2	6.47	133.28	118.40
1	C	170	GLU	CA-C-O	-6.47	114.04	120.70
1	C	96	HIS	CA-CB-CG	-6.45	107.35	113.80
1	C	172	ARG	NE-CZ-NH1	6.45	127.95	121.50
1	D	320	GLU	CA-CB-CG	6.45	127.00	114.10
1	A	207	GLU	CA-CB-CG	6.44	126.98	114.10
1	C	194	PRO	N-CA-C	6.39	121.85	113.86
1	D	255	ASP	CA-CB-CG	6.39	118.99	112.60
1	C	80	ASP	CA-CB-CG	-6.34	106.26	112.60
1	D	389	HIS	CA-CB-CG	-6.34	107.46	113.80
1	A	181	GLN	O-C-N	6.32	127.13	121.19
1	B	57	ASP	N-CA-C	-6.32	103.92	111.69
1	C	177	ARG	N-CA-C	-6.32	99.91	109.95
1	C	328	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	328	ASP	CA-CB-CG	6.30	118.91	112.60
1	D	96	HIS	CA-CB-CG	-6.28	107.52	113.80
1	D	21	GLN	CB-CG-CD	-6.27	101.94	112.60
1	B	172	ARG	NE-CZ-NH2	-6.24	113.58	119.20
1	A	240	LYS	CA-C-O	-6.22	112.14	119.48
1	A	244	ILE	O-C-N	6.21	130.29	123.09
1	A	79	LEU	CA-C-O	6.20	127.12	120.55
1	C	177	ARG	N-CA-CB	6.20	120.77	110.85
1	C	328	ASP	CA-C-N	6.19	126.09	119.28
1	C	328	ASP	C-N-CA	6.19	126.09	119.28
1	B	394	ARG	CD-NE-CZ	-6.18	115.75	124.40
1	B	107	ASN	N-CA-C	-6.15	104.58	111.28
1	C	117	ARG	NE-CZ-NH1	6.13	127.63	121.50
1	C	215	ASN	CA-CB-CG	-6.13	106.47	112.60
1	D	255	ASP	CA-C-O	-6.12	113.34	120.62
1	B	229	THR	CA-CB-OG1	-6.11	100.44	109.60
1	A	177	ARG	N-CA-C	-6.11	99.95	109.72
1	A	320	GLU	CB-CG-CD	6.10	122.97	112.60
1	C	278	GLY	CA-C-N	6.09	127.45	119.84
1	C	278	GLY	C-N-CA	6.09	127.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ARG	CA-C-O	-6.08	114.07	120.58
1	B	276	GLU	N-CA-C	6.07	120.82	113.41
1	C	394	ARG	CD-NE-CZ	-6.07	115.91	124.40
1	A	243	HIS	CA-CB-CG	6.06	119.86	113.80
1	C	331	VAL	N-CA-C	-6.05	104.84	110.53
1	A	216	PRO	CA-C-O	-6.05	114.29	121.67
1	D	95	THR	N-CA-C	6.05	118.78	111.40
1	B	77	LYS	O-C-N	6.05	128.30	122.07
1	C	328	ASP	CB-CA-C	6.02	119.17	109.41
1	D	309	LYS	CA-C-O	-6.01	114.17	120.55
1	B	330	GLU	OE1-CD-OE2	6.01	137.33	122.90
1	B	45	GLU	CB-CG-CD	6.00	122.79	112.60
1	D	342	GLU	CB-CG-CD	5.99	122.78	112.60
1	C	23	ARG	N-CA-C	-5.98	98.79	108.41
1	D	312	ILE	CA-C-O	-5.94	114.56	120.85
1	A	306	GLU	CB-CA-C	-5.91	101.60	110.88
1	A	231	GLY	CA-C-N	5.91	128.81	120.42
1	A	231	GLY	C-N-CA	5.91	128.81	120.42
1	C	81	GLU	CB-CG-CD	5.89	122.62	112.60
1	C	203	VAL	N-CA-CB	-5.89	102.53	110.54
1	B	158	TYR	N-CA-C	-5.88	104.78	111.14
1	B	90	THR	CA-CB-OG1	-5.88	100.78	109.60
1	D	328	ASP	CB-CA-C	5.87	117.83	109.38
1	C	247	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	D	195	THR	CA-CB-OG1	-5.86	100.81	109.60
1	B	54	HIS	N-CA-C	-5.85	100.75	110.17
1	C	389	HIS	CA-CB-CG	-5.85	107.95	113.80
1	C	219	GLY	CA-C-O	-5.84	114.73	120.75
1	A	295	PRO	N-CA-C	-5.84	101.98	110.80
1	C	354	TYR	CA-C-O	-5.83	113.51	120.10
1	A	345	THR	O-C-N	5.83	127.60	121.42
1	B	77	LYS	CB-CA-C	-5.81	101.76	110.88
1	B	281	GLY	CA-C-N	5.80	130.14	120.86
1	B	281	GLY	C-N-CA	5.80	130.14	120.86
1	B	328	ASP	CA-C-O	5.80	123.93	119.46
1	D	54	HIS	N-CA-CB	5.78	119.83	110.41
1	B	253	LYS	CA-C-O	-5.78	114.95	121.25
1	A	340	VAL	O-C-N	5.78	127.47	121.87
1	A	180	ILE	CB-CA-C	-5.76	103.66	111.15
1	D	10	LYS	O-C-N	5.74	129.67	122.55
1	C	66	GLN	N-CA-C	-5.73	104.94	111.07
1	B	178	PHE	O-C-N	5.72	130.10	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	96	HIS	CA-CB-CG	-5.71	108.08	113.80
1	D	239	LYS	O-C-N	5.70	130.00	122.47
1	B	141	GLU	CB-CG-CD	5.68	122.26	112.60
1	D	338	SER	CA-CB-OG	-5.68	99.73	111.10
1	C	349	ASN	N-CA-C	-5.68	101.95	110.24
1	B	68	ARG	NE-CZ-NH1	-5.67	115.83	121.50
1	B	31	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	C	155	LEU	CB-CA-C	5.66	120.18	110.79
1	B	280	ASP	N-CA-C	-5.65	103.48	111.56
1	A	8	GLU	CA-CB-CG	-5.64	102.82	114.10
1	A	394	ARG	NE-CZ-NH1	-5.63	115.86	121.50
1	D	59	VAL	O-C-N	5.63	126.10	120.92
1	D	299	GLU	N-CA-C	5.62	119.13	110.42
1	B	157	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	D	76	LYS	O-C-N	5.62	128.79	122.22
1	D	143	ALA	O-C-N	5.62	129.02	123.46
1	A	319	LYS	CA-C-O	5.61	126.91	120.90
1	B	54	HIS	N-CA-CB	5.61	119.77	110.63
1	B	103	GLY	N-CA-C	-5.61	105.11	110.21
1	A	10	LYS	CB-CA-C	-5.60	104.35	111.86
1	D	349	ASN	CA-CB-CG	-5.59	107.01	112.60
1	A	284	ALA	N-CA-C	-5.58	106.31	113.23
1	B	216	PRO	CB-CA-C	5.57	118.60	110.63
1	B	210	GLU	CB-CG-CD	5.56	122.06	112.60
1	A	146	ASP	CA-C-O	-5.55	114.67	120.55
1	A	69	ASP	CA-CB-CG	-5.54	107.06	112.60
1	B	146	ASP	CA-C-O	-5.53	114.69	120.55
1	C	41	HIS	CA-C-O	-5.52	115.01	120.70
1	C	322	ALA	N-CA-C	-5.52	105.34	111.36
1	D	229	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	204	GLN	CB-CG-CD	5.52	121.98	112.60
1	D	94	PHE	CA-C-O	-5.51	112.19	118.47
1	D	220	HIS	O-C-N	5.51	127.96	122.12
1	B	144	GLU	N-CA-C	-5.50	107.11	113.88
1	A	46	ILE	CA-C-O	-5.49	112.41	119.39
1	B	63	SER	O-C-N	5.49	129.62	123.19
1	C	64	ASP	N-CA-C	-5.49	103.14	110.55
1	D	188	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	A	340	VAL	CA-C-O	-5.48	115.25	120.95
1	A	328	ASP	CA-C-O	5.48	124.91	119.49
1	D	277	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	B	193	LEU	O-C-N	5.47	127.61	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	GLU	N-CA-C	5.47	118.98	110.17
1	B	10	LYS	CB-CA-C	-5.47	104.12	111.89
1	A	331	VAL	N-CA-C	-5.47	105.20	110.72
1	B	177	ARG	N-CA-C	-5.46	101.26	109.95
1	B	379	PHE	CA-CB-CG	5.46	119.27	113.80
1	C	281	GLY	N-CA-C	-5.46	100.23	113.18
1	B	218	THR	CA-C-N	5.46	126.04	119.98
1	B	218	THR	C-N-CA	5.46	126.04	119.98
1	A	394	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	A	80	ASP	O-C-N	5.44	127.69	122.03
1	D	212	PHE	N-CA-C	5.44	118.27	109.40
1	A	54	HIS	N-CA-C	-5.44	101.41	110.17
1	A	260	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	45	GLU	CA-CB-CG	5.44	124.98	114.10
1	C	335	LEU	O-C-N	5.44	128.35	122.15
1	C	15	LEU	CA-C-O	5.44	126.31	120.55
1	A	276	GLU	N-CA-C	5.43	120.00	112.45
1	C	306	GLU	CG-CD-OE1	5.43	130.89	118.40
1	D	194	PRO	N-CA-C	5.42	120.68	113.57
1	B	340	VAL	CB-CA-C	5.41	118.89	111.97
1	C	225	ASN	OD1-CG-ND2	-5.40	117.20	122.60
1	C	276	GLU	CG-CD-OE2	5.40	130.82	118.40
1	C	294	LYS	CB-CA-C	-5.40	102.97	110.16
1	A	313	ARG	N-CA-CB	-5.40	102.18	110.01
1	D	52	THR	CA-C-O	-5.40	115.32	121.58
1	B	389	HIS	CA-CB-CG	-5.40	108.40	113.80
1	C	71	ILE	O-C-N	5.39	127.19	121.91
1	C	379	PHE	CA-CB-CG	5.39	119.19	113.80
1	B	80	ASP	O-C-N	5.38	127.83	122.08
1	B	54	HIS	CB-CA-C	-5.37	100.42	109.50
1	D	45	GLU	CA-C-O	-5.37	114.03	120.10
1	B	177	ARG	CA-C-O	-5.37	115.10	121.16
1	B	303	GLY	N-CA-C	-5.36	106.30	112.73
1	D	204	GLN	CB-CG-CD	5.35	121.69	112.60
1	D	210	GLU	CB-CG-CD	5.35	121.69	112.60
1	B	138	GLY	CA-C-N	5.34	126.82	120.14
1	B	138	GLY	C-N-CA	5.34	126.82	120.14
1	A	185	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	B	394	ARG	NH1-CZ-NH2	5.34	126.24	119.30
1	C	82	THR	CA-CB-OG1	-5.34	101.59	109.60
1	B	244	ILE	CA-C-O	-5.34	115.19	120.90
1	D	377	PHE	CA-C-O	-5.34	113.07	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	185	ASN	CA-C-O	-5.33	115.58	121.28
1	A	286	ASP	N-CA-C	5.32	120.43	113.30
1	B	41	HIS	CA-CB-CG	-5.32	108.48	113.80
1	B	124	ASP	O-C-N	5.32	127.55	122.07
1	B	320	GLU	CB-CG-CD	5.32	121.64	112.60
1	C	253	LYS	CA-C-O	-5.31	115.46	121.25
1	D	358	LEU	CA-C-O	5.31	126.10	120.10
1	A	394	ARG	CD-NE-CZ	-5.30	116.97	124.40
1	A	247	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	B	102	GLY	CA-C-O	-5.29	118.50	122.37
1	B	394	ARG	CB-CA-C	-5.29	100.05	110.10
1	D	143	ALA	N-CA-CB	-5.29	103.52	111.56
1	D	346	PRO	CA-C-O	-5.28	115.51	121.43
1	D	302	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	144	GLU	N-CA-C	-5.27	107.22	113.97
1	A	240	LYS	O-C-N	5.27	128.56	122.19
1	A	191	ILE	CA-C-O	-5.27	114.73	120.84
1	C	222	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	A	64	ASP	N-CA-C	-5.26	103.94	110.41
1	A	42	LYS	CB-CG-CD	-5.26	99.21	111.30
1	C	220	HIS	CA-C-O	-5.25	114.85	120.42
1	B	171	ASP	N-CA-CB	5.25	117.93	110.16
1	C	223	MET	N-CA-C	-5.25	106.14	112.54
1	D	64	ASP	N-CA-C	-5.25	103.61	110.53
1	D	151	VAL	N-CA-C	5.24	115.97	110.62
1	C	41	HIS	CA-CB-CG	-5.22	108.58	113.80
1	B	202	PHE	CA-C-N	5.21	128.71	120.47
1	B	202	PHE	C-N-CA	5.21	128.71	120.47
1	C	360	ASP	CA-C-O	5.21	126.34	120.92
1	D	374	ALA	CA-C-O	-5.21	112.98	119.18
1	B	177	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	D	306	GLU	CB-CA-C	-5.20	102.72	110.88
1	B	96	HIS	CA-C-O	-5.20	114.77	120.17
1	D	177	ARG	N-CA-C	-5.19	101.42	109.72
1	C	202	PHE	CA-C-N	5.19	127.56	120.46
1	C	202	PHE	C-N-CA	5.19	127.56	120.46
1	D	117	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	D	86	VAL	O-C-N	5.18	127.01	121.10
1	A	286	ASP	CB-CA-C	-5.18	101.42	110.17
1	C	171	ASP	CA-CB-CG	-5.18	107.42	112.60
1	B	143	ALA	N-CA-CB	-5.17	102.88	111.57
1	A	107	ASN	N-CA-C	-5.17	105.83	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	GLY	N-CA-C	-5.16	103.30	112.54
1	B	313	ARG	CA-C-N	5.16	127.15	120.44
1	B	313	ARG	C-N-CA	5.16	127.15	120.44
1	B	331	VAL	N-CA-C	-5.16	105.51	110.72
1	D	203	VAL	N-CA-CB	-5.16	104.03	110.47
1	B	305	TRP	CA-CB-CG	-5.15	103.81	113.60
1	B	91	THR	CA-C-O	-5.15	115.14	120.70
1	A	208	ARG	CA-CB-CG	5.14	124.38	114.10
1	C	23	ARG	CA-C-O	-5.14	115.08	120.58
1	C	331	VAL	CB-CA-C	5.13	118.75	112.02
1	C	311	ASN	O-C-N	5.13	127.35	122.07
1	D	302	ASP	CA-C-O	-5.12	115.45	120.82
1	D	349	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	C	221	GLU	CB-CG-CD	5.11	121.29	112.60
1	A	158	TYR	CA-C-N	5.11	127.08	120.44
1	A	158	TYR	C-N-CA	5.11	127.08	120.44
1	C	185	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	308	ALA	N-CA-C	-5.11	105.63	111.14
1	A	44	ALA	CA-C-O	5.10	125.96	120.55
1	D	215	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	126	GLY	CA-C-N	5.09	127.11	120.28
1	A	126	GLY	C-N-CA	5.09	127.11	120.28
1	A	286	ASP	CA-C-O	-5.09	113.26	119.32
1	A	24	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	35	ASP	CB-CA-C	5.09	117.66	109.41
1	C	172	ARG	CB-CG-CD	-5.08	99.60	111.30
1	A	14	GLY	N-CA-C	-5.08	103.44	112.54
1	A	220	HIS	O-C-N	5.08	127.31	122.07
1	B	366	ASP	CA-C-O	-5.08	113.96	119.95
1	C	13	PHE	CA-C-O	-5.08	115.17	121.06
1	C	230	GLN	CA-C-O	-5.07	115.18	120.55
1	A	205	GLU	CG-CD-OE2	5.07	130.05	118.40
1	C	361	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	C	332	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	B	57	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	177	ARG	CB-CG-CD	-5.05	99.68	111.30
1	C	158	TYR	N-CA-C	-5.05	105.86	111.36
1	B	284	ALA	N-CA-C	-5.05	106.63	112.89
1	B	302	ASP	O-C-N	5.04	127.90	122.15
1	C	207	GLU	CA-C-O	-5.04	115.51	120.70
1	A	86	VAL	O-C-N	5.04	126.84	121.10
1	D	146	ASP	O-C-N	5.03	127.45	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	GLU	CA-C-O	-5.03	115.54	120.82
1	D	273	ASP	CA-CB-CG	5.03	117.62	112.60
1	B	282	ALA	N-CA-C	5.02	117.29	110.01
1	D	314	MET	N-CA-CB	5.02	117.42	109.94
1	D	207	GLU	CA-CB-CG	5.02	124.14	114.10
1	D	225	ASN	OD1-CG-ND2	-5.01	117.58	122.60
1	A	47	GLY	N-CA-C	5.01	122.21	115.00
1	C	205	GLU	CG-CD-OE2	5.01	129.92	118.40
1	D	32	THR	CA-CB-OG1	-5.00	102.10	109.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	2956	29	0
1	B	3053	0	2956	29	0
1	C	3053	0	2956	23	0
1	D	3053	0	2956	28	0
2	A	229	0	0	1	0
2	B	221	0	0	0	0
2	C	238	0	0	1	0
2	D	216	0	0	4	0
All	All	13116	0	11824	96	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 (96) 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:204:GLN:OE1	1:D:204:GLN:OE1	1.59	1.18
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.61	1.15
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.17	0.92
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.19	0.86
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.22	0.82
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.25	0.82
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.68	0.75
1:B:3:VAL:HG12	1:B:4:GLN:H	1.57	0.69
1:D:3:VAL:HG23	2:D:591:HOH:O	1.96	0.65
1:A:204:GLN:HG2	2:A:546:HOH:O	1.99	0.63
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.80	0.62
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.83	0.61
1:A:36:PRO:O	1:A:40:VAL:HG23	2.02	0.59
1:B:77:LYS:O	1:B:80:ASP:HB2	2.01	0.59
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.86	0.58
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.85	0.58
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.87	0.57
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.09	0.57
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.85	0.56
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.89	0.56
1:B:164:LEU:C	1:B:164:LEU:HD23	2.31	0.55
1:A:238:HIS:O	1:A:239:LYS:HB2	2.06	0.54
1:B:7:ARG:HG2	1:B:49:TYR:HB2	1.88	0.54
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.42	0.54
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.90	0.53
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.44	0.53
1:C:72:ILE:O	1:C:76:LYS:HG3	2.10	0.52
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.74	0.52
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.92	0.52
1:B:216:PRO:HG2	1:B:232:ILE:HD11	1.93	0.50
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.93	0.50
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.93	0.49
1:C:41:HIS:HE1	2:C:517:HOH:O	1.95	0.49
1:B:152:SER:HB2	2:D:563:HOH:O	2.11	0.49
1:A:305:TRP:O	1:A:309:LYS:HG3	2.13	0.48
1:A:65:ALA:O	1:A:69:ASP:HB2	2.14	0.48
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.43	0.48
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.49	0.48
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.96	0.47
1:C:161:ALA:O	1:C:165:LEU:HG	2.15	0.46
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.50	0.46
1:A:186:GLU:HA	1:A:187:PRO:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.51	0.46
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.97	0.46
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.31	0.46
1:A:164:LEU:C	1:A:164:LEU:HD23	2.41	0.46
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.97	0.46
1:B:216:PRO:HG2	1:B:232:ILE:CD1	2.46	0.45
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.79	0.45
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.98	0.45
1:B:101:ASP:CG	1:B:101:ASP:O	2.59	0.45
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.52	0.44
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.00	0.44
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.99	0.44
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.53	0.44
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.17	0.44
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.54	0.43
1:B:203:VAL:HG22	1:B:212:PHE:HB3	2.00	0.43
1:B:278:GLY:CA	1:B:282:ALA:O	2.66	0.43
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.95	0.43
1:D:72:ILE:O	1:D:76:LYS:HG3	2.19	0.43
1:B:37:VAL:HG13	1:B:78:ALA:HB2	2.01	0.43
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.89	0.43
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.47	0.43
1:B:280:ASP:C	1:B:282:ALA:H	2.25	0.43
1:B:219:GLY:O	1:B:223:MET:HG3	2.19	0.42
1:B:278:GLY:HA3	1:B:282:ALA:O	2.18	0.42
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.73	0.42
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.85	0.42
1:D:330:GLU:OE1	2:D:604:HOH:O	2.21	0.42
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.86	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.88	0.42
1:A:6:THR:O	1:A:9:ASP:HB2	2.20	0.42
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.55	0.42
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.80	0.42
1:A:183:LYS:HG2	1:A:184:PRO:HD2	2.02	0.42
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.54	0.42
1:A:326:ARG:HA	1:A:326:ARG:HD3	1.92	0.41
1:D:219:GLY:O	1:D:223:MET:HG3	2.21	0.41
1:A:42:LYS:O	1:A:45:GLU:HB3	2.20	0.41
1:C:234:GLN:HE21	1:C:238:HIS:CE1	2.12	0.41
1:D:178:PHE:HB2	1:D:212:PHE:CD1	2.56	0.41
1:A:60:PRO:O	1:A:61:PHE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.85	0.41
1:A:299:GLU:HB3	1:A:303:GLY:HA3	2.01	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.16	0.41
1:D:88:MET:HA	1:D:133:THR:O	2.21	0.41
1:D:181:GLN:NE2	1:D:245:ASP:OD2	2.53	0.41
1:A:77:LYS:O	1:A:80:ASP:CB	2.69	0.41
1:A:161:ALA:O	1:A:165:LEU:HG	2.21	0.40
1:A:181:GLN:NE2	1:A:245:ASP:OD2	2.54	0.40
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.87	0.40
1:D:278:GLY:HA2	2:D:505:HOH:O	2.21	0.40
1:D:186:GLU:HA	1:D:187:PRO:HA	1.79	0.40
1:C:186:GLU:HA	1:C:187:PRO:HA	1.92	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	46
1	B	390/393 (99%)	375 (96%)	13 (3%)	2 (0%)	24	31
1	C	390/393 (99%)	376 (96%)	10 (3%)	4 (1%)	12	15
1	D	390/393 (99%)	375 (96%)	13 (3%)	2 (0%)	24	31
All	All	1560/1572 (99%)	1502 (96%)	49 (3%)	9 (1%)	21	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	280	ASP
1	A	186	GLU

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Mol	Chain	Res	Type
1	B	186	GLU
1	C	186	GLU
1	C	279	PRO
1	C	364	PHE
1	D	186	GLU
1	D	280	ASP
1	B	281	GLY

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%)	296 (97%)	10 (3%)	33	50
1	B	306/310 (99%)	302 (99%)	4 (1%)	61	77
1	C	306/310 (99%)	302 (99%)	4 (1%)	61	77
1	D	306/310 (99%)	297 (97%)	9 (3%)	37	55
All	All	1224/1240 (99%)	1197 (98%)	27 (2%)	45	65

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	23	ARG
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	203	VAL
1	A	208	ARG
1	B	49	TYR
1	B	81	GLU
1	B	203	VAL
1	B	394	ARG

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Mol	Chain	Res	Type
1	C	3	VAL
1	C	49	TYR
1	C	80	ASP
1	C	203	VAL
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	180	ILE
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 (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	204	GLN
1	A	238	HIS
1	B	204	GLN
1	B	222	GLN
1	B	230	GLN
1	B	238	HIS
1	B	256	GLN
1	C	181	GLN
1	C	185	ASN
1	C	222	GLN
1	C	238	HIS
1	D	181	GLN
1	D	185	ASN
1	D	222	GLN
1	D	238	HIS

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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.