



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:52 AM UTC

PDB ID : 6XIM / pdb_00006xim
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 : 1992-04-03
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

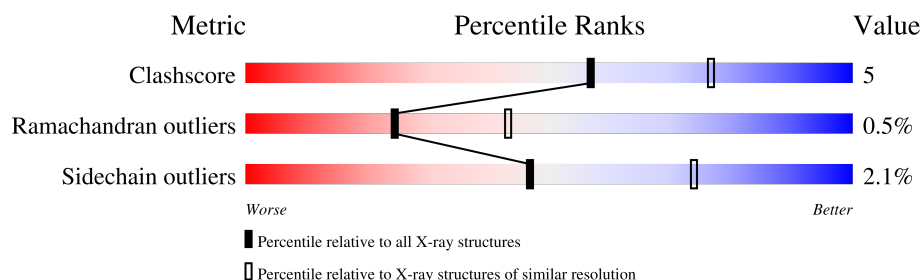
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



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

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	393	74% 22% .
1	B	393	72% 23% 5%
1	C	393	74% 22% .
1	D	393	76% 22% .

2 Entry composition [i](#)

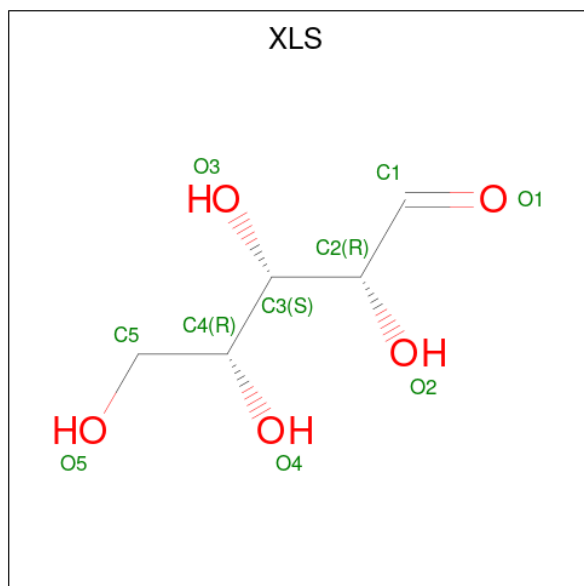
There are 4 unique types of molecules in this entry. The entry contains 13141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-xylose (CCD ID: XLS) (formula: C₅H₁₀O₅).



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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

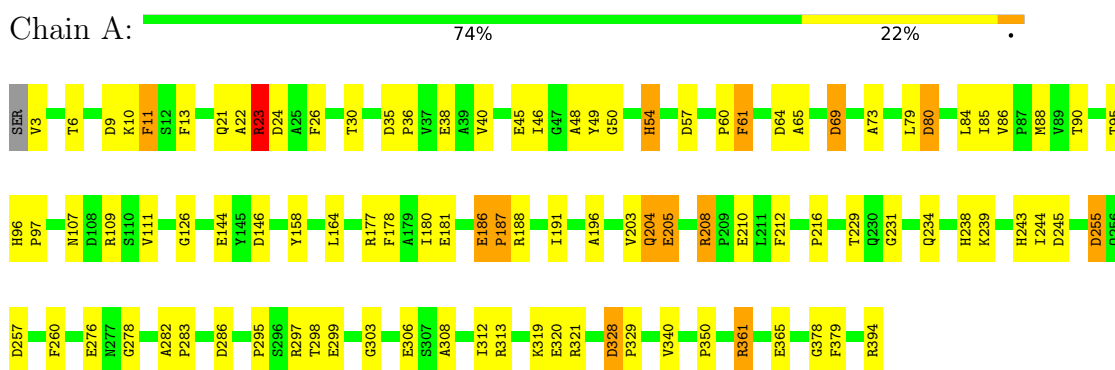
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	213	Total	O	0	0
			213	213		
4	C	231	Total	O	0	0
			231	231		
4	D	212	Total	O	0	0
			212	212		

3 Residue-property plots [i](#)

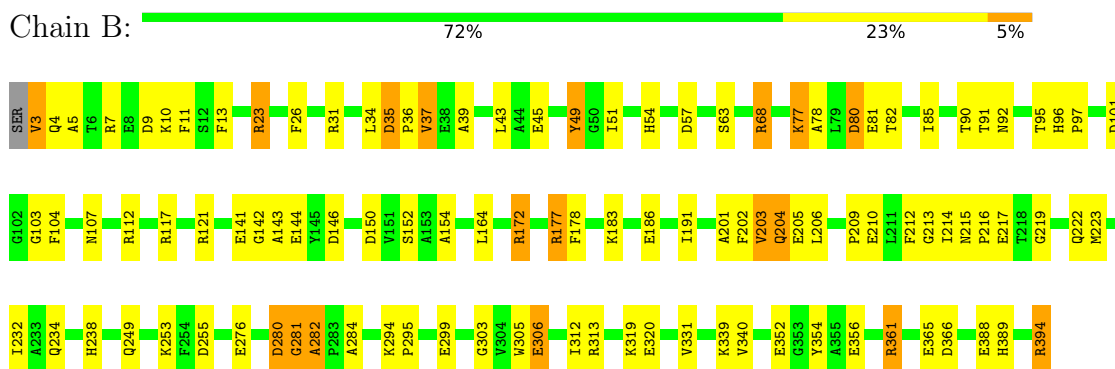
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

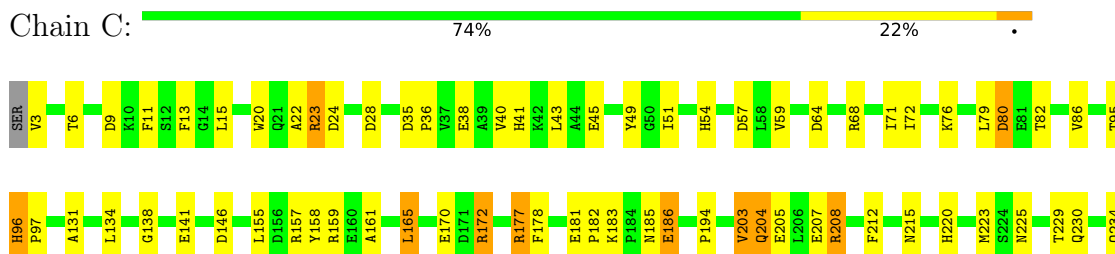
• Molecule 1: D-XYLOSE ISOMERASE

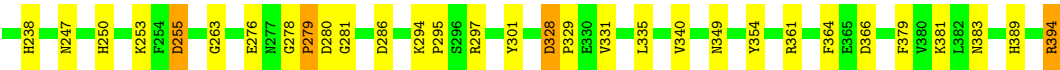


• Molecule 1: D-XYLOSE ISOMERASE

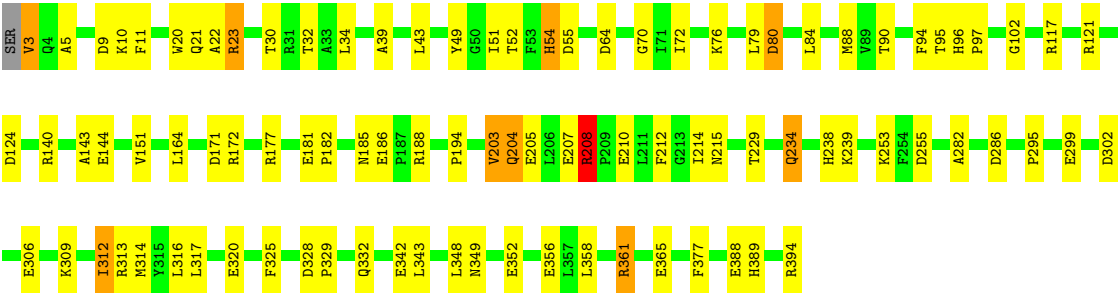


• Molecule 1: D-XYLOSE ISOMERASE





● 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) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13141	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, XLS

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	0.95	0/3125	1.97	92/4233 (2.2%)
1	B	0.94	1/3125 (0.0%)	1.92	79/4233 (1.9%)
1	C	0.95	0/3125	1.92	75/4233 (1.8%)
1	D	0.96	0/3125	1.96	80/4233 (1.9%)
All	All	0.95	1/12500 (0.0%)	1.94	326/16932 (1.9%)

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	2
1	C	0	2
1	D	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	GLY	CA-C	5.70	1.55	1.51

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	CA-CB-CG	-13.60	99.00	112.60
1	D	204	GLN	OE1-CD-NE2	-12.98	109.62	122.60
1	C	204	GLN	OE1-CD-NE2	-12.00	110.60	122.60
1	B	204	GLN	OE1-CD-NE2	-11.62	110.98	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLN	OE1-CD-NE2	-9.71	112.89	122.60
1	A	286	ASP	CA-CB-CG	-8.94	103.66	112.60
1	A	107	ASN	CA-CB-CG	8.86	121.46	112.60
1	A	379	PHE	CA-CB-CG	8.60	122.40	113.80
1	A	394	ARG	NH1-CZ-NH2	8.37	130.18	119.30
1	D	255	ASP	CA-CB-CG	8.33	120.93	112.60
1	B	394	ARG	N-CA-CB	8.26	124.55	110.50
1	D	172	ARG	CD-NE-CZ	8.20	135.88	124.40
1	B	13	PHE	CA-CB-CG	8.16	121.96	113.80
1	B	95	THR	N-CA-C	8.10	120.02	111.03
1	D	313	ARG	NE-CZ-NH2	8.08	126.47	119.20
1	D	286	ASP	CA-CB-CG	-8.05	104.55	112.60
1	A	188	ARG	CD-NE-CZ	8.03	135.64	124.40
1	D	328	ASP	CA-CB-CG	7.99	120.58	112.60
1	D	54	HIS	N-CA-C	-7.89	97.77	110.32
1	D	171	ASP	CA-C-O	-7.87	112.07	120.42
1	A	13	PHE	CA-C-O	-7.78	112.04	121.06
1	A	244	ILE	CA-C-O	-7.76	112.60	120.90
1	A	394	ARG	CA-CB-CG	7.74	129.59	114.10
1	D	389	HIS	CA-CB-CG	-7.62	106.19	113.80
1	C	80	ASP	CA-CB-CG	-7.60	105.00	112.60
1	B	112	ARG	NE-CZ-NH1	-7.59	113.91	121.50
1	C	328	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	57	ASP	CA-CB-CG	7.47	120.07	112.60
1	B	117	ARG	NE-CZ-NH1	7.47	128.97	121.50
1	A	320	GLU	CB-CG-CD	7.46	125.27	112.60
1	A	26	PHE	CA-C-O	-7.41	110.74	119.48
1	B	320	GLU	CB-CG-CD	7.36	125.11	112.60
1	B	96	HIS	CA-CB-CG	-7.35	106.45	113.80
1	D	349	ASN	CA-CB-CG	-7.31	105.29	112.60
1	D	95	THR	N-CA-C	7.25	118.97	111.14
1	D	144	GLU	N-CA-C	-7.25	104.70	113.97
1	A	95	THR	N-CA-C	7.21	118.93	111.14
1	B	141	GLU	CB-CG-CD	7.20	124.85	112.60
1	A	319	LYS	CA-C-O	7.20	128.38	120.82
1	A	255	ASP	CA-CB-CG	7.10	119.70	112.60
1	C	225	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	D	144	GLU	N-CA-CB	7.04	120.46	110.67
1	C	172	ARG	CD-NE-CZ	-7.01	114.58	124.40
1	A	73	ALA	CA-C-N	7.01	127.71	120.00
1	A	73	ALA	C-N-CA	7.01	127.71	120.00
1	B	150	ASP	CA-CB-CG	-6.98	105.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ARG	NE-CZ-NH2	-6.97	112.92	119.20
1	D	80	ASP	CA-CB-CG	-6.97	105.63	112.60
1	B	80	ASP	CA-CB-CG	-6.91	105.69	112.60
1	C	64	ASP	CA-CB-CG	-6.89	105.71	112.60
1	A	328	ASP	CA-CB-CG	6.87	119.47	112.60
1	C	54	HIS	N-CA-C	-6.86	100.37	110.52
1	C	45	GLU	CA-CB-CG	6.85	127.81	114.10
1	C	340	VAL	CB-CA-C	6.85	120.65	111.88
1	C	379	PHE	CA-CB-CG	6.82	120.62	113.80
1	C	335	LEU	O-C-N	6.80	129.32	122.12
1	D	255	ASP	CB-CG-OD1	6.79	134.02	118.40
1	D	320	GLU	CA-CB-CG	6.78	127.66	114.10
1	C	157	ARG	CA-C-O	-6.77	113.24	120.42
1	C	24	ASP	CA-CB-CG	6.77	119.37	112.60
1	D	253	LYS	CA-C-O	-6.74	113.90	121.25
1	B	394	ARG	NE-CZ-NH2	-6.72	113.15	119.20
1	B	389	HIS	CA-CB-CG	-6.72	107.08	113.80
1	C	354	TYR	CA-C-O	-6.69	113.46	120.55
1	A	394	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	C	278	GLY	CA-C-N	6.61	128.10	119.84
1	C	278	GLY	C-N-CA	6.61	128.10	119.84
1	B	142	GLY	CA-C-O	-6.57	116.38	120.91
1	C	13	PHE	CA-C-O	-6.55	113.46	121.06
1	B	77	LYS	O-C-N	6.55	128.81	122.07
1	A	204	GLN	CB-CG-CD	6.53	123.70	112.60
1	B	177	ARG	NE-CZ-NH2	-6.52	113.33	119.20
1	D	358	LEU	CA-C-O	6.49	127.44	120.10
1	B	57	ASP	N-CA-C	-6.45	103.76	111.69
1	C	229	THR	CA-CB-OG1	-6.44	99.94	109.60
1	D	32	THR	CA-CB-OG1	-6.42	99.97	109.60
1	C	172	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	B	85	ILE	CA-C-O	-6.37	115.61	121.72
1	D	54	HIS	N-CA-CB	6.36	120.77	110.41
1	D	377	PHE	CA-C-O	-6.33	111.93	119.15
1	C	383	ASN	OD1-CG-ND2	6.31	128.91	122.60
1	D	21	GLN	CB-CG-CD	-6.29	101.90	112.60
1	D	313	ARG	N-CA-CB	6.26	119.09	110.01
1	B	295	PRO	CA-C-O	-6.26	114.53	121.23
1	A	255	ASP	CB-CA-C	6.23	120.14	110.67
1	A	23	ARG	CA-C-O	-6.23	113.91	120.58
1	A	54	HIS	CA-C-O	-6.23	113.93	121.28
1	C	194	PRO	N-CA-C	6.21	121.62	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	GLU	CA-C-O	-6.20	114.32	120.70
1	C	146	ASP	CA-C-O	-6.18	114.00	120.55
1	B	31	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	A	181	GLU	O-C-N	6.16	126.98	121.19
1	C	23	ARG	N-CA-C	-6.15	98.51	108.41
1	A	340	VAL	CA-C-O	-6.14	114.57	120.95
1	C	15	LEU	CA-C-O	6.13	127.05	120.55
1	B	210	GLU	CB-CG-CD	6.11	122.98	112.60
1	A	216	PRO	CA-C-O	-6.08	114.25	121.67
1	D	312	ILE	CA-C-O	-6.08	114.41	120.85
1	A	243	HIS	CA-CB-CG	6.07	119.87	113.80
1	D	55	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	86	VAL	O-C-N	6.06	128.01	121.10
1	C	253	LYS	CA-C-O	-6.06	114.64	121.25
1	A	295	PRO	N-CA-C	-6.05	101.66	110.80
1	D	286	ASP	CA-C-O	-6.05	112.34	119.48
1	A	177	ARG	N-CA-C	-6.03	100.07	109.72
1	B	57	ASP	CA-CB-CG	6.03	118.62	112.60
1	C	172	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	C	95	THR	N-CA-C	6.02	117.64	111.14
1	C	28	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	188	ARG	NE-CZ-NH2	5.98	124.59	119.20
1	B	366	ASP	CA-C-O	-5.95	112.93	119.95
1	A	61	PHE	CA-C-O	-5.94	115.01	120.95
1	C	177	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	D	328	ASP	CB-CA-C	5.93	117.92	109.38
1	B	178	PHE	O-C-N	5.92	130.35	123.30
1	C	394	ARG	CD-NE-CZ	-5.92	116.11	124.40
1	A	79	LEU	CA-C-O	5.92	126.82	120.55
1	A	13	PHE	O-C-N	5.91	130.12	123.27
1	A	257	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	340	VAL	O-C-N	5.88	127.57	121.87
1	C	215	ASN	CA-CB-CG	-5.88	106.72	112.60
1	B	10	LYS	CB-CA-C	-5.87	103.99	111.86
1	D	10	LYS	CB-CA-C	-5.87	103.99	111.86
1	C	71	ILE	O-C-N	5.86	127.56	121.87
1	D	239	LYS	O-C-N	5.85	129.28	122.67
1	A	231	GLY	CA-C-N	5.85	128.72	120.42
1	A	231	GLY	C-N-CA	5.85	128.72	120.42
1	D	349	ASN	O-C-N	5.84	127.79	121.60
1	C	366	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	177	ARG	N-CA-CB	5.83	120.97	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	295	PRO	CB-CA-C	5.82	118.97	111.64
1	B	90	THR	CA-CB-OG1	-5.82	100.88	109.60
1	C	159	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	C	281	GLY	N-CA-C	-5.80	99.42	113.18
1	B	107	ASN	N-CA-C	-5.80	105.04	111.71
1	D	204	GLN	CB-CG-CD	5.79	122.44	112.60
1	C	389	HIS	CA-CB-CG	-5.79	108.01	113.80
1	A	45	GLU	CA-C-O	-5.78	114.42	120.55
1	D	94	PHE	CA-C-O	-5.78	111.88	118.47
1	B	183	LYS	O-C-N	5.77	126.34	121.84
1	B	68	ARG	NE-CZ-NH1	-5.77	115.73	121.50
1	C	82	THR	CA-CB-OG1	-5.77	100.95	109.60
1	D	212	PHE	N-CA-C	5.76	118.80	109.40
1	B	45	GLU	CB-CG-CD	5.76	122.40	112.60
1	A	276	GLU	N-CA-C	5.76	120.46	112.45
1	B	340	VAL	CB-CA-C	5.75	119.24	111.88
1	D	194	PRO	N-CA-C	5.73	121.07	113.57
1	D	79	LEU	CA-C-O	5.72	126.62	120.55
1	D	210	GLU	CB-CG-CD	5.71	122.30	112.60
1	C	165	LEU	O-C-N	5.70	128.17	122.12
1	A	205	GLU	CB-CG-CD	5.69	122.27	112.60
1	A	278	GLY	N-CA-C	-5.69	105.34	112.23
1	B	54	HIS	N-CA-C	-5.69	101.02	110.17
1	B	201	ALA	CA-C-N	5.68	127.83	120.44
1	B	201	ALA	C-N-CA	5.68	127.83	120.44
1	A	24	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	361	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	D	94	PHE	O-C-N	5.68	128.62	121.64
1	A	244	ILE	O-C-N	5.67	129.67	123.09
1	B	281	GLY	CA-C-N	5.66	129.92	120.86
1	B	281	GLY	C-N-CA	5.66	129.92	120.86
1	C	79	LEU	CA-C-O	5.66	126.76	120.82
1	B	276	GLU	N-CA-C	5.65	120.31	113.41
1	C	208	ARG	CD-NE-CZ	-5.65	116.49	124.40
1	D	332	GLN	CA-C-O	5.64	126.53	120.55
1	A	26	PHE	O-C-N	5.64	129.02	122.19
1	A	21	GLN	CB-CG-CD	-5.62	103.04	112.60
1	A	205	GLU	CG-CD-OE2	5.62	131.34	118.40
1	C	223	MET	N-CA-C	-5.62	105.68	112.54
1	D	30	THR	O-C-N	5.62	128.84	122.20
1	B	319	LYS	CA-C-N	5.62	127.75	120.44
1	B	319	LYS	C-N-CA	5.62	127.75	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	LYS	CA-C-O	-5.62	115.15	121.05
1	B	282	ALA	N-CA-C	5.62	118.15	110.01
1	D	171	ASP	O-C-N	5.61	128.54	122.15
1	B	339	LYS	CB-CA-C	-5.60	102.66	111.51
1	B	177	ARG	N-CA-C	-5.59	101.06	109.95
1	A	298	THR	CA-CB-CG2	5.59	120.01	110.50
1	D	21	GLN	OE1-CD-NE2	5.59	128.19	122.60
1	A	46	ILE	CA-C-O	-5.58	112.30	119.39
1	A	69	ASP	O-C-N	5.58	128.03	122.12
1	B	82	THR	CA-C-O	-5.58	112.75	119.27
1	C	207	GLU	CG-CD-OE2	-5.57	105.60	118.40
1	B	313	ARG	CA-C-N	5.56	127.66	120.44
1	B	313	ARG	C-N-CA	5.56	127.66	120.44
1	B	77	LYS	CB-CA-C	-5.55	102.16	110.88
1	A	308	ALA	N-CA-C	-5.54	105.15	111.14
1	B	215	ASN	CA-CB-CG	-5.54	107.06	112.60
1	B	144	GLU	N-CA-C	-5.52	107.09	113.88
1	C	331	VAL	N-CA-C	-5.52	105.34	110.53
1	D	328	ASP	CA-C-O	5.51	123.40	119.32
1	B	37	VAL	O-C-N	5.51	127.50	121.83
1	A	54	HIS	N-CA-C	-5.51	101.30	110.17
1	C	141	GLU	CB-CG-CD	5.51	121.96	112.60
1	A	158	TYR	CA-C-O	5.50	126.25	120.42
1	D	70	GLY	O-C-N	5.48	127.45	122.19
1	B	299	GLU	N-CA-C	5.48	119.00	110.17
1	A	109	ARG	CA-C-N	5.47	127.61	120.28
1	A	109	ARG	C-N-CA	5.47	127.61	120.28
1	D	306	GLU	CB-CA-C	-5.47	102.30	110.88
1	C	155	LEU	CB-CA-C	5.46	119.86	110.79
1	A	48	ALA	CA-C-O	-5.46	115.61	121.56
1	D	210	GLU	CA-C-O	-5.46	112.89	119.49
1	C	57	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	143	ALA	N-CA-CB	-5.45	102.42	111.57
1	B	217	GLU	CA-C-O	-5.45	114.48	120.36
1	C	23	ARG	CA-C-O	-5.44	114.76	120.58
1	C	361	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	D	299	GLU	N-CA-C	5.44	118.86	110.42
1	D	124	ASP	O-C-N	5.44	127.67	122.07
1	C	328	ASP	CB-CA-C	5.43	118.21	109.41
1	C	185	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	95	THR	CA-C-O	-5.43	115.11	120.70
1	B	26	PHE	CA-C-O	-5.43	113.07	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	TYR	CA-C-N	5.42	127.81	120.44
1	A	158	TYR	C-N-CA	5.42	127.81	120.44
1	C	6	THR	N-CA-CB	5.42	119.98	111.20
1	D	342	GLU	CG-CD-OE2	5.41	130.84	118.40
1	C	331	VAL	CB-CA-C	5.41	119.10	112.02
1	D	342	GLU	CB-CG-CD	5.39	121.77	112.60
1	B	177	ARG	CB-CG-CD	-5.39	98.91	111.30
1	D	215	ASN	CB-CG-ND2	5.39	124.48	116.40
1	A	126	GLY	CA-C-N	5.38	127.44	120.44
1	A	126	GLY	C-N-CA	5.38	127.44	120.44
1	A	245	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	35	ASP	CB-CA-C	5.37	118.11	109.41
1	C	96	HIS	CA-CB-CG	-5.37	108.43	113.80
1	D	215	ASN	CA-CB-CG	-5.37	107.23	112.60
1	D	117	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	D	314	MET	N-CA-CB	5.36	117.92	109.94
1	B	284	ALA	N-CA-C	-5.35	106.70	113.18
1	D	388	GLU	CA-CB-CG	-5.35	103.39	114.10
1	C	255	ASP	CA-CB-CG	5.35	117.95	112.60
1	D	309	LYS	CA-C-O	-5.35	114.88	120.55
1	B	112	ARG	NE-CZ-NH2	5.33	124.00	119.20
1	C	394	ARG	NE-CZ-NH1	-5.33	116.17	121.50
1	D	302	ASP	CA-CB-CG	-5.33	107.27	112.60
1	B	388	GLU	CG-CD-OE2	5.32	130.63	118.40
1	A	191	ILE	CA-C-O	-5.31	114.68	120.84
1	C	255	ASP	CB-CA-C	5.31	118.75	110.67
1	B	63	SER	O-C-N	5.31	129.40	123.19
1	B	255	ASP	N-CA-CB	-5.30	101.53	110.49
1	D	282	ALA	N-CA-C	5.30	117.83	110.20
1	A	95	THR	O-C-N	5.30	127.81	122.09
1	A	146	ASP	N-CA-C	5.30	117.05	111.28
1	C	134	LEU	CA-C-O	-5.30	114.50	120.32
1	C	158	TYR	CA-CB-CG	5.29	123.41	113.90
1	B	331	VAL	N-CA-C	-5.28	105.57	110.53
1	A	361	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	D	239	LYS	CB-CA-C	-5.28	105.07	111.82
1	D	151	VAL	N-CA-C	5.27	116.00	110.62
1	D	325	PHE	CA-C-O	5.26	126.35	120.82
1	C	138	GLY	CA-C-N	5.26	126.71	120.14
1	C	138	GLY	C-N-CA	5.26	126.71	120.14
1	A	313	ARG	N-CA-CB	-5.24	102.41	110.01
1	C	230	GLN	CA-C-O	-5.24	114.99	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	ASP	CA-C-N	5.24	125.55	119.47
1	C	328	ASP	C-N-CA	5.24	125.55	119.47
1	B	202	PHE	CA-C-N	5.23	128.73	120.47
1	B	202	PHE	C-N-CA	5.23	128.73	120.47
1	B	280	ASP	N-CA-C	-5.22	104.09	111.56
1	A	79	LEU	CA-C-N	5.22	127.54	120.65
1	A	79	LEU	C-N-CA	5.22	127.54	120.65
1	A	180	ILE	CB-CA-C	-5.22	104.37	111.15
1	D	143	ALA	N-CA-CB	-5.22	103.63	111.56
1	D	124	ASP	CA-C-O	-5.21	115.34	120.82
1	B	361	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	D	316	LEU	CB-CA-C	5.20	119.43	110.79
1	A	11	PHE	CA-C-O	-5.20	114.76	120.69
1	A	306	GLU	CB-CA-C	-5.20	102.72	110.88
1	B	191	ILE	CA-C-O	-5.19	114.89	121.48
1	A	111	VAL	O-C-N	5.19	127.17	121.83
1	A	10	LYS	CB-CA-C	-5.19	104.91	111.86
1	C	247	ASN	OD1-CG-ND2	-5.19	117.41	122.60
1	B	23	ARG	N-CA-C	-5.18	100.07	108.41
1	A	378	GLY	CA-C-N	5.18	127.64	120.29
1	A	378	GLY	C-N-CA	5.18	127.64	120.29
1	C	301	TYR	CA-C-O	-5.17	114.25	120.10
1	A	321	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	A	229	THR	CA-CB-OG1	-5.17	101.85	109.60
1	D	88	MET	CA-CB-CG	5.17	124.44	114.10
1	B	303	GLY	N-CA-C	-5.17	106.53	112.73
1	B	388	GLU	CG-CD-OE1	-5.16	106.53	118.40
1	A	260	PHE	CA-CB-CG	-5.15	108.65	113.80
1	D	95	THR	O-C-N	5.14	127.64	122.09
1	A	107	ASN	N-CA-C	-5.14	105.86	111.82
1	D	23	ARG	N-CA-C	-5.14	100.13	108.41
1	D	121	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	C	349	ASN	N-CA-C	-5.13	102.75	110.24
1	D	234	GLN	CA-C-O	-5.13	114.98	120.42
1	B	103	GLY	N-CA-C	-5.13	105.54	110.21
1	D	329	PRO	N-CA-C	-5.12	106.74	113.65
1	B	305	TRP	CA-CB-CG	-5.12	103.88	113.60
1	C	276	GLU	CG-CD-OE2	5.12	130.16	118.40
1	A	144	GLU	N-CA-CB	5.11	117.38	110.59
1	A	350	PRO	CB-CA-C	5.11	118.08	111.64
1	D	177	ARG	N-CA-C	-5.11	101.55	109.72
1	D	203	VAL	CB-CA-C	5.11	118.73	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	THR	CA-C-O	-5.10	115.19	120.70
1	A	394	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	D	64	ASP	CA-CB-CG	-5.09	107.51	112.60
1	B	104	PHE	CA-C-O	-5.09	114.35	120.10
1	D	229	THR	CA-CB-OG1	-5.09	101.97	109.60
1	B	146	ASP	CA-C-O	-5.08	115.16	120.55
1	A	298	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	394	ARG	CG-CD-NE	-5.06	100.86	112.00
1	A	64	ASP	N-CA-C	-5.06	104.18	110.41
1	C	64	ASP	N-CA-C	-5.06	103.85	110.53
1	A	196	ALA	CA-C-N	5.05	125.55	119.94
1	A	196	ALA	C-N-CA	5.05	125.55	119.94
1	A	109	ARG	N-CA-C	5.05	116.78	111.28
1	B	213	GLY	O-C-N	5.04	129.25	122.70
1	C	79	LEU	CA-C-N	5.03	127.34	120.54
1	C	79	LEU	C-N-CA	5.03	127.34	120.54
1	C	286	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	312	ILE	CA-C-N	5.03	126.98	120.44
1	A	312	ILE	C-N-CA	5.03	126.98	120.44
1	C	203	VAL	N-CA-CB	-5.02	103.71	110.54
1	D	208	ARG	CG-CD-NE	5.02	123.05	112.00
1	C	177	ARG	N-CA-C	-5.02	101.22	109.40
1	A	88	MET	CA-C-O	-5.01	115.38	120.99
1	D	207	GLU	CA-CB-CG	5.01	124.13	114.10
1	D	52	THR	CA-C-O	-5.01	115.77	121.58
1	B	306	GLU	CA-C-O	5.01	126.08	120.82
1	D	214	ILE	O-C-N	5.00	128.59	123.04
1	B	394	ARG	NH1-CZ-NH2	5.00	125.80	119.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	B	172	ARG	Sidechain
1	B	177	ARG	Sidechain
1	C	172	ARG	Sidechain
1	C	177	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	27	0
1	B	3053	0	2954	38	0
1	C	3053	0	2954	28	0
1	D	3053	0	2954	31	0
2	A	10	0	9	0	0
2	B	10	0	9	0	0
2	C	10	0	9	0	0
2	D	10	0	9	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	225	0	0	1	0
4	B	213	0	0	3	0
4	C	231	0	0	1	0
4	D	212	0	0	6	0
All	All	13141	0	11852	111	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 (111) 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	1.68	1.10
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.70	1.08
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.21	0.88
1:A:204:GLN:HG2	4:A:552:HOH:O	1.76	0.84
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.24	0.84
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.23	0.81
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.25	0.80
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.65	0.78
1:D:3:VAL:HG23	4:D:595:HOH:O	1.83	0.78
1:B:294:LYS:HE2	4:B:585:HOH:O	1.93	0.67
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.79	0.64
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.81	0.63
1:A:36:PRO:O	1:A:40:VAL:HG23	2.03	0.59
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.85	0.57
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.85	0.57
1:C:59:VAL:HG11	1:C:68:ARG:HG3	1.87	0.57
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.87	0.57
1:B:219:GLY:O	1:B:223:MET:HG3	2.05	0.56
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.71	0.56
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.88	0.56
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.43	0.54
1:D:394:ARG:NH1	4:D:604:HOH:O	2.08	0.54
1:B:3:VAL:HG12	1:B:4:GLN:H	1.73	0.54
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.91	0.53
1:D:3:VAL:CG2	4:D:595:HOH:O	2.51	0.53
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.91	0.53
1:C:72:ILE:O	1:C:76:LYS:HG3	2.09	0.52
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.13	0.51
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.46	0.51
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.17	0.51
1:A:65:ALA:O	1:A:69:ASP:HB2	2.12	0.50
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.92	0.49
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.95	0.49
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.94	0.49
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.48	0.48
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.43	0.48
1:B:77:LYS:O	1:B:80:ASP:HB2	2.14	0.48
1:D:3:VAL:HB	4:D:595:HOH:O	2.13	0.47
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.96	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.96	0.47
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.75	0.47
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.50	0.47
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.28	0.47
1:A:186:GLU:OE1	1:A:255:ASP:HB3	2.15	0.46
1:A:238:HIS:O	1:A:239:LYS:HB2	2.15	0.46
1:B:152:SER:HB2	4:D:566:HOH:O	2.16	0.46
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.74	0.46
1:D:72:ILE:O	1:D:76:LYS:HG3	2.15	0.46
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.51	0.45
1:C:186:GLU:OE1	1:C:255:ASP:HB3	2.17	0.45
1:D:3:VAL:CB	4:D:595:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.50	0.45
1:A:6:THR:O	1:A:9:ASP:HB2	2.17	0.45
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.52	0.45
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.99	0.44
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.17	0.43
1:B:164:LEU:C	1:B:164:LEU:HD23	2.42	0.43
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.53	0.43
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.53	0.43
1:C:86:VAL:O	1:C:131:ALA:HA	2.19	0.43
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.48	0.43
1:D:361:ARG:HB3	1:D:365:GLU:HB2	2.01	0.43
1:B:34:LEU:HD21	1:B:39:ALA:HB2	2.01	0.43
1:A:164:LEU:C	1:A:164:LEU:HD23	2.43	0.43
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.54	0.43
1:C:41:HIS:HE1	4:C:521:HOH:O	2.00	0.43
1:C:161:ALA:O	1:C:165:LEU:HG	2.19	0.43
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.32	0.43
1:B:7:ARG:HD3	4:B:497:HOH:O	2.18	0.43
1:B:280:ASP:C	1:B:282:ALA:H	2.26	0.43
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.95	0.43
1:B:101:ASP:CG	1:B:101:ASP:O	2.62	0.42
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.84	0.42
1:A:186:GLU:HA	1:A:187:PRO:HA	1.74	0.42
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.92	0.42
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.48	0.42
1:B:214:ILE:HG13	1:B:216:PRO:HD3	2.01	0.42
1:B:354:TYR:HB3	1:D:164:LEU:HD21	2.01	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.42
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.79	0.42
1:D:20:TRP:CE2	1:D:22:ALA:HA	2.54	0.42
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.86	0.42
1:D:5:ALA:HB2	1:D:312:ILE:CG2	2.50	0.42
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.55	0.41
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.87	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:B:92:ASN:OD1	1:B:92:ASN:C	2.63	0.41
1:D:34:LEU:HD21	1:D:39:ALA:HB2	2.01	0.41
1:B:232:ILE:HD13	1:B:232:ILE:HA	1.87	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.90	0.41
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.92	0.41
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:HG13	1:B:78:ALA:HB2	2.03	0.41
1:A:30:THR:HG22	1:B:97:PRO:HB3	2.02	0.41
1:C:36:PRO:O	1:C:40:VAL:HG23	2.21	0.41
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.56	0.41
1:D:181:GLU:HA	1:D:182:PRO:HD3	1.90	0.41
1:A:60:PRO:O	1:A:61:PHE:C	2.64	0.41
1:B:5:ALA:HB2	1:B:312:ILE:HG21	2.02	0.41
1:B:121:ARG:HD3	4:B:442:HOH:O	2.20	0.41
1:B:203:VAL:HG22	1:B:212:PHE:HB3	2.03	0.41
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.92	0.40
1:A:50:GLY:HA2	1:A:85:ILE:O	2.21	0.40
1:B:206:LEU:O	1:B:209:PRO:HD3	2.20	0.40
1:D:9:ASP:HB3	1:D:11:PHE:CE2	2.56	0.40
1:B:35:ASP:HA	1:B:36:PRO:HD3	1.93	0.40
1:C:250:HIS:CE1	1:C:263:GLY:HA2	2.57	0.40
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.03	0.40
1:B:352:GLU:HG2	1:B:356:GLU:HB2	2.03	0.40
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/393 (99%)	377 (97%)	12 (3%)	1 (0%)	36	55
1	B	390/393 (99%)	375 (96%)	13 (3%)	2 (0%)	24	43
1	C	390/393 (99%)	373 (96%)	13 (3%)	4 (1%)	12	24
1	D	390/393 (99%)	377 (97%)	12 (3%)	1 (0%)	36	55
All	All	1560/1572 (99%)	1502 (96%)	50 (3%)	8 (0%)	24	43

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	C	364	PHE
1	D	186	GLU
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%)	298 (97%)	8 (3%)	40	68
1	B	306/310 (99%)	301 (98%)	5 (2%)	55	79
1	C	306/310 (99%)	300 (98%)	6 (2%)	48	75
1	D	306/310 (99%)	299 (98%)	7 (2%)	44	72
All	All	1224/1240 (99%)	1198 (98%)	26 (2%)	47	74

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	38	GLU
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	187	PRO
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

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Mol	Chain	Res	Type
1	C	38	GLU
1	C	49	TYR
1	C	80	ASP
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
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	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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 12 ligands modelled in this entry, 8 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	XLS	A	397	3	8,9,9	2.15	1 (12%)	10,11,11	1.21	1 (10%)
2	XLS	C	397	3	8,9,9	2.24	1 (12%)	10,11,11	1.59	2 (20%)
2	XLS	B	397	3	8,9,9	2.32	1 (12%)	10,11,11	1.67	3 (30%)
2	XLS	D	397	3	8,9,9	2.32	1 (12%)	10,11,11	2.26	5 (50%)

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	XLS	A	397	3	-	4/11/12/12	-
2	XLS	C	397	3	-	1/11/12/12	-
2	XLS	B	397	3	-	5/11/12/12	-
2	XLS	D	397	3	-	5/11/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	397	XLS	O1-C1	6.50	1.44	1.20
2	D	397	XLS	O1-C1	6.41	1.44	1.20
2	C	397	XLS	O1-C1	6.18	1.43	1.20
2	A	397	XLS	O1-C1	5.91	1.42	1.20

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	397	XLS	O2-C2-C1	-3.72	102.03	110.48
2	D	397	XLS	O3-C3-C2	3.14	114.97	109.13
2	B	397	XLS	O4-C4-C3	3.03	116.34	109.25
2	D	397	XLS	O5-C5-C4	2.91	117.26	111.16
2	B	397	XLS	O2-C2-C1	-2.74	104.24	110.48
2	C	397	XLS	O5-C5-C4	-2.64	105.61	111.16
2	D	397	XLS	O2-C2-C3	2.56	115.46	109.46
2	D	397	XLS	C5-C4-C3	2.49	117.25	112.17
2	B	397	XLS	C3-C2-C1	2.34	118.14	111.03
2	C	397	XLS	C5-C4-C3	-2.21	107.67	112.17
2	A	397	XLS	O3-C3-C2	2.07	112.99	109.13

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	397	XLS	O1-C1-C2-C3
2	A	397	XLS	C1-C2-C3-C4
2	B	397	XLS	O1-C1-C2-C3
2	C	397	XLS	O1-C1-C2-C3
2	D	397	XLS	O1-C1-C2-C3
2	B	397	XLS	O4-C4-C5-O5
2	A	397	XLS	O4-C4-C5-O5
2	B	397	XLS	O2-C2-C3-O3
2	B	397	XLS	C1-C2-C3-C4
2	B	397	XLS	O2-C2-C3-C4
2	D	397	XLS	C1-C2-C3-C4
2	D	397	XLS	O2-C2-C3-C4
2	D	397	XLS	O2-C2-C3-O3
2	A	397	XLS	C1-C2-C3-O3
2	D	397	XLS	C1-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.