



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:50 PM UTC

PDB ID : 9XIM / pdb_00009xim
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 : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

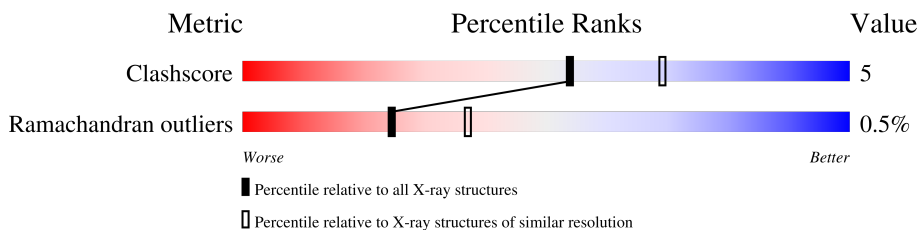
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)

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	75% 22% .
1	B	393	71% 26% .
1	C	393	73% 23% ..
1	D	393	73% 25% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13214 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.

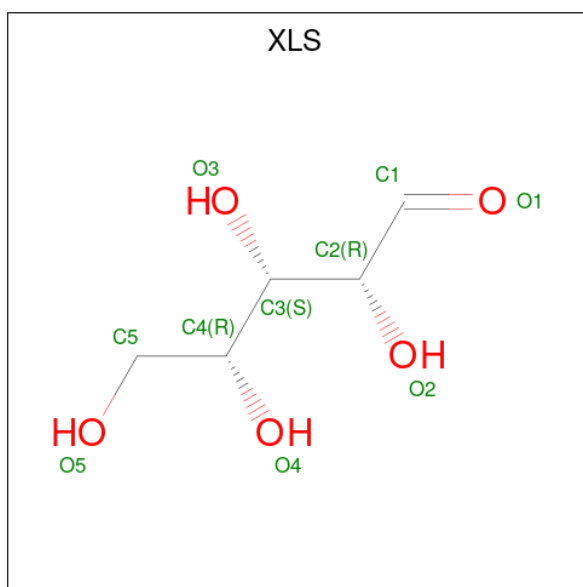
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3049	1937	533	575	4			
1	B	392	Total	C	N	O	S	0	0	0
			3049	1937	533	575	4			
1	C	391	Total	C	N	O	S	0	0	0
			3042	1932	532	574	4			
1	D	392	Total	C	N	O	S	0	0	0
			3048	1936	533	575	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	GLN	GLU	conflict	UNP P12851
B	186	GLN	GLU	conflict	UNP P12851
C	186	GLN	GLU	conflict	UNP P12851
D	186	GLN	GLU	conflict	UNP P12851

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	242	Total	O	0	0
			242	242		

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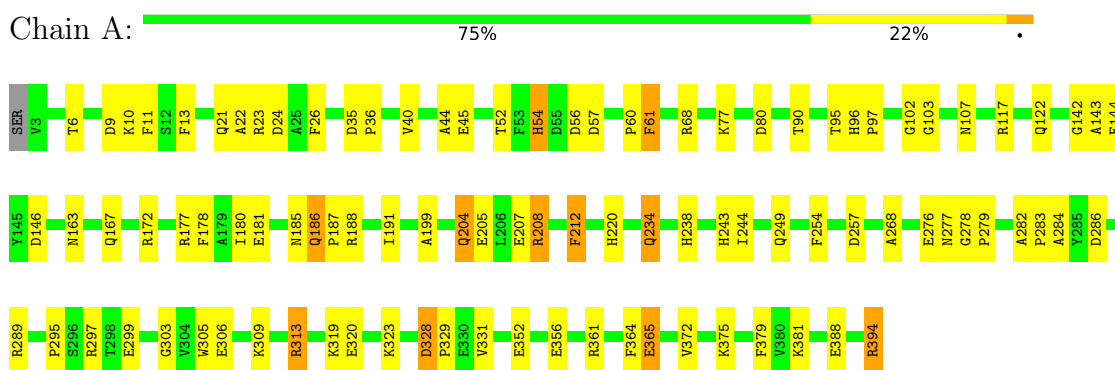
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	240	Total 240	O 240	0	0
4	C	257	Total 257	O 257	0	0
4	D	239	Total 239	O 239	0	0

3 Residue-property plots

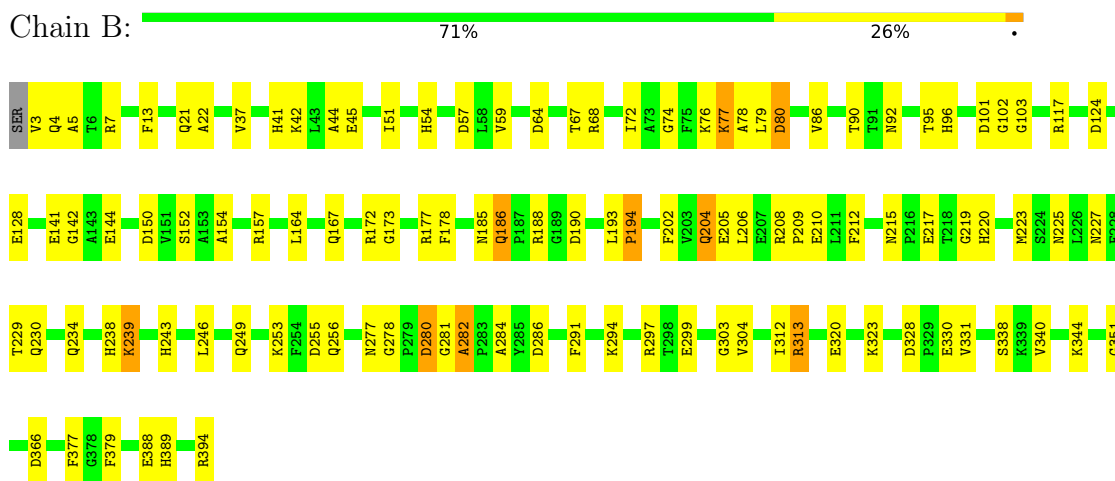
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

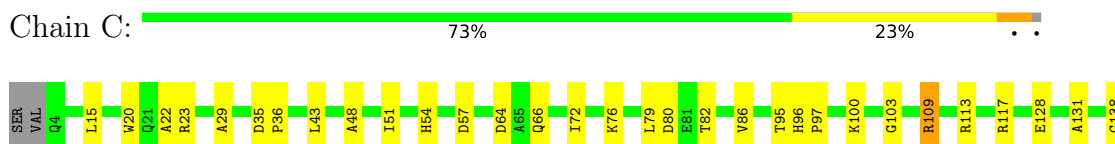
• Molecule 1: D-XYLOSE ISOMERASE

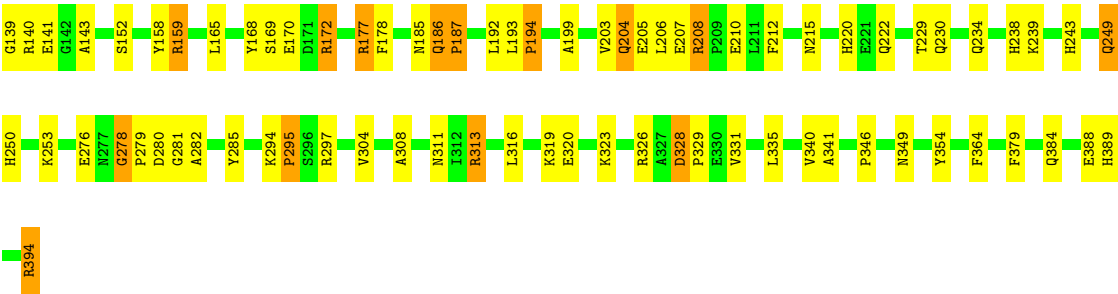


• Molecule 1: D-XYLOSE ISOMERASE

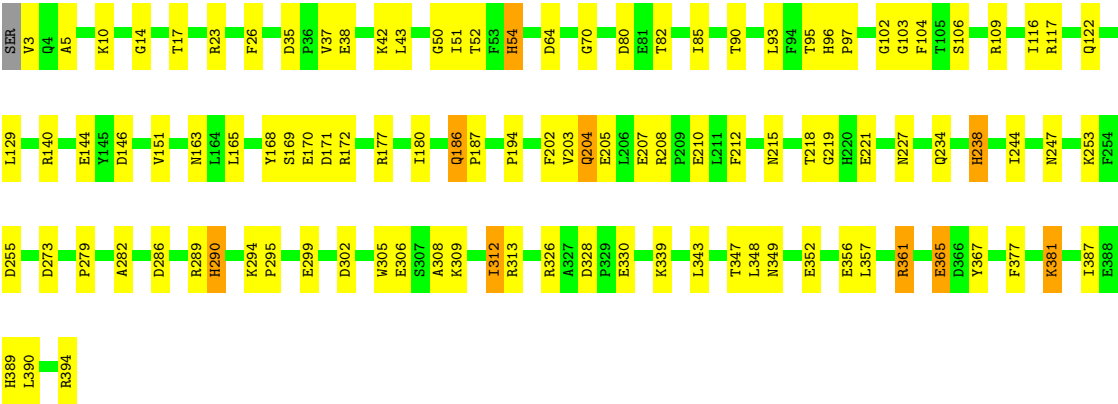


• Molecule 1: D-XYLOSE ISOMERASE





● Molecule 1: D-XYLOSE ISOMERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.144 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13214	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: XLS, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	3/3121 (0.1%)	1.97	79/4228 (1.9%)
1	B	0.97	1/3121 (0.0%)	1.95	87/4228 (2.1%)
1	C	0.97	0/3114	1.99	99/4218 (2.3%)
1	D	1.03	3/3119 (0.1%)	1.98	94/4224 (2.2%)
All	All	0.99	7/12475 (0.1%)	1.97	359/16898 (2.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	SER	C-N	-15.58	1.14	1.33
1	A	103	GLY	CA-C	6.06	1.55	1.51
1	B	103	GLY	CA-C	5.93	1.55	1.51
1	A	142	GLY	C-O	5.88	1.27	1.23
1	D	103	GLY	N-CA	5.29	1.49	1.45
1	D	170	GLU	N-CA	-5.12	1.40	1.46
1	A	103	GLY	N-CA	5.05	1.49	1.45

All (359) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	ARG	CD-NE-CZ	19.08	151.11	124.40
1	C	313	ARG	CD-NE-CZ	17.93	149.50	124.40
1	C	204	GLN	OE1-CD-NE2	-14.76	107.84	122.60
1	D	204	GLN	OE1-CD-NE2	-13.43	109.17	122.60
1	A	80	ASP	CA-CB-CG	-12.07	100.53	112.60
1	D	169	SER	CA-C-O	-11.27	108.99	120.82
1	B	204	GLN	OE1-CD-NE2	-10.67	111.93	122.60
1	D	247	ASN	OD1-CG-ND2	10.65	133.25	122.60
1	A	204	GLN	OE1-CD-NE2	-10.52	112.08	122.60
1	D	122	GLN	OE1-CD-NE2	-9.75	112.85	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	ARG	CD-NE-CZ	-9.74	110.76	124.40
1	B	394	ARG	NE-CZ-NH2	-8.69	111.38	119.20
1	A	199	ALA	CB-CA-C	8.65	125.56	110.85
1	B	313	ARG	NE-CZ-NH2	8.62	126.96	119.20
1	A	57	ASP	CA-CB-CG	8.22	120.83	112.60
1	C	379	PHE	CA-CB-CG	8.16	121.96	113.80
1	A	23	ARG	CD-NE-CZ	8.16	135.82	124.40
1	C	253	LYS	CA-C-O	-8.02	112.51	121.25
1	D	218	THR	CA-C-O	-8.01	112.26	121.07
1	C	64	ASP	CA-CB-CG	-7.99	104.61	112.60
1	B	394	ARG	N-CA-CB	7.92	123.95	110.50
1	D	95	THR	N-CA-C	7.90	119.67	111.14
1	A	319	LYS	CA-C-O	7.89	129.34	120.90
1	A	379	PHE	CA-CB-CG	7.82	121.62	113.80
1	C	326	ARG	NE-CZ-NH2	7.75	126.17	119.20
1	B	286	ASP	CA-C-O	-7.74	110.34	119.48
1	C	340	VAL	CB-CA-C	7.68	121.70	111.88
1	D	302	ASP	CA-CB-CG	-7.67	104.93	112.60
1	D	326	ARG	NE-CZ-NH2	7.67	126.10	119.20
1	D	165	LEU	CA-C-O	-7.64	112.80	120.82
1	D	23	ARG	CA-C-O	-7.62	112.42	120.58
1	D	302	ASP	CA-C-O	-7.58	112.86	120.82
1	A	68	ARG	CD-NE-CZ	7.54	134.96	124.40
1	C	23	ARG	CA-C-O	-7.53	112.09	120.60
1	A	188	ARG	CD-NE-CZ	7.45	134.83	124.40
1	C	54	HIS	N-CA-C	-7.41	98.54	110.32
1	B	117	ARG	NE-CZ-NH1	7.40	128.90	121.50
1	B	57	ASP	CA-CB-CG	7.38	119.98	112.60
1	D	170	GLU	N-CA-CB	7.36	120.91	109.94
1	B	217	GLU	CA-C-O	-7.31	112.81	120.70
1	B	77	LYS	O-C-N	7.25	129.53	122.07
1	B	394	ARG	NH1-CZ-NH2	7.18	128.64	119.30
1	C	335	LEU	O-C-N	7.17	129.73	122.12
1	C	141	GLU	CB-CG-CD	7.16	124.76	112.60
1	C	389	HIS	CA-CB-CG	-7.15	106.65	113.80
1	A	191	ILE	CA-C-O	-7.15	112.40	121.48
1	D	210	GLU	CB-CG-CD	7.08	124.64	112.60
1	C	313	ARG	NE-CZ-NH1	7.06	128.56	121.50
1	D	328	ASP	CA-CB-CG	7.05	119.66	112.60
1	C	128	GLU	CB-CG-CD	7.04	124.57	112.60
1	A	257	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	44	ALA	CA-C-O	7.01	127.98	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	GLY	CA-C-N	6.97	128.85	120.14
1	C	138	GLY	C-N-CA	6.97	128.85	120.14
1	B	59	VAL	O-C-N	6.96	127.60	121.12
1	D	54	HIS	N-CA-C	-6.96	98.96	110.17
1	C	208	ARG	NE-CZ-NH1	-6.92	114.58	121.50
1	C	170	GLU	CA-C-O	-6.92	113.09	120.42
1	D	144	GLU	N-CA-C	-6.91	105.12	113.97
1	B	124	ASP	O-C-N	6.86	129.14	122.07
1	B	255	ASP	CA-CB-CG	-6.86	105.74	112.60
1	D	365	GLU	CA-C-O	-6.85	113.57	120.90
1	A	107	ASN	CA-CB-CG	6.84	119.44	112.60
1	C	29	ALA	CA-C-O	-6.84	113.50	121.16
1	D	349	ASN	CA-CB-CG	-6.83	105.77	112.60
1	A	172	ARG	CD-NE-CZ	6.83	133.97	124.40
1	C	109	ARG	NE-CZ-NH1	-6.82	114.68	121.50
1	D	286	ASP	CA-C-O	-6.82	111.44	119.48
1	A	249	GLN	OE1-CD-NE2	6.81	129.41	122.60
1	A	24	ASP	CA-CB-CG	6.80	119.40	112.60
1	A	102	GLY	CA-C-O	-6.78	117.42	122.37
1	D	80	ASP	CA-CB-CG	-6.76	105.84	112.60
1	A	244	ILE	CA-C-O	-6.75	113.68	120.90
1	A	244	ILE	O-C-N	6.75	130.91	123.09
1	D	313	ARG	CA-CB-CG	6.74	127.59	114.10
1	B	394	ARG	CD-NE-CZ	-6.66	115.08	124.40
1	B	80	ASP	CA-CB-CG	-6.62	105.97	112.60
1	B	95	THR	N-CA-C	6.58	119.43	111.40
1	B	256	GLN	CB-CG-CD	-6.58	101.41	112.60
1	B	13	PHE	CA-CB-CG	6.57	120.37	113.80
1	C	281	GLY	N-CA-C	-6.57	97.60	113.18
1	C	48	ALA	CA-C-O	-6.55	114.42	121.56
1	D	357	LEU	O-C-N	6.52	129.03	122.12
1	B	54	HIS	N-CA-C	-6.51	99.97	110.32
1	C	194	PRO	N-CA-C	6.50	121.98	113.86
1	C	185	ASN	O-C-N	6.49	129.78	123.29
1	C	222	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	A	286	ASP	CA-C-O	-6.46	111.64	119.32
1	A	61	PHE	CA-C-O	-6.44	114.51	120.95
1	D	194	PRO	N-CA-C	6.42	121.98	113.57
1	C	313	ARG	NH1-CZ-NH2	-6.42	110.96	119.30
1	D	306	GLU	CB-CA-C	-6.42	100.81	110.88
1	D	330	GLU	CG-CD-OE2	-6.39	103.71	118.40
1	D	208	ARG	CD-NE-CZ	-6.35	115.51	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	GLU	CG-CD-OE2	-6.33	103.84	118.40
1	D	349	ASN	OD1-CG-ND2	6.33	128.93	122.60
1	C	185	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	220	HIS	CA-C-O	-6.30	114.20	120.82
1	A	45	GLU	CA-C-O	-6.30	113.87	120.55
1	D	93	LEU	CA-C-O	-6.30	113.90	121.34
1	B	253	LYS	CA-C-O	-6.29	114.58	121.31
1	A	295	PRO	N-CA-C	-6.29	101.30	110.80
1	C	80	ASP	CA-CB-CG	-6.26	106.34	112.60
1	C	354	TYR	CA-C-O	-6.26	113.03	120.10
1	A	103	GLY	O-C-N	6.21	125.33	121.85
1	C	328	ASP	CB-CA-C	6.21	119.44	109.51
1	C	204	GLN	CG-CD-NE2	6.18	125.67	116.40
1	B	90	THR	CA-CB-OG1	-6.18	100.33	109.60
1	C	95	THR	N-CA-C	6.17	117.80	111.14
1	C	165	LEU	O-C-N	6.17	128.42	122.07
1	B	286	ASP	CA-CB-CG	-6.15	106.45	112.60
1	D	177	ARG	N-CA-C	-6.15	99.38	109.40
1	B	185	ASN	OD1-CG-ND2	-6.14	116.45	122.60
1	C	341	ALA	CA-C-O	-6.12	112.94	119.97
1	C	143	ALA	O-C-N	6.11	129.40	123.29
1	B	45	GLU	CA-CB-CG	6.10	126.31	114.10
1	C	328	ASP	CA-C-O	6.10	124.16	119.46
1	B	96	HIS	CA-CB-CG	-6.08	107.72	113.80
1	C	249	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	D	212	PHE	N-CA-C	6.07	118.79	108.90
1	D	106	SER	CA-C-O	-6.07	115.12	121.55
1	C	192	LEU	CA-C-O	-6.06	114.96	121.56
1	C	349	ASN	N-CA-C	-6.05	101.40	110.24
1	A	375	LYS	CA-C-O	-6.03	114.41	121.16
1	A	204	GLN	CB-CG-CD	6.02	122.84	112.60
1	D	215	ASN	CA-CB-CG	-6.01	106.58	112.60
1	B	95	THR	CA-CB-OG1	-6.00	100.60	109.60
1	D	146	ASP	O-C-N	6.00	128.48	122.12
1	A	185	ASN	CA-C-O	-5.99	115.03	121.38
1	A	394	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	D	52	THR	CA-C-O	-5.99	114.63	121.58
1	A	172	ARG	NE-CZ-NH1	5.98	127.48	121.50
1	D	312	ILE	O-C-N	5.98	128.12	121.90
1	C	158	TYR	N-CA-C	-5.97	104.86	111.36
1	A	57	ASP	N-CA-CB	5.96	119.08	110.20
1	D	221	GLU	CB-CG-CD	5.95	122.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	GLU	OE1-CD-OE2	5.95	137.17	122.90
1	C	335	LEU	CA-C-O	-5.93	114.27	120.55
1	C	64	ASP	N-CA-C	-5.91	102.73	110.53
1	B	54	HIS	N-CA-CB	5.90	120.02	110.41
1	B	331	VAL	N-CA-C	-5.89	104.99	110.53
1	D	302	ASP	O-C-N	5.88	128.13	122.07
1	B	303	GLY	N-CA-C	-5.88	105.24	112.77
1	C	100	LYS	CA-C-O	-5.87	112.39	119.49
1	A	95	THR	N-CA-C	5.87	117.54	111.03
1	B	351	GLY	CA-C-O	-5.87	112.51	119.02
1	A	177	ARG	CB-CA-C	5.86	120.56	109.37
1	D	151	VAL	N-CA-C	5.86	116.59	110.62
1	A	180	ILE	N-CA-CB	5.85	116.91	110.53
1	D	387	ILE	CA-C-O	-5.85	114.86	120.95
1	B	41	HIS	CA-CB-CG	-5.85	107.95	113.80
1	B	323	LYS	N-CA-CB	5.83	118.46	110.01
1	D	207	GLU	CA-C-O	-5.82	114.25	120.42
1	D	227	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	D	117	ARG	NE-CZ-NH2	-5.82	113.97	119.20
1	D	117	ARG	NE-CZ-NH1	5.81	127.31	121.50
1	D	180	ILE	O-C-N	5.80	129.25	122.81
1	D	203	VAL	CB-CA-C	5.79	119.63	112.04
1	D	299	GLU	N-CA-C	5.79	119.39	110.42
1	C	199	ALA	CA-C-O	-5.79	114.28	120.42
1	A	117	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	B	68	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	A	144	GLU	N-CA-CB	5.78	118.27	110.59
1	D	289	ARG	CD-NE-CZ	5.78	132.49	124.40
1	D	313	ARG	CD-NE-CZ	-5.77	116.32	124.40
1	A	328	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	229	THR	CA-CB-OG1	-5.74	100.98	109.60
1	B	215	ASN	CA-CB-CG	-5.74	106.86	112.60
1	B	256	GLN	OE1-CD-NE2	5.74	128.34	122.60
1	B	225	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	A	163	ASN	O-C-N	5.71	128.17	122.12
1	A	394	ARG	NH1-CZ-NH2	5.71	126.72	119.30
1	A	52	THR	CA-CB-OG1	-5.71	101.04	109.60
1	C	139	GLY	CA-C-O	-5.70	114.24	120.40
1	B	74	GLY	O-C-N	5.70	127.71	122.19
1	C	328	ASP	CA-C-N	5.69	125.53	119.28
1	C	328	ASP	C-N-CA	5.69	125.53	119.28
1	A	313	ARG	NH1-CZ-NH2	-5.68	111.92	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ALA	CA-C-O	5.67	126.56	120.55
1	D	328	ASP	CA-C-O	5.66	123.51	119.32
1	D	180	ILE	CB-CA-C	-5.66	103.80	111.15
1	A	276	GLU	N-CA-C	5.65	120.31	112.45
1	B	243	HIS	CA-C-O	-5.65	115.39	121.38
1	C	109	ARG	CD-NE-CZ	-5.63	116.52	124.40
1	C	384	GLN	CA-C-O	-5.63	114.58	120.55
1	B	328	ASP	CA-C-O	5.62	123.79	119.46
1	D	238	HIS	CA-CB-CG	5.62	119.42	113.80
1	C	207	GLU	CG-CD-OE2	-5.62	105.48	118.40
1	A	102	GLY	O-C-N	5.62	129.10	123.48
1	C	57	ASP	N-CA-CB	5.61	118.56	110.20
1	A	243	HIS	CA-CB-CG	5.61	119.41	113.80
1	B	45	GLU	CB-CG-CD	5.61	122.14	112.60
1	C	113	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	A	13	PHE	CA-C-O	-5.61	114.56	121.06
1	B	202	PHE	CA-C-N	5.59	128.12	120.46
1	B	202	PHE	C-N-CA	5.59	128.12	120.46
1	B	230	GLN	CA-C-O	-5.58	114.64	120.55
1	B	204	GLN	CG-CD-OE1	5.57	131.94	120.80
1	C	207	GLU	CA-C-O	-5.57	114.97	120.70
1	C	320	GLU	CB-CG-CD	5.56	122.05	112.60
1	B	320	GLU	CB-CG-CD	5.55	122.04	112.60
1	B	366	ASP	CA-C-O	-5.55	113.40	119.95
1	A	286	ASP	CA-CB-CG	-5.55	107.05	112.60
1	C	285	TYR	CA-C-O	5.54	126.47	120.32
1	A	144	GLU	N-CA-C	-5.54	107.06	113.88
1	A	103	GLY	N-CA-C	-5.54	105.17	110.21
1	A	177	ARG	N-CA-C	-5.53	100.39	109.40
1	B	157	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	B	280	ASP	N-CA-C	-5.51	103.68	111.56
1	D	70	GLY	O-C-N	5.50	127.47	122.19
1	A	208	ARG	CD-NE-CZ	-5.50	116.71	124.40
1	A	234	GLN	CA-C-O	-5.49	115.05	120.70
1	A	365	GLU	CA-C-O	-5.49	115.03	120.90
1	D	146	ASP	CA-C-O	-5.48	114.74	120.55
1	D	203	VAL	N-CA-CB	-5.47	103.64	110.47
1	B	124	ASP	CA-CB-CG	5.46	118.06	112.60
1	D	14	GLY	N-CA-C	-5.46	102.76	112.54
1	C	229	THR	CA-CB-OG1	-5.46	101.41	109.60
1	A	181	GLU	O-C-N	5.46	127.34	121.12
1	C	328	ASP	CA-CB-CG	5.45	118.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	GLN	CA-C-O	-5.45	114.77	120.55
1	C	79	LEU	CA-C-O	5.45	126.54	120.82
1	D	104	PHE	O-C-N	5.45	129.47	122.39
1	B	64	ASP	N-CA-C	-5.44	103.34	110.53
1	C	82	THR	CA-CB-OG1	-5.44	101.44	109.60
1	A	364	PHE	CA-C-N	5.44	127.88	120.54
1	A	364	PHE	C-N-CA	5.44	127.88	120.54
1	D	328	ASP	CB-CA-C	5.44	117.21	109.38
1	B	299	GLU	N-CA-C	5.43	118.84	110.42
1	D	10	LYS	CB-CA-C	-5.43	104.18	111.89
1	C	177	ARG	CB-CG-CD	5.42	123.77	111.30
1	C	208	ARG	NH1-CZ-NH2	5.42	126.34	119.30
1	A	372	VAL	CA-C-O	-5.42	115.11	120.85
1	D	347	THR	CA-C-O	5.42	126.25	120.24
1	B	313	ARG	CA-CB-CG	5.42	124.93	114.10
1	D	361	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	B	210	GLU	CB-CG-CD	5.40	121.78	112.60
1	B	239	LYS	CB-CA-C	-5.40	104.29	111.63
1	A	57	ASP	N-CA-C	-5.39	105.06	111.69
1	B	379	PHE	CA-CB-CG	5.39	119.19	113.80
1	D	290	HIS	CA-C-O	-5.39	114.45	120.54
1	B	103	GLY	N-CA-C	-5.39	105.31	110.21
1	D	109	ARG	N-CA-C	5.38	117.15	111.28
1	C	165	LEU	CA-C-O	-5.38	115.17	120.82
1	B	96	HIS	CA-C-O	-5.38	114.58	120.17
1	C	215	ASN	CA-CB-CG	-5.38	107.22	112.60
1	C	66	GLN	O-C-N	5.37	127.60	122.07
1	C	117	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	C	276	GLU	CG-CD-OE2	5.37	130.75	118.40
1	C	172	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	C	394	ARG	NH1-CZ-NH2	5.37	126.28	119.30
1	B	389	HIS	CA-CB-CG	-5.36	108.44	113.80
1	A	220	HIS	CA-CB-CG	-5.36	108.44	113.80
1	D	279	PRO	CB-CA-C	5.36	117.95	111.46
1	B	188	ARG	CA-C-O	-5.36	115.49	121.81
1	A	381	LYS	CA-C-O	-5.35	115.20	120.82
1	D	306	GLU	O-C-N	5.34	127.57	122.07
1	A	21	GLN	CB-CG-CD	-5.34	103.53	112.60
1	A	207	GLU	CA-C-O	-5.33	115.20	120.70
1	B	177	ARG	N-CA-C	-5.33	101.48	109.95
1	C	169	SER	O-C-N	5.32	127.55	122.07
1	D	26	PHE	CA-C-O	-5.32	113.31	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PHE	CA-C-O	-5.32	112.90	119.18
1	D	54	HIS	N-CA-CB	5.32	119.30	110.63
1	B	284	ALA	N-CA-C	-5.32	106.75	113.18
1	A	220	HIS	O-C-N	5.31	127.54	122.07
1	C	159	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	D	377	PHE	CA-C-O	-5.30	112.87	119.18
1	B	227	ASN	OD1-CG-ND2	5.30	127.90	122.60
1	C	57	ASP	N-CA-C	-5.30	105.17	111.69
1	D	389	HIS	CA-CB-CG	-5.30	108.50	113.80
1	C	210	GLU	CB-CG-CD	5.29	121.59	112.60
1	D	330	GLU	OE1-CD-OE2	5.28	135.58	122.90
1	D	365	GLU	O-C-N	5.28	127.58	122.09
1	C	331	VAL	N-CA-C	-5.28	105.57	110.53
1	D	171	ASP	CA-C-O	-5.27	114.83	120.42
1	D	104	PHE	CA-C-O	-5.27	113.11	119.49
1	C	187	PRO	N-CA-C	5.27	125.79	112.10
1	A	284	ALA	N-CA-C	-5.26	106.86	113.28
1	D	255	ASP	CA-C-O	-5.26	114.97	121.02
1	C	304	VAL	CA-C-O	-5.25	115.60	121.17
1	A	319	LYS	CA-C-N	5.25	127.26	120.44
1	A	319	LYS	C-N-CA	5.25	127.26	120.44
1	B	67	THR	O-C-N	5.24	127.47	122.07
1	C	177	ARG	N-CA-C	-5.24	101.16	109.59
1	C	203	VAL	N-CA-CB	-5.24	101.70	110.65
1	D	279	PRO	CA-C-O	5.24	127.00	121.03
1	B	220	HIS	CA-CB-CG	-5.23	108.57	113.80
1	B	79	LEU	CA-C-O	5.23	125.97	120.42
1	C	23	ARG	N-CA-C	-5.23	100.57	108.67
1	A	10	LYS	CB-CA-C	-5.22	104.86	111.86
1	D	207	GLU	CB-CG-CD	-5.21	103.74	112.60
1	A	77	LYS	O-C-N	5.21	127.43	122.07
1	D	163	ASN	CA-CB-CG	-5.20	107.40	112.60
1	A	212	PHE	N-CA-C	5.20	117.96	109.59
1	D	253	LYS	CA-C-O	-5.20	115.75	121.31
1	D	282	ALA	N-CA-C	5.20	117.68	110.20
1	A	44	ALA	N-CA-C	-5.19	105.62	111.28
1	B	141	GLU	CB-CG-CD	5.18	121.41	112.60
1	B	344	LYS	CA-CB-CG	-5.18	103.74	114.10
1	C	220	HIS	CA-C-O	-5.18	114.93	120.42
1	C	308	ALA	N-CA-CB	5.18	117.52	110.01
1	B	249	GLN	CA-C-O	-5.17	115.21	120.89
1	B	304	VAL	CA-CB-CG2	5.17	119.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	LEU	CA-C-O	-5.16	114.80	120.43
1	C	295	PRO	N-CA-C	-5.16	103.01	110.80
1	B	194	PRO	N-CA-C	5.15	120.30	113.86
1	B	144	GLU	N-CA-C	-5.15	107.38	113.97
1	D	82	THR	CA-CB-OG1	-5.15	101.88	109.60
1	D	170	GLU	CA-C-O	5.15	126.41	120.90
1	A	146	ASP	N-CA-C	5.14	116.89	111.28
1	D	339	LYS	CB-CA-C	-5.14	104.43	111.73
1	D	308	ALA	N-CA-C	-5.13	105.58	111.07
1	D	93	LEU	O-C-N	5.13	128.87	121.95
1	B	255	ASP	CA-C-O	-5.12	115.13	121.02
1	B	340	VAL	CB-CA-C	5.12	118.43	111.88
1	C	349	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	C	394	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	B	291	PHE	CA-C-O	-5.12	115.22	120.54
1	A	268	ALA	N-CA-C	-5.11	105.79	111.36
1	A	143	ALA	N-CA-CB	-5.11	102.98	111.57
1	A	56	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	64	ASP	N-CA-C	-5.11	104.13	110.41
1	D	367	TYR	O-C-N	5.11	129.01	123.04
1	A	54	HIS	CA-C-O	-5.10	115.05	120.92
1	C	208	ARG	CB-CG-CD	-5.10	99.57	111.30
1	C	346	PRO	CA-C-O	-5.10	115.72	121.43
1	A	289	ARG	CD-NE-CZ	5.10	131.54	124.40
1	A	320	GLU	CB-CG-CD	5.09	121.25	112.60
1	C	207	GLU	CG-CD-OE1	5.09	130.11	118.40
1	B	277	ASN	N-CA-C	-5.09	102.53	109.71
1	B	150	ASP	CA-CB-CG	-5.08	107.52	112.60
1	C	168	TYR	CA-C-N	5.08	127.05	120.44
1	C	168	TYR	C-N-CA	5.08	127.05	120.44
1	D	390	LEU	CA-C-O	-5.08	115.16	120.55
1	C	158	TYR	CA-CB-CG	5.08	123.04	113.90
1	D	273	ASP	CA-C-N	5.07	127.03	120.44
1	D	273	ASP	C-N-CA	5.07	127.03	120.44
1	D	313	ARG	N-CA-C	-5.07	105.64	111.07
1	D	202	PHE	CA-C-N	5.07	127.68	120.53
1	D	202	PHE	C-N-CA	5.07	127.68	120.53
1	D	219	GLY	CA-C-O	-5.07	114.93	120.40
1	B	102	GLY	N-CA-C	-5.06	106.97	112.08
1	C	389	HIS	N-CA-CB	5.05	117.64	110.16
1	B	68	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	A	331	VAL	N-CA-C	-5.05	105.62	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	381	LYS	CA-CB-CG	-5.05	104.00	114.10
1	C	316	LEU	CA-C-O	-5.04	115.20	120.55
1	C	278	GLY	CA-C-N	5.04	126.14	119.84
1	C	278	GLY	C-N-CA	5.04	126.14	119.84
1	C	243	HIS	CA-CB-CG	5.04	118.84	113.80
1	B	57	ASP	N-CA-C	-5.03	105.50	111.69
1	D	17	THR	CB-CA-C	5.03	120.42	110.42
1	B	282	ALA	N-CA-C	5.02	117.29	110.01
1	B	173	GLY	CA-C-O	-5.02	114.10	119.82
1	A	122	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	C	311	ASN	O-C-N	5.01	127.23	122.07
1	C	103	GLY	N-CA-C	-5.01	101.31	113.18
1	C	140	ARG	CD-NE-CZ	5.00	131.41	124.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3049	0	2952	28	0
1	B	3049	0	2952	40	0
1	C	3042	0	2943	32	0
1	D	3048	0	2946	30	0
2	A	10	0	8	0	0
2	B	10	0	8	0	0
2	C	10	0	8	0	0
2	D	10	0	8	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	242	0	0	3	0
4	B	240	0	0	3	0
4	C	257	0	0	1	0
4	D	239	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13214	0	11825	117	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 (117) 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	1.56	1.24
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.64	1.15
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.18	0.86
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.23	0.86
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.24	0.85
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.68	0.75
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.34	0.73
1:B:388:GLU:CD	1:C:313:ARG:HH11	1.98	0.72
1:D:3:VAL:HG23	4:D:579:HOH:O	1.90	0.71
1:C:177:ARG:HD3	4:C:612:HOH:O	1.92	0.70
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.75	0.69
1:A:277:ASN:OD1	1:A:323:LYS:HE3	1.93	0.69
1:A:313:ARG:HG3	4:A:639:HOH:O	1.94	0.66
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.79	0.65
1:B:294:LYS:HE2	4:B:547:HOH:O	1.99	0.62
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.83	0.61
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.83	0.61
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.84	0.60
1:B:388:GLU:OE2	1:C:313:ARG:HD3	2.00	0.60
1:A:167:GLN:OE1	1:A:208:ARG:NH2	2.36	0.58
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.86	0.58
1:B:7:ARG:HD3	4:B:496:HOH:O	2.06	0.56
1:D:394:ARG:NH1	4:D:610:HOH:O	2.08	0.55
1:B:152:SER:HB2	4:D:411:HOH:O	2.07	0.54
1:A:279:PRO:HG2	4:A:614:HOH:O	2.08	0.54
1:C:319:LYS:O	1:C:323:LYS:HG2	2.08	0.53
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.89	0.53
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.44	0.53
1:A:305:TRP:O	1:A:309:LYS:HG3	2.10	0.52
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.91	0.52
4:A:542:HOH:O	1:C:152:SER:HB2	2.09	0.51
1:A:254:PHE:HB3	1:B:186:GLN:NE2	2.25	0.51
1:D:168:TYR:CE1	1:D:172:ARG:HD3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLU:HB3	1:A:394:ARG:HG2	1.92	0.50
1:B:313:ARG:HH21	1:C:388:GLU:CD	2.19	0.50
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.93	0.49
1:B:77:LYS:O	1:B:80:ASP:HB2	2.13	0.49
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.15	0.49
1:B:3:VAL:HG12	1:B:4:GLN:H	1.79	0.48
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.12	0.48
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.13	0.48
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.10	0.47
1:C:238:HIS:O	1:C:239:LYS:HB2	2.14	0.47
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.50	0.47
1:A:352:GLU:HG3	1:A:356:GLU:HB2	1.96	0.47
1:B:164:LEU:C	1:B:164:LEU:HD23	2.39	0.47
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.50	0.47
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.48	0.46
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.42	0.46
1:D:35:ASP:OD1	1:D:37:VAL:HB	2.16	0.46
1:A:6:THR:O	1:A:9:ASP:HB2	2.17	0.45
1:C:86:VAL:O	1:C:131:ALA:HA	2.17	0.45
1:D:168:TYR:O	1:D:172:ARG:HG3	2.17	0.45
1:B:294:LYS:HE2	4:B:563:HOH:O	2.16	0.45
1:B:219:GLY:O	1:B:223:MET:HG3	2.17	0.45
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.52	0.45
1:C:72:ILE:O	1:C:76:LYS:HG3	2.17	0.45
1:D:42:LYS:HD2	4:D:578:HOH:O	2.17	0.45
1:B:280:ASP:C	1:B:282:ALA:H	2.24	0.44
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.79	0.44
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.31	0.44
1:A:36:PRO:O	1:A:40:VAL:HG23	2.18	0.44
1:C:278:GLY:HA3	1:C:282:ALA:O	2.18	0.44
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.52	0.44
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.32	0.44
1:D:50:GLY:HA2	1:D:85:ILE:O	2.18	0.43
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.88	0.43
1:B:154:ALA:HB2	1:D:343:LEU:HD21	2.01	0.43
1:B:193:LEU:N	1:B:194:PRO:HD3	2.34	0.43
1:C:109:ARG:HH11	1:C:109:ARG:HD3	1.49	0.43
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.58	0.42
1:C:159:ARG:HG3	1:C:206:LEU:HD23	2.01	0.42
1:D:352:GLU:HG3	1:D:356:GLU:HB2	2.02	0.42
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.87	0.42
1:D:186:GLN:HA	1:D:187:PRO:HA	1.80	0.42
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.88	0.42
1:C:294:LYS:HE2	4:D:424:HOH:O	2.19	0.42
1:C:193:LEU:N	1:C:194:PRO:HD3	2.35	0.42
1:D:43:LEU:HD12	1:D:51:ILE:HD12	2.02	0.42
1:D:116:ILE:HD13	1:D:116:ILE:HG21	1.88	0.41
1:B:101:ASP:CG	1:B:101:ASP:O	2.62	0.41
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.55	0.41
1:A:60:PRO:O	1:A:61:PHE:C	2.62	0.41
1:D:129:LEU:HD23	1:D:129:LEU:HA	1.93	0.41
1:A:186:GLN:HA	1:A:187:PRO:HA	1.72	0.41
1:B:21:GLN:O	1:B:22:ALA:HB3	2.20	0.41
1:B:193:LEU:N	1:B:194:PRO:CD	2.83	0.41
1:D:5:ALA:HB2	1:D:312:ILE:HG21	2.02	0.41
1:C:249:GLN:HG3	1:C:250:HIS:N	2.36	0.41
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.55	0.41
1:D:172:ARG:HE	1:D:172:ARG:HB3	1.62	0.41
1:D:244:ILE:O	1:D:290:HIS:HB3	2.21	0.41
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.89	0.41
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.89	0.41
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.83	0.41
1:B:238:HIS:O	1:B:239:LYS:HB2	2.20	0.41
1:C:43:LEU:HD12	1:C:51:ILE:HD12	2.03	0.41
1:B:72:ILE:O	1:B:76:LYS:HG3	2.21	0.41
1:B:92:ASN:OD1	1:B:92:ASN:C	2.63	0.41
1:B:338:SER:HA	1:B:377:PHE:O	2.21	0.41
1:B:5:ALA:HB2	1:B:312:ILE:HG21	2.02	0.41
1:B:51:ILE:O	1:B:86:VAL:HA	2.20	0.41
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.82	0.41
1:B:206:LEU:O	1:B:209:PRO:HD3	2.20	0.41
1:B:278:GLY:CA	1:B:282:ALA:O	2.69	0.41
1:D:38:GLU:O	1:D:42:LYS:HG2	2.21	0.41
1:D:305:TRP:O	1:D:309:LYS:HG3	2.21	0.41
1:C:15:LEU:HD12	1:C:15:LEU:HA	1.81	0.40
1:B:142:GLY:HA3	1:B:190:ASP:O	2.20	0.40
1:A:278:GLY:CA	1:A:282:ALA:O	2.69	0.40
1:A:306:GLU:HG2	1:D:381:LYS:HB2	2.03	0.40
1:C:172:ARG:HE	1:C:172:ARG:HB3	1.14	0.40
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.86	0.40
1:B:37:VAL:HG13	1:B:78:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLN:HA	1:C:187:PRO:HA	1.86	0.40
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.94	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%)	12 (3%)	1 (0%)	36	50
1	B	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	24	37
1	C	389/393 (99%)	373 (96%)	12 (3%)	4 (1%)	12	20
1	D	390/393 (99%)	375 (96%)	14 (4%)	1 (0%)	36	50
All	All	1559/1572 (99%)	1503 (96%)	48 (3%)	8 (0%)	24	37

All (8) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	B	397	3	8,9,9	2.16	1 (12%)	10,11,11	1.09	1 (10%)
2	XLS	A	397	3	8,9,9	2.29	1 (12%)	10,11,11	1.87	1 (10%)
2	XLS	C	397	3	8,9,9	2.10	1 (12%)	10,11,11	1.36	2 (20%)
2	XLS	D	397	3	8,9,9	2.27	1 (12%)	10,11,11	0.95	0

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	397	XLS	O1-C1	6.24	1.43	1.20
2	D	397	XLS	O1-C1	6.20	1.43	1.20
2	B	397	XLS	O1-C1	6.03	1.42	1.20
2	C	397	XLS	O1-C1	5.90	1.42	1.20

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	397	XLS	O4-C4-C3	4.09	118.82	109.25
2	B	397	XLS	O4-C4-C3	2.78	115.75	109.25
2	C	397	XLS	O5-C5-C4	-2.54	105.81	111.16
2	C	397	XLS	O4-C4-C3	2.28	114.59	109.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	169:SER	C	170:GLU	N	1.14

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.