



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:33 PM UTC

PDB ID : 2XIM / pdb_00002xim
Title : ARGININE RESIDUES AS STABILIZING ELEMENTS IN PROTEINS
Authors : Mrabet, N.T.; Van Denbroek, A.; Van Den Brande, I.; Stanssens, P.; Laroche, Y.; Lambeir, A.-M.; Matthyssens, G.; Jenkins, J.; Chiadmi, M.; Vantilbeurgh, H.; Rey, F.; Janin, J.; Quax, W.J.; Lasters, I.; Demaeyer, M.; Wodak, S.J.
Deposited on : 1991-05-29
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
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

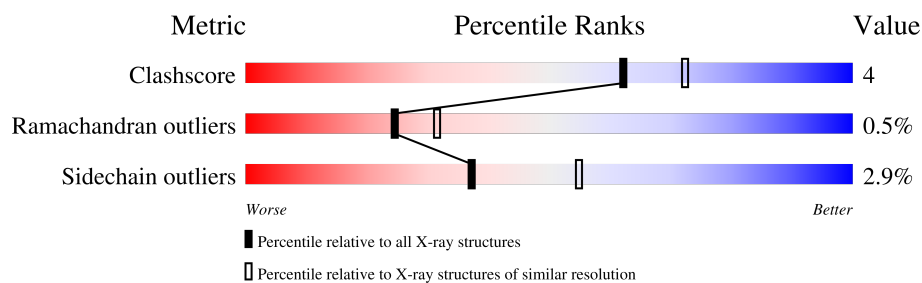
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	78% 18% .
1	C	393	76% 19% . .
1	D	393	78% 18% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13187 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.

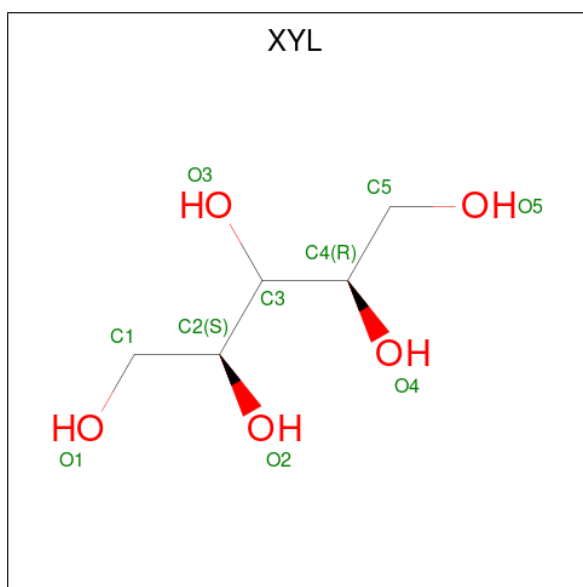
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3055	1939	534	578	4			
1	B	392	Total	C	N	O	S	0	0	0
			3055	1939	534	578	4			
1	C	392	Total	C	N	O	S	0	0	0
			3055	1939	534	578	4			
1	D	392	Total	C	N	O	S	0	0	0
			3055	1939	534	578	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	253	ARG	LYS	conflict	UNP P12851
B	253	ARG	LYS	conflict	UNP P12851
C	253	ARG	LYS	conflict	UNP P12851
D	253	ARG	LYS	conflict	UNP P12851

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	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	230	Total	O	0	0
			230	230		

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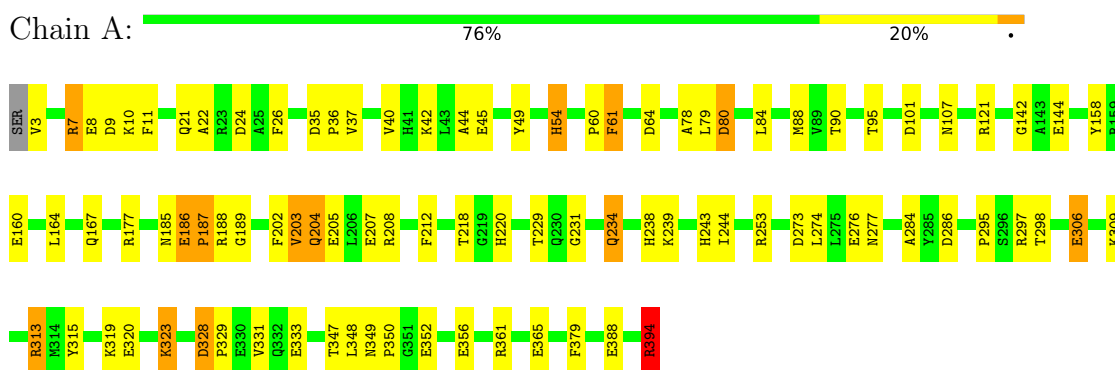
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	231	Total 231	O 231	0	0
4	C	236	Total 236	O 236	0	0
4	D	222	Total 222	O 222	0	0

3 Residue-property plots [i](#)

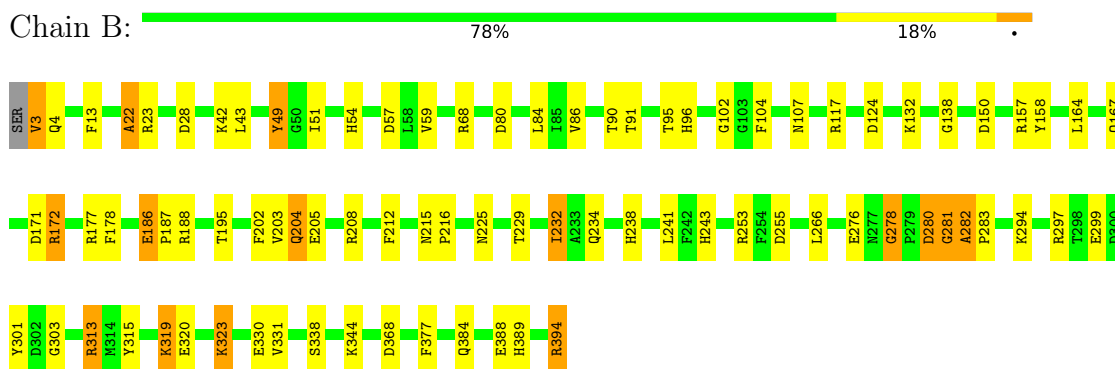
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

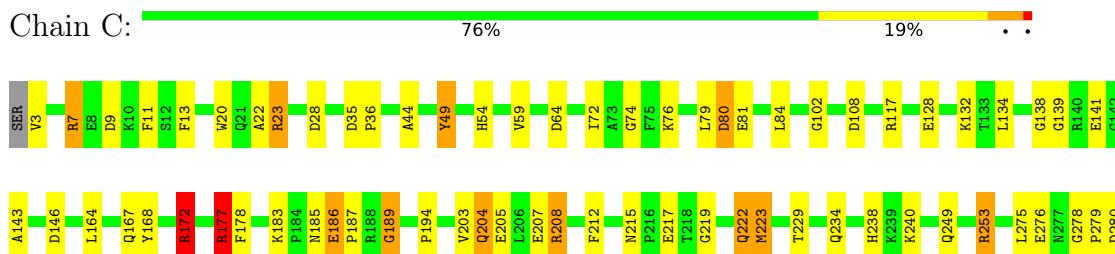
• Molecule 1: D-XYLOSE ISOMERASE



• Molecule 1: D-XYLOSE ISOMERASE

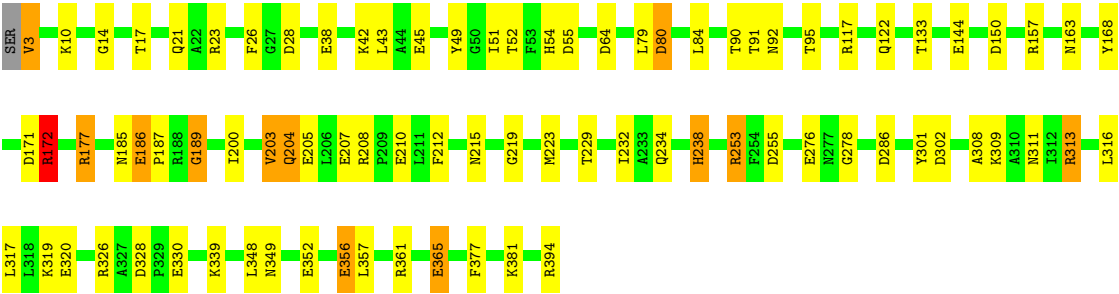
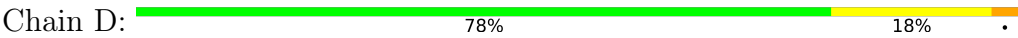


• Molecule 1: D-XYLOSE ISOMERASE





● 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) – 2.30	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}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13187	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: MG, XYZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.95	0/3127	1.96	71/4236 (1.7%)
1	B	0.96	1/3127 (0.0%)	1.95	76/4236 (1.8%)
1	C	0.98	0/3127	2.03	84/4236 (2.0%)
1	D	0.97	0/3127	1.91	73/4236 (1.7%)
All	All	0.97	1/12508 (0.0%)	1.96	304/16944 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	102	GLY	C-N	-7.05	1.27	1.33

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	ARG	CD-NE-CZ	33.59	171.43	124.40
1	B	313	ARG	CD-NE-CZ	20.47	153.06	124.40
1	A	204	GLN	OE1-CD-NE2	-15.25	107.35	122.60
1	A	80	ASP	CA-CB-CG	-13.80	98.80	112.60
1	D	204	GLN	OE1-CD-NE2	-13.32	109.28	122.60
1	C	204	GLN	OE1-CD-NE2	-12.91	109.69	122.60
1	B	204	GLN	OE1-CD-NE2	-10.74	111.86	122.60
1	B	102	GLY	N-CA-C	-10.22	101.75	112.08
1	A	286	ASP	CA-CB-CG	-9.89	102.71	112.60
1	C	208	ARG	CD-NE-CZ	-9.80	110.69	124.40
1	B	313	ARG	NE-CZ-NH2	9.66	127.90	119.20
1	B	80	ASP	CA-CB-CG	-9.08	103.52	112.60
1	A	95	THR	N-CA-C	8.76	120.60	111.14
1	B	320	GLU	CB-CG-CD	8.43	126.93	112.60
1	A	45	GLU	CA-C-O	-8.38	111.66	120.55
1	C	313	ARG	NE-CZ-NH2	8.34	126.71	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	335	LEU	O-C-N	8.33	130.95	122.12
1	B	389	HIS	CA-CB-CG	-8.27	105.53	113.80
1	D	286	ASP	CA-CB-CG	-8.09	104.52	112.60
1	C	28	ASP	CA-CB-CG	8.08	120.68	112.60
1	D	122	GLN	OE1-CD-NE2	-8.08	114.52	122.60
1	A	188	ARG	CD-NE-CZ	8.05	135.66	124.40
1	A	142	GLY	CA-C-O	-7.93	115.44	120.91
1	A	313	ARG	CD-NE-CZ	-7.86	113.40	124.40
1	C	128	GLU	CB-CG-CD	7.83	125.91	112.60
1	C	64	ASP	CA-CB-CG	-7.81	104.79	112.60
1	A	7	ARG	CD-NE-CZ	7.79	135.31	124.40
1	B	117	ARG	NE-CZ-NH1	7.77	129.27	121.50
1	D	172	ARG	CD-NE-CZ	7.64	135.10	124.40
1	B	394	ARG	CD-NE-CZ	-7.63	113.72	124.40
1	C	54	HIS	N-CA-C	-7.43	98.51	110.32
1	C	379	PHE	CA-CB-CG	7.42	121.22	113.80
1	D	328	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	379	PHE	CA-CB-CG	7.23	121.03	113.80
1	B	202	PHE	CA-C-N	7.23	130.37	120.46
1	B	202	PHE	C-N-CA	7.23	130.37	120.46
1	C	313	ARG	NH1-CZ-NH2	-7.22	109.91	119.30
1	C	44	ALA	CA-C-O	7.22	128.20	120.55
1	D	10	LYS	CB-CA-C	-7.15	102.28	111.86
1	D	208	ARG	CD-NE-CZ	-7.08	114.49	124.40
1	C	208	ARG	NE-CZ-NH1	-7.08	114.42	121.50
1	C	229	THR	CA-CB-OG1	-7.08	98.99	109.60
1	D	171	ASP	CA-C-O	-7.04	112.96	120.42
1	B	95	THR	N-CA-C	7.01	119.95	111.40
1	D	286	ASP	CA-C-O	-6.97	111.26	119.48
1	A	244	ILE	CA-C-O	-6.93	113.48	120.90
1	C	349	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	B	57	ASP	CA-CB-CG	6.91	119.51	112.60
1	C	326	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	D	95	THR	N-CA-C	6.90	119.82	111.40
1	D	54	HIS	N-CA-C	-6.90	99.06	110.17
1	A	231	GLY	CA-C-N	6.88	130.19	120.42
1	A	231	GLY	C-N-CA	6.88	130.19	120.42
1	D	328	ASP	CB-CA-C	6.87	117.68	109.85
1	C	172	ARG	NE-CZ-NH1	-6.85	114.65	121.50
1	A	204	GLN	CB-CG-CD	6.85	124.25	112.60
1	C	340	VAL	CB-CA-C	6.78	120.56	111.88
1	C	335	LEU	CA-C-O	-6.75	113.39	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	ASP	O-C-N	6.74	130.54	122.85
1	A	229	THR	CA-CB-OG1	-6.74	99.49	109.60
1	B	278	GLY	N-CA-C	-6.71	104.11	112.23
1	A	64	ASP	N-CA-C	-6.69	101.90	110.53
1	B	150	ASP	CA-CB-CG	-6.67	105.93	112.60
1	A	394	ARG	NH1-CZ-NH2	6.66	127.96	119.30
1	B	138	GLY	CA-C-N	6.65	128.51	120.13
1	B	138	GLY	C-N-CA	6.65	128.51	120.13
1	C	80	ASP	CA-CB-CG	-6.61	105.99	112.60
1	A	24	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	309	LYS	CA-C-O	-6.51	112.48	119.97
1	B	96	HIS	CA-CB-CG	-6.51	107.28	113.80
1	D	278	GLY	N-CA-C	-6.51	104.35	112.23
1	C	13	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	61	PHE	CA-C-O	-6.49	114.47	120.95
1	A	79	LEU	CA-C-O	6.48	127.42	120.55
1	D	80	ASP	CA-CB-CG	-6.46	106.14	112.60
1	D	255	ASP	CA-CB-CG	6.46	119.06	112.60
1	C	146	ASP	CA-C-O	-6.46	113.71	120.55
1	B	280	ASP	N-CA-C	-6.45	103.28	111.92
1	D	238	HIS	CA-CB-CG	6.43	120.23	113.80
1	A	21	GLN	CB-CG-CD	-6.42	101.69	112.60
1	D	377	PHE	CA-C-O	-6.40	111.56	119.18
1	D	215	ASN	CA-CB-CG	-6.40	106.20	112.60
1	C	253	ARG	NE-CZ-NH1	6.38	127.88	121.50
1	A	177	ARG	CD-NE-CZ	-6.37	115.48	124.40
1	A	253	ARG	CD-NE-CZ	6.34	133.28	124.40
1	D	52	THR	CA-C-O	-6.32	114.25	121.58
1	B	177	ARG	CA-C-O	-6.31	114.03	121.16
1	D	349	ASN	OD1-CG-ND2	6.29	128.89	122.60
1	B	68	ARG	NE-CZ-NH1	-6.27	115.23	121.50
1	D	313	ARG	CA-CB-CG	6.26	126.62	114.10
1	A	320	GLU	CB-CG-CD	6.24	123.21	112.60
1	D	253	ARG	CD-NE-CZ	6.24	133.13	124.40
1	B	54	HIS	N-CA-CB	6.21	120.54	110.41
1	A	177	ARG	CB-CA-C	6.20	121.21	109.37
1	B	229	THR	CA-CB-OG1	-6.20	100.30	109.60
1	B	54	HIS	N-CA-C	-6.19	100.48	110.32
1	C	7	ARG	CB-CG-CD	6.19	125.53	111.30
1	A	144	GLU	N-CA-C	-6.18	106.28	113.88
1	C	301	TYR	CA-C-O	-6.17	113.12	120.10
1	C	328	ASP	CA-CB-CG	6.17	118.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	394	ARG	NE-CZ-NH2	-6.14	113.67	119.20
1	D	55	ASP	CA-CB-CG	6.14	118.74	112.60
1	D	339	LYS	CB-CA-C	-6.13	103.02	111.73
1	B	102	GLY	CA-C-N	6.12	133.13	123.95
1	B	102	GLY	C-N-CA	6.12	133.13	123.95
1	D	212	PHE	N-CA-C	6.11	118.86	108.90
1	A	284	ALA	N-CA-C	-6.11	105.66	113.23
1	C	177	ARG	N-CA-C	-6.10	100.25	109.95
1	B	13	PHE	CA-C-O	-6.09	113.99	121.06
1	B	23	ARG	CD-NE-CZ	6.08	132.91	124.40
1	C	7	ARG	NH1-CZ-NH2	-6.08	111.40	119.30
1	C	207	GLU	CA-C-O	-6.07	113.99	120.42
1	B	59	VAL	O-C-N	6.07	126.50	120.92
1	B	232	ILE	N-CA-C	-6.07	104.59	110.72
1	C	143	ALA	O-C-N	6.06	129.35	123.29
1	D	203	VAL	CA-CB-CG1	6.05	120.68	110.40
1	B	158	TYR	N-CA-C	-6.03	104.63	111.14
1	C	79	LEU	CA-C-O	6.02	127.14	120.82
1	C	194	PRO	N-CA-C	6.01	121.37	113.86
1	D	21	GLN	OE1-CD-NE2	6.00	128.60	122.60
1	C	328	ASP	CB-CA-C	5.99	118.00	109.38
1	D	14	GLY	N-CA-C	-5.97	104.02	112.37
1	D	144	GLU	N-CA-C	-5.92	106.39	113.97
1	A	44	ALA	CA-C-O	5.90	126.80	120.55
1	C	253	ARG	CA-C-O	-5.90	114.82	121.25
1	B	241	LEU	CA-C-O	-5.89	114.98	121.58
1	C	354	TYR	CA-C-O	-5.88	114.32	120.55
1	A	243	HIS	CA-CB-CG	5.83	119.63	113.80
1	D	150	ASP	CA-CB-CG	-5.81	106.79	112.60
1	D	79	LEU	CA-C-O	5.80	126.70	120.55
1	A	8	GLU	CA-CB-CG	-5.79	102.51	114.10
1	D	163	ASN	CA-CB-CG	-5.79	106.81	112.60
1	D	203	VAL	CB-CA-C	5.79	119.95	112.14
1	C	389	HIS	CA-CB-CG	-5.78	108.02	113.80
1	C	294	LYS	O-C-N	5.77	126.92	121.38
1	A	26	PHE	CA-C-O	-5.76	112.38	119.18
1	B	225	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	C	134	LEU	CA-C-O	-5.74	114.32	120.46
1	C	276	GLU	CG-CD-OE2	5.74	131.59	118.40
1	A	273	ASP	CA-CB-CG	5.73	118.33	112.60
1	C	223	MET	N-CA-C	-5.73	105.39	112.38
1	B	331	VAL	N-CA-C	-5.72	105.15	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	ARG	N-CA-C	-5.72	99.86	108.96
1	C	141	GLU	CB-CG-CD	5.71	122.31	112.60
1	C	167	GLN	CA-C-O	5.71	126.81	120.82
1	D	311	ASN	CA-CB-CG	5.69	118.29	112.60
1	D	320	GLU	CB-CG-CD	5.69	122.27	112.60
1	C	102	GLY	CA-C-O	-5.69	118.22	122.37
1	B	315	TYR	CA-C-O	-5.67	114.86	120.82
1	C	215	ASN	CA-CB-CG	-5.67	106.93	112.60
1	C	281	GLY	N-CA-C	-5.67	99.75	113.18
1	D	330	GLU	O-C-N	5.66	128.60	122.15
1	B	283	PRO	N-CA-CB	5.65	108.34	103.31
1	C	349	ASN	N-CA-C	-5.65	101.99	110.24
1	D	308	ALA	N-CA-C	-5.65	105.04	111.14
1	C	49	TYR	N-CA-C	-5.64	106.75	113.97
1	C	297	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	B	281	GLY	CA-C-N	5.64	130.05	121.03
1	B	281	GLY	C-N-CA	5.64	130.05	121.03
1	B	107	ASN	N-CA-C	-5.63	105.23	111.71
1	A	158	TYR	CA-C-N	5.63	128.09	120.44
1	A	158	TYR	C-N-CA	5.63	128.09	120.44
1	C	189	GLY	N-CA-C	-5.63	105.83	112.64
1	B	104	PHE	CA-CB-CG	5.62	119.42	113.80
1	C	222	GLN	OE1-CD-NE2	-5.62	116.97	122.60
1	C	138	GLY	CA-C-N	5.62	127.17	120.14
1	C	138	GLY	C-N-CA	5.62	127.17	120.14
1	A	333	GLU	CB-CG-CD	-5.62	103.05	112.60
1	C	7	ARG	NE-CZ-NH1	5.60	127.10	121.50
1	A	244	ILE	O-C-N	5.59	129.57	123.09
1	C	64	ASP	N-CA-C	-5.58	103.16	110.53
1	A	177	ARG	N-CA-C	-5.58	100.31	109.40
1	C	177	ARG	CB-CG-CD	5.55	124.08	111.30
1	A	234	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	D	330	GLU	CG-CD-OE2	-5.55	105.63	118.40
1	C	204	GLN	CB-CG-CD	5.54	122.01	112.60
1	B	282	ALA	N-CA-C	5.53	118.17	110.20
1	D	45	GLU	CA-C-O	-5.53	113.61	119.97
1	B	215	ASN	CA-CB-CG	-5.52	107.08	112.60
1	B	330	GLU	CG-CD-OE2	-5.51	105.72	118.40
1	A	207	GLU	CA-C-O	-5.51	115.02	120.70
1	C	394	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	D	189	GLY	N-CA-C	-5.51	106.11	112.50
1	A	101	ASP	CA-CB-CG	5.50	118.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	167	GLN	OE1-CD-NE2	-5.50	117.10	122.60
1	B	255	ASP	N-CA-CB	-5.49	100.60	109.60
1	A	394	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	D	356	GLU	CA-C-O	-5.48	115.05	120.70
1	A	88	MET	CA-C-O	-5.48	114.85	120.99
1	A	220	HIS	CA-C-O	-5.48	115.06	120.82
1	C	81	GLU	CB-CG-CD	5.47	121.89	112.60
1	B	303	GLY	N-CA-C	-5.46	106.18	112.73
1	D	330	GLU	OE1-CD-OE2	5.46	135.99	122.90
1	C	275	LEU	CA-C-O	-5.44	114.66	120.42
1	A	203	VAL	N-CA-CB	-5.43	103.15	110.54
1	C	80	ASP	O-C-N	5.43	127.74	122.09
1	A	218	THR	CA-C-N	5.43	126.00	119.98
1	A	218	THR	C-N-CA	5.43	126.00	119.98
1	B	13	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	160	GLU	CA-C-N	5.41	127.48	120.44
1	A	160	GLU	C-N-CA	5.41	127.48	120.44
1	B	344	LYS	CA-CB-CG	-5.41	103.28	114.10
1	A	212	PHE	N-CA-C	5.41	118.30	109.59
1	B	323	LYS	CB-CA-C	-5.40	102.36	110.90
1	C	278	GLY	CA-C-N	5.40	126.59	119.84
1	C	278	GLY	C-N-CA	5.40	126.59	119.84
1	B	188	ARG	CD-NE-CZ	5.39	131.95	124.40
1	A	306	GLU	CB-CA-C	-5.39	101.84	110.79
1	D	91	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	202	PHE	CA-C-N	5.37	127.82	120.46
1	A	202	PHE	C-N-CA	5.37	127.82	120.46
1	D	326	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	144	GLU	N-CA-CB	5.37	117.73	110.59
1	B	86	VAL	CA-C-N	5.37	124.88	119.19
1	B	86	VAL	C-N-CA	5.37	124.88	119.19
1	D	157	ARG	NE-CZ-NH2	5.36	124.03	119.20
1	C	217	GLU	CA-C-O	-5.36	114.57	120.36
1	D	365	GLU	CA-C-O	-5.36	115.16	120.90
1	D	28	ASP	CA-C-O	-5.35	115.49	121.81
1	C	323	LYS	CB-CA-C	-5.35	102.48	110.88
1	B	157	ARG	NE-CZ-NH1	5.35	126.85	121.50
1	A	54	HIS	N-CA-C	-5.34	101.57	110.17
1	B	330	GLU	OE1-CD-OE2	5.34	135.71	122.90
1	C	207	GLU	CG-CD-OE2	-5.33	106.13	118.40
1	A	295	PRO	N-CA-C	-5.33	102.75	110.80
1	C	322	ALA	N-CA-C	-5.33	105.39	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	LYS	CB-CA-C	-5.32	104.74	111.86
1	D	210	GLU	CB-CG-CD	5.31	121.63	112.60
1	B	319	LYS	CA-C-O	5.31	126.39	120.82
1	D	302	ASP	CA-CB-CG	-5.31	107.29	112.60
1	C	294	LYS	CB-CA-C	-5.30	102.07	110.02
1	B	243	HIS	CA-CB-CG	5.30	119.10	113.80
1	D	349	ASN	O-C-N	5.30	127.22	121.60
1	D	301	TYR	CB-CA-C	5.29	120.42	110.63
1	D	320	GLU	CA-CB-CG	5.29	124.68	114.10
1	A	107	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	26	PHE	CA-CB-CG	-5.28	108.52	113.80
1	C	23	ARG	N-CA-C	-5.28	99.92	108.41
1	D	316	LEU	CB-CA-C	5.27	119.81	110.85
1	C	108	ASP	CA-C-N	5.27	127.34	120.28
1	C	108	ASP	C-N-CA	5.27	127.34	120.28
1	D	17	THR	CB-CA-C	5.26	120.90	110.42
1	C	240	LYS	O-C-N	5.26	128.56	122.19
1	B	42	LYS	O-C-N	5.26	127.69	122.12
1	A	121	ARG	NE-CZ-NH2	-5.25	114.47	119.20
1	C	59	VAL	O-C-N	5.23	125.73	120.92
1	D	177	ARG	N-CA-C	-5.23	101.17	109.59
1	D	21	GLN	CB-CG-CD	-5.23	103.72	112.60
1	A	203	VAL	CB-CA-C	5.22	119.18	112.14
1	A	328	ASP	CA-C-N	5.21	125.01	119.28
1	A	328	ASP	C-N-CA	5.21	125.01	119.28
1	D	117	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	D	278	GLY	O-C-N	5.20	127.38	122.18
1	A	331	VAL	N-CA-C	-5.20	105.65	110.53
1	B	90	THR	CA-CB-OG1	-5.19	101.81	109.60
1	D	229	THR	CA-CB-OG1	-5.19	101.82	109.60
1	D	133	THR	CA-CB-CG2	5.18	119.31	110.50
1	B	394	ARG	NH1-CZ-NH2	5.18	126.03	119.30
1	B	368	ASP	CA-C-O	-5.17	116.42	122.37
1	D	210	GLU	CA-C-O	-5.17	114.25	120.10
1	B	49	TYR	N-CA-C	-5.17	107.35	113.97
1	A	347	THR	CA-CB-OG1	-5.17	101.84	109.60
1	B	195	THR	CA-CB-OG1	-5.17	101.85	109.60
1	C	54	HIS	N-CA-CB	5.16	118.82	110.41
1	B	57	ASP	N-CA-C	-5.15	105.35	111.69
1	D	80	ASP	O-C-N	5.14	127.37	122.07
1	C	253	ARG	NH1-CZ-NH2	-5.14	112.61	119.30
1	C	177	ARG	CB-CA-C	5.14	118.78	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	207	GLU	CA-CB-CG	5.13	124.36	114.10
1	B	171	ASP	CA-C-O	-5.12	115.13	120.55
1	B	22	ALA	N-CA-C	5.10	118.75	111.92
1	B	323	LYS	N-CA-CB	5.10	117.46	110.07
1	B	177	ARG	N-CA-C	-5.10	101.85	109.95
1	D	357	LEU	O-C-N	5.09	127.31	122.07
1	C	208	ARG	NH1-CZ-NH2	5.09	125.92	119.30
1	A	187	PRO	N-CA-C	5.08	125.32	112.10
1	A	45	GLU	O-C-N	5.08	127.50	122.12
1	B	91	THR	CA-C-O	-5.07	115.22	120.70
1	C	332	GLN	CA-C-O	5.07	125.92	120.55
1	D	317	LEU	CA-C-O	-5.07	115.50	120.82
1	B	299	GLU	N-CA-C	5.07	118.33	110.17
1	D	90	THR	CA-CB-CG2	5.06	119.11	110.50
1	B	301	TYR	CA-CB-CG	-5.06	104.80	113.90
1	C	74	GLY	CA-C-O	5.06	125.96	120.75
1	C	117	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	274	LEU	CA-C-O	-5.06	115.51	120.82
1	B	28	ASP	O-C-N	5.05	128.87	122.65
1	D	204	GLN	CG-CD-NE2	5.05	123.98	116.40
1	B	303	GLY	O-C-N	5.05	127.04	122.19
1	A	315	TYR	CA-C-O	-5.04	115.52	120.82
1	B	394	ARG	N-CA-CB	5.04	119.08	110.50
1	C	13	PHE	CA-C-O	-5.04	115.21	121.06
1	C	289	ARG	N-CA-C	-5.04	97.79	107.57
1	D	64	ASP	N-CA-C	-5.04	104.21	110.41
1	D	26	PHE	CA-C-O	-5.04	113.54	119.48
1	B	124	ASP	O-C-N	5.03	127.25	122.07
1	C	383	ASN	CA-CB-CG	-5.03	107.57	112.60
1	B	276	GLU	N-CA-C	5.02	119.53	113.41
1	B	177	ARG	CA-CB-CG	-5.02	104.07	114.10
1	C	139	GLY	CA-C-O	-5.01	114.98	120.40
1	A	298	THR	CA-CB-CG2	5.01	119.01	110.50
1	D	309	LYS	CA-C-O	-5.01	115.24	120.55
1	A	95	THR	CA-CB-OG1	-5.00	102.09	109.60
1	D	200	ILE	N-CA-CB	5.00	116.40	110.55

There are no chirality outliers.

There are no planarity outliers.

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	3055	0	2954	27	0
1	B	3055	0	2954	27	0
1	C	3055	0	2954	36	0
1	D	3055	0	2954	22	0
2	A	10	0	12	1	0
2	B	10	0	11	1	0
2	C	10	0	11	1	0
2	D	10	0	12	1	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	230	0	0	2	0
4	B	231	0	0	2	0
4	C	236	0	0	4	0
4	D	222	0	0	5	0
All	All	13187	0	11862	99	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 (99) 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	1.57	1.19
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.61	1.18
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.12	0.98
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.26	0.83
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.25	0.83
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.64	0.80
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.28	0.79
1:C:177:ARG:HD3	4:C:605:HOH:O	1.85	0.77
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.71	0.71
1:C:372:VAL:HA	1:C:375:LYS:HD2	1.77	0.67
1:A:313:ARG:HG3	4:A:627:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:VAL:HG23	4:D:569:HOH:O	1.93	0.67
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.78	0.66
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.79	0.64
1:A:36:PRO:O	1:A:40:VAL:HG23	1.99	0.63
1:A:167:GLN:OE1	1:A:208:ARG:NH2	2.28	0.62
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.82	0.61
1:D:38:GLU:O	1:D:42:LYS:HG2	2.02	0.60
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.83	0.60
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.04	0.60
1:B:164:LEU:C	1:B:164:LEU:HD23	2.28	0.58
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.87	0.57
1:D:394:ARG:HD2	4:D:598:HOH:O	2.05	0.57
2:C:397:XYL:H12	4:C:575:HOH:O	2.03	0.57
1:C:294:LYS:HE2	4:D:420:HOH:O	2.04	0.55
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.41	0.55
1:B:294:LYS:HE2	4:B:547:HOH:O	2.07	0.55
1:B:3:VAL:HG12	1:B:4:GLN:H	1.71	0.55
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.88	0.54
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.89	0.53
1:C:168:TYR:O	1:C:172:ARG:HG2	2.10	0.52
1:D:394:ARG:NH1	4:D:598:HOH:O	2.07	0.51
1:D:168:TYR:O	1:D:172:ARG:HG2	2.11	0.50
1:A:277:ASN:OD1	1:A:323:LYS:HE3	2.13	0.49
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.45	0.49
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.95	0.49
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.49	0.48
1:A:204:GLN:CD	1:C:204:GLN:OE1	2.48	0.48
1:C:72:ILE:O	1:C:76:LYS:HG3	2.14	0.48
2:D:397:XYL:H12	4:D:540:HOH:O	2.14	0.48
1:A:189:GLY:O	1:B:253:ARG:NH1	2.47	0.47
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.32	0.47
1:B:216:PRO:HG2	1:B:232:ILE:HD11	1.96	0.47
1:C:183:LYS:HE2	1:C:185:ASN:O	2.14	0.47
1:C:189:GLY:O	1:D:253:ARG:NH1	2.47	0.47
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.50	0.47
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.50	0.47
1:C:253:ARG:NH1	1:D:189:GLY:O	2.48	0.46
1:A:388:GLU:HB3	1:A:394:ARG:HG2	1.98	0.46
1:C:177:ARG:NH2	4:C:585:HOH:O	2.30	0.46
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.97	0.46
2:B:397:XYL:H12	4:B:563:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.80	0.45
2:A:397:XYL:H3	4:A:593:HOH:O	2.15	0.45
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.25	0.45
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.16	0.45
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.76	0.44
1:C:164:LEU:C	1:C:164:LEU:HD23	2.42	0.44
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.18	0.44
1:D:219:GLY:O	1:D:223:MET:HG3	2.17	0.44
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.98	0.44
1:A:276:GLU:HG3	1:A:319:LYS:HG3	1.98	0.44
1:A:352:GLU:HG3	1:A:356:GLU:HB2	1.99	0.44
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.51	0.44
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.18	0.43
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.54	0.43
1:C:168:TYR:O	1:C:172:ARG:CG	2.66	0.43
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.53	0.43
1:D:352:GLU:HG3	1:D:356:GLU:HB2	2.01	0.43
1:D:92:ASN:C	1:D:92:ASN:OD1	2.61	0.42
1:B:384:GLN:O	1:B:388:GLU:HG3	2.19	0.42
1:B:394:ARG:HH11	1:B:394:ARG:HD3	1.55	0.42
1:C:219:GLY:O	1:C:223:MET:HG3	2.19	0.42
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.55	0.42
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.90	0.42
1:A:348:LEU:HD11	1:C:164:LEU:HD12	2.01	0.42
1:C:172:ARG:HE	1:C:172:ARG:HB3	1.04	0.42
1:B:186:GLU:HA	1:B:187:PRO:HA	1.88	0.42
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.77	0.42
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.89	0.42
1:D:186:GLU:HA	1:D:187:PRO:HA	1.82	0.42
1:A:349:ASN:HB3	1:A:350:PRO:HD2	2.02	0.42
1:B:388:GLU:CD	1:C:313:ARG:HH21	2.28	0.41
1:B:338:SER:HA	1:B:377:PHE:O	2.20	0.41
1:C:186:GLU:HA	1:C:187:PRO:HA	1.92	0.41
1:B:280:ASP:C	1:B:282:ALA:H	2.27	0.41
1:C:23:ARG:HD2	4:C:614:HOH:O	2.19	0.41
1:B:313:ARG:HH21	1:C:388:GLU:CD	2.28	0.41
1:D:276:GLU:HG3	1:D:319:LYS:HG3	2.01	0.41
1:A:37:VAL:HG13	1:A:78:ALA:HB2	2.02	0.41
1:B:313:ARG:NH2	1:C:388:GLU:OE1	2.54	0.41
1:B:319:LYS:O	1:B:323:LYS:HG2	2.21	0.41
1:D:232:ILE:HD13	1:D:232:ILE:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLY:CA	1:B:282:ALA:O	2.70	0.40
1:A:60:PRO:O	1:A:61:PHE:C	2.63	0.40
1:A:238:HIS:O	1:A:239:LYS:HB2	2.21	0.40
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.83	0.40
1:A:186:GLU:HA	1:A:187:PRO:HA	1.78	0.40
1:B:266:LEU:HD23	1:B:266:LEU:HA	1.88	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%)	377 (97%)	11 (3%)	2 (0%)	24	31
1	C	390/393 (99%)	376 (96%)	10 (3%)	4 (1%)	12	15
1	D	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	46
All	All	1560/1572 (99%)	1505 (96%)	47 (3%)	8 (0%)	24	31

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	D	186	GLU
1	C	364	PHE
1	C	279	PRO
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%)	300 (98%)	6 (2%)	48	67
1	C	306/310 (99%)	296 (97%)	10 (3%)	33	50
1	D	306/310 (99%)	297 (97%)	9 (3%)	37	55
All	All	1224/1240 (99%)	1189 (97%)	35 (3%)	37	55

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	ARG
1	A	42	LYS
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	185	ASN
1	A	203	VAL
1	A	323	LYS
1	A	394	ARG
1	B	3	VAL
1	B	49	TYR
1	B	84	LEU
1	B	132	LYS
1	B	172	ARG
1	B	203	VAL
1	C	3	VAL
1	C	7	ARG
1	C	49	TYR
1	C	80	ASP
1	C	84	LEU
1	C	132	LYS
1	C	172	ARG
1	C	177	ARG

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Mol	Chain	Res	Type
1	C	203	VAL
1	C	375	LYS
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	172	ARG
1	D	177	ARG
1	D	185	ASN
1	D	203	VAL
1	D	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	XYL	C	397	3	9,9,9	0.44	0	11,11,11	1.67	4 (36%)
2	XYL	A	397	3	9,9,9	0.57	0	11,11,11	1.05	1 (9%)
2	XYL	D	397	3	9,9,9	0.82	0	11,11,11	1.38	2 (18%)
2	XYL	B	397	3	9,9,9	0.54	0	11,11,11	2.31	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XYL	C	397	3	-	0/12/12/12	-
2	XYL	A	397	3	-	1/12/12/12	-
2	XYL	D	397	3	-	1/12/12/12	-
2	XYL	B	397	3	-	4/12/12/12	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XYL	O4-C4-C3	6.42	124.28	109.25
2	C	397	XYL	O4-C4-C3	3.31	116.99	109.25
2	D	397	XYL	C5-C4-C3	2.58	117.44	112.17
2	D	397	XYL	C4-C3-C2	-2.50	109.41	113.57
2	C	397	XYL	O5-C5-C4	-2.40	106.11	111.16
2	B	397	XYL	C1-C2-C3	2.39	117.05	112.17
2	A	397	XYL	O4-C4-C3	2.27	114.56	109.25
2	C	397	XYL	C1-C2-C3	2.25	116.75	112.17
2	B	397	XYL	O5-C5-C4	-2.11	106.73	111.16
2	C	397	XYL	C4-C3-C2	-2.01	110.22	113.57

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.