



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:48 PM UTC

PDB ID : 1XIM / pdb_00001xim
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 : 2.20 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

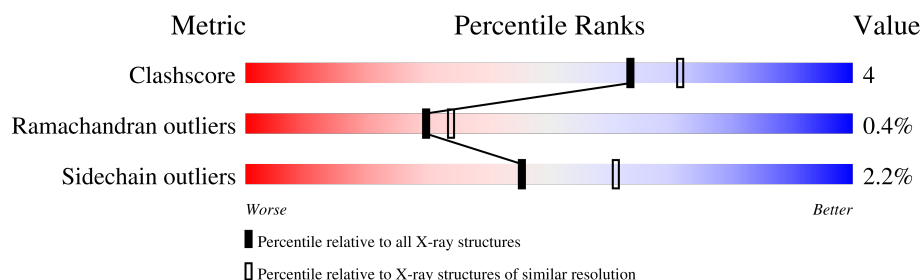
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	
1	B	393	
1	C	393	
1	D	393	

2 Entry composition [i](#)

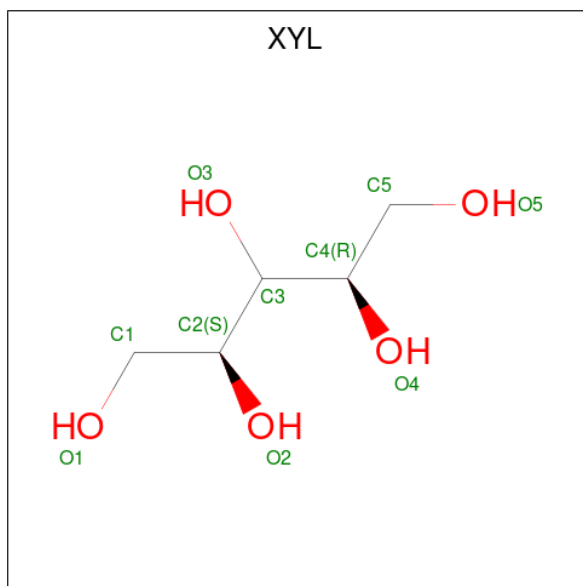
There are 4 unique types of molecules in this entry. The entry contains 13141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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		

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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 COBALT (II) ION (CCD ID: CO) (formula: Co).

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

- Molecule 4 is water.

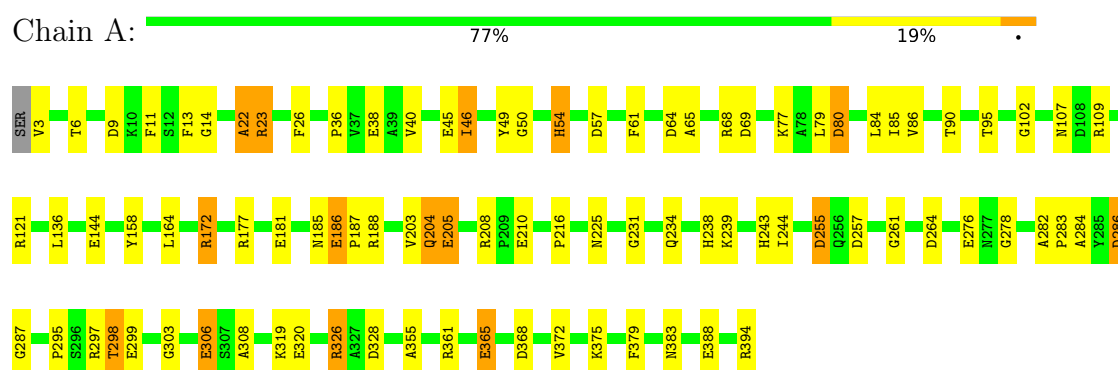
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total	O	0	0
			225	225		
4	B	212	Total	O	0	0
			212	212		
4	C	233	Total	O	0	0
			233	233		
4	D	211	Total	O	0	0
			211	211		

3 Residue-property plots [i](#)

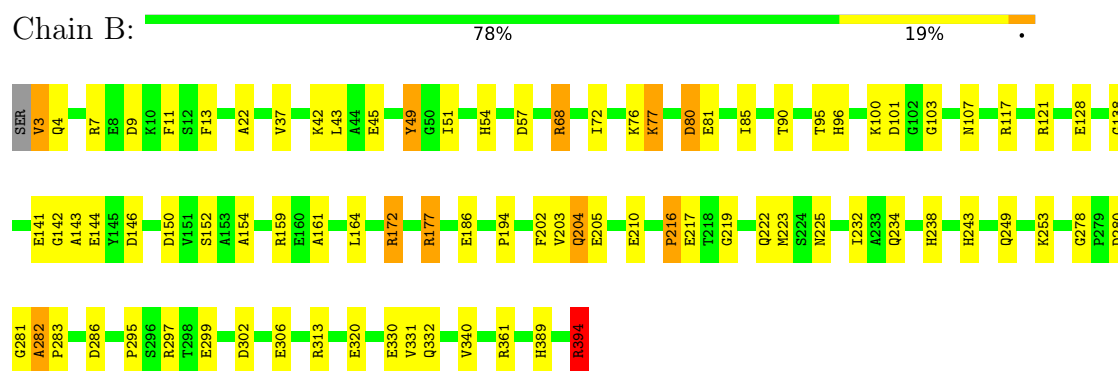
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

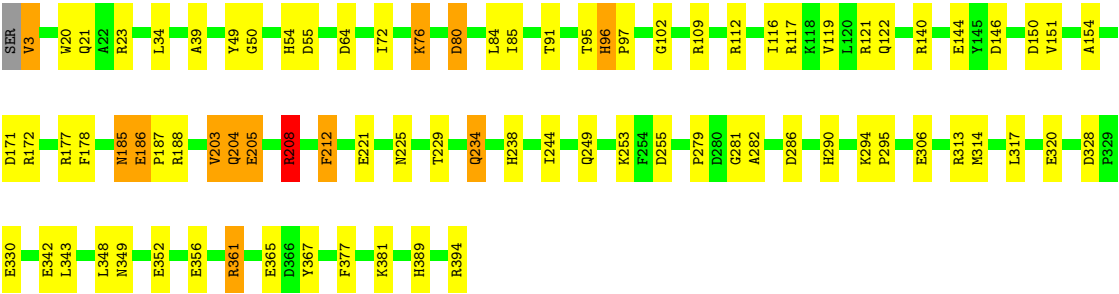
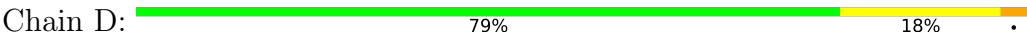


• Molecule 1: D-XYLOSE ISOMERASE





● 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) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13141	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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: CO, 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	0/3125	1.94	73/4233 (1.7%)
1	B	0.94	1/3125 (0.0%)	1.91	66/4233 (1.6%)
1	C	0.94	0/3125	1.90	75/4233 (1.8%)
1	D	0.97	0/3125	1.92	67/4233 (1.6%)
All	All	0.95	1/12500 (0.0%)	1.92	281/16932 (1.7%)

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	2
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	7

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 (281) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	CA-CB-CG	-15.48	97.11	112.60
1	C	204	GLN	OE1-CD-NE2	-13.27	109.33	122.60
1	D	204	GLN	OE1-CD-NE2	-13.26	109.34	122.60
1	B	204	GLN	OE1-CD-NE2	-12.64	109.96	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLN	OE1-CD-NE2	-11.70	110.90	122.60
1	D	255	ASP	CA-CB-CG	10.38	122.98	112.60
1	B	172	ARG	NE-CZ-NH2	-9.37	110.77	119.20
1	C	172	ARG	NE-CZ-NH2	-9.22	110.90	119.20
1	B	177	ARG	NE-CZ-NH2	-9.11	111.00	119.20
1	A	188	ARG	CD-NE-CZ	8.65	136.51	124.40
1	A	320	GLU	CB-CG-CD	8.34	126.78	112.60
1	C	225	ASN	OD1-CG-ND2	-8.26	114.34	122.60
1	B	95	THR	N-CA-C	8.26	120.20	111.03
1	A	255	ASP	CA-CB-CG	8.12	120.72	112.60
1	B	172	ARG	NE-CZ-NH1	8.06	129.56	121.50
1	A	286	ASP	CA-CB-CG	-8.03	104.58	112.60
1	C	172	ARG	NE-CZ-NH1	8.00	129.50	121.50
1	B	13	PHE	CA-CB-CG	7.89	121.69	113.80
1	B	80	ASP	CA-CB-CG	-7.87	104.73	112.60
1	B	394	ARG	N-CA-CB	7.80	123.76	110.50
1	C	64	ASP	CA-CB-CG	-7.80	104.80	112.60
1	B	225	ASN	OD1-CG-ND2	-7.66	114.94	122.60
1	C	80	ASP	CA-CB-CG	-7.63	104.97	112.60
1	B	320	GLU	CB-CG-CD	7.62	125.56	112.60
1	A	107	ASN	CA-CB-CG	7.62	120.22	112.60
1	A	379	PHE	CA-CB-CG	7.61	121.41	113.80
1	D	208	ARG	CG-CD-NE	7.61	128.74	112.00
1	D	208	ARG	NE-CZ-NH1	7.58	129.08	121.50
1	A	394	ARG	CA-CB-CG	7.55	129.21	114.10
1	A	394	ARG	NH1-CZ-NH2	7.48	129.02	119.30
1	B	394	ARG	NE-CZ-NH2	-7.48	112.47	119.20
1	D	54	HIS	N-CA-C	-7.45	98.47	110.32
1	C	54	HIS	N-CA-C	-7.45	99.50	110.52
1	C	13	PHE	CA-C-O	-7.43	112.44	121.06
1	D	144	GLU	N-CA-C	-7.39	104.50	113.97
1	D	328	ASP	CA-CB-CG	7.36	119.96	112.60
1	C	134	LEU	CA-C-O	-7.34	112.44	120.30
1	D	349	ASN	OD1-CG-ND2	7.27	129.87	122.60
1	D	286	ASP	CA-CB-CG	-7.25	105.35	112.60
1	D	349	ASN	CA-CB-CG	-7.24	105.36	112.60
1	D	122	GLN	OE1-CD-NE2	-7.22	115.38	122.60
1	D	203	VAL	CB-CA-C	7.18	121.44	112.04
1	A	244	ILE	CA-C-O	-7.17	113.23	120.90
1	D	188	ARG	NE-CZ-NH2	7.15	125.63	119.20
1	D	117	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	B	389	HIS	CA-CB-CG	-7.10	106.70	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ASP	CA-CB-CG	7.09	119.69	112.60
1	C	28	ASP	CA-CB-CG	7.00	119.60	112.60
1	D	389	HIS	CA-CB-CG	-6.93	106.86	113.80
1	C	332	GLN	OE1-CD-NE2	-6.93	115.67	122.60
1	B	332	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	A	181	GLU	O-C-N	6.87	127.64	121.19
1	C	146	ASP	CA-C-O	-6.81	113.33	120.55
1	A	394	ARG	NE-CZ-NH1	-6.80	114.70	121.50
1	B	210	GLU	CB-CG-CD	6.80	124.17	112.60
1	D	255	ASP	CB-CG-OD1	6.79	134.02	118.40
1	C	177	ARG	NE-CZ-NH1	6.71	128.22	121.50
1	B	150	ASP	CA-CB-CG	-6.69	105.91	112.60
1	B	117	ARG	NE-CZ-NH1	6.69	128.19	121.50
1	C	159	ARG	NE-CZ-NH1	-6.69	114.81	121.50
1	C	172	ARG	CD-NE-CZ	-6.67	115.06	124.40
1	B	282	ALA	N-CA-C	6.63	119.63	110.01
1	B	286	ASP	CA-CB-CG	-6.60	106.00	112.60
1	C	255	ASP	CA-CB-CG	6.53	119.13	112.60
1	A	326	ARG	NE-CZ-NH1	6.52	128.02	121.50
1	C	349	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	A	158	TYR	CA-C-N	6.49	129.26	120.44
1	A	158	TYR	C-N-CA	6.49	129.26	120.44
1	C	229	THR	CA-CB-OG1	-6.48	99.87	109.60
1	D	55	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	253	LYS	CA-C-O	-6.43	114.30	121.05
1	D	154	ALA	CA-C-O	-6.42	113.75	120.55
1	C	253	LYS	CA-C-O	-6.39	114.28	121.25
1	A	61	PHE	CA-C-O	-6.38	114.57	120.95
1	D	54	HIS	N-CA-CB	6.37	120.79	110.41
1	C	138	GLY	CA-C-N	6.36	128.09	120.14
1	C	138	GLY	C-N-CA	6.36	128.09	120.14
1	A	45	GLU	CA-C-O	-6.34	113.69	120.42
1	B	313	ARG	CA-C-N	6.30	128.63	120.44
1	B	313	ARG	C-N-CA	6.30	128.63	120.44
1	B	394	ARG	CD-NE-CZ	-6.27	115.62	124.40
1	C	185	ASN	OD1-CG-ND2	-6.25	116.34	122.60
1	C	95	THR	N-CA-C	6.21	118.98	111.40
1	D	313	ARG	NE-CZ-NH2	6.20	124.78	119.20
1	B	340	VAL	CB-CA-C	6.20	119.81	111.88
1	D	306	GLU	CB-CA-C	-6.19	100.51	110.79
1	A	26	PHE	CA-C-O	-6.18	111.89	119.18
1	A	95	THR	N-CA-C	6.17	117.80	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	VAL	N-CA-CB	-6.16	102.16	110.54
1	A	13	PHE	CA-C-O	-6.15	113.93	121.06
1	A	308	ALA	N-CA-C	-6.15	104.50	111.14
1	D	144	GLU	N-CA-CB	6.14	119.20	110.67
1	D	171	ASP	CA-CB-CG	-6.11	106.49	112.60
1	C	340	VAL	CB-CA-C	6.09	119.68	111.88
1	B	96	HIS	CA-CB-CG	-6.07	107.73	113.80
1	A	287	GLY	O-C-N	6.06	127.83	121.77
1	A	23	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	B	68	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	D	121	ARG	NE-CZ-NH2	-6.05	113.76	119.20
1	D	112	ARG	CD-NE-CZ	6.05	132.87	124.40
1	C	331	VAL	N-CA-C	-6.00	104.89	110.53
1	D	328	ASP	CA-C-O	5.99	123.75	119.32
1	A	205	GLU	CG-CD-OE2	5.99	132.18	118.40
1	C	278	GLY	CA-C-N	5.98	127.32	119.84
1	C	278	GLY	C-N-CA	5.98	127.32	119.84
1	B	217	GLU	CA-C-O	-5.97	113.91	120.36
1	B	361	ARG	CD-NE-CZ	-5.97	116.04	124.40
1	A	177	ARG	N-CA-C	-5.97	100.17	109.72
1	D	320	GLU	CA-CB-CG	5.97	126.04	114.10
1	B	243	HIS	CA-C-O	-5.95	114.92	121.28
1	A	54	HIS	N-CA-C	-5.92	100.91	110.32
1	C	79	LEU	CA-C-O	5.91	127.03	120.82
1	B	77	LYS	O-C-N	5.89	128.14	122.07
1	A	319	LYS	CA-C-O	5.89	127.01	120.82
1	A	26	PHE	CA-CB-CG	-5.89	107.91	113.80
1	B	57	ASP	N-CA-C	-5.89	104.45	111.69
1	C	45	GLU	CA-CB-CG	5.88	125.87	114.10
1	C	177	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	D	342	GLU	CG-CD-OE2	5.84	131.84	118.40
1	A	64	ASP	N-CA-C	-5.84	103.23	110.41
1	C	167	GLN	OE1-CD-NE2	-5.84	116.76	122.60
1	A	79	LEU	CA-C-O	5.82	126.72	120.55
1	B	54	HIS	N-CA-C	-5.82	100.80	110.17
1	A	109	ARG	N-CA-C	5.82	117.62	111.28
1	D	367	TYR	O-C-N	5.79	129.82	123.04
1	C	41	HIS	CA-C-O	-5.79	114.74	120.70
1	A	216	PRO	CA-C-O	-5.78	114.61	121.67
1	A	255	ASP	CB-CA-C	5.77	119.44	110.67
1	A	46	ILE	CA-C-O	-5.77	112.07	119.39
1	C	301	TYR	CA-C-O	-5.77	113.58	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	354	TYR	CA-C-O	-5.76	114.45	120.55
1	D	282	ALA	N-CA-C	5.75	118.47	110.20
1	A	261	GLY	CA-C-O	-5.71	112.66	119.06
1	B	280	ASP	N-CA-C	-5.71	103.39	111.56
1	D	328	ASP	CB-CA-C	5.71	117.61	109.38
1	C	194	PRO	N-CA-C	5.70	120.98	113.86
1	C	81	GLU	CB-CG-CD	5.68	122.26	112.60
1	D	64	ASP	CA-CB-CG	-5.68	106.92	112.60
1	B	57	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	136	LEU	CA-C-O	-5.67	114.45	120.40
1	A	80	ASP	O-C-N	5.65	127.91	122.03
1	A	26	PHE	O-C-N	5.65	128.86	122.20
1	C	215	ASN	CA-CB-CG	-5.64	106.96	112.60
1	C	141	GLU	CB-CG-CD	5.64	122.19	112.60
1	A	278	GLY	N-CA-C	-5.64	105.41	112.23
1	C	170	GLU	CA-C-O	-5.63	114.90	120.70
1	D	171	ASP	CA-C-O	-5.63	114.58	120.55
1	A	57	ASP	N-CA-CB	5.62	118.57	110.20
1	A	57	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	257	ASP	CA-CB-CG	5.61	118.20	112.60
1	C	349	ASN	N-CA-C	-5.60	102.00	110.39
1	C	379	PHE	CA-CB-CG	5.59	119.39	113.80
1	B	146	ASP	CA-C-O	-5.59	114.62	120.55
1	A	158	TYR	CA-C-O	5.59	126.34	120.42
1	A	375	LYS	CA-C-O	-5.59	114.90	121.16
1	B	90	THR	CA-CB-OG1	-5.58	101.24	109.60
1	B	144	GLU	N-CA-C	-5.56	106.85	113.97
1	C	328	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	76	LYS	O-C-N	5.54	127.99	122.12
1	A	295	PRO	N-CA-C	-5.53	102.45	110.80
1	D	279	PRO	CA-C-O	5.51	127.32	121.03
1	A	172	ARG	NE-CZ-NH1	5.51	127.01	121.50
1	B	143	ALA	N-CA-CB	-5.50	102.33	111.57
1	D	172	ARG	CD-NE-CZ	5.49	132.09	124.40
1	C	80	ASP	N-CA-CB	-5.49	101.76	109.94
1	B	281	GLY	CA-C-N	5.49	129.64	120.86
1	B	281	GLY	C-N-CA	5.49	129.64	120.86
1	C	230	GLN	CA-C-O	-5.49	114.74	120.55
1	B	295	PRO	CA-C-O	-5.48	115.37	121.23
1	C	281	GLY	CA-C-N	5.45	128.96	120.68
1	C	281	GLY	C-N-CA	5.45	128.96	120.68
1	A	68	ARG	NE-CZ-NH2	5.44	124.10	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	LYS	CA-C-O	-5.43	115.34	121.25
1	D	151	VAL	N-CA-C	5.42	116.15	110.62
1	C	64	ASP	N-CA-C	-5.42	103.38	110.53
1	D	95	THR	N-CA-C	5.41	118.00	111.40
1	A	102	GLY	CA-C-O	-5.41	118.56	122.45
1	C	320	GLU	CB-CG-CD	5.41	121.79	112.60
1	D	109	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	C	372	VAL	CA-C-O	-5.39	115.34	120.95
1	A	57	ASP	N-CA-C	-5.39	105.06	111.69
1	B	177	ARG	N-CA-C	-5.39	101.39	109.95
1	C	389	HIS	CA-CB-CG	-5.39	108.41	113.80
1	C	328	ASP	CB-CA-C	5.38	118.13	109.41
1	C	157	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	B	194	PRO	CA-C-O	-5.37	111.48	119.00
1	B	138	GLY	CA-C-N	5.37	126.85	120.14
1	B	138	GLY	C-N-CA	5.37	126.85	120.14
1	A	243	HIS	CA-CB-CG	5.36	119.16	113.80
1	B	159	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	C	204	GLN	CG-CD-NE2	5.36	124.44	116.40
1	A	306	GLU	CB-CA-C	-5.35	102.47	110.88
1	C	143	ALA	N-CA-CB	-5.35	103.22	111.46
1	B	37	VAL	O-C-N	5.35	127.34	121.83
1	C	292	ASP	O-C-N	5.35	128.31	122.64
1	B	161	ALA	CA-C-O	-5.34	114.76	120.42
1	C	276	GLU	CG-CD-OE2	5.33	130.67	118.40
1	D	330	GLU	CB-CG-CD	-5.33	103.55	112.60
1	D	21	GLN	CB-CG-CD	-5.32	103.55	112.60
1	D	361	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	77	LYS	O-C-N	5.32	127.84	122.09
1	D	177	ARG	N-CA-C	-5.32	101.49	109.95
1	A	144	GLU	N-CA-CB	5.32	118.23	110.47
1	D	255	ASP	CA-C-O	-5.31	114.30	120.62
1	B	299	GLU	N-CA-C	5.31	118.72	110.17
1	D	234	GLN	CA-C-O	-5.31	114.79	120.42
1	D	96	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	121	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	C	361	ARG	NE-CZ-NH2	5.31	123.97	119.20
1	D	150	ASP	CA-CB-CG	-5.30	107.30	112.60
1	D	225	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	D	281	GLY	CA-C-N	5.29	129.50	121.03
1	D	281	GLY	C-N-CA	5.29	129.50	121.03
1	B	45	GLU	CB-CG-CD	5.29	121.59	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	185	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	23	ARG	NE-CZ-NH2	-5.27	114.45	119.20
1	B	85	ILE	CA-C-O	-5.27	116.66	121.72
1	B	77	LYS	CB-CA-C	-5.27	102.61	110.88
1	C	23	ARG	CA-C-O	-5.27	114.94	120.58
1	C	335	LEU	O-C-N	5.26	128.15	122.15
1	D	367	TYR	CA-C-O	-5.26	114.69	120.69
1	A	365	GLU	O-C-N	5.25	127.55	122.09
1	D	249	GLN	CA-CB-CG	5.24	124.58	114.10
1	C	383	ASN	OD1-CG-ND2	5.24	127.84	122.60
1	C	82	THR	CA-CB-OG1	-5.24	101.75	109.60
1	A	298	THR	CA-CB-CG2	5.23	119.39	110.50
1	A	383	ASN	CA-CB-CG	-5.23	107.37	112.60
1	D	119	VAL	CA-C-O	-5.22	115.25	121.05
1	D	212	PHE	N-CA-C	5.21	117.89	109.40
1	D	146	ASP	O-C-N	5.20	127.64	122.12
1	B	330	GLU	OE1-CD-OE2	5.20	135.38	122.90
1	D	314	MET	N-CA-CB	5.20	117.55	110.01
1	B	302	ASP	O-C-N	5.20	128.07	122.15
1	C	185	ASN	O-C-N	5.20	128.49	123.29
1	A	14	GLY	N-CA-C	-5.19	103.25	112.54
1	A	231	GLY	CA-C-N	5.19	127.79	120.42
1	A	231	GLY	C-N-CA	5.19	127.79	120.42
1	B	177	ARG	CA-C-O	-5.18	115.30	121.16
1	A	225	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	C	177	ARG	N-CA-C	-5.18	101.25	109.59
1	C	223	MET	N-CA-C	-5.18	106.22	112.54
1	D	377	PHE	CA-C-O	-5.17	113.25	119.15
1	C	134	LEU	O-C-N	5.17	129.27	123.27
1	C	222	GLN	CG-CD-NE2	5.17	124.15	116.40
1	B	68	ARG	CD-NE-CZ	-5.17	117.17	124.40
1	B	313	ARG	CB-CA-C	5.16	118.98	110.88
1	A	22	ALA	N-CA-C	5.15	118.82	111.92
1	A	276	GLU	N-CA-C	5.15	119.60	112.45
1	B	142	GLY	CA-C-O	-5.15	117.36	120.91
1	C	328	ASP	CA-C-N	5.15	124.94	119.28
1	C	328	ASP	C-N-CA	5.15	124.94	119.28
1	D	109	ARG	NE-CZ-NH2	-5.14	114.57	119.20
1	D	203	VAL	CA-CB-CG1	5.14	119.14	110.40
1	C	23	ARG	N-CA-C	-5.14	100.14	108.41
1	B	331	VAL	N-CA-C	-5.13	105.71	110.53
1	A	23	ARG	CA-C-O	-5.13	115.20	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	GLU	CG-CD-OE2	-5.11	106.64	118.40
1	D	204	GLN	CB-CG-CD	5.11	121.29	112.60
1	A	355	ALA	CA-C-O	-5.09	115.16	120.55
1	D	80	ASP	CA-CB-CG	-5.09	107.51	112.60
1	D	286	ASP	CA-C-O	-5.08	113.48	119.48
1	C	117	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	B	202	PHE	CA-C-N	5.08	128.49	120.47
1	B	202	PHE	C-N-CA	5.08	128.49	120.47
1	C	56	ASP	CA-C-O	-5.07	112.45	119.05
1	B	107	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	A	328	ASP	CA-C-O	5.06	124.50	119.49
1	B	283	PRO	N-CA-CB	5.05	107.80	103.31
1	A	86	VAL	O-C-N	5.04	126.85	121.10
1	A	388	GLU	CA-CB-CG	-5.04	104.01	114.10
1	C	112	ARG	CG-CD-NE	5.04	123.09	112.00
1	D	221	GLU	CG-CD-OE1	5.04	130.00	118.40
1	A	264	ASP	CB-CA-C	5.04	119.86	111.30
1	C	221	GLU	CB-CG-CD	5.03	121.15	112.60
1	B	216	PRO	CA-C-O	-5.02	115.73	121.86
1	A	284	ALA	N-CA-C	-5.02	107.00	113.23
1	D	205	GLU	CG-CD-OE2	5.02	129.95	118.40
1	D	229	THR	CA-CB-OG1	-5.02	102.07	109.60
1	B	141	GLU	CB-CG-CD	5.02	121.13	112.60
1	C	281	GLY	N-CA-C	-5.01	101.31	113.18
1	B	172	ARG	CD-NE-CZ	-5.00	117.40	124.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	ARG	Sidechain
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	25	0
1	B	3053	0	2954	29	0
1	C	3053	0	2954	25	0
1	D	3053	0	2954	27	0
2	A	10	0	11	1	0
2	B	10	0	11	1	0
2	C	10	0	11	1	0
2	D	10	0	11	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	225	0	0	2	0
4	B	212	0	0	3	0
4	C	233	0	0	2	0
4	D	211	0	0	4	0
All	All	13141	0	11860	97	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 (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.54	1.21
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.58	1.17
2:C:397:XYL:H12	4:C:610:HOH:O	1.52	1.08
2:B:397:XYL:H12	4:B:589:HOH:O	1.60	1.00
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.22	0.86
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.23	0.82
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.81
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.26	0.80
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.62	0.80
1:A:204:GLN:HG2	4:A:553:HOH:O	1.84	0.76
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:397:XYL:H12	4:D:598:HOH:O	1.92	0.70
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.80	0.63
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.81	0.63
2:A:397:XYL:H12	4:A:592:HOH:O	1.99	0.61
1:B:3:VAL:HG12	1:B:4:GLN:H	1.66	0.60
1:D:3:VAL:HG23	4:D:593:HOH:O	2.04	0.57
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.87	0.57
1:A:36:PRO:O	1:A:40:VAL:HG23	2.06	0.56
1:A:65:ALA:O	1:A:69:ASP:HB2	2.06	0.56
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.87	0.55
1:B:164:LEU:C	1:B:164:LEU:HD23	2.32	0.54
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.91	0.53
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.91	0.53
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.44	0.53
1:D:72:ILE:O	1:D:76:LYS:HG3	2.09	0.51
1:A:298:THR:HA	1:B:100:LYS:HD2	1.92	0.51
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.44	0.50
1:D:34:LEU:HD21	1:D:39:ALA:HB2	1.94	0.50
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.47	0.49
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.93	0.49
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.94	0.49
1:B:152:SER:HB2	4:D:564:HOH:O	2.13	0.49
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.94	0.49
1:B:77:LYS:O	1:B:80:ASP:HB2	2.13	0.48
1:A:6:THR:O	1:A:9:ASP:HB2	2.14	0.48
1:B:278:GLY:CA	1:B:282:ALA:O	2.63	0.47
1:B:278:GLY:HA3	1:B:282:ALA:O	2.14	0.47
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.96	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.97	0.47
1:C:41:HIS:HE1	4:C:521:HOH:O	1.99	0.46
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.96	0.46
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.46	0.46
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.51	0.46
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.14	0.45
1:A:186:GLU:HA	1:A:187:PRO:HA	1.75	0.45
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.51	0.45
1:B:121:ARG:HD3	4:B:440:HOH:O	2.16	0.45
1:D:20:TRP:CE3	1:D:294:LYS:HB3	2.52	0.44
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.47	0.44
1:C:72:ILE:O	1:C:76:LYS:HG3	2.18	0.44
1:D:178:PHE:HB2	1:D:212:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:ARG:NH1	4:D:603:HOH:O	2.34	0.44
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.44	0.44
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.99	0.44
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.52	0.43
1:B:101:ASP:CG	1:B:101:ASP:O	2.61	0.43
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.79	0.43
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.84	0.43
1:B:216:PRO:HG2	1:B:232:ILE:HD11	2.01	0.42
1:C:161:ALA:O	1:C:165:LEU:HG	2.19	0.42
1:C:186:GLU:HA	1:C:187:PRO:HA	1.90	0.42
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.54	0.42
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.96	0.42
1:B:22:ALA:HB1	1:B:297:ARG:HG3	2.00	0.42
1:A:164:LEU:C	1:A:164:LEU:HD23	2.44	0.42
1:A:186:GLU:OE1	1:A:255:ASP:HB3	2.19	0.42
1:B:219:GLY:O	1:B:223:MET:HG3	2.20	0.42
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.85	0.42
1:C:86:VAL:O	1:C:131:ALA:HA	2.20	0.42
1:D:244:ILE:O	1:D:290:HIS:HB3	2.20	0.42
1:C:278:GLY:HA3	1:C:282:ALA:O	2.20	0.42
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.19	0.41
1:A:368:ASP:O	1:A:372:VAL:HG23	2.21	0.41
1:C:192:LEU:HA	1:C:192:LEU:HD23	1.85	0.41
1:D:116:ILE:HD13	1:D:116:ILE:HG21	1.84	0.41
1:B:100:LYS:NZ	4:B:401:HOH:O	2.51	0.41
1:A:164:LEU:HD12	1:C:348:LEU:HD11	2.02	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.21	0.41
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.56	0.41
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.87	0.41
1:B:394:ARG:HH11	1:B:394:ARG:HD3	1.69	0.41
1:A:238:HIS:O	1:A:239:LYS:HB2	2.21	0.41
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.94	0.41
1:C:164:LEU:C	1:C:164:LEU:HD23	2.46	0.41
1:A:50:GLY:HA2	1:A:85:ILE:O	2.21	0.40
1:B:72:ILE:O	1:B:76:LYS:HG3	2.21	0.40
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.57	0.40
1:D:186:GLU:HA	1:D:187:PRO:HA	1.80	0.40
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.56	0.40
1:A:326:ARG:HA	1:A:326:ARG:HD3	1.91	0.40
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.99	0.40
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.90	0.40
1:A:306:GLU:HG2	1:D:381:LYS:HB2	2.03	0.40
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.03	0.40
1:D:50:GLY:HA2	1:D:85:ILE:O	2.21	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%)	376 (96%)	13 (3%)	1 (0%)	36	42
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	42
1	C	390/393 (99%)	375 (96%)	11 (3%)	4 (1%)	12	11
1	D	390/393 (99%)	375 (96%)	14 (4%)	1 (0%)	36	42
All	All	1560/1572 (99%)	1502 (96%)	51 (3%)	7 (0%)	30	34

All (7) 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

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%)	297 (97%)	9 (3%)	37	51
1	B	306/310 (99%)	301 (98%)	5 (2%)	55	71
1	C	306/310 (99%)	301 (98%)	5 (2%)	55	71
1	D	306/310 (99%)	298 (97%)	8 (3%)	40	55
All	All	1224/1240 (99%)	1197 (98%)	27 (2%)	45	61

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

Mol	Chain	Res	Type
1	A	3	VAL
1	A	38	GLU
1	A	46	ILE
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	185	ASN
1	A	203	VAL
1	A	286	ASP
1	B	3	VAL
1	B	49	TYR
1	B	81	GLU
1	B	203	VAL
1	B	394	ARG
1	C	3	VAL
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	91	THR

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Mol	Chain	Res	Type
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	GLN
1	A	238	HIS
1	B	204	GLN
1	B	222	GLN
1	B	230	GLN
1	B	238	HIS
1	C	222	GLN
1	C	238	HIS
1	D	185	ASN
1	D	234	GLN
1	D	238	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	B	397	3	9,9,9	0.53	0	11,11,11	2.13	3 (27%)
2	XYL	C	397	3	9,9,9	0.52	0	11,11,11	2.04	5 (45%)
2	XYL	D	397	3	9,9,9	0.51	0	11,11,11	1.61	1 (9%)
2	XYL	A	397	3	9,9,9	0.55	0	11,11,11	1.34	2 (18%)

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	B	397	3	-	2/12/12/12	-
2	XYL	C	397	3	-	0/12/12/12	-
2	XYL	D	397	3	-	0/12/12/12	-
2	XYL	A	397	3	-	1/12/12/12	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XYL	O4-C4-C3	4.99	120.94	109.25
2	C	397	XYL	C1-C2-C3	4.00	120.31	112.17
2	B	397	XYL	C1-C2-C3	3.66	119.63	112.17
2	D	397	XYL	O2-C2-C1	-3.35	101.41	109.03
2	C	397	XYL	O4-C4-C3	2.81	115.83	109.25
2	B	397	XYL	O2-C2-C1	-2.67	102.96	109.03
2	A	397	XYL	O4-C4-C3	2.54	115.20	109.25
2	C	397	XYL	O5-C5-C4	-2.47	105.98	111.16
2	A	397	XYL	O2-C2-C1	-2.23	103.95	109.03
2	C	397	XYL	C5-C4-C3	-2.16	107.78	112.17
2	C	397	XYL	O2-C2-C1	-2.01	104.46	109.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	397	XYL	O4-C4-C5-O5
2	A	397	XYL	O4-C4-C5-O5
2	B	397	XYL	C3-C4-C5-O5

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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