



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:10 AM UTC

PDB ID : 5XIN / pdb_00005xin
Title : PROTEIN ENGINEERING OF XYLOSE (GLUCOSE) ISOMERASE FROM ACTINOPLANES MISSOURIENSIS. 1. CRYSTALLOGRAPHY AND SITE-DIRECTED MUTAGENESIS OF METAL BINDING SITES
Authors : Janin, J.
Deposited on : 1992-04-06
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

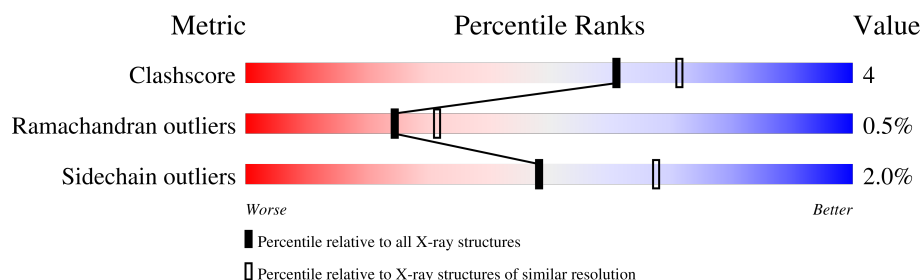
1 Overall quality at a glance

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	
1	B	393	
1	C	393	
1	D	393	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13125 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.

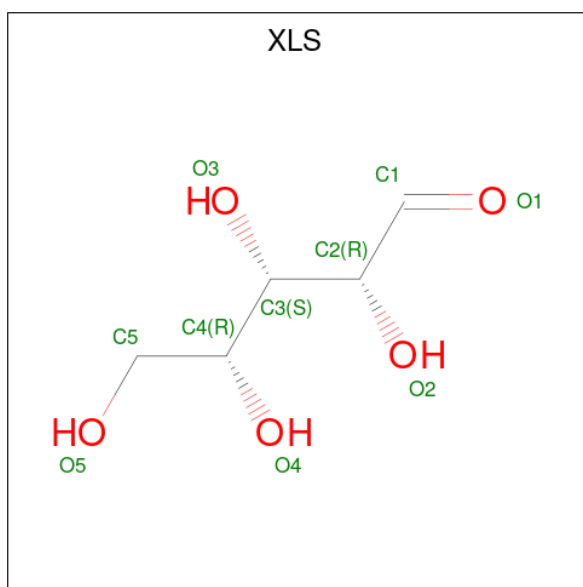
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			
1	B	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			
1	C	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			
1	D	392	Total	C	N	O	S	0	0	0
			3050	1938	532	576	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	ALA	ASP	conflict	UNP P12851
B	255	ALA	ASP	conflict	UNP P12851
C	255	ALA	ASP	conflict	UNP P12851
D	255	ALA	ASP	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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

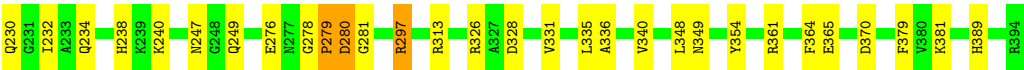
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	224	Total	O	0	0
			224	224		

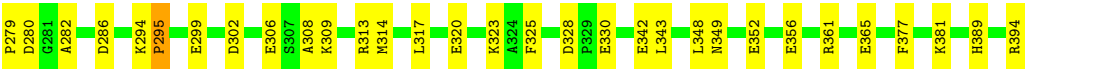
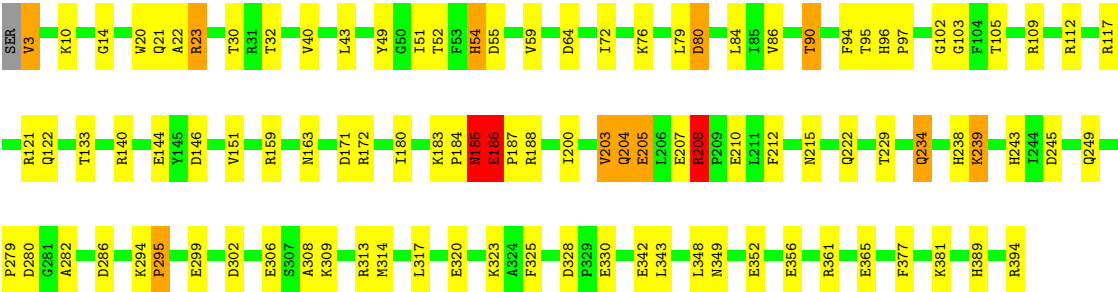
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	214	Total 214	O 214	0	0
4	C	232	Total 232	O 232	0	0
4	D	211	Total 211	O 211	0	0



● 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}	0.152 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13125	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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, MG

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	0.98	0/3122	2.00	85/4229 (2.0%)
1	B	0.97	1/3122 (0.0%)	1.94	78/4229 (1.8%)
1	C	0.97	0/3122	1.98	95/4229 (2.2%)
1	D	0.99	1/3122 (0.0%)	2.01	93/4229 (2.2%)
All	All	0.98	2/12488 (0.0%)	1.98	351/16916 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	GLY	CA-C	6.13	1.55	1.51
1	D	103	GLY	N-CA	5.53	1.49	1.45

All (351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	GLN	OE1-CD-NE2	-15.99	106.61	122.60
1	A	80	ASP	CA-CB-CG	-15.52	97.08	112.60
1	B	204	GLN	OE1-CD-NE2	-13.92	108.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLN	OE1-CD-NE2	-11.60	111.00	122.60
1	C	204	GLN	OE1-CD-NE2	-9.63	112.97	122.60
1	A	107	ASN	CA-CB-CG	9.42	122.02	112.60
1	D	172	ARG	CD-NE-CZ	9.32	137.45	124.40
1	A	286	ASP	CA-CB-CG	-9.10	103.50	112.60
1	A	379	PHE	CA-CB-CG	8.58	122.38	113.80
1	A	244	ILE	CA-C-O	-8.55	111.76	120.90
1	C	80	ASP	CA-CB-CG	-8.34	104.26	112.60
1	B	394	ARG	N-CA-CB	8.21	124.45	110.50
1	B	172	ARG	NE-CZ-NH2	-8.15	111.86	119.20
1	B	13	PHE	CA-CB-CG	8.12	121.92	113.80
1	C	172	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	D	54	HIS	N-CA-C	-8.07	97.48	110.32
1	D	328	ASP	CA-CB-CG	8.07	120.67	112.60
1	B	172	ARG	NE-CZ-NH1	8.05	129.55	121.50
1	A	394	ARG	CA-CB-CG	8.03	130.16	114.10
1	A	394	ARG	NH1-CZ-NH2	8.00	129.70	119.30
1	A	320	GLU	CB-CG-CD	7.97	126.15	112.60
1	C	177	ARG	N-CA-CB	7.89	123.39	110.69
1	B	177	ARG	NE-CZ-NH2	-7.83	112.15	119.20
1	C	15	LEU	CA-C-O	7.79	128.81	120.55
1	A	79	LEU	CA-C-O	7.65	128.66	120.55
1	D	122	GLN	OE1-CD-NE2	-7.65	114.95	122.60
1	D	328	ASP	CA-C-O	7.64	124.98	119.32
1	C	64	ASP	CA-CB-CG	-7.64	104.96	112.60
1	A	23	ARG	CA-C-O	-7.61	113.00	120.92
1	B	95	THR	N-CA-C	7.53	119.27	111.14
1	D	144	GLU	N-CA-C	-7.37	104.54	113.97
1	A	231	GLY	CA-C-N	7.35	130.86	120.42
1	A	231	GLY	C-N-CA	7.35	130.86	120.42
1	D	342	GLU	CB-CG-CD	7.29	125.00	112.60
1	A	319	LYS	CA-C-O	7.25	128.66	120.90
1	D	80	ASP	CA-CB-CG	-7.24	105.36	112.60
1	C	172	ARG	CD-NE-CZ	-7.19	114.34	124.40
1	C	54	HIS	N-CA-C	-7.18	99.89	110.52
1	B	320	GLU	CB-CG-CD	7.16	124.78	112.60
1	A	26	PHE	CA-C-O	-7.14	110.75	119.18
1	D	95	THR	N-CA-C	7.12	118.83	111.14
1	D	313	ARG	NE-CZ-NH2	7.12	125.61	119.20
1	C	208	ARG	CD-NE-CZ	-7.08	114.49	124.40
1	D	342	GLU	CG-CD-OE2	7.02	134.55	118.40
1	B	117	ARG	NE-CZ-NH1	6.93	128.43	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	204	GLN	CB-CG-CD	6.92	124.36	112.60
1	C	222	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	D	212	PHE	N-CA-C	6.86	120.09	108.90
1	D	171	ASP	CA-C-O	-6.84	113.30	120.55
1	B	394	ARG	NE-CZ-NH2	-6.84	113.05	119.20
1	C	340	VAL	CB-CA-C	6.83	120.62	111.88
1	B	80	ASP	CA-CB-CG	-6.79	105.81	112.60
1	D	349	ASN	CA-CB-CG	-6.75	105.85	112.60
1	B	202	PHE	CA-C-N	6.72	129.67	120.46
1	B	202	PHE	C-N-CA	6.72	129.67	120.46
1	D	109	ARG	CD-NE-CZ	6.72	133.81	124.40
1	B	248	GLY	O-C-N	6.71	129.27	123.37
1	A	244	ILE	O-C-N	6.69	130.85	123.09
1	A	14	GLY	N-CA-C	-6.66	103.05	112.37
1	B	141	GLU	CB-CG-CD	6.63	123.88	112.60
1	D	286	ASP	CA-CB-CG	-6.62	105.98	112.60
1	C	328	ASP	CA-CB-CG	6.60	119.20	112.60
1	B	45	GLU	CB-CG-CD	6.57	123.77	112.60
1	D	10	LYS	CB-CA-C	-6.54	103.09	111.86
1	C	229	THR	CA-CB-OG1	-6.54	99.79	109.60
1	C	15	LEU	O-C-N	-6.51	115.22	122.12
1	D	313	ARG	N-CA-CB	6.51	119.45	110.01
1	C	185	ASN	O-C-N	6.50	129.78	123.29
1	B	218	THR	CA-C-N	6.48	127.17	119.98
1	B	218	THR	C-N-CA	6.48	127.17	119.98
1	C	230	GLN	CA-C-O	-6.47	113.69	120.55
1	B	57	ASP	CA-CB-CG	6.45	119.05	112.60
1	C	335	LEU	O-C-N	6.43	128.94	122.12
1	B	185	ASN	OD1-CG-ND2	-6.39	116.21	122.60
1	A	199	ALA	CB-CA-C	6.38	121.70	110.85
1	C	202	PHE	CA-C-N	6.37	129.19	120.46
1	C	202	PHE	C-N-CA	6.37	129.19	120.46
1	C	117	ARG	NE-CZ-NH1	6.37	127.86	121.50
1	B	394	ARG	CD-NE-CZ	-6.35	115.51	124.40
1	D	295	PRO	CB-CA-C	6.35	119.14	111.46
1	B	150	ASP	CA-CB-CG	-6.35	106.25	112.60
1	C	389	HIS	CA-CB-CG	-6.34	107.45	113.80
1	D	185	ASN	CA-C-O	-6.34	114.50	121.28
1	B	295	PRO	CA-C-O	-6.33	114.46	121.23
1	C	45	GLU	CA-CB-CG	6.33	126.76	114.10
1	C	336	ALA	CA-C-O	-6.33	114.19	120.70
1	C	379	PHE	CA-CB-CG	6.32	120.12	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	PRO	N-CA-C	6.32	121.75	113.86
1	D	151	VAL	CA-C-O	6.29	127.49	120.95
1	B	57	ASP	N-CA-C	-6.29	103.96	111.69
1	A	26	PHE	O-C-N	6.26	129.59	122.20
1	A	188	ARG	CD-NE-CZ	6.25	133.15	124.40
1	A	11	PHE	CA-C-O	-6.25	113.48	120.54
1	D	207	GLU	CA-CB-CG	6.24	126.58	114.10
1	D	21	GLN	CB-CG-CD	-6.22	102.03	112.60
1	C	146	ASP	CA-C-O	-6.21	113.97	120.55
1	D	54	HIS	N-CA-CB	6.21	120.53	110.41
1	A	95	THR	N-CA-C	6.21	117.84	111.14
1	C	95	THR	N-CA-C	6.21	117.84	111.14
1	D	59	VAL	O-C-N	6.18	126.61	120.92
1	D	55	ASP	CA-CB-CG	6.15	118.75	112.60
1	D	151	VAL	N-CA-C	6.15	116.89	110.62
1	D	203	VAL	CB-CA-C	6.15	120.09	112.04
1	D	105	THR	CA-C-O	-6.14	112.52	119.95
1	D	306	GLU	CB-CA-C	-6.13	101.25	110.88
1	A	204	GLN	CB-CG-CD	6.13	123.02	112.60
1	C	140	ARG	CD-NE-CZ	6.13	132.98	124.40
1	D	286	ASP	CA-C-O	-6.12	112.26	119.48
1	B	63	SER	O-C-N	6.11	130.34	123.19
1	A	57	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	210	GLU	CB-CG-CD	6.08	122.93	112.60
1	D	144	GLU	N-CA-CB	6.08	119.11	110.67
1	A	172	ARG	CD-NE-CZ	6.06	132.88	124.40
1	A	383	ASN	CA-CB-CG	-6.05	106.55	112.60
1	B	107	ASN	N-CA-C	-6.04	104.70	111.28
1	D	243	HIS	CA-C-O	-6.03	114.99	121.38
1	C	172	ARG	NE-CZ-NH1	6.02	127.52	121.50
1	B	331	VAL	N-CA-C	-6.01	104.88	110.53
1	A	312	ILE	CA-C-N	6.01	128.25	120.44
1	A	312	ILE	C-N-CA	6.01	128.25	120.44
1	A	180	ILE	N-CA-CB	6.00	117.07	110.53
1	A	13	PHE	CA-C-O	-5.97	114.13	121.06
1	D	117	ARG	NE-CZ-NH1	5.97	127.47	121.50
1	C	23	ARG	N-CA-C	-5.96	98.81	108.41
1	D	279	PRO	CA-C-O	5.96	127.83	121.03
1	B	389	HIS	CA-CB-CG	-5.95	107.85	113.80
1	A	61	PHE	CA-C-O	-5.94	115.01	120.95
1	C	207	GLU	CA-C-O	-5.94	114.58	120.82
1	D	55	ASP	O-C-N	5.94	128.27	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	314	MET	N-CA-CB	5.92	118.60	110.01
1	C	165	LEU	O-C-N	5.92	128.39	122.12
1	C	185	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	B	82	THR	CA-C-O	-5.91	112.36	119.27
1	C	57	ASP	CA-CB-CG	5.90	118.50	112.60
1	D	389	HIS	CA-CB-CG	-5.87	107.93	113.80
1	D	377	PHE	CA-C-O	-5.87	112.46	119.15
1	B	248	GLY	CA-C-O	-5.86	116.47	121.57
1	A	313	ARG	N-CA-CB	-5.86	101.52	110.01
1	C	313	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	68	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	79	LEU	CA-C-N	5.83	128.34	120.65
1	A	79	LEU	C-N-CA	5.83	128.34	120.65
1	C	365	GLU	CA-C-O	-5.83	114.37	120.55
1	A	46	ILE	CA-C-O	-5.82	112.00	119.39
1	C	222	GLN	CG-CD-NE2	5.82	125.12	116.40
1	A	309	LYS	CA-C-O	-5.80	113.30	119.97
1	C	127	ALA	CA-C-N	5.78	128.03	120.28
1	C	127	ALA	C-N-CA	5.78	128.03	120.28
1	A	276	GLU	N-CA-C	5.77	120.47	112.45
1	B	303	GLY	N-CA-C	-5.77	105.80	112.73
1	C	281	GLY	N-CA-C	-5.77	99.51	113.18
1	D	302	ASP	CA-C-O	-5.76	114.76	120.70
1	C	225	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	A	10	LYS	CB-CA-C	-5.75	103.73	111.89
1	D	328	ASP	CB-CA-C	5.74	117.64	109.38
1	B	282	ALA	N-CA-C	5.73	118.32	110.01
1	A	102	GLY	O-C-N	5.73	130.03	123.21
1	A	177	ARG	N-CA-C	-5.72	100.56	109.72
1	B	340	VAL	CB-CA-C	5.72	119.20	111.88
1	D	188	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	68	ARG	CD-NE-CZ	5.67	132.34	124.40
1	D	94	PHE	O-C-N	5.67	128.61	121.64
1	D	32	THR	CA-CB-OG1	-5.66	101.11	109.60
1	D	215	ASN	CB-CG-ND2	5.65	124.88	116.40
1	A	102	GLY	CA-C-O	-5.64	118.39	122.45
1	A	394	ARG	NE-CZ-NH2	-5.63	114.13	119.20
1	C	278	GLY	CA-C-N	5.63	126.88	119.84
1	C	278	GLY	C-N-CA	5.63	126.88	119.84
1	B	117	ARG	NE-CZ-NH2	-5.63	114.14	119.20
1	A	284	ALA	N-CA-C	-5.62	106.25	113.23
1	A	155	LEU	CB-CA-C	5.62	120.40	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	GLU	N-CA-C	5.61	119.21	110.17
1	B	96	HIS	CA-CB-CG	-5.60	108.20	113.80
1	C	349	ASN	N-CA-C	-5.60	102.07	110.24
1	A	205	GLU	CG-CD-OE2	5.59	131.27	118.40
1	B	161	ALA	CA-C-O	-5.59	114.49	120.42
1	B	305	TRP	CA-CB-CG	-5.59	102.97	113.60
1	A	64	ASP	N-CA-C	-5.59	103.53	110.41
1	B	122	GLN	OE1-CD-NE2	-5.59	117.01	122.60
1	A	295	PRO	N-CA-C	-5.58	102.37	110.80
1	D	52	THR	CA-C-O	-5.58	115.10	121.58
1	D	133	THR	O-C-N	5.57	130.07	123.27
1	D	86	VAL	O-C-N	5.57	127.45	121.10
1	C	331	VAL	N-CA-C	-5.57	105.30	110.53
1	B	210	GLU	CA-CB-CG	5.57	125.23	114.10
1	C	141	GLU	CB-CG-CD	5.56	122.06	112.60
1	C	276	GLU	CG-CD-OE2	5.56	131.20	118.40
1	B	54	HIS	N-CA-C	-5.56	101.21	110.17
1	D	79	LEU	CA-C-O	5.56	126.44	120.55
1	C	64	ASP	N-CA-C	-5.56	103.20	110.53
1	B	313	ARG	CA-C-N	5.55	127.66	120.44
1	B	313	ARG	C-N-CA	5.55	127.66	120.44
1	B	171	ASP	N-CA-CB	5.54	118.37	110.16
1	B	45	GLU	CA-CB-CG	5.54	125.18	114.10
1	B	191	ILE	CA-C-O	-5.54	114.41	120.84
1	A	185	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	126	GLY	CA-C-N	5.52	127.68	120.28
1	A	126	GLY	C-N-CA	5.52	127.68	120.28
1	D	40	VAL	CA-C-N	5.52	127.61	120.44
1	D	40	VAL	C-N-CA	5.52	127.61	120.44
1	A	306	GLU	CB-CA-C	-5.52	102.22	110.88
1	C	165	LEU	CA-C-O	-5.52	114.70	120.55
1	C	144	GLU	N-CA-CB	5.51	118.64	110.53
1	C	138	GLY	CA-C-N	5.50	127.01	120.14
1	C	138	GLY	C-N-CA	5.50	127.01	120.14
1	D	94	PHE	CA-C-O	-5.49	112.21	118.47
1	C	170	GLU	CA-C-O	-5.49	115.04	120.70
1	B	171	ASP	CA-C-O	-5.49	114.60	120.42
1	B	112	ARG	NE-CZ-NH1	-5.49	116.02	121.50
1	D	349	ASN	O-C-N	5.49	127.41	121.60
1	A	243	HIS	CA-CB-CG	5.48	119.28	113.80
1	C	297	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	B	177	ARG	CB-CG-CD	-5.48	98.70	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	28	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	54	HIS	N-CA-C	-5.45	101.39	110.17
1	D	299	GLU	N-CA-C	5.45	118.86	110.42
1	B	277	ASN	OD1-CG-ND2	5.43	128.03	122.60
1	D	23	ARG	N-CA-C	-5.43	99.67	108.41
1	D	249	GLN	CA-CB-CG	5.43	124.95	114.10
1	B	87	PRO	O-C-N	5.42	129.59	122.27
1	C	180	ILE	N-CA-CB	5.42	117.69	110.26
1	D	239	LYS	CB-CA-C	-5.42	104.88	111.82
1	A	381	LYS	CA-CB-CG	-5.41	103.28	114.10
1	D	234	GLN	CA-C-O	-5.40	114.69	120.42
1	B	158	TYR	N-CA-C	-5.40	105.31	111.14
1	B	31	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	C	66	GLN	N-CA-C	-5.40	105.29	111.07
1	A	86	VAL	O-C-N	5.40	127.25	121.10
1	B	146	ASP	CA-C-O	-5.39	114.83	120.55
1	D	90	THR	CA-CB-CG2	5.39	119.67	110.50
1	A	308	ALA	N-CA-C	-5.39	105.32	111.14
1	C	218	THR	CA-C-N	5.39	125.96	119.98
1	C	218	THR	C-N-CA	5.39	125.96	119.98
1	B	180	ILE	N-CA-CB	5.38	116.40	110.53
1	B	144	GLU	N-CA-C	-5.37	107.27	113.88
1	A	264	ASP	CB-CA-C	5.37	120.42	111.30
1	C	177	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	C	207	GLU	CG-CD-OE2	-5.37	106.06	118.40
1	C	328	ASP	CA-C-N	5.36	125.69	119.47
1	C	328	ASP	C-N-CA	5.36	125.69	119.47
1	A	234	GLN	CA-C-O	-5.36	115.18	120.70
1	B	44	ALA	CA-C-O	5.35	126.22	120.55
1	A	394	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	B	138	GLY	CA-C-N	5.34	126.82	120.14
1	B	138	GLY	C-N-CA	5.34	126.82	120.14
1	D	186	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	216	PRO	CA-C-O	-5.33	115.16	121.67
1	C	313	ARG	NH1-CZ-NH2	-5.33	112.37	119.30
1	A	54	HIS	CA-C-O	-5.33	114.99	121.28
1	B	245	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	198	HIS	O-C-N	5.32	127.76	122.12
1	B	177	ARG	CA-C-O	-5.32	115.15	121.16
1	C	159	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	C	177	ARG	N-CA-C	-5.32	101.03	109.59
1	C	155	LEU	CB-CA-C	5.30	119.59	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	C	203	VAL	N-CA-CB	-5.30	103.34	110.54
1	D	309	LYS	CA-C-O	-5.30	114.94	120.55
1	B	281	GLY	CA-C-N	5.29	129.33	120.86
1	B	281	GLY	C-N-CA	5.29	129.33	120.86
1	C	75	PHE	O-C-N	5.28	127.51	122.07
1	D	64	ASP	N-CA-C	-5.28	103.56	110.53
1	D	205	GLU	CG-CD-OE2	5.28	130.54	118.40
1	D	210	GLU	CB-CG-CD	5.28	121.57	112.60
1	D	171	ASP	O-C-N	5.27	127.71	122.12
1	D	163	ASN	O-C-N	5.27	127.70	122.12
1	C	349	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	C	212	PHE	N-CA-C	5.26	118.07	109.59
1	C	326	ARG	NE-CZ-NH2	5.26	123.94	119.20
1	D	325	PHE	CA-C-N	5.26	128.30	120.31
1	D	325	PHE	C-N-CA	5.26	128.30	120.31
1	A	42	LYS	CB-CG-CD	-5.24	99.24	111.30
1	A	345	THR	O-C-N	5.24	126.97	121.42
1	D	30	THR	O-C-N	5.24	128.38	122.20
1	A	80	ASP	O-C-N	5.24	127.48	122.03
1	C	223	MET	N-CA-C	-5.24	106.15	112.54
1	D	325	PHE	CA-C-O	5.24	126.50	120.90
1	B	77	LYS	CB-CA-C	-5.23	102.67	110.88
1	B	330	GLU	OE1-CD-OE2	5.22	135.43	122.90
1	B	142	GLY	CA-C-O	-5.22	117.31	120.91
1	D	14	GLY	N-CA-C	-5.22	103.20	112.54
1	C	240	LYS	CA-C-O	-5.22	113.32	119.48
1	B	107	ASN	N-CA-CB	5.22	117.79	110.12
1	D	112	ARG	CD-NE-CZ	5.22	131.70	124.40
1	C	328	ASP	CB-CA-C	5.21	117.85	109.51
1	B	85	ILE	CA-C-O	-5.21	116.15	121.67
1	A	322	ALA	N-CA-C	-5.21	105.69	111.36
1	B	23	ARG	N-CA-C	-5.20	100.03	108.41
1	C	361	ARG	NE-CZ-NH2	5.19	123.87	119.20
1	B	243	HIS	CA-C-O	-5.18	115.89	121.38
1	D	10	LYS	O-C-N	5.18	128.79	122.58
1	A	328	ASP	CA-CB-CG	5.16	117.76	112.60
1	D	222	GLN	CG-CD-NE2	5.16	124.14	116.40
1	B	103	GLY	N-CA-C	-5.15	105.52	110.21
1	C	80	ASP	N-CA-CB	-5.15	102.26	109.94
1	A	171	ASP	CA-C-O	-5.15	114.96	120.42
1	A	355	ALA	CA-C-O	-5.15	115.09	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	ALA	N-CA-CB	-5.15	102.92	111.57
1	C	23	ARG	CA-C-O	-5.15	115.07	120.58
1	C	81	GLU	CB-CG-CD	5.15	121.35	112.60
1	D	64	ASP	CA-CB-CG	-5.14	107.46	112.60
1	D	215	ASN	CA-CB-CG	-5.14	107.46	112.60
1	C	365	GLU	O-C-N	5.14	127.57	122.12
1	C	209	PRO	O-C-N	5.14	128.85	122.22
1	B	243	HIS	CA-CB-CG	5.13	118.93	113.80
1	D	239	LYS	O-C-N	5.13	128.47	122.67
1	C	215	ASN	CA-CB-CG	-5.13	107.47	112.60
1	D	308	ALA	N-CA-C	-5.12	105.59	111.07
1	D	95	THR	O-C-N	5.12	127.62	122.09
1	A	45	GLU	CA-C-O	-5.12	115.12	120.55
1	A	110	SER	O-C-N	5.11	127.54	122.12
1	D	229	THR	CA-CB-OG1	-5.11	101.94	109.60
1	D	282	ALA	N-CA-C	5.10	117.55	110.20
1	D	320	GLU	CA-CB-CG	5.10	124.31	114.10
1	B	79	LEU	CA-C-O	5.10	125.96	120.55
1	C	370	ASP	O-C-N	5.10	127.53	122.12
1	A	73	ALA	CA-C-N	5.10	125.61	120.00
1	A	73	ALA	C-N-CA	5.10	125.61	120.00
1	A	260	PHE	CA-CB-CG	-5.10	108.70	113.80
1	D	146	ASP	N-CA-C	5.10	116.84	111.28
1	A	205	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	205	GLU	OE1-CD-OE2	-5.08	110.70	122.90
1	B	178	PHE	O-C-N	5.08	129.34	123.30
1	C	15	LEU	CA-C-N	5.07	131.23	121.18
1	C	15	LEU	C-N-CA	5.07	131.23	121.18
1	C	207	GLU	CB-CA-C	5.07	118.83	110.88
1	C	208	ARG	NE-CZ-NH1	-5.07	116.44	121.50
1	A	243	HIS	CA-C-N	-5.06	114.30	122.25
1	A	243	HIS	C-N-CA	-5.06	114.30	122.25
1	C	354	TYR	CA-C-O	-5.06	114.38	120.10
1	D	208	ARG	CG-CD-NE	5.06	123.13	112.00
1	A	287	GLY	O-C-N	5.05	126.82	121.77
1	C	172	ARG	CB-CG-CD	-5.05	99.68	111.30
1	C	185	ASN	CA-C-O	-5.05	115.88	121.28
1	D	121	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	A	181	GLU	O-C-N	5.04	126.87	121.12
1	B	35	ASP	CB-CA-C	5.04	117.58	109.41
1	A	302	ASP	CA-C-N	5.04	125.57	119.98
1	A	302	ASP	C-N-CA	5.04	125.57	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	ARG	CA-CB-CG	5.04	124.17	114.10
1	C	219	GLY	CA-C-O	-5.04	115.56	120.75
1	D	55	ASP	CA-C-O	-5.03	115.51	120.90
1	D	245	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	276	GLU	N-CA-C	5.03	119.55	113.41
1	C	102	GLY	CA-C-O	-5.03	118.70	122.37
1	A	220	HIS	CA-C-O	-5.02	115.55	120.82
1	C	220	HIS	CA-C-O	-5.01	115.24	120.55
1	D	54	HIS	CB-CA-C	-5.00	100.95	109.51
1	D	200	ILE	N-CA-CB	5.00	116.41	110.55
1	D	159	ARG	CA-C-N	5.00	126.98	120.28
1	D	159	ARG	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	B	172	ARG	Sidechain
1	B	177	ARG	Sidechain
1	C	172	ARG	Sidechain
1	D	208	ARG	Sidechain

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	3050	0	2955	25	0
1	B	3050	0	2955	32	0
1	C	3050	0	2955	27	0
1	D	3050	0	2955	29	0
2	A	10	0	10	0	0
2	B	10	0	9	0	0
2	C	10	0	9	0	0
2	D	10	0	10	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	224	0	0	1	0
4	B	214	0	0	1	0
4	C	232	0	0	1	0
4	D	211	0	0	6	0
All	All	13125	0	11858	101	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 (101) 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	1.61	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	1.10	0.96
1:D:3:VAL:HG23	4:D:594:HOH:O	1.73	0.86
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.20	0.86
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.22	0.85
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.25	0.82
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.66	0.76
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.02	0.74
1:A:204:GLN:HG2	4:A:551:HOH:O	1.92	0.70
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.74	0.68
1:D:330:GLU:OE1	4:D:606:HOH:O	2.13	0.65
1:D:394:ARG:NH1	4:D:603:HOH:O	2.16	0.60
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.83	0.60
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.37	0.59
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.84	0.59
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.85	0.59
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.85	0.59
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.85	0.58
1:B:7:ARG:HG2	1:B:49:TYR:HB2	1.85	0.57
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.89	0.55
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.88	0.55
1:A:65:ALA:O	1:A:69:ASP:HB2	2.07	0.54
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.88	0.54
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.90	0.53
1:A:238:HIS:O	1:A:239:LYS:HB2	2.08	0.53
1:C:183:LYS:HE2	1:C:185:ASN:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.45	0.51
1:A:36:PRO:O	1:A:40:VAL:HG23	2.11	0.51
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.93	0.51
1:B:77:LYS:O	1:B:80:ASP:HB2	2.11	0.50
1:A:306:GLU:HG2	1:D:381:LYS:HB2	1.93	0.50
1:C:72:ILE:O	1:C:76:LYS:HG3	2.12	0.49
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.47	0.49
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.47	0.49
1:C:228:PHE:CE1	1:C:232:ILE:HD11	2.48	0.48
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.94	0.48
1:C:41:HIS:HE1	4:C:521:HOH:O	1.96	0.48
1:D:238:HIS:O	1:D:239:LYS:HB2	2.13	0.47
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.49	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.95	0.46
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.98	0.46
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.96	0.46
1:A:164:LEU:C	1:A:164:LEU:HD23	2.41	0.45
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.81	0.45
1:D:72:ILE:O	1:D:76:LYS:HG3	2.16	0.45
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.93	0.45
1:B:219:GLY:O	1:B:223:MET:HG3	2.17	0.45
1:D:3:VAL:CB	4:D:594:HOH:O	2.65	0.44
1:D:3:VAL:CG2	4:D:594:HOH:O	2.47	0.44
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.87	0.44
1:B:181:GLU:HA	1:B:182:PRO:HD3	1.90	0.44
1:D:361:ARG:HB3	1:D:365:GLU:HB2	1.99	0.44
1:A:164:LEU:HD12	1:C:348:LEU:HD11	2.00	0.44
1:B:3:VAL:HG12	1:B:4:GLN:H	1.82	0.44
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.53	0.44
1:B:164:LEU:C	1:B:164:LEU:HD23	2.43	0.43
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.78	0.43
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.49	0.43
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.90	0.43
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.00	0.43
1:A:305:TRP:O	1:A:309:LYS:HG3	2.19	0.43
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.54	0.43
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.19	0.43
1:D:317:LEU:HD23	1:D:317:LEU:HA	1.84	0.42
1:A:6:THR:O	1:A:9:ASP:HB2	2.20	0.42
1:A:234:GLN:HE21	1:A:238:HIS:CE1	2.13	0.42
1:B:352:GLU:HG2	1:B:356:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:GLU:HA	1:C:187:PRO:HA	1.92	0.42
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.83	0.42
1:D:186:GLU:HA	1:D:187:PRO:HA	1.80	0.42
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.88	0.42
1:D:185:ASN:HD22	1:D:186:GLU:HB2	1.84	0.42
1:B:278:GLY:CA	1:B:282:ALA:O	2.68	0.42
1:C:106:SER:O	1:C:112:ARG:HD3	2.19	0.42
1:D:183:LYS:HG2	1:D:184:PRO:HD2	2.02	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.88	0.42
1:A:326:ARG:HA	1:A:326:ARG:HD3	1.89	0.42
1:B:22:ALA:HB1	1:B:297:ARG:HG3	2.01	0.42
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.42
1:C:279:PRO:HB2	1:C:280:ASP:H	1.75	0.42
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.55	0.41
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.55	0.41
1:A:14:GLY:HA2	1:A:52:THR:OG1	2.20	0.41
1:B:49:TYR:CE2	1:B:85:ILE:HD11	2.55	0.41
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.42	0.41
1:B:101:ASP:CG	1:B:101:ASP:O	2.63	0.41
1:B:280:ASP:C	1:B:282:ALA:H	2.28	0.41
1:C:161:ALA:O	1:C:165:LEU:HG	2.20	0.41
1:D:20:TRP:CE2	1:D:22:ALA:HA	2.55	0.41
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.93	0.41
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.80	0.41
1:B:217:GLU:HA	1:B:245:ASP:O	2.21	0.41
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.17	0.41
1:B:152:SER:HB2	4:D:565:HOH:O	2.21	0.41
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.56	0.40
1:B:100:LYS:NZ	4:B:402:HOH:O	2.49	0.40
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.21	0.40
1:B:186:GLU:HA	1:B:187:PRO:HA	1.89	0.40
1:C:79:LEU:HD23	1:C:79:LEU:HA	1.96	0.40
1:B:206:LEU:O	1:B:209:PRO:HD3	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%)	377 (97%)	12 (3%)	1 (0%)	36	46
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	36	46
1	C	390/393 (99%)	374 (96%)	12 (3%)	4 (1%)	12	15
1	D	390/393 (99%)	376 (96%)	12 (3%)	2 (0%)	24	31
All	All	1560/1572 (99%)	1503 (96%)	49 (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	C	279	PRO
1	C	364	PHE
1	D	186	GLU
1	D	280	ASP

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	305/309 (99%)	299 (98%)	6 (2%)	48	67
1	B	305/309 (99%)	300 (98%)	5 (2%)	55	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	305/309 (99%)	301 (99%)	4 (1%)	61 77
1	D	305/309 (99%)	296 (97%)	9 (3%)	36 53
All	All	1220/1236 (99%)	1196 (98%)	24 (2%)	48 67

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	49	TYR
1	A	80	ASP
1	A	84	LEU
1	A	203	VAL
1	A	208	ARG
1	B	3	VAL
1	B	49	TYR
1	B	81	GLU
1	B	203	VAL
1	B	394	ARG
1	C	3	VAL
1	C	49	TYR
1	C	80	ASP
1	C	203	VAL
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	180	ILE
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG
1	D	323	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	238	HIS
1	B	204	GLN
1	B	222	GLN
1	B	230	GLN

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Mol	Chain	Res	Type
1	B	238	HIS
1	C	41	HIS
1	C	222	GLN
1	C	238	HIS
1	D	41	HIS
1	D	185	ASN
1	D	238	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 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	D	397	3	8,9,9	2.55	1 (12%)	10,11,11	1.51	2 (20%)
2	XLS	A	397	3	8,9,9	2.54	1 (12%)	10,11,11	1.52	1 (10%)
2	XLS	B	397	3	8,9,9	2.53	1 (12%)	10,11,11	2.39	3 (30%)
2	XLS	C	397	3	8,9,9	2.54	1 (12%)	10,11,11	1.73	2 (20%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	397	XLS	O1-C1	7.16	1.47	1.20
2	A	397	XLS	O1-C1	7.11	1.47	1.20
2	D	397	XLS	O1-C1	7.04	1.46	1.20
2	B	397	XLS	O1-C1	7.02	1.46	1.20

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XLS	O4-C4-C3	5.66	122.50	109.25
2	C	397	XLS	O4-C4-C3	4.15	118.95	109.25
2	A	397	XLS	O4-C4-C3	4.02	118.67	109.25
2	B	397	XLS	O2-C2-C3	-2.80	102.90	109.46
2	D	397	XLS	O2-C2-C1	-2.65	104.46	110.48
2	B	397	XLS	O3-C3-C2	-2.65	104.22	109.13
2	D	397	XLS	C5-C4-C3	2.15	116.56	112.17
2	C	397	XLS	O5-C5-C4	-2.04	106.88	111.16

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	B	397	XLS	O4-C4-C5-O5
2	A	397	XLS	O4-C4-C5-O5
2	B	397	XLS	O3-C3-C4-C5
2	D	397	XLS	O3-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.