



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:35 AM UTC

PDB ID : 4XIM / pdb_00004xim
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 : 1992-03-11
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
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

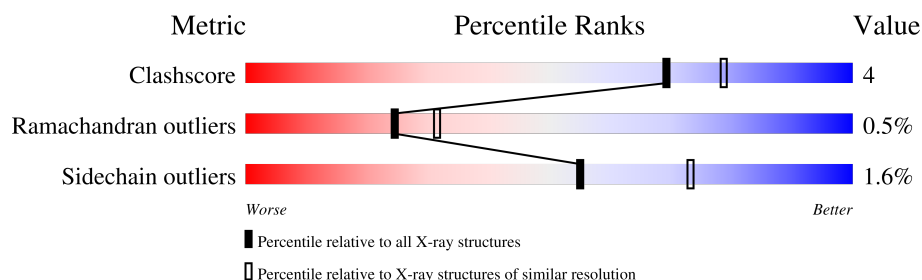
1 Overall quality at a glance

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	 77% 19% . .
1	B	393	 73% 25% . .
1	C	393	 75% 22% . .
1	D	393	 77% 20% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12995 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	391	Total	C	N	O	S	0	0	0
			3041	1934	529	574	4			
1	B	391	Total	C	N	O	S	0	0	0
			3037	1932	527	574	4			
1	C	391	Total	C	N	O	S	0	0	0
			3035	1931	525	575	4			
1	D	391	Total	C	N	O	S	0	0	0
			3037	1931	527	575	4			

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	209	Total	O	0	0
			209	209		
3	B	207	Total	O	0	0
			207	207		
3	C	217	Total	O	0	0
			217	217		
3	D	204	Total	O	0	0
			204	204		

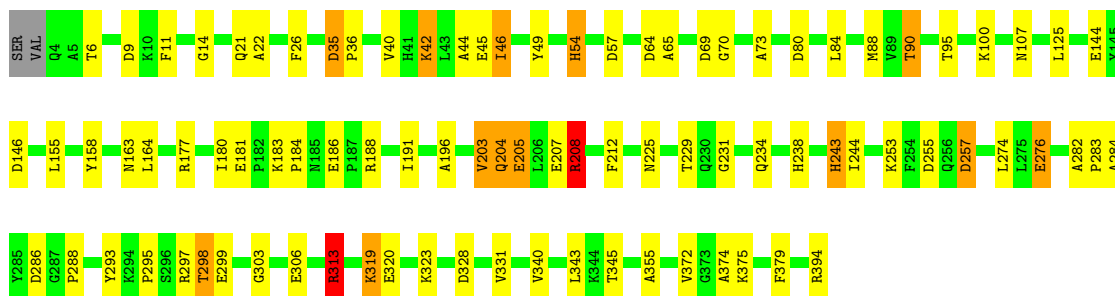
3 Residue-property plots

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

Note EDS was not executed.

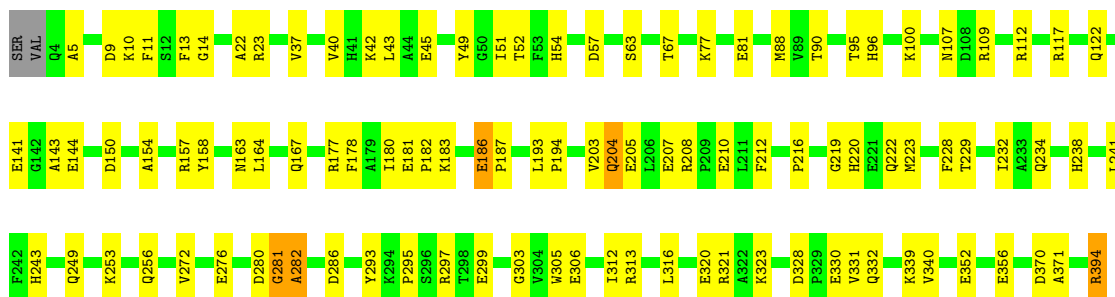
• Molecule 1: D-XYLOSE ISOMERASE

Chain A: 



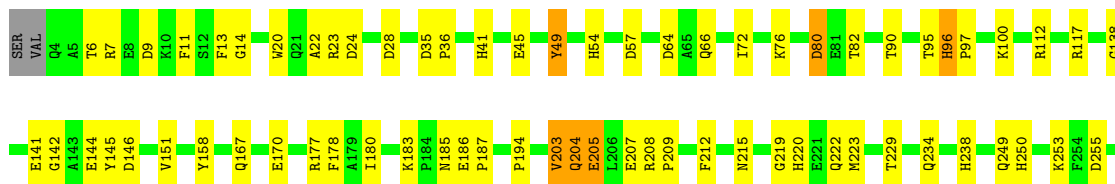
• Molecule 1: D-XYLOSE ISOMERASE

Chain B: 



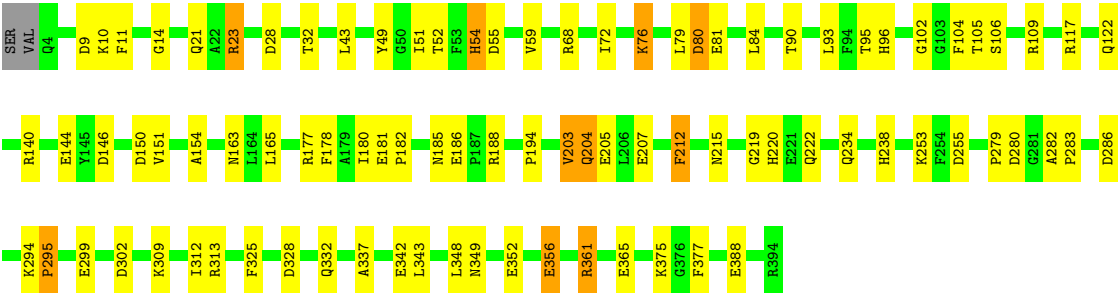
• Molecule 1: D-XYLOSE ISOMERASE

Chain C: 





● 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}	0.158 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12995	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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

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	0.96	0/3113	1.99	89/4216 (2.1%)
1	B	0.97	0/3109	1.93	78/4211 (1.9%)
1	C	0.97	0/3107	1.92	79/4208 (1.9%)
1	D	0.97	1/3109 (0.0%)	1.95	81/4211 (1.9%)
All	All	0.97	1/12438 (0.0%)	1.95	327/16846 (1.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	105	THR	CA-CB	5.06	1.60	1.53

All (327) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	GLN	OE1-CD-NE2	-13.71	108.89	122.60
1	D	204	GLN	OE1-CD-NE2	-13.29	109.31	122.60
1	A	204	GLN	OE1-CD-NE2	-13.04	109.56	122.60
1	C	204	GLN	OE1-CD-NE2	-12.28	110.33	122.60
1	A	257	ASP	CA-CB-CG	9.64	122.24	112.60
1	B	394	ARG	N-CA-CB	9.50	126.66	110.50
1	D	286	ASP	CA-CB-CG	-9.44	103.16	112.60
1	A	379	PHE	CA-CB-CG	9.07	122.87	113.80
1	C	64	ASP	CA-CB-CG	-9.02	103.58	112.60
1	B	394	ARG	NE-CZ-NH2	-8.82	111.27	119.20
1	A	107	ASN	CA-CB-CG	8.58	121.18	112.60
1	D	255	ASP	CA-CB-CG	8.37	120.97	112.60
1	B	95	THR	N-CA-C	8.05	119.84	111.14
1	B	150	ASP	CA-CB-CG	-8.01	104.59	112.60
1	D	54	HIS	N-CA-C	-7.98	97.62	110.32
1	D	95	THR	N-CA-C	7.98	119.76	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	NH1-CZ-NH2	7.83	129.48	119.30
1	C	301	TYR	CA-C-O	-7.82	111.26	120.10
1	B	117	ARG	NE-CZ-NH1	7.68	129.18	121.50
1	C	361	ARG	NE-CZ-NH2	7.64	126.08	119.20
1	A	274	LEU	CA-C-O	-7.58	112.86	120.82
1	A	244	ILE	CA-C-O	-7.43	112.94	120.90
1	C	41	HIS	CA-C-O	-7.36	113.12	120.70
1	A	286	ASP	CA-CB-CG	-7.32	105.28	112.60
1	C	117	ARG	NE-CZ-NH1	7.25	128.75	121.50
1	C	335	LEU	O-C-N	7.23	129.78	122.12
1	D	313	ARG	CG-CD-NE	7.22	127.89	112.00
1	B	394	ARG	CD-NE-CZ	-7.22	114.29	124.40
1	A	45	GLU	CA-C-O	-7.20	112.92	120.55
1	C	219	GLY	CA-C-O	-7.19	112.63	120.40
1	C	229	THR	CA-CB-OG1	-7.16	98.86	109.60
1	D	122	GLN	OE1-CD-NE2	-7.14	115.46	122.60
1	D	313	ARG	CA-CB-CG	7.14	128.38	114.10
1	B	286	ASP	CA-C-O	-7.13	111.07	119.48
1	C	146	ASP	CA-C-O	-7.11	113.02	120.55
1	D	146	ASP	CA-C-O	-7.09	113.03	120.55
1	A	394	ARG	CA-CB-CG	7.09	128.27	114.10
1	C	320	GLU	CB-CG-CD	7.08	124.64	112.60
1	A	26	PHE	CA-C-O	-7.07	111.25	119.59
1	D	188	ARG	NE-CZ-NH2	7.05	125.55	119.20
1	D	328	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	37	VAL	O-C-N	7.01	129.05	121.83
1	C	255	ASP	CA-CB-CG	7.00	119.61	112.60
1	A	320	GLU	CB-CG-CD	6.99	124.49	112.60
1	A	243	HIS	CA-CB-CG	6.98	120.78	113.80
1	C	170	GLU	CA-C-O	-6.93	113.56	120.70
1	A	180	ILE	N-CA-CB	6.92	118.07	110.53
1	B	57	ASP	CA-CB-CG	6.88	119.48	112.60
1	A	180	ILE	CB-CA-C	-6.86	102.24	111.15
1	D	80	ASP	CA-CB-CG	-6.83	105.77	112.60
1	D	23	ARG	CA-C-O	-6.81	113.29	120.58
1	A	394	ARG	NE-CZ-NH1	-6.80	114.70	121.50
1	D	144	GLU	N-CA-C	-6.79	105.27	113.97
1	B	23	ARG	CD-NE-CZ	6.76	133.87	124.40
1	D	328	ASP	CA-C-O	6.76	124.32	119.32
1	B	321	ARG	NE-CZ-NH2	-6.74	113.14	119.20
1	C	208	ARG	CD-NE-CZ	-6.71	115.00	124.40
1	B	320	GLU	CB-CG-CD	6.69	123.98	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ILE	N-CA-CB	6.69	117.82	110.53
1	A	207	GLU	CG-CD-OE1	6.68	133.78	118.40
1	C	389	HIS	CA-CB-CG	-6.63	107.17	113.80
1	A	57	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	80	ASP	O-C-N	6.62	128.88	122.07
1	A	204	GLN	CB-CG-CD	6.62	123.85	112.60
1	A	100	LYS	CA-C-O	-6.52	112.73	120.10
1	A	205	GLU	CB-CG-CD	6.51	123.67	112.60
1	C	54	HIS	N-CA-C	-6.50	99.98	110.32
1	A	229	THR	CA-CB-OG1	-6.50	99.86	109.60
1	A	191	ILE	CA-C-O	-6.48	113.32	120.84
1	B	96	HIS	CA-CB-CG	-6.48	107.32	113.80
1	A	73	ALA	CA-C-N	6.45	126.97	119.94
1	A	73	ALA	C-N-CA	6.45	126.97	119.94
1	D	117	ARG	NE-CZ-NH1	6.44	127.94	121.50
1	C	177	ARG	CG-CD-NE	6.40	126.07	112.00
1	A	26	PHE	CA-CB-CG	-6.39	107.41	113.80
1	B	303	GLY	N-CA-C	-6.37	104.62	112.77
1	C	328	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	203	VAL	N-CA-CB	-6.35	99.79	110.65
1	D	255	ASP	CA-C-O	-6.34	113.08	120.62
1	B	122	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	B	332	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	C	13	PHE	CA-C-O	-6.33	113.72	121.06
1	D	163	ASN	OD1-CG-ND2	6.31	128.91	122.60
1	C	95	THR	N-CA-C	6.30	117.94	111.14
1	D	279	PRO	CB-CA-C	6.30	119.08	111.46
1	D	312	ILE	CA-C-O	-6.29	114.07	121.05
1	D	165	LEU	CA-C-O	-6.29	113.89	120.55
1	C	80	ASP	CA-CB-CG	-6.28	106.32	112.60
1	A	95	THR	N-CA-C	6.28	117.92	111.14
1	D	80	ASP	O-C-N	6.27	128.52	122.07
1	C	185	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	B	328	ASP	CA-C-O	6.25	124.27	119.46
1	B	77	LYS	O-C-N	6.25	128.50	122.07
1	A	45	GLU	O-C-N	6.23	128.72	122.12
1	D	10	LYS	CB-CA-C	-6.23	103.05	111.89
1	B	253	LYS	CA-C-O	-6.22	114.52	121.05
1	A	46	ILE	CA-C-O	-6.21	111.50	119.39
1	D	81	GLU	CA-C-O	-6.21	112.83	119.97
1	D	253	LYS	CA-C-O	-6.20	114.49	121.25
1	B	229	THR	CA-CB-OG1	-6.20	100.30	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	THR	CA-CB-OG1	-6.19	100.32	109.60
1	B	295	PRO	CA-C-O	-6.17	114.63	121.23
1	A	375	LYS	CA-C-O	-6.16	114.02	121.05
1	B	13	PHE	CA-CB-CG	6.16	119.96	113.80
1	C	281	GLY	N-CA-C	-6.15	98.61	113.18
1	A	306	GLU	CB-CA-C	-6.14	101.24	110.88
1	A	177	ARG	N-CA-C	-6.13	99.92	109.72
1	A	340	VAL	O-C-N	6.13	127.81	121.87
1	D	96	HIS	CA-CB-CG	-6.12	107.68	113.80
1	D	207	GLU	CA-CB-CG	6.11	126.32	114.10
1	C	354	TYR	CA-C-O	-6.11	113.20	120.10
1	A	44	ALA	CA-C-O	6.09	127.00	120.55
1	C	205	GLU	CG-CD-OE2	6.08	132.38	118.40
1	A	188	ARG	CD-NE-CZ	6.06	132.88	124.40
1	C	331	VAL	N-CA-C	-6.05	104.84	110.53
1	D	194	PRO	N-CA-C	6.04	121.48	113.57
1	A	21	GLN	CB-CG-CD	-6.03	102.35	112.60
1	B	370	ASP	CA-C-O	-6.03	114.16	120.55
1	C	328	ASP	CA-C-N	6.01	125.89	119.28
1	C	328	ASP	C-N-CA	6.01	125.89	119.28
1	D	55	ASP	CA-CB-CG	6.00	118.60	112.60
1	C	82	THR	CA-CB-OG1	-6.00	100.61	109.60
1	D	295	PRO	CB-CA-C	5.99	118.71	111.46
1	D	309	LYS	CA-C-O	-5.99	114.20	120.55
1	B	54	HIS	N-CA-CB	5.98	120.38	110.63
1	A	255	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	163	ASN	OD1-CG-ND2	5.95	128.55	122.60
1	D	342	GLU	CB-CG-CD	5.94	122.70	112.60
1	A	355	ALA	CA-C-O	-5.92	114.27	120.55
1	A	207	GLU	CG-CD-OE2	-5.92	104.78	118.40
1	B	57	ASP	N-CA-C	-5.91	104.42	111.69
1	D	212	PHE	N-CA-C	5.91	119.03	109.40
1	C	64	ASP	N-CA-C	-5.91	102.73	110.53
1	D	32	THR	CA-CB-OG1	-5.90	100.75	109.60
1	C	138	GLY	CA-C-N	5.90	127.51	120.14
1	C	138	GLY	C-N-CA	5.90	127.51	120.14
1	A	345	THR	O-C-N	5.89	127.66	121.42
1	C	194	PRO	N-CA-C	5.88	121.22	113.86
1	B	241	LEU	CA-C-O	-5.88	114.99	121.58
1	A	295	PRO	N-CA-C	-5.86	101.96	110.80
1	B	52	THR	CA-C-O	-5.86	114.79	121.58
1	C	340	VAL	CB-CA-C	5.84	119.36	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	PHE	CA-C-O	5.84	126.95	120.82
1	B	282	ALA	N-CA-C	5.83	118.12	110.08
1	B	331	VAL	N-CA-C	-5.83	105.05	110.53
1	C	209	PRO	O-C-N	5.83	129.73	122.22
1	D	203	VAL	CA-CB-CG1	5.83	120.30	110.40
1	A	144	GLU	N-CA-CB	5.82	118.33	110.59
1	D	302	ASP	O-C-N	5.82	128.06	122.07
1	D	349	ASN	CA-CB-CG	-5.81	106.79	112.60
1	A	313	ARG	CG-CD-NE	5.80	124.77	112.00
1	D	144	GLU	N-CA-CB	5.80	118.73	110.67
1	C	6	THR	N-CA-CB	5.80	120.59	111.20
1	B	54	HIS	N-CA-C	-5.79	100.84	110.17
1	A	88	MET	CA-C-O	-5.79	114.50	120.99
1	D	203	VAL	N-CA-CB	-5.79	103.23	110.47
1	D	302	ASP	CA-C-O	-5.78	114.75	120.82
1	B	339	LYS	CB-CA-C	-5.75	102.42	111.51
1	C	144	GLU	N-CA-C	-5.75	106.61	113.97
1	A	64	ASP	N-CA-C	-5.74	103.35	110.41
1	A	90	THR	CA-CB-OG1	-5.74	101.00	109.60
1	C	141	GLU	CB-CG-CD	5.73	122.35	112.60
1	C	180	ILE	CA-CB-CG1	5.72	120.12	110.40
1	A	225	ASN	OD1-CG-ND2	-5.72	116.88	122.60
1	C	142	GLY	CA-C-O	-5.71	116.97	120.91
1	B	210	GLU	CB-CG-CD	5.71	122.30	112.60
1	C	276	GLU	CG-CD-OE2	5.71	131.52	118.40
1	C	23	ARG	N-CA-C	-5.70	99.23	108.41
1	B	10	LYS	CB-CA-C	-5.70	104.22	111.86
1	D	23	ARG	N-CA-C	-5.70	99.24	108.41
1	B	158	TYR	N-CA-C	-5.69	104.99	111.14
1	C	335	LEU	CA-C-O	-5.69	114.52	120.55
1	A	244	ILE	O-C-N	5.69	129.69	123.09
1	A	208	ARG	CB-CG-CD	5.69	124.38	111.30
1	D	328	ASP	CB-CA-C	5.68	117.56	109.38
1	D	332	GLN	CA-C-O	5.67	126.78	120.82
1	A	163	ASN	O-C-N	5.67	128.13	122.12
1	D	286	ASP	CA-C-O	-5.67	112.80	119.48
1	B	63	SER	O-C-N	5.65	129.72	123.16
1	C	45	GLU	CA-CB-CG	5.65	125.40	114.10
1	D	151	VAL	CA-C-O	5.65	126.82	120.95
1	B	316	LEU	CA-C-O	-5.64	114.45	120.42
1	A	54	HIS	N-CA-C	-5.63	101.10	110.17
1	B	54	HIS	CB-CA-C	-5.63	99.98	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	154	ALA	CA-C-O	-5.63	114.58	120.55
1	C	100	LYS	CA-C-O	-5.63	112.68	119.49
1	D	104	PHE	CA-C-O	-5.62	113.75	120.10
1	A	328	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	76	LYS	O-C-N	5.61	128.07	122.12
1	C	207	GLU	CG-CD-OE2	-5.61	105.50	118.40
1	B	63	SER	N-CA-C	-5.61	100.54	109.96
1	B	157	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	A	95	THR	O-C-N	5.60	128.14	122.09
1	D	203	VAL	CB-CA-C	5.60	119.37	112.04
1	B	54	HIS	CA-CB-CG	-5.59	108.21	113.80
1	A	319	LYS	CA-C-O	5.58	126.47	120.55
1	B	394	ARG	NH1-CZ-NH2	5.58	126.55	119.30
1	C	313	ARG	CA-CB-CG	5.57	125.25	114.10
1	C	306	GLU	CG-CD-OE1	5.57	131.21	118.40
1	D	14	GLY	N-CA-C	-5.57	102.58	112.54
1	A	177	ARG	CD-NE-CZ	5.56	132.18	124.40
1	A	331	VAL	N-CA-C	-5.56	105.11	110.72
1	A	345	THR	CA-C-O	-5.55	114.82	119.76
1	A	298	THR	CA-CB-CG2	5.55	119.93	110.50
1	D	104	PHE	O-C-N	5.54	128.70	122.22
1	C	28	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	374	ALA	CA-C-O	-5.53	112.80	119.27
1	A	107	ASN	N-CA-C	-5.53	105.41	111.82
1	B	243	HIS	CA-CB-CG	5.52	119.32	113.80
1	D	377	PHE	CA-C-O	-5.51	112.86	119.15
1	B	207	GLU	CG-CD-OE1	5.51	131.07	118.40
1	B	323	LYS	CA-CB-CG	-5.51	103.09	114.10
1	C	207	GLU	CA-C-O	-5.50	115.05	120.82
1	D	375	LYS	CA-C-N	5.49	126.14	120.60
1	D	375	LYS	C-N-CA	5.49	126.14	120.60
1	B	299	GLU	N-CA-C	5.48	119.00	110.17
1	D	93	LEU	CA-C-O	-5.47	113.92	120.65
1	D	68	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	323	LYS	CB-CA-C	-5.45	102.32	110.88
1	C	177	ARG	N-CA-CB	5.45	119.46	110.69
1	C	313	ARG	CA-C-O	-5.45	115.10	120.82
1	B	112	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	D	177	ARG	N-CA-C	-5.44	101.02	109.72
1	D	356	GLU	CA-C-O	-5.44	114.66	120.42
1	B	313	ARG	CA-C-N	5.44	127.51	120.44
1	B	313	ARG	C-N-CA	5.44	127.51	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	LEU	CA-C-O	5.43	126.31	120.55
1	A	70	GLY	O-C-N	5.42	127.39	122.18
1	C	253	LYS	CA-C-O	-5.42	115.34	121.25
1	C	96	HIS	CA-CB-CG	-5.42	108.38	113.80
1	D	255	ASP	O-C-N	5.42	130.09	122.77
1	D	21	GLN	CB-CG-CD	-5.41	103.40	112.60
1	C	215	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	45	GLU	CB-CG-CD	5.40	121.78	112.60
1	C	177	ARG	N-CA-C	-5.40	100.90	109.59
1	C	328	ASP	CB-CA-C	5.40	118.15	109.41
1	C	187	PRO	N-CA-C	5.39	126.12	112.10
1	B	67	THR	O-C-N	5.38	127.62	122.07
1	B	371	ALA	CA-C-O	-5.38	114.71	120.42
1	C	14	GLY	N-CA-C	-5.38	104.83	112.37
1	A	95	THR	CA-C-O	-5.36	115.18	120.70
1	B	228	PHE	CA-C-O	-5.35	115.38	121.00
1	A	57	ASP	N-CA-CB	5.35	118.17	110.20
1	A	57	ASP	CA-C-O	-5.34	114.31	120.24
1	D	52	THR	CA-CB-OG1	-5.33	101.61	109.60
1	B	370	ASP	O-C-N	5.32	127.76	122.12
1	D	299	GLU	N-CA-C	5.32	118.73	110.17
1	C	284	ALA	N-CA-C	-5.31	106.64	113.23
1	C	278	GLY	CA-C-N	5.31	126.48	119.84
1	C	278	GLY	C-N-CA	5.31	126.48	119.84
1	D	106	SER	CA-C-O	-5.31	115.92	121.55
1	B	330	GLU	CG-CD-OE2	-5.30	106.20	118.40
1	A	14	GLY	N-CA-C	-5.30	104.95	112.37
1	C	66	GLN	N-CA-C	-5.29	105.41	111.07
1	B	293	TYR	CA-C-O	-5.28	115.54	121.40
1	D	220	HIS	CA-CB-CG	-5.28	108.52	113.80
1	C	145	TYR	CA-C-O	-5.27	114.60	120.66
1	B	340	VAL	CB-CA-C	5.26	118.71	111.97
1	C	316	LEU	CA-C-O	-5.26	114.97	120.55
1	C	365	GLU	CA-C-O	-5.26	114.97	120.55
1	D	215	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	D	312	ILE	O-C-N	5.25	127.36	121.90
1	A	57	ASP	N-CA-C	-5.24	105.24	111.69
1	B	143	ALA	N-CA-CB	-5.24	102.77	111.57
1	B	40	VAL	O-C-N	5.23	127.03	121.91
1	C	57	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	144	GLU	N-CA-C	-5.21	107.30	113.97
1	A	196	ALA	CA-C-N	5.21	125.72	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ALA	C-N-CA	5.21	125.72	119.94
1	C	158	TYR	N-CA-C	-5.21	105.68	111.36
1	C	223	MET	N-CA-C	-5.21	106.18	112.54
1	B	141	GLU	CB-CG-CD	5.21	121.45	112.60
1	C	112	ARG	CG-CD-NE	5.21	123.45	112.00
1	C	250	HIS	CA-C-O	-5.21	115.12	121.58
1	B	109	ARG	N-CA-C	5.21	117.70	111.71
1	C	294	LYS	O-C-N	5.19	126.36	121.38
1	A	253	LYS	N-CA-C	-5.19	101.39	108.24
1	C	203	VAL	N-CA-CB	-5.18	102.41	110.54
1	A	146	ASP	CA-C-O	-5.18	115.06	120.55
1	C	90	THR	CA-C-N	5.17	130.70	122.94
1	C	90	THR	C-N-CA	5.17	130.70	122.94
1	A	158	TYR	CA-C-N	5.17	127.47	120.44
1	A	158	TYR	C-N-CA	5.17	127.47	120.44
1	A	394	ARG	CG-CD-NE	-5.17	100.63	112.00
1	D	52	THR	CA-C-O	-5.16	115.59	121.58
1	A	181	GLU	O-C-N	5.16	127.00	121.12
1	D	151	VAL	N-CA-C	5.16	115.88	110.62
1	D	222	GLN	CG-CD-NE2	5.16	124.13	116.40
1	A	181	GLU	CG-CD-OE1	5.14	130.22	118.40
1	A	35	ASP	CB-CA-C	5.14	117.73	109.41
1	B	281	GLY	CA-C-N	5.14	128.49	120.68
1	B	281	GLY	C-N-CA	5.14	128.49	120.68
1	D	28	ASP	O-C-N	5.13	128.64	122.79
1	A	42	LYS	CB-CG-CD	-5.12	99.51	111.30
1	B	180	ILE	CB-CA-C	-5.12	104.49	111.15
1	B	14	GLY	N-CA-C	-5.12	105.20	112.37
1	D	150	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	394	ARG	CD-NE-CZ	-5.11	117.24	124.40
1	B	177	ARG	NE-CZ-NH2	-5.11	114.60	119.20
1	C	151	VAL	O-C-N	5.11	126.83	121.87
1	D	342	GLU	CG-CD-OE2	5.11	130.15	118.40
1	D	356	GLU	CG-CD-OE2	5.11	130.15	118.40
1	B	330	GLU	OE1-CD-OE2	5.10	135.15	122.90
1	D	109	ARG	N-CA-C	5.10	116.84	111.28
1	C	354	TYR	O-C-N	5.09	128.18	122.22
1	A	231	GLY	CA-C-N	5.09	127.65	120.42
1	A	231	GLY	C-N-CA	5.09	127.65	120.42
1	A	276	GLU	N-CA-C	5.09	119.53	112.45
1	B	88	MET	N-CA-CB	-5.07	103.19	111.66
1	D	388	GLU	CA-CB-CG	-5.07	103.96	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	ALA	N-CA-C	-5.07	106.95	113.23
1	B	371	ALA	O-C-N	5.06	127.92	122.15
1	B	276	GLU	N-CA-C	5.06	119.48	112.45
1	B	107	ASN	N-CA-C	-5.06	105.89	111.71
1	C	167	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	D	361	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	C	41	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	372	VAL	O-C-N	5.04	127.02	121.83
1	A	155	LEU	CB-CA-C	5.04	119.42	110.85
1	A	298	THR	CA-C-O	-5.03	112.53	119.12
1	B	305	TRP	CA-CB-CG	-5.03	104.05	113.60
1	D	59	VAL	O-C-N	5.03	125.54	120.92
1	A	212	PHE	N-CA-C	5.02	117.59	109.40
1	D	219	GLY	CA-C-O	-5.02	114.98	120.40
1	D	337	ALA	CA-C-O	-5.01	115.23	120.55
1	B	256	GLN	CB-CG-CD	-5.01	104.08	112.60
1	B	272	VAL	CA-C-O	5.01	126.16	120.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3041	0	2942	28	0
1	B	3037	0	2935	26	0
1	C	3035	0	2930	22	0
1	D	3037	0	2933	20	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	209	0	0	1	0
3	B	207	0	0	0	0
3	C	217	0	0	0	0
3	D	204	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12995	0	11740	84	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 (84) 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	1.57	1.20
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.61	1.18
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.17	0.86
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.23	0.86
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.25	0.83
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.82
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.76	0.67
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.78	0.66
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.79	0.64
1:A:276:GLU:HG3	1:A:319:LYS:HG3	1.82	0.62
1:C:24:ASP:O	1:D:23:ARG:NH2	2.33	0.62
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.82	0.60
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.83	0.60
1:A:36:PRO:O	1:A:40:VAL:HG23	2.01	0.60
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.83	0.59
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.86	0.58
1:A:204:GLN:HG2	3:A:541:HOH:O	2.03	0.58
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.41	0.56
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.08	0.53
1:C:72:ILE:O	1:C:76:LYS:HG3	2.11	0.51
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.45	0.50
1:D:72:ILE:O	1:D:76:LYS:HG3	2.11	0.50
1:A:257:ASP:HB3	1:A:293:TYR:HA	1.95	0.49
1:A:313:ARG:HG3	1:A:313:ARG:HH11	1.78	0.49
1:B:164:LEU:C	1:B:164:LEU:HD23	2.37	0.49
1:B:216:PRO:HG2	1:B:232:ILE:HD11	1.96	0.47
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.97	0.47
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.96	0.47
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.50	0.47
1:A:298:THR:HA	1:B:100:LYS:HD2	1.97	0.47
1:A:6:THR:O	1:A:9:ASP:HB2	2.16	0.46
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.96	0.46
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.96	0.46
1:C:278:GLY:HA3	1:C:282:ALA:O	2.15	0.46
1:B:280:ASP:C	1:B:282:ALA:H	2.22	0.46
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.98	0.46
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.98	0.45
1:A:313:ARG:HH11	1:A:313:ARG:CG	2.29	0.45
1:C:234:GLN:HE21	1:C:238:HIS:CE1	2.10	0.44
1:D:178:PHE:HB2	1:D:212:PHE:CD2	2.53	0.44
1:A:65:ALA:O	1:A:69:ASP:HB2	2.17	0.44
1:D:361:ARG:HB3	1:D:365:GLU:HB2	2.00	0.44
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.52	0.44
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.84	0.43
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.84	0.43
1:A:243:HIS:CD2	1:A:288:PRO:HG2	2.53	0.43
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.84	0.43
1:B:154:ALA:HB2	1:D:343:LEU:HD21	2.01	0.43
1:C:7:ARG:HD2	1:C:49:TYR:HB2	2.00	0.43
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.64	0.43
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.89	0.42
1:B:193:LEU:N	1:B:194:PRO:CD	2.81	0.42
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.54	0.42
1:D:282:ALA:HA	1:D:283:PRO:HD3	1.90	0.42
1:D:9:ASP:HB3	1:D:11:PHE:CE2	2.54	0.42
1:C:368:ASP:O	1:C:372:VAL:HG23	2.20	0.42
1:A:183:LYS:HG2	1:A:184:PRO:HD2	2.02	0.42
1:B:186:GLU:HA	1:B:187:PRO:HA	1.87	0.42
1:A:42:LYS:HD3	1:A:42:LYS:HA	1.84	0.42
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.55	0.41
1:B:219:GLY:O	1:B:223:MET:HG3	2.20	0.41
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.88	0.41
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.55	0.41
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.15	0.41
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.84	0.41
1:A:343:LEU:HD12	1:A:343:LEU:HA	1.95	0.41
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.56	0.41
1:A:164:LEU:C	1:A:164:LEU:HD23	2.46	0.41
1:B:352:GLU:HG2	1:B:356:GLU:HB2	2.03	0.41
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.56	0.41
1:B:43:LEU:HD12	1:B:51:ILE:HD12	2.03	0.41
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.56	0.41
1:B:183:LYS:HG3	1:B:220:HIS:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.17	0.41
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.54	0.41
1:B:181:GLU:HA	1:B:182:PRO:HD3	1.91	0.41
1:A:125:LEU:HD12	1:A:125:LEU:HA	1.76	0.40
1:B:5:ALA:HB2	1:B:312:ILE:HG21	2.02	0.40
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.82	0.40
1:D:181:GLU:HA	1:D:182:PRO:HD3	1.92	0.40
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.93	0.40
1:A:313:ARG:C	1:A:313:ARG:HD3	2.40	0.40
1:D:102:GLY:HA2	1:D:140:ARG:HB2	2.03	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	389/393 (99%)	376 (97%)	12 (3%)	1 (0%)	36	46
1	B	389/393 (99%)	375 (96%)	12 (3%)	2 (0%)	24	31
1	C	389/393 (99%)	375 (96%)	11 (3%)	3 (1%)	16	20
1	D	389/393 (99%)	375 (96%)	12 (3%)	2 (0%)	24	31
All	All	1556/1572 (99%)	1501 (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	C	364	PHE

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Mol	Chain	Res	Type
1	D	186	GLU
1	D	280	ASP
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	303/310 (98%)	297 (98%)	6 (2%)	48	67
1	B	302/310 (97%)	298 (99%)	4 (1%)	61	77
1	C	301/310 (97%)	298 (99%)	3 (1%)	68	82
1	D	302/310 (97%)	296 (98%)	6 (2%)	48	67
All	All	1208/1240 (97%)	1189 (98%)	19 (2%)	55	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	TYR
1	A	84	LEU
1	A	203	VAL
1	A	208	ARG
1	A	313	ARG
1	B	49	TYR
1	B	81	GLU
1	B	203	VAL
1	B	394	ARG
1	C	49	TYR
1	C	80	ASP
1	C	203	VAL
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	180	ILE
1	D	185	ASN

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Mol	Chain	Res	Type
1	D	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
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	B	256	GLN
1	C	41	HIS
1	C	222	GLN
1	C	238	HIS
1	D	41	HIS
1	D	185	ASN
1	D	222	GLN
1	D	238	HIS

5.3.3 RNA [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 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.