Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 01:06 AM EST

PDB ID	:	8XIM
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	:	1992-04-01
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

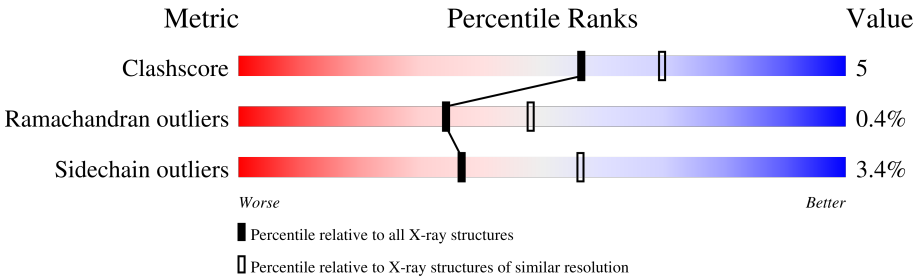
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	393	80% 17%
1	B	393	83% 15%
1	C	393	80% 16%
1	D	393	80% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13203 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

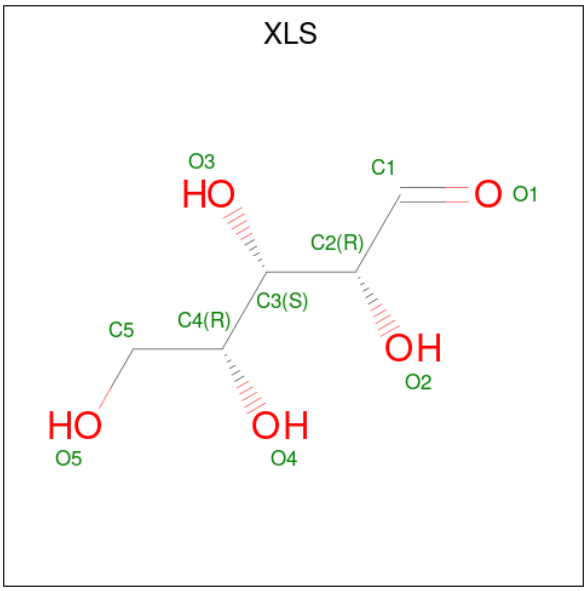
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

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

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is D-xylose (three-letter code: XLS) (formula: $C_5H_{10}O_5$).



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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	240	Total O 240 240	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	235	Total O 235 235	0	0
4	C	254	Total O 254 254	0	0
4	D	242	Total O 242 242	0	0

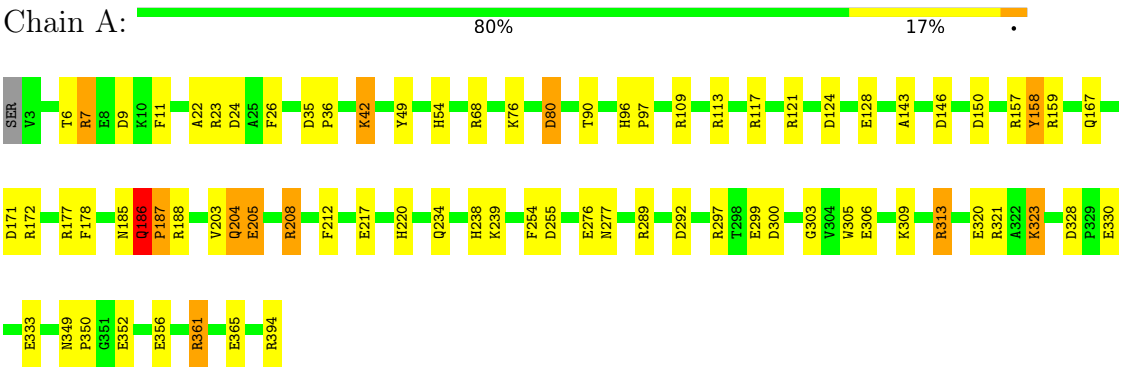
3 Residue-property plots (i)

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

Note EDS was not executed.

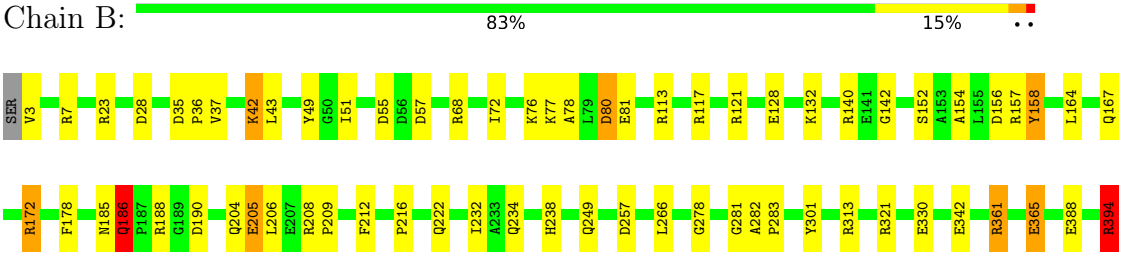
• Molecule 1: D-XYLOSE ISOMERASE

Chain A:



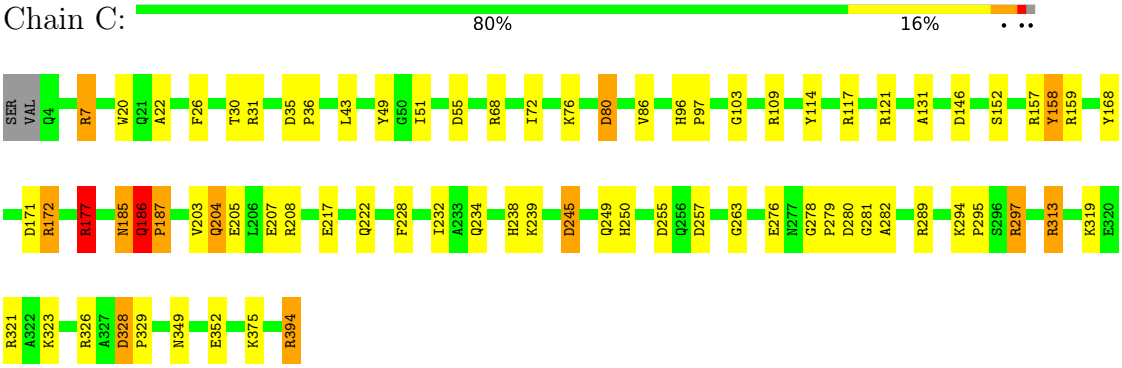
• Molecule 1: D-XYLOSE ISOMERASE

Chain B:



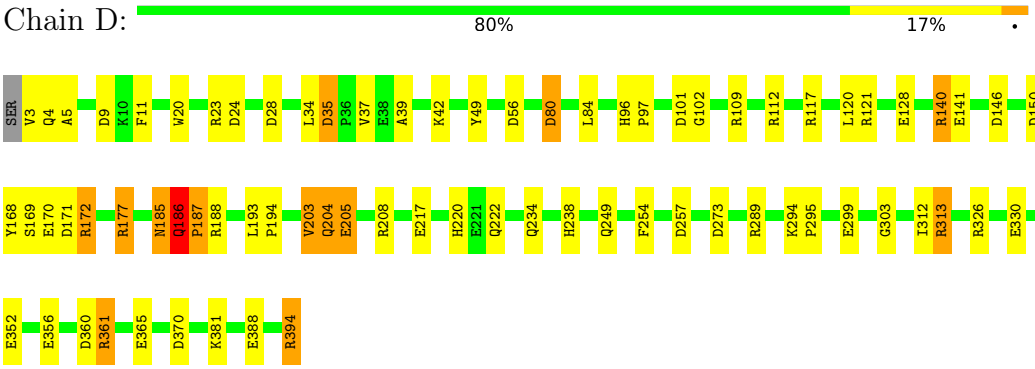
• Molecule 1: D-XYLOSE ISOMERASE

Chain C:



• Molecule 1: D-XYLOSE ISOMERASE

Chain D:


80%
17%
SER V3 Q4 A5 D9 K10 F11 W20 R23 D24 D28 L34 D35 P36 V37 E38 A39 K42 Y49 D56 D80 L84 H96 P97 D101 G102 R109 R112 R117 L120 R121 E128 R140 E141 D146 D150 R157 Y158
Y168 S169 E170 D171 R172 R177 N185 Q186 P187 R188 L193 P194 V203 Q204 E205 R208 E217 H220 E221 Q222 Q234 H238 Q249 F254 D257 D273 R289 K294 P295 E299 G303 I312 R313 R326 E330 L343 L348
E352 E356 D360 R361 E365 D370 K381 E388 R394

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.45Å 143.45Å 231.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.146 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13203	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.78	0/3121	1.58	54/4228 (1.3%)
1	B	0.78	0/3121	1.58	38/4228 (0.9%)
1	C	0.78	0/3114	1.58	41/4218 (1.0%)
1	D	0.81	1/3119 (0.0%)	1.57	50/4224 (1.2%)
All	All	0.79	1/12475 (0.0%)	1.58	183/16898 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	SER	C-N	-9.31	1.12	1.34

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	117	ARG	NE-CZ-NH1	18.94	129.77	120.30
1	B	313	ARG	CD-NE-CZ	16.50	146.71	123.60
1	C	313	ARG	NE-CZ-NH1	16.47	128.53	120.30
1	C	117	ARG	NE-CZ-NH1	16.00	128.30	120.30
1	B	313	ARG	NE-CZ-NH1	15.85	128.23	120.30
1	C	313	ARG	CD-NE-CZ	14.38	143.74	123.60
1	B	394	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	A	117	ARG	NE-CZ-NH1	13.50	127.05	120.30
1	D	117	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	B	117	ARG	NE-CZ-NH2	-12.34	114.13	120.30
1	D	109	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	A	394	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	D	109	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	A	117	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	D	35	ASP	CB-CG-OD1	11.79	128.91	118.30
1	C	326	ARG	NE-CZ-NH2	11.77	126.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	188	ARG	NE-CZ-NH2	11.75	126.17	120.30
1	D	112	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	D	117	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	C	117	ARG	NE-CZ-NH2	-10.58	115.01	120.30
1	C	394	ARG	NE-CZ-NH1	-10.39	115.10	120.30
1	B	157	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	B	330	GLU	OE1-CD-OE2	10.08	135.39	123.30
1	A	394	ARG	NE-CZ-NH1	-9.96	115.32	120.30
1	D	330	GLU	OE1-CD-OE2	9.96	135.25	123.30
1	A	394	ARG	NH1-CZ-NH2	9.86	130.25	119.40
1	A	146	ASP	CB-CG-OD1	9.71	127.04	118.30
1	C	157	ARG	NE-CZ-NH1	9.27	124.93	120.30
1	A	205	GLU	OE1-CD-OE2	-9.18	112.29	123.30
1	B	80	ASP	CB-CG-OD1	-9.09	110.12	118.30
1	B	321	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	A	80	ASP	CB-CG-OD1	-9.00	110.20	118.30
1	C	321	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	121	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	C	313	ARG	NH1-CZ-NH2	-8.80	109.72	119.40
1	D	257	ASP	CB-CG-OD1	8.77	126.19	118.30
1	A	157	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	121	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	D	23	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	23	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	C	80	ASP	CB-CG-OD1	-8.43	110.71	118.30
1	A	113	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	C	257	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	394	ARG	N-CA-CB	8.29	125.51	110.60
1	A	150	ASP	CB-CG-OD1	8.24	125.72	118.30
1	B	140	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	172	ARG	CD-NE-CZ	8.21	135.09	123.60
1	A	188	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	109	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	31	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	C	208	ARG	CD-NE-CZ	-8.09	112.28	123.60
1	D	361	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	D	121	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	113	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	B	313	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	394	ARG	CD-NE-CZ	-7.79	112.69	123.60
1	A	23	ARG	CD-NE-CZ	7.76	134.46	123.60
1	D	394	ARG	NE-CZ-NH2	-7.60	116.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	140	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	361	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	361	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	156	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	B	158	TYR	CB-CG-CD2	7.46	125.48	121.00
1	A	172	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	C	68	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	D	150	ASP	CB-CG-OD1	7.35	124.91	118.30
1	A	109	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	C	289	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	B	257	ASP	CB-CG-OD2	7.29	124.86	118.30
1	C	208	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	D	330	GLU	CG-CD-OE2	-7.18	103.94	118.30
1	D	370	ASP	CB-CG-OD2	7.15	124.74	118.30
1	D	273	ASP	CB-CG-OD2	7.13	124.72	118.30
1	A	330	GLU	OE1-CD-OE2	7.12	131.85	123.30
1	C	121	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	328	ASP	CB-CG-OD2	7.01	124.61	118.30
1	D	170	GLU	N-CA-CB	6.95	123.11	110.60
1	A	24	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	313	ARG	CA-CB-CG	6.90	128.58	113.40
1	C	158	TYR	CB-CG-CD2	6.89	125.13	121.00
1	A	159	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	23	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	292	ASP	CB-CG-OD2	6.83	124.45	118.30
1	B	394	ARG	NH1-CZ-NH2	6.68	126.75	119.40
1	C	328	ASP	CB-CG-OD2	6.64	124.28	118.30
1	C	281	GLY	N-CA-C	-6.63	96.52	113.10
1	A	361	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	24	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	C	159	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	D	289	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	C	297	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	C	146	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	297	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	C	245	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	321	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	330	GLU	CG-CD-OE2	-6.39	105.52	118.30
1	C	109	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	55	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	121	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	140	ARG	NE-CZ-NH2	-6.29	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	28	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	C	394	ARG	NH1-CZ-NH2	6.26	126.29	119.40
1	D	24	ASP	CB-CG-OD1	6.26	123.93	118.30
1	D	157	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	26	PHE	CB-CG-CD1	-6.22	116.45	120.80
1	D	205	GLU	CG-CD-OE2	6.22	130.74	118.30
1	B	68	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	D	208	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	171	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	55	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	188	ARG	CD-NE-CZ	5.99	131.99	123.60
1	C	276	GLU	CG-CD-OE2	5.98	130.26	118.30
1	C	394	ARG	CD-NE-CZ	-5.97	115.25	123.60
1	C	204	GLN	OE1-CD-NE2	-5.96	108.19	121.90
1	C	114	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	300	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	205	GLU	OE1-CD-OE2	-5.91	116.21	123.30
1	A	205	GLU	CG-CD-OE2	5.88	130.06	118.30
1	D	150	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	255	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	D	360	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	D	101	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	301	TYR	CB-CG-CD1	-5.81	117.51	121.00
1	C	31	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	113	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	171	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	D	56	ASP	CB-CG-OD2	5.75	123.48	118.30
1	D	208	ARG	CD-NE-CZ	-5.75	115.56	123.60
1	D	9	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	D	35	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	255	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	333	GLU	OE1-CD-OE2	5.67	130.11	123.30
1	D	313	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	D	326	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	A	143	ALA	N-CA-CB	-5.62	102.24	110.10
1	D	80	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	B	158	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	D	146	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	207	GLU	CG-CD-OE2	-5.51	107.27	118.30
1	A	7	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	23	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	187	PRO	N-CA-C	5.46	126.30	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	ASP	CA-CB-CG	-5.46	101.39	113.40
1	A	289	ARG	CD-NE-CZ	5.42	131.19	123.60
1	C	208	ARG	NH1-CZ-NH2	5.40	125.34	119.40
1	C	171	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	388	GLU	CG-CD-OE1	-5.40	107.50	118.30
1	B	365	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	A	208	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	124	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	57	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	289	ARG	CD-NE-CZ	5.32	131.05	123.60
1	D	121	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	326	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	342	GLU	CG-CD-OE2	5.28	128.87	118.30
1	D	177	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	276	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	D	169	SER	CA-C-O	-5.26	109.05	120.10
1	C	187	PRO	N-CA-C	5.25	125.75	112.10
1	B	188	ARG	CD-NE-CZ	5.24	130.94	123.60
1	B	156	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	68	ARG	CD-NE-CZ	5.21	130.90	123.60
1	A	158	TYR	CB-CG-CD2	5.21	124.13	121.00
1	A	204	GLN	OE1-CD-NE2	-5.20	109.93	121.90
1	B	321	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	208	ARG	CD-NE-CZ	-5.19	116.33	123.60
1	A	320	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	C	177	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	204	GLN	OE1-CD-NE2	-5.18	109.99	121.90
1	D	205	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	D	203	VAL	CA-CB-CG1	5.13	118.59	110.90
1	C	158	TYR	CA-CB-CG	5.12	123.13	113.40
1	A	128	GLU	CG-CD-OE1	-5.12	108.07	118.30
1	B	140	ARG	CD-NE-CZ	5.11	130.75	123.60
1	A	177	ARG	CB-CA-C	5.09	120.59	110.40
1	D	28	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	103	GLY	N-CA-C	-5.08	100.40	113.10
1	A	146	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	109	ARG	CD-NE-CZ	5.04	130.66	123.60
1	A	394	ARG	N-CA-CB	5.04	119.66	110.60
1	B	81	GLU	CA-CB-CG	5.03	124.48	113.40
1	B	121	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	D	128	GLU	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3049	0	2952	26	0
1	B	3049	0	2952	33	0
1	C	3042	0	2943	39	0
1	D	3048	0	2946	37	0
2	A	10	0	8	0	0
2	B	10	0	8	0	0
2	C	10	0	8	1	0
2	D	10	0	9	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	240	0	0	3	0
4	B	235	0	0	1	0
4	C	254	0	0	3	0
4	D	242	0	0	8	0
All	All	13203	0	11826	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (119) 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	1.54	1.26
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.66	1.13
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.19	0.90
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.18	0.89
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.21	0.88
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.29	0.79
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.71	0.71
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:PHE:HE2	1:D:186:GLN:NE2	1.90	0.69
1:A:277:ASN:OD1	1:A:323:LYS:HE3	1.93	0.69
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.77	0.68
1:B:388:GLU:CD	1:C:313:ARG:HH11	1.98	0.67
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.80	0.65
1:D:217:GLU:OE2	4:D:429:HOH:O	2.14	0.64
1:A:313:ARG:HG3	4:A:637:HOH:O	2.00	0.62
1:B:77:LYS:O	1:B:80:ASP:HB2	2.01	0.61
1:D:185:ASN:HD22	1:D:186:GLN:HB2	1.65	0.61
1:D:3:VAL:HG12	1:D:4:GLN:H	1.65	0.61
1:B:76:LYS:NZ	1:B:128:GLU:OE2	2.35	0.60
1:B:388:GLU:OE2	1:C:313:ARG:HD3	2.03	0.59
1:D:141:GLU:OE2	4:D:595:HOH:O	2.17	0.59
1:A:167:GLN:OE1	1:A:208:ARG:NH2	2.36	0.58
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.86	0.58
1:C:26:PHE:CE2	1:D:186:GLN:NE2	2.67	0.58
1:D:394:ARG:NH1	4:D:614:HOH:O	2.14	0.56
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.89	0.55
1:C:177:ARG:HD3	4:C:613:HOH:O	2.06	0.54
1:D:220:HIS:NE2	4:D:429:HOH:O	2.33	0.53
2:C:397:XLS:H1	4:C:581:HOH:O	2.08	0.53
1:D:168:TYR:CE1	1:D:172:ARG:HD3	2.44	0.53
1:B:72:ILE:O	1:B:76:LYS:HG3	2.09	0.53
1:C:7:ARG:HH11	1:C:7:ARG:HG3	1.74	0.52
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.91	0.52
1:D:35:ASP:OD1	1:D:37:VAL:HB	2.10	0.52
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.14	0.51
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.45	0.51
1:C:168:TYR:O	1:C:172:ARG:HG2	2.10	0.51
1:B:152:SER:HB2	4:D:413:HOH:O	2.10	0.51
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.10	0.51
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.93	0.51
1:A:6:THR:O	1:A:9:ASP:HB2	2.11	0.51
1:C:72:ILE:O	1:C:76:LYS:HG3	2.11	0.50
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.92	0.50
1:C:7:ARG:HH11	1:C:7:ARG:CG	2.25	0.50
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.47	0.49
1:A:254:PHE:CD1	1:B:186:GLN:HG2	2.48	0.49
1:A:217:GLU:OE2	4:A:398:HOH:O	2.20	0.48
1:C:349:ASN:O	1:C:352:GLU:HB2	2.14	0.48
1:D:3:VAL:HG23	4:D:582:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.27	0.48
1:D:3:VAL:N	4:D:582:HOH:O	2.46	0.48
1:C:186:GLN:HG2	1:D:254:PHE:CD1	2.49	0.47
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.48	0.46
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.79	0.46
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.97	0.46
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.12	0.46
1:A:352:GLU:HG3	1:A:356:GLU:HB2	1.96	0.46
1:B:206:LEU:O	1:B:209:PRO:HD3	2.16	0.46
1:B:278:GLY:CA	1:B:282:ALA:O	2.64	0.45
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.52	0.45
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.99	0.44
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.98	0.44
4:A:542:HOH:O	1:C:152:SER:HB2	2.17	0.44
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.52	0.44
1:C:185:ASN:HD22	1:C:186:GLN:HB2	1.81	0.44
1:B:278:GLY:HA3	1:B:282:ALA:O	2.17	0.44
1:C:278:GLY:HA3	1:C:282:ALA:O	2.18	0.44
1:B:394:ARG:HH11	1:B:394:ARG:HD3	1.55	0.44
1:C:186:GLN:HA	1:C:187:PRO:HA	1.86	0.44
1:B:142:GLY:HA3	1:B:190:ASP:O	2.18	0.44
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.17	0.44
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.99	0.44
1:C:30:THR:HG22	1:D:97:PRO:HB3	2.00	0.44
1:D:42:LYS:HD2	4:D:581:HOH:O	2.18	0.43
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.99	0.43
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.79	0.43
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.53	0.43
1:B:178:PHE:HB2	1:B:212:PHE:CD2	2.53	0.43
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.45	0.43
1:C:319:LYS:O	1:C:323:LYS:HG2	2.19	0.43
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.83	0.43
1:C:43:LEU:HD12	1:C:51:ILE:HD12	2.01	0.43
1:A:42:LYS:HB3	1:A:42:LYS:HE2	1.65	0.43
1:C:7:ARG:CG	1:C:7:ARG:NH1	2.82	0.43
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.80	0.43
1:C:86:VAL:O	1:C:131:ALA:HA	2.19	0.43
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.89	0.43
1:D:186:GLN:HA	1:D:187:PRO:HA	1.80	0.43
1:B:42:LYS:HE2	1:B:42:LYS:HB3	1.64	0.43
1:C:217:GLU:HA	1:C:245:ASP:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:GLU:HB3	1:D:303:GLY:HA3	2.01	0.43
1:B:216:PRO:HG2	1:B:232:ILE:HD11	2.01	0.42
1:C:238:HIS:O	1:C:239:LYS:HB2	2.18	0.42
1:D:120:LEU:HD22	1:D:168:TYR:CD2	2.54	0.42
1:D:34:LEU:HD21	1:D:39:ALA:HB2	2.02	0.42
1:A:305:TRP:O	1:A:309:LYS:HG3	2.20	0.42
1:A:186:GLN:HA	1:A:187:PRO:HA	1.77	0.42
1:D:222:GLN:HE21	1:D:249:GLN:HB3	1.83	0.42
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.19	0.42
1:A:217:GLU:HB3	1:A:220:HIS:CG	2.54	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.91	0.41
1:B:7:ARG:HD3	4:B:497:HOH:O	2.21	0.41
1:D:20:TRP:CE3	1:D:294:LYS:HB3	2.55	0.41
1:A:306:GLU:HG2	1:D:381:LYS:HB2	2.03	0.41
1:A:238:HIS:O	1:A:239:LYS:HB2	2.20	0.41
1:B:388:GLU:OE1	1:C:313:ARG:NH1	2.52	0.41
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.91	0.41
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.90	0.41
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.55	0.41
1:B:35:ASP:HA	1:B:36:PRO:HD3	1.91	0.41
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.90	0.41
1:D:193:LEU:N	1:D:194:PRO:CD	2.84	0.41
1:B:266:LEU:HD23	1:B:266:LEU:HA	1.80	0.41
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.97	0.41
1:C:250:HIS:CE1	1:C:263:GLY:HA2	2.56	0.41
1:A:349:ASN:HB3	1:A:350:PRO:CD	2.51	0.40
1:C:177:ARG:NH2	4:C:590:HOH:O	2.40	0.40
1:B:282:ALA:HB1	1:B:283:PRO:HD2	2.03	0.40
1:C:278:GLY:CA	1:C:282:ALA:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	41	55
1	B	390/393 (99%)	378 (97%)	10 (3%)	2 (0%)	29	41
1	C	389/393 (99%)	374 (96%)	12 (3%)	3 (1%)	19	29
1	D	390/393 (99%)	377 (97%)	12 (3%)	1 (0%)	41	55
All	All	1559/1572 (99%)	1505 (96%)	47 (3%)	7 (0%)	34	48

All (7) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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	305/310 (98%)	294 (96%)	11 (4%)	35	54
1	B	305/310 (98%)	296 (97%)	9 (3%)	41	61
1	C	304/310 (98%)	293 (96%)	11 (4%)	35	54
1	D	304/310 (98%)	293 (96%)	11 (4%)	35	54
All	All	1218/1240 (98%)	1176 (97%)	42 (3%)	37	56

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	42	LYS
1	A	49	TYR
1	A	76	LYS

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Mol	Chain	Res	Type
1	A	80	ASP
1	A	158	TYR
1	A	185	ASN
1	A	186	GLN
1	A	203	VAL
1	A	313	ARG
1	A	323	LYS
1	B	3	VAL
1	B	42	LYS
1	B	49	TYR
1	B	132	LYS
1	B	158	TYR
1	B	172	ARG
1	B	185	ASN
1	B	186	GLN
1	B	394	ARG
1	C	7	ARG
1	C	49	TYR
1	C	80	ASP
1	C	158	TYR
1	C	172	ARG
1	C	177	ARG
1	C	185	ASN
1	C	186	GLN
1	C	203	VAL
1	C	255	ASP
1	C	375	LYS
1	D	49	TYR
1	D	80	ASP
1	D	84	LEU
1	D	158	TYR
1	D	172	ARG
1	D	177	ARG
1	D	185	ASN
1	D	186	GLN
1	D	187	PRO
1	D	203	VAL
1	D	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

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

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 monosaccharides 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	1.98	1 (12%)	10,11,11	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	XLS	C	397	3	8,9,9	1.97	1 (12%)	10,11,11	1.35	1 (10%)
2	XLS	B	397	3	8,9,9	2.12	1 (12%)	10,11,11	1.21	1 (10%)
2	XLS	A	397	3	8,9,9	2.06	1 (12%)	10,11,11	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XLS	D	397	3	-	0/10/12/12	-
2	XLS	C	397	3	-	0/10/12/12	-
2	XLS	B	397	3	-	1/10/12/12	-
2	XLS	A	397	3	-	1/10/12/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	397	XLS	O1-C1	5.89	1.43	1.19
2	A	397	XLS	O1-C1	5.77	1.43	1.19
2	C	397	XLS	O1-C1	5.50	1.41	1.19
2	D	397	XLS	O1-C1	5.48	1.41	1.19

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	397	XLS	O4-C4-C3	2.59	115.40	109.10
2	C	397	XLS	O3-C3-C2	2.08	112.99	109.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	397	XLS	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	169:SER	C	170:GLU	N	1.12

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.