Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:59 PM GMT

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PDB ID	:	6XIM
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	:	1992-04-03
Resolution	:	2.50 Å(reported)

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 2.50 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	Percentile Ranks	Value
Clashscore		4
Ramachandran outliers		0.5%
Sidechain outliers		2.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
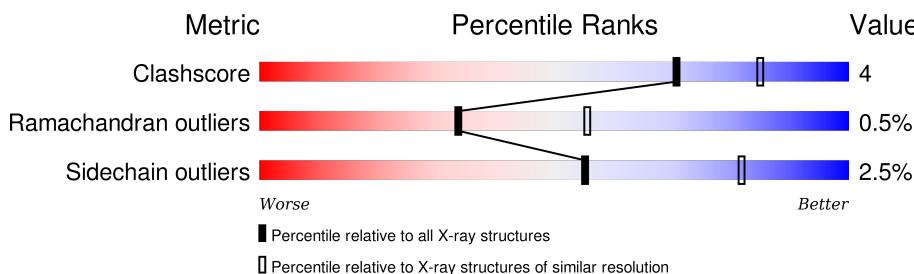
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	393	81% 16% •
1	B	393	80% 16% •
1	C	393	80% 17% •
1	D	393	82% 16% •
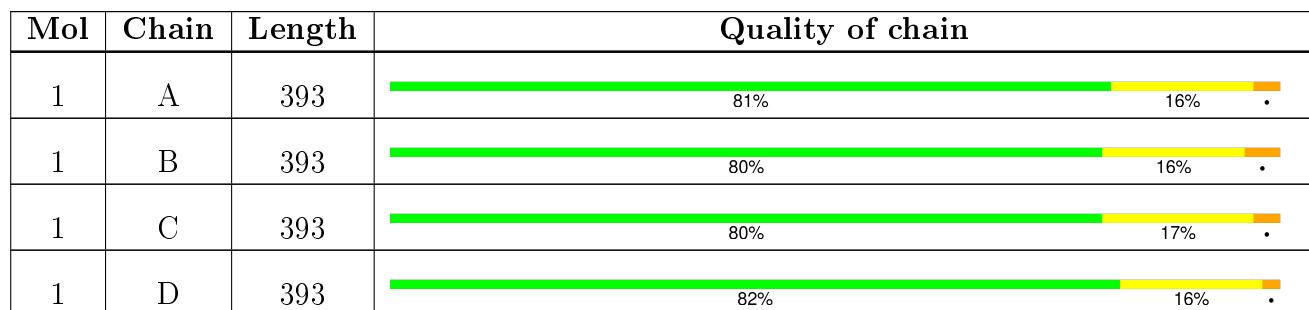
2 Entry composition (i)

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 3053	C 1939	N 532	O 578	S 4	0	0	0
1	B	392	Total 3053	C 1939	N 532	O 578	S 4	0	0	0
1	C	392	Total 3053	C 1939	N 532	O 578	S 4	0	0	0
1	D	392	Total 3053	C 1939	N 532	O 578	S 4	0	0	0

- Molecule 2 is SUGAR (D-XYLOSE (LINEAR FORM)) (three-letter code: XLS) (formula: $C_5H_{10}O_5$).
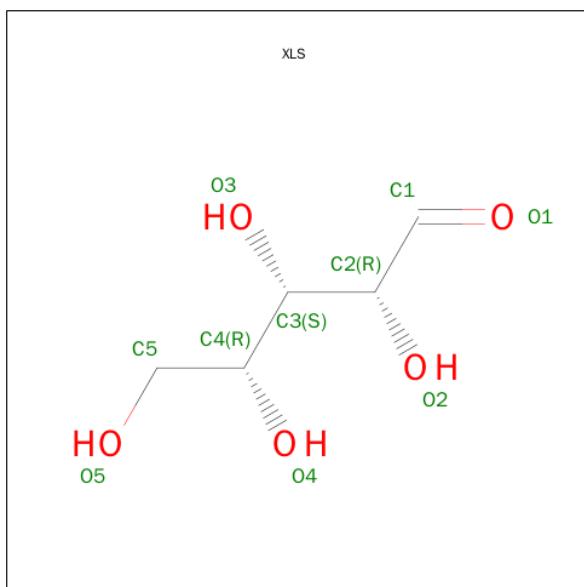
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 10	C 5	O 5	0	0
2	B	1	Total 10	C 5	O 5	0	0

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	225	Total 225	O 225	0	0
4	B	213	Total 213	O 213	0	0
4	C	231	Total 231	O 231	0	0
4	D	212	Total 212	O 212	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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
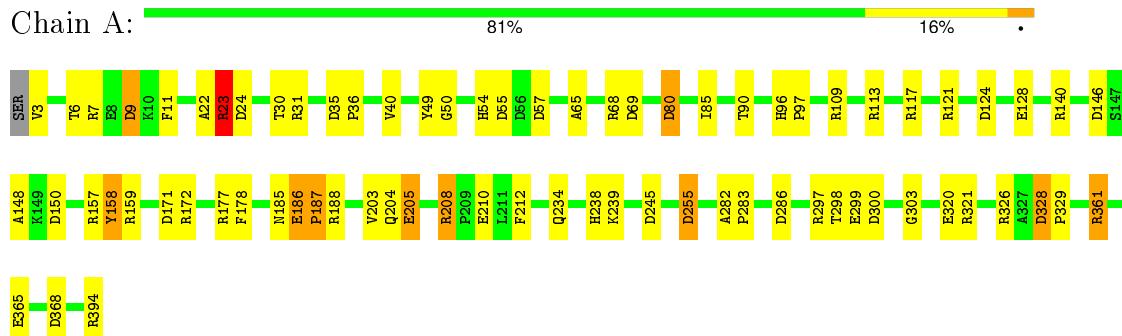
- Molecule 1: D-XYLOSE ISOMERASE

- Molecule 1: D-XYLOSE ISOMERASE

• Molecule 1: D-XYLOSE ISOMERASE

Chain D:
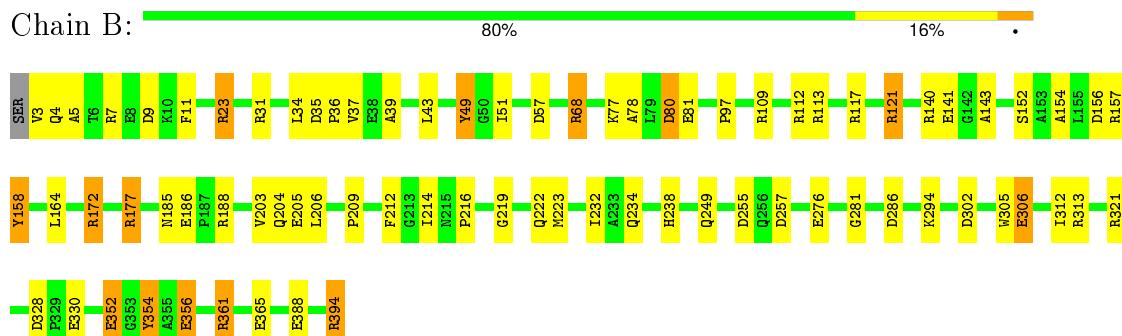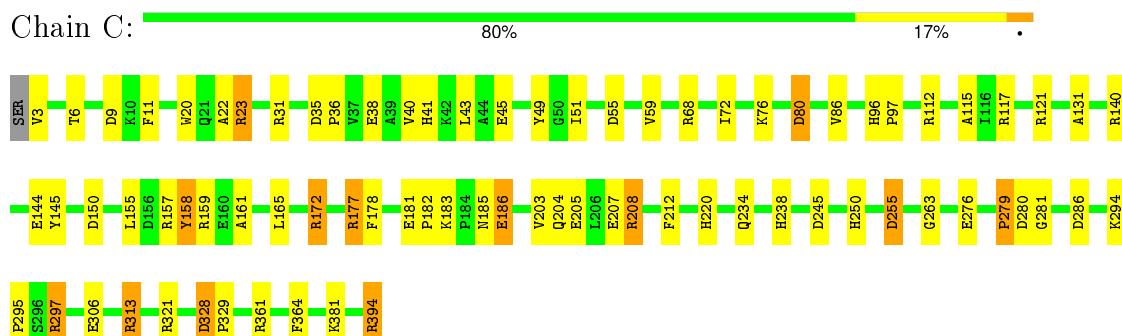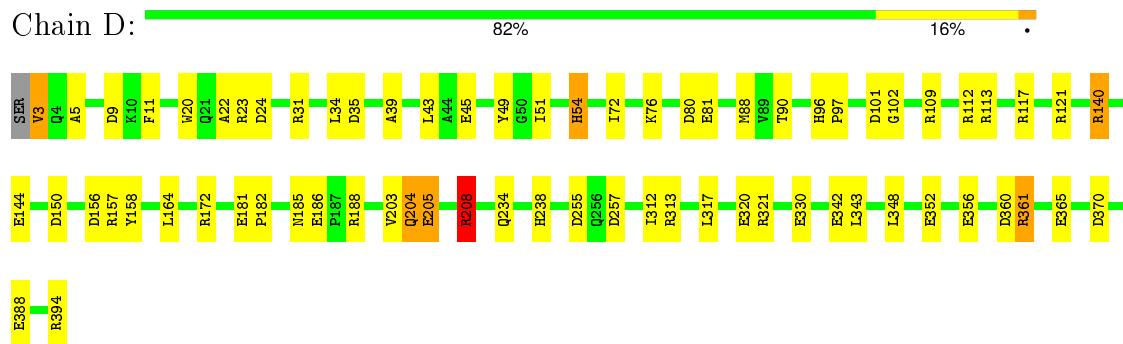
4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13141	wwPDB-VP
Average B, all atoms (Å²)	19.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, XLS

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	0.80	0/3125	1.64	52/4233 (1.2%)
1	B	0.80	0/3125	1.65	50/4233 (1.2%)
1	C	0.80	0/3125	1.61	52/4233 (1.2%)
1	D	0.80	0/3125	1.63	44/4233 (1.0%)
All	All	0.80	0/12500	1.63	198/16932 (1.2%)

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	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (198) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ASP	CB-CG-OD1	17.47	134.02	118.30
1	B	117	ARG	NE-CZ-NH1	17.34	128.97	120.30
1	B	172	ARG	NE-CZ-NH2	-14.75	112.92	120.30
1	C	172	ARG	NE-CZ-NH1	14.45	127.53	120.30
1	B	394	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	C	177	ARG	NE-CZ-NH1	14.26	127.43	120.30
1	B	177	ARG	NE-CZ-NH2	-13.93	113.33	120.30
1	C	172	ARG	NE-CZ-NH2	-13.69	113.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	A	361	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	B	112	ARG	NE-CZ-NH1	-12.79	113.91	120.30
1	A	321	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	C	117	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	D	313	ARG	NE-CZ-NH2	12.34	126.47	120.30
1	D	121	ARG	NE-CZ-NH2	-11.45	114.57	120.30
1	D	112	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	B	321	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	B	172	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	A	394	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	B	117	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	394	ARG	NE-CZ-NH2	-10.67	114.97	120.30
1	C	177	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	D	255	ASP	CB-CG-OD2	-10.32	109.01	118.30
1	B	158	TYR	CB-CG-CD2	10.29	127.18	121.00
1	B	113	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	172	ARG	NE-CZ-NH1	9.89	125.25	120.30
1	C	255	ASP	CB-CG-OD1	9.82	127.14	118.30
1	A	394	ARG	NH1-CZ-NH2	9.80	130.18	119.40
1	A	326	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	A	146	ASP	CB-CG-OD1	9.32	126.69	118.30
1	D	35	ASP	CB-CG-OD1	9.26	126.63	118.30
1	A	80	ASP	CB-CG-OD1	-9.26	109.97	118.30
1	A	23	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	C	159	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	C	313	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	C	158	TYR	CB-CG-CD2	9.14	126.48	121.00
1	B	68	ARG	NE-CZ-NH1	-9.14	115.73	120.30
1	B	121	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	D	208	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	D	109	ARG	NE-CZ-NH1	9.01	124.80	120.30
1	B	31	ARG	NE-CZ-NH2	8.91	124.75	120.30
1	A	328	ASP	CB-CG-OD2	8.82	126.24	118.30
1	D	150	ASP	CB-CG-OD1	8.81	126.23	118.30
1	D	172	ARG	CD-NE-CZ	8.77	135.88	123.60
1	B	177	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	B	156	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	A	188	ARG	CD-NE-CZ	8.60	135.64	123.60
1	A	117	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	B	330	GLU	OE1-CD-OE2	8.58	133.60	123.30
1	D	188	ARG	NE-CZ-NH2	8.57	124.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ASP	CB-CG-OD1	8.52	125.97	118.30
1	D	117	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	205	GLU	OE1-CD-OE2	-8.32	113.31	123.30
1	A	157	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	124	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	255	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	C	394	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	C	80	ASP	CB-CG-OD1	-8.24	110.88	118.30
1	A	113	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	255	ASP	CB-CG-OD1	8.03	125.52	118.30
1	D	361	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	B	80	ASP	CB-CG-OD1	-7.99	111.11	118.30
1	B	157	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	150	ASP	CB-CG-OD1	7.86	125.37	118.30
1	A	121	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C	328	ASP	CB-CG-OD2	7.80	125.32	118.30
1	B	158	TYR	CB-CG-CD1	-7.79	116.33	121.00
1	C	55	ASP	CB-CG-OD1	7.78	125.30	118.30
1	B	328	ASP	CB-CG-OD2	7.75	125.28	118.30
1	B	394	ARG	N-CA-CB	7.75	124.55	110.60
1	C	361	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	A	158	TYR	CB-CG-CD2	7.49	125.50	121.00
1	C	23	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	B	361	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	B	112	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	394	ARG	CA-CB-CG	7.36	129.59	113.40
1	D	330	GLU	OE1-CD-OE2	7.34	132.10	123.30
1	A	326	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	C	297	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	A	117	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	B	140	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	D	360	ASP	CB-CG-OD1	-7.25	111.77	118.30
1	C	31	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	D	113	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	C	145	TYR	CB-CG-CD2	7.20	125.32	121.00
1	C	321	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	159	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	321	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	D	101	ASP	CB-CG-OD2	6.93	124.53	118.30
1	A	31	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	D	205	GLU	OE1-CD-OE2	-6.90	115.02	123.30
1	C	121	ARG	NE-CZ-NH1	6.88	123.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	ASP	CB-CG-OD1	6.84	124.46	118.30
1	A	146	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	C	276	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	C	245	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	23	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	C	117	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	D	140	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	D	109	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	9	ASP	CB-CG-OD2	6.67	124.31	118.30
1	C	208	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	A	368	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	245	ASP	CB-CG-OD1	6.57	124.22	118.30
1	D	88	MET	CA-CB-CG	6.55	124.44	113.30
1	C	45	GLU	CA-CB-CG	6.55	127.81	113.40
1	A	80	ASP	CA-CB-CG	-6.54	99.00	113.40
1	A	205	GLU	CG-CD-OE2	6.52	131.34	118.30
1	D	320	GLU	CA-CB-CG	6.48	127.66	113.40
1	D	257	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	245	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	C	172	ARG	CD-NE-CZ	-6.44	114.58	123.60
1	C	23	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	55	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	157	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	C	207	GLU	CG-CD-OE2	-6.35	105.60	118.30
1	A	7	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	109	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	302	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	342	GLU	CG-CD-OE2	6.27	130.84	118.30
1	C	145	TYR	CB-CG-CD1	-6.26	117.24	121.00
1	A	23	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	255	ASP	CB-CG-OD1	6.24	123.91	118.30
1	D	31	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	388	GLU	CG-CD-OE2	6.16	130.63	118.30
1	B	141	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	A	24	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	57	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	C	150	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	121	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	276	GLU	CG-CD-OE2	5.93	130.16	118.30
1	A	320	GLU	OE1-CD-OE2	-5.92	116.19	123.30
1	C	321	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	388	GLU	CG-CD-OE1	-5.88	106.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	257	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	35	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	321	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	361	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	394	ARG	NH1-CZ-NH2	5.82	125.80	119.40
1	D	370	ASP	CB-CG-OD2	5.81	123.53	118.30
1	D	313	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
1	C	177	ARG	N-CA-CB	5.76	120.97	110.60
1	B	313	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	171	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	45	GLU	OE1-CD-OE2	5.70	130.13	123.30
1	B	109	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	54	HIS	N-CA-CB	5.65	120.77	110.60
1	B	354	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	C	207	GLU	CG-CD-OE1	5.55	129.41	118.30
1	D	150	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	68	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	A	300	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	143	ALA	N-CA-CB	-5.49	102.42	110.10
1	D	144	GLU	N-CA-CB	5.48	120.46	110.60
1	C	281	GLY	N-CA-C	-5.47	99.42	113.10
1	D	205	GLU	CG-CD-OE2	5.47	129.23	118.30
1	C	255	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	57	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	298	THR	CA-CB-CG2	5.43	120.01	112.40
1	B	356	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	A	140	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	286	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	150	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	D	342	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	D	208	ARG	CG-CD-NE	5.36	123.05	111.80
1	C	394	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	B	188	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	204	GLN	OE1-CD-NE2	-5.34	109.62	121.90
1	B	302	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	D	388	GLU	CG-CD-OE1	-5.31	107.67	118.30
1	A	55	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	81	GLU	OE1-CD-OE2	5.29	129.64	123.30
1	C	313	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
1	C	158	TYR	CA-CB-CG	5.27	123.41	113.40
1	B	352	GLU	OE1-CD-OE2	5.25	129.60	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	140	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	394	ARG	CG-CD-NE	-5.21	100.86	111.80
1	B	305	TRP	CA-CB-CG	-5.17	103.88	113.70
1	C	306	GLU	CG-CD-OE1	5.17	128.63	118.30
1	D	157	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	128	GLU	CG-CD-OE1	-5.16	107.99	118.30
1	D	156	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	113	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	112	ARG	CG-CD-NE	5.13	122.58	111.80
1	B	306	GLU	OE1-CD-OE2	5.11	129.43	123.30
1	A	128	GLU	CG-CD-OE2	5.10	128.49	118.30
1	B	113	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	6	THR	N-CA-CB	5.09	119.98	110.30
1	C	144	GLU	CG-CD-OE1	5.09	128.49	118.30
1	C	155	LEU	CB-CA-C	5.08	119.86	110.20
1	C	208	ARG	CD-NE-CZ	-5.08	116.49	123.60
1	D	81	GLU	CG-CD-OE1	-5.06	108.18	118.30
1	B	255	ASP	N-CA-CB	-5.04	101.53	110.60
1	A	148	ALA	N-CA-CB	-5.03	103.05	110.10
1	C	208	ARG	NH1-CZ-NH2	5.03	124.94	119.40
1	C	115	ALA	CB-CA-C	5.03	117.65	110.10
1	B	276	GLU	CG-CD-OE1	-5.03	108.24	118.30

There are no chirality outliers.

All (6) 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	C	177	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	3053	0	2954	25	0
1	B	3053	0	2954	34	0
1	C	3053	0	2954	28	0
1	D	3053	0	2954	33	0
2	A	10	0	9	0	0
2	B	10	0	9	0	0
2	C	10	0	9	0	0
2	D	10	0	9	0	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	1	0
4	B	213	0	0	3	0
4	C	231	0	0	1	0
4	D	212	0	0	6	0
All	All	13141	0	11852	107	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 (107) 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	1.68	1.10
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.70	1.08
1:D:208:ARG:HH11	1:D:208:ARG:HG2	1.33	0.94
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.21	0.88
1:A:204:GLN:HG2	4:A:552:HOH:O	1.76	0.84
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.24	0.84
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.23	0.81
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.25	0.80
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.65	0.78
1:D:3:VAL:HG23	4:D:595:HOH:O	1.83	0.78
1:B:294:LYS:HE2	4:B:585:HOH:O	1.93	0.67
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.78	0.65
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.79	0.64
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.81	0.63
1:A:36:PRO:O	1:A:40:VAL:HG23	2.03	0.59
1:C:43:LEU:HD12	1:C:51:ILE:HD12	1.85	0.57
1:C:59:VAL:HG11	1:C:68:ARG:HG3	1.87	0.57
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.87	0.57
1:B:219:GLY:O	1:B:223:MET:HG3	2.05	0.56
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.88	0.56
1:B:68:ARG:HH11	1:B:68:ARG:HG2	1.71	0.56
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.43	0.54
1:D:394:ARG:NH1	4:D:604:HOH:O	2.08	0.54
1:B:3:VAL:HG12	1:B:4:GLN:H	1.73	0.54
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.91	0.53
1:D:3:VAL:CG2	4:D:595:HOH:O	2.51	0.53
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.91	0.53
1:C:72:ILE:O	1:C:76:LYS:HG3	2.09	0.52
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.13	0.51
1:D:208:ARG:NH1	1:D:208:ARG:HG2	2.08	0.51
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.46	0.51
1:B:234:GLN:HE21	1:B:238:HIS:CE1	2.17	0.51
1:A:65:ALA:O	1:A:69:ASP:HB2	2.12	0.50
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.92	0.49
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.95	0.49
1:A:299:GLU:HB3	1:A:303:GLY:HA3	1.94	0.49
1:C:23:ARG:CZ	1:D:23:ARG:HD2	2.43	0.48
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.48	0.48
1:B:77:LYS:O	1:B:80:ASP:HB2	2.14	0.48
1:D:3:VAL:HB	4:D:595:HOH:O	2.13	0.47
1:D:5:ALA:HB2	1:D:312:ILE:HG21	1.96	0.47
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.96	0.47
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.75	0.47
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.50	0.47
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.28	0.47
1:A:238:HIS:O	1:A:239:LYS:HB2	2.15	0.47
1:A:186:GLU:OE1	1:A:255:ASP:HB3	2.15	0.46
1:B:152:SER:HB2	4:D:566:HOH:O	2.16	0.46
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.74	0.46
1:D:72:ILE:O	1:D:76:LYS:HG3	2.15	0.46
1:C:208:ARG:HD3	1:C:208:ARG:HH11	1.51	0.45
1:D:3:VAL:CB	4:D:595:HOH:O	2.64	0.45
1:C:186:GLU:OE1	1:C:255:ASP:HB3	2.17	0.45
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.50	0.45
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.52	0.45
1:A:6:THR:O	1:A:9:ASP:HB2	2.17	0.45
1:D:352:GLU:HG3	1:D:356:GLU:HB2	1.99	0.44
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ASP:HB3	1:C:11:PHE:CE2	2.53	0.43
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.53	0.43
1:C:86:VAL:O	1:C:131:ALA:HA	2.19	0.43
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.48	0.43
1:D:361:ARG:HB3	1:D:365:GLU:HB2	2.01	0.43
1:B:34:LEU:HD21	1:B:39:ALA:HB2	2.01	0.43
1:B:9:ASP:HB3	1:B:11:PHE:CE2	2.54	0.43
1:C:161:ALA:O	1:C:165:LEU:HG	2.19	0.43
1:C:41:HIS:HE1	4:C:521:HOH:O	2.00	0.43
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.32	0.43
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.95	0.43
1:B:7:ARG:HD3	4:B:497:HOH:O	2.18	0.43
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.84	0.42
1:A:186:GLU:HA	1:A:187:PRO:HA	1.74	0.42
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.92	0.42
1:C:394:ARG:HH11	1:C:394:ARG:HD3	1.48	0.42
1:B:214:ILE:HG13	1:B:216:PRO:HD3	2.01	0.42
1:B:354:TYR:HB3	1:D:164:LEU:HD21	2.01	0.42
1:D:20:TRP:CE2	1:D:22:ALA:HA	2.54	0.42
1:A:328:ASP:HA	1:A:329:PRO:HD2	1.79	0.42
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.42
1:D:317:LEU:HA	1:D:317:LEU:HD23	1.86	0.42
1:D:5:ALA:HB2	1:D:312:ILE:CG2	2.50	0.42
1:D:11:PHE:CE2	1:D:312:ILE:HG23	2.55	0.41
1:A:35:ASP:HA	1:A:36:PRO:HD3	1.87	0.41
1:D:34:LEU:HD21	1:D:39:ALA:HB2	2.01	0.41
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.20	0.41
1:B:232:ILE:HA	1:B:232:ILE:HD13	1.87	0.41
1:C:294:LYS:HA	1:C:295:PRO:HD3	1.92	0.41
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.90	0.41
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.56	0.41
1:B:37:VAL:HG13	1:B:78:ALA:HB2	2.03	0.41
1:C:36:PRO:O	1:C:40:VAL:HG23	2.21	0.41
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.56	0.41
1:A:30:THR:HG22	1:B:97:PRO:HB3	2.02	0.41
1:D:181:GLU:HA	1:D:182:PRO:HD3	1.90	0.41
1:B:121:ARG:HD3	4:B:442:HOH:O	2.20	0.41
1:B:5:ALA:HB2	1:B:312:ILE:HG21	2.02	0.41
1:B:203:VAL:HG22	1:B:212:PHE:HB3	2.03	0.41
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.92	0.40
1:D:9:ASP:HB3	1:D:11:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLY:HA2	1:A:85:ILE:O	2.21	0.40
1:B:206:LEU:O	1:B:209:PRO:HD3	2.20	0.40
1:B:35:ASP:HA	1:B:36:PRO:HD3	1.93	0.40
1:C:250:HIS:CE1	1:C:263:GLY:HA2	2.57	0.40
1:B:7:ARG:HG2	1:B:49:TYR:HB2	2.03	0.40
1:B:352:GLU:HG2	1:B:356:GLU:HB2	2.03	0.40
1:B:361:ARG:HA	1:B:365:GLU:OE1	2.20	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%)	377 (97%)	12 (3%)	1 (0%)	46	68
1	B	390/393 (99%)	375 (96%)	13 (3%)	2 (0%)	34	55
1	C	390/393 (99%)	373 (96%)	13 (3%)	4 (1%)	19	34
1	D	390/393 (99%)	377 (97%)	12 (3%)	1 (0%)	46	68
All	All	1560/1572 (99%)	1502 (96%)	50 (3%)	8 (0%)	34	55

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	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	306/310 (99%)	296 (97%)	10 (3%)	45	73
1	B	306/310 (99%)	301 (98%)	5 (2%)	70	90
1	C	306/310 (99%)	297 (97%)	9 (3%)	50	77
1	D	306/310 (99%)	299 (98%)	7 (2%)	58	83
All	All	1224/1240 (99%)	1193 (98%)	31 (2%)	55	82

All (31) 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	158	TYR
1	A	177	ARG
1	A	185	ASN
1	A	187	PRO
1	A	203	VAL
1	A	208	ARG
1	A	286	ASP
1	B	49	TYR
1	B	81	GLU
1	B	158	TYR
1	B	185	ASN
1	B	394	ARG
1	C	3	VAL
1	C	38	GLU
1	C	49	TYR
1	C	80	ASP
1	C	158	TYR
1	C	185	ASN
1	C	203	VAL
1	C	279	PRO
1	C	313	ARG

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Mol	Chain	Res	Type
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	158	TYR
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG

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

Mol	Chain	Res	Type
1	A	185	ASN
1	A	204	GLN
1	A	238	HIS
1	B	185	ASN
1	B	204	GLN
1	B	222	GLN
1	B	238	HIS
1	C	41	HIS
1	C	185	ASN
1	C	238	HIS
1	D	185	ASN
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 carbohydrates 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	XLS	A	397	3	9,9,9	1.71	1 (11%)	11,11,11	2.19	2 (18%)
2	XLS	B	397	3	9,9,9	1.85	1 (11%)	11,11,11	2.64	4 (36%)
2	XLS	C	397	3	9,9,9	1.76	1 (11%)	11,11,11	2.17	5 (45%)
2	XLS	D	397	3	9,9,9	1.90	1 (11%)	11,11,11	2.89	6 (54%)

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	A	397	3	-	0/10/12/12	0/0/0/0
2	XLS	B	397	3	-	0/10/12/12	0/0/0/0
2	XLS	C	397	3	-	0/10/12/12	0/0/0/0
2	XLS	D	397	3	-	0/10/12/12	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	397	XLS	O1-C1	4.89	1.42	1.19
2	C	397	XLS	O1-C1	5.11	1.43	1.19
2	D	397	XLS	O1-C1	5.30	1.44	1.19
2	B	397	XLS	O1-C1	5.38	1.44	1.19

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	397	XLS	O1-C1-C2	-6.51	106.63	125.60
2	B	397	XLS	O1-C1-C2	-6.18	107.60	125.60
2	A	397	XLS	O1-C1-C2	-6.12	107.77	125.60
2	C	397	XLS	O1-C1-C2	-4.27	113.14	125.60
2	D	397	XLS	O2-C2-C1	-3.43	102.03	110.22
2	C	397	XLS	O5-C5-C4	-2.52	105.61	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	XLS	O2-C2-C1	-2.50	104.24	110.22
2	C	397	XLS	C5-C4-C3	-2.05	107.67	112.48
2	D	397	XLS	C5-C4-C3	2.04	117.25	112.48
2	C	397	XLS	O3-C3-C2	2.15	112.73	108.93
2	A	397	XLS	O3-C3-C2	2.30	112.99	108.93
2	D	397	XLS	O2-C2-C3	2.62	115.46	109.45
2	D	397	XLS	O5-C5-C4	2.84	117.26	111.10
2	B	397	XLS	O4-C4-C3	2.92	116.34	109.02
2	D	397	XLS	O3-C3-C2	3.42	114.97	108.93
2	C	397	XLS	C3-C2-C1	3.63	117.04	111.68
2	B	397	XLS	C3-C2-C1	4.38	118.14	111.68

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 (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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.