



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 11:52 PM EST

PDB ID : 3XIM  
Title : ARGININE RESIDUES AS STABILIZING ELEMENTS IN PROTEINS  
Authors : Mrabet, N.T.; Van Denbroek, A.; Van Den Brande, I.; Stanssens, P.; Laroche, Y.; Lambeir, A.-M.; Matthyssens, G.; Jenkins, J.; Chiadmi, M.; Vantilbeurgh, H.; Rey, F.; Janin, J.; Quax, W.J.; Lasters, I.; Demaeyer, M.; Wodak, S.J.  
Deposited on : 1991-05-29  
Resolution : 2.30 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](mailto: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>.

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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)  
Xtrriage (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

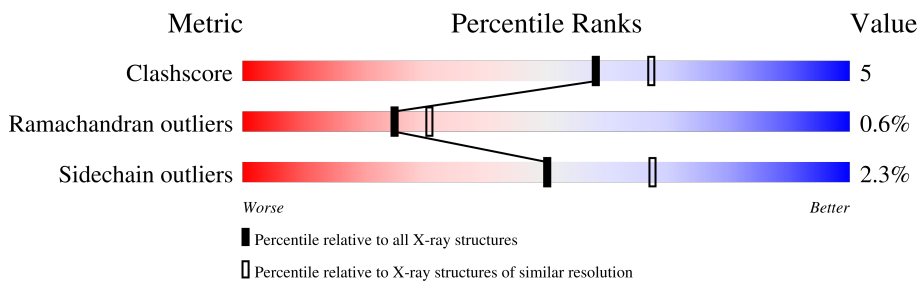
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (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  $\geq 3$ , 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	80% 16% ..
1	B	393	79% 19% .
1	C	393	80% 17% ..
1	D	393	79% 19% .

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13147 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.

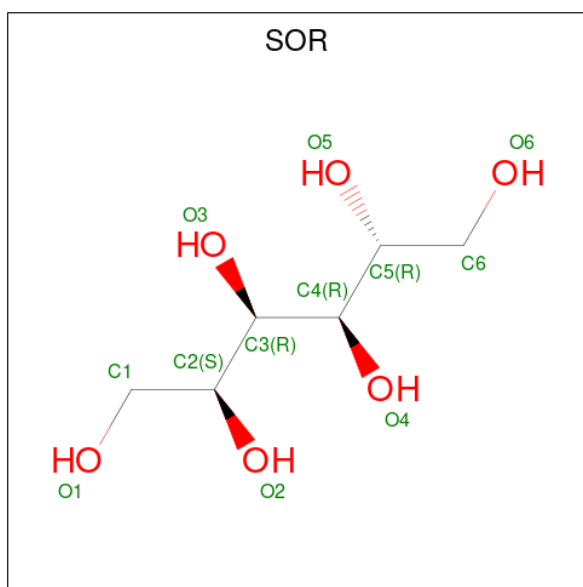
- Molecule 1 is a protein called D-XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	3052	1934	537	577	4	0	0	0
1	B	392	3059	1939	538	578	4	0	0	0
1	C	390	3047	1931	536	576	4	0	0	0
1	D	392	3062	1940	538	580	4	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	ARG	LYS	conflict	UNP P12851
A	319	ARG	LYS	conflict	UNP P12851
A	323	ARG	LYS	conflict	UNP P12851
B	309	ARG	LYS	conflict	UNP P12851
B	319	ARG	LYS	conflict	UNP P12851
B	323	ARG	LYS	conflict	UNP P12851
C	309	ARG	LYS	conflict	UNP P12851
C	319	ARG	LYS	conflict	UNP P12851
C	323	ARG	LYS	conflict	UNP P12851
D	309	ARG	LYS	conflict	UNP P12851
D	319	ARG	LYS	conflict	UNP P12851
D	323	ARG	LYS	conflict	UNP P12851

- Molecule 2 is sorbitol (three-letter code: SOR) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	206	Total 206	O 206	0	0
4	C	232	Total 232	O 232	0	0
4	D	211	Total 211	O 211	0	0

### 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.

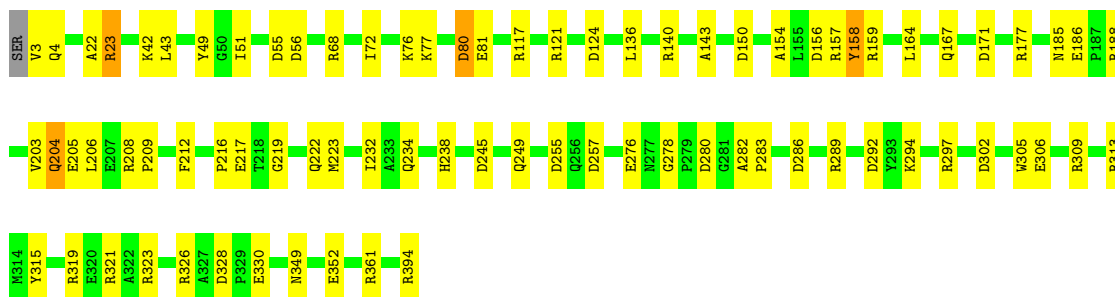
- Molecule 1: D-XYLOSE ISOMERASE

Chain A: 




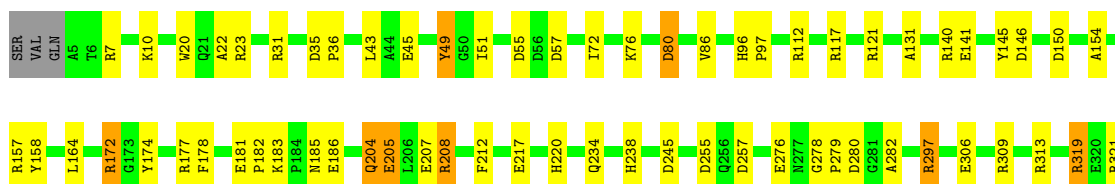
- Molecule 1: D-XYLOSE ISOMERASE

Chain B: 



- Molecule 1: D-XYLOSE ISOMERASE

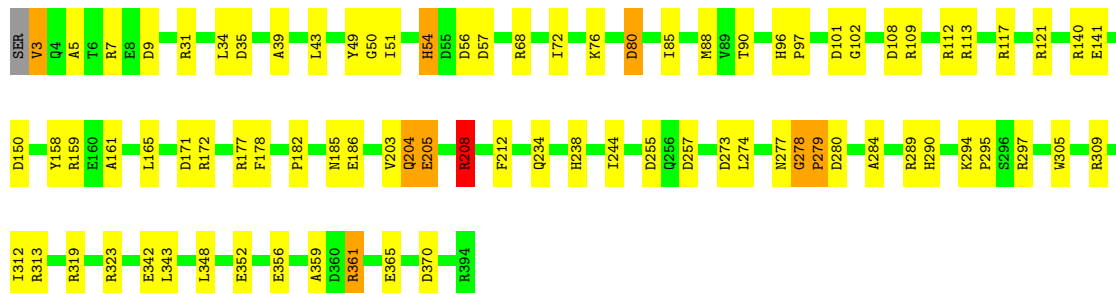
Chain C: 





- Molecule 1: D-XYLOSE ISOMERASE

Chain D: 79% 19%



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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, $R_{free}$	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	13147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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, SOR

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	0.82	0/3124	1.79	59/4232 (1.4%)
1	B	0.81	0/3131	1.75	56/4242 (1.3%)
1	C	0.81	0/3119	1.65	56/4225 (1.3%)
1	D	0.82	0/3134	1.77	52/4246 (1.2%)
All	All	0.81	0/12508	1.74	223/16945 (1.3%)

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

There are no bond length outliers.

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	ASP	CB-CG-OD1	40.60	154.84	118.30
1	A	255	ASP	CB-CG-OD1	34.34	149.21	118.30
1	B	255	ASP	CB-CG-OD1	26.19	141.87	118.30
1	D	255	ASP	CB-CG-OD2	-25.32	95.51	118.30
1	A	255	ASP	CB-CG-OD2	-20.97	99.42	118.30
1	B	117	ARG	NE-CZ-NH1	19.75	130.18	120.30
1	B	394	ARG	NE-CZ-NH2	-18.66	110.97	120.30
1	B	319	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	A	394	ARG	NE-CZ-NH2	-17.16	111.72	120.30
1	B	255	ASP	CB-CG-OD2	-16.34	103.59	118.30
1	B	177	ARG	NE-CZ-NH2	-15.91	112.34	120.30
1	A	255	ASP	CA-CB-CG	13.98	144.15	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ARG	NE-CZ-NH1	13.97	127.28	120.30
1	C	117	ARG	NE-CZ-NH1	13.90	127.25	120.30
1	C	361	ARG	NE-CZ-NH2	13.70	127.15	120.30
1	C	23	ARG	NE-CZ-NH2	-13.65	113.48	120.30
1	A	394	ARG	NH1-CZ-NH2	13.48	134.23	119.40
1	C	255	ASP	CB-CG-OD2	13.47	130.42	118.30
1	D	150	ASP	CB-CG-OD1	13.41	130.37	118.30
1	A	313	ARG	NE-CZ-NH1	13.31	126.96	120.30
1	C	31	ARG	NE-CZ-NH1	12.89	126.75	120.30
1	B	157	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	D	257	ASP	CB-CG-OD1	12.56	129.60	118.30
1	A	394	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	C	319	ARG	NE-CZ-NH2	-12.25	114.18	120.30
1	B	117	ARG	NE-CZ-NH2	-11.33	114.64	120.30
1	D	35	ASP	CB-CG-OD1	11.25	128.43	118.30
1	D	208	ARG	NE-CZ-NH1	11.23	125.92	120.30
1	A	121	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	C	321	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	C	23	ARG	NE-CZ-NH1	10.83	125.72	120.30
1	A	361	ARG	NE-CZ-NH1	10.71	125.65	120.30
1	C	257	ASP	CB-CG-OD1	10.53	127.77	118.30
1	A	321	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	D	313	ARG	NE-CZ-NH2	10.27	125.44	120.30
1	D	121	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	D	255	ASP	CA-CB-CG	9.97	135.33	113.40
1	D	117	ARG	NE-CZ-NH1	9.79	125.20	120.30
1	A	177	ARG	CA-CB-CG	9.66	134.65	113.40
1	A	124	ASP	CB-CG-OD1	9.52	126.87	118.30
1	B	330	GLU	OE1-CD-OE2	9.52	134.72	123.30
1	B	323	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	A	157	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	B	255	ASP	CA-CB-CG	9.34	133.96	113.40
1	C	80	ASP	CB-CG-OD1	-9.34	109.89	118.30
1	A	112	ARG	NE-CZ-NH2	-9.31	115.65	120.30
1	C	255	ASP	OD1-CG-OD2	-9.27	105.69	123.30
1	B	121	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	205	GLU	OE1-CD-OE2	-9.21	112.25	123.30
1	A	326	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	C	121	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	323	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	326	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	68	ARG	NE-CZ-NH2	8.97	124.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	313	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	B	361	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	C	177	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	D	257	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	A	109	ARG	NE-CZ-NH1	-8.48	116.06	120.30
1	C	7	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	B	257	ASP	CB-CG-OD1	8.44	125.90	118.30
1	A	326	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	B	309	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	A	150	ASP	CB-CG-OD1	8.33	125.80	118.30
1	B	289	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	C	31	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	A	117	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	D	172	ARG	CD-NE-CZ	8.14	135.00	123.60
1	D	150	ASP	CB-CG-OD2	-8.13	110.99	118.30
1	C	157	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	D	297	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	D	370	ASP	CB-CG-OD2	7.94	125.45	118.30
1	C	177	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	A	121	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	55	ASP	CB-CG-OD1	7.89	125.40	118.30
1	B	188	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	D	57	ASP	CB-CG-OD2	7.85	125.37	118.30
1	B	177	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	C	208	ARG	CD-NE-CZ	-7.78	112.71	123.60
1	D	31	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	D	172	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	C	174	TYR	CB-CG-CD2	-7.64	116.42	121.00
1	A	146	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	80	ASP	CB-CG-OD1	-7.61	111.45	118.30
1	C	321	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	109	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	101	ASP	CB-CG-OD2	7.58	125.12	118.30
1	A	159	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	A	306	GLU	OE1-CD-OE2	7.42	132.20	123.30
1	A	113	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	150	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	D	112	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	B	150	ASP	CB-CG-OD1	7.26	124.83	118.30
1	D	255	ASP	OD1-CG-OD2	-7.23	109.56	123.30
1	C	245	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	279	PRO	C-N-CA	7.12	139.49	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASP	CB-CG-OD1	7.10	124.69	118.30
1	A	80	ASP	CB-CG-OD1	-6.98	112.02	118.30
1	C	326	ARG	NE-CZ-NH2	6.97	123.79	120.30
1	D	319	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	D	172	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	121	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	D	204	GLN	OE1-CD-NE2	-6.76	106.34	121.90
1	C	150	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	56	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	23	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	205	GLU	CG-CD-OE2	6.73	131.75	118.30
1	D	342	GLU	OE1-CD-OE2	-6.71	115.24	123.30
1	D	342	GLU	CG-CD-OE2	6.71	131.73	118.30
1	C	207	GLU	CG-CD-OE2	-6.65	105.01	118.30
1	A	150	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	204	GLN	OE1-CD-NE2	-6.62	106.67	121.90
1	C	208	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	A	109	ARG	NH1-CZ-NH2	6.56	126.61	119.40
1	A	45	GLU	OE1-CD-OE2	6.55	131.16	123.30
1	A	177	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	D	113	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	361	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	313	ARG	NH1-CZ-NH2	-6.45	112.30	119.40
1	D	88	MET	CA-CB-CG	6.39	124.17	113.30
1	B	23	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	255	ASP	OD1-CG-OD2	-6.31	111.31	123.30
1	B	394	ARG	N-CA-CB	6.30	121.94	110.60
1	C	146	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	394	ARG	CD-NE-CZ	-6.28	114.81	123.60
1	B	302	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	328	ASP	CB-CG-OD2	6.22	123.89	118.30
1	C	255	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	205	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	C	117	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	217	GLU	CG-CD-OE1	-6.16	105.97	118.30
1	B	156	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	217	GLU	OE1-CD-OE2	6.12	130.64	123.30
1	A	217	GLU	CG-CD-OE2	6.08	130.47	118.30
1	C	205	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	C	297	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	C	245	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	C	309	ARG	NE-CZ-NH2	-6.06	117.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	GLU	CG-CD-OE2	-6.06	106.18	118.30
1	C	141	GLU	OE1-CD-OE2	-6.05	116.04	123.30
1	B	188	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	140	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	109	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	145	TYR	CB-CG-CD2	6.02	124.61	121.00
1	C	23	ARG	CD-NE-CZ	6.01	132.01	123.60
1	D	177	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	305	TRP	CA-CB-CG	-5.99	102.33	113.70
1	B	68	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	C	174	TYR	CB-CG-CD1	5.97	124.58	121.00
1	D	56	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	313	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	273	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	217	GLU	OE1-CD-OE2	5.88	130.35	123.30
1	B	159	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	323	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	394	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	286	ASP	CB-CG-OD1	5.76	123.48	118.30
1	C	207	GLU	CG-CD-OE1	5.76	129.81	118.30
1	D	205	GLU	CG-CD-OE2	5.74	129.77	118.30
1	B	204	GLN	OE1-CD-NE2	-5.73	108.72	121.90
1	B	394	ARG	NH1-CZ-NH2	5.73	125.71	119.40
1	A	394	ARG	CG-CD-NE	-5.72	99.78	111.80
1	D	7	ARG	CD-NE-CZ	-5.70	115.62	123.60
1	D	171	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	188	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	205	GLU	CG-CD-OE2	5.67	129.65	118.30
1	C	356	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	B	245	ASP	CB-CG-OD1	5.58	123.33	118.30
1	D	121	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	156	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	286	ASP	CA-CB-CG	-5.52	101.26	113.40
1	B	326	ARG	NH1-CZ-NH2	-5.49	113.36	119.40
1	D	108	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	171	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	68	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	B	158	TYR	CB-CG-CD2	5.44	124.26	121.00
1	A	24	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	112	ARG	CG-CD-NE	5.41	123.17	111.80
1	B	171	ASP	CB-CG-OD1	5.37	123.14	118.30
1	B	302	ASP	CB-CG-OD1	5.37	123.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ASN	CA-C-N	-5.37	105.47	116.20
1	C	330	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	B	121	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	9	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	57	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	55	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	7	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	217	GLU	CG-CD-OE1	-5.29	107.73	118.30
1	D	361	ARG	CA-CB-CG	5.28	125.01	113.40
1	D	9	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	D	80	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	C	45	GLU	CA-CB-CG	5.26	124.97	113.40
1	C	306	GLU	CG-CD-OE2	-5.25	107.80	118.30
1	A	24	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	68	ARG	CD-NE-CZ	5.24	130.93	123.60
1	A	80	ASP	CA-CB-CG	-5.23	101.89	113.40
1	A	42	LYS	CB-CG-CD	-5.19	98.10	111.60
1	C	313	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	D	109	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	187	PRO	N-CA-C	5.17	125.54	112.10
1	C	276	GLU	CG-CD-OE2	5.16	128.62	118.30
1	C	297	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	368	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	143	ALA	N-CA-CB	-5.13	102.92	110.10
1	C	204	GLN	OE1-CD-NE2	-5.12	110.12	121.90
1	B	124	ASP	CB-CG-OD1	5.11	122.89	118.30
1	C	140	ARG	CD-NE-CZ	5.10	130.75	123.60
1	D	68	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	314	MET	CG-SD-CE	5.08	108.33	100.20
1	B	323	ARG	CG-CD-NE	5.08	122.46	111.80
1	B	394	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	D	35	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	D	54	HIS	N-CA-CB	5.06	119.71	110.60
1	D	289	ARG	N-CA-C	-5.06	97.34	111.00
1	B	321	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	158	TYR	CB-CG-CD2	5.05	124.03	121.00
1	B	292	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	159	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	319	ARG	NH1-CZ-NH2	5.04	124.94	119.40
1	B	143	ALA	N-CA-CB	-5.03	103.06	110.10
1	A	156	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	117	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ARG	CD-NE-CZ	5.00	130.60	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	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	3052	0	2945	30	0
1	B	3059	0	2954	32	0
1	C	3047	0	2943	28	0
1	D	3062	0	2956	37	0
2	A	12	0	13	0	0
2	B	12	0	14	0	0
2	C	12	0	13	0	0
2	D	12	0	14	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	222	0	0	3	0
4	B	206	0	0	2	0
4	C	232	0	0	2	0
4	D	211	0	0	4	0
All	All	13147	0	11852	115	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 (115) 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:D:278:GLY:HA2	4:D:509:HOH:O	1.21	1.26
1:B:204:GLN:OE1	1:D:204:GLN:OE1	1.66	1.10
1:A:204:GLN:OE1	1:C:204:GLN:OE1	1.69	1.09
1:D:208:ARG:HG2	1:D:208:ARG:HH11	1.22	1.02
1:D:277:ASN:HD21	1:D:323:ARG:HE	1.12	0.97
1:D:279:PRO:HD3	1:D:284:ALA:HB2	1.55	0.89
1:D:234:GLN:HE21	1:D:238:HIS:HE1	1.20	0.89
1:D:278:GLY:HA3	1:D:284:ALA:HB2	1.55	0.89
1:A:234:GLN:HE21	1:A:238:HIS:HE1	1.25	0.82
1:C:234:GLN:HE21	1:C:238:HIS:HE1	1.28	0.82
1:C:278:GLY:HA3	1:C:282:ALA:O	1.81	0.81
1:B:234:GLN:HE21	1:B:238:HIS:HE1	1.30	0.77
1:C:278:GLY:CA	1:C:282:ALA:O	2.36	0.73
1:A:319:ARG:NH1	4:A:565:HOH:O	2.15	0.73
1:D:208:ARG:HG2	1:D:208:ARG:NH1	1.96	0.72
1:A:204:GLN:HG2	4:A:549:HOH:O	1.91	0.71
1:A:238:HIS:HD2	1:C:205:GLU:OE2	1.74	0.70
1:A:278:GLY:HA3	1:A:282:ALA:O	1.92	0.70
1:B:3:VAL:HG12	1:B:4:GLN:H	1.56	0.70
1:D:279:PRO:HD3	1:D:284:ALA:CB	2.23	0.68
1:B:278:GLY:CA	1:B:282:ALA:O	2.43	0.67
1:A:205:GLU:OE2	1:C:238:HIS:HD2	1.76	0.67
1:A:279:PRO:HG2	4:A:509:HOH:O	1.95	0.66
1:B:278:GLY:HA3	1:B:282:ALA:O	1.96	0.65
1:A:278:GLY:CA	1:A:282:ALA:O	2.46	0.63
1:A:22:ALA:HB1	1:A:297:ARG:HG3	1.81	0.62
1:B:164:LEU:HD12	1:D:348:LEU:HD11	1.83	0.60
1:B:72:ILE:O	1:B:76:LYS:HG3	2.02	0.60
1:A:65:ALA:O	1:A:69:ASP:HB2	2.02	0.59
1:B:306:GLU:HG2	1:C:381:LYS:HB2	1.82	0.59
1:C:22:ALA:HB1	1:C:297:ARG:HG3	1.86	0.58
1:D:277:ASN:ND2	1:D:323:ARG:HE	1.92	0.58
1:B:72:ILE:HG22	1:B:76:LYS:HE3	1.85	0.58
1:B:43:LEU:HD12	1:B:51:ILE:HD12	1.87	0.56
1:B:22:ALA:HB1	1:B:297:ARG:HG3	1.86	0.55
1:D:102:GLY:HA2	1:D:140:ARG:HB2	1.89	0.55
1:D:274:LEU:HD12	4:D:509:HOH:O	2.07	0.55
1:D:43:LEU:HD12	1:D:51:ILE:HD12	1.89	0.55
1:D:277:ASN:HD21	1:D:323:ARG:NE	1.95	0.54
1:C:278:GLY:HA2	4:C:510:HOH:O	2.08	0.54
1:B:205:GLU:OE2	1:D:238:HIS:HD2	1.91	0.54
1:D:234:GLN:HE21	1:D:238:HIS:CE1	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:NH1	1:A:210:GLU:OE2	2.41	0.53
1:D:72:ILE:O	1:D:76:LYS:HG3	2.08	0.53
1:D:279:PRO:HD3	1:D:284:ALA:CA	2.40	0.52
1:B:282:ALA:HB1	1:B:283:PRO:HD2	1.93	0.51
1:A:9:ASP:HB3	1:A:11:PHE:CE2	2.46	0.50
1:B:238:HIS:HD2	1:D:205:GLU:OE2	1.95	0.50
1:C:183:LYS:HG3	1:C:220:HIS:CG	2.47	0.50
1:C:86:VAL:O	1:C:131:ALA:HA	2.11	0.50
1:B:203:VAL:HG22	1:B:212:PHE:HB3	1.94	0.50
1:A:164:LEU:HD12	1:C:348:LEU:HD11	1.93	0.50
1:B:278:GLY:HA2	4:B:496:HOH:O	2.10	0.49
1:B:206:LEU:O	1:B:209:PRO:HD3	2.11	0.49
1:A:36:PRO:O	1:A:40:VAL:HG23	2.13	0.49
1:B:294:LYS:HE2	4:B:583:HOH:O	2.14	0.48
1:D:141:GLU:OE2	4:D:574:HOH:O	2.20	0.47
1:C:35:ASP:HA	1:C:36:PRO:HD3	1.72	0.47
1:A:186:GLU:HA	1:A:187:PRO:HA	1.71	0.46
1:B:77:LYS:O	1:B:80:ASP:HB2	2.16	0.46
1:A:54:HIS:CD2	1:A:90:THR:HG23	2.50	0.46
1:C:20:TRP:CZ2	1:C:22:ALA:HA	2.51	0.46
1:D:178:PHE:HB2	1:D:212:PHE:CD2	2.51	0.46
1:B:154:ALA:HB2	1:D:343:LEU:HD21	1.99	0.45
1:B:216:PRO:HG2	1:B:232:ILE:HD11	1.99	0.45
1:B:3:VAL:HG12	1:B:4:GLN:N	2.28	0.44
1:D:34:LEU:CD2	1:D:39:ALA:HB2	2.47	0.44
1:C:172:ARG:HE	1:C:172:ARG:HB3	1.33	0.44
1:D:3:VAL:HG23	4:D:594:HOH:O	2.17	0.44
1:D:244:ILE:O	1:D:290:HIS:HB3	2.17	0.44
1:C:164:LEU:C	1:C:164:LEU:HD23	2.38	0.44
1:A:282:ALA:HA	1:A:283:PRO:HD3	1.87	0.44
1:C:328:ASP:HA	1:C:329:PRO:HD3	1.81	0.44
1:B:276:GLU:OE2	1:B:315:TYR:OH	2.34	0.44
1:B:219:GLY:O	1:B:223:MET:HG3	2.18	0.43
1:C:10:LYS:HA	1:C:49:TYR:CD1	2.54	0.43
1:D:161:ALA:O	1:D:165:LEU:HG	2.19	0.43
1:C:20:TRP:CE2	1:C:22:ALA:HA	2.53	0.43
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.82	0.43
1:D:305:TRP:O	1:D:309:ARG:HG3	2.19	0.42
1:A:361:ARG:HA	1:A:365:GLU:OE1	2.19	0.42
1:D:96:HIS:HA	1:D:97:PRO:HD3	1.96	0.42
1:D:54:HIS:CD2	1:D:90:THR:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:HB3	1:A:303:GLY:HA3	2.01	0.42
1:D:50:GLY:HA2	1:D:85:ILE:O	2.19	0.42
1:C:43:LEU:HD12	1:C:51:ILE:HD12	2.01	0.42
1:C:96:HIS:HA	1:C:97:PRO:HD3	1.95	0.42
1:D:356:GLU:O	1:D:359:ALA:HB3	2.20	0.42
1:A:343:LEU:HD21	1:C:154:ALA:HB2	2.02	0.41
1:C:338:SER:HB3	1:C:379:PHE:CE1	2.56	0.41
1:A:164:LEU:C	1:A:164:LEU:HD23	2.41	0.41
1:A:178:PHE:HB2	1:A:212:PHE:CD2	2.55	0.41
1:B:164:LEU:C	1:B:164:LEU:HD23	2.40	0.41
1:C:319:ARG:NH2	4:C:583:HOH:O	2.53	0.41
1:A:94:PHE:HA	1:A:140:ARG:HG3	2.00	0.41
1:A:326:ARG:HA	1:A:326:ARG:HD3	1.93	0.41
1:D:352:GLU:HG3	1:D:356:GLU:HB2	2.01	0.41
1:A:23:ARG:HG2	1:B:23:ARG:NH1	2.36	0.41
1:B:167:GLN:OE1	1:B:208:ARG:NH2	2.52	0.41
1:A:276:GLU:HG3	1:A:319:ARG:HG3	2.01	0.41
1:C:181:GLU:HA	1:C:182:PRO:HD3	1.91	0.41
1:B:232:ILE:HD13	1:B:232:ILE:HA	1.89	0.41
1:B:280:ASP:C	1:B:282:ALA:H	2.24	0.41
1:A:106:SER:O	1:A:112:ARG:HD3	2.21	0.41
1:B:349:ASN:N	1:B:352:GLU:OE1	2.47	0.41
1:D:294:LYS:HA	1:D:295:PRO:HD3	1.87	0.41
1:C:72:ILE:O	1:C:76:LYS:HG3	2.21	0.41
1:D:5:ALA:HB2	1:D:312:ILE:HG21	2.01	0.40
1:D:34:LEU:HD21	1:D:39:ALA:HB2	2.02	0.40
1:A:86:VAL:O	1:A:131:ALA:HA	2.20	0.40
1:A:238:HIS:O	1:A:239:LYS:HB2	2.20	0.40
1:B:42:LYS:HD3	1:B:42:LYS:HA	1.78	0.40
1:D:361:ARG:HA	1:D:365:GLU:OE1	2.21	0.40
1:C:208:ARG:HH11	1:C:208:ARG:HD3	1.43	0.40
1:C:178:PHE:HB2	1:C:212:PHE:CD2	2.57	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%)	374 (96%)	14 (4%)	1 (0%)	41	50
1	B	390/393 (99%)	376 (96%)	13 (3%)	1 (0%)	41	50
1	C	388/393 (99%)	370 (95%)	14 (4%)	4 (1%)	15	17
1	D	390/393 (99%)	376 (96%)	11 (3%)	3 (1%)	19	23
All	All	1557/1572 (99%)	1496 (96%)	52 (3%)	9 (1%)	25	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	279	PRO
1	D	278	GLY
1	D	280	ASP
1	C	280	ASP
1	A	186	GLU
1	B	186	GLU
1	C	186	GLU
1	C	364	PHE
1	D	186	GLU

### 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%)	295 (97%)	10 (3%)	38	53
1	B	306/310 (99%)	301 (98%)	5 (2%)	62	78
1	C	305/310 (98%)	300 (98%)	5 (2%)	62	78
1	D	307/310 (99%)	299 (97%)	8 (3%)	46	63
All	All	1223/1240 (99%)	1195 (98%)	28 (2%)	50	67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	TYR
1	A	80	ASP
1	A	158	TYR
1	A	185	ASN
1	A	203	VAL
1	A	208	ARG
1	A	286	ASP
1	A	323	ARG
1	A	394	ARG
1	B	49	TYR
1	B	81	GLU
1	B	136	LEU
1	B	158	TYR
1	B	185	ASN
1	C	49	TYR
1	C	80	ASP
1	C	158	TYR
1	C	172	ARG
1	C	185	ASN
1	D	3	VAL
1	D	49	TYR
1	D	80	ASP
1	D	158	TYR
1	D	182	PRO
1	D	185	ASN
1	D	203	VAL
1	D	208	ARG

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

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

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Mol	Chain	Res	Type
1	D	277	ASN

### 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 monosaccharides 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	SOR	B	397	3	11,11,11	0.92	0	14,14,14	1.76	4 (28%)
2	SOR	A	397	3	11,11,11	0.88	0	14,14,14	1.53	3 (21%)
2	SOR	D	397	3	11,11,11	1.21	1 (9%)	14,14,14	2.19	7 (50%)
2	SOR	C	397	3	11,11,11	0.88	0	14,14,14	1.24	2 (14%)

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	SOR	B	397	3	-	3/16/16/16	-
2	SOR	A	397	3	-	1/16/16/16	-
2	SOR	D	397	3	-	4/16/16/16	-
2	SOR	C	397	3	-	3/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	397	SOR	C1-C2	2.39	1.58	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	397	SOR	O4-C4-C3	4.51	119.97	109.47
2	D	397	SOR	O6-C6-C5	-3.79	102.81	111.07
2	D	397	SOR	O2-C2-C3	3.39	117.34	109.10
2	D	397	SOR	C1-C2-C3	-3.28	105.30	112.41
2	A	397	SOR	O4-C4-C3	2.80	115.99	109.47
2	D	397	SOR	O2-C2-C1	-2.65	102.92	109.14
2	D	397	SOR	O5-C5-C4	2.58	115.36	109.10
2	A	397	SOR	O6-C6-C5	-2.43	105.77	111.07
2	B	397	SOR	C5-C4-C3	2.41	116.24	112.47
2	C	397	SOR	C6-C5-C4	-2.33	107.36	112.41
2	D	397	SOR	C6-C5-C4	-2.21	107.62	112.41
2	B	397	SOR	C6-C5-C4	-2.16	107.73	112.41
2	D	397	SOR	O1-C1-C2	-2.15	106.39	111.07
2	C	397	SOR	O4-C4-C3	2.11	114.39	109.47
2	A	397	SOR	C1-C2-C3	-2.05	107.98	112.41
2	B	397	SOR	O3-C3-C4	2.00	114.14	109.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	397	SOR	C4-C5-C6-O6
2	D	397	SOR	O5-C5-C6-O6
2	C	397	SOR	C4-C5-C6-O6
2	C	397	SOR	O5-C5-C6-O6
2	B	397	SOR	O5-C5-C6-O6
2	B	397	SOR	C4-C5-C6-O6
2	B	397	SOR	C2-C3-C4-C5

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
2	A	397	SOR	O5-C5-C6-O6
2	C	397	SOR	C2-C3-C4-C5
2	D	397	SOR	O1-C1-C2-O2
2	D	397	SOR	O2-C2-C3-C4

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

### 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.