



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2024 – 09:04 PM EST

PDB ID : 1DOT  
Title : CRYSTALLOGRAPHIC STRUCTURE OF DUCK OVOTRANSFERRIN AT  
2.3 ANGSTROMS RESOLUTION  
Authors : Rawas, A.; Muirhead, H.  
Deposited on : 1995-08-03  
Resolution : 2.35 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

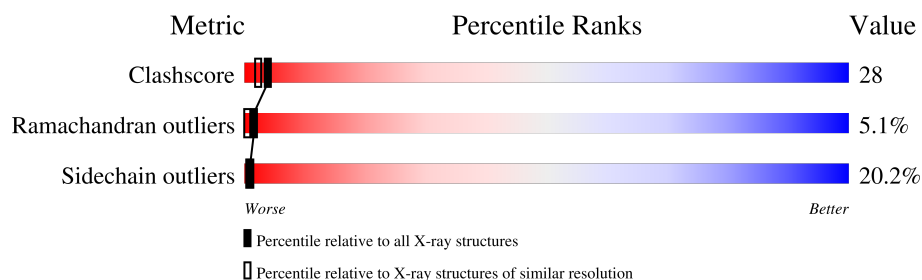
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)

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	686	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	691	-	-	X	-
2	NAG	A	692	-	-	X	-
5	CO3	A	689	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5665 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 DUCK OVOTRANSFERRIN.

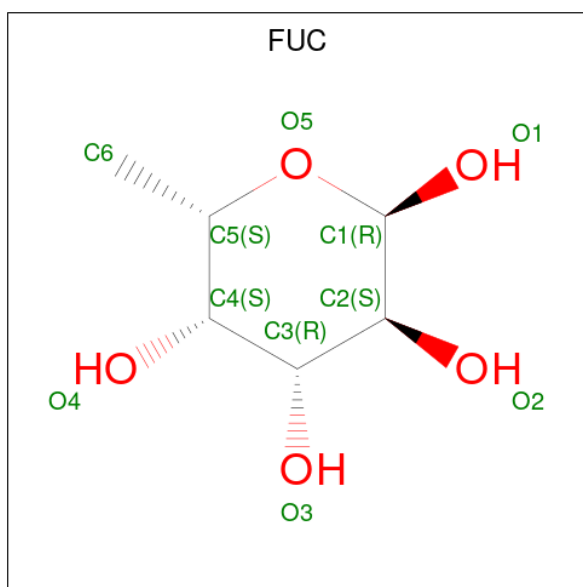
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	686	5299	3325	903	1032	39	0	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is alpha-L-fucopyranose (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).

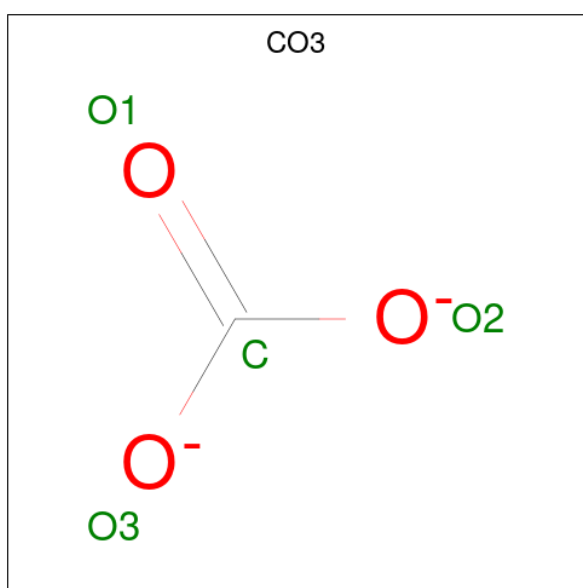


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is water.

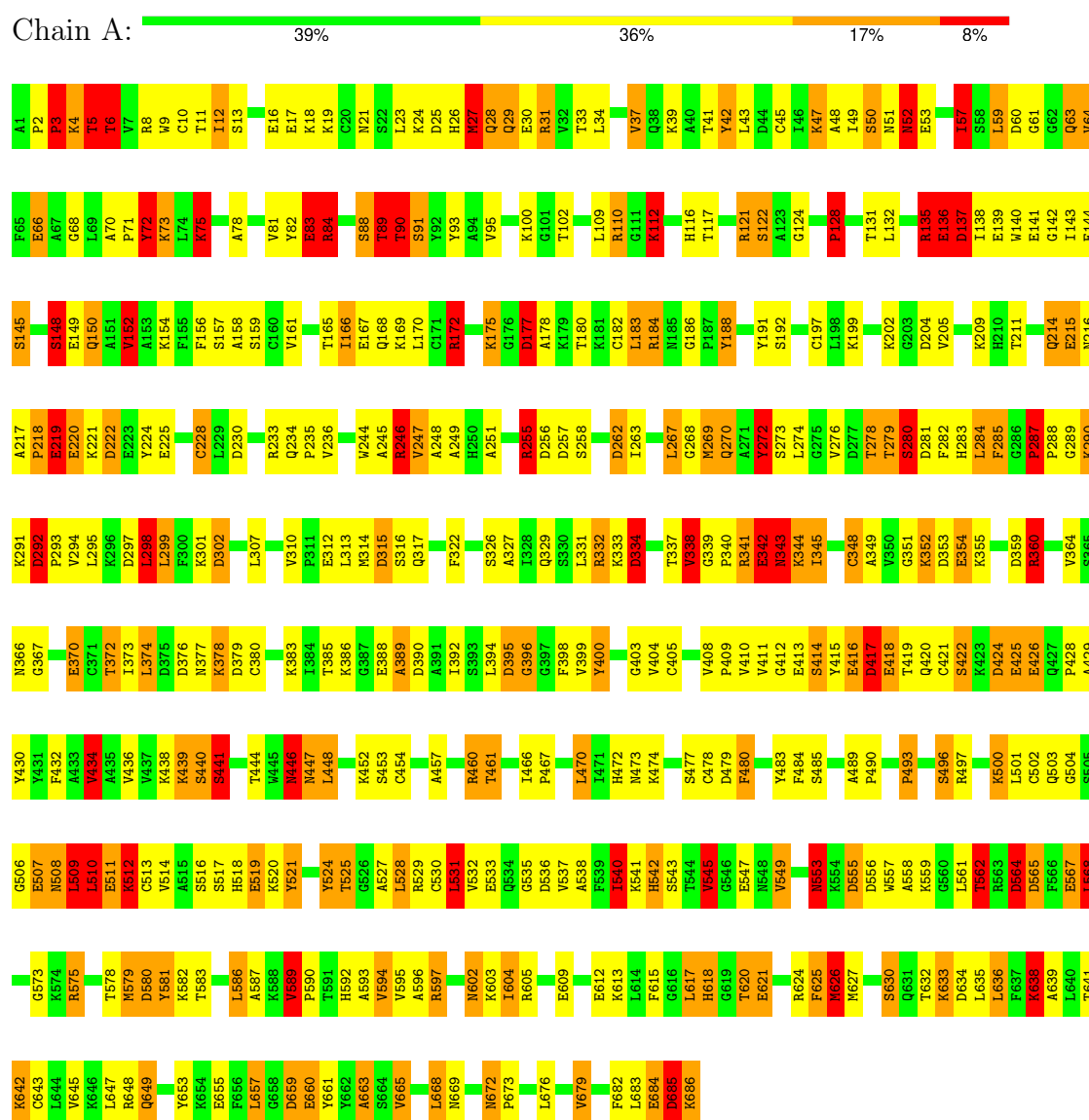
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	318	Total	O	0	0
			318	318		

### 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: DUCK OVOTRANSFERRIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.60Å 85.60Å 178.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.35)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.230 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5665	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	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: NAG, FE, FUC, CO3

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	1.29	23/5402 (0.4%)	2.36	300/7292 (4.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	ILE	N-CA	-12.24	1.21	1.46
1	A	136	GLU	N-CA	11.25	1.68	1.46
1	A	148	SER	CA-CB	8.58	1.65	1.52
1	A	405	CYS	CB-SG	-7.51	1.69	1.82
1	A	82	TYR	C-O	7.30	1.37	1.23
1	A	70	ALA	CA-C	-7.12	1.34	1.52
1	A	418	GLU	N-CA	-6.97	1.32	1.46
1	A	141	GLU	CG-CD	-6.62	1.42	1.51
1	A	354	GLU	CD-OE2	-5.99	1.19	1.25
1	A	337	THR	CA-CB	5.72	1.68	1.53
1	A	135	ARG	CD-NE	-5.65	1.36	1.46
1	A	135	ARG	NE-CZ	-5.65	1.25	1.33
1	A	4	LYS	N-CA	5.43	1.57	1.46
1	A	91	SER	CB-OG	-5.39	1.35	1.42
1	A	684	GLU	CD-OE1	-5.29	1.19	1.25
1	A	639	ALA	C-O	5.27	1.33	1.23
1	A	142	GLY	N-CA	-5.24	1.38	1.46
1	A	506	GLY	N-CA	5.21	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	418	GLU	CG-CD	-5.20	1.44	1.51
1	A	337	THR	C-O	5.19	1.33	1.23
1	A	71	PRO	CA-CB	-5.15	1.43	1.53
1	A	5	THR	CA-CB	5.15	1.66	1.53
1	A	417	ASP	C-N	-5.02	1.22	1.34

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ARG	CD-NE-CZ	26.09	160.12	123.60
1	A	417	ASP	C-N-CA	19.85	171.32	121.70
1	A	70	ALA	N-CA-CB	-18.71	83.90	110.10
1	A	597	ARG	CD-NE-CZ	18.64	149.70	123.60
1	A	31	ARG	NE-CZ-NH1	15.74	128.17	120.30
1	A	344	LYS	O-C-N	-15.20	98.39	122.70
1	A	385	THR	CA-CB-CG2	14.68	132.96	112.40
1	A	344	LYS	C-N-CA	14.52	157.99	121.70
1	A	360	ARG	CD-NE-CZ	13.78	142.89	123.60
1	A	344	LYS	CA-C-N	13.06	145.93	117.20
1	A	418	GLU	CB-CG-CD	12.91	149.07	114.20
1	A	597	ARG	NE-CZ-NH2	12.56	126.58	120.30
1	A	141	GLU	CB-CG-CD	12.50	147.94	114.20
1	A	148	SER	N-CA-C	11.57	142.25	111.00
1	A	172	ARG	NE-CZ-NH2	-11.54	114.53	120.30
1	A	517	SER	C-N-CA	11.51	150.47	121.70
1	A	144	GLU	C-N-CA	10.97	149.12	121.70
1	A	28	GLN	C-N-CA	10.90	148.95	121.70
1	A	390	ASP	CB-CG-OD1	-10.78	108.59	118.30
1	A	135	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	334	ASP	CA-CB-CG	10.68	136.88	113.40
1	A	511	GLU	CA-CB-CG	10.55	136.61	113.40
1	A	25	ASP	CA-CB-CG	10.47	136.43	113.40
1	A	639	ALA	CA-C-N	10.23	139.72	117.20
1	A	84	ARG	CA-CB-CG	10.22	135.87	113.40
1	A	136	GLU	N-CA-CB	-9.87	92.84	110.60
1	A	148	SER	N-CA-CB	-9.80	95.79	110.50
1	A	184	ARG	NE-CZ-NH2	-9.73	115.44	120.30
1	A	426	GLU	CA-CB-CG	9.72	134.78	113.40
1	A	344	LYS	CB-CA-C	9.71	129.82	110.40
1	A	112	LYS	CA-CB-CG	9.68	134.69	113.40
1	A	184	ARG	CD-NE-CZ	9.61	137.06	123.60
1	A	13	SER	N-CA-CB	9.53	124.80	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ASN	CB-CA-C	9.41	129.21	110.40
1	A	507	GLU	N-CA-CB	9.38	127.49	110.60
1	A	390	ASP	CB-CG-OD2	9.28	126.66	118.30
1	A	121	ARG	NE-CZ-NH2	9.22	124.91	120.30
1	A	184	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	222	ASP	CB-CG-OD2	9.15	126.54	118.30
1	A	255	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	31	ARG	CA-CB-CG	8.78	132.70	113.40
1	A	634	ASP	N-CA-CB	-8.67	94.99	110.60
1	A	17	GLU	CA-CB-CG	8.62	132.37	113.40
1	A	89	THR	N-CA-CB	8.61	126.66	110.30
1	A	204	ASP	CB-CG-OD1	-8.55	110.61	118.30
1	A	31	ARG	CD-NE-CZ	8.53	135.54	123.60
1	A	82	TYR	CA-C-N	8.47	135.84	117.20
1	A	302	ASP	CA-CB-CG	8.46	132.02	113.40
1	A	71	PRO	CA-N-CD	-8.40	99.74	111.50
1	A	660	GLU	CA-CB-CG	8.38	131.84	113.40
1	A	6	THR	N-CA-C	8.37	133.61	111.00
1	A	568	LEU	CA-CB-CG	8.36	134.52	115.30
1	A	416	GLU	C-N-CA	8.31	142.47	121.70
1	A	626	MET	CA-CB-CG	8.23	127.29	113.30
1	A	2	PRO	N-CA-C	8.13	133.25	112.10
1	A	299	LEU	C-N-CA	8.09	141.93	121.70
1	A	342	GLU	C-N-CA	8.06	141.84	121.70
1	A	425	GLU	CA-CB-CG	8.05	131.10	113.40
1	A	344	LYS	N-CA-C	-8.02	89.36	111.00
1	A	575	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	48	ALA	N-CA-CB	7.99	121.28	110.10
1	A	353	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	71	PRO	N-CA-CB	7.88	112.76	103.30
1	A	70	ALA	CB-CA-C	7.88	121.92	110.10
1	A	307	LEU	CA-CB-CG	7.81	133.25	115.30
1	A	258	SER	C-N-CA	7.78	141.15	121.70
1	A	593	ALA	CB-CA-C	7.76	121.74	110.10
1	A	315	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	64	VAL	CA-CB-CG1	7.68	122.42	110.90
1	A	110	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	A	25	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	215	GLU	CA-CB-CG	7.57	130.04	113.40
1	A	31	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	579	MET	C-N-CA	7.52	140.51	121.70
1	A	478	CYS	C-N-CA	7.50	140.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	O-C-N	-7.46	110.76	122.70
1	A	567	GLU	CA-CB-CG	7.44	129.78	113.40
1	A	657	LEU	CA-CB-CG	7.44	132.41	115.30
1	A	150	GLN	C-N-CA	7.42	140.25	121.70
1	A	27	MET	CG-SD-CE	-7.34	88.46	100.20
1	A	419	THR	CA-CB-CG2	7.31	122.64	112.40
1	A	639	ALA	CB-CA-C	7.28	121.02	110.10
1	A	4	LYS	C-N-CA	7.27	139.87	121.70
1	A	338	VAL	CA-CB-CG2	7.26	121.79	110.90
1	A	609	GLU	OE1-CD-OE2	7.23	131.98	123.30
1	A	332	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	83	GLU	C-N-CA	7.15	139.58	121.70
1	A	233	ARG	CD-NE-CZ	7.13	133.58	123.60
1	A	345	ILE	N-CA-C	-7.13	91.75	111.00
1	A	633	LYS	CA-C-O	-7.13	105.13	120.10
1	A	172	ARG	NH1-CZ-NH2	7.11	127.22	119.40
1	A	145	SER	N-CA-CB	7.09	121.14	110.50
1	A	90	THR	CA-CB-CG2	7.09	122.32	112.40
1	A	50	SER	CA-CB-OG	7.06	130.27	111.20
1	A	270	GLN	CA-CB-CG	7.06	128.92	113.40
1	A	337	THR	N-CA-C	7.06	130.05	111.00
1	A	424	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	A	509	LEU	CA-CB-CG	7.03	131.47	115.30
1	A	29	GLN	CB-CG-CD	7.02	129.84	111.60
1	A	549	VAL	CA-CB-CG1	7.01	121.41	110.90
1	A	512	LYS	CA-C-N	7.00	132.60	117.20
1	A	334	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	581	TYR	CA-CB-CG	-6.99	100.13	113.40
1	A	332	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	A	661	TYR	CB-CG-CD1	6.96	125.18	121.00
1	A	218	PRO	C-N-CA	6.93	139.02	121.70
1	A	685	ASP	CB-CG-OD1	-6.92	112.07	118.30
1	A	136	GLU	CA-CB-CG	6.91	128.60	113.40
1	A	489	ALA	N-CA-CB	6.86	119.70	110.10
1	A	287	PRO	N-CA-CB	-6.83	95.08	102.60
1	A	31	ARG	N-CA-CB	6.82	122.87	110.60
1	A	441	SER	CA-CB-OG	6.79	129.53	111.20
1	A	82	TYR	CA-C-O	-6.77	105.88	120.10
1	A	542	HIS	CA-CB-CG	6.73	125.03	113.60
1	A	360	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	8	ARG	CD-NE-CZ	6.72	133.01	123.60
1	A	418	GLU	OE1-CD-OE2	-6.69	115.27	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	396	GLY	C-N-CA	6.68	136.32	122.30
1	A	524	TYR	CB-CG-CD1	6.68	125.01	121.00
1	A	150	GLN	CB-CG-CD	6.67	128.95	111.60
1	A	341	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	425	GLU	CB-CG-CD	6.66	132.19	114.20
1	A	110	ARG	CA-CB-CG	6.64	128.02	113.40
1	A	135	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	589	VAL	CG1-CB-CG2	6.64	121.53	110.90
1	A	389	ALA	N-CA-CB	6.64	119.39	110.10
1	A	298	LEU	CA-CB-CG	6.63	130.56	115.30
1	A	642	LYS	CG-CD-CE	6.62	131.76	111.90
1	A	110	ARG	CD-NE-CZ	6.62	132.87	123.60
1	A	270	GLN	CB-CG-CD	6.59	128.75	111.60
1	A	425	GLU	CG-CD-OE1	6.55	131.41	118.30
1	A	580	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	617	LEU	C-N-CA	6.54	138.05	121.70
1	A	655	GLU	CA-CB-CG	6.54	127.78	113.40
1	A	506	GLY	N-CA-C	-6.52	96.81	113.10
1	A	418	GLU	CA-CB-CG	6.51	127.72	113.40
1	A	659	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	50	SER	N-CA-CB	6.44	120.16	110.50
1	A	353	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	72	TYR	CB-CG-CD1	-6.42	117.14	121.00
1	A	256	ASP	N-CA-CB	6.39	122.11	110.60
1	A	338	VAL	N-CA-CB	6.39	125.56	111.50
1	A	281	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	287	PRO	N-CA-C	6.37	128.65	112.10
1	A	639	ALA	O-C-N	-6.35	112.54	122.70
1	A	137	ASP	CB-CA-C	6.30	123.00	110.40
1	A	639	ALA	CA-C-O	-6.28	106.91	120.10
1	A	177	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	57	ILE	N-CA-CB	6.26	125.19	110.80
1	A	137	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	83	GLU	N-CA-C	6.25	127.89	111.00
1	A	613	LYS	C-N-CA	6.23	137.28	121.70
1	A	618	HIS	N-CA-CB	6.23	121.81	110.60
1	A	327	ALA	N-CA-CB	6.22	118.81	110.10
1	A	540	ILE	CA-CB-CG2	6.22	123.35	110.90
1	A	564	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	400	TYR	CB-CG-CD2	6.22	124.73	121.00
1	A	516	SER	N-CA-CB	6.21	119.81	110.50
1	A	385	THR	CA-CB-OG1	-6.19	95.99	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	LEU	CB-CA-C	6.16	121.91	110.20
1	A	618	HIS	CA-CB-CG	6.15	124.06	113.60
1	A	4	LYS	CA-C-O	6.13	132.97	120.10
1	A	60	ASP	CB-CG-OD2	6.13	123.81	118.30
1	A	82	TYR	N-CA-C	6.12	127.53	111.00
1	A	60	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	A	136	GLU	CG-CD-OE2	-6.12	106.06	118.30
1	A	272	TYR	CA-CB-CG	6.12	125.03	113.40
1	A	337	THR	CA-C-N	6.10	130.62	117.20
1	A	75	LYS	CD-CE-NZ	6.10	125.72	111.70
1	A	28	GLN	O-C-N	-6.08	112.96	122.70
1	A	150	GLN	CB-CA-C	6.07	122.53	110.40
1	A	479	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	51	ASN	O-C-N	-6.03	113.06	122.70
1	A	66	GLU	CG-CD-OE1	-6.01	106.28	118.30
1	A	394	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	641	THR	N-CA-CB	5.99	121.68	110.30
1	A	279	THR	CA-CB-CG2	5.98	120.77	112.40
1	A	144	GLU	CA-CB-CG	5.97	126.53	113.40
1	A	512	LYS	O-C-N	-5.94	113.20	122.70
1	A	25	ASP	N-CA-CB	5.94	121.28	110.60
1	A	136	GLU	CG-CD-OE1	5.93	130.16	118.30
1	A	6	THR	N-CA-CB	-5.92	99.06	110.30
1	A	634	ASP	N-CA-C	-5.92	95.02	111.00
1	A	417	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	337	THR	O-C-N	-5.89	113.27	122.70
1	A	683	LEU	CA-C-N	5.88	130.14	117.20
1	A	396	GLY	CA-C-N	5.88	127.95	116.20
1	A	139	GLU	CG-CD-OE1	5.87	130.04	118.30
1	A	21	ASN	CA-CB-CG	5.87	126.32	113.40
1	A	102	THR	CA-C-N	5.87	130.12	117.20
1	A	562	THR	CA-CB-CG2	5.87	120.62	112.40
1	A	148	SER	CA-C-N	5.87	130.10	117.20
1	A	57	ILE	CA-CB-CG2	5.84	122.58	110.90
1	A	538	ALA	N-CA-CB	5.83	118.27	110.10
1	A	632	THR	N-CA-CB	5.83	121.38	110.30
1	A	267	LEU	CB-CA-C	5.82	121.27	110.20
1	A	246	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	633	LYS	CB-CA-C	5.79	121.98	110.40
1	A	84	ARG	N-CA-CB	5.77	120.99	110.60
1	A	285	PHE	CA-CB-CG	5.76	127.73	113.90
1	A	668	LEU	CA-CB-CG	5.76	128.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	VAL	N-CA-CB	-5.75	98.84	111.50
1	A	110	ARG	CB-CG-CD	5.75	126.55	111.60
1	A	267	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	95	VAL	CA-CB-CG1	5.73	119.49	110.90
1	A	403	GLY	C-N-CA	5.72	136.00	121.70
1	A	524	TYR	CA-CB-CG	5.71	124.25	113.40
1	A	479	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	553	ASN	CA-CB-CG	5.70	125.94	113.40
1	A	509	LEU	C-N-CA	5.70	135.95	121.70
1	A	31	ARG	CB-CG-CD	5.69	126.40	111.60
1	A	388	GLU	C-N-CA	5.69	135.93	121.70
1	A	580	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	51	ASN	CA-C-N	5.67	129.68	117.20
1	A	370	GLU	CA-CB-CG	5.66	125.86	113.40
1	A	460	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	A	624	ARG	N-CA-CB	5.66	120.78	110.60
1	A	672	ASN	CB-CA-C	5.65	121.70	110.40
1	A	617	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	42	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	A	524	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	A	3	PRO	CA-C-O	5.60	133.65	120.20
1	A	660	GLU	N-CA-CB	5.60	120.68	110.60
1	A	429	ALA	CB-CA-C	5.60	118.50	110.10
1	A	483	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	222	ASP	C-N-CA	5.57	135.61	121.70
1	A	302	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	90	THR	CA-CB-OG1	-5.54	97.36	109.00
1	A	400	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	A	663	ALA	CB-CA-C	5.51	118.36	110.10
1	A	434	VAL	CG1-CB-CG2	5.51	119.71	110.90
1	A	341	ARG	CA-CB-CG	5.50	125.50	113.40
1	A	422	SER	C-N-CA	5.50	135.45	121.70
1	A	661	TYR	CB-CG-CD2	-5.49	117.70	121.00
1	A	507	GLU	CB-CG-CD	5.47	128.97	114.20
1	A	73	LYS	CA-CB-CG	5.47	125.43	113.40
1	A	292	ASP	CB-CA-C	5.47	121.34	110.40
1	A	510	LEU	CB-CA-C	5.43	120.53	110.20
1	A	152	VAL	CB-CA-C	5.43	121.72	111.40
1	A	68	GLY	C-N-CA	5.43	135.27	121.70
1	A	262	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	A	293	PRO	C-N-CA	5.41	135.23	121.70
1	A	359	ASP	CA-CB-CG	5.39	125.25	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	LYS	N-CA-C	5.38	125.54	111.00
1	A	121	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	150	GLN	CA-C-O	5.36	131.36	120.10
1	A	66	GLU	OE1-CD-OE2	5.36	129.73	123.30
1	A	625	PHE	CB-CA-C	5.34	121.08	110.40
1	A	219	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	519	GLU	C-N-CA	5.33	135.02	121.70
1	A	270	GLN	N-CA-CB	5.32	120.18	110.60
1	A	136	GLU	N-CA-C	-5.32	96.64	111.00
1	A	568	LEU	CB-CG-CD1	5.32	120.04	111.00
1	A	297	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	348	CYS	CA-CB-SG	-5.31	104.44	114.00
1	A	531	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	404	VAL	C-N-CA	5.30	134.95	121.70
1	A	446	ASN	C-N-CA	5.29	134.92	121.70
1	A	638	LYS	CB-CG-CD	5.28	125.32	111.60
1	A	679	VAL	C-N-CA	5.26	134.85	121.70
1	A	413	GLU	CA-CB-CG	5.25	124.96	113.40
1	A	220	GLU	CB-CG-CD	5.25	128.38	114.20
1	A	141	GLU	CB-CA-C	5.25	120.90	110.40
1	A	434	VAL	N-CA-CB	-5.25	99.96	111.50
1	A	272	TYR	CB-CA-C	5.24	120.88	110.40
1	A	256	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	665	VAL	CB-CA-C	5.23	121.34	111.40
1	A	327	ALA	CB-CA-C	-5.22	102.28	110.10
1	A	37	VAL	CA-CB-CG2	5.21	118.71	110.90
1	A	594	VAL	CA-CB-CG2	5.21	118.71	110.90
1	A	71	PRO	CB-CA-C	-5.17	99.06	112.00
1	A	649	GLN	CA-CB-CG	5.17	124.77	113.40
1	A	132	LEU	CB-CA-C	5.16	120.01	110.20
1	A	582	LYS	C-N-CA	5.16	134.59	121.70
1	A	128	PRO	CA-C-N	5.15	128.53	117.20
1	A	352	LYS	CG-CD-CE	5.14	127.31	111.90
1	A	508	ASN	CA-CB-CG	5.14	124.70	113.40
1	A	683	LEU	CA-C-O	-5.13	109.32	120.10
1	A	84	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	565	ASP	CB-CG-OD1	5.13	122.91	118.30
1	A	83	GLU	O-C-N	-5.12	114.50	122.70
1	A	414	SER	N-CA-CB	5.12	118.17	110.50
1	A	248	ALA	CB-CA-C	5.08	117.72	110.10
1	A	280	SER	N-CA-C	5.08	124.71	111.00
1	A	352	LYS	CD-CE-NZ	5.07	123.36	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	GLU	CG-CD-OE2	-5.06	108.18	118.30
1	A	64	VAL	N-CA-CB	5.05	122.61	111.50
1	A	48	ALA	O-C-N	5.04	130.77	122.70
1	A	348	CYS	C-N-CA	5.04	134.29	121.70
1	A	10	CYS	CA-CB-SG	5.03	123.06	114.00
1	A	597	ARG	CA-CB-CG	5.03	124.47	113.40
1	A	474	LYS	C-N-CA	5.03	134.28	121.70
1	A	388	GLU	CA-CB-CG	5.03	124.46	113.40
1	A	141	GLU	OE1-CD-OE2	-5.02	117.27	123.30
1	A	507	GLU	CA-CB-CG	5.02	124.44	113.40
1	A	122	SER	N-CA-CB	5.02	118.03	110.50
1	A	553	ASN	N-CA-CB	5.01	119.62	110.60
1	A	370	GLU	N-CA-CB	5.01	119.62	110.60
1	A	417	ASP	CA-CB-CG	5.01	124.42	113.40
1	A	385	THR	N-CA-CB	5.00	119.81	110.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	SER	Mainchain
1	A	152	VAL	Mainchain
1	A	188	TYR	Mainchain
1	A	27	MET	Mainchain
1	A	3	PRO	Peptide
1	A	338	VAL	Mainchain
1	A	5	THR	Peptide
1	A	521	TYR	Mainchain
1	A	528	LEU	Mainchain
1	A	545	VAL	Mainchain

## 5.2 Too-close contacts ⓘ

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	5299	0	5179	286	0
2	A	28	0	25	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	9	3	0
4	A	2	0	0	0	0
5	A	8	0	0	2	0
6	A	318	0	0	27	0
All	All	5665	0	5213	292	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 28.

All (292) 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:322:PHE:CB	1:A:597:ARG:HH22	1.23	1.51
1:A:136:GLU:N	1:A:136:GLU:CA	1.68	1.50
1:A:322:PHE:CB	1:A:597:ARG:NH2	1.85	1.40
2:A:692:NAG:C4	3:A:693:FUC:O3	1.72	1.21
1:A:192:SER:HB2	6:A:966:HOH:O	1.41	1.20
1:A:322:PHE:CG	1:A:597:ARG:NH2	2.13	1.16
1:A:649:GLN:HB2	6:A:863:HOH:O	1.53	1.07
1:A:510:LEU:HD11	6:A:758:HOH:O	1.56	1.04
1:A:177:ASP:OD2	6:A:782:HOH:O	1.76	1.04
1:A:473:ASN:ND2	2:A:691:NAG:O4	1.90	1.03
2:A:692:NAG:H4	3:A:693:FUC:O3	1.57	1.02
1:A:322:PHE:HB3	1:A:597:ARG:HH22	0.84	1.00
1:A:322:PHE:HB2	1:A:597:ARG:NH2	1.76	1.00
1:A:140:TRP:HE1	1:A:148:SER:HB2	1.27	0.99
1:A:344:LYS:HE2	1:A:367:GLY:O	1.62	0.98
1:A:663:ALA:HB1	2:A:692:NAG:H2	1.46	0.96
1:A:473:ASN:HD21	2:A:691:NAG:H3	1.27	0.96
1:A:246:ARG:NH1	1:A:685:ASP:O	1.98	0.96
1:A:287:PRO:HB3	1:A:302:ASP:HB3	1.50	0.93
1:A:374:LEU:HD22	1:A:379:ASP:HB3	1.49	0.93
1:A:136:GLU:N	1:A:136:GLU:CB	2.33	0.90
1:A:322:PHE:HB3	1:A:597:ARG:NH2	1.63	0.89
1:A:202:LYS:HE3	6:A:774:HOH:O	1.71	0.89
1:A:621:GLU:OE2	6:A:730:HOH:O	1.91	0.89
1:A:473:ASN:ND2	2:A:691:NAG:H3	1.88	0.88
1:A:473:ASN:HD21	2:A:691:NAG:C3	1.86	0.87
1:A:136:GLU:H	1:A:137:ASP:H	1.24	0.85
1:A:378:LYS:HE2	1:A:676:LEU:HD23	1.59	0.85
2:A:692:NAG:O4	3:A:693:FUC:O3	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD11	1:A:383:LYS:HG3	1.60	0.84
1:A:135:ARG:C	1:A:136:GLU:CA	2.46	0.84
1:A:473:ASN:HD21	2:A:691:NAG:C4	1.92	0.83
1:A:9:TRP:HB2	1:A:34:LEU:HD11	1.63	0.80
1:A:177:ASP:CG	6:A:782:HOH:O	2.16	0.79
1:A:434:VAL:HG21	1:A:581:TYR:HE1	1.49	0.78
1:A:355:LYS:HB2	1:A:373:ILE:HD13	1.66	0.77
1:A:322:PHE:HB2	1:A:597:ARG:HH22	1.32	0.77
1:A:434:VAL:HG21	1:A:581:TYR:CE1	2.20	0.77
1:A:420:GLN:HB3	1:A:425:GLU:HA	1.65	0.77
1:A:216:ASN:HD22	1:A:290:LYS:HG3	1.49	0.76
1:A:136:GLU:N	1:A:137:ASP:H	1.82	0.76
1:A:136:GLU:N	1:A:136:GLU:HB3	2.01	0.76
1:A:221:LYS:HD3	6:A:879:HOH:O	1.87	0.75
1:A:136:GLU:N	1:A:137:ASP:N	2.35	0.74
1:A:510:LEU:CD1	6:A:758:HOH:O	2.24	0.73
1:A:136:GLU:N	1:A:136:GLU:C	2.41	0.73
1:A:417:ASP:HA	1:A:642:LYS:HB3	1.71	0.73
1:A:165:THR:H	1:A:166:ILE:HD13	1.52	0.73
1:A:50:SER:HB3	1:A:72:TYR:HB3	1.70	0.72
1:A:344:LYS:HB3	1:A:370:GLU:OE2	1.89	0.72
1:A:27:MET:HA	1:A:29:GLN:HG2	1.71	0.72
1:A:633:LYS:HA	1:A:633:LYS:HE2	1.71	0.71
1:A:527:ALA:HB3	1:A:540:ILE:HD11	1.73	0.71
1:A:83:GLU:HG2	1:A:84:ARG:H	1.56	0.71
1:A:470:LEU:HD13	2:A:691:NAG:H81	1.72	0.70
1:A:89:THR:HG22	1:A:685:ASP:OD1	1.91	0.70
1:A:374:LEU:HD13	1:A:380:CYS:HA	1.73	0.70
1:A:274:LEU:HA	1:A:278:THR:HG23	1.73	0.70
1:A:329:GLN:HE22	1:A:333:LYS:NZ	1.89	0.70
1:A:221:LYS:HE3	6:A:937:HOH:O	1.91	0.70
1:A:422:SER:H	1:A:425:GLU:H	1.40	0.69
1:A:282:PHE:HE2	1:A:284:LEU:HD22	1.56	0.69
1:A:310:VAL:HG22	1:A:682:PHE:CZ	2.28	0.69
1:A:341:ARG:HD3	1:A:603:LYS:HE2	1.75	0.69
1:A:620:THR:HG23	6:A:730:HOH:O	1.92	0.69
1:A:341:ARG:HD2	1:A:343:ASN:HD22	1.58	0.68
1:A:214:GLN:HE22	1:A:221:LYS:NZ	1.93	0.66
1:A:425:GLU:HB2	1:A:645:VAL:HG13	1.77	0.66
2:A:691:NAG:O3	6:A:772:HOH:O	1.95	0.66
1:A:288:PRO:HD2	1:A:291:LYS:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:HG11	1:A:604:ILE:HG22	1.77	0.65
1:A:620:THR:HG22	1:A:621:GLU:HG2	1.78	0.65
1:A:378:LYS:HE3	1:A:398:PHE:HE1	1.61	0.65
1:A:448:LEU:HG	1:A:484:PHE:HE1	1.62	0.65
1:A:326:SER:HB3	6:A:959:HOH:O	1.95	0.65
1:A:136:GLU:H	1:A:137:ASP:N	1.93	0.64
1:A:620:THR:CG2	6:A:730:HOH:O	2.46	0.64
1:A:417:ASP:CA	1:A:642:LYS:HB3	2.28	0.64
1:A:341:ARG:HD2	1:A:343:ASN:ND2	2.14	0.63
1:A:470:LEU:CD1	2:A:691:NAG:C8	2.77	0.62
1:A:344:LYS:CB	1:A:370:GLU:OE2	2.47	0.62
1:A:617:LEU:HD12	1:A:626:MET:HE1	1.82	0.61
1:A:4:LYS:O	1:A:4:LYS:HG2	1.99	0.61
1:A:322:PHE:CB	1:A:597:ARG:HH21	2.07	0.61
1:A:345:ILE:HD12	1:A:604:ILE:HG13	1.81	0.61
1:A:313:LEU:HB3	1:A:679:VAL:CG1	2.31	0.61
1:A:472:HIS:HB2	1:A:480:PHE:HE1	1.66	0.60
1:A:344:LYS:HG2	1:A:367:GLY:O	2.01	0.60
1:A:372:THR:HG21	1:A:389:ALA:HB2	1.83	0.60
1:A:528:LEU:HD23	1:A:557:TRP:HH2	1.65	0.60
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.01	0.59
1:A:349:ALA:O	1:A:373:ILE:HD12	2.02	0.59
1:A:420:GLN:CB	1:A:425:GLU:HA	2.33	0.59
1:A:75:LYS:HE3	1:A:314:MET:O	2.01	0.59
1:A:374:LEU:HD11	1:A:383:LYS:CG	2.32	0.59
1:A:663:ALA:CB	2:A:692:NAG:H2	2.26	0.59
1:A:313:LEU:HB3	1:A:679:VAL:HG11	1.85	0.59
1:A:339:GLY:N	1:A:340:PRO:HD3	2.18	0.58
1:A:217:ALA:HB1	1:A:220:GLU:HG2	1.86	0.58
1:A:150:GLN:HE21	1:A:166:ILE:HG13	1.66	0.58
1:A:470:LEU:HD13	2:A:691:NAG:C8	2.34	0.58
1:A:344:LYS:CE	1:A:367:GLY:O	2.44	0.58
1:A:452:LYS:HG2	1:A:501:LEU:HD11	1.86	0.58
1:A:376:ASP:HB2	1:A:379:ASP:HB2	1.84	0.57
1:A:432:PHE:H	1:A:542:HIS:HD2	1.49	0.57
1:A:417:ASP:HB3	1:A:642:LYS:HD2	1.85	0.57
1:A:615:PHE:HB2	1:A:627:MET:HG3	1.85	0.57
1:A:216:ASN:ND2	1:A:290:LYS:HG3	2.20	0.57
1:A:602:ASN:ND2	1:A:605:ARG:HE	2.04	0.56
1:A:140:TRP:NE1	1:A:148:SER:HB2	2.09	0.56
1:A:152:VAL:HG23	1:A:156:PHE:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:VAL:HG23	1:A:594:VAL:HG13	1.87	0.56
1:A:502:CYS:HB3	1:A:519:GLU:OE1	2.06	0.56
1:A:470:LEU:CD1	2:A:691:NAG:H81	2.35	0.56
1:A:3:PRO:HB2	1:A:5:THR:HG23	1.88	0.56
1:A:49:ILE:O	1:A:255:ARG:HD3	2.06	0.56
1:A:396:GLY:O	1:A:399:VAL:HB	2.06	0.56
1:A:42:TYR:HB2	1:A:59:LEU:HD11	1.88	0.55
1:A:211:THR:O	1:A:215:GLU:HG3	2.06	0.55
1:A:45:CYS:HB3	1:A:57:ILE:HD13	1.87	0.55
1:A:50:SER:CB	1:A:72:TYR:HB3	2.34	0.55
1:A:109:LEU:O	1:A:112:LYS:HB2	2.07	0.55
1:A:23:LEU:HD22	1:A:284:LEU:HD21	1.88	0.55
1:A:568:LEU:HD13	1:A:578:THR:HA	1.89	0.55
1:A:553:ASN:HD21	1:A:555:ASP:HB2	1.72	0.54
1:A:152:VAL:HG23	1:A:156:PHE:HD2	1.73	0.54
1:A:348:CYS:SG	1:A:374:LEU:HD12	2.48	0.54
1:A:351:GLY:O	1:A:373:ILE:HD11	2.07	0.54
1:A:436:VAL:HG12	1:A:531:LEU:HD11	1.89	0.54
1:A:23:LEU:HB2	1:A:282:PHE:CZ	2.44	0.53
1:A:617:LEU:HD11	1:A:642:LYS:NZ	2.24	0.53
1:A:191:TYR:OH	5:A:689:CO3:O2	2.27	0.53
1:A:109:LEU:HA	1:A:112:LYS:HD2	1.89	0.53
1:A:263:ILE:O	1:A:267:LEU:HB2	2.09	0.53
1:A:360:ARG:HH11	1:A:625:PHE:HB2	1.74	0.53
1:A:400:TYR:HB2	1:A:657:LEU:HD11	1.91	0.52
1:A:121:ARG:NE	5:A:689:CO3:O1	2.37	0.52
1:A:457:ALA:HB3	1:A:460:ARG:HD3	1.91	0.52
1:A:421:CYS:H	1:A:425:GLU:N	2.08	0.52
1:A:165:THR:N	1:A:166:ILE:HD13	2.21	0.52
1:A:511:GLU:HB3	1:A:514:VAL:HG23	1.92	0.52
1:A:180:THR:HA	1:A:183:LEU:HG	1.91	0.51
1:A:282:PHE:CE2	1:A:284:LEU:HD22	2.42	0.51
1:A:553:ASN:ND2	1:A:555:ASP:HB2	2.26	0.51
1:A:23:LEU:HD13	1:A:282:PHE:CE2	2.45	0.51
1:A:61:GLY:HA3	6:A:948:HOH:O	2.10	0.51
1:A:378:LYS:HG2	6:A:805:HOH:O	2.11	0.50
1:A:395:ASP:OD2	1:A:460:ARG:HA	2.11	0.50
1:A:128:PRO:HA	1:A:244:TRP:CZ3	2.47	0.50
1:A:408:VAL:O	1:A:595:VAL:HA	2.11	0.50
1:A:273:SER:O	1:A:278:THR:HG23	2.12	0.50
1:A:497:ARG:HA	1:A:500:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:TYR:CE1	1:A:541:LYS:HG2	2.47	0.50
1:A:131:THR:O	1:A:135:ARG:HG3	2.12	0.50
1:A:676:LEU:HA	1:A:679:VAL:HG22	1.93	0.49
1:A:3:PRO:HG3	1:A:262:ASP:OD1	2.13	0.49
1:A:292:ASP:O	1:A:295:LEU:HB2	2.12	0.49
1:A:408:VAL:HG12	1:A:596:ALA:O	2.11	0.49
1:A:527:ALA:HB3	1:A:540:ILE:CD1	2.41	0.49
1:A:660:GLU:HB3	6:A:746:HOH:O	2.12	0.49
1:A:27:MET:HA	1:A:29:GLN:CG	2.40	0.49
1:A:649:GLN:CB	6:A:863:HOH:O	2.33	0.49
1:A:263:ILE:HG22	1:A:267:LEU:HD22	1.95	0.49
1:A:543:SER:O	1:A:547:GLU:HB2	2.12	0.49
1:A:158:ALA:HB1	1:A:172:ARG:HB3	1.95	0.49
1:A:199:LYS:HG3	1:A:224:TYR:OH	2.13	0.49
1:A:414:SER:HB2	1:A:645:VAL:HG23	1.93	0.49
1:A:89:THR:CG2	1:A:685:ASP:OD1	2.60	0.49
1:A:412:GLY:HA3	1:A:428:PRO:HG3	1.94	0.49
1:A:11:THR:HG22	1:A:16:GLU:HG2	1.95	0.49
1:A:461:THR:HG21	1:A:589:VAL:CG1	2.43	0.48
1:A:497:ARG:HA	1:A:500:LYS:CE	2.43	0.48
1:A:49:ILE:CD1	1:A:57:ILE:HG12	2.43	0.48
1:A:322:PHE:CD2	1:A:597:ARG:NH2	2.77	0.48
1:A:497:ARG:O	1:A:500:LYS:HB2	2.13	0.48
1:A:420:GLN:CA	1:A:425:GLU:HA	2.44	0.48
1:A:440:SER:O	1:A:575:ARG:NH2	2.45	0.48
1:A:209:LYS:NZ	1:A:301:LYS:NZ	2.62	0.48
1:A:521:TYR:HE1	1:A:529:ARG:HG2	1.78	0.48
1:A:19:LYS:NZ	6:A:946:HOH:O	2.46	0.48
1:A:470:LEU:CD1	2:A:691:NAG:H83	2.44	0.48
1:A:567:GLU:HG3	1:A:575:ARG:NH1	2.29	0.48
1:A:91:SER:HB2	1:A:247:VAL:O	2.13	0.47
1:A:100:LYS:HE2	1:A:225:GLU:HG3	1.96	0.47
1:A:283:HIS:HE1	6:A:886:HOH:O	1.96	0.47
1:A:167:GLU:HB2	1:A:170:LEU:HD12	1.95	0.47
1:A:415:TYR:CE1	1:A:638:LYS:HG2	2.49	0.47
1:A:52:ASN:HA	1:A:255:ARG:NH1	2.29	0.47
1:A:411:VAL:CG2	1:A:594:VAL:HG13	2.45	0.47
1:A:317:GLN:HG2	6:A:961:HOH:O	2.14	0.47
1:A:466:ILE:HB	1:A:467:PRO:HD3	1.96	0.47
1:A:503:GLN:O	1:A:507:GLU:HA	2.14	0.47
1:A:175:LYS:HD3	6:A:833:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:CZ	1:A:685:ASP:O	2.61	0.47
1:A:409:PRO:HB2	1:A:647:LEU:CD1	2.44	0.47
1:A:395:ASP:OD2	1:A:460:ARG:HG2	2.14	0.47
1:A:12:ILE:HA	1:A:39:LYS:O	2.15	0.47
1:A:457:ALA:HA	1:A:490:PRO:HD2	1.97	0.47
1:A:116:HIS:CD2	1:A:161:VAL:HG22	2.50	0.46
1:A:93:TYR:HA	1:A:245:ALA:O	2.16	0.46
1:A:525:THR:HG21	1:A:633:LYS:HG3	1.97	0.46
1:A:557:TRP:CE2	1:A:558:ALA:HB2	2.49	0.46
1:A:461:THR:CG2	1:A:589:VAL:HG21	2.44	0.46
1:A:214:GLN:HE22	1:A:221:LYS:CE	2.29	0.46
1:A:420:GLN:HB3	1:A:426:GLU:H	1.81	0.46
1:A:216:ASN:O	1:A:290:LYS:HE3	2.15	0.46
1:A:6:THR:HA	1:A:33:THR:O	2.15	0.46
1:A:294:VAL:HA	6:A:900:HOH:O	2.15	0.46
1:A:317:GLN:HB3	1:A:386:LYS:HE2	1.97	0.46
1:A:177:ASP:HB3	1:A:178:ALA:H	1.55	0.46
1:A:274:LEU:HA	1:A:278:THR:CG2	2.45	0.46
1:A:140:TRP:CH2	1:A:331:LEU:HA	2.50	0.45
1:A:630:SER:HB3	1:A:635:LEU:HB2	1.97	0.45
1:A:269:MET:HA	1:A:272:TYR:HD2	1.82	0.45
1:A:157:SER:O	1:A:169:LYS:HD3	2.17	0.45
1:A:416:GLU:HB3	1:A:418:GLU:HB2	1.98	0.45
1:A:567:GLU:HG3	1:A:575:ARG:HH11	1.81	0.45
1:A:219:GLU:HG2	6:A:857:HOH:O	2.17	0.45
1:A:521:TYR:CD1	1:A:530:CYS:HB2	2.52	0.44
1:A:329:GLN:HE22	1:A:333:LYS:HZ2	1.65	0.44
1:A:348:CYS:SG	1:A:372:THR:HG22	2.58	0.44
1:A:612:GLU:OE2	1:A:643:CYS:HA	2.17	0.44
1:A:90:THR:HG22	1:A:685:ASP:HB3	2.00	0.44
1:A:218:PRO:HD2	1:A:219:GLU:HG3	1.98	0.44
1:A:395:ASP:HA	1:A:592:HIS:CD2	2.52	0.44
1:A:504:GLY:O	1:A:520:LYS:HB2	2.17	0.44
1:A:461:THR:HG21	1:A:589:VAL:HG11	1.98	0.44
1:A:580:ASP:HB2	6:A:761:HOH:O	2.17	0.44
1:A:59:LEU:HG	1:A:63:GLN:HB2	2.00	0.44
1:A:246:ARG:NH1	1:A:686:LYS:HD2	2.33	0.43
1:A:284:LEU:HD12	1:A:284:LEU:O	2.17	0.43
1:A:684:GLU:O	1:A:685:ASP:HB2	2.17	0.43
1:A:202:LYS:CE	6:A:774:HOH:O	2.49	0.43
1:A:290:LYS:HG2	1:A:291:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:O	1:A:251:ALA:HB1	2.19	0.43
1:A:444:THR:OG1	1:A:447:ASN:HB3	2.19	0.43
1:A:49:ILE:HD11	1:A:57:ILE:HG12	2.00	0.43
1:A:417:ASP:OD1	1:A:418:GLU:HG3	2.18	0.43
1:A:438:LYS:HB3	1:A:439:LYS:H	1.56	0.43
1:A:421:CYS:N	1:A:425:GLU:HB3	2.34	0.43
1:A:542:HIS:HB2	1:A:581:TYR:CG	2.53	0.43
1:A:556:ASP:HA	1:A:559:LYS:HB2	2.00	0.43
1:A:589:VAL:HG22	1:A:590:PRO:HD2	1.99	0.43
1:A:441:SER:HA	1:A:575:ARG:NH2	2.34	0.43
1:A:562:THR:CG2	1:A:564:ASP:HB3	2.48	0.43
1:A:602:ASN:ND2	1:A:605:ARG:HH21	2.16	0.43
1:A:89:THR:HG22	1:A:90:THR:H	1.84	0.43
1:A:352:LYS:N	1:A:518:HIS:NE2	2.59	0.43
1:A:354:GLU:HB3	1:A:636:LEU:HD23	2.01	0.42
1:A:283:HIS:CE1	6:A:886:HOH:O	2.70	0.42
1:A:528:LEU:HD11	1:A:545:VAL:HG13	2.01	0.42
1:A:27:MET:HB2	1:A:30:GLU:HG2	2.02	0.42
1:A:532:VAL:HG11	1:A:557:TRP:HE3	1.83	0.42
1:A:617:LEU:HD12	1:A:626:MET:CE	2.48	0.42
1:A:12:ILE:HG22	1:A:45:CYS:SG	2.60	0.42
1:A:653:TYR:O	1:A:657:LEU:HG	2.20	0.42
1:A:228:CYS:HB2	1:A:230:ASP:OD1	2.20	0.42
1:A:529:ARG:O	1:A:533:GLU:HG3	2.20	0.42
1:A:313:LEU:HB3	1:A:679:VAL:HG13	2.01	0.41
1:A:380:CYS:HB3	1:A:392:ILE:HD12	2.01	0.41
1:A:47:LYS:H	1:A:47:LYS:HG2	1.74	0.41
1:A:298:LEU:O	1:A:299:LEU:HB2	2.20	0.41
1:A:378:LYS:HE2	1:A:676:LEU:CD2	2.38	0.41
1:A:452:LYS:H	1:A:536:ASP:HB2	1.85	0.41
1:A:586:LEU:O	1:A:587:ALA:HB2	2.20	0.41
1:A:234:GLN:HA	1:A:235:PRO:HD3	1.82	0.41
2:A:691:NAG:H62	2:A:692:NAG:C7	2.50	0.41
1:A:63:GLN:HA	1:A:66:GLU:HG2	2.02	0.41
1:A:217:ALA:HB1	1:A:220:GLU:CG	2.48	0.41
1:A:314:MET:HG3	1:A:315:ASP:O	2.20	0.41
1:A:341:ARG:O	1:A:342:GLU:C	2.59	0.41
1:A:417:ASP:CG	1:A:418:GLU:HG3	2.40	0.41
1:A:425:GLU:CB	1:A:645:VAL:HG13	2.48	0.41
1:A:81:VAL:CG1	1:A:88:SER:HB2	2.50	0.41
1:A:493:PRO:O	1:A:496:SER:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:LEU:HD11	1:A:642:LYS:HZ2	1.86	0.41
1:A:138:ILE:HD13	1:A:152:VAL:HB	2.03	0.41
1:A:246:ARG:NH1	1:A:686:LYS:NZ	2.68	0.41
1:A:159:SER:HB2	1:A:170:LEU:HA	2.02	0.41
1:A:188:TYR:CZ	1:A:197:CYS:HA	2.56	0.41
1:A:209:LYS:HZ2	1:A:301:LYS:NZ	2.19	0.41
1:A:466:ILE:N	1:A:467:PRO:HD2	2.36	0.41
1:A:446:ASN:HD21	1:A:573:GLY:HA2	1.85	0.41
1:A:380:CYS:CB	1:A:392:ILE:HD12	2.51	0.40
2:A:691:NAG:H62	2:A:692:NAG:N2	2.35	0.40
1:A:41:THR:HG22	1:A:43:LEU:H	1.86	0.40
1:A:669:ASN:O	1:A:673:PRO:HG3	2.21	0.40
1:A:26:HIS:O	1:A:27:MET:HB3	2.20	0.40
1:A:57:ILE:HD12	1:A:59:LEU:CD1	2.52	0.40
1:A:268:GLY:O	1:A:272:TYR:HB3	2.21	0.40
1:A:295:LEU:O	1:A:298:LEU:HD22	2.21	0.40
1:A:454:CYS:SG	1:A:535:GLY:HA3	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	684/686 (100%)	567 (83%)	82 (12%)	35 (5%)	<b>1</b> <b>0</b>

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	145	SER
1	A	177	ASP
1	A	280	SER

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Mol	Chain	Res	Type
1	A	287	PRO
1	A	290	LYS
1	A	334	ASP
1	A	338	VAL
1	A	343	ASN
1	A	480	PHE
1	A	509	LEU
1	A	510	LEU
1	A	512	LYS
1	A	561	LEU
1	A	579	MET
1	A	685	ASP
1	A	257	ASP
1	A	289	GLY
1	A	342	GLU
1	A	453	SER
1	A	461	THR
1	A	508	ASN
1	A	122	SER
1	A	136	GLU
1	A	249	ALA
1	A	27	MET
1	A	83	GLU
1	A	366	ASN
1	A	439	LYS
1	A	440	SER
1	A	513	CYS
1	A	618	HIS
1	A	636	LEU
1	A	137	ASP
1	A	186	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	578/578 (100%)	461 (80%)	117 (20%)	<b>1</b> <b>1</b>

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	6	THR
1	A	12	ILE
1	A	18	LYS
1	A	24	LYS
1	A	27	MET
1	A	28	GLN
1	A	31	ARG
1	A	37	VAL
1	A	47	LYS
1	A	52	ASN
1	A	53	GLU
1	A	57	ILE
1	A	59	LEU
1	A	63	GLN
1	A	64	VAL
1	A	72	TYR
1	A	73	LYS
1	A	75	LYS
1	A	84	ARG
1	A	88	SER
1	A	89	THR
1	A	90	THR
1	A	110	ARG
1	A	112	LYS
1	A	128	PRO
1	A	135	ARG
1	A	136	GLU
1	A	143	ILE
1	A	149	GLU
1	A	152	VAL
1	A	154	LYS
1	A	166	ILE
1	A	168	GLN
1	A	172	ARG

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Mol	Chain	Res	Type
1	A	175	LYS
1	A	182	CYS
1	A	184	ARG
1	A	205	VAL
1	A	214	GLN
1	A	219	GLU
1	A	222	ASP
1	A	228	CYS
1	A	236	VAL
1	A	246	ARG
1	A	247	VAL
1	A	255	ARG
1	A	269	MET
1	A	270	GLN
1	A	272	TYR
1	A	276	VAL
1	A	278	THR
1	A	279	THR
1	A	280	SER
1	A	284	LEU
1	A	285	PHE
1	A	287	PRO
1	A	292	ASP
1	A	298	LEU
1	A	312	GLU
1	A	316	SER
1	A	332	ARG
1	A	334	ASP
1	A	338	VAL
1	A	343	ASN
1	A	360	ARG
1	A	364	VAL
1	A	372	THR
1	A	374	LEU
1	A	377	ASN
1	A	378	LYS
1	A	395	ASP
1	A	417	ASP
1	A	424	ASP
1	A	430	TYR
1	A	434	VAL
1	A	441	SER

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Mol	Chain	Res	Type
1	A	446	ASN
1	A	447	ASN
1	A	448	LEU
1	A	470	LEU
1	A	477	SER
1	A	485	SER
1	A	493	PRO
1	A	496	SER
1	A	500	LYS
1	A	509	LEU
1	A	510	LEU
1	A	512	LYS
1	A	525	THR
1	A	531	LEU
1	A	537	VAL
1	A	540	ILE
1	A	545	VAL
1	A	549	VAL
1	A	553	ASN
1	A	555	ASP
1	A	562	THR
1	A	564	ASP
1	A	565	ASP
1	A	568	LEU
1	A	583	THR
1	A	586	LEU
1	A	589	VAL
1	A	602	ASN
1	A	604	ILE
1	A	620	THR
1	A	621	GLU
1	A	626	MET
1	A	630	SER
1	A	638	LYS
1	A	648	ARG
1	A	659	ASP
1	A	665	VAL
1	A	668	LEU
1	A	672	ASN
1	A	686	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	126	ASN
1	A	150	GLN
1	A	210	HIS
1	A	214	GLN
1	A	216	ASN
1	A	283	HIS
1	A	317	GLN
1	A	329	GLN
1	A	343	ASN
1	A	346	GLN
1	A	377	ASN
1	A	446	ASN
1	A	449	GLN
1	A	472	HIS
1	A	473	ASN
1	A	542	HIS
1	A	553	ASN
1	A	669	ASN
1	A	678	GLN

### 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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	NAG	A	691	-	14,14,15	1.59	4 (28%)	17,19,21	1.86	6 (35%)
3	FUC	A	693	-	10,10,11	0.89	0	14,14,16	2.13	6 (42%)
5	CO3	A	689	4	3,3,3	1.74	1 (33%)	2,3,3	0.75	0
2	NAG	A	692	-	14,14,15	1.44	3 (21%)	17,19,21	1.94	4 (23%)
5	CO3	A	690	4	3,3,3	1.82	1 (33%)	2,3,3	1.53	1 (50%)

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
3	FUC	A	693	-	-	-	0/1/1/1
2	NAG	A	692	-	-	1/6/23/26	0/1/1/1
2	NAG	A	691	-	-	3/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	691	NAG	O7-C7	-3.65	1.15	1.23
2	A	692	NAG	O7-C7	-3.33	1.15	1.23
5	A	690	CO3	O1-C	3.13	1.36	1.25
5	A	689	CO3	O1-C	2.98	1.36	1.25
2	A	691	NAG	C3-C2	-2.55	1.47	1.52
2	A	691	NAG	C1-C2	-2.47	1.49	1.52
2	A	692	NAG	C2-N2	2.29	1.50	1.46
2	A	692	NAG	O4-C4	2.09	1.48	1.43
2	A	691	NAG	C2-N2	2.03	1.49	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	692	NAG	C3-C4-C5	4.59	118.55	110.23
3	A	693	FUC	O3-C3-C2	4.34	118.92	110.05
2	A	692	NAG	O5-C1-C2	-3.97	105.15	111.29
3	A	693	FUC	O3-C3-C4	3.67	119.04	110.38
2	A	691	NAG	C1-O5-C5	3.23	116.52	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	693	FUC	O2-C2-C3	3.15	116.68	110.15
2	A	692	NAG	O5-C5-C4	2.92	117.93	110.83
2	A	691	NAG	C4-C3-C2	2.84	115.18	111.02
3	A	693	FUC	C3-C4-C5	-2.77	105.60	109.81
2	A	691	NAG	C1-C2-N2	2.63	114.58	110.43
2	A	691	NAG	O3-C3-C2	2.44	114.47	109.40
2	A	692	NAG	C2-N2-C7	-2.31	119.81	122.90
2	A	691	NAG	O5-C5-C6	2.17	111.89	107.66
2	A	691	NAG	O3-C3-C4	2.11	115.36	110.38
3	A	693	FUC	C1-O5-C5	2.05	117.80	112.97
5	A	690	CO3	O3-C-O1	2.05	124.92	119.68
3	A	693	FUC	C1-C2-C3	-2.01	106.71	109.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	691	NAG	C4-C5-C6-O6
2	A	691	NAG	O5-C5-C6-O6
2	A	692	NAG	O5-C5-C6-O6
2	A	691	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	691	NAG	13	0
3	A	693	FUC	3	0
5	A	689	CO3	2	0
2	A	692	NAG	7	0

## 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.