



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:40 PM GMT

PDB ID : 1LFG  
Title : Structure of diferric human lactoferrin  
Authors : Baker, E.N.; Anderson, B.F.; Haridas, M.  
Deposited on : 1992-02-05  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

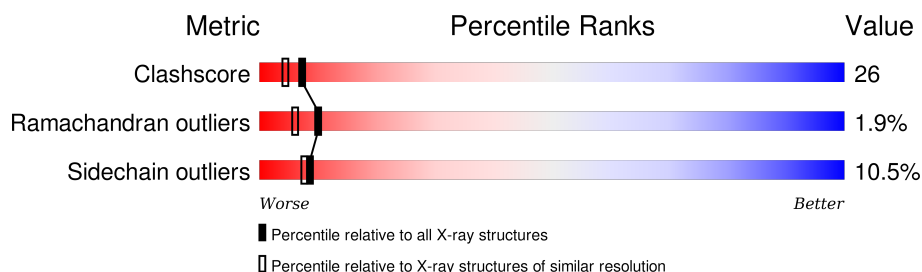
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	691	

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
3	NAG	A	941	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5886 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 LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5322	3327	947	1011	37			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	CONFLICT	UNP P02788
A	200	LYS	ARG	CONFLICT	UNP P02788
A	418	ALA	GLN	CONFLICT	UNP P02788
A	500	ALA	ARG	CONFLICT	UNP P02788
A	512	GLU	GLN	CONFLICT	UNP P02788

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

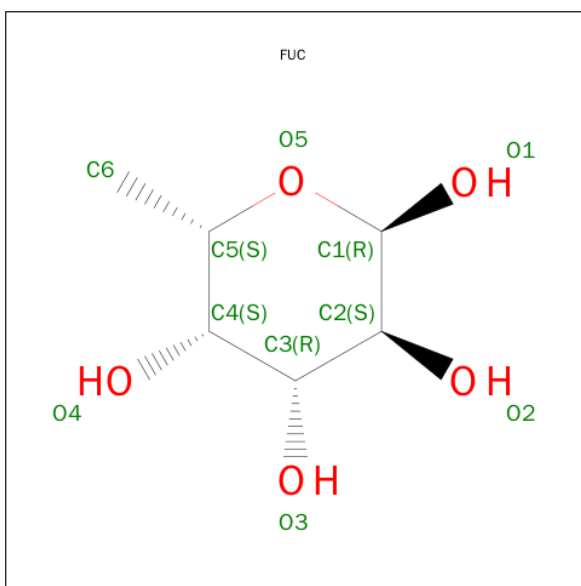
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 3 is SUGAR (3-MER) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).

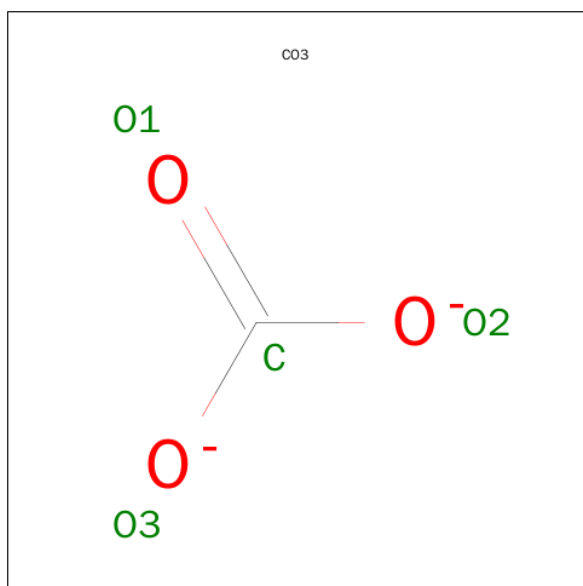


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 6 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

- Molecule 7 is water.

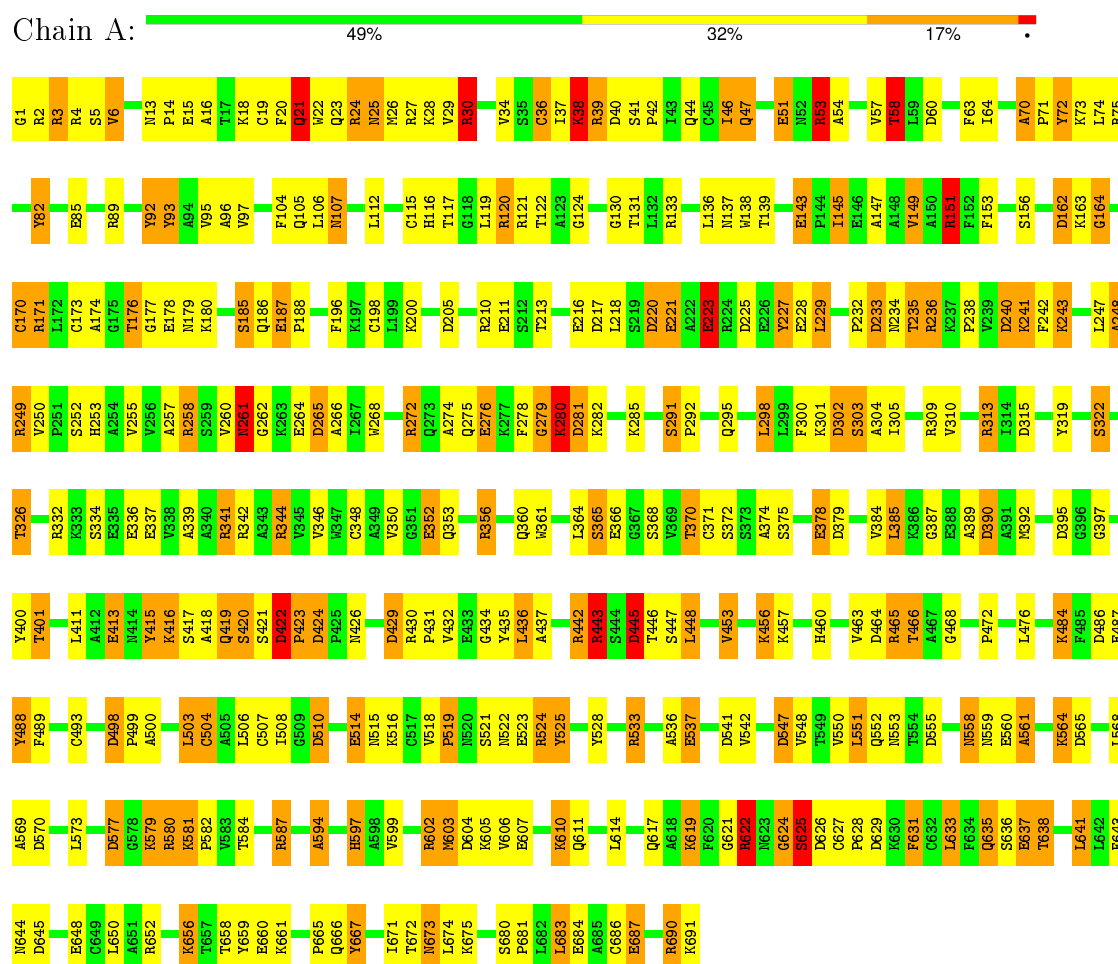
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	493	Total	O	0	0
			493	493		

### 3 Residue-property plots

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: LACTOFERRIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.26 Å 97.40 Å 55.85 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, $R_{free}$	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5886	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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: FUC, CO3, FE, NAG

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	0.94	2/5436 (0.0%)	2.36	263/7354 (3.6%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	VAL	C-N	-5.55	1.21	1.34
1	A	242	PHE	C-N	-5.21	1.22	1.34

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	ARG	NE-CZ-NH1	25.17	132.89	120.30
1	A	39	ARG	NE-CZ-NH2	-20.09	110.25	120.30
1	A	465	ARG	NE-CZ-NH2	19.33	129.97	120.30
1	A	75	ARG	NE-CZ-NH2	18.43	129.51	120.30
1	A	342	ARG	CD-NE-CZ	18.25	149.14	123.60
1	A	39	ARG	NE-CZ-NH1	17.53	129.06	120.30
1	A	151	ARG	NE-CZ-NH2	-16.96	111.82	120.30
1	A	587	ARG	NE-CZ-NH2	-16.35	112.12	120.30
1	A	272	ARG	NE-CZ-NH2	-15.95	112.33	120.30
1	A	602	ARG	NE-CZ-NH2	-15.40	112.60	120.30
1	A	249	ARG	NE-CZ-NH1	-15.19	112.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ARG	NE-CZ-NH2	-15.15	112.72	120.30
1	A	604	ASP	CB-CG-OD2	14.83	131.64	118.30
1	A	151	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	A	233	ASP	CB-CG-OD2	13.34	130.30	118.30
1	A	217	ASP	CB-CG-OD1	12.85	129.86	118.30
1	A	464	ASP	CB-CG-OD1	12.77	129.79	118.30
1	A	442	ARG	NE-CZ-NH1	-12.40	114.10	120.30
1	A	70	ALA	CB-CA-C	11.81	127.82	110.10
1	A	326	THR	CA-CB-CG2	11.81	128.94	112.40
1	A	89	ARG	NE-CZ-NH1	11.75	126.17	120.30
1	A	537	GLU	OE1-CD-OE2	-11.62	109.35	123.30
1	A	510	ASP	CB-CG-OD2	-11.61	107.85	118.30
1	A	24	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	A	30	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	A	356	ARG	NE-CZ-NH2	11.32	125.96	120.30
1	A	443	ARG	CD-NE-CZ	-11.17	107.97	123.60
1	A	602	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	510	ASP	CB-CG-OD1	10.80	128.02	118.30
1	A	27	ARG	NE-CZ-NH1	10.63	125.62	120.30
1	A	315	ASP	CB-CG-OD2	-10.57	108.79	118.30
1	A	645	ASP	CB-CG-OD1	-10.56	108.80	118.30
1	A	342	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	A	464	ASP	CB-CG-OD2	-10.29	109.03	118.30
1	A	309	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	A	392	MET	CA-CB-CG	-10.25	95.87	113.30
1	A	27	ARG	CD-NE-CZ	10.21	137.89	123.60
1	A	258	ARG	NE-CZ-NH2	9.97	125.28	120.30
1	A	265	ASP	CB-CG-OD2	-9.83	109.46	118.30
1	A	272	ARG	NE-CZ-NH1	9.81	125.20	120.30
1	A	30	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	171	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	A	210	ARG	NE-CZ-NH2	9.71	125.16	120.30
1	A	53	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	A	261	ASN	CA-CB-CG	9.66	134.66	113.40
1	A	89	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	240	ASP	CB-CG-OD1	9.46	126.82	118.30
1	A	660	GLU	OE1-CD-OE2	9.33	134.49	123.30
1	A	133	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	622	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	687	GLU	CB-CG-CD	9.10	138.76	114.20
1	A	309	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	A	422	ASP	CB-CG-OD1	8.97	126.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	594	ALA	N-CA-CB	-8.76	97.84	110.10
1	A	344	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	233	ASP	CB-CG-OD1	-8.70	110.47	118.30
1	A	684	GLU	CA-CB-CG	8.65	132.43	113.40
1	A	422	ASP	CA-CB-CG	8.60	132.33	113.40
1	A	54	ALA	N-CA-CB	8.58	122.11	110.10
1	A	533	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	435	TYR	CB-CG-CD1	8.40	126.04	121.00
1	A	96	ALA	N-CA-CB	8.37	121.81	110.10
1	A	220	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	249	ARG	NH1-CZ-NH2	7.95	128.14	119.40
1	A	577	ASP	CB-CG-OD1	-7.92	111.18	118.30
1	A	258	ARG	CD-NE-CZ	-7.91	112.52	123.60
1	A	315	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	537	GLU	CG-CD-OE1	7.87	134.04	118.30
1	A	205	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	555	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	493	CYS	N-CA-CB	7.84	124.72	110.60
1	A	36	CYS	CA-CB-SG	-7.83	99.90	114.00
1	A	313	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	587	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	264	GLU	OE1-CD-OE2	7.71	132.56	123.30
1	A	18	LYS	N-CA-CB	7.69	124.44	110.60
1	A	547	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	A	541	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	75	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	A	604	ASP	OD1-CG-OD2	-7.39	109.25	123.30
1	A	227	TYR	CB-CG-CD1	-7.37	116.58	121.00
1	A	24	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	435	TYR	CB-CG-CD2	-7.33	116.61	121.00
1	A	528	TYR	CB-CG-CD1	7.27	125.36	121.00
1	A	93	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	635	GLN	CB-CA-C	7.16	124.72	110.40
1	A	430	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	652	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	498	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	53	ARG	NH1-CZ-NH2	-7.04	111.65	119.40
1	A	659	TYR	CB-CG-CD2	7.04	125.22	121.00
1	A	291	SER	N-CA-CB	-7.02	99.97	110.50
1	A	424	ASP	CB-CG-OD1	-6.98	112.01	118.30
1	A	645	ASP	CB-CG-OD2	6.96	124.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	690	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	121	ARG	CG-CD-NE	6.88	126.24	111.80
1	A	365	SER	CA-C-O	-6.82	105.77	120.10
1	A	360	GLN	CA-CB-CG	6.81	128.38	113.40
1	A	684	GLU	CG-CD-OE2	-6.79	104.71	118.30
1	A	587	ARG	CD-NE-CZ	-6.78	114.11	123.60
1	A	635	GLN	CB-CG-CD	6.75	129.16	111.60
1	A	133	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	390	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	337	GLU	OE1-CD-OE2	6.69	131.32	123.30
1	A	488	TYR	CB-CG-CD2	6.66	125.00	121.00
1	A	227	TYR	CB-CG-CD2	6.66	125.00	121.00
1	A	365	SER	O-C-N	6.65	133.33	122.70
1	A	249	ARG	CD-NE-CZ	-6.62	114.33	123.60
1	A	486	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	75	ARG	CB-CG-CD	6.62	128.80	111.60
1	A	322	SER	O-C-N	6.61	134.44	123.20
1	A	389	ALA	CB-CA-C	6.60	120.00	110.10
1	A	255	VAL	CG1-CB-CG2	6.60	121.46	110.90
1	A	524	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	488	TYR	CB-CG-CD1	-6.59	117.04	121.00
1	A	149	VAL	CB-CA-C	6.54	123.83	111.40
1	A	429	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	A	332	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	413	GLU	CA-CB-CG	6.51	127.73	113.40
1	A	242	PHE	C-N-CA	6.49	137.91	121.70
1	A	570	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	465	ARG	CD-NE-CZ	-6.45	114.58	123.60
1	A	514	GLU	OE1-CD-OE2	-6.44	115.57	123.30
1	A	163	LYS	C-N-CA	6.37	135.67	122.30
1	A	163	LYS	CA-C-O	6.35	133.43	120.10
1	A	223	GLU	CA-CB-CG	6.27	127.19	113.40
1	A	257	ALA	CB-CA-C	6.23	119.45	110.10
1	A	131	THR	CA-CB-CG2	6.20	121.08	112.40
1	A	463	VAL	CG1-CB-CG2	-6.17	101.04	110.90
1	A	465	ARG	NH1-CZ-NH2	-6.16	112.63	119.40
1	A	453	VAL	CA-CB-CG1	6.13	120.10	110.90
1	A	672	THR	O-C-N	6.13	132.52	122.70
1	A	528	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	A	587	ARG	CB-CG-CD	-6.09	95.78	111.60
1	A	228	GLU	CA-CB-CG	6.08	126.77	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	GLN	OE1-CD-NE2	6.05	135.81	121.90
1	A	156	SER	CB-CA-C	-6.04	98.63	110.10
1	A	234	ASN	CB-CA-C	6.03	122.46	110.40
1	A	171	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	281	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	498	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	542	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	A	217	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	24	ARG	CA-CB-CG	5.94	126.46	113.40
1	A	516	LYS	CA-CB-CG	5.94	126.46	113.40
1	A	465	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	72	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	A	569	ALA	CB-CA-C	5.92	118.98	110.10
1	A	504	CYS	CA-C-O	-5.91	107.69	120.10
1	A	415	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	A	92	TYR	CZ-CE2-CD2	-5.83	114.55	119.80
1	A	484	LYS	O-C-N	5.83	132.03	122.70
1	A	584	THR	O-C-N	-5.83	113.37	122.70
1	A	378	GLU	OE1-CD-OE2	-5.82	116.32	123.30
1	A	82	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	A	463	VAL	CA-CB-CG1	5.79	119.59	110.90
1	A	570	ASP	OD1-CG-OD2	5.79	134.29	123.30
1	A	216	GLU	OE1-CD-OE2	-5.75	116.39	123.30
1	A	514	GLU	CA-CB-CG	5.75	126.06	113.40
1	A	120	ARG	CB-CG-CD	5.75	126.55	111.60
1	A	304	ALA	N-CA-CB	5.73	118.13	110.10
1	A	390	ASP	CB-CG-OD1	-5.73	113.15	118.30
1	A	162	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	A	420	SER	C-N-CA	5.72	136.01	121.70
1	A	240	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	570	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	210	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	A	63	PHE	CA-C-O	-5.67	108.20	120.10
1	A	302	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	21	GLN	CA-CB-CG	5.65	125.83	113.40
1	A	558	ASN	CA-C-O	5.64	131.95	120.10
1	A	371	CYS	CA-CB-SG	-5.64	103.84	114.00
1	A	220	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	187	GLU	CB-CG-CD	5.63	129.40	114.20
1	A	38	LYS	O-C-N	5.62	131.70	122.70
1	A	211	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	A	436	LEU	CA-CB-CG	5.60	128.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	CYS	C-N-CA	5.59	135.69	121.70
1	A	366	GLU	C-N-CA	5.59	134.04	122.30
1	A	74	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	503	LEU	O-C-N	5.58	131.63	122.70
1	A	356	ARG	NH1-CZ-NH2	-5.57	113.27	119.40
1	A	687	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	A	216	GLU	CG-CD-OE2	5.56	129.42	118.30
1	A	336	GLU	CG-CD-OE2	-5.56	107.18	118.30
1	A	379	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	687	GLU	CA-C-O	5.55	131.75	120.10
1	A	170	CYS	CA-CB-SG	5.53	123.95	114.00
1	A	581	LYS	N-CA-CB	5.52	120.53	110.60
1	A	581	LYS	O-C-N	5.49	131.53	121.10
1	A	432	VAL	O-C-N	5.47	131.46	122.70
1	A	401	THR	CA-CB-OG1	-5.46	97.53	109.00
1	A	445	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	A	553	ASN	O-C-N	5.46	131.44	122.70
1	A	667	TYR	CB-CG-CD2	5.46	124.28	121.00
1	A	53	ARG	CD-NE-CZ	5.45	131.23	123.60
1	A	310	VAL	CA-CB-CG1	5.43	119.05	110.90
1	A	599	VAL	CG1-CB-CG2	5.43	119.59	110.90
1	A	303	SER	N-CA-CB	-5.42	102.37	110.50
1	A	120	ARG	N-CA-C	5.42	125.63	111.00
1	A	178	GLU	CB-CA-C	5.42	121.23	110.40
1	A	423	PRO	C-N-CA	5.41	135.23	121.70
1	A	652	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	A	519	PRO	CA-CB-CG	-5.41	93.73	104.00
1	A	525	TYR	CB-CG-CD2	-5.41	117.76	121.00
1	A	385	LEU	CB-CG-CD1	-5.40	101.82	111.00
1	A	51	GLU	OE1-CD-OE2	5.40	129.78	123.30
1	A	384	VAL	CG1-CB-CG2	5.39	119.53	110.90
1	A	58	THR	CB-CA-C	5.37	126.11	111.60
1	A	370	THR	C-N-CA	5.37	135.13	121.70
1	A	559	ASN	CA-CB-CG	-5.37	101.59	113.40
1	A	607	GLU	CG-CD-OE2	-5.37	107.56	118.30
1	A	560	GLU	CG-CD-OE2	-5.34	107.61	118.30
1	A	248	ALA	N-CA-CB	5.33	117.56	110.10
1	A	198	CYS	CA-CB-SG	5.32	123.57	114.00
1	A	281	ASP	C-N-CA	5.31	134.99	121.70
1	A	104	PHE	CB-CA-C	5.31	121.03	110.40
1	A	233	ASP	CA-CB-CG	-5.31	101.71	113.40
1	A	339	ALA	N-CA-CB	5.31	117.54	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	660	GLU	CG-CD-OE1	-5.28	107.74	118.30
1	A	350	VAL	CA-CB-CG1	5.28	118.81	110.90
1	A	611	GLN	N-CA-CB	5.27	120.09	110.60
1	A	272	ARG	N-CA-CB	-5.27	101.11	110.60
1	A	243	LYS	CB-CA-C	-5.26	99.87	110.40
1	A	684	GLU	OE1-CD-OE2	5.25	129.60	123.30
1	A	341	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	205	ASP	OD1-CG-OD2	5.25	133.27	123.30
1	A	104	PHE	N-CA-C	-5.24	96.86	111.00
1	A	411	LEU	O-C-N	5.23	131.07	122.70
1	A	434	GLY	CA-C-N	5.22	128.68	117.20
1	A	673	ASN	CB-CA-C	5.21	120.82	110.40
1	A	366	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	A	561	ALA	CB-CA-C	-5.20	102.30	110.10
1	A	63	PHE	O-C-N	5.20	131.01	122.70
1	A	683	LEU	CB-CA-C	5.19	120.06	110.20
1	A	242	PHE	O-C-N	-5.18	114.41	122.70
1	A	319	TYR	O-C-N	5.18	130.99	122.70
1	A	597	HIS	CA-CB-CG	-5.18	104.80	113.60
1	A	57	VAL	CA-CB-CG2	5.18	118.67	110.90
1	A	1	GLY	O-C-N	5.17	130.98	122.70
1	A	624	GLY	N-CA-C	5.16	126.00	113.10
1	A	445	ASP	N-CA-CB	-5.16	101.31	110.60
1	A	536	ALA	CB-CA-C	5.16	117.83	110.10
1	A	64	ILE	CB-CG1-CD1	5.13	128.27	113.90
1	A	177	GLY	O-C-N	5.13	130.91	122.70
1	A	374	ALA	N-CA-CB	5.12	117.27	110.10
1	A	631	PHE	CD1-CE1-CZ	-5.12	113.96	120.10
1	A	365	SER	N-CA-CB	5.11	118.17	110.50
1	A	93	TYR	CB-CG-CD1	5.11	124.06	121.00
1	A	200	LYS	CG-CD-CE	5.11	127.22	111.90
1	A	46	ILE	CA-C-O	5.07	130.75	120.10
1	A	236	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	A	276	GLU	CA-CB-CG	5.07	124.55	113.40
1	A	466	THR	CA-CB-CG2	5.06	119.48	112.40
1	A	38	LYS	CA-C-N	-5.05	106.08	117.20
1	A	121	ARG	CD-NE-CZ	5.05	130.67	123.60
1	A	75	ARG	NH1-CZ-NH2	-5.05	113.85	119.40
1	A	650	LEU	N-CA-C	-5.04	97.39	111.00
1	A	229	LEU	CB-CG-CD1	5.04	119.56	111.00
1	A	279	GLY	O-C-N	-5.03	114.66	122.70
1	A	437	ALA	CB-CA-C	5.01	117.62	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain

## 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	5322	0	5172	257	0
2	A	24	0	21	6	0
3	A	28	0	24	9	0
4	A	9	0	9	3	0
5	A	2	0	0	0	0
6	A	8	0	0	0	0
7	A	493	0	0	14	0
All	All	5886	0	5226	273	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 26.

All (273) 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:36:CYS:C	1:A:37:ILE:HD12	1.69	1.11
1:A:138:TRP:CD2	1:A:145:ILE:HD13	1.90	1.06
4:A:961:FUC:C1	4:A:961:FUC:C5	2.30	1.05
1:A:422:ASP:HB3	1:A:423:PRO:HD3	1.35	1.05
3:A:941:NAG:H83	3:A:941:NAG:H3	1.47	0.95
1:A:26:MET:CE	1:A:278:PHE:HE2	1.80	0.94
1:A:686:CYS:O	1:A:690:ARG:HG2	1.69	0.91
1:A:38:LYS:O	1:A:39:ARG:HG2	1.70	0.91
1:A:302:ASP:O	1:A:303:SER:HB2	1.69	0.88
1:A:346:VAL:HG22	1:A:370:THR:CG2	2.04	0.88
1:A:26:MET:HE2	1:A:278:PHE:HE2	1.37	0.87
1:A:25:ASN:HA	1:A:28:LYS:HE3	1.56	0.87
3:A:941:NAG:C6	4:A:961:FUC:C1	2.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LYS:NZ	1:A:565:ASP:OD2	2.08	0.86
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.58	0.84
1:A:26:MET:CE	1:A:278:PHE:CE2	2.61	0.83
1:A:26:MET:HE2	1:A:278:PHE:CE2	2.13	0.83
1:A:622:ARG:C	1:A:622:ARG:HD3	1.99	0.83
1:A:29:VAL:HG12	1:A:29:VAL:O	1.79	0.82
1:A:295:GLN:CB	1:A:298:LEU:HD21	2.12	0.80
1:A:417:SER:C	1:A:419:GLN:H	1.84	0.79
1:A:637:GLU:O	1:A:638:THR:HG23	1.82	0.79
1:A:241:LYS:N	1:A:241:LYS:HD2	1.97	0.79
1:A:422:ASP:CB	1:A:423:PRO:HD3	2.10	0.79
1:A:220:ASP:O	1:A:223:GLU:HG2	1.82	0.78
1:A:58:THR:HG21	1:A:300:PHE:CD1	2.20	0.77
1:A:581:LYS:HB3	1:A:582:PRO:HD2	1.64	0.77
1:A:279:GLY:HA3	1:A:282:LYS:NZ	2.00	0.77
1:A:279:GLY:HA3	1:A:282:LYS:HZ2	1.49	0.76
1:A:346:VAL:HG22	1:A:370:THR:HG23	1.68	0.76
1:A:37:ILE:HD12	1:A:37:ILE:N	2.01	0.75
1:A:25:ASN:H	1:A:25:ASN:HD22	1.33	0.75
1:A:280:LYS:O	1:A:282:LYS:HE3	1.87	0.75
3:A:941:NAG:H82	3:A:941:NAG:C1	2.17	0.74
1:A:422:ASP:CB	1:A:423:PRO:CD	2.65	0.74
1:A:658:THR:HB	7:A:1122:HOH:O	1.88	0.73
2:A:901:NAG:H5	2:A:921:FUC:H5	1.71	0.73
1:A:422:ASP:HB3	1:A:423:PRO:CD	2.15	0.72
2:A:901:NAG:H82	7:A:1309:HOH:O	1.89	0.72
1:A:107:ASN:HD22	1:A:107:ASN:H	1.35	0.72
1:A:176:THR:HG22	1:A:176:THR:O	1.90	0.71
1:A:295:GLN:HB2	1:A:298:LEU:HD21	1.70	0.71
1:A:577:ASP:OD1	1:A:579:LYS:HB2	1.90	0.71
1:A:58:THR:HG21	1:A:300:PHE:CE1	2.25	0.71
1:A:637:GLU:C	1:A:638:THR:HG23	2.11	0.71
1:A:260:VAL:HG13	1:A:261:ASN:N	2.05	0.71
1:A:515:ASN:O	1:A:518:VAL:HG12	1.91	0.70
1:A:47:GLN:HG2	1:A:72:TYR:CE1	2.27	0.70
2:A:901:NAG:C6	2:A:921:FUC:H5	2.22	0.69
1:A:13:ASN:N	1:A:14:PRO:HD2	2.07	0.69
1:A:26:MET:HE3	1:A:278:PHE:CE2	2.27	0.69
2:A:901:NAG:C5	2:A:921:FUC:H5	2.22	0.69
1:A:564:LYS:CE	1:A:565:ASP:OD2	2.41	0.69
1:A:6:VAL:O	1:A:34:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HD2	1:A:285:LYS:NZ	2.08	0.68
1:A:36:CYS:O	1:A:37:ILE:HD12	1.93	0.68
1:A:322:SER:HB3	1:A:385:LEU:O	1.93	0.68
1:A:26:MET:HE3	1:A:278:PHE:HE2	1.59	0.68
1:A:456:LYS:O	1:A:489:PHE:HB3	1.94	0.68
1:A:20:PHE:CE1	1:A:36:CYS:HB2	2.29	0.68
1:A:326:THR:HG22	7:A:1252:HOH:O	1.95	0.67
1:A:138:TRP:CE3	1:A:145:ILE:HD13	2.29	0.67
1:A:233:ASP:OD2	1:A:235:THR:HG23	1.94	0.67
1:A:25:ASN:N	1:A:25:ASN:HD22	1.92	0.67
1:A:551:LEU:H	1:A:551:LEU:HD13	1.60	0.66
3:A:941:NAG:C8	3:A:941:NAG:C1	2.71	0.65
1:A:484:LYS:HB3	1:A:487:GLU:HG3	1.77	0.65
1:A:603:MET:HE2	7:A:1148:HOH:O	1.97	0.65
1:A:610:LYS:O	1:A:614:LEU:HG	1.95	0.65
1:A:47:GLN:O	1:A:51:GLU:HG2	1.95	0.64
1:A:176:THR:CG2	1:A:176:THR:O	2.45	0.64
1:A:147:ALA:O	1:A:151:ARG:HG3	1.98	0.64
1:A:421:SER:HB2	1:A:424:ASP:HB2	1.79	0.64
1:A:395:ASP:OD2	1:A:465:ARG:HA	1.97	0.64
1:A:138:TRP:CG	1:A:145:ILE:HD13	2.32	0.64
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.12	0.63
1:A:105:GLN:HA	1:A:105:GLN:HE21	1.64	0.63
1:A:619:LYS:HE2	1:A:626:ASP:OD2	1.99	0.63
1:A:681:PRO:HD2	7:A:1392:HOH:O	1.99	0.62
1:A:561:ALA:O	1:A:564:LYS:HG2	2.00	0.62
1:A:344:ARG:HD3	1:A:370:THR:HG21	1.82	0.61
1:A:260:VAL:HG13	1:A:261:ASN:H	1.64	0.61
1:A:218:LEU:HD11	1:A:227:TYR:CE2	2.34	0.61
1:A:21:GLN:O	1:A:22:TRP:C	2.38	0.61
1:A:573:LEU:O	1:A:580:ARG:HA	2.00	0.61
1:A:220:ASP:HB3	1:A:223:GLU:OE2	2.01	0.60
1:A:220:ASP:O	1:A:223:GLU:CG	2.50	0.60
1:A:38:LYS:HD3	1:A:39:ARG:O	2.02	0.60
3:A:942:NAG:H83	3:A:942:NAG:H3	1.82	0.60
1:A:13:ASN:H	1:A:14:PRO:HD2	1.67	0.60
1:A:97:VAL:HG22	1:A:229:LEU:HD23	1.83	0.60
3:A:941:NAG:C8	3:A:941:NAG:H3	2.18	0.59
1:A:26:MET:HE1	1:A:274:ALA:HA	1.82	0.59
1:A:38:LYS:O	1:A:39:ARG:NH1	2.24	0.59
1:A:107:ASN:ND2	1:A:107:ASN:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLY:HA3	7:A:1000:HOH:O	2.02	0.59
1:A:581:LYS:HB3	1:A:582:PRO:CD	2.31	0.59
1:A:29:VAL:O	1:A:29:VAL:CG1	2.49	0.59
1:A:218:LEU:HD11	1:A:227:TYR:HE2	1.68	0.59
1:A:401:THR:HG23	1:A:683:LEU:HD13	1.85	0.59
1:A:13:ASN:N	1:A:14:PRO:CD	2.65	0.59
1:A:551:LEU:CD1	1:A:551:LEU:N	2.66	0.59
1:A:548:VAL:O	1:A:552:GLN:HG3	2.03	0.59
1:A:21:GLN:HA	1:A:24:ARG:CG	2.33	0.58
1:A:220:ASP:OD1	1:A:221:GLU:N	2.37	0.58
1:A:37:ILE:N	1:A:37:ILE:CD1	2.67	0.58
1:A:690:ARG:O	1:A:691:LYS:C	2.42	0.58
1:A:295:GLN:HB3	1:A:298:LEU:HD21	1.86	0.58
1:A:116:HIS:N	1:A:116:HIS:CD2	2.67	0.58
1:A:51:GLU:OE2	1:A:53:ARG:HD2	2.03	0.58
1:A:518:VAL:HG23	1:A:519:PRO:HD2	1.86	0.57
1:A:280:LYS:O	1:A:282:LYS:HG3	2.05	0.56
1:A:361:TRP:CD1	1:A:361:TRP:O	2.58	0.56
1:A:70:ALA:CB	1:A:73:LYS:HE3	2.36	0.56
1:A:23:GLN:HB2	1:A:34:VAL:O	2.06	0.56
1:A:233:ASP:N	1:A:233:ASP:OD1	2.23	0.56
2:A:901:NAG:H62	2:A:921:FUC:H5	1.88	0.56
1:A:680:SER:HB2	1:A:681:PRO:CD	2.36	0.56
1:A:551:LEU:HD13	1:A:551:LEU:N	2.21	0.55
1:A:352:GLU:H	1:A:352:GLU:CD	2.05	0.55
1:A:507:CYS:HB3	1:A:523:GLU:OE1	2.06	0.55
1:A:240:ASP:C	1:A:241:LYS:HD2	2.26	0.55
1:A:322:SER:O	1:A:326:THR:HG23	2.07	0.55
1:A:445:ASP:OD1	1:A:448:LEU:HD23	2.06	0.55
1:A:457:LYS:HB3	1:A:506:LEU:HD11	1.89	0.54
1:A:579:LYS:HD2	1:A:579:LYS:N	2.23	0.54
1:A:423:PRO:HB2	7:A:1101:HOH:O	2.09	0.53
1:A:138:TRP:HE1	1:A:143:GLU:HG2	1.73	0.53
1:A:637:GLU:C	1:A:638:THR:CG2	2.76	0.53
1:A:417:SER:C	1:A:419:GLN:N	2.60	0.52
1:A:3:ARG:HE	1:A:266:ALA:HB2	1.72	0.52
1:A:260:VAL:CG1	1:A:261:ASN:N	2.72	0.52
1:A:656:LYS:HE2	1:A:661:LYS:O	2.09	0.52
1:A:28:LYS:HD2	1:A:285:LYS:HZ3	1.74	0.52
1:A:3:ARG:O	1:A:3:ARG:HG3	2.10	0.52
1:A:38:LYS:C	1:A:39:ARG:HG2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:901:NAG:C6	2:A:921:FUC:C5	2.88	0.51
1:A:16:ALA:O	1:A:20:PHE:CD2	2.64	0.51
1:A:28:LYS:HD2	1:A:285:LYS:HZ2	1.74	0.51
1:A:233:ASP:OD2	1:A:235:THR:CG2	2.58	0.51
1:A:445:ASP:OD1	1:A:448:LEU:CD2	2.59	0.51
1:A:13:ASN:HB3	1:A:14:PRO:HD3	1.93	0.51
1:A:105:GLN:HB2	1:A:107:ASN:ND2	2.26	0.50
3:A:942:NAG:C8	3:A:942:NAG:H3	2.31	0.50
1:A:633:LEU:HD22	1:A:643:PHE:CE2	2.46	0.50
1:A:21:GLN:O	1:A:24:ARG:N	2.44	0.50
1:A:51:GLU:HG3	1:A:53:ARG:HG3	1.92	0.50
1:A:508:ILE:HD11	1:A:524:ARG:HB2	1.94	0.49
1:A:20:PHE:HE1	7:A:1301:HOH:O	1.96	0.49
1:A:238:PRO:HB2	1:A:240:ASP:OD1	2.13	0.49
1:A:60:ASP:HA	1:A:253:HIS:CD2	2.47	0.49
1:A:40:ASP:HB2	1:A:44:GLN:OE1	2.13	0.49
1:A:313:ARG:O	1:A:313:ARG:HG3	2.12	0.49
1:A:92:TYR:O	1:A:250:VAL:HG22	2.13	0.49
1:A:21:GLN:HA	1:A:24:ARG:HG2	1.93	0.49
1:A:625:SER:OG	1:A:626:ASP:OD1	2.30	0.49
1:A:138:TRP:CG	1:A:145:ILE:CD1	2.96	0.48
1:A:260:VAL:CG1	1:A:261:ASN:H	2.25	0.48
1:A:665:PRO:HG2	1:A:666:GLN:OE1	2.13	0.48
1:A:353:GLN:HG3	1:A:356:ARG:HH12	1.77	0.48
1:A:268:TRP:O	1:A:272:ARG:HB2	2.13	0.48
1:A:25:ASN:N	1:A:25:ASN:ND2	2.61	0.48
1:A:170:CYS:O	1:A:171:ARG:C	2.51	0.48
1:A:112:LEU:O	1:A:153:PHE:HB3	2.13	0.48
1:A:364:LEU:CD2	1:A:631:PHE:HB2	2.44	0.48
1:A:667:TYR:CE2	1:A:671:ILE:HD11	2.49	0.47
1:A:390:ASP:OD2	1:A:605:LYS:HE2	2.14	0.47
1:A:429:ASP:O	1:A:431:PRO:HD3	2.14	0.47
1:A:375:SER:HB3	7:A:1232:HOH:O	2.14	0.47
1:A:472:PRO:O	1:A:476:LEU:HG	2.15	0.47
1:A:424:ASP:HB3	1:A:648:GLU:OE2	2.14	0.47
1:A:617:GLN:O	1:A:621:GLY:HA3	2.16	0.46
1:A:34:VAL:O	1:A:34:VAL:HG13	2.14	0.46
1:A:185:SER:C	1:A:187:GLU:N	2.68	0.46
1:A:238:PRO:HD2	1:A:241:LYS:HG2	1.98	0.46
1:A:105:GLN:HB2	1:A:107:ASN:HD21	1.81	0.46
1:A:424:ASP:C	1:A:424:ASP:OD1	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HA	1:A:73:LYS:HE3	1.97	0.46
1:A:221:GLU:HG2	1:A:221:GLU:H	1.32	0.46
1:A:341:ARG:HG3	1:A:341:ARG:O	2.16	0.46
1:A:499:PRO:HA	1:A:504:CYS:SG	2.56	0.46
1:A:20:PHE:O	1:A:24:ARG:HG2	2.14	0.46
1:A:93:TYR:CZ	1:A:243:LYS:HE2	2.51	0.46
1:A:38:LYS:O	1:A:39:ARG:CG	2.55	0.46
1:A:6:VAL:HG12	1:A:6:VAL:O	2.14	0.46
1:A:352:GLU:OE1	1:A:352:GLU:N	2.29	0.46
1:A:247:LEU:O	1:A:248:ALA:HB2	2.16	0.46
1:A:279:GLY:O	1:A:280:LYS:C	2.53	0.46
1:A:518:VAL:CG2	1:A:519:PRO:HD2	2.45	0.46
1:A:422:ASP:HB2	1:A:423:PRO:CD	2.46	0.45
1:A:624:GLY:O	1:A:626:ASP:N	2.49	0.45
1:A:51:GLU:HG3	1:A:53:ARG:HD2	1.98	0.45
1:A:498:ASP:OD1	1:A:500:ALA:HB3	2.15	0.45
1:A:3:ARG:CG	1:A:3:ARG:O	2.63	0.45
1:A:21:GLN:HA	1:A:24:ARG:HG3	1.97	0.45
1:A:136:LEU:O	1:A:137:ASN:C	2.54	0.45
1:A:514:GLU:O	1:A:515:ASN:HB2	2.17	0.45
1:A:627:CYS:HA	1:A:628:PRO:HA	1.67	0.45
1:A:420:SER:OG	1:A:421:SER:N	2.35	0.45
1:A:258:ARG:HB2	1:A:262:GLY:HA2	1.98	0.45
1:A:173:CYS:HB3	1:A:187:GLU:OE1	2.17	0.45
1:A:180:LYS:HE2	1:A:180:LYS:HB3	1.81	0.45
1:A:488:TYR:HD1	1:A:488:TYR:N	2.15	0.44
1:A:413:GLU:OE1	1:A:644:ASN:ND2	2.48	0.44
1:A:533:ARG:NE	1:A:537:GLU:OE2	2.48	0.44
1:A:279:GLY:H	1:A:282:LYS:HD2	1.83	0.44
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.18	0.44
1:A:41:SER:HB2	1:A:42:PRO:HD2	1.99	0.44
1:A:19:CYS:O	1:A:36:CYS:SG	2.75	0.44
1:A:365:SER:HB2	1:A:368:SER:OG	2.17	0.44
1:A:443:ARG:HD3	1:A:443:ARG:HH11	1.25	0.44
1:A:30:ARG:HH11	1:A:30:ARG:HG2	1.83	0.44
1:A:42:PRO:O	1:A:46:ILE:HG13	2.17	0.44
1:A:58:THR:CG2	1:A:300:PHE:CE1	2.98	0.44
1:A:525:TYR:CE1	1:A:533:ARG:HG2	2.53	0.43
1:A:240:ASP:OD1	1:A:240:ASP:N	2.44	0.43
1:A:507:CYS:HB3	1:A:523:GLU:CD	2.37	0.43
1:A:442:ARG:HD3	1:A:442:ARG:HH11	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:SER:O	1:A:419:GLN:N	2.50	0.43
1:A:70:ALA:HB1	1:A:73:LYS:HE3	2.01	0.43
1:A:258:ARG:HH11	1:A:258:ARG:HD2	1.50	0.43
1:A:14:PRO:O	1:A:15:GLU:C	2.57	0.43
1:A:105:GLN:HE22	1:A:236:ARG:HG3	1.83	0.43
1:A:162:ASP:OD1	1:A:164:GLY:HA3	2.19	0.43
1:A:275:GLN:O	1:A:279:GLY:HA3	2.19	0.43
1:A:378:GLU:HG3	7:A:1121:HOH:O	2.19	0.43
1:A:503:LEU:HD23	1:A:503:LEU:HA	1.84	0.43
1:A:680:SER:HB2	1:A:681:PRO:HD2	2.00	0.42
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.79	0.42
1:A:291:SER:HA	1:A:292:PRO:HD3	1.78	0.42
3:A:941:NAG:C8	3:A:941:NAG:C3	2.89	0.42
1:A:547:ASP:OD1	1:A:547:ASP:N	2.51	0.42
1:A:397:GLY:O	1:A:400:TYR:HB3	2.19	0.42
3:A:941:NAG:O6	4:A:961:FUC:C5	2.67	0.42
1:A:26:MET:HE1	1:A:274:ALA:CA	2.49	0.42
1:A:488:TYR:CD1	1:A:488:TYR:N	2.87	0.42
1:A:122:THR:CG2	1:A:250:VAL:HG11	2.49	0.42
1:A:395:ASP:HA	1:A:597:HIS:CD2	2.55	0.42
1:A:279:GLY:CA	1:A:282:LYS:NZ	2.78	0.42
1:A:499:PRO:HG3	7:A:1240:HOH:O	2.19	0.42
1:A:466:THR:HG21	1:A:594:ALA:HB1	2.01	0.42
1:A:346:VAL:HG22	1:A:370:THR:HG22	1.97	0.42
1:A:97:VAL:HG22	1:A:229:LEU:CD2	2.48	0.42
1:A:106:LEU:HD23	1:A:232:PRO:HA	2.02	0.42
1:A:82:TYR:CE2	1:A:252:SER:HB2	2.54	0.42
1:A:279:GLY:N	1:A:282:LYS:HD2	2.35	0.41
1:A:415:TYR:C	1:A:416:LYS:O	2.56	0.41
1:A:196:PHE:HB2	1:A:213:THR:HG21	2.02	0.41
1:A:179:ASN:ND2	1:A:186:GLN:OE1	2.54	0.41
1:A:510:ASP:HA	1:A:522:ASN:O	2.20	0.41
1:A:179:ASN:O	1:A:180:LYS:C	2.58	0.41
1:A:641:LEU:HD23	7:A:1285:HOH:O	2.20	0.41
1:A:419:GLN:HA	7:A:1250:HOH:O	2.21	0.41
1:A:550:VAL:HG12	1:A:568:LEU:HD12	2.01	0.41
1:A:352:GLU:CD	1:A:352:GLU:N	2.71	0.41
1:A:508:ILE:HD11	1:A:524:ARG:CB	2.50	0.41
1:A:42:PRO:HG3	7:A:1168:HOH:O	2.20	0.41
1:A:145:ILE:HA	1:A:145:ILE:HD12	1.82	0.41
1:A:285:LYS:HE3	1:A:285:LYS:HB2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:O	1:A:282:LYS:HD3	2.21	0.41
1:A:95:VAL:H	1:A:95:VAL:HG22	1.70	0.41
1:A:249:ARG:HD3	1:A:249:ARG:HH11	1.52	0.41
1:A:460:HIS:ND1	1:A:468:GLY:O	2.51	0.41
1:A:448:LEU:O	1:A:580:ARG:HD2	2.21	0.41
1:A:387:GLY:HA2	1:A:602:ARG:NH1	2.36	0.41
1:A:143:GLU:OE1	1:A:151:ARG:NH2	2.54	0.40
1:A:115:CYS:C	1:A:116:HIS:CD2	2.94	0.40
1:A:220:ASP:OD1	1:A:220:ASP:C	2.60	0.40
1:A:453:VAL:O	1:A:456:LYS:HB2	2.22	0.40
1:A:617:GLN:O	1:A:621:GLY:N	2.52	0.40
1:A:558:ASN:OD1	1:A:558:ASN:C	2.60	0.40
1:A:564:LYS:HG3	1:A:565:ASP:H	1.86	0.40
1:A:675:LYS:HA	1:A:675:LYS:HD3	1.87	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	689/691 (100%)	618 (90%)	58 (8%)	13 (2%)	<b>10</b> <b>6</b>

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	ASP
1	A	280	LYS
1	A	416	LYS
1	A	625	SER
1	A	637	GLU
1	A	418	ALA
1	A	564	LYS

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Mol	Chain	Res	Type
1	A	281	ASP
1	A	164	GLY
1	A	446	THR
1	A	521	SER
1	A	606	VAL
1	A	636	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	570/572 (100%)	510 (90%)	60 (10%)	<b>8</b> <b>8</b>

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	ARG
1	A	4	ARG
1	A	5	SER
1	A	21	GLN
1	A	25	ASN
1	A	30	ARG
1	A	38	LYS
1	A	53	ARG
1	A	58	THR
1	A	71	PRO
1	A	85	GLU
1	A	107	ASN
1	A	120	ARG
1	A	139	THR
1	A	143	GLU
1	A	145	ILE
1	A	149	VAL
1	A	176	THR
1	A	185	SER

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Mol	Chain	Res	Type
1	A	221	GLU
1	A	223	GLU
1	A	225	ASP
1	A	235	THR
1	A	241	LYS
1	A	261	ASN
1	A	265	ASP
1	A	280	LYS
1	A	298	LEU
1	A	301	LYS
1	A	305	ILE
1	A	334	SER
1	A	352	GLU
1	A	372	SER
1	A	419	GLN
1	A	426	ASN
1	A	436	LEU
1	A	443	ARG
1	A	445	ASP
1	A	447	SER
1	A	448	LEU
1	A	456	LYS
1	A	551	LEU
1	A	579	LYS
1	A	580	ARG
1	A	587	ARG
1	A	603	MET
1	A	610	LYS
1	A	619	LYS
1	A	622	ARG
1	A	625	SER
1	A	629	ASP
1	A	633	LEU
1	A	635	GLN
1	A	638	THR
1	A	641	LEU
1	A	656	LYS
1	A	673	ASN
1	A	674	LEU
1	A	687	GLU

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



Mol	Chain	Res	Type
1	A	21	GLN
1	A	23	GLN
1	A	25	ASN
1	A	47	GLN
1	A	91	HIS
1	A	105	GLN
1	A	107	ASN
1	A	179	ASN
1	A	186	GLN
1	A	329	GLN
1	A	330	ASN
1	A	353	GLN
1	A	419	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

2 carbohydrates are modelled in this entry.

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	901	1,2	14,14,15	2.16	4 (28%)	15,19,21	4.81	12 (80%)
2	FUC	A	921	2	10,10,11	0.96	0	14,14,16	1.48	3 (21%)

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	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	FUC	A	921	2	-	0/0/17/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAG	C2-N2	-5.43	1.36	1.46
2	A	901	NAG	O7-C7	-3.59	1.14	1.23
2	A	901	NAG	C6-C5	-2.95	1.41	1.51
2	A	901	NAG	O5-C1	2.65	1.48	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	NAG	C1-O5-C5	-8.04	102.04	112.25
2	A	901	NAG	C6-C5-C4	-6.16	97.83	113.02
2	A	901	NAG	O7-C7-N2	-4.99	111.69	121.86
2	A	901	NAG	O4-C4-C5	-3.93	98.84	109.24
2	A	901	NAG	O3-C3-C4	-3.26	102.99	110.34
2	A	901	NAG	C4-C3-C2	-3.17	106.31	111.23
2	A	921	FUC	C1-C2-C3	-2.86	106.15	109.54
2	A	901	NAG	C3-C4-C5	-2.50	105.84	110.20
2	A	921	FUC	O2-C2-C1	-2.05	105.09	109.21
2	A	921	FUC	O4-C4-C3	3.50	118.21	110.34
2	A	901	NAG	O6-C6-C5	4.25	125.36	111.33
2	A	901	NAG	C3-C2-N2	4.38	121.05	110.56
2	A	901	NAG	C8-C7-N2	4.41	124.54	116.11
2	A	901	NAG	C2-N2-C7	7.29	132.41	123.04
2	A	901	NAG	O3-C3-C2	8.03	125.03	109.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	6	0
2	A	921	FUC	5	0

## 5.6 Ligand geometry

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$
6	CO3	A	695	5	0,3,3	0.00	-	0,3,3	0.00	-
6	CO3	A	696	5	0,3,3	0.00	-	0,3,3	0.00	-
3	NAG	A	941	1,3,4	14,14,15	2.03	3 (21%)	15,19,21	3.85	8 (53%)
3	NAG	A	942	3	14,14,15	1.31	2 (14%)	15,19,21	6.15	8 (53%)
4	FUC	A	961	3	7,8,11	0.36	0	6,10,16	1.11	1 (16%)

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
6	CO3	A	695	5	-	0/0/0/0	0/0/0/0
6	CO3	A	696	5	-	0/0/0/0	0/0/0/0
3	NAG	A	941	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	A	942	3	-	0/6/23/26	0/1/1/1
4	FUC	A	961	3	-	0/10/10/20	0/0/0/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	941	NAG	O6-C6	-6.37	1.14	1.42
3	A	942	NAG	O7-C7	-3.26	1.15	1.23
3	A	941	NAG	O7-C7	-2.36	1.17	1.23
3	A	942	NAG	C1-C2	2.29	1.55	1.52
3	A	941	NAG	C1-C2	2.49	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	942	NAG	O7-C7-N2	-11.38	98.67	121.86
3	A	941	NAG	C2-N2-C7	-7.38	113.56	123.04
3	A	942	NAG	C3-C2-N2	-6.33	95.40	110.56
3	A	942	NAG	C3-C4-C5	-4.30	102.70	110.20
3	A	941	NAG	O7-C7-N2	-2.87	116.00	121.86
3	A	942	NAG	C6-C5-C4	-2.76	106.20	113.02
3	A	941	NAG	O7-C7-C8	-2.63	117.23	122.06
3	A	941	NAG	O3-C3-C2	-2.49	104.17	109.11
4	A	961	FUC	C4-C3-C2	-2.08	109.08	112.47
3	A	942	NAG	O4-C4-C3	2.06	114.98	110.34
3	A	941	NAG	C4-C3-C2	2.45	115.04	111.23
3	A	942	NAG	O5-C5-C6	2.59	112.96	107.35
3	A	941	NAG	C1-O5-C5	5.35	119.04	112.25
3	A	941	NAG	C8-C7-N2	5.57	126.76	116.11
3	A	941	NAG	O6-C6-C5	8.69	140.04	111.33
3	A	942	NAG	C8-C7-N2	12.30	139.64	116.11
3	A	942	NAG	C1-O5-C5	14.24	130.32	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	941	NAG	7	0
3	A	942	NAG	2	0
4	A	961	FUC	3	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 will therefore be empty.

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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