Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2024 – 04:47 AM EDT

PDB ID	:	1LFI
Title	:	METAL SUBSTITUTION IN TRANSFERRINS: THE CRYSTAL STRUCTURE OF HUMAN COPPER-LACTOFERRIN AT 2.1 ANGSTROMS RESOLUTION
Authors	:	Smith, C.A.; Anderson, B.F.; Baker, H.M.; Baker, E.N.
Deposited on	:	1992-02-10
Resolution	:	2.10 Å(reported)

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

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

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

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

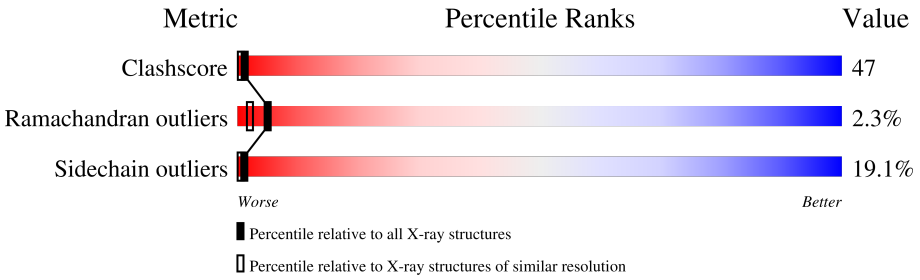
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.10 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	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	691	28% 43% 21% 8%
2	B	3	33% 67%
3	C	2	100%

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	B	1	-	-	X	-
2	NAG	B	2	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1	-	-	X	-
3	FUC	C	2	X	-	-	-
5	CO3	A	695	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5695 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.

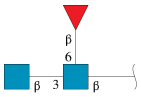
- Molecule 1 is a protein called LACTOFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	0	0
			5322	3326	946	1013	37			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	GLN	conflict	UNP P02788
A	512	GLU	GLN	conflict	UNP P02788

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			

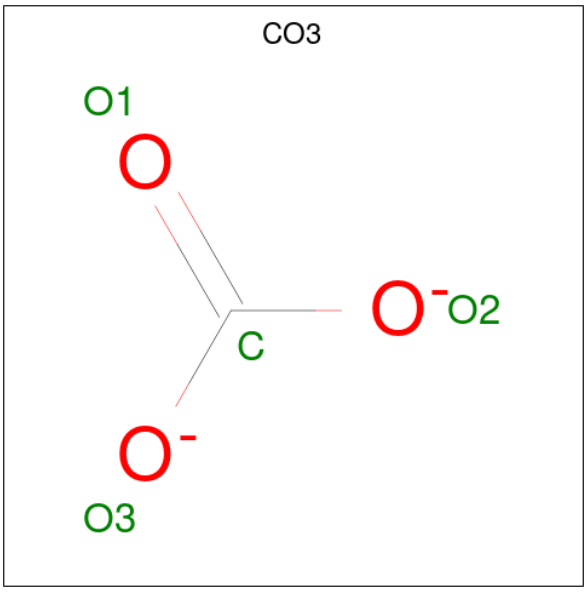
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	301	Total O 301 301	0	0

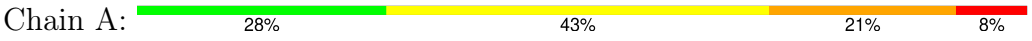
3 Residue-property plots (i)

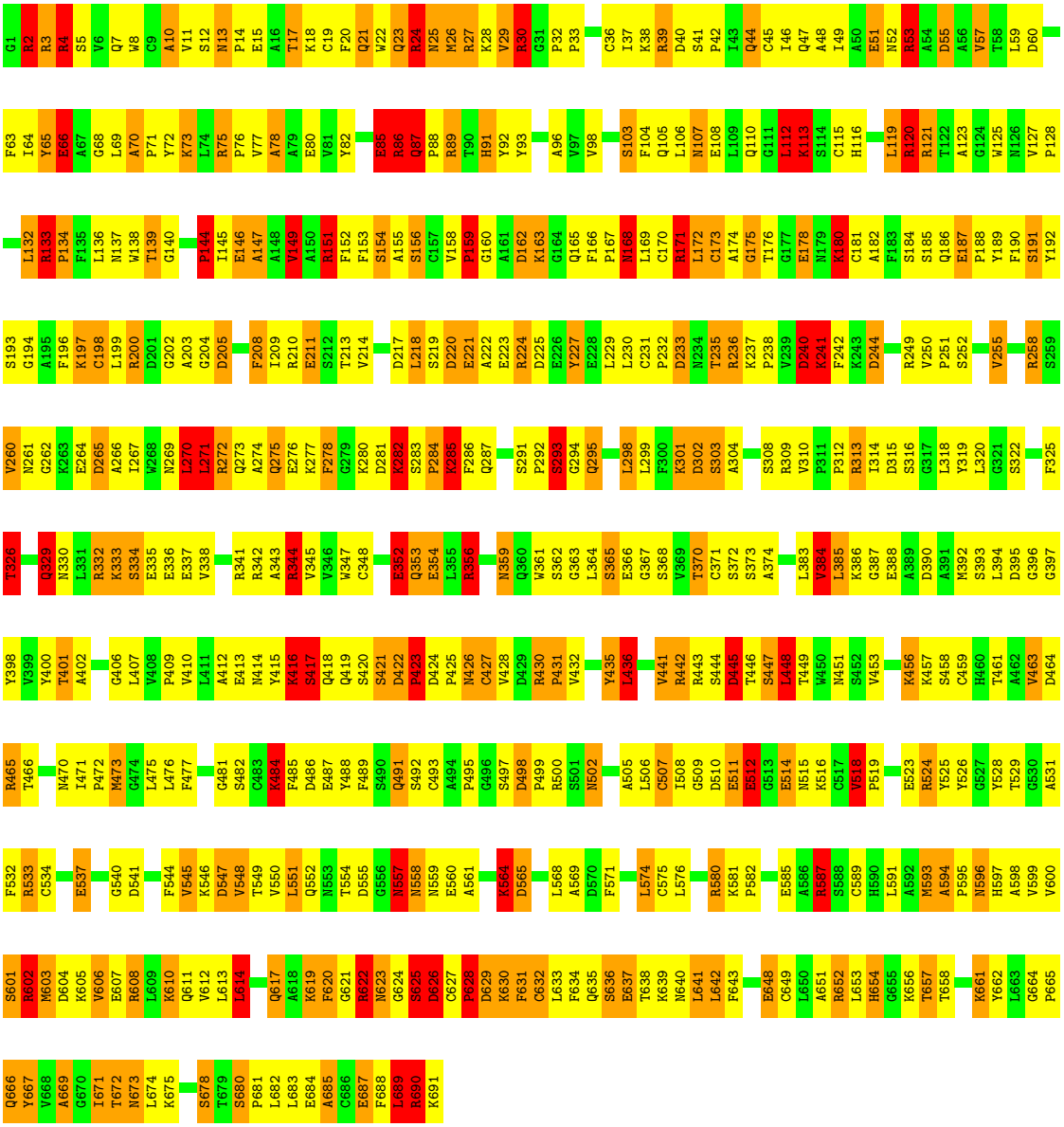
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: LACTOFERRIN

Chain A:





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-[beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

• Molecule 3: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

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, α, β, γ	155.90Å 97.00Å 56.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5695	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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: FUL, FUC, CU, NAG, 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	1.14	3/5436 (0.1%)	2.77	398/7355 (5.4%)

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	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	TYR	CB-CG	-7.48	1.40	1.51
1	A	2	ARG	N-CA	6.32	1.58	1.46
1	A	335	GLU	CD-OE1	5.60	1.31	1.25

All (398) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	602	ARG	NE-CZ-NH2	-40.71	99.94	120.30
1	A	210	ARG	NE-CZ-NH1	-31.09	104.75	120.30
1	A	602	ARG	NE-CZ-NH1	28.77	134.69	120.30
1	A	27	ARG	NE-CZ-NH1	26.32	133.46	120.30
1	A	344	ARG	CD-NE-CZ	23.84	156.98	123.60
1	A	342	ARG	NE-CZ-NH1	22.31	131.46	120.30
1	A	430	ARG	NE-CZ-NH1	-21.48	109.56	120.30
1	A	249	ARG	NE-CZ-NH2	-20.54	110.03	120.30
1	A	27	ARG	NE-CZ-NH2	-17.19	111.71	120.30
1	A	313	ARG	NE-CZ-NH1	17.10	128.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	302	ASP	CB-CG-OD1	16.70	133.32	118.30
1	A	341	ARG	NE-CZ-NH2	-16.31	112.15	120.30
1	A	24	ARG	NE-CZ-NH1	16.28	128.44	120.30
1	A	205	ASP	CB-CG-OD1	-15.70	104.17	118.30
1	A	342	ARG	CD-NE-CZ	15.54	145.36	123.60
1	A	133	ARG	NE-CZ-NH2	-15.48	112.56	120.30
1	A	133	ARG	CD-NE-CZ	15.18	144.85	123.60
1	A	86	ARG	N-CA-CB	15.11	137.80	110.60
1	A	53	ARG	NE-CZ-NH1	-15.02	112.79	120.30
1	A	210	ARG	NE-CZ-NH2	14.82	127.71	120.30
1	A	302	ASP	CB-CG-OD2	-14.76	105.02	118.30
1	A	93	TYR	CB-CG-CD1	-14.68	112.19	121.00
1	A	486	ASP	CB-CG-OD1	14.29	131.16	118.30
1	A	89	ARG	CD-NE-CZ	14.27	143.58	123.60
1	A	465	ARG	NE-CZ-NH2	14.24	127.42	120.30
1	A	86	ARG	CD-NE-CZ	14.03	143.25	123.60
1	A	315	ASP	CB-CG-OD2	-14.03	105.67	118.30
1	A	430	ARG	NE-CZ-NH2	13.75	127.17	120.30
1	A	53	ARG	NE-CZ-NH2	13.26	126.93	120.30
1	A	233	ASP	CB-CG-OD2	13.25	130.23	118.30
1	A	315	ASP	CB-CG-OD1	13.17	130.16	118.30
1	A	27	ARG	CD-NE-CZ	13.13	141.99	123.60
1	A	332	ARG	NE-CZ-NH2	-13.11	113.75	120.30
1	A	93	TYR	CB-CG-CD2	12.83	128.70	121.00
1	A	53	ARG	CD-NE-CZ	-12.60	105.97	123.60
1	A	587	ARG	CD-NE-CZ	12.37	140.91	123.60
1	A	86	ARG	NE-CZ-NH1	12.31	126.46	120.30
1	A	604	ASP	CB-CG-OD1	11.73	128.86	118.30
1	A	608	ARG	NE-CZ-NH2	-11.63	114.49	120.30
1	A	443	ARG	CD-NE-CZ	-11.51	107.48	123.60
1	A	533	ARG	CD-NE-CZ	11.34	139.48	123.60
1	A	690	ARG	NE-CZ-NH2	-11.29	114.65	120.30
1	A	240	ASP	CB-CG-OD2	-11.26	108.17	118.30
1	A	89	ARG	NE-CZ-NH2	-11.21	114.69	120.30
1	A	265	ASP	CB-CG-OD2	-11.21	108.21	118.30
1	A	92	TYR	CB-CG-CD2	-11.05	114.37	121.00
1	A	547	ASP	CB-CG-OD2	-10.97	108.43	118.30
1	A	533	ARG	NE-CZ-NH1	10.89	125.75	120.30
1	A	565	ASP	CB-CG-OD1	10.89	128.10	118.30
1	A	444	SER	N-CA-CB	-10.83	94.25	110.50
1	A	435	TYR	CB-CG-CD1	10.63	127.38	121.00
1	A	332	ARG	NH1-CZ-NH2	10.59	131.05	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	272	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	A	332	ARG	NE-CZ-NH1	-10.35	115.12	120.30
1	A	587	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	690	ARG	NE-CZ-NH1	-9.94	115.33	120.30
1	A	565	ASP	CB-CG-OD2	-9.88	109.41	118.30
1	A	149	VAL	CA-CB-CG1	9.88	125.72	110.90
1	A	445	ASP	CB-CG-OD1	-9.88	109.41	118.30
1	A	430	ARG	CD-NE-CZ	-9.77	109.93	123.60
1	A	498	ASP	CB-CG-OD1	9.76	127.08	118.30
1	A	160	GLY	CA-C-O	-9.71	103.12	120.60
1	A	365	SER	O-C-N	9.70	138.22	122.70
1	A	272	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	A	690	ARG	NH1-CZ-NH2	9.61	129.97	119.40
1	A	224	ARG	NE-CZ-NH1	-9.53	115.54	120.30
1	A	447	SER	N-CA-CB	-9.40	96.40	110.50
1	A	342	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	A	486	ASP	CB-CG-OD2	-9.35	109.89	118.30
1	A	488	TYR	CB-CG-CD1	9.31	126.59	121.00
1	A	370	THR	CA-CB-OG1	-9.30	89.47	109.00
1	A	667	TYR	CB-CG-CD2	9.24	126.54	121.00
1	A	365	SER	CA-C-O	-9.18	100.82	120.10
1	A	70	ALA	CB-CA-C	8.94	123.50	110.10
1	A	673	ASN	CB-CG-OD1	-8.90	103.79	121.60
1	A	309	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	456	LYS	CA-CB-CG	8.79	132.75	113.40
1	A	374	ALA	N-CA-CB	8.71	122.30	110.10
1	A	325	PHE	O-C-N	-8.67	108.83	122.70
1	A	626	ASP	O-C-N	8.59	136.45	122.70
1	A	133	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	685	ALA	N-CA-CB	-8.51	98.18	110.10
1	A	121	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	A	524	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	29	VAL	CB-CA-C	8.37	127.31	111.40
1	A	220	ASP	CB-CG-OD1	8.36	125.83	118.30
1	A	325	PHE	CA-C-O	8.35	137.64	120.10
1	A	617	GLN	O-C-N	8.33	136.03	122.70
1	A	249	ARG	NH1-CZ-NH2	8.32	128.55	119.40
1	A	370	THR	CA-CB-CG2	8.31	124.04	112.40
1	A	547	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	672	THR	CA-CB-CG2	-8.27	100.82	112.40
1	A	265	ASP	OD1-CG-OD2	8.26	138.99	123.30
1	A	344	ARG	NE-CZ-NH1	8.24	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	91	HIS	O-C-N	8.14	135.72	122.70
1	A	30	ARG	CD-NE-CZ	8.10	134.93	123.60
1	A	236	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	113	LYS	CD-CE-NZ	8.05	130.21	111.70
1	A	366	GLU	C-N-CA	8.00	139.09	122.30
1	A	139	THR	CA-CB-CG2	7.84	123.38	112.40
1	A	211	GLU	OE1-CD-OE2	-7.80	113.94	123.30
1	A	352	GLU	O-C-N	7.78	135.14	122.70
1	A	672	THR	OG1-CB-CG2	7.66	127.62	110.00
1	A	313	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	A	648	GLU	CG-CD-OE2	7.58	133.45	118.30
1	A	372	SER	O-C-N	7.54	134.76	122.70
1	A	156	SER	CB-CA-C	-7.50	95.85	110.10
1	A	255	VAL	CA-CB-CG2	7.48	122.11	110.90
1	A	518	VAL	CA-CB-CG1	7.47	122.10	110.90
1	A	654	HIS	CA-CB-CG	-7.46	100.92	113.60
1	A	151	ARG	CD-NE-CZ	-7.44	113.18	123.60
1	A	4	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	A	332	ARG	CG-CD-NE	-7.40	96.26	111.80
1	A	39	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	119	LEU	CB-CG-CD2	-7.39	98.43	111.00
1	A	210	ARG	NH1-CZ-NH2	7.39	127.53	119.40
1	A	673	ASN	CA-CB-CG	-7.39	97.15	113.40
1	A	448	LEU	CA-CB-CG	7.38	132.27	115.30
1	A	326	THR	CA-CB-OG1	-7.35	93.57	109.00
1	A	271	LEU	CB-CG-CD2	-7.33	98.53	111.00
1	A	465	ARG	CD-NE-CZ	7.32	133.85	123.60
1	A	162	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	489	PHE	CB-CG-CD1	-7.32	115.68	120.80
1	A	502	ASN	O-C-N	7.31	134.40	122.70
1	A	629	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	629	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	514	GLU	OE1-CD-OE2	7.19	131.92	123.30
1	A	661	LYS	CB-CA-C	-7.18	96.04	110.40
1	A	356	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	427	CYS	CA-CB-SG	7.14	126.86	114.00
1	A	512	GLU	CB-CA-C	-7.13	96.15	110.40
1	A	446	THR	N-CA-CB	-7.11	96.80	110.30
1	A	465	ARG	NH1-CZ-NH2	-7.11	111.58	119.40
1	A	444	SER	C-N-CA	7.10	139.44	121.70
1	A	549	THR	CA-CB-CG2	7.09	122.33	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	A	537	GLU	OE1-CD-OE2	7.06	131.78	123.30
1	A	146	GLU	CG-CD-OE2	7.04	132.37	118.30
1	A	629	ASP	CA-CB-CG	7.01	128.83	113.40
1	A	93	TYR	CA-CB-CG	-7.01	100.08	113.40
1	A	555	ASP	CA-CB-CG	6.99	128.78	113.40
1	A	392	MET	CA-CB-CG	-6.98	101.43	113.30
1	A	149	VAL	CB-CA-C	6.98	124.66	111.40
1	A	548	VAL	N-CA-CB	-6.96	96.19	111.50
1	A	160	GLY	CA-C-N	6.95	132.49	117.20
1	A	353	GLN	CG-CD-OE1	6.91	135.41	121.60
1	A	580	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	A	308	SER	CA-CB-OG	-6.89	92.60	111.20
1	A	45	CYS	CB-CA-C	6.88	124.17	110.40
1	A	147	ALA	CB-CA-C	6.87	120.41	110.10
1	A	383	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	A	103	SER	N-CA-C	-6.86	92.47	111.00
1	A	24	ARG	CA-CB-CG	6.86	128.49	113.40
1	A	413	GLU	CG-CD-OE2	6.84	131.98	118.30
1	A	337	GLU	O-C-N	-6.81	111.80	122.70
1	A	341	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	648	GLU	CG-CD-OE1	-6.80	104.70	118.30
1	A	678	SER	CA-C-O	6.78	134.33	120.10
1	A	309	ARG	CD-NE-CZ	6.77	133.07	123.60
1	A	617	GLN	N-CA-CB	6.77	122.78	110.60
1	A	662	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	A	689	LEU	CB-CG-CD2	-6.75	99.52	111.00
1	A	333	LYS	CA-CB-CG	-6.74	98.56	113.40
1	A	120	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	A	319	TYR	CB-CG-CD2	6.73	125.04	121.00
1	A	200	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	335	GLU	CG-CD-OE2	6.67	131.64	118.30
1	A	632	CYS	CA-CB-SG	-6.64	102.05	114.00
1	A	171	ARG	NE-CZ-NH2	6.64	123.62	120.30
1	A	210	ARG	CA-CB-CG	6.62	127.97	113.40
1	A	451	ASN	CB-CG-OD1	6.59	134.78	121.60
1	A	224	ARG	NH1-CZ-NH2	6.58	126.64	119.40
1	A	623	ASN	CB-CA-C	6.56	123.51	110.40
1	A	631	PHE	CA-C-O	6.54	133.82	120.10
1	A	569	ALA	N-CA-CB	-6.53	100.95	110.10
1	A	65	TYR	CB-CG-CD2	6.53	124.92	121.00
1	A	528	TYR	CB-CG-CD1	-6.52	117.09	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	601	SER	N-CA-CB	6.51	120.27	110.50
1	A	249	ARG	CG-CD-NE	6.51	125.46	111.80
1	A	623	ASN	CA-CB-CG	6.49	127.68	113.40
1	A	220	ASP	N-CA-CB	6.42	122.16	110.60
1	A	75	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	280	LYS	CA-CB-CG	6.39	127.46	113.40
1	A	51	GLU	CA-CB-CG	6.39	127.45	113.40
1	A	371	CYS	CB-CA-C	-6.38	97.64	110.40
1	A	402	ALA	CA-C-N	-6.38	103.45	116.20
1	A	335	GLU	CG-CD-OE1	-6.37	105.55	118.30
1	A	119	LEU	O-C-N	6.37	132.90	122.70
1	A	92	TYR	CB-CG-CD1	6.36	124.82	121.00
1	A	443	ARG	CA-C-N	-6.36	103.21	117.20
1	A	144	PRO	CB-CA-C	-6.34	96.14	112.00
1	A	557	ASN	N-CA-C	-6.34	93.89	111.00
1	A	10	ALA	CB-CA-C	6.33	119.59	110.10
1	A	104	PHE	O-C-N	6.29	132.76	122.70
1	A	205	ASP	OD1-CG-OD2	6.28	135.22	123.30
1	A	491	GLN	N-CA-CB	6.26	121.87	110.60
1	A	151	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	211	GLU	CG-CD-OE1	6.25	130.79	118.30
1	A	623	ASN	N-CA-CB	-6.24	99.37	110.60
1	A	265	ASP	N-CA-CB	6.24	121.83	110.60
1	A	626	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	473	MET	CA-CB-CG	6.21	123.86	113.30
1	A	661	LYS	N-CA-CB	6.18	121.72	110.60
1	A	151	ARG	CB-CG-CD	6.17	127.63	111.60
1	A	488	TYR	CB-CG-CD2	-6.16	117.30	121.00
1	A	614	LEU	CB-CA-C	6.16	121.90	110.20
1	A	492	SER	CA-C-O	6.16	133.03	120.10
1	A	93	TYR	N-CA-CB	-6.15	99.52	110.60
1	A	230	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	65	TYR	CA-CB-CG	-6.15	101.72	113.40
1	A	89	ARG	CG-CD-NE	6.13	124.67	111.80
1	A	303	SER	N-CA-CB	-6.13	101.31	110.50
1	A	557	ASN	O-C-N	6.12	132.50	122.70
1	A	265	ASP	CB-CG-OD1	-6.12	112.80	118.30
1	A	213	THR	CA-CB-OG1	-6.11	96.17	109.00
1	A	29	VAL	N-CA-CB	-6.10	98.08	111.50
1	A	406	GLY	CA-C-O	-6.09	109.64	120.60
1	A	571	PHE	O-C-N	6.09	132.44	122.70
1	A	493	CYS	N-CA-CB	6.08	121.54	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	443	ARG	CA-C-O	6.06	132.83	120.10
1	A	87	GLN	CA-CB-CG	-6.06	100.07	113.40
1	A	412	ALA	N-CA-CB	-6.05	101.62	110.10
1	A	606	VAL	N-CA-C	6.05	127.35	111.00
1	A	144	PRO	O-C-N	6.05	132.37	122.70
1	A	548	VAL	CB-CA-C	6.05	122.89	111.40
1	A	685	ALA	CB-CA-C	6.03	119.14	110.10
1	A	602	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	A	514	GLU	CA-CB-CG	6.00	126.61	113.40
1	A	127	VAL	CA-CB-CG1	5.99	119.88	110.90
1	A	484	LYS	O-C-N	5.96	132.24	122.70
1	A	384	VAL	CA-CB-CG1	5.96	119.83	110.90
1	A	601	SER	CB-CA-C	-5.96	98.78	110.10
1	A	500	ARG	CB-CA-C	5.93	122.27	110.40
1	A	66	GLU	OE1-CD-OE2	5.93	130.42	123.30
1	A	262	GLY	N-CA-C	5.93	127.92	113.10
1	A	103	SER	O-C-N	5.93	132.18	122.70
1	A	342	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
1	A	26	MET	CG-SD-CE	5.91	109.65	100.20
1	A	680	SER	N-CA-CB	5.89	119.34	110.50
1	A	528	TYR	CD1-CG-CD2	5.89	124.38	117.90
1	A	91	HIS	N-CA-CB	5.89	121.20	110.60
1	A	622	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	192	TYR	CA-C-O	5.87	132.42	120.10
1	A	511	GLU	CB-CG-CD	5.87	130.04	114.20
1	A	608	ARG	CG-CD-NE	-5.87	99.48	111.80
1	A	180	LYS	CA-CB-CG	-5.86	100.51	113.40
1	A	104	PHE	N-CA-CB	5.85	121.13	110.60
1	A	319	TYR	O-C-N	5.84	132.05	122.70
1	A	11	VAL	CG1-CB-CG2	5.84	120.24	110.90
1	A	552	GLN	CA-C-O	-5.83	107.86	120.10
1	A	620	PHE	O-C-N	5.83	133.11	123.20
1	A	329	GLN	CA-C-N	5.83	130.01	117.20
1	A	52	ASN	OD1-CG-ND2	5.81	135.26	121.90
1	A	416	LYS	O-C-N	5.80	131.99	122.70
1	A	132	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	A	163	LYS	CA-C-N	-5.80	104.60	116.20
1	A	393	SER	N-CA-CB	5.79	119.19	110.50
1	A	47	GLN	CA-CB-CG	5.79	126.14	113.40
1	A	163	LYS	CB-CA-C	-5.78	98.83	110.40
1	A	623	ASN	CA-C-N	-5.78	104.64	116.20
1	A	270	LEU	CA-CB-CG	5.77	128.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	ASP	CA-C-O	-5.76	108.01	120.10
1	A	303	SER	CB-CA-C	5.75	121.03	110.10
1	A	23	GLN	C-N-CA	5.74	136.05	121.70
1	A	598	ALA	N-CA-CB	5.74	118.13	110.10
1	A	178	GLU	CB-CG-CD	5.72	129.65	114.20
1	A	309	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	426	ASN	CB-CA-C	5.72	121.84	110.40
1	A	630	LYS	CA-CB-CG	-5.71	100.83	113.40
1	A	337	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	A	348	CYS	C-N-CA	5.69	135.93	121.70
1	A	491	GLN	CB-CA-C	-5.69	99.02	110.40
1	A	634	PHE	CG-CD2-CE2	5.68	127.05	120.80
1	A	86	ARG	CA-C-N	-5.68	104.71	117.20
1	A	623	ASN	O-C-N	5.67	132.84	123.20
1	A	187	GLU	CA-C-O	5.67	132.00	120.10
1	A	244	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	198	CYS	CA-CB-SG	5.66	124.19	114.00
1	A	652	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	298	LEU	CB-CA-C	5.65	120.93	110.20
1	A	227	TYR	CA-C-O	5.64	131.95	120.10
1	A	233	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	667	TYR	CG-CD1-CE1	5.64	125.81	121.30
1	A	526	TYR	CD1-CE1-CZ	5.63	124.87	119.80
1	A	396	GLY	CA-C-O	-5.62	110.48	120.60
1	A	304	ALA	N-CA-C	-5.62	95.84	111.00
1	A	525	TYR	CB-CG-CD1	5.61	124.37	121.00
1	A	168	ASN	O-C-N	5.59	131.65	122.70
1	A	487	GLU	CG-CD-OE1	-5.59	107.11	118.30
1	A	178	GLU	CG-CD-OE1	5.59	129.48	118.30
1	A	546	LYS	CD-CE-NZ	-5.58	98.86	111.70
1	A	363	GLY	C-N-CA	5.58	135.65	121.70
1	A	451	ASN	CB-CA-C	5.58	121.55	110.40
1	A	136	LEU	CA-C-O	-5.57	108.41	120.10
1	A	240	ASP	CA-CB-CG	-5.57	101.16	113.40
1	A	173	CYS	CA-CB-SG	-5.55	104.00	114.00
1	A	352	GLU	CB-CA-C	-5.55	99.29	110.40
1	A	224	ARG	CG-CD-NE	-5.55	100.14	111.80
1	A	173	CYS	CB-CA-C	5.54	121.48	110.40
1	A	421	SER	O-C-N	5.53	131.55	122.70
1	A	316	SER	O-C-N	5.52	132.58	123.20
1	A	564	LYS	N-CA-C	5.52	125.90	111.00
1	A	96	ALA	N-CA-CB	5.51	117.82	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	65	TYR	CG-CD1-CE1	5.50	125.70	121.30
1	A	628	PRO	N-CA-CB	-5.50	96.55	102.60
1	A	217	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	489	PHE	CD1-CG-CD2	5.48	125.43	118.30
1	A	104	PHE	N-CA-C	-5.46	96.26	111.00
1	A	423	PRO	N-CA-C	-5.46	97.90	112.10
1	A	612	VAL	CA-CB-CG2	5.45	119.08	110.90
1	A	197	LYS	O-C-N	5.45	131.41	122.70
1	A	282	LYS	C-N-CA	5.44	135.30	121.70
1	A	285	LYS	N-CA-CB	-5.43	100.83	110.60
1	A	603	MET	CB-CG-SD	-5.42	96.13	112.40
1	A	625	SER	CA-C-N	5.42	129.12	117.20
1	A	185	SER	N-CA-CB	-5.41	102.39	110.50
1	A	518	VAL	CB-CA-C	5.41	121.67	111.40
1	A	601	SER	O-C-N	5.40	131.34	122.70
1	A	574	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	558	ASN	N-CA-CB	5.38	120.29	110.60
1	A	373	SER	C-N-CA	5.38	135.16	121.70
1	A	184	SER	O-C-N	5.37	131.29	122.70
1	A	242	PHE	CA-C-O	-5.37	108.83	120.10
1	A	436	LEU	CA-C-O	-5.36	108.84	120.10
1	A	241	LYS	CB-CA-C	-5.36	99.69	110.40
1	A	24	ARG	CD-NE-CZ	5.35	131.09	123.60
1	A	507	CYS	CA-CB-SG	-5.35	104.37	114.00
1	A	267	ILE	O-C-N	5.35	131.25	122.70
1	A	511	GLU	CB-CA-C	5.34	121.08	110.40
1	A	491	GLN	CG-CD-OE1	-5.34	110.93	121.60
1	A	8	TRP	N-CA-CB	5.33	120.20	110.60
1	A	320	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	A	224	ARG	N-CA-CB	5.32	120.17	110.60
1	A	224	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	407	LEU	CA-C-O	-5.30	108.96	120.10
1	A	388	GLU	CG-CD-OE1	-5.30	107.70	118.30
1	A	104	PHE	CA-CB-CG	5.29	126.59	113.90
1	A	445	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	548	VAL	CA-CB-CG1	5.27	118.80	110.90
1	A	680	SER	O-C-N	5.26	131.10	121.10
1	A	281	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	642	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	A	690	ARG	CG-CD-NE	-5.25	100.77	111.80
1	A	386	LYS	CA-CB-CG	-5.25	101.84	113.40
1	A	371	CYS	CA-CB-SG	-5.25	104.56	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	431	PRO	N-CA-CB	5.25	109.59	103.30
1	A	98	VAL	CA-CB-CG1	5.24	118.76	110.90
1	A	619	LYS	CA-C-O	-5.24	109.11	120.10
1	A	691	LYS	CA-C-O	-5.21	109.15	120.10
1	A	596	ASN	O-C-N	5.19	131.01	122.70
1	A	512	GLU	N-CA-CB	5.19	119.94	110.60
1	A	528	TYR	CG-CD2-CE2	-5.19	117.15	121.30
1	A	312	PRO	O-C-N	5.18	131.00	122.70
1	A	24	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	559	ASN	CB-CG-OD1	5.17	131.94	121.60
1	A	628	PRO	O-C-N	5.17	130.97	122.70
1	A	354	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	52	ASN	CB-CG-OD1	-5.16	111.29	121.60
1	A	44	GLN	O-C-N	5.15	130.94	122.70
1	A	559	ASN	CA-C-O	-5.15	109.29	120.10
1	A	493	CYS	CA-C-N	-5.14	105.88	117.20
1	A	175	GLY	CA-C-O	5.14	129.85	120.60
1	A	78	ALA	N-CA-CB	-5.14	102.91	110.10
1	A	287	GLN	N-CA-CB	5.14	119.85	110.60
1	A	347	TRP	CG-CD1-NE1	-5.13	104.97	110.10
1	A	278	PHE	N-CA-C	5.13	124.85	111.00
1	A	55	ASP	O-C-N	5.12	130.90	122.70
1	A	545	VAL	CA-CB-CG1	5.12	118.59	110.90
1	A	594	ALA	CB-CA-C	5.12	117.79	110.10
1	A	8	TRP	CB-CA-C	-5.11	100.17	110.40
1	A	489	PHE	CA-C-O	-5.11	109.37	120.10
1	A	24	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	A	76	PRO	N-CA-CB	5.10	109.42	103.30
1	A	315	ASP	N-CA-CB	-5.10	101.42	110.60
1	A	571	PHE	CA-CB-CG	-5.10	101.66	113.90
1	A	236	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	347	TRP	CD1-NE1-CE2	5.10	113.59	109.00
1	A	413	GLU	OE1-CD-OE2	-5.09	117.20	123.30
1	A	112	LEU	CB-CA-C	5.08	119.86	110.20
1	A	669	ALA	CA-C-N	-5.08	106.03	116.20
1	A	139	THR	CA-CB-OG1	-5.08	98.33	109.00
1	A	302	ASP	CB-CA-C	5.08	120.56	110.40
1	A	208	PHE	CA-C-N	-5.07	106.04	117.20
1	A	318	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	372	SER	CA-C-O	-5.07	109.46	120.10
1	A	672	THR	CB-CA-C	-5.07	97.92	111.60
1	A	430	ARG	CG-CD-NE	5.05	122.41	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	359	ASN	CA-C-N	-5.05	106.09	117.20
1	A	602	ARG	CA-C-O	-5.04	109.51	120.10
1	A	441	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	A	146	GLU	CG-CD-OE1	-5.03	108.24	118.30
1	A	514	GLU	CG-CD-OE2	-5.03	108.24	118.30
1	A	87	GLN	CB-CA-C	5.02	120.44	110.40
1	A	385	LEU	CB-CA-C	5.02	119.74	110.20
1	A	255	VAL	CB-CA-C	5.02	120.93	111.40
1	A	57	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	497	SER	N-CA-CB	5.01	118.01	110.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	ARG	Sidechain
1	A	442	ARG	Sidechain
1	A	602	ARG	Sidechain
1	A	690	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	5322	0	5163	487	0
2	B	38	0	34	13	0
3	C	24	0	22	7	0
4	A	2	0	0	0	0
5	A	8	0	0	3	0
6	A	301	0	0	18	0
All	All	5695	0	5219	497	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 47.

All (497) 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:87:GLN:H	1:A:88:PRO:CD	1.43	1.28
2:B:1:NAG:O4	2:B:2:NAG:N2	1.68	1.24
1:A:295:GLN:HE21	1:A:295:GLN:N	1.47	1.12
1:A:87:GLN:H	1:A:88:PRO:HD3	0.99	1.12
1:A:283:SER:HB3	1:A:285:LYS:HD3	1.25	1.10
1:A:13:ASN:HB3	1:A:14:PRO:HD3	1.32	1.10
1:A:427:CYS:O	1:A:649:CYS:SG	2.12	1.08
1:A:283:SER:O	1:A:285:LYS:HG3	1.54	1.08
1:A:564:LYS:HE3	1:A:565:ASP:OD2	1.51	1.07
1:A:278:PHE:HE1	1:A:285:LYS:HE2	1.20	1.07
1:A:231:CYS:SG	1:A:235:THR:HG22	1.94	1.06
1:A:4:ARG:HD3	1:A:5:SER:N	1.70	1.06
1:A:295:GLN:HE21	1:A:295:GLN:CA	1.70	1.04
1:A:278:PHE:HE1	1:A:285:LYS:CE	1.71	1.03
1:A:71:PRO:HA	1:A:73:LYS:HE3	1.42	1.01
1:A:422:ASP:HB3	1:A:423:PRO:CD	1.91	1.00
1:A:4:ARG:CD	1:A:5:SER:H	1.75	0.99
1:A:475:LEU:CD2	3:C:1:NAG:H81	1.92	0.98
1:A:4:ARG:CD	1:A:5:SER:N	2.26	0.98
1:A:137:ASN:HD22	2:B:1:NAG:H83	1.26	0.98
1:A:278:PHE:CE1	1:A:285:LYS:HE2	1.97	0.97
1:A:417:SER:C	1:A:419:GLN:H	1.56	0.96
1:A:295:GLN:HA	1:A:295:GLN:NE2	1.81	0.95
1:A:87:GLN:N	1:A:88:PRO:HD3	1.82	0.95
1:A:436:LEU:HD12	1:A:593:MET:HE3	1.48	0.94
1:A:436:LEU:CD1	1:A:593:MET:HE3	2.00	0.91
1:A:622:ARG:HD3	1:A:622:ARG:O	1.70	0.91
1:A:561:ALA:HA	1:A:564:LYS:CG	1.99	0.91
1:A:294:GLY:C	1:A:295:GLN:HE21	1.74	0.91
2:B:1:NAG:O4	2:B:2:NAG:C2	2.18	0.91
1:A:70:ALA:HA	1:A:73:LYS:HD2	1.52	0.90
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.34	0.90
1:A:283:SER:HB3	1:A:285:LYS:CD	2.01	0.90
1:A:687:GLU:HG3	1:A:688:PHE:H	1.38	0.88
1:A:25:ASN:H	1:A:25:ASN:HD22	1.18	0.88
1:A:3:ARG:HA	1:A:266:ALA:HB2	1.57	0.87
1:A:87:GLN:N	1:A:88:PRO:CD	2.23	0.86
1:A:427:CYS:SG	1:A:648:GLU:HG2	2.15	0.86
1:A:25:ASN:HD22	1:A:25:ASN:N	1.68	0.85
1:A:295:GLN:CA	1:A:295:GLN:NE2	2.31	0.85
1:A:322:SER:O	1:A:326:THR:HB	1.77	0.85
2:B:1:NAG:C3	2:B:2:NAG:C1	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASP:O	1:A:424:ASP:N	2.11	0.84
1:A:25:ASN:OD1	1:A:286:PHE:HB2	1.78	0.83
1:A:295:GLN:CB	1:A:298:LEU:HD11	2.07	0.83
1:A:314:ILE:HD13	1:A:689:LEU:CD1	2.09	0.83
1:A:220:ASP:HB3	1:A:223:GLU:HG3	1.61	0.83
1:A:119:LEU:O	1:A:120:ARG:HB2	1.77	0.83
1:A:436:LEU:CD1	1:A:593:MET:CE	2.57	0.83
1:A:13:ASN:HB3	1:A:14:PRO:CD	2.08	0.82
1:A:421:SER:HB3	1:A:424:ASP:HB2	1.61	0.82
1:A:344:ARG:CD	1:A:370:THR:HG22	2.09	0.82
1:A:564:LYS:CE	1:A:565:ASP:OD2	2.28	0.82
1:A:137:ASN:ND2	2:B:1:NAG:H83	1.93	0.82
1:A:4:ARG:HD2	1:A:5:SER:H	1.41	0.81
1:A:344:ARG:HD2	1:A:370:THR:CG2	2.08	0.81
1:A:658:THR:OG1	1:A:661:LYS:HG3	1.80	0.81
1:A:417:SER:C	1:A:419:GLN:N	2.32	0.81
1:A:687:GLU:HG3	1:A:688:PHE:N	1.95	0.80
1:A:475:LEU:CD2	3:C:1:NAG:C8	2.60	0.80
1:A:105:GLN:HB2	1:A:107:ASN:ND2	1.97	0.79
1:A:417:SER:HB2	1:A:420:SER:H	1.47	0.79
1:A:475:LEU:HD22	3:C:1:NAG:C8	2.13	0.78
1:A:442:ARG:O	1:A:445:ASP:HB2	1.83	0.78
1:A:155:ALA:HB2	1:A:171:ARG:NH1	1.98	0.78
1:A:333:LYS:HB3	1:A:338:VAL:HG23	1.65	0.78
1:A:17:THR:O	1:A:21:GLN:HG3	1.84	0.78
1:A:219:SER:HA	6:A:1201:HOH:O	1.83	0.77
1:A:295:GLN:N	1:A:295:GLN:NE2	2.29	0.77
1:A:105:GLN:HB2	1:A:107:ASN:HD21	1.48	0.77
1:A:3:ARG:HA	1:A:266:ALA:CB	2.14	0.77
1:A:293:SER:HA	6:A:1052:HOH:O	1.84	0.77
1:A:295:GLN:HB2	1:A:298:LEU:HD11	1.67	0.77
1:A:3:ARG:CA	1:A:266:ALA:HB2	2.16	0.76
1:A:314:ILE:HD13	1:A:689:LEU:HD13	1.65	0.76
1:A:171:ARG:HG2	1:A:171:ARG:NH1	1.93	0.76
1:A:475:LEU:HD22	3:C:1:NAG:H81	1.65	0.76
1:A:238:PRO:HB2	1:A:240:ASP:OD1	1.86	0.76
1:A:175:GLY:O	1:A:180:LYS:HG3	1.86	0.76
1:A:620:PHE:HB3	1:A:631:PHE:O	1.85	0.76
1:A:38:LYS:O	1:A:39:ARG:NH1	2.16	0.76
1:A:107:ASN:H	1:A:107:ASN:HD22	1.33	0.75
1:A:463:VAL:O	1:A:464:ASP:HB2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:NAG:C4	2:B:2:NAG:C1	2.63	0.74
1:A:115:CYS:SG	1:A:204:GLY:HA3	2.27	0.74
1:A:608:ARG:HA	1:A:611:GLN:HG2	1.67	0.74
1:A:533:ARG:O	1:A:537:GLU:HG3	1.86	0.74
1:A:409:PRO:HB2	1:A:653:LEU:HD11	1.69	0.74
1:A:422:ASP:HB3	1:A:423:PRO:HD3	1.67	0.74
1:A:238:PRO:HG2	1:A:241:LYS:HD2	1.70	0.74
1:A:684:GLU:O	1:A:687:GLU:CG	2.36	0.74
1:A:688:PHE:HD1	1:A:689:LEU:CD1	2.02	0.73
1:A:231:CYS:SG	1:A:235:THR:CG2	2.75	0.73
1:A:322:SER:HB3	1:A:385:LEU:O	1.88	0.73
1:A:171:ARG:HH11	1:A:171:ARG:CG	2.01	0.73
1:A:390:ASP:OD2	1:A:605:LYS:HE2	1.88	0.73
1:A:4:ARG:HD3	1:A:5:SER:HB3	1.71	0.73
1:A:241:LYS:HA	1:A:241:LYS:HZ2	1.52	0.72
1:A:187:GLU:OE2	1:A:189:TYR:HB2	1.89	0.72
1:A:12:SER:OG	1:A:14:PRO:HD2	1.88	0.72
1:A:235:THR:CG2	1:A:237:LYS:HD2	2.19	0.72
1:A:436:LEU:HD13	1:A:593:MET:CE	2.19	0.72
1:A:475:LEU:HD23	3:C:1:NAG:H81	1.71	0.72
1:A:292:PRO:O	1:A:294:GLY:N	2.23	0.71
1:A:235:THR:HG21	1:A:237:LYS:HD2	1.72	0.71
1:A:548:VAL:HA	1:A:551:LEU:HD12	1.73	0.71
1:A:422:ASP:HB3	1:A:423:PRO:HD2	1.71	0.71
1:A:38:LYS:O	1:A:39:ARG:HG2	1.90	0.71
1:A:229:LEU:O	1:A:236:ARG:HA	1.90	0.71
1:A:260:VAL:CG1	1:A:261:ASN:N	2.54	0.70
1:A:260:VAL:CG1	1:A:261:ASN:H	2.04	0.70
1:A:283:SER:CB	1:A:285:LYS:HD3	2.14	0.70
1:A:445:ASP:O	1:A:580:ARG:NH1	2.25	0.70
1:A:231:CYS:CB	1:A:235:THR:HG22	2.20	0.70
1:A:352:GLU:OE1	1:A:352:GLU:N	2.21	0.69
1:A:156:SER:CA	1:A:172:LEU:HD12	2.22	0.69
1:A:344:ARG:HD2	1:A:370:THR:HG22	1.70	0.69
1:A:684:GLU:O	1:A:687:GLU:HG2	1.92	0.69
1:A:344:ARG:CD	1:A:370:THR:CG2	2.67	0.69
1:A:196:PHE:CZ	1:A:200:ARG:HD2	2.28	0.69
1:A:554:THR:O	1:A:557:ASN:HB2	1.92	0.69
1:A:624:GLY:O	1:A:626:ASP:N	2.26	0.68
1:A:137:ASN:HD22	2:B:1:NAG:C8	2.02	0.68
1:A:561:ALA:HA	1:A:564:LYS:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:O	1:A:237:LYS:HG3	1.94	0.68
1:A:485:PHE:CZ	1:A:674:LEU:HD22	2.28	0.68
1:A:638:THR:HA	6:A:1223:HOH:O	1.93	0.68
1:A:4:ARG:HD3	1:A:5:SER:CB	2.24	0.67
1:A:119:LEU:O	1:A:120:ARG:CB	2.43	0.67
1:A:409:PRO:HB2	1:A:653:LEU:CD1	2.24	0.67
1:A:13:ASN:O	1:A:17:THR:HG23	1.95	0.67
1:A:260:VAL:HG13	1:A:261:ASN:N	2.09	0.67
1:A:105:GLN:N	1:A:108:GLU:OE1	2.26	0.66
1:A:510:ASP:HB3	1:A:515:ASN:HD22	1.61	0.66
1:A:14:PRO:HB2	1:A:298:LEU:HD21	1.76	0.66
1:A:436:LEU:HD13	1:A:593:MET:HE1	1.78	0.66
1:A:622:ARG:HD3	1:A:622:ARG:C	2.15	0.66
1:A:395:ASP:HA	1:A:597:HIS:CD2	2.31	0.66
1:A:688:PHE:HD1	1:A:689:LEU:HD13	1.58	0.65
1:A:220:ASP:O	1:A:223:GLU:HB2	1.95	0.65
1:A:241:LYS:HZ3	1:A:241:LYS:N	1.94	0.65
1:A:367:GLY:HA2	6:A:1191:HOH:O	1.96	0.65
1:A:278:PHE:CE1	1:A:285:LYS:CE	2.62	0.65
1:A:314:ILE:CD1	1:A:689:LEU:HD13	2.26	0.65
1:A:294:GLY:C	1:A:295:GLN:NE2	2.48	0.64
1:A:14:PRO:O	1:A:298:LEU:HD22	1.97	0.64
1:A:22:TRP:HB2	1:A:286:PHE:CZ	2.32	0.64
2:B:1:NAG:O4	2:B:2:NAG:C1	2.45	0.64
1:A:344:ARG:HD3	1:A:370:THR:HG22	1.79	0.64
1:A:295:GLN:HE21	1:A:295:GLN:HA	1.43	0.63
1:A:237:LYS:HB3	1:A:238:PRO:HD2	1.80	0.63
1:A:387:GLY:HA2	1:A:602:ARG:NH1	2.14	0.63
1:A:295:GLN:HB2	1:A:298:LEU:CD1	2.29	0.63
1:A:510:ASP:C	1:A:510:ASP:OD1	2.36	0.63
1:A:241:LYS:CA	1:A:241:LYS:NZ	2.62	0.62
1:A:314:ILE:HD13	1:A:689:LEU:HD11	1.80	0.62
1:A:69:LEU:O	1:A:72:TYR:HB2	1.98	0.62
1:A:231:CYS:HB2	1:A:235:THR:HG22	1.81	0.62
1:A:106:LEU:HG	1:A:106:LEU:O	2.00	0.62
1:A:422:ASP:CB	1:A:423:PRO:CD	2.70	0.62
1:A:610:LYS:O	1:A:614:LEU:HB2	2.00	0.62
1:A:155:ALA:HB1	1:A:171:ARG:HG2	1.80	0.62
1:A:502:ASN:O	1:A:505:ALA:HB3	2.00	0.62
1:A:14:PRO:HA	1:A:17:THR:HG23	1.82	0.62
1:A:18:LYS:HG2	1:A:299:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:NAG:O3	2:B:2:NAG:O5	2.17	0.61
1:A:12:SER:HB3	1:A:15:GLU:HG3	1.81	0.61
1:A:134:PRO:HB3	6:A:1253:HOH:O	1.98	0.61
1:A:667:TYR:HB2	6:A:1143:HOH:O	2.00	0.61
1:A:684:GLU:O	1:A:687:GLU:HG3	2.00	0.61
1:A:669:ALA:O	1:A:672:THR:HB	2.01	0.61
1:A:125:TRP:CH2	1:A:149:VAL:HG11	2.34	0.61
1:A:688:PHE:CD1	1:A:689:LEU:CD1	2.84	0.61
1:A:86:ARG:CA	1:A:88:PRO:HD3	2.29	0.61
1:A:344:ARG:HD2	1:A:370:THR:HG21	1.81	0.61
1:A:313:ARG:O	1:A:313:ARG:HG3	2.01	0.61
1:A:133:ARG:NH2	1:A:330:ASN:O	2.34	0.61
1:A:608:ARG:HA	1:A:611:GLN:CG	2.30	0.61
1:A:51:GLU:OE1	1:A:53:ARG:HD2	2.01	0.60
2:B:1:NAG:C4	2:B:2:NAG:HN2	2.10	0.60
1:A:170:CYS:O	1:A:171:ARG:C	2.39	0.60
1:A:271:LEU:O	1:A:275:GLN:HB3	2.01	0.60
1:A:25:ASN:N	1:A:25:ASN:ND2	2.44	0.60
1:A:41:SER:OG	1:A:44:GLN:HG3	2.01	0.60
1:A:532:PHE:CE1	1:A:550:VAL:HG22	2.37	0.60
1:A:457:LYS:HB3	1:A:506:LEU:HD11	1.83	0.60
1:A:200:ARG:HG2	1:A:227:TYR:OH	2.02	0.60
1:A:283:SER:C	1:A:285:LYS:HG3	2.22	0.59
1:A:361:TRP:CD1	1:A:361:TRP:C	2.75	0.59
1:A:548:VAL:CA	1:A:551:LEU:HD12	2.32	0.59
1:A:24:ARG:O	1:A:28:LYS:HB3	2.02	0.59
1:A:361:TRP:CD1	1:A:361:TRP:O	2.56	0.59
1:A:637:GLU:HG2	1:A:638:THR:HG23	1.85	0.58
1:A:509:GLY:CA	1:A:516:LYS:HA	2.32	0.58
1:A:485:PHE:HZ	1:A:674:LEU:HD22	1.66	0.58
1:A:55:ASP:OD1	1:A:258:ARG:NH2	2.35	0.58
1:A:295:GLN:CB	1:A:298:LEU:CD1	2.81	0.58
1:A:162:ASP:HB3	1:A:166:PHE:CD2	2.39	0.58
1:A:470:ASN:ND2	1:A:671:ILE:HD13	2.18	0.58
1:A:561:ALA:HA	1:A:564:LYS:HG2	1.84	0.58
1:A:38:LYS:C	1:A:39:ARG:HG2	2.24	0.57
1:A:218:LEU:HD23	1:A:224:ARG:HA	1.85	0.57
1:A:241:LYS:HA	1:A:241:LYS:NZ	2.17	0.57
1:A:688:PHE:CD1	1:A:689:LEU:HD12	2.39	0.57
1:A:4:ARG:CD	1:A:5:SER:HB3	2.34	0.57
1:A:41:SER:HB2	1:A:42:PRO:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:PRO:HB3	1:A:146:GLU:OE1	2.04	0.57
1:A:514:GLU:O	1:A:515:ASN:HB2	2.05	0.57
1:A:146:GLU:OE1	1:A:146:GLU:N	2.34	0.57
1:A:51:GLU:O	1:A:53:ARG:HG2	2.05	0.57
1:A:384:VAL:O	1:A:602:ARG:HD3	2.04	0.56
1:A:475:LEU:HD23	3:C:1:NAG:C8	2.30	0.56
1:A:191:SER:HB3	6:A:1221:HOH:O	2.04	0.56
1:A:154:SER:O	1:A:168:ASN:ND2	2.39	0.56
1:A:4:ARG:CD	1:A:5:SER:CB	2.82	0.56
1:A:10:ALA:HB1	1:A:15:GLU:HB3	1.87	0.56
1:A:680:SER:HB2	1:A:681:PRO:CD	2.35	0.56
1:A:173:CYS:CB	1:A:181:CYS:HB2	2.35	0.56
1:A:173:CYS:HB2	1:A:181:CYS:HB2	1.86	0.56
1:A:260:VAL:HG12	1:A:261:ASN:H	1.69	0.56
1:A:344:ARG:HG3	1:A:345:VAL:N	2.21	0.56
1:A:502:ASN:O	1:A:505:ALA:CB	2.53	0.56
1:A:4:ARG:HD3	1:A:5:SER:CA	2.36	0.56
1:A:445:ASP:OD1	1:A:448:LEU:HD23	2.05	0.56
1:A:165:GLN:C	1:A:167:PRO:HD3	2.25	0.56
1:A:417:SER:O	1:A:419:GLN:N	2.36	0.56
1:A:547:ASP:OD1	1:A:547:ASP:N	2.38	0.56
1:A:29:VAL:HG21	1:A:285:LYS:NZ	2.22	0.55
1:A:26:MET:CE	1:A:278:PHE:HE2	2.18	0.55
1:A:155:ALA:CB	1:A:171:ARG:HG2	2.36	0.55
1:A:220:ASP:OD2	1:A:222:ALA:HB3	2.07	0.55
1:A:13:ASN:CB	1:A:14:PRO:CD	2.78	0.55
1:A:459:CYS:SG	1:A:540:GLY:HA3	2.47	0.55
1:A:398:TYR:HA	1:A:401:THR:HG23	1.89	0.55
1:A:458:SER:HB2	1:A:544:PHE:HE2	1.71	0.55
1:A:680:SER:HB2	1:A:681:PRO:HD2	1.89	0.55
1:A:581:LYS:HD2	1:A:589:CYS:HB2	1.89	0.54
1:A:561:ALA:HA	1:A:564:LYS:CD	2.36	0.54
1:A:672:THR:HG22	1:A:673:ASN:N	2.16	0.54
1:A:359:ASN:O	1:A:362:SER:HB3	2.08	0.54
1:A:110:GLN:HB2	1:A:152:PHE:CE1	2.43	0.53
1:A:390:ASP:HB3	1:A:605:LYS:HG2	1.90	0.53
1:A:241:LYS:N	1:A:241:LYS:NZ	2.56	0.53
1:A:26:MET:HE2	1:A:278:PHE:HE2	1.73	0.53
1:A:112:LEU:O	1:A:153:PHE:HB3	2.08	0.53
1:A:666:GLN:H	1:A:666:GLN:NE2	2.06	0.53
1:A:27:ARG:HE	1:A:33:PRO:HB3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:CD1	1:A:57:VAL:HG12	2.39	0.53
1:A:14:PRO:HA	1:A:17:THR:CG2	2.39	0.53
1:A:352:GLU:HG2	6:A:1179:HOH:O	2.09	0.53
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.74	0.53
1:A:582:PRO:HD2	1:A:585:GLU:HB2	1.91	0.53
1:A:365:SER:HB2	1:A:368:SER:OG	2.08	0.52
1:A:561:ALA:O	1:A:564:LYS:HG3	2.09	0.52
1:A:401:THR:CG2	6:A:1166:HOH:O	2.57	0.52
1:A:466:THR:HG22	1:A:471:ILE:HD12	1.91	0.52
1:A:123:ALA:HB3	5:A:695:CO3:O1	2.10	0.52
1:A:241:LYS:HZ3	1:A:241:LYS:CA	2.23	0.52
1:A:531:ALA:HB3	1:A:545:VAL:CG1	2.40	0.52
1:A:561:ALA:CA	1:A:564:LYS:HG3	2.40	0.52
1:A:165:GLN:O	1:A:167:PRO:HD3	2.10	0.52
1:A:657:THR:HB	6:A:1138:HOH:O	2.10	0.52
1:A:22:TRP:HB2	1:A:286:PHE:HZ	1.73	0.52
1:A:132:LEU:C	1:A:134:PRO:HD2	2.29	0.51
1:A:531:ALA:O	1:A:534:CYS:HB3	2.11	0.51
1:A:133:ARG:N	1:A:134:PRO:CD	2.73	0.51
1:A:295:GLN:CG	1:A:298:LEU:HD11	2.40	0.51
1:A:410:VAL:HG13	1:A:606:VAL:HG13	1.93	0.51
1:A:636:SER:O	1:A:637:GLU:O	2.27	0.51
1:A:427:CYS:O	1:A:427:CYS:SG	2.69	0.51
1:A:587:ARG:HH11	1:A:587:ARG:HB2	1.74	0.51
1:A:628:PRO:HB3	1:A:632:CYS:SG	2.50	0.51
1:A:510:ASP:OD1	1:A:512:GLU:N	2.41	0.51
1:A:14:PRO:CB	1:A:295:GLN:HG3	2.41	0.51
1:A:435:TYR:HE1	1:A:595:PRO:O	1.94	0.51
1:A:470:ASN:ND2	1:A:671:ILE:CD1	2.74	0.51
1:A:529:THR:HG21	6:A:1181:HOH:O	2.11	0.51
1:A:278:PHE:HE1	1:A:285:LYS:HE3	1.69	0.50
1:A:435:TYR:O	1:A:593:MET:CE	2.58	0.50
1:A:17:THR:O	1:A:21:GLN:CG	2.58	0.50
1:A:42:PRO:O	1:A:46:ILE:HG13	2.11	0.50
1:A:113:LYS:O	1:A:205:ASP:HB2	2.11	0.50
1:A:430:ARG:NH2	1:A:648:GLU:CD	2.65	0.50
1:A:133:ARG:NH1	1:A:138:TRP:CZ3	2.80	0.50
1:A:428:VAL:HG12	1:A:652:ARG:HG3	1.94	0.50
1:A:430:ARG:HH21	1:A:648:GLU:CD	2.14	0.50
1:A:561:ALA:C	1:A:564:LYS:HG3	2.32	0.50
1:A:395:ASP:OD2	1:A:465:ARG:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG12	1:A:264:GLU:HG2	1.93	0.50
1:A:353:GLN:HE22	1:A:639:LYS:NZ	2.10	0.50
1:A:86:ARG:HA	1:A:88:PRO:HD3	1.92	0.50
1:A:334:SER:HB2	1:A:336:GLU:H	1.76	0.50
1:A:156:SER:N	1:A:172:LEU:HD12	2.27	0.49
1:A:330:ASN:N	1:A:330:ASN:HD22	2.07	0.49
1:A:86:ARG:HB2	1:A:86:ARG:NH1	2.26	0.49
1:A:485:PHE:HZ	1:A:674:LEU:CD2	2.24	0.49
1:A:20:PHE:O	1:A:23:GLN:HB3	2.12	0.49
1:A:233:ASP:OD1	1:A:235:THR:HB	2.12	0.49
1:A:531:ALA:HB3	1:A:545:VAL:HG12	1.93	0.49
1:A:593:MET:HE3	1:A:593:MET:HA	1.93	0.49
1:A:607:GLU:O	1:A:611:GLN:HG2	2.12	0.49
1:A:12:SER:OG	1:A:14:PRO:CD	2.58	0.49
1:A:75:ARG:HH12	1:A:310:VAL:HG12	1.77	0.49
1:A:168:ASN:HA	1:A:171:ARG:HB2	1.95	0.49
1:A:3:ARG:CB	1:A:266:ALA:HB2	2.43	0.48
1:A:48:ALA:O	1:A:49:ILE:C	2.51	0.48
1:A:174:ALA:HB3	1:A:188:PRO:HG2	1.95	0.48
1:A:218:LEU:HG	1:A:223:GLU:HB3	1.95	0.48
1:A:344:ARG:HD3	1:A:370:THR:CG2	2.40	0.48
1:A:477:PHE:HD1	1:A:482:SER:O	1.96	0.48
1:A:197:LYS:O	1:A:200:ARG:N	2.46	0.48
1:A:227:TYR:CD1	1:A:227:TYR:N	2.82	0.48
1:A:466:THR:HG21	1:A:594:ALA:CB	2.43	0.48
1:A:601:SER:OG	1:A:602:ARG:N	2.47	0.48
1:A:105:GLN:HA	1:A:105:GLN:NE2	2.29	0.48
1:A:162:ASP:CG	1:A:165:GLN:HG3	2.34	0.48
1:A:238:PRO:CG	1:A:241:LYS:HD2	2.40	0.48
1:A:518:VAL:HG22	1:A:519:PRO:HD2	1.94	0.48
1:A:624:GLY:O	1:A:627:CYS:N	2.36	0.48
1:A:85:GLU:O	1:A:86:ARG:NH1	2.45	0.48
1:A:123:ALA:CB	5:A:695:CO3:O1	2.61	0.48
1:A:441:VAL:HG21	1:A:574:LEU:CD1	2.44	0.48
1:A:558:ASN:OD1	1:A:560:GLU:HG3	2.14	0.48
1:A:15:GLU:HG2	1:A:298:LEU:HD23	1.95	0.48
1:A:173:CYS:HB3	1:A:181:CYS:N	2.29	0.48
1:A:561:ALA:HA	1:A:564:LYS:HD3	1.94	0.48
1:A:636:SER:HB2	1:A:641:LEU:HD22	1.95	0.48
1:A:485:PHE:CZ	1:A:674:LEU:CD2	2.95	0.48
1:A:21:GLN:O	1:A:25:ASN:ND2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:VAL:HG21	1:A:574:LEU:HD11	1.96	0.47
1:A:70:ALA:HA	1:A:73:LYS:CD	2.35	0.47
1:A:138:TRP:CZ2	1:A:140:GLY:HA2	2.49	0.47
1:A:71:PRO:HA	1:A:73:LYS:CE	2.28	0.47
1:A:550:VAL:HG12	1:A:568:LEU:HD12	1.96	0.47
1:A:13:ASN:N	1:A:14:PRO:HD2	2.29	0.47
1:A:397:GLY:HA3	1:A:464:ASP:O	2.14	0.47
1:A:617:GLN:O	1:A:621:GLY:N	2.46	0.47
1:A:624:GLY:C	1:A:626:ASP:H	2.18	0.47
1:A:628:PRO:CB	1:A:632:CYS:SG	3.03	0.47
1:A:639:LYS:O	1:A:640:ASN:HB2	2.13	0.47
1:A:277:LYS:HA	1:A:277:LYS:HD3	1.63	0.47
1:A:352:GLU:H	1:A:352:GLU:CD	2.13	0.47
1:A:687:GLU:O	1:A:690:ARG:HB2	2.14	0.47
1:A:14:PRO:CA	1:A:17:THR:HG23	2.44	0.47
1:A:82:TYR:CE2	1:A:252:SER:HB2	2.50	0.47
1:A:162:ASP:HB3	1:A:166:PHE:HD2	1.79	0.47
1:A:173:CYS:SG	1:A:181:CYS:SG	3.13	0.47
1:A:231:CYS:N	1:A:235:THR:O	2.32	0.47
1:A:397:GLY:O	1:A:400:TYR:HB3	2.14	0.47
1:A:78:ALA:HB3	1:A:255:VAL:HB	1.97	0.46
1:A:137:ASN:ND2	2:B:1:NAG:C8	2.69	0.46
1:A:353:GLN:HE22	1:A:639:LYS:HZ3	1.64	0.46
1:A:631:PHE:HE2	1:A:633:LEU:HD13	1.80	0.46
1:A:145:ILE:O	1:A:149:VAL:HG12	2.14	0.46
1:A:431:PRO:HG3	1:A:654:HIS:CD2	2.51	0.46
1:A:86:ARG:HB2	1:A:86:ARG:CZ	2.45	0.46
1:A:116:HIS:N	1:A:116:HIS:CD2	2.83	0.46
1:A:163:LYS:HE2	1:A:180:LYS:HE2	1.95	0.46
1:A:548:VAL:HA	1:A:551:LEU:CD1	2.42	0.46
1:A:627:CYS:HA	1:A:628:PRO:HA	1.67	0.46
1:A:221:GLU:HB3	1:A:224:ARG:HH11	1.79	0.46
1:A:576:LEU:HD21	1:A:591:LEU:HD22	1.97	0.46
1:A:26:MET:CE	1:A:274:ALA:HA	2.45	0.46
1:A:86:ARG:O	1:A:87:GLN:HB2	2.15	0.46
1:A:272:ARG:CD	6:A:1237:HOH:O	2.62	0.46
1:A:424:ASP:HB3	1:A:648:GLU:OE2	2.16	0.46
1:A:156:SER:HB2	1:A:169:LEU:HA	1.97	0.46
1:A:282:LYS:HE2	1:A:283:SER:OG	2.15	0.46
1:A:394:LEU:HD12	1:A:600:VAL:HG21	1.98	0.46
1:A:60:ASP:O	1:A:64:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLY:O	1:A:197:LYS:HB3	2.15	0.46
1:A:196:PHE:O	1:A:199:LEU:HB3	2.16	0.46
1:A:587:ARG:HA	1:A:587:ARG:HD3	1.70	0.46
1:A:333:LYS:CB	1:A:338:VAL:HG23	2.42	0.46
1:A:284:PRO:O	1:A:285:LYS:C	2.52	0.45
1:A:7:GLN:HB3	1:A:37:ILE:HD13	1.98	0.45
1:A:344:ARG:CD	1:A:370:THR:HG21	2.43	0.45
1:A:675:LYS:HD3	1:A:675:LYS:HA	1.80	0.45
1:A:187:GLU:HA	1:A:188:PRO:HD2	1.62	0.45
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.61	0.45
1:A:40:ASP:HB2	1:A:44:GLN:OE1	2.17	0.45
1:A:180:LYS:HE2	1:A:180:LYS:HB3	1.52	0.45
1:A:147:ALA:O	1:A:151:ARG:HG3	2.16	0.45
1:A:313:ARG:HB3	1:A:685:ALA:HB2	1.97	0.45
1:A:463:VAL:O	1:A:464:ASP:CB	2.57	0.45
1:A:27:ARG:O	1:A:30:ARG:HA	2.17	0.45
1:A:613:LEU:HD23	1:A:613:LEU:HA	1.75	0.45
1:A:509:GLY:HA3	1:A:514:GLU:O	2.16	0.45
1:A:29:VAL:HG21	1:A:285:LYS:HZ3	1.80	0.45
1:A:238:PRO:HD2	1:A:241:LYS:HD2	1.99	0.45
1:A:507:CYS:HB3	1:A:523:GLU:OE1	2.17	0.45
1:A:107:ASN:ND2	1:A:107:ASN:H	2.06	0.45
1:A:666:GLN:H	1:A:666:GLN:CD	2.19	0.45
1:A:68:GLY:O	1:A:73:LYS:HA	2.17	0.44
1:A:491:GLN:HB3	1:A:505:ALA:HB3	1.99	0.44
1:A:107:ASN:HD22	1:A:107:ASN:N	2.03	0.44
1:A:196:PHE:CE2	1:A:200:ARG:HD2	2.52	0.44
1:A:39:ARG:HD2	1:A:44:GLN:HB3	1.99	0.44
1:A:134:PRO:CB	6:A:1253:HOH:O	2.60	0.44
1:A:432:VAL:HB	1:A:596:ASN:OD1	2.17	0.44
1:A:302:ASP:HB2	6:A:1271:HOH:O	2.17	0.44
1:A:86:ARG:HA	1:A:86:ARG:HH11	1.82	0.44
1:A:173:CYS:HB3	1:A:181:CYS:H	1.81	0.44
1:A:591:LEU:N	1:A:591:LEU:HD23	2.29	0.44
1:A:189:TYR:C	1:A:194:GLY:HA3	2.37	0.44
1:A:273:GLN:O	1:A:276:GLU:N	2.51	0.44
1:A:354:GLU:HB3	1:A:642:LEU:HD23	2.00	0.44
1:A:390:ASP:CG	1:A:605:LYS:HE2	2.37	0.44
1:A:461:THR:HG21	5:A:696:CO3:O3	2.17	0.44
1:A:14:PRO:HB2	1:A:295:GLN:HG3	1.99	0.44
1:A:330:ASN:N	1:A:330:ASN:ND2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:THR:HG21	1:A:594:ALA:HB1	1.99	0.44
1:A:593:MET:CE	1:A:593:MET:HA	2.48	0.44
1:A:291:SER:OG	1:A:298:LEU:HB2	2.17	0.43
1:A:80:GLU:OE1	1:A:301:LYS:HB2	2.18	0.43
1:A:159:PRO:HG2	1:A:190:PHE:HA	2.00	0.43
1:A:236:ARG:C	1:A:237:LYS:HG3	2.39	0.43
1:A:238:PRO:HG2	1:A:241:LYS:CD	2.44	0.43
1:A:40:ASP:N	1:A:44:GLN:OE1	2.51	0.43
1:A:155:ALA:HB1	1:A:171:ARG:HB3	2.01	0.43
1:A:158:VAL:O	1:A:159:PRO:C	2.57	0.43
1:A:581:LYS:HB3	1:A:582:PRO:HD2	2.01	0.43
1:A:197:LYS:O	1:A:198:CYS:C	2.56	0.43
1:A:285:LYS:H	1:A:285:LYS:HG2	1.31	0.43
1:A:30:ARG:HG3	1:A:30:ARG:HH11	1.84	0.43
1:A:128:PRO:HB3	1:A:208:PHE:CD1	2.54	0.43
1:A:509:GLY:HA2	1:A:516:LYS:HA	1.98	0.43
1:A:673:ASN:ND2	6:A:1145:HOH:O	2.51	0.43
1:A:272:ARG:HD3	6:A:1237:HOH:O	2.19	0.43
1:A:664:GLY:HA2	1:A:665:PRO:HD2	1.72	0.43
1:A:187:GLU:O	1:A:189:TYR:N	2.51	0.42
1:A:641:LEU:C	1:A:643:PHE:H	2.20	0.42
1:A:63:PHE:HA	1:A:66:GLU:HB2	2.01	0.42
1:A:146:GLU:HA	1:A:149:VAL:HG13	2.00	0.42
1:A:353:GLN:NE2	1:A:639:LYS:NZ	2.66	0.42
1:A:156:SER:C	1:A:172:LEU:HD12	2.40	0.42
1:A:219:SER:O	1:A:220:ASP:C	2.57	0.42
1:A:495:PRO:HB3	1:A:518:VAL:O	2.20	0.42
1:A:10:ALA:HB1	1:A:15:GLU:CB	2.49	0.42
1:A:622:ARG:C	1:A:622:ARG:CD	2.86	0.42
1:A:89:ARG:NH2	1:A:211:GLU:OE2	2.51	0.42
1:A:498:ASP:HA	1:A:499:PRO:HD2	1.65	0.42
1:A:231:CYS:HB3	1:A:232:PRO:HD2	2.02	0.42
1:A:477:PHE:O	1:A:481:GLY:HA2	2.20	0.42
1:A:343:ALA:O	1:A:608:ARG:NH2	2.52	0.42
1:A:414:ASN:O	1:A:648:GLU:N	2.47	0.42
1:A:619:LYS:NZ	6:A:1066:HOH:O	2.53	0.42
1:A:29:VAL:CG2	1:A:285:LYS:NZ	2.82	0.42
1:A:19:CYS:O	1:A:36:CYS:SG	2.78	0.42
1:A:91:HIS:HB2	1:A:250:VAL:O	2.20	0.42
1:A:214:VAL:H	1:A:214:VAL:HG12	1.40	0.42
1:A:430:ARG:HA	1:A:431:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.89	0.42
1:A:594:ALA:HA	1:A:595:PRO:HD3	1.83	0.42
3:C:1:NAG:H4	3:C:2:FUC:C1	2.50	0.42
1:A:2:ARG:O	1:A:3:ARG:CB	2.67	0.42
1:A:441:VAL:HG12	1:A:541:ASP:O	2.20	0.42
1:A:5:SER:HA	1:A:33:PRO:O	2.20	0.41
1:A:231:CYS:HB2	1:A:233:ASP:OD1	2.20	0.41
1:A:302:ASP:O	1:A:303:SER:HB2	2.20	0.41
1:A:352:GLU:N	1:A:352:GLU:CD	2.73	0.41
1:A:37:ILE:HG12	1:A:53:ARG:O	2.20	0.41
1:A:162:ASP:OD1	1:A:162:ASP:C	2.59	0.41
1:A:250:VAL:HB	1:A:251:PRO:HD2	2.03	0.41
1:A:165:GLN:HB2	1:A:166:PHE:CD2	2.55	0.41
1:A:202:GLY:O	1:A:203:ALA:C	2.56	0.41
1:A:631:PHE:CE2	1:A:633:LEU:HD13	2.55	0.41
1:A:221:GLU:HB3	1:A:224:ARG:NH1	2.35	0.41
1:A:511:GLU:N	6:A:1082:HOH:O	2.45	0.41
2:B:1:NAG:O4	2:B:2:NAG:H2	2.15	0.41
1:A:361:TRP:HB2	1:A:631:PHE:CZ	2.56	0.41
1:A:125:TRP:CH2	1:A:149:VAL:CG1	3.03	0.41
1:A:196:PHE:HZ	1:A:218:LEU:HD22	1.85	0.41
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.34	0.41
1:A:508:ILE:HG13	1:A:524:ARG:HB2	2.02	0.41
1:A:547:ASP:O	1:A:551:LEU:HD12	2.21	0.41
1:A:628:PRO:CA	1:A:632:CYS:SG	3.09	0.41
1:A:12:SER:OG	1:A:13:ASN:N	2.54	0.41
1:A:32:PRO:HA	1:A:33:PRO:HD3	1.85	0.41
1:A:65:TYR:OH	1:A:329:GLN:HG2	2.21	0.41
1:A:159:PRO:HB3	1:A:182:ALA:O	2.20	0.41
1:A:220:ASP:CG	1:A:221:GLU:N	2.74	0.41
1:A:353:GLN:NE2	1:A:639:LYS:HZ2	2.19	0.41
1:A:424:ASP:OD1	1:A:425:PRO:HD2	2.20	0.41
2:B:1:NAG:C4	2:B:2:NAG:N2	2.75	0.41
1:A:509:GLY:N	1:A:516:LYS:HA	2.36	0.40
1:A:658:THR:OG1	1:A:661:LYS:CG	2.61	0.40
1:A:672:THR:CG2	1:A:673:ASN:N	2.74	0.40
1:A:163:LYS:HE3	1:A:180:LYS:O	2.21	0.40
1:A:269:ASN:O	1:A:270:LEU:C	2.57	0.40
1:A:414:ASN:HD22	1:A:651:ALA:HB2	1.85	0.40
1:A:484:LYS:HB2	1:A:484:LYS:HE3	1.63	0.40
1:A:636:SER:CB	1:A:641:LEU:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:O	1:A:417:SER:O	2.39	0.40
1:A:38:LYS:O	1:A:39:ARG:CG	2.66	0.40
1:A:133:ARG:CB	1:A:134:PRO:HD3	2.52	0.40
1:A:472:PRO:O	1:A:476:LEU:HG	2.21	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%)	590 (86%)	83 (12%)	16 (2%)	5 2

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	3	ARG
1	A	4	ARG
1	A	87	GLN
1	A	293	SER
1	A	417	SER
1	A	625	SER
1	A	637	GLU
1	A	85	GLU
1	A	418	GLN
1	A	678	SER
1	A	423	PRO
1	A	416	LYS
1	A	284	PRO
1	A	422	ASP
1	A	159	PRO

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	570/574 (99%)	461 (81%)	109 (19%)	1 0

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	13	ASN
1	A	17	THR
1	A	21	GLN
1	A	24	ARG
1	A	25	ASN
1	A	30	ARG
1	A	53	ARG
1	A	59	LEU
1	A	66	GLU
1	A	73	LYS
1	A	85	GLU
1	A	86	ARG
1	A	87	GLN
1	A	103	SER
1	A	107	ASN
1	A	112	LEU
1	A	113	LYS
1	A	120	ARG
1	A	121	ARG
1	A	133	ARG
1	A	134	PRO
1	A	139	THR
1	A	144	PRO
1	A	149	VAL
1	A	151	ARG
1	A	154	SER
1	A	159	PRO
1	A	168	ASN
1	A	171	ARG

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Mol	Chain	Res	Type
1	A	172	LEU
1	A	176	THR
1	A	178	GLU
1	A	180	LYS
1	A	186	GLN
1	A	191	SER
1	A	193	SER
1	A	209	ILE
1	A	218	LEU
1	A	221	GLU
1	A	225	ASP
1	A	235	THR
1	A	240	ASP
1	A	241	LYS
1	A	244	ASP
1	A	260	VAL
1	A	265	ASP
1	A	270	LEU
1	A	271	LEU
1	A	275	GLN
1	A	282	LYS
1	A	285	LYS
1	A	293	SER
1	A	295	GLN
1	A	301	LYS
1	A	326	THR
1	A	329	GLN
1	A	332	ARG
1	A	334	SER
1	A	344	ARG
1	A	352	GLU
1	A	356	ARG
1	A	364	LEU
1	A	384	VAL
1	A	401	THR
1	A	415	TYR
1	A	417	SER
1	A	426	ASN
1	A	436	LEU
1	A	445	ASP
1	A	447	SER
1	A	448	LEU

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Mol	Chain	Res	Type
1	A	449	THR
1	A	453	VAL
1	A	456	LYS
1	A	463	VAL
1	A	473	MET
1	A	484	LYS
1	A	512	GLU
1	A	518	VAL
1	A	551	LEU
1	A	557	ASN
1	A	564	LYS
1	A	575	CYS
1	A	587	ARG
1	A	593	MET
1	A	599	VAL
1	A	603	MET
1	A	610	LYS
1	A	614	LEU
1	A	622	ARG
1	A	623	ASN
1	A	625	SER
1	A	626	ASP
1	A	628	PRO
1	A	629	ASP
1	A	630	LYS
1	A	635	GLN
1	A	636	SER
1	A	641	LEU
1	A	656	LYS
1	A	657	THR
1	A	666	GLN
1	A	671	ILE
1	A	682	LEU
1	A	683	LEU
1	A	687	GLU
1	A	689	LEU
1	A	690	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN

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Mol	Chain	Res	Type
1	A	13	ASN
1	A	23	GLN
1	A	25	ASN
1	A	91	HIS
1	A	105	GLN
1	A	107	ASN
1	A	168	ASN
1	A	234	ASN
1	A	295	GLN
1	A	330	ASN
1	A	353	GLN
1	A	426	ASN
1	A	515	ASN
1	A	666	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

5 monosaccharides 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	B	1	2,1	14,14,15	1.64	2 (14%)	17,19,21	2.99	7 (41%)
2	NAG	B	2	2	14,14,15	2.04	4 (28%)	17,19,21	5.25	8 (47%)
2	FUL	B	3	2	10,10,11	1.73	2 (20%)	14,14,16	3.80	11 (78%)
3	NAG	C	1	3,1	14,14,15	1.44	1 (7%)	17,19,21	3.41	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FUC	C	2	3	10,10,11	1.47	2 (20%)	14,14,16	2.96	7 (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
2	NAG	B	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	B	2	2	-	3/6/23/26	0/1/1/1
2	FUL	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	5/6/23/26	0/1/1/1
3	FUC	C	2	3	1/1/4/5	-	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	-4.93	1.45	1.52
2	B	1	NAG	C2-N2	-4.44	1.38	1.46
2	B	3	FUL	O5-C5	4.02	1.51	1.43
3	C	1	NAG	O7-C7	-4.00	1.14	1.23
2	B	2	NAG	O5-C1	3.13	1.49	1.43
2	B	1	NAG	C3-C2	2.50	1.57	1.52
3	C	2	FUC	O5-C5	2.49	1.48	1.43
2	B	3	FUL	C2-C3	2.48	1.56	1.52
2	B	2	NAG	O7-C7	-2.43	1.17	1.23
3	C	2	FUC	O2-C2	2.30	1.48	1.43
2	B	2	NAG	C4-C5	2.09	1.57	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	C1-O5-C5	-14.08	93.32	112.19
3	C	1	NAG	C2-N2-C7	10.47	136.93	122.90
2	B	2	NAG	C1-C2-N2	10.29	126.64	110.43
2	B	1	NAG	C2-N2-C7	-9.10	110.70	122.90
2	B	2	NAG	O7-C7-N2	-7.78	108.23	121.98
3	C	2	FUC	C2-C3-C4	7.35	123.78	110.86
2	B	3	FUL	C1-C2-C3	-6.57	100.08	109.64
2	B	2	NAG	C8-C7-N2	5.99	126.05	116.12
2	B	3	FUL	C1-O5-C5	-5.47	100.07	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	NAG	O5-C1-C2	-5.22	103.21	111.29
2	B	3	FUL	O3-C3-C2	5.14	120.55	110.05
2	B	3	FUL	O2-C2-C1	5.13	120.98	109.22
2	B	1	NAG	C1-C2-N2	-4.85	102.79	110.43
2	B	3	FUL	O5-C1-C2	-4.56	99.92	110.79
3	C	1	NAG	C4-C3-C2	-4.53	104.38	111.02
2	B	3	FUL	C2-C3-C4	-4.45	103.04	110.86
2	B	2	NAG	C3-C4-C5	4.21	117.86	110.23
3	C	2	FUC	C1-C2-C3	4.01	115.49	109.64
3	C	1	NAG	O7-C7-C8	3.88	128.97	122.05
2	B	1	NAG	O4-C4-C5	-3.78	100.02	109.32
3	C	1	NAG	C6-C5-C4	-3.60	104.19	113.02
3	C	2	FUC	O2-C2-C3	3.38	117.16	110.15
3	C	1	NAG	O4-C4-C3	3.23	117.99	110.38
3	C	2	FUC	O4-C4-C5	3.22	116.85	109.74
2	B	1	NAG	C8-C7-N2	3.19	121.40	116.12
2	B	3	FUL	O2-C2-C3	3.14	116.65	110.15
2	B	3	FUL	O4-C4-C5	2.90	116.13	109.74
3	C	1	NAG	C1-C2-N2	2.89	114.98	110.43
3	C	2	FUC	O5-C1-C2	2.85	117.59	110.79
3	C	2	FUC	C1-O5-C5	2.80	119.56	112.97
3	C	1	NAG	C1-O5-C5	2.61	115.69	112.19
2	B	1	NAG	C1-O5-C5	2.45	115.47	112.19
2	B	2	NAG	O4-C4-C3	2.42	116.07	110.38
2	B	1	NAG	O7-C7-N2	-2.36	117.81	121.98
3	C	1	NAG	O7-C7-N2	-2.34	117.85	121.98
2	B	3	FUL	O5-C5-C4	2.32	113.72	109.55
3	C	2	FUC	O5-C5-C4	2.31	113.70	109.55
2	B	3	FUL	O5-C5-C6	-2.23	102.56	107.40
2	B	3	FUL	C6-C5-C4	2.09	116.91	113.08
2	B	2	NAG	O7-C7-C8	2.06	125.72	122.05
2	B	1	NAG	O5-C5-C6	-2.05	103.67	107.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	2	FUC	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C3-C2-N2-C7

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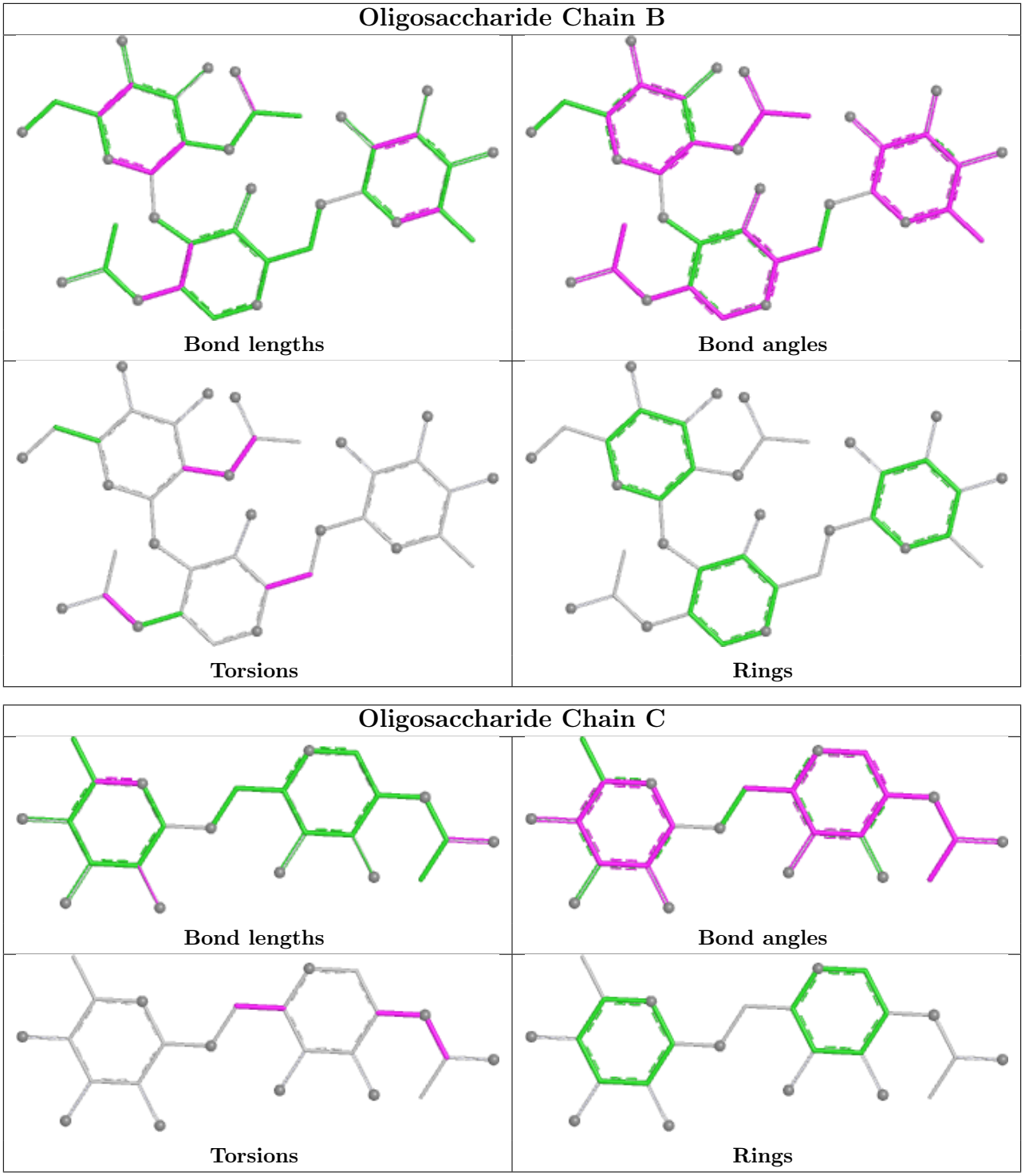
Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	B	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	C4-C5-C6-O6
3	C	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	13	0
3	C	1	NAG	7	0
3	C	2	FUC	1	0
2	B	2	NAG	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	CO3	A	696	4	3,3,3	0.85	0	2,3,3	1.48	0
5	CO3	A	695	4	3,3,3	0.87	0	2,3,3	2.14	1 (50%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	695	CO3	O3-C-O1	2.47	125.99	119.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	696	CO3	1	0
5	A	695	CO3	2	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.