



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:32 PM UTC

PDB ID : 1DOT / pdb_00001dot
Title : CRYSTALLOGRAPHIC STRUCTURE OF DUCK OVOTRANSFERRIN AT
2.3 ANGSTROMS RESOLUTION
Authors : Rawas, A.; Muirhead, H.
Deposited on : 1995-08-03
Resolution : 2.35 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

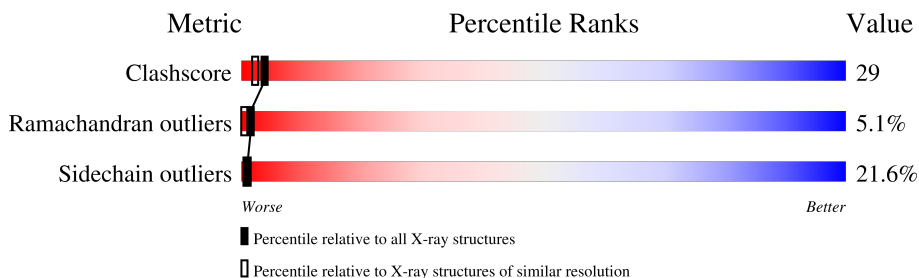
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	686	

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

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

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5665 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DUCK OVOTRANSFERRIN.

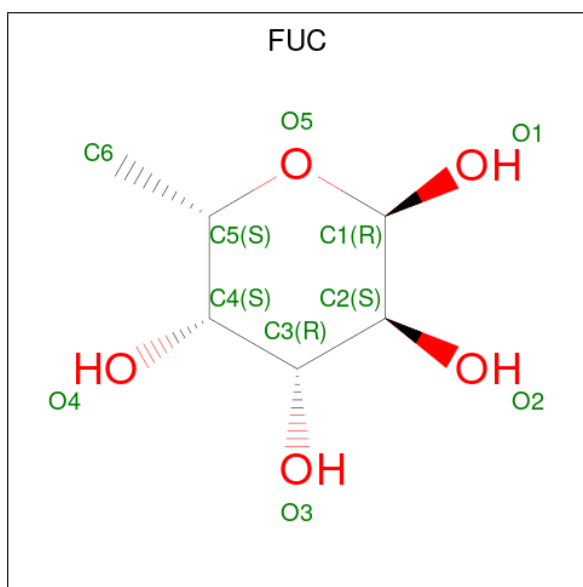
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	686	5299	3325	903	1032	39	0	0	0

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



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

- Molecule 3 is alpha-L-fucopyranose (CCD ID: FUC) (formula: $C_6H_{12}O_5$).

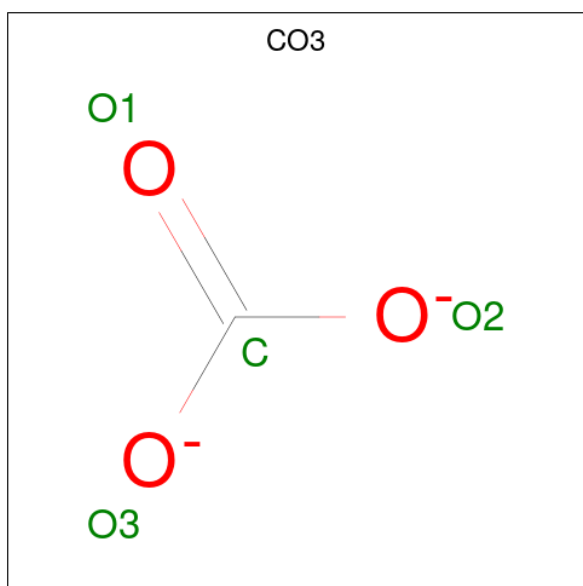


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



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

- Molecule 6 is water.

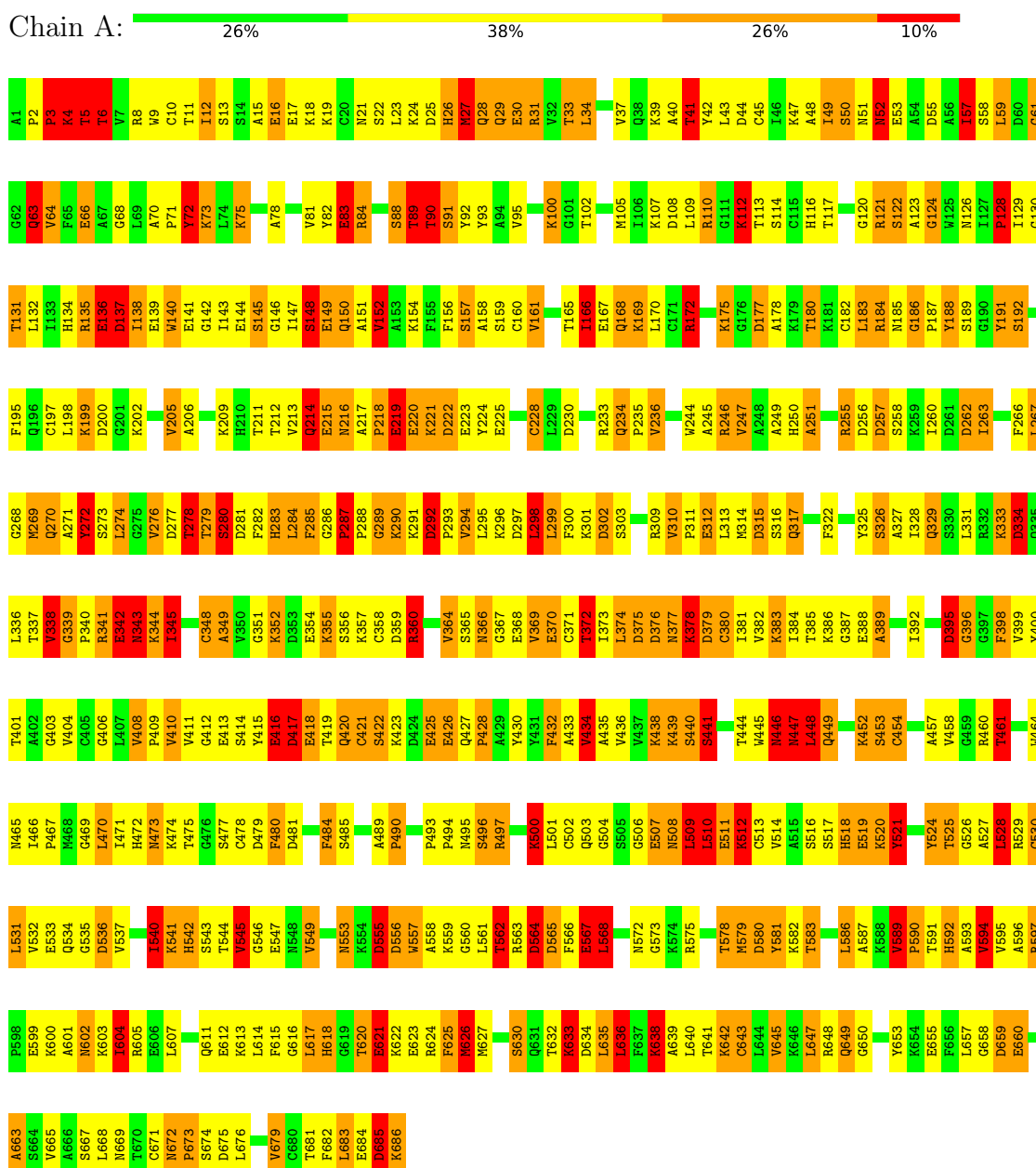
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	318	Total	O	0	0
			318	318		

3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: DUCK OVOTRANSFERRIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.60Å 85.60Å 178.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.35	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.35)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.230 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5665	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: FE, FUC, CO3, 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	1.69	60/5402 (1.1%)	3.20	707/7292 (9.7%)

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

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

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	ILE	N-CA	-20.34	1.21	1.46
1	A	70	ALA	CA-C	-18.36	1.34	1.53
1	A	136	GLU	N-CA	17.57	1.68	1.46
1	A	82	TYR	C-O	12.99	1.37	1.24
1	A	337	THR	CA-CB	11.12	1.68	1.53
1	A	4	LYS	N-CA	10.96	1.57	1.46
1	A	418	GLU	N-CA	-10.68	1.32	1.46
1	A	344	LYS	C-N	7.99	1.44	1.33
1	A	417	ASP	C-N	-7.98	1.22	1.33
1	A	5	THR	CA-CB	7.98	1.66	1.53
1	A	639	ALA	C-O	7.42	1.33	1.24
1	A	148	SER	CA-CB	7.31	1.65	1.53
1	A	349	ALA	C-N	-7.26	1.26	1.33
1	A	337	THR	C-O	7.26	1.33	1.23
1	A	148	SER	C-O	6.93	1.32	1.24
1	A	614	LEU	N-CA	-6.87	1.38	1.46
1	A	135	ARG	CD-NE	-6.72	1.36	1.46
1	A	135	ARG	NE-CZ	-6.67	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	597	ARG	N-CA	6.62	1.54	1.45
1	A	635	LEU	CA-C	-6.59	1.44	1.52
1	A	52	ASN	N-CA	6.57	1.56	1.46
1	A	180	THR	CA-CB	6.27	1.63	1.53
1	A	148	SER	CA-C	-6.03	1.44	1.52
1	A	5	THR	N-CA	6.02	1.53	1.46
1	A	206	ALA	N-CA	6.01	1.53	1.46
1	A	29	GLN	N-CA	-6.00	1.38	1.46
1	A	512	LYS	C-O	5.96	1.31	1.24
1	A	506	GLY	N-CA	5.86	1.53	1.45
1	A	71	PRO	CA-CB	-5.84	1.43	1.53
1	A	287	PRO	CA-CB	5.78	1.61	1.54
1	A	518	HIS	N-CA	-5.73	1.39	1.46
1	A	146	GLY	CA-C	5.71	1.56	1.52
1	A	41	THR	CA-CB	5.67	1.62	1.53
1	A	640	LEU	N-CA	5.58	1.53	1.46
1	A	475	THR	CA-CB	5.54	1.62	1.53
1	A	549	VAL	C-O	5.53	1.30	1.24
1	A	82	TYR	C-N	-5.52	1.25	1.33
1	A	435	ALA	N-CA	5.48	1.52	1.46
1	A	446	ASN	C-N	-5.44	1.25	1.33
1	A	583	THR	CA-CB	5.40	1.62	1.53
1	A	157	SER	N-CA	5.37	1.52	1.46
1	A	517	SER	C-N	-5.34	1.26	1.33
1	A	219	GLU	N-CA	-5.28	1.40	1.46
1	A	102	THR	C-O	5.28	1.30	1.23
1	A	58	SER	CA-CB	-5.26	1.46	1.53
1	A	89	THR	C-N	-5.25	1.26	1.33
1	A	71	PRO	CB-CG	-5.24	1.30	1.51
1	A	145	SER	N-CA	-5.24	1.39	1.46
1	A	29	GLN	CA-CB	5.23	1.61	1.53
1	A	123	ALA	C-N	-5.22	1.27	1.33
1	A	593	ALA	N-CA	5.19	1.52	1.45
1	A	172	ARG	C-O	5.18	1.30	1.24
1	A	257	ASP	C-O	5.16	1.30	1.24
1	A	286	GLY	N-CA	5.15	1.51	1.44
1	A	434	VAL	N-CA	5.15	1.51	1.46
1	A	82	TYR	CA-CB	5.12	1.63	1.53
1	A	3	PRO	C-N	5.08	1.43	1.34
1	A	591	THR	CA-CB	5.08	1.60	1.53
1	A	147	ILE	N-CA	5.05	1.52	1.46
1	A	300	PHE	N-CA	-5.01	1.39	1.45

All (707) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	LYS	CA-C-N	27.04	157.99	123.10
1	A	344	LYS	C-N-CA	27.04	157.99	123.10
1	A	417	ASP	CA-C-N	26.06	171.32	121.54
1	A	417	ASP	C-N-CA	26.06	171.32	121.54
1	A	135	ARG	CD-NE-CZ	25.52	160.12	124.40
1	A	334	ASP	CA-CB-CG	24.28	136.88	112.60
1	A	25	ASP	CA-CB-CG	23.83	136.43	112.60
1	A	344	LYS	O-C-N	-22.41	98.39	123.48
1	A	418	GLU	CB-CG-CD	21.45	149.07	112.60
1	A	141	GLU	CB-CG-CD	20.79	147.94	112.60
1	A	302	ASP	CA-CB-CG	19.42	132.02	112.60
1	A	2	PRO	N-CA-C	18.48	133.25	110.70
1	A	597	ARG	CD-NE-CZ	18.07	149.70	124.40
1	A	517	SER	CA-C-N	16.64	150.47	121.52
1	A	517	SER	C-N-CA	16.64	150.47	121.52
1	A	70	ALA	N-CA-CB	-16.61	83.90	109.98
1	A	28	GLN	CA-C-N	15.84	148.95	122.65
1	A	28	GLN	C-N-CA	15.84	148.95	122.65
1	A	6	THR	N-CA-C	15.78	133.61	110.10
1	A	396	GLY	CA-C-N	14.84	136.32	120.00
1	A	396	GLY	C-N-CA	14.84	136.32	120.00
1	A	148	SER	N-CA-C	14.76	142.25	110.80
1	A	287	PRO	N-CA-C	14.71	128.65	110.70
1	A	144	GLU	CA-C-N	14.44	149.12	121.54
1	A	144	GLU	C-N-CA	14.44	149.12	121.54
1	A	285	PHE	CA-CB-CG	13.93	127.73	113.80
1	A	21	ASN	CA-CB-CG	13.72	126.32	112.60
1	A	416	GLU	CA-C-N	13.67	142.47	120.60
1	A	416	GLU	C-N-CA	13.67	142.47	120.60
1	A	218	PRO	CA-C-N	13.66	139.02	120.44
1	A	218	PRO	C-N-CA	13.66	139.02	120.44
1	A	337	THR	N-CA-C	13.48	130.05	112.26
1	A	553	ASN	CA-CB-CG	13.34	125.94	112.60
1	A	385	THR	CA-CB-CG2	13.21	132.96	110.50
1	A	360	ARG	CD-NE-CZ	13.20	142.89	124.40
1	A	4	LYS	CA-C-N	12.96	139.87	120.82
1	A	4	LYS	C-N-CA	12.96	139.87	120.82
1	A	4	LYS	CA-C-O	12.94	132.97	119.51
1	A	258	SER	CA-C-N	12.80	141.15	122.21
1	A	258	SER	C-N-CA	12.80	141.15	122.21
1	A	359	ASP	CA-CB-CG	12.65	125.25	112.60
1	A	507	GLU	N-CA-CB	12.40	127.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	LEU	CA-C-N	12.38	141.93	122.62
1	A	299	LEU	C-N-CA	12.38	141.93	122.62
1	A	344	LYS	N-CA-C	-12.28	89.36	108.76
1	A	508	ASN	CA-CB-CG	12.10	124.70	112.60
1	A	417	ASP	CA-CB-CG	11.82	124.42	112.60
1	A	639	ALA	CA-C-O	-11.67	106.91	120.10
1	A	150	GLN	CA-C-N	11.63	140.25	121.18
1	A	150	GLN	C-N-CA	11.63	140.25	121.18
1	A	52	ASN	CB-CA-C	11.58	129.21	112.07
1	A	345	ILE	N-CA-C	-11.57	91.75	108.53
1	A	425	GLU	CB-CG-CD	11.52	132.19	112.60
1	A	507	GLU	N-CA-C	-11.45	100.02	114.56
1	A	82	TYR	N-CA-C	11.32	127.53	114.62
1	A	511	GLU	CA-CB-CG	11.26	136.61	114.10
1	A	542	HIS	CA-CB-CG	11.23	125.03	113.80
1	A	579	MET	CA-C-N	11.22	140.51	123.23
1	A	579	MET	C-N-CA	11.22	140.51	123.23
1	A	150	GLN	OE1-CD-NE2	-10.91	111.69	122.60
1	A	84	ARG	CA-CB-CG	10.89	135.87	114.10
1	A	633	LYS	CA-C-O	-10.75	105.13	120.51
1	A	344	LYS	CB-CA-C	10.74	129.82	110.16
1	A	315	ASP	CA-CB-CG	10.67	123.27	112.60
1	A	352	LYS	N-CA-C	10.65	125.54	112.54
1	A	342	GLU	CA-C-N	10.63	141.84	121.54
1	A	342	GLU	C-N-CA	10.63	141.84	121.54
1	A	136	GLU	N-CA-CB	-10.44	92.84	110.49
1	A	672	ASN	CA-CB-CG	10.40	123.00	112.60
1	A	426	GLU	CA-CB-CG	10.34	134.78	114.10
1	A	112	LYS	CA-CB-CG	10.30	134.69	114.10
1	A	297	ASP	CA-CB-CG	10.26	122.86	112.60
1	A	618	HIS	CA-CB-CG	10.26	124.06	113.80
1	A	29	GLN	CB-CG-CD	10.14	129.84	112.60
1	A	82	TYR	CA-C-O	-10.05	105.88	118.54
1	A	48	ALA	CA-C-O	-10.01	110.31	120.82
1	A	478	CYS	CA-C-N	9.99	140.46	122.38
1	A	478	CYS	C-N-CA	9.99	140.46	122.38
1	A	474	LYS	CA-C-N	9.85	134.28	120.29
1	A	474	LYS	C-N-CA	9.85	134.28	120.29
1	A	292	ASP	CB-CA-C	9.78	121.34	109.31
1	A	634	ASP	N-CA-CB	-9.75	94.99	110.69
1	A	658	GLY	CA-C-O	-9.73	114.83	122.52
1	A	375	ASP	CA-CB-CG	9.66	122.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	GLU	CB-CG-CD	9.63	128.97	112.60
1	A	199	LYS	CA-C-N	9.62	133.57	120.38
1	A	199	LYS	C-N-CA	9.62	133.57	120.38
1	A	150	GLN	CB-CG-CD	9.62	128.95	112.60
1	A	48	ALA	N-CA-C	-9.61	100.79	111.07
1	A	50	SER	CA-CB-OG	9.59	130.27	111.10
1	A	403	GLY	CA-C-N	9.57	136.00	120.30
1	A	403	GLY	C-N-CA	9.57	136.00	120.30
1	A	270	GLN	CB-CG-CD	9.50	128.75	112.60
1	A	83	GLU	CA-C-N	9.44	139.58	121.54
1	A	83	GLU	C-N-CA	9.44	139.58	121.54
1	A	31	ARG	CA-CB-CG	9.30	132.70	114.10
1	A	220	GLU	CB-CG-CD	9.28	128.38	112.60
1	A	71	PRO	N-CA-CB	9.23	112.76	102.60
1	A	601	ALA	N-CA-C	9.22	123.63	112.38
1	A	441	SER	CA-CB-OG	9.22	129.53	111.10
1	A	446	ASN	CA-CB-CG	9.20	121.80	112.60
1	A	17	GLU	CA-CB-CG	9.13	132.37	114.10
1	A	385	THR	CA-CB-OG1	-9.07	95.99	109.60
1	A	634	ASP	N-CA-C	-9.05	95.02	109.59
1	A	184	ARG	CD-NE-CZ	9.04	137.06	124.40
1	A	64	VAL	N-CA-C	-9.01	101.18	111.00
1	A	169	LYS	CA-C-N	8.97	133.95	120.31
1	A	169	LYS	C-N-CA	8.97	133.95	120.31
1	A	447	ASN	CA-CB-CG	8.92	121.52	112.60
1	A	642	LYS	CG-CD-CE	8.90	131.76	111.30
1	A	31	ARG	N-CA-CB	8.88	122.87	109.91
1	A	660	GLU	CA-CB-CG	8.87	131.84	114.10
1	A	526	GLY	CA-C-O	-8.86	111.63	120.75
1	A	377	ASN	CA-C-N	8.86	133.10	120.79
1	A	377	ASN	C-N-CA	8.86	133.10	120.79
1	A	589	VAL	N-CA-CB	-8.84	98.84	111.21
1	A	114	SER	CA-C-O	8.83	130.24	120.70
1	A	580	ASP	CA-CB-CG	8.82	121.42	112.60
1	A	423	LYS	CA-C-O	8.82	129.20	119.24
1	A	3	PRO	O-C-N	-8.80	110.76	122.64
1	A	191	TYR	CA-C-N	8.80	132.07	120.28
1	A	191	TYR	C-N-CA	8.80	132.07	120.28
1	A	293	PRO	CA-C-N	8.79	135.23	120.64
1	A	293	PRO	C-N-CA	8.79	135.23	120.64
1	A	216	ASN	OD1-CG-ND2	-8.76	113.84	122.60
1	A	563	ARG	CA-C-N	8.73	132.69	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	ARG	C-N-CA	8.73	132.69	120.29
1	A	123	ALA	CA-C-N	8.71	129.58	120.00
1	A	123	ALA	C-N-CA	8.71	129.58	120.00
1	A	148	SER	N-CA-CB	-8.70	95.79	110.49
1	A	519	GLU	CA-C-N	8.70	135.02	121.19
1	A	519	GLU	C-N-CA	8.70	135.02	121.19
1	A	338	VAL	N-CA-CB	8.69	125.56	111.23
1	A	617	LEU	CA-C-N	8.64	138.05	121.54
1	A	617	LEU	C-N-CA	8.64	138.05	121.54
1	A	475	THR	N-CA-C	8.62	120.76	111.36
1	A	49	ILE	CA-C-O	-8.62	111.72	120.85
1	A	423	LYS	CA-C-N	8.57	132.09	120.44
1	A	423	LYS	C-N-CA	8.57	132.09	120.44
1	A	135	ARG	CA-C-O	-8.54	111.92	120.89
1	A	13	SER	N-CA-CB	8.54	124.80	111.56
1	A	425	GLU	CA-CB-CG	8.50	131.10	114.10
1	A	600	LYS	CA-C-N	8.49	134.19	120.60
1	A	600	LYS	C-N-CA	8.49	134.19	120.60
1	A	57	ILE	N-CA-CB	8.46	125.19	111.23
1	A	376	ASP	CA-C-O	-8.46	112.04	121.51
1	A	679	VAL	CA-C-N	8.46	134.85	120.72
1	A	679	VAL	C-N-CA	8.46	134.85	120.72
1	A	613	LYS	CA-C-N	8.46	137.28	121.81
1	A	613	LYS	C-N-CA	8.46	137.28	121.81
1	A	378	LYS	CA-C-N	8.45	132.72	120.38
1	A	378	LYS	C-N-CA	8.45	132.72	120.38
1	A	325	TYR	CA-C-N	8.45	133.15	120.31
1	A	325	TYR	C-N-CA	8.45	133.15	120.31
1	A	48	ALA	O-C-N	8.45	130.77	122.07
1	A	683	LEU	CA-C-O	-8.41	109.32	119.49
1	A	71	PRO	CA-N-CD	-8.40	99.74	111.50
1	A	256	ASP	N-CA-CB	8.30	122.11	110.07
1	A	658	GLY	N-CA-C	-8.30	102.28	112.33
1	A	500	LYS	N-CA-C	8.29	120.40	111.36
1	A	51	ASN	O-C-N	-8.28	113.06	122.75
1	A	604	ILE	N-CA-C	-8.28	102.79	110.82
1	A	639	ALA	O-C-N	-8.28	112.54	122.22
1	A	287	PRO	N-CA-CB	-8.25	95.08	103.08
1	A	528	LEU	N-CA-C	-8.24	101.55	111.69
1	A	597	ARG	NE-CZ-NH2	8.20	126.58	119.20
1	A	28	GLN	CA-C-O	8.19	129.59	119.11
1	A	90	THR	CA-CB-OG1	-8.16	97.36	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	HIS	CA-CB-CG	-8.15	105.65	113.80
1	A	89	THR	N-CA-CB	8.13	126.66	111.53
1	A	266	PHE	CA-C-N	8.09	130.96	120.44
1	A	266	PHE	C-N-CA	8.09	130.96	120.44
1	A	328	ILE	CA-C-N	8.08	132.94	120.82
1	A	328	ILE	C-N-CA	8.08	132.94	120.82
1	A	446	ASN	CA-C-N	8.08	134.92	122.08
1	A	446	ASN	C-N-CA	8.08	134.92	122.08
1	A	303	SER	CA-C-N	8.06	132.23	120.95
1	A	303	SER	C-N-CA	8.06	132.23	120.95
1	A	348	CYS	CA-C-N	8.03	134.29	123.05
1	A	348	CYS	C-N-CA	8.03	134.29	123.05
1	A	83	GLU	N-CA-C	8.02	127.89	110.80
1	A	270	GLN	OE1-CD-NE2	-8.01	114.59	122.60
1	A	149	GLU	CA-C-N	8.00	134.16	122.16
1	A	149	GLU	C-N-CA	8.00	134.16	122.16
1	A	172	ARG	N-CA-C	7.99	121.00	111.33
1	A	417	ASP	CA-C-O	7.98	129.14	119.49
1	A	215	GLU	CA-CB-CG	7.97	130.04	114.10
1	A	31	ARG	CD-NE-CZ	7.96	135.54	124.40
1	A	144	GLU	N-CA-C	-7.91	101.46	112.45
1	A	469	GLY	CA-C-N	7.90	130.71	120.44
1	A	469	GLY	C-N-CA	7.90	130.71	120.44
1	A	70	ALA	CB-CA-C	7.85	121.92	109.52
1	A	567	GLU	CA-CB-CG	7.84	129.78	114.10
1	A	30	GLU	CB-CG-CD	7.83	125.91	112.60
1	A	388	GLU	CA-C-N	7.82	135.93	121.62
1	A	388	GLU	C-N-CA	7.82	135.93	121.62
1	A	536	ASP	N-CA-C	-7.82	104.26	113.88
1	A	150	GLN	CA-C-O	7.81	131.36	122.37
1	A	423	LYS	N-CA-C	-7.78	104.31	113.88
1	A	48	ALA	N-CA-CB	7.77	121.28	110.01
1	A	222	ASP	CA-C-N	7.72	135.61	122.26
1	A	222	ASP	C-N-CA	7.72	135.61	122.26
1	A	151	ALA	CA-C-O	7.70	127.01	119.08
1	A	270	GLN	CA-C-N	7.68	131.34	120.28
1	A	270	GLN	C-N-CA	7.68	131.34	120.28
1	A	621	GLU	CB-CG-CD	7.67	125.64	112.60
1	A	433	ALA	CA-C-O	-7.67	111.95	120.69
1	A	581	TYR	CA-CB-CG	-7.65	100.13	113.90
1	A	594	VAL	CB-CA-C	7.65	120.39	110.91
1	A	422	SER	CA-C-N	7.61	135.45	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	SER	C-N-CA	7.61	135.45	122.36
1	A	300	PHE	CA-CB-CG	-7.59	106.21	113.80
1	A	604	ILE	N-CA-CB	7.58	121.44	110.52
1	A	641	THR	N-CA-CB	7.57	121.68	109.95
1	A	540	ILE	CA-CB-CG2	7.56	123.35	110.50
1	A	509	LEU	CA-C-N	7.54	135.95	121.54
1	A	509	LEU	C-N-CA	7.54	135.95	121.54
1	A	21	ASN	N-CA-C	-7.54	103.03	112.90
1	A	15	ALA	CA-C-N	7.52	131.73	120.31
1	A	15	ALA	C-N-CA	7.52	131.73	120.31
1	A	286	GLY	CA-C-N	7.45	128.05	120.38
1	A	286	GLY	C-N-CA	7.45	128.05	120.38
1	A	68	GLY	CA-C-N	7.43	135.27	122.64
1	A	68	GLY	C-N-CA	7.43	135.27	122.64
1	A	434	VAL	N-CA-CB	-7.43	99.96	112.44
1	A	144	GLU	CB-CG-CD	7.43	125.23	112.60
1	A	270	GLN	CA-CB-CG	7.41	128.92	114.10
1	A	624	ARG	N-CA-CB	7.38	120.78	110.07
1	A	660	GLU	N-CA-CB	7.38	120.68	109.91
1	A	168	GLN	CA-C-N	7.37	130.15	120.28
1	A	168	GLN	C-N-CA	7.37	130.15	120.28
1	A	565	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	464	TRP	CA-C-N	7.33	130.40	120.44
1	A	464	TRP	C-N-CA	7.33	130.40	120.44
1	A	582	LYS	CA-C-N	7.32	134.59	121.92
1	A	582	LYS	C-N-CA	7.32	134.59	121.92
1	A	292	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	25	ASP	N-CA-CB	7.30	121.28	110.33
1	A	144	GLU	CA-C-O	7.30	128.91	120.00
1	A	607	LEU	N-CA-C	-7.25	103.06	110.97
1	A	511	GLU	CB-CG-CD	7.25	124.93	112.60
1	A	136	GLU	CA-CB-CG	7.25	128.60	114.10
1	A	2	PRO	CA-C-N	7.24	128.89	119.84
1	A	2	PRO	C-N-CA	7.24	128.89	119.84
1	A	590	PRO	CA-C-O	-7.24	113.16	121.56
1	A	187	PRO	N-CA-C	7.22	123.23	113.84
1	A	64	VAL	N-CA-CB	7.21	122.61	110.56
1	A	398	PHE	CA-C-N	7.21	130.66	120.42
1	A	398	PHE	C-N-CA	7.21	130.66	120.42
1	A	31	ARG	N-CA-C	-7.21	103.11	110.97
1	A	147	ILE	N-CA-C	-7.20	99.61	109.55
1	A	572	ASN	CA-CB-CG	7.18	119.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LYS	CA-C-O	7.17	129.17	120.92
1	A	3	PRO	CA-C-O	7.17	133.65	120.60
1	A	219	GLU	CB-CG-CD	7.17	124.78	112.60
1	A	152	VAL	CB-CA-C	7.14	121.72	111.65
1	A	419	THR	CA-CB-CG2	7.14	122.64	110.50
1	A	57	ILE	CA-CB-CG2	7.11	122.58	110.50
1	A	149	GLU	N-CA-C	7.10	120.84	111.75
1	A	296	LYS	CA-C-N	7.09	132.71	122.35
1	A	296	LYS	C-N-CA	7.09	132.71	122.35
1	A	64	VAL	CA-CB-CG1	7.07	122.42	110.40
1	A	512	LYS	O-C-N	-7.06	113.20	122.59
1	A	349	ALA	CA-C-N	7.04	133.66	122.33
1	A	349	ALA	C-N-CA	7.04	133.66	122.33
1	A	371	CYS	N-CA-C	7.03	120.98	109.24
1	A	213	VAL	N-CA-CB	7.02	118.77	110.55
1	A	481	ASP	CA-CB-CG	7.02	119.62	112.60
1	A	31	ARG	O-C-N	7.00	129.31	122.03
1	A	544	THR	CA-C-N	7.00	129.94	120.77
1	A	544	THR	C-N-CA	7.00	129.94	120.77
1	A	312	GLU	N-CA-C	6.99	119.75	111.71
1	A	337	THR	O-C-N	-6.97	113.27	122.20
1	A	352	LYS	CG-CD-CE	6.96	127.31	111.30
1	A	110	ARG	CA-CB-CG	6.96	128.02	114.10
1	A	90	THR	CA-CB-CG2	6.95	122.32	110.50
1	A	6	THR	N-CA-CB	-6.95	99.06	109.69
1	A	107	LYS	CA-C-N	6.95	134.19	122.65
1	A	107	LYS	C-N-CA	6.95	134.19	122.65
1	A	404	VAL	CA-C-N	6.95	134.95	122.38
1	A	404	VAL	C-N-CA	6.95	134.95	122.38
1	A	461	THR	CA-C-N	6.95	129.47	120.44
1	A	461	THR	C-N-CA	6.95	129.47	120.44
1	A	55	ASP	CA-CB-CG	6.93	119.53	112.60
1	A	161	VAL	O-C-N	6.92	128.99	121.10
1	A	521	TYR	CA-C-O	-6.92	110.53	119.80
1	A	506	GLY	N-CA-C	-6.91	96.81	113.18
1	A	518	HIS	N-CA-C	-6.88	106.08	114.75
1	A	61	GLY	CA-C-N	6.88	127.73	120.03
1	A	61	GLY	C-N-CA	6.88	127.73	120.03
1	A	276	VAL	N-CA-C	6.86	117.56	110.36
1	A	278	THR	N-CA-C	-6.86	101.68	110.53
1	A	359	ASP	CA-C-N	6.86	129.76	120.44
1	A	359	ASP	C-N-CA	6.86	129.76	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	GLU	CA-CB-CG	6.84	127.78	114.10
1	A	453	SER	CA-C-O	6.83	130.27	120.51
1	A	200	ASP	CA-C-N	6.82	131.40	122.26
1	A	200	ASP	C-N-CA	6.82	131.40	122.26
1	A	102	THR	CA-C-O	-6.81	114.11	121.94
1	A	418	GLU	CA-CB-CG	6.81	127.72	114.10
1	A	581	TYR	CA-C-N	6.77	130.03	120.28
1	A	581	TYR	C-N-CA	6.77	130.03	120.28
1	A	180	THR	N-CA-C	6.75	121.22	112.92
1	A	287	PRO	CB-CA-C	-6.75	102.69	110.92
1	A	150	GLN	CB-CA-C	6.73	122.53	112.03
1	A	416	GLU	CA-C-O	6.73	128.73	120.25
1	A	495	ASN	CA-CB-CG	6.72	119.32	112.60
1	A	338	VAL	CA-CB-CG2	6.70	121.79	110.40
1	A	618	HIS	N-CA-CB	6.70	121.81	110.49
1	A	102	THR	CB-CA-C	6.70	124.27	110.40
1	A	216	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	31	ARG	NE-CZ-NH1	6.67	128.17	121.50
1	A	166	ILE	CB-CG1-CD1	6.67	127.80	113.80
1	A	136	GLU	N-CA-C	-6.65	96.64	110.80
1	A	44	ASP	CA-C-N	6.64	129.72	120.29
1	A	44	ASP	C-N-CA	6.64	129.72	120.29
1	A	110	ARG	CB-CG-CD	6.63	126.55	111.30
1	A	183	LEU	CB-CA-C	6.62	121.91	110.45
1	A	625	PHE	CB-CA-C	6.62	121.08	109.89
1	A	267	LEU	CB-CA-C	6.62	121.27	110.88
1	A	607	LEU	N-CA-CB	6.62	119.57	109.91
1	A	626	MET	CA-CB-CG	6.59	127.29	114.10
1	A	385	THR	N-CA-CB	6.59	119.81	110.12
1	A	279	THR	CB-CA-C	6.58	121.79	110.94
1	A	591	THR	N-CA-C	6.57	118.33	110.19
1	A	31	ARG	CB-CG-CD	6.57	126.40	111.30
1	A	233	ARG	CD-NE-CZ	6.56	133.58	124.40
1	A	263	ILE	CA-C-O	-6.55	114.23	121.17
1	A	280	SER	N-CA-C	6.53	124.71	110.80
1	A	655	GLU	CA-C-N	6.52	128.92	120.44
1	A	655	GLU	C-N-CA	6.52	128.92	120.44
1	A	185	ASN	CA-C-N	6.52	132.11	121.87
1	A	185	ASN	C-N-CA	6.52	132.11	121.87
1	A	52	ASN	N-CA-CB	-6.51	103.06	110.35
1	A	494	PRO	CA-C-N	6.51	131.75	120.68
1	A	494	PRO	C-N-CA	6.51	131.75	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	ALA	CA-C-O	-6.49	114.28	121.23
1	A	34	LEU	CA-C-O	6.49	129.14	121.36
1	A	28	GLN	O-C-N	-6.48	112.96	122.43
1	A	549	VAL	CA-CB-CG1	6.48	121.41	110.40
1	A	256	ASP	N-CA-C	-6.47	104.16	111.14
1	A	645	VAL	CA-C-N	6.45	130.53	121.24
1	A	645	VAL	C-N-CA	6.45	130.53	121.24
1	A	632	THR	N-CA-CB	6.44	121.38	110.49
1	A	214	GLN	N-CA-C	6.44	120.24	112.38
1	A	594	VAL	N-CA-CB	6.44	117.74	110.72
1	A	541	LYS	CA-C-N	6.43	130.89	120.60
1	A	541	LYS	C-N-CA	6.43	130.89	120.60
1	A	638	LYS	CG-CD-CE	6.43	126.10	111.30
1	A	449	GLN	CA-C-O	-6.43	113.86	120.80
1	A	490	PRO	CA-C-O	6.42	128.66	121.34
1	A	126	ASN	CA-C-O	-6.38	114.06	121.07
1	A	643	CYS	CA-C-N	6.37	132.16	123.11
1	A	643	CYS	C-N-CA	6.37	132.16	123.11
1	A	298	LEU	CA-C-O	6.36	127.73	120.54
1	A	458	VAL	CA-C-N	6.36	132.44	121.07
1	A	458	VAL	C-N-CA	6.36	132.44	121.07
1	A	121	ARG	NE-CZ-NH2	6.35	124.91	119.20
1	A	137	ASP	CB-CA-C	6.32	123.00	110.42
1	A	520	LYS	CA-C-O	6.32	128.41	121.02
1	A	145	SER	N-CA-CB	6.30	121.14	110.49
1	A	57	ILE	CA-C-O	-6.26	112.95	120.78
1	A	557	TRP	CA-C-N	6.26	133.09	122.26
1	A	557	TRP	C-N-CA	6.26	133.09	122.26
1	A	124	GLY	CA-C-O	-6.25	114.03	120.66
1	A	138	ILE	CB-CA-C	6.25	118.40	111.08
1	A	685	ASP	CA-C-N	6.25	132.96	121.70
1	A	685	ASP	C-N-CA	6.25	132.96	121.70
1	A	365	SER	CA-C-N	6.25	133.48	121.54
1	A	365	SER	C-N-CA	6.25	133.48	121.54
1	A	120	GLY	CA-C-N	6.24	131.33	122.09
1	A	120	GLY	C-N-CA	6.24	131.33	122.09
1	A	489	ALA	O-C-N	6.24	128.50	121.32
1	A	89	THR	CA-C-N	6.24	132.84	122.54
1	A	89	THR	C-N-CA	6.24	132.84	122.54
1	A	135	ARG	CA-C-N	-6.24	109.62	121.54
1	A	135	ARG	C-N-CA	-6.24	109.62	121.54
1	A	329	GLN	CA-C-N	6.24	131.10	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	GLN	C-N-CA	6.24	131.10	121.19
1	A	16	GLU	CB-CG-CD	6.23	123.19	112.60
1	A	189	SER	CA-C-O	6.22	129.25	121.66
1	A	144	GLU	CA-CB-CG	6.22	126.53	114.10
1	A	377	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	84	ARG	N-CA-CB	6.21	120.99	110.49
1	A	267	LEU	N-CA-CB	-6.21	101.00	110.01
1	A	100	LYS	N-CA-C	-6.21	101.74	110.50
1	A	280	SER	CA-C-O	-6.21	111.63	120.51
1	A	604	ILE	CA-C-N	6.20	128.87	120.38
1	A	604	ILE	C-N-CA	6.20	128.87	120.38
1	A	272	TYR	CA-CB-CG	6.18	125.03	113.90
1	A	270	GLN	N-CA-CB	6.15	120.18	109.72
1	A	8	ARG	CD-NE-CZ	6.15	133.01	124.40
1	A	622	LYS	CA-C-N	6.13	129.00	120.29
1	A	622	LYS	C-N-CA	6.13	129.00	120.29
1	A	553	ASN	CA-C-O	6.12	127.10	120.43
1	A	448	LEU	N-CA-C	6.12	118.92	111.82
1	A	410	VAL	CA-C-N	6.11	131.48	122.99
1	A	410	VAL	C-N-CA	6.11	131.48	122.99
1	A	540	ILE	N-CA-CB	-6.11	101.15	111.23
1	A	129	ILE	CA-C-N	6.10	126.89	119.99
1	A	129	ILE	C-N-CA	6.10	126.89	119.99
1	A	638	LYS	CB-CG-CD	6.09	125.32	111.30
1	A	368	GLU	N-CA-CB	6.09	119.28	110.20
1	A	452	LYS	CA-C-N	6.09	133.18	121.54
1	A	452	LYS	C-N-CA	6.09	133.18	121.54
1	A	172	ARG	NH1-CZ-NH2	6.09	127.22	119.30
1	A	408	VAL	N-CA-CB	-6.09	102.69	111.21
1	A	83	GLU	O-C-N	-6.08	114.50	122.59
1	A	146	GLY	CA-C-O	-6.07	115.39	120.92
1	A	395	ASP	CB-CA-C	6.07	120.03	109.65
1	A	356	SER	CA-CB-OG	6.06	123.21	111.10
1	A	381	ILE	CA-C-O	-6.06	113.93	120.47
1	A	674	SER	CA-C-N	6.05	128.38	120.28
1	A	674	SER	C-N-CA	6.05	128.38	120.28
1	A	110	ARG	CD-NE-CZ	6.05	132.87	124.40
1	A	317	GLN	CA-C-N	6.05	128.38	120.28
1	A	317	GLN	C-N-CA	6.05	128.38	120.28
1	A	542	HIS	N-CA-C	6.04	119.75	112.38
1	A	294	VAL	CA-C-N	6.04	132.29	121.66
1	A	294	VAL	C-N-CA	6.04	132.29	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	THR	CA-CB-CG2	6.04	120.77	110.50
1	A	438	LYS	CA-C-N	6.04	133.07	121.54
1	A	438	LYS	C-N-CA	6.04	133.07	121.54
1	A	509	LEU	CA-C-O	6.03	129.14	120.51
1	A	90	THR	N-CA-CB	-6.02	101.58	110.49
1	A	13	SER	O-C-N	6.01	129.85	123.42
1	A	635	LEU	CA-C-O	-6.01	112.81	120.14
1	A	616	GLY	CA-C-O	-6.00	115.98	122.47
1	A	555	ASP	N-CA-C	-6.00	101.89	110.59
1	A	92	TYR	CA-C-N	5.99	130.74	122.77
1	A	92	TYR	C-N-CA	5.99	130.74	122.77
1	A	102	THR	O-C-N	-5.99	115.28	122.65
1	A	218	PRO	CA-C-O	5.99	128.15	119.34
1	A	497	ARG	CA-C-N	5.99	133.93	121.94
1	A	497	ARG	C-N-CA	5.99	133.93	121.94
1	A	611	GLN	N-CA-C	5.99	119.42	111.75
1	A	339	GLY	CA-C-N	5.97	127.31	119.84
1	A	339	GLY	C-N-CA	5.97	127.31	119.84
1	A	383	LYS	CA-C-N	5.96	128.19	120.56
1	A	383	LYS	C-N-CA	5.96	128.19	120.56
1	A	384	ILE	CA-C-N	5.96	128.27	120.28
1	A	384	ILE	C-N-CA	5.96	128.27	120.28
1	A	562	THR	CA-CB-CG2	5.95	120.62	110.50
1	A	146	GLY	N-CA-C	-5.95	100.60	111.25
1	A	236	VAL	CB-CA-C	5.94	120.16	112.14
1	A	134	HIS	N-CA-CB	5.93	118.83	110.12
1	A	343	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	368	GLU	N-CA-C	-5.91	104.43	111.69
1	A	25	ASP	N-CA-C	-5.90	105.17	112.90
1	A	102	THR	N-CA-C	-5.90	102.92	110.53
1	A	191	TYR	CA-C-O	5.88	127.00	120.82
1	A	671	CYS	N-CA-C	5.88	120.51	112.04
1	A	370	GLU	CA-CB-CG	5.88	125.86	114.10
1	A	132	LEU	CA-C-N	5.87	127.96	120.56
1	A	132	LEU	C-N-CA	5.87	127.96	120.56
1	A	277	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	72	TYR	CA-C-O	-5.85	114.03	120.24
1	A	212	THR	CA-C-O	-5.85	114.21	120.42
1	A	113	THR	CA-CB-OG1	-5.85	100.82	109.60
1	A	672	ASN	CB-CA-C	5.85	121.70	110.17
1	A	327	ALA	N-CA-CB	5.85	118.81	110.16
1	A	200	ASP	N-CA-C	5.84	118.40	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	ASP	CA-C-N	5.83	132.68	121.54
1	A	479	ASP	C-N-CA	5.83	132.68	121.54
1	A	186	GLY	CA-C-N	5.83	125.50	119.56
1	A	186	GLY	C-N-CA	5.83	125.50	119.56
1	A	352	LYS	CA-C-N	5.82	128.55	120.29
1	A	352	LYS	C-N-CA	5.82	128.55	120.29
1	A	633	LYS	CB-CA-C	5.81	121.98	110.42
1	A	659	ASP	CA-C-O	-5.81	114.26	120.42
1	A	51	ASN	CA-C-N	-5.80	113.99	122.06
1	A	51	ASN	C-N-CA	-5.80	113.99	122.06
1	A	152	VAL	N-CA-C	-5.80	104.17	112.35
1	A	10	CYS	CB-CA-C	5.80	119.79	110.16
1	A	128	PRO	CB-CA-C	5.80	120.58	112.11
1	A	659	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	379	ASP	CA-C-N	5.80	130.54	120.68
1	A	379	ASP	C-N-CA	5.80	130.54	120.68
1	A	673	PRO	CA-C-O	-5.79	114.81	121.36
1	A	205	VAL	CA-C-N	-5.78	114.26	122.94
1	A	205	VAL	C-N-CA	-5.78	114.26	122.94
1	A	315	ASP	N-CA-C	-5.78	100.97	109.18
1	A	510	LEU	CA-C-O	-5.78	112.24	120.51
1	A	369	VAL	CB-CA-C	5.78	119.59	110.81
1	A	617	LEU	O-C-N	-5.78	114.98	122.37
1	A	34	LEU	CA-C-N	5.77	131.81	122.29
1	A	34	LEU	C-N-CA	5.77	131.81	122.29
1	A	147	ILE	N-CA-CB	5.76	120.57	110.49
1	A	157	SER	CA-C-N	5.75	132.68	121.63
1	A	157	SER	C-N-CA	5.75	132.68	121.63
1	A	343	ASN	CA-C-N	5.75	132.67	121.63
1	A	343	ASN	C-N-CA	5.75	132.67	121.63
1	A	524	TYR	CA-CB-CG	5.75	124.25	113.90
1	A	681	THR	CA-C-N	5.75	128.24	120.65
1	A	681	THR	C-N-CA	5.75	128.24	120.65
1	A	454	CYS	CA-C-O	5.74	127.34	120.28
1	A	141	GLU	CA-C-N	5.74	132.66	121.41
1	A	141	GLU	C-N-CA	5.74	132.66	121.41
1	A	635	LEU	CA-C-N	5.73	132.49	121.54
1	A	635	LEU	C-N-CA	5.73	132.49	121.54
1	A	250	HIS	CA-CB-CG	5.73	119.53	113.80
1	A	50	SER	N-CA-CB	5.72	120.16	110.49
1	A	271	ALA	CA-C-N	5.72	130.40	120.68
1	A	271	ALA	C-N-CA	5.72	130.40	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	PHE	N-CA-C	-5.72	102.06	110.52
1	A	566	PHE	CA-C-N	5.72	131.51	122.36
1	A	566	PHE	C-N-CA	5.72	131.51	122.36
1	A	341	ARG	CA-CB-CG	5.70	125.50	114.10
1	A	453	SER	N-CA-C	5.70	122.94	110.80
1	A	562	THR	CB-CA-C	5.70	121.22	110.62
1	A	445	TRP	N-CA-C	-5.70	104.76	110.97
1	A	195	PHE	CA-CB-CG	-5.69	108.11	113.80
1	A	519	GLU	CA-C-O	5.68	126.57	120.32
1	A	73	LYS	CA-CB-CG	5.67	125.43	114.10
1	A	660	GLU	CB-CA-C	-5.66	102.24	110.96
1	A	169	LYS	CG-CD-CE	5.66	124.31	111.30
1	A	27	MET	CG-SD-CE	-5.66	88.46	100.90
1	A	425	GLU	CG-CD-OE1	5.66	131.41	118.40
1	A	553	ASN	N-CA-CB	5.64	119.62	110.43
1	A	358	CYS	CA-C-N	5.63	128.10	120.38
1	A	358	CYS	C-N-CA	5.63	128.10	120.38
1	A	151	ALA	CA-C-N	5.62	129.53	120.82
1	A	151	ALA	C-N-CA	5.62	129.53	120.82
1	A	639	ALA	CB-CA-C	5.62	121.02	110.63
1	A	578	THR	O-C-N	-5.61	116.07	122.08
1	A	591	THR	N-CA-CB	5.59	117.86	110.25
1	A	122	SER	CA-C-N	5.59	128.23	120.29
1	A	122	SER	C-N-CA	5.59	128.23	120.29
1	A	549	VAL	N-CA-CB	-5.59	102.00	111.23
1	A	310	VAL	CB-CA-C	5.59	116.45	110.53
1	A	647	LEU	CB-CA-C	5.59	118.98	109.53
1	A	469	GLY	N-CA-C	-5.58	106.03	112.50
1	A	663	ALA	CA-C-O	-5.58	113.55	119.97
1	A	545	VAL	CB-CA-C	5.58	118.84	111.70
1	A	148	SER	O-C-N	-5.58	115.17	122.59
1	A	516	SER	CA-C-N	5.58	132.19	121.54
1	A	516	SER	C-N-CA	5.58	132.19	121.54
1	A	419	THR	CA-CB-OG1	-5.58	101.24	109.60
1	A	150	GLN	O-C-N	-5.57	115.83	122.46
1	A	380	CYS	N-CA-CB	5.57	118.88	110.30
1	A	556	ASP	CA-C-N	5.57	128.20	120.29
1	A	556	ASP	C-N-CA	5.57	128.20	120.29
1	A	33	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	333	LYS	CA-C-N	5.57	132.17	121.54
1	A	333	LYS	C-N-CA	5.57	132.17	121.54
1	A	511	GLU	N-CA-C	5.56	119.36	108.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	LYS	N-CA-C	5.56	122.64	110.80
1	A	473	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	372	THR	CA-C-O	-5.55	114.84	121.56
1	A	205	VAL	O-C-N	5.55	129.33	123.00
1	A	530	CYS	CB-CA-C	5.55	119.66	110.90
1	A	428	PRO	CB-CA-C	5.54	120.70	111.56
1	A	432	PHE	O-C-N	5.53	130.02	123.27
1	A	387	GLY	O-C-N	-5.53	115.51	122.70
1	A	581	TYR	N-CA-C	5.53	120.03	113.12
1	A	396	GLY	O-C-N	-5.51	115.53	122.70
1	A	672	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	A	90	THR	CB-CA-C	5.50	119.28	110.09
1	A	149	GLU	O-C-N	-5.50	115.93	122.20
1	A	149	GLU	CA-C-O	5.50	126.36	120.20
1	A	22	SER	CA-CB-OG	5.49	122.08	111.10
1	A	326	SER	CA-CB-OG	5.49	122.08	111.10
1	A	593	ALA	CB-CA-C	5.49	121.74	109.56
1	A	223	GLU	CB-CG-CD	5.49	121.92	112.60
1	A	418	GLU	N-CA-C	5.47	122.46	110.80
1	A	490	PRO	CA-C-N	5.47	129.39	122.00
1	A	490	PRO	C-N-CA	5.47	129.39	122.00
1	A	355	LYS	CA-C-N	5.45	127.58	120.28
1	A	355	LYS	C-N-CA	5.45	127.58	120.28
1	A	553	ASN	CA-C-N	5.45	131.19	122.86
1	A	553	ASN	C-N-CA	5.45	131.19	122.86
1	A	105	MET	N-CA-C	-5.44	102.11	109.95
1	A	517	SER	O-C-N	-5.44	115.36	122.59
1	A	413	GLU	CA-CB-CG	5.43	124.96	114.10
1	A	516	SER	N-CA-CB	5.43	119.81	111.56
1	A	22	SER	CA-C-N	5.43	130.63	121.14
1	A	22	SER	C-N-CA	5.43	130.63	121.14
1	A	382	VAL	O-C-N	-5.42	116.14	121.94
1	A	311	PRO	CA-C-N	5.42	128.09	120.28
1	A	311	PRO	C-N-CA	5.42	128.09	120.28
1	A	160	CYS	N-CA-CB	5.42	119.21	110.65
1	A	215	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	124	GLY	N-CA-C	5.41	119.69	112.77
1	A	578	THR	N-CA-CB	5.41	118.04	109.82
1	A	597	ARG	N-CA-C	-5.41	102.33	109.84
1	A	611	GLN	CA-C-N	5.41	129.87	120.68
1	A	611	GLN	C-N-CA	5.41	129.87	120.68
1	A	341	ARG	CB-CG-CD	5.41	123.73	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ILE	CA-C-N	5.41	129.87	122.84
1	A	345	ILE	C-N-CA	5.41	129.87	122.84
1	A	401	THR	CA-C-N	5.40	129.86	120.68
1	A	401	THR	C-N-CA	5.40	129.86	120.68
1	A	421	CYS	N-CA-C	5.38	122.25	110.80
1	A	114	SER	N-CA-C	5.38	118.16	109.40
1	A	148	SER	CA-C-O	-5.38	112.82	120.51
1	A	549	VAL	CB-CA-C	5.38	120.11	111.29
1	A	192	SER	CA-CB-OG	-5.37	100.36	111.10
1	A	406	GLY	CA-C-O	-5.37	113.05	119.06
1	A	471	ILE	CA-C-N	5.37	127.73	120.38
1	A	471	ILE	C-N-CA	5.37	127.73	120.38
1	A	136	GLU	CG-CD-OE2	-5.36	106.06	118.40
1	A	52	ASN	OD1-CG-ND2	5.36	127.96	122.60
1	A	634	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	490	PRO	CB-CA-C	5.36	118.37	111.46
1	A	221	LYS	CA-C-N	5.35	131.78	121.18
1	A	221	LYS	C-N-CA	5.35	131.78	121.18
1	A	147	ILE	CB-CA-C	5.35	119.01	111.63
1	A	82	TYR	CB-CA-C	-5.35	102.17	109.28
1	A	95	VAL	CA-CB-CG1	5.35	119.49	110.40
1	A	283	HIS	CA-C-O	-5.35	114.55	120.38
1	A	649	GLN	CA-CB-CG	5.33	124.77	114.10
1	A	667	SER	CA-C-O	-5.33	112.89	120.51
1	A	357	LYS	CB-CG-CD	5.33	123.56	111.30
1	A	336	LEU	CA-C-N	5.33	131.01	122.86
1	A	336	LEU	C-N-CA	5.33	131.01	122.86
1	A	73	LYS	CB-CA-C	5.31	119.56	111.70
1	A	546	GLY	CA-C-N	5.29	130.18	122.08
1	A	546	GLY	C-N-CA	5.29	130.18	122.08
1	A	40	ALA	CA-C-N	5.29	132.49	123.03
1	A	40	ALA	C-N-CA	5.29	132.49	123.03
1	A	642	LYS	N-CA-CB	-5.28	102.76	110.47
1	A	592	HIS	CA-C-N	-5.28	113.58	122.29
1	A	592	HIS	C-N-CA	-5.28	113.58	122.29
1	A	66	GLU	CG-CD-OE1	-5.27	106.28	118.40
1	A	366	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	72	TYR	CA-C-N	-5.26	115.94	123.20
1	A	72	TYR	C-N-CA	-5.26	115.94	123.20
1	A	271	ALA	CA-C-O	5.26	126.04	120.10
1	A	281	ASP	CA-C-O	-5.26	113.38	119.64
1	A	387	GLY	CA-C-N	5.26	131.83	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	GLY	C-N-CA	5.26	131.83	121.58
1	A	130	GLY	CA-C-N	5.26	127.85	120.28
1	A	130	GLY	C-N-CA	5.26	127.85	120.28
1	A	140	TRP	CA-C-N	-5.26	115.30	122.87
1	A	140	TRP	C-N-CA	-5.26	115.30	122.87
1	A	292	ASP	N-CA-C	-5.25	102.00	109.62
1	A	112	LYS	N-CA-C	-5.25	102.39	109.95
1	A	260	ILE	CA-C-N	5.24	129.55	120.58
1	A	260	ILE	C-N-CA	5.24	129.55	120.58
1	A	381	ILE	CA-C-N	5.24	127.12	120.72
1	A	381	ILE	C-N-CA	5.24	127.12	120.72
1	A	63	GLN	CA-C-O	5.24	125.48	119.35
1	A	489	ALA	N-CA-CB	5.24	119.70	110.37
1	A	142	GLY	CA-C-N	5.24	131.40	121.97
1	A	142	GLY	C-N-CA	5.24	131.40	121.97
1	A	416	GLU	N-CA-CB	5.24	119.07	110.90
1	A	636	LEU	N-CA-C	5.24	121.95	110.80
1	A	650	GLY	CA-C-N	5.24	128.10	120.98
1	A	650	GLY	C-N-CA	5.24	128.10	120.98
1	A	447	ASN	N-CA-CB	-5.23	102.59	111.27
1	A	426	GLU	CB-CG-CD	5.22	121.47	112.60
1	A	91	SER	CA-C-O	5.21	127.03	121.45
1	A	398	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	568	LEU	CA-CB-CG	5.21	134.52	116.30
1	A	172	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	597	ARG	CA-CB-CG	5.19	124.47	114.10
1	A	564	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	364	VAL	N-CA-C	5.18	115.91	110.62
1	A	388	GLU	CA-CB-CG	5.18	124.46	114.10
1	A	541	LYS	N-CA-CB	5.18	118.48	110.46
1	A	71	PRO	CB-CA-C	-5.17	99.06	112.00
1	A	507	GLU	CA-CB-CG	5.17	124.44	114.10
1	A	251	ALA	CA-C-O	-5.16	115.21	120.89
1	A	270	GLN	CA-C-O	-5.16	114.98	121.02
1	A	572	ASN	CA-C-N	5.16	131.52	121.41
1	A	572	ASN	C-N-CA	5.16	131.52	121.41
1	A	650	GLY	N-CA-C	5.16	122.85	114.90
1	A	420	GLN	N-CA-CB	5.15	118.87	110.37
1	A	289	GLY	CA-C-N	5.15	131.38	121.54
1	A	289	GLY	C-N-CA	5.15	131.38	121.54
1	A	272	TYR	CB-CA-C	5.15	120.88	110.38
1	A	251	ALA	CA-C-N	5.14	129.00	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	ALA	C-N-CA	5.14	129.00	121.80
1	A	70	ALA	N-CA-C	5.13	116.16	109.64
1	A	198	LEU	CA-C-N	5.13	127.11	120.44
1	A	198	LEU	C-N-CA	5.13	127.11	120.44
1	A	674	SER	N-CA-C	-5.12	103.93	110.53
1	A	136	GLU	CG-CD-OE1	5.11	130.16	118.40
1	A	130	GLY	O-C-N	-5.11	117.07	122.13
1	A	28	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	131	THR	CA-C-O	-5.11	114.33	120.10
1	A	128	PRO	CA-C-N	5.11	127.09	120.56
1	A	128	PRO	C-N-CA	5.11	127.09	120.56
1	A	549	VAL	N-CA-C	5.11	119.96	109.34
1	A	560	GLY	CA-C-N	5.10	131.29	121.54
1	A	560	GLY	C-N-CA	5.10	131.29	121.54
1	A	293	PRO	O-C-N	-5.10	115.75	122.64
1	A	329	GLN	OE1-CD-NE2	5.10	127.70	122.60
1	A	29	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	132	LEU	CB-CA-C	5.09	120.01	110.70
1	A	510	LEU	CB-CA-C	5.08	120.53	110.42
1	A	465	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	593	ALA	CA-C-O	-5.07	115.18	121.06
1	A	139	GLU	CG-CD-OE1	5.06	130.04	118.40
1	A	389	ALA	N-CA-CB	5.05	119.39	111.56
1	A	4	LYS	N-CA-C	5.05	120.17	112.54
1	A	108	ASP	N-CA-C	5.05	118.58	112.93
1	A	327	ALA	CB-CA-C	-5.04	102.28	110.85
1	A	427	GLN	O-C-N	5.04	127.23	121.94
1	A	112	LYS	CB-CG-CD	5.04	122.89	111.30
1	A	675	ASP	CA-C-O	-5.04	115.21	120.55
1	A	34	LEU	O-C-N	-5.03	117.43	123.06
1	A	262	ASP	CA-CB-CG	-5.03	107.58	112.60
1	A	223	GLU	CA-C-O	5.02	124.88	119.15
1	A	309	ARG	CA-C-O	5.01	126.70	121.19
1	A	418	GLU	N-CA-CB	-5.01	102.03	110.49
1	A	553	ASN	OD1-CG-ND2	-5.00	117.60	122.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	SER	Mainchain
1	A	152	VAL	Mainchain

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

5.2 Too-close contacts [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	5299	0	5186	295	0
2	A	28	0	25	18	0
3	A	10	0	9	3	0
4	A	2	0	0	0	0
5	A	8	0	0	2	0
6	A	318	0	0	27	0
All	All	5665	0	5220	301	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 29.

All (301) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PHE:CB	1:A:597:ARG:HH22	1.23	1.51
1:A:136:GLU:N	1:A:136:GLU:CA	1.68	1.50
1:A:322:PHE:CB	1:A:597:ARG:NH2	1.85	1.40
2:A:692:NAG:C4	3:A:693:FUC:O3	1.72	1.21
1:A:192:SER:HB2	6:A:966:HOH:O	1.41	1.20
1:A:322:PHE:CG	1:A:597:ARG:NH2	2.13	1.16
1:A:649:GLN:HB2	6:A:863:HOH:O	1.53	1.07
1:A:510:LEU:HD11	6:A:758:HOH:O	1.56	1.04
1:A:177:ASP:OD2	6:A:782:HOH:O	1.76	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ASN:ND2	2:A:691:NAG:O4	1.90	1.03
2:A:692:NAG:H4	3:A:693:FUC:O3	1.57	1.02
1:A:322:PHE:HB3	1:A:597:ARG:HH22	0.84	1.00
1:A:322:PHE:HB2	1:A:597:ARG:NH2	1.76	1.00
1:A:140:TRP:HE1	1:A:148:SER:HB2	1.27	0.99
1:A:344:LYS:HE2	1:A:367:GLY:O	1.62	0.98
1:A:663:ALA:HB1	2:A:692:NAG:H2	1.46	0.96
1:A:473:ASN:HD21	2:A:691:NAG:H3	1.27	0.96
1:A:246:ARG:NH1	1:A:685:ASP:O	1.98	0.96
1:A:287:PRO:HB3	1:A:302:ASP:HB3	1.50	0.93
1:A:374:LEU:HD22	1:A:379:ASP:HB3	1.49	0.93
1:A:136:GLU:N	1:A:136:GLU:CB	2.33	0.90
1:A:322:PHE:HB3	1:A:597:ARG:NH2	1.63	0.89
1:A:202:LYS:HE3	6:A:774:HOH:O	1.71	0.89
1:A:621:GLU:OE2	6:A:730:HOH:O	1.91	0.89
1:A:135:ARG:C	1:A:136:GLU:CA	2.46	0.89
1:A:473:ASN:ND2	2:A:691:NAG:H3	1.88	0.88
1:A:177:ASP:CG	6:A:782:HOH:O	2.16	0.87
1:A:473:ASN:HD21	2:A:691:NAG:C3	1.86	0.87
1:A:136:GLU:H	1:A:137:ASP:H	1.24	0.85
1:A:378:LYS:HE2	1:A:676:LEU:HD23	1.59	0.85
2:A:692:NAG:O4	3:A:693:FUC:O3	1.95	0.84
1:A:374:LEU:HD11	1:A:383:LYS:HG3	1.60	0.84
1:A:473:ASN:HD21	2:A:691:NAG:C4	1.92	0.83
1:A:9:TRP:HB2	1:A:34:LEU:HD11	1.63	0.80
1:A:136:GLU:N	1:A:136:GLU:C	2.41	0.78
1:A:434:VAL:HG21	1:A:581:TYR:HE1	1.49	0.78
1:A:355:LYS:HB2	1:A:373:ILE:HD13	1.66	0.77
1:A:322:PHE:HB2	1:A:597:ARG:HH22	1.32	0.77
1:A:434:VAL:HG21	1:A:581:TYR:CE1	2.20	0.77
1:A:420:GLN:HB3	1:A:425:GLU:HA	1.65	0.77
1:A:216:ASN:HD22	1:A:290:LYS:HG3	1.49	0.76
1:A:136:GLU:N	1:A:137:ASP:H	1.82	0.76
1:A:136:GLU:N	1:A:136:GLU:HB3	2.01	0.76
1:A:221:LYS:HD3	6:A:879:HOH:O	1.87	0.75
1:A:136:GLU:N	1:A:137:ASP:N	2.35	0.74
1:A:510:LEU:CD1	6:A:758:HOH:O	2.24	0.73
1:A:417:ASP:HA	1:A:642:LYS:HB3	1.71	0.73
1:A:165:THR:H	1:A:166:ILE:HD13	1.52	0.73
1:A:50:SER:HB3	1:A:72:TYR:HB3	1.70	0.72
1:A:344:LYS:HB3	1:A:370:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:MET:HA	1:A:29:GLN:HG2	1.71	0.72
1:A:633:LYS:HA	1:A:633:LYS:HE2	1.71	0.71
1:A:527:ALA:HB3	1:A:540:ILE:HD11	1.73	0.71
1:A:83:GLU:HG2	1:A:84:ARG:H	1.56	0.71
1:A:470:LEU:HD13	2:A:691:NAG:H81	1.72	0.70
1:A:89:THR:HG22	1:A:685:ASP:OD1	1.91	0.70
1:A:374:LEU:HD13	1:A:380:CYS:HA	1.73	0.70
1:A:274:LEU:HA	1:A:278:THR:HG23	1.73	0.70
1:A:329:GLN:HE22	1:A:333:LYS:NZ	1.89	0.70
1:A:221:LYS:HE3	6:A:937:HOH:O	1.91	0.70
1:A:422:SER:H	1:A:425:GLU:H	1.40	0.69
1:A:282:PHE:HE2	1:A:284:LEU:HD22	1.56	0.69
1:A:310:VAL:HG22	1:A:682:PHE:CZ	2.28	0.69
1:A:341:ARG:HD3	1:A:603:LYS:HE2	1.75	0.69
1:A:620:THR:HG23	6:A:730:HOH:O	1.92	0.69
1:A:341:ARG:HD2	1:A:343:ASN:HD22	1.58	0.68
1:A:214:GLN:HE22	1:A:221:LYS:NZ	1.93	0.66
1:A:425:GLU:HB2	1:A:645:VAL:HG13	1.77	0.66
2:A:691:NAG:O3	6:A:772:HOH:O	1.95	0.66
1:A:288:PRO:HD2	1:A:291:LYS:HD2	1.78	0.65
1:A:410:VAL:HG11	1:A:604:ILE:HG22	1.77	0.65
1:A:620:THR:HG22	1:A:621:GLU:HG2	1.78	0.65
1:A:378:LYS:HE3	1:A:398:PHE:HE1	1.61	0.65
1:A:448:LEU:HG	1:A:484:PHE:HE1	1.62	0.65
1:A:326:SER:HB3	6:A:959:HOH:O	1.95	0.65
1:A:136:GLU:H	1:A:137:ASP:N	1.93	0.64
1:A:617:LEU:HD12	1:A:626:MET:HE1	1.79	0.64
1:A:620:THR:CG2	6:A:730:HOH:O	2.46	0.64
1:A:417:ASP:CA	1:A:642:LYS:HB3	2.28	0.64
1:A:341:ARG:HD2	1:A:343:ASN:ND2	2.14	0.63
1:A:470:LEU:CD1	2:A:691:NAG:C8	2.77	0.62
1:A:344:LYS:CB	1:A:370:GLU:OE2	2.47	0.62
1:A:4:LYS:O	1:A:4:LYS:HG2	1.99	0.61
1:A:322:PHE:CB	1:A:597:ARG:HH21	2.07	0.61
1:A:345:ILE:HD12	1:A:604:ILE:HG13	1.81	0.61
1:A:313:LEU:HB3	1:A:679:VAL:CG1	2.31	0.61
1:A:472:HIS:HB2	1:A:480:PHE:HE1	1.66	0.60
1:A:344:LYS:HG2	1:A:367:GLY:O	2.01	0.60
1:A:372:THR:HG21	1:A:389:ALA:HB2	1.83	0.60
1:A:528:LEU:HD23	1:A:557:TRP:HH2	1.65	0.60
1:A:117:THR:OG1	1:A:124:GLY:HA3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ALA:O	1:A:373:ILE:HD12	2.02	0.59
1:A:420:GLN:CB	1:A:425:GLU:HA	2.33	0.59
1:A:75:LYS:HE3	1:A:314:MET:O	2.01	0.59
1:A:374:LEU:HD11	1:A:383:LYS:CG	2.32	0.59
1:A:663:ALA:CB	2:A:692:NAG:H2	2.26	0.59
1:A:313:LEU:HB3	1:A:679:VAL:HG11	1.85	0.59
1:A:339:GLY:N	1:A:340:PRO:HD3	2.18	0.58
1:A:217:ALA:HB1	1:A:220:GLU:HG2	1.86	0.58
1:A:150:GLN:HE21	1:A:166:ILE:HG13	1.66	0.58
1:A:470:LEU:HD13	2:A:691:NAG:C8	2.34	0.58
1:A:344:LYS:CE	1:A:367:GLY:O	2.44	0.58
1:A:452:LYS:HG2	1:A:501:LEU:HD11	1.86	0.58
1:A:376:ASP:HB2	1:A:379:ASP:HB2	1.84	0.57
1:A:432:PHE:H	1:A:542:HIS:HD2	1.49	0.57
1:A:417:ASP:HB3	1:A:642:LYS:HD2	1.85	0.57
1:A:615:PHE:HB2	1:A:627:MET:HG3	1.85	0.57
1:A:216:ASN:ND2	1:A:290:LYS:HG3	2.20	0.57
1:A:602:ASN:ND2	1:A:605:ARG:HE	2.04	0.56
1:A:140:TRP:NE1	1:A:148:SER:HB2	2.09	0.56
1:A:152:VAL:HG23	1:A:156:PHE:CD2	2.41	0.56
1:A:411:VAL:HG23	1:A:594:VAL:HG13	1.87	0.56
1:A:502:CYS:HB3	1:A:519:GLU:OE1	2.06	0.56
1:A:470:LEU:CD1	2:A:691:NAG:H81	2.35	0.56
1:A:3:PRO:HB2	1:A:5:THR:HG23	1.88	0.56
1:A:49:ILE:O	1:A:255:ARG:HD3	2.06	0.56
1:A:396:GLY:O	1:A:399:VAL:HB	2.06	0.56
1:A:42:TYR:HB2	1:A:59:LEU:HD11	1.88	0.55
1:A:211:THR:O	1:A:215:GLU:HG3	2.06	0.55
1:A:45:CYS:HB3	1:A:57:ILE:HD13	1.87	0.55
1:A:50:SER:CB	1:A:72:TYR:HB3	2.34	0.55
1:A:109:LEU:O	1:A:112:LYS:HB2	2.07	0.55
1:A:23:LEU:HD22	1:A:284:LEU:HD21	1.88	0.55
1:A:568:LEU:HD13	1:A:578:THR:HA	1.89	0.55
1:A:553:ASN:HD21	1:A:555:ASP:HB2	1.72	0.54
1:A:152:VAL:HG23	1:A:156:PHE:HD2	1.73	0.54
1:A:348:CYS:SG	1:A:374:LEU:HD12	2.48	0.54
1:A:351:GLY:O	1:A:373:ILE:HD11	2.07	0.54
1:A:436:VAL:HG12	1:A:531:LEU:HD11	1.89	0.54
1:A:23:LEU:HB2	1:A:282:PHE:CZ	2.44	0.53
1:A:617:LEU:HD11	1:A:642:LYS:NZ	2.24	0.53
1:A:191:TYR:OH	5:A:689:CO3:O2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HA	1:A:112:LYS:HD2	1.89	0.53
1:A:263:ILE:O	1:A:267:LEU:HB2	2.09	0.53
1:A:360:ARG:HH11	1:A:625:PHE:HB2	1.74	0.53
1:A:400:TYR:HB2	1:A:657:LEU:HD11	1.91	0.52
1:A:121:ARG:NE	5:A:689:CO3:O1	2.37	0.52
1:A:457:ALA:HB3	1:A:460:ARG:HD3	1.91	0.52
1:A:421:CYS:H	1:A:425:GLU:N	2.08	0.52
1:A:165:THR:N	1:A:166:ILE:HD13	2.21	0.52
1:A:511:GLU:HB3	1:A:514:VAL:HG23	1.92	0.52
1:A:180:THR:HA	1:A:183:LEU:HG	1.91	0.51
1:A:282:PHE:CE2	1:A:284:LEU:HD22	2.42	0.51
1:A:553:ASN:ND2	1:A:555:ASP:HB2	2.26	0.51
1:A:23:LEU:HD13	1:A:282:PHE:CE2	2.45	0.51
1:A:61:GLY:HA3	6:A:948:HOH:O	2.10	0.51
1:A:378:LYS:HG2	6:A:805:HOH:O	2.11	0.50
1:A:395:ASP:OD2	1:A:460:ARG:HA	2.11	0.50
1:A:209:LYS:NZ	1:A:301:LYS:HZ1	2.09	0.50
1:A:128:PRO:HA	1:A:244:TRP:CZ3	2.47	0.50
1:A:408:VAL:O	1:A:595:VAL:HA	2.11	0.50
1:A:273:SER:O	1:A:278:THR:HG23	2.12	0.50
1:A:497:ARG:HA	1:A:500:LYS:HE2	1.92	0.50
1:A:524:TYR:CE1	1:A:541:LYS:HG2	2.47	0.50
1:A:131:THR:O	1:A:135:ARG:HG3	2.12	0.50
1:A:676:LEU:HA	1:A:679:VAL:HG22	1.93	0.49
1:A:3:PRO:HG3	1:A:262:ASP:OD1	2.13	0.49
1:A:292:ASP:O	1:A:295:LEU:HB2	2.12	0.49
1:A:408:VAL:HG12	1:A:596:ALA:O	2.11	0.49
1:A:527:ALA:HB3	1:A:540:ILE:CD1	2.41	0.49
1:A:660:GLU:HB3	6:A:746:HOH:O	2.12	0.49
1:A:27:MET:HA	1:A:29:GLN:CG	2.40	0.49
1:A:649:GLN:CB	6:A:863:HOH:O	2.33	0.49
1:A:263:ILE:HG22	1:A:267:LEU:HD22	1.95	0.49
1:A:543:SER:O	1:A:547:GLU:HB2	2.12	0.49
1:A:158:ALA:HB1	1:A:172:ARG:HB3	1.95	0.49
1:A:199:LYS:HG3	1:A:224:TYR:OH	2.13	0.49
1:A:414:SER:HB2	1:A:645:VAL:HG23	1.93	0.49
1:A:89:THR:CG2	1:A:685:ASP:OD1	2.60	0.49
1:A:412:GLY:HA3	1:A:428:PRO:HG3	1.94	0.49
1:A:11:THR:HG22	1:A:16:GLU:HG2	1.95	0.49
1:A:461:THR:HG21	1:A:589:VAL:CG1	2.43	0.48
1:A:497:ARG:HA	1:A:500:LYS:CE	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:CD1	1:A:57:ILE:HG12	2.43	0.48
1:A:322:PHE:CD2	1:A:597:ARG:NH2	2.77	0.48
1:A:343:ASN:ND2	1:A:343:ASN:H	2.09	0.48
1:A:497:ARG:O	1:A:500:LYS:HB2	2.13	0.48
1:A:420:GLN:CA	1:A:425:GLU:HA	2.44	0.48
1:A:23:LEU:HD12	1:A:27:MET:HE1	1.95	0.48
1:A:440:SER:O	1:A:575:ARG:NH2	2.45	0.48
1:A:209:LYS:NZ	1:A:301:LYS:NZ	2.62	0.48
1:A:521:TYR:HE1	1:A:529:ARG:HG2	1.78	0.48
1:A:19:LYS:NZ	6:A:946:HOH:O	2.46	0.48
1:A:470:LEU:CD1	2:A:691:NAG:H83	2.44	0.48
1:A:567:GLU:HG3	1:A:575:ARG:NH1	2.29	0.48
1:A:91:SER:HB2	1:A:247:VAL:O	2.13	0.47
1:A:100:LYS:HE2	1:A:225:GLU:HG3	1.96	0.47
1:A:283:HIS:HE1	6:A:886:HOH:O	1.96	0.47
1:A:167:GLU:HB2	1:A:170:LEU:HD12	1.95	0.47
1:A:415:TYR:CE1	1:A:638:LYS:HG2	2.49	0.47
1:A:52:ASN:HA	1:A:255:ARG:NH1	2.29	0.47
1:A:411:VAL:CG2	1:A:594:VAL:HG13	2.45	0.47
1:A:317:GLN:HG2	6:A:961:HOH:O	2.14	0.47
1:A:466:ILE:HB	1:A:467:PRO:HD3	1.96	0.47
1:A:503:GLN:O	1:A:507:GLU:HA	2.14	0.47
1:A:175:LYS:HD3	6:A:833:HOH:O	2.14	0.47
1:A:246:ARG:CZ	1:A:685:ASP:O	2.61	0.47
1:A:409:PRO:HB2	1:A:647:LEU:CD1	2.44	0.47
1:A:395:ASP:OD2	1:A:460:ARG:HG2	2.14	0.47
1:A:12:ILE:HA	1:A:39:LYS:O	2.15	0.47
1:A:457:ALA:HA	1:A:490:PRO:HD2	1.97	0.47
1:A:116:HIS:CD2	1:A:161:VAL:HG22	2.50	0.46
1:A:93:TYR:HA	1:A:245:ALA:O	2.16	0.46
1:A:525:THR:HG21	1:A:633:LYS:HG3	1.97	0.46
1:A:557:TRP:CE2	1:A:558:ALA:HB2	2.49	0.46
1:A:461:THR:CG2	1:A:589:VAL:HG21	2.44	0.46
1:A:214:GLN:HE22	1:A:221:LYS:CE	2.29	0.46
1:A:420:GLN:HB3	1:A:426:GLU:H	1.81	0.46
1:A:216:ASN:O	1:A:290:LYS:HE3	2.15	0.46
1:A:417:ASP:CG	1:A:418:GLU:HG3	2.40	0.46
1:A:6:THR:HA	1:A:33:THR:O	2.15	0.46
1:A:294:VAL:HA	6:A:900:HOH:O	2.15	0.46
1:A:317:GLN:HB3	1:A:386:LYS:HE2	1.97	0.46
1:A:177:ASP:HB3	1:A:178:ALA:H	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HA	1:A:278:THR:CG2	2.45	0.46
1:A:140:TRP:CH2	1:A:331:LEU:HA	2.50	0.45
1:A:341:ARG:O	1:A:342:GLU:C	2.59	0.45
1:A:630:SER:HB3	1:A:635:LEU:HB2	1.97	0.45
1:A:269:MET:HA	1:A:272:TYR:HD2	1.82	0.45
1:A:157:SER:O	1:A:169:LYS:HD3	2.17	0.45
1:A:416:GLU:HB3	1:A:418:GLU:HB2	1.98	0.45
1:A:567:GLU:HG3	1:A:575:ARG:HH11	1.81	0.45
1:A:219:GLU:HG2	6:A:857:HOH:O	2.17	0.45
1:A:521:TYR:CD1	1:A:530:CYS:HB2	2.52	0.44
1:A:23:LEU:CD1	1:A:27:MET:HE1	2.47	0.44
1:A:329:GLN:HE22	1:A:333:LYS:HZ2	1.65	0.44
1:A:348:CYS:SG	1:A:372:THR:HG22	2.58	0.44
1:A:612:GLU:OE2	1:A:643:CYS:HA	2.17	0.44
1:A:90:THR:HG22	1:A:685:ASP:HB3	2.00	0.44
1:A:218:PRO:HD2	1:A:219:GLU:HG3	1.98	0.44
1:A:395:ASP:HA	1:A:592:HIS:CD2	2.52	0.44
1:A:504:GLY:O	1:A:520:LYS:HB2	2.17	0.44
1:A:461:THR:HG21	1:A:589:VAL:HG11	1.98	0.44
1:A:580:ASP:HB2	6:A:761:HOH:O	2.17	0.44
1:A:59:LEU:HG	1:A:63:GLN:HB2	2.00	0.44
1:A:246:ARG:NH1	1:A:686:LYS:HD2	2.33	0.43
1:A:284:LEU:HD12	1:A:284:LEU:O	2.17	0.43
1:A:617:LEU:HD11	1:A:642:LYS:HZ2	1.83	0.43
1:A:684:GLU:O	1:A:685:ASP:HB2	2.17	0.43
1:A:246:ARG:NH1	1:A:686:LYS:C	2.77	0.43
1:A:314:MET:HE1	1:A:683:LEU:HG	1.99	0.43
1:A:202:LYS:CE	6:A:774:HOH:O	2.49	0.43
1:A:290:LYS:HG2	1:A:291:LYS:O	2.19	0.43
1:A:78:ALA:O	1:A:251:ALA:HB1	2.19	0.43
1:A:444:THR:OG1	1:A:447:ASN:HB3	2.19	0.43
1:A:360:ARG:C	1:A:360:ARG:HD3	2.43	0.43
1:A:49:ILE:HD11	1:A:57:ILE:HG12	2.00	0.43
1:A:417:ASP:OD1	1:A:418:GLU:HG3	2.18	0.43
1:A:438:LYS:HB3	1:A:439:LYS:H	1.56	0.43
1:A:421:CYS:N	1:A:425:GLU:HB3	2.34	0.43
1:A:542:HIS:HB2	1:A:581:TYR:CG	2.53	0.43
1:A:556:ASP:HA	1:A:559:LYS:HB2	2.00	0.43
1:A:589:VAL:HG22	1:A:590:PRO:HD2	1.99	0.43
1:A:441:SER:HA	1:A:575:ARG:NH2	2.34	0.43
1:A:562:THR:CG2	1:A:564:ASP:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ASN:ND2	1:A:605:ARG:HH21	2.16	0.43
1:A:89:THR:HG22	1:A:90:THR:H	1.84	0.43
1:A:352:LYS:N	1:A:518:HIS:NE2	2.59	0.43
1:A:686:LYS:HD2	1:A:686:LYS:C	2.43	0.43
1:A:354:GLU:HB3	1:A:636:LEU:HD23	2.01	0.42
1:A:283:HIS:CE1	6:A:886:HOH:O	2.70	0.42
1:A:528:LEU:HD11	1:A:545:VAL:HG13	2.01	0.42
1:A:27:MET:HB2	1:A:30:GLU:HG2	2.02	0.42
1:A:532:VAL:HG11	1:A:557:TRP:HE3	1.83	0.42
1:A:617:LEU:HD12	1:A:626:MET:CE	2.48	0.42
1:A:12:ILE:HG22	1:A:45:CYS:SG	2.60	0.42
1:A:653:TYR:O	1:A:657:LEU:HG	2.20	0.42
1:A:214:GLN:HE22	1:A:221:LYS:HZ1	1.62	0.42
1:A:228:CYS:HB2	1:A:230:ASP:OD1	2.20	0.42
1:A:529:ARG:O	1:A:533:GLU:HG3	2.20	0.42
1:A:313:LEU:HB3	1:A:679:VAL:HG13	2.01	0.41
1:A:380:CYS:HB3	1:A:392:ILE:HD12	2.01	0.41
1:A:47:LYS:H	1:A:47:LYS:HG2	1.74	0.41
1:A:298:LEU:O	1:A:299:LEU:HB2	2.20	0.41
1:A:378:LYS:HE2	1:A:676:LEU:CD2	2.38	0.41
1:A:452:LYS:H	1:A:536:ASP:HB2	1.85	0.41
1:A:586:LEU:O	1:A:587:ALA:HB2	2.20	0.41
1:A:234:GLN:HA	1:A:235:PRO:HD3	1.82	0.41
2:A:691:NAG:H62	2:A:692:NAG:C7	2.50	0.41
1:A:63:GLN:HA	1:A:66:GLU:HG2	2.02	0.41
1:A:217:ALA:HB1	1:A:220:GLU:CG	2.48	0.41
1:A:314:MET:HG3	1:A:315:ASP:O	2.20	0.41
1:A:425:GLU:CB	1:A:645:VAL:HG13	2.48	0.41
1:A:81:VAL:CG1	1:A:88:SER:HB2	2.50	0.41
1:A:448:LEU:O	1:A:449:GLN:C	2.63	0.41
1:A:493:PRO:O	1:A:496:SER:HB2	2.19	0.41
1:A:138:ILE:HD13	1:A:152:VAL:HB	2.03	0.41
1:A:246:ARG:NH1	1:A:686:LYS:NZ	2.68	0.41
1:A:159:SER:HB2	1:A:170:LEU:HA	2.02	0.41
1:A:188:TYR:CZ	1:A:197:CYS:HA	2.56	0.41
1:A:466:ILE:N	1:A:467:PRO:HD2	2.36	0.41
1:A:446:ASN:HD21	1:A:573:GLY:HA2	1.85	0.41
1:A:380:CYS:CB	1:A:392:ILE:HD12	2.51	0.40
2:A:691:NAG:H62	2:A:692:NAG:N2	2.35	0.40
1:A:41:THR:HG22	1:A:43:LEU:H	1.86	0.40
1:A:669:ASN:O	1:A:673:PRO:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:HIS:O	1:A:27:MET:HB3	2.20	0.40
1:A:57:ILE:HD12	1:A:59:LEU:CD1	2.52	0.40
1:A:268:GLY:O	1:A:272:TYR:HB3	2.21	0.40
1:A:295:LEU:O	1:A:298:LEU:HD22	2.21	0.40
1:A:454:CYS:SG	1:A:535:GLY:HA3	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [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	684/686 (100%)	567 (83%)	82 (12%)	35 (5%)	1 0

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	145	SER
1	A	177	ASP
1	A	280	SER
1	A	287	PRO
1	A	290	LYS
1	A	334	ASP
1	A	338	VAL
1	A	343	ASN
1	A	480	PHE
1	A	509	LEU
1	A	510	LEU
1	A	512	LYS
1	A	561	LEU
1	A	579	MET
1	A	685	ASP

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Mol	Chain	Res	Type
1	A	257	ASP
1	A	289	GLY
1	A	342	GLU
1	A	453	SER
1	A	461	THR
1	A	508	ASN
1	A	122	SER
1	A	136	GLU
1	A	249	ALA
1	A	27	MET
1	A	83	GLU
1	A	366	ASN
1	A	439	LYS
1	A	440	SER
1	A	513	CYS
1	A	618	HIS
1	A	636	LEU
1	A	137	ASP
1	A	186	GLY

5.3.2 Protein sidechains [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	578/578 (100%)	453 (78%)	125 (22%)	1 1

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	4	LYS
1	A	6	THR
1	A	12	ILE
1	A	18	LYS
1	A	24	LYS
1	A	27	MET

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Mol	Chain	Res	Type
1	A	28	GLN
1	A	31	ARG
1	A	37	VAL
1	A	41	THR
1	A	52	ASN
1	A	53	GLU
1	A	57	ILE
1	A	59	LEU
1	A	63	GLN
1	A	64	VAL
1	A	72	TYR
1	A	73	LYS
1	A	75	LYS
1	A	88	SER
1	A	89	THR
1	A	90	THR
1	A	110	ARG
1	A	112	LYS
1	A	128	PRO
1	A	136	GLU
1	A	143	ILE
1	A	149	GLU
1	A	152	VAL
1	A	154	LYS
1	A	166	ILE
1	A	168	GLN
1	A	172	ARG
1	A	175	LYS
1	A	182	CYS
1	A	184	ARG
1	A	205	VAL
1	A	214	GLN
1	A	219	GLU
1	A	222	ASP
1	A	228	CYS
1	A	234	GLN
1	A	236	VAL
1	A	246	ARG
1	A	247	VAL
1	A	255	ARG
1	A	269	MET
1	A	270	GLN

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Mol	Chain	Res	Type
1	A	272	TYR
1	A	274	LEU
1	A	276	VAL
1	A	278	THR
1	A	279	THR
1	A	280	SER
1	A	284	LEU
1	A	285	PHE
1	A	287	PRO
1	A	292	ASP
1	A	298	LEU
1	A	312	GLU
1	A	316	SER
1	A	334	ASP
1	A	338	VAL
1	A	343	ASN
1	A	345	ILE
1	A	360	ARG
1	A	364	VAL
1	A	369	VAL
1	A	372	THR
1	A	374	LEU
1	A	375	ASP
1	A	377	ASN
1	A	378	LYS
1	A	395	ASP
1	A	416	GLU
1	A	417	ASP
1	A	430	TYR
1	A	434	VAL
1	A	441	SER
1	A	446	ASN
1	A	447	ASN
1	A	448	LEU
1	A	470	LEU
1	A	477	SER
1	A	485	SER
1	A	496	SER
1	A	500	LYS
1	A	509	LEU
1	A	510	LEU
1	A	512	LYS

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Mol	Chain	Res	Type
1	A	525	THR
1	A	531	LEU
1	A	534	GLN
1	A	537	VAL
1	A	540	ILE
1	A	545	VAL
1	A	549	VAL
1	A	555	ASP
1	A	562	THR
1	A	564	ASP
1	A	565	ASP
1	A	567	GLU
1	A	568	LEU
1	A	583	THR
1	A	586	LEU
1	A	589	VAL
1	A	594	VAL
1	A	599	GLU
1	A	602	ASN
1	A	604	ILE
1	A	620	THR
1	A	621	GLU
1	A	623	GLU
1	A	626	MET
1	A	630	SER
1	A	633	LYS
1	A	636	LEU
1	A	638	LYS
1	A	648	ARG
1	A	659	ASP
1	A	665	VAL
1	A	668	LEU
1	A	672	ASN
1	A	686	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	150	GLN
1	A	210	HIS
1	A	214	GLN

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Mol	Chain	Res	Type
1	A	216	ASN
1	A	243	ASN
1	A	283	HIS
1	A	317	GLN
1	A	329	GLN
1	A	343	ASN
1	A	377	ASN
1	A	446	ASN
1	A	449	GLN
1	A	472	HIS
1	A	473	ASN
1	A	542	HIS
1	A	553	ASN
1	A	669	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CO3	A	689	4	3,3,3	1.74	1 (33%)	2,3,3	0.75	0
2	NAG	A	692	-	14,14,15	1.44	3 (21%)	17,19,21	1.94	4 (23%)
2	NAG	A	691	-	14,14,15	1.59	4 (28%)	17,19,21	1.86	6 (35%)
3	FUC	A	693	-	10,10,11	0.89	0	14,14,16	2.13	6 (42%)
5	CO3	A	690	4	3,3,3	1.82	1 (33%)	2,3,3	1.53	1 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	691	-	-	3/6/23/26	0/1/1/1
2	NAG	A	692	-	-	1/6/23/26	0/1/1/1
3	FUC	A	693	-	-	-	0/1/1/1

All (9) bond length outliers are listed below:

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

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	692	NAG	C3-C4-C5	4.59	118.55	110.23
3	A	693	FUC	O3-C3-C2	4.34	118.92	110.05
2	A	692	NAG	O5-C1-C2	-3.97	105.15	111.29
3	A	693	FUC	O3-C3-C4	3.67	119.04	110.38
2	A	691	NAG	C1-O5-C5	3.23	116.52	112.19
3	A	693	FUC	O2-C2-C3	3.15	116.68	110.15
2	A	692	NAG	O5-C5-C4	2.92	117.93	110.83
2	A	691	NAG	C4-C3-C2	2.84	115.18	111.02
3	A	693	FUC	C3-C4-C5	-2.77	105.60	109.81

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

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	689	CO3	2	0
2	A	692	NAG	7	0
2	A	691	NAG	13	0
3	A	693	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.