



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:27 AM UTC

PDB ID : 1KSI / pdb_00001ksi
Title : CRYSTAL STRUCTURE OF A EUKARYOTIC (PEA SEEDLING)
COPPER-CONTAINING AMINE OXIDASE AT 2.2Å RESOLUTION
Authors : Wilce, M.C.J.; Kumar, V.; Freeman, H.C.; Guss, J.M.
Deposited on : 1996-07-20
Resolution : 2.20 Å(reported)

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

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

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)
Xtriage (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

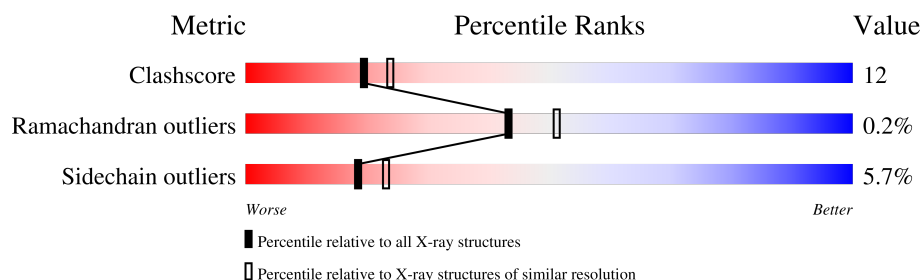
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	642	58% 35% 7%
1	B	642	62% 32% 6%
2	C	2	100%
2	D	2	50% 50%

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	C	1	X	-	X	-
2	NAG	C	2	-	-	X	-
2	NAG	D	1	X	-	-	-
3	NAG	A	701	-	-	X	-
3	NAG	B	701	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10995 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 COPPER AMINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	10	1	0
			5168	3319	877	961	11			
1	B	642	Total	C	N	O	S	12	1	0
			5168	3319	877	961	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	387	TPQ	TYR	modified residue	UNP Q43077
B	387	TPQ	TYR	modified residue	UNP Q43077

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		
4	B	1	Total	Cu	0	0
			1	1		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	B	1	Total	Mn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	272	Total	O	0	0
			272	272		

Continued on next page...

Continued from previous page...

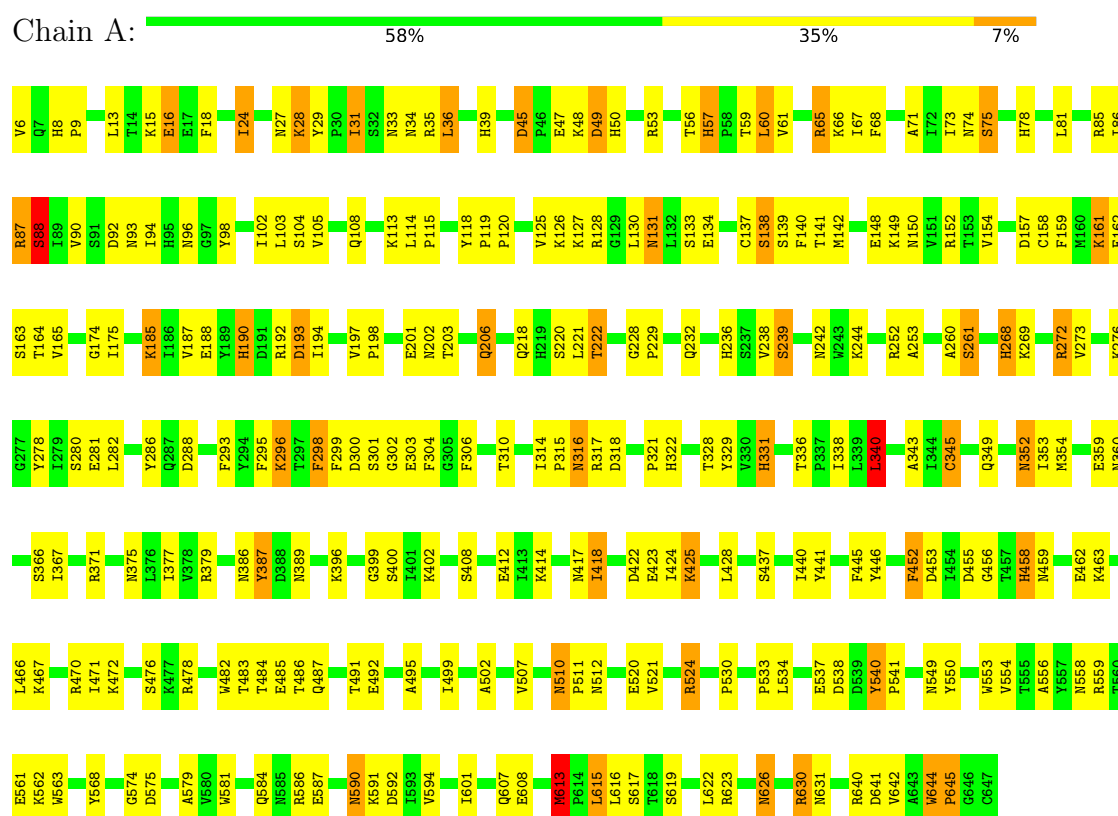
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	299	Total 299	O 299	0	0

3 Residue-property plots

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

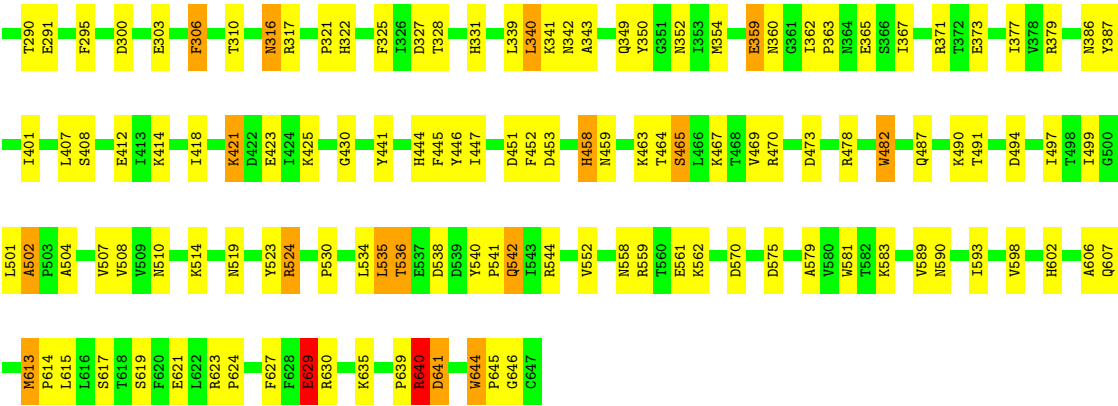
Note EDS was not executed.

• Molecule 1: COPPER AMINE OXIDASE

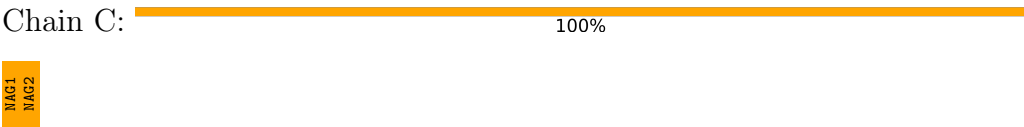


• Molecule 1: COPPER AMINE OXIDASE





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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	85.37Å 114.64Å 199.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20	Depositor
% Data completeness (in resolution range)	86.5 (7.00-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10995	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: NAG, MN, TPQ, CU

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	1.02	4/5297 (0.1%)	2.08	186/7211 (2.6%)
1	B	1.03	5/5297 (0.1%)	2.02	168/7211 (2.3%)
All	All	1.03	9/10594 (0.1%)	2.05	354/14422 (2.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	640	ARG	NE-CZ	12.85	1.47	1.33
1	B	148	GLU	CA-CB	10.43	1.70	1.53
1	B	640	ARG	CD-NE	7.85	1.57	1.46
1	A	162	GLU	N-CA	6.59	1.54	1.46
1	B	640	ARG	CA-CB	-5.50	1.44	1.53
1	A	149	LYS	CA-CB	5.40	1.62	1.53
1	B	277	GLY	N-CA	5.29	1.51	1.45
1	A	152	ARG	CD-NE	-5.18	1.39	1.46
1	A	616	LEU	N-CA	-5.11	1.39	1.46

All (354) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ARG	CD-NE-CZ	19.55	151.76	124.40
1	A	85	ARG	CD-NE-CZ	13.08	142.71	124.40
1	A	623	ARG	CD-NE-CZ	11.65	140.71	124.40
1	B	39	HIS	CA-CB-CG	-11.14	102.66	113.80
1	A	300	ASP	CA-C-O	-11.10	109.02	120.90
1	B	148	GLU	N-CA-CB	11.10	126.80	110.26
1	A	459	ASN	OD1-CG-ND2	-10.40	112.20	122.60
1	B	300	ASP	CA-C-O	-9.70	110.15	120.63
1	A	193	ASP	CA-CB-CG	-9.41	103.19	112.60
1	B	161	LYS	CA-C-N	-9.23	108.88	121.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	LYS	C-N-CA	-9.23	108.88	121.71
1	A	252	ARG	NE-CZ-NH2	9.18	127.46	119.20
1	A	53	ARG	CA-C-O	9.17	130.27	120.55
1	B	140	PHE	CA-C-O	-9.13	110.50	120.36
1	B	253	ALA	CA-C-N	9.13	130.74	120.42
1	B	253	ALA	C-N-CA	9.13	130.74	120.42
1	B	220	SER	CA-C-O	9.07	131.54	122.01
1	A	150	ASN	CA-CB-CG	9.06	121.66	112.60
1	A	268	HIS	CA-CB-CG	-8.95	104.85	113.80
1	B	238	VAL	CA-C-O	8.78	129.96	120.57
1	A	575	ASP	CA-CB-CG	8.75	121.35	112.60
1	A	458	HIS	CA-CB-CG	-8.74	105.06	113.80
1	B	193	ASP	CA-CB-CG	-8.53	104.07	112.60
1	A	87	ARG	CD-NE-CZ	8.51	136.31	124.40
1	A	317	ARG	NE-CZ-NH1	8.51	130.01	121.50
1	A	252	ARG	NE-CZ-NH1	-8.50	113.00	121.50
1	A	232	GLN	CB-CG-CD	8.41	126.90	112.60
1	B	640	ARG	CA-CB-CG	8.34	130.78	114.10
1	B	239	SER	CA-CB-OG	-8.32	94.45	111.10
1	A	161	LYS	CA-C-N	-8.18	105.91	121.54
1	A	161	LYS	C-N-CA	-8.18	105.91	121.54
1	B	257	ILE	CA-C-N	-8.14	109.02	122.21
1	B	257	ILE	C-N-CA	-8.14	109.02	122.21
1	A	459	ASN	CB-CG-ND2	8.11	128.56	116.40
1	A	549	ASN	CB-CG-ND2	8.05	128.48	116.40
1	A	298	PHE	N-CA-C	8.00	121.23	110.35
1	A	175	ILE	N-CA-C	7.98	119.39	107.75
1	B	641	ASP	CA-CB-CG	-7.96	104.64	112.60
1	B	640	ARG	CB-CA-C	7.92	122.86	109.72
1	A	149	LYS	CB-CA-C	7.91	122.24	109.90
1	A	239	SER	CA-CB-OG	-7.90	95.30	111.10
1	A	478	ARG	NE-CZ-NH2	-7.84	112.14	119.20
1	B	232	GLN	CB-CG-CD	7.83	125.91	112.60
1	A	533	PRO	CA-C-O	-7.82	111.92	121.31
1	A	549	ASN	CA-CB-CG	7.76	120.36	112.60
1	B	255	ILE	CA-C-O	7.73	130.31	121.11
1	B	85	ARG	CD-NE-CZ	7.72	135.20	124.40
1	A	218	GLN	OE1-CD-NE2	-7.69	114.91	122.60
1	A	641	ASP	CA-CB-CG	-7.66	104.94	112.60
1	B	640	ARG	NH1-CZ-NH2	-7.64	109.37	119.30
1	A	49	ASP	O-C-N	7.62	131.65	122.27
1	A	478	ARG	NE-CZ-NH1	7.61	129.11	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	MET	CA-C-O	7.58	128.66	120.24
1	A	502	ALA	N-CA-CB	-7.57	104.15	111.27
1	A	268	HIS	CB-CA-C	-7.57	101.15	111.89
1	B	49	ASP	CB-CA-C	-7.51	97.91	110.68
1	A	157	ASP	CA-C-O	-7.50	112.69	121.16
1	A	131	ASN	OD1-CG-ND2	-7.49	115.11	122.60
1	B	316	ASN	OD1-CG-ND2	-7.48	115.12	122.60
1	A	45	ASP	O-C-N	7.40	127.24	121.47
1	A	579	ALA	O-C-N	-7.37	114.31	122.12
1	A	422	ASP	CB-CA-C	-7.33	98.22	110.68
1	B	317	ARG	NE-CZ-NH2	-7.31	112.62	119.20
1	B	131	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	A	159	PHE	CA-C-O	-7.26	112.64	121.06
1	A	502	ALA	CA-C-O	-7.22	113.92	120.13
1	A	640	ARG	NE-CZ-NH1	-7.18	114.32	121.50
1	A	644	TRP	CA-C-N	7.13	127.45	119.32
1	A	644	TRP	C-N-CA	7.13	127.45	119.32
1	B	624	PRO	O-C-N	-7.13	113.83	122.89
1	A	331	HIS	CA-C-O	-7.07	113.16	121.44
1	B	102	ILE	CA-C-O	-7.07	112.92	121.13
1	B	154	VAL	CA-C-O	-7.07	114.63	121.63
1	B	377	ILE	CA-C-O	7.06	128.09	120.53
1	A	203	THR	CA-C-O	7.04	127.49	119.18
1	B	268	HIS	CB-CA-C	-7.04	101.89	111.89
1	B	316	ASN	CB-CG-ND2	7.00	126.91	116.40
1	B	150	ASN	CB-CG-ND2	6.96	126.84	116.40
1	A	329	TYR	CA-CB-CG	-6.94	101.40	113.90
1	B	629	GLU	CB-CG-CD	6.93	124.38	112.60
1	A	617	SER	N-CA-CB	-6.92	99.50	111.55
1	A	232	GLN	OE1-CD-NE2	-6.92	115.68	122.60
1	A	49	ASP	CB-CA-C	-6.88	97.45	110.67
1	B	159	PHE	CA-C-O	-6.88	113.08	121.06
1	A	619	SER	N-CA-CB	-6.87	100.33	111.24
1	A	35	ARG	NE-CZ-NH2	6.84	125.35	119.20
1	B	268	HIS	CA-CB-CG	-6.83	106.97	113.80
1	A	34	ASN	OD1-CG-ND2	6.83	129.43	122.60
1	A	631	ASN	OD1-CG-ND2	-6.80	115.80	122.60
1	B	123	ASP	CA-CB-CG	6.80	119.40	112.60
1	B	362	ILE	CA-C-O	6.78	124.41	119.25
1	B	42	GLY	O-C-N	-6.75	117.79	123.73
1	B	276	LYS	CA-C-N	-6.74	115.06	121.46
1	B	276	LYS	C-N-CA	-6.74	115.06	121.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	487	GLN	OE1-CD-NE2	6.72	129.32	122.60
1	B	290	THR	CA-C-N	6.68	129.22	120.28
1	B	290	THR	C-N-CA	6.68	129.22	120.28
1	A	154	VAL	CA-C-O	-6.67	114.78	121.45
1	A	452	PHE	CA-C-O	-6.64	113.72	121.16
1	A	128	ARG	NE-CZ-NH2	6.61	125.15	119.20
1	A	295	PHE	CA-CB-CG	-6.61	107.19	113.80
1	B	310	THR	CA-C-O	-6.61	113.16	120.69
1	A	90	VAL	N-CA-C	-6.59	106.82	113.47
1	A	579	ALA	CA-C-O	6.58	127.53	120.55
1	A	50	HIS	N-CA-C	-6.58	104.19	111.36
1	B	458	HIS	CA-CB-CG	-6.58	107.22	113.80
1	A	244	LYS	CA-C-O	-6.57	112.20	120.28
1	A	459	ASN	CA-CB-CG	6.56	119.16	112.60
1	B	478	ARG	CA-C-O	-6.56	113.81	121.16
1	B	195	GLU	CA-C-O	-6.54	113.14	120.66
1	B	641	ASP	CA-C-O	-6.53	113.11	120.43
1	A	521	VAL	O-C-N	-6.52	115.91	122.62
1	A	440	ILE	CA-C-O	-6.49	114.90	121.59
1	A	185	LYS	N-CA-CB	-6.49	99.51	111.13
1	B	349	GLN	OE1-CD-NE2	6.47	129.07	122.60
1	A	75	SER	N-CA-C	6.44	120.72	112.86
1	A	575	ASP	CB-CG-OD1	6.42	133.17	118.40
1	B	220	SER	N-CA-CB	6.42	118.99	110.25
1	A	49	ASP	N-CA-CB	6.41	120.22	110.28
1	B	150	ASN	OD1-CG-ND2	-6.39	116.21	122.60
1	A	316	ASN	CB-CG-ND2	6.38	125.97	116.40
1	A	417	ASN	CA-CB-CG	6.38	118.98	112.60
1	A	304	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	45	ASP	CA-CB-CG	-6.37	106.23	112.60
1	B	430	GLY	CA-C-O	-6.33	114.73	121.38
1	B	365	GLU	CB-CG-CD	-6.33	101.84	112.60
1	A	175	ILE	N-CA-CB	-6.33	103.42	111.64
1	B	236	HIS	CA-CB-CG	-6.32	107.48	113.80
1	B	290	THR	CA-C-O	6.31	129.19	121.99
1	A	568	TYR	CA-C-N	-6.30	116.55	122.66
1	A	568	TYR	C-N-CA	-6.30	116.55	122.66
1	B	85	ARG	N-CA-C	-6.30	104.33	111.14
1	B	606	ALA	CA-C-O	-6.29	114.29	121.40
1	B	478	ARG	CD-NE-CZ	6.28	133.19	124.40
1	B	593	ILE	CA-C-O	6.27	128.32	121.67
1	B	172	ILE	CA-C-O	-6.27	113.51	120.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	640	ARG	CD-NE-CZ	6.27	133.18	124.40
1	B	180	ASP	CA-C-O	-6.23	113.64	120.43
1	B	350	TYR	N-CA-C	6.21	119.77	110.14
1	B	206	GLN	OE1-CD-NE2	6.20	128.80	122.60
1	A	641	ASP	CA-C-N	-6.20	114.05	122.91
1	A	641	ASP	C-N-CA	-6.20	114.05	122.91
1	B	535	LEU	CA-C-O	-6.19	113.93	121.36
1	B	342	ASN	CB-CA-C	-6.19	103.10	111.89
1	A	487	GLN	CB-CG-CD	6.19	123.12	112.60
1	B	98	TYR	CA-CB-CG	-6.19	102.76	113.90
1	B	236	HIS	CA-C-O	6.17	126.77	119.48
1	A	456	GLY	CA-C-O	-6.17	117.10	122.16
1	A	39	HIS	CA-CB-CG	-6.17	107.63	113.80
1	A	642	VAL	CB-CA-C	6.16	119.66	110.98
1	B	201	GLU	N-CA-CB	-6.15	100.23	109.71
1	B	359	GLU	CA-C-N	-6.12	113.05	122.60
1	B	359	GLU	C-N-CA	-6.12	113.05	122.60
1	A	445	PHE	O-C-N	-6.12	116.02	123.30
1	A	640	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	A	590	ASN	OD1-CG-ND2	-6.09	116.51	122.60
1	A	33	ASN	CA-CB-CG	-6.08	106.52	112.60
1	A	278	TYR	CA-C-O	-6.06	114.79	121.28
1	A	238	VAL	CA-C-O	6.06	127.05	120.57
1	B	327	ASP	CA-CB-CG	-6.06	106.54	112.60
1	B	53	ARG	CA-C-O	6.05	126.84	120.42
1	A	242	ASN	CA-C-O	6.05	126.72	119.59
1	A	260	ALA	CA-C-O	6.04	127.19	120.43
1	A	613	MET	N-CA-C	6.03	119.05	109.64
1	A	340	LEU	CB-CA-C	6.01	121.63	111.41
1	A	389	ASN	CA-C-O	-6.01	113.84	120.33
1	A	206	GLN	O-C-N	6.00	130.12	123.16
1	A	140	PHE	CA-C-O	-5.99	113.89	120.36
1	B	35	ARG	CD-NE-CZ	5.99	132.78	124.40
1	A	16	GLU	CA-CB-CG	5.99	126.08	114.10
1	A	613	MET	CB-CA-C	5.98	116.53	109.47
1	B	414	LYS	CA-C-N	5.98	126.02	120.34
1	B	414	LYS	C-N-CA	5.98	126.02	120.34
1	A	399	GLY	CA-C-O	5.97	125.63	119.01
1	A	310	THR	CA-CB-CG2	5.96	120.64	110.50
1	A	445	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	550	TYR	CA-CB-CG	-5.92	103.25	113.90
1	B	229	PRO	CA-C-O	-5.92	114.51	122.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	627	PHE	CA-C-O	5.92	126.88	120.55
1	B	514	LYS	CA-CB-CG	-5.91	102.27	114.10
1	A	574	GLY	CA-C-O	5.91	126.93	119.72
1	B	379	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	B	583	LYS	N-CA-C	-5.89	105.36	112.54
1	A	345	CYS	CA-C-O	5.89	127.76	121.11
1	B	613	MET	N-CA-C	5.87	118.80	109.64
1	B	451	ASP	CA-C-O	5.86	128.14	121.58
1	B	482	TRP	CA-CB-CG	5.85	124.72	113.60
1	B	83	ASN	CA-C-O	-5.83	114.06	120.70
1	B	67	ILE	CB-CG1-CD1	5.82	126.03	113.80
1	B	283	PHE	CB-CA-C	5.82	118.39	110.94
1	B	182	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	472	LYS	N-CA-CB	5.78	118.92	110.47
1	A	594	VAL	CA-C-O	-5.76	114.42	120.76
1	A	626	ASN	CA-CB-CG	-5.76	106.84	112.60
1	B	644	TRP	CA-C-N	5.75	125.22	119.24
1	B	644	TRP	C-N-CA	5.75	125.22	119.24
1	A	317	ARG	CD-NE-CZ	-5.73	116.38	124.40
1	B	238	VAL	O-C-N	-5.72	116.68	123.03
1	A	27	ASN	CA-CB-CG	-5.71	106.89	112.60
1	B	255	ILE	O-C-N	-5.70	115.99	122.72
1	A	318	ASP	N-CA-C	-5.70	106.17	113.23
1	B	444	HIS	CA-CB-CG	5.68	119.48	113.80
1	B	544	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	A	360	ASN	CA-CB-CG	-5.67	106.93	112.60
1	B	639	PRO	CA-C-N	5.66	128.74	120.71
1	B	639	PRO	C-N-CA	5.66	128.74	120.71
1	A	96	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	371	ARG	NE-CZ-NH1	5.65	127.15	121.50
1	B	617	SER	N-CA-CB	-5.64	102.16	110.85
1	B	14	THR	N-CA-CB	-5.62	102.40	110.44
1	A	228	GLY	CA-C-N	5.61	125.56	119.78
1	A	228	GLY	C-N-CA	5.61	125.56	119.78
1	A	28	LYS	N-CA-C	-5.61	106.60	113.50
1	B	508	VAL	CA-C-O	-5.61	114.48	120.59
1	B	14	THR	CA-CB-OG1	-5.61	101.19	109.60
1	B	29	TYR	O-C-N	5.60	125.93	121.17
1	A	302	GLY	N-CA-C	5.59	120.87	113.37
1	B	68	PHE	CA-CB-CG	5.59	119.39	113.80
1	B	619	SER	N-CA-CB	-5.59	101.12	111.52
1	A	138	SER	N-CA-CB	-5.59	101.12	111.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	VAL	O-C-N	5.58	126.43	121.57
1	B	421	LYS	CA-C-N	5.58	128.07	120.54
1	B	421	LYS	C-N-CA	5.58	128.07	120.54
1	B	598	VAL	CA-C-N	5.58	130.11	123.19
1	B	598	VAL	C-N-CA	5.58	130.11	123.19
1	A	556	ALA	CA-C-O	-5.58	114.91	121.16
1	B	49	ASP	O-C-N	5.57	128.03	122.12
1	A	98	TYR	CA-CB-CG	-5.57	103.88	113.90
1	A	65	ARG	CD-NE-CZ	5.56	132.18	124.40
1	A	377	ILE	CA-C-O	5.56	126.37	120.48
1	A	24	ILE	O-C-N	-5.55	116.45	121.89
1	B	447	ILE	N-CA-CB	5.55	119.21	112.10
1	A	128	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	B	325	PHE	CA-CB-CG	-5.53	108.27	113.80
1	B	617	SER	N-CA-C	5.52	118.70	110.14
1	A	232	GLN	CA-CB-CG	5.52	125.13	114.10
1	B	27	ASN	CA-C-O	-5.51	114.58	120.42
1	B	469	VAL	CA-C-O	-5.50	114.67	120.39
1	B	510	ASN	CB-CA-C	5.50	115.39	110.44
1	A	202	ASN	CA-CB-CG	5.49	118.09	112.60
1	B	295	PHE	CA-CB-CG	-5.48	108.32	113.80
1	B	88	SER	N-CA-CB	-5.47	101.35	111.52
1	A	239	SER	CA-C-O	-5.46	114.46	120.30
1	A	88	SER	N-CA-C	5.46	118.08	108.75
1	B	33	ASN	OD1-CG-ND2	5.46	128.06	122.60
1	B	265	LEU	CA-C-N	5.45	129.82	120.71
1	B	265	LEU	C-N-CA	5.45	129.82	120.71
1	B	523	TYR	CA-C-N	-5.45	114.04	122.59
1	B	523	TYR	C-N-CA	-5.45	114.04	122.59
1	A	92	ASP	CA-CB-CG	5.44	118.04	112.60
1	B	322	HIS	CA-CB-CG	5.44	119.24	113.80
1	A	50	HIS	O-C-N	5.43	128.34	122.15
1	B	371	ARG	CD-NE-CZ	5.43	132.00	124.40
1	B	140	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	57	HIS	CA-C-N	5.42	124.88	119.24
1	A	57	HIS	C-N-CA	5.42	124.88	119.24
1	A	229	PRO	O-C-N	5.42	129.73	123.01
1	B	42	GLY	CA-C-O	5.42	127.22	121.31
1	A	75	SER	CA-CB-OG	-5.40	100.30	111.10
1	B	15	LYS	CA-C-O	5.39	126.67	120.90
1	B	138	SER	CA-C-O	-5.39	114.80	121.06
1	A	164	THR	CA-C-O	-5.39	115.02	121.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	SER	CA-C-O	-5.38	114.96	120.99
1	B	190	HIS	CA-CB-CG	-5.38	108.42	113.80
1	A	478	ARG	CD-NE-CZ	5.38	131.93	124.40
1	B	221	LEU	CA-C-O	5.37	127.13	121.33
1	A	142	MET	CA-CB-CG	5.37	124.83	114.10
1	B	640	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	B	579	ALA	CA-C-O	5.34	126.13	120.10
1	A	645	PRO	CB-CA-C	-5.33	103.36	112.64
1	A	386	ASN	CA-C-O	-5.33	111.75	120.80
1	B	445	PHE	CA-CB-CG	5.33	119.13	113.80
1	A	301	SER	CA-C-N	5.32	126.98	120.22
1	A	301	SER	C-N-CA	5.32	126.98	120.22
1	B	152	ARG	CD-NE-CZ	5.30	131.82	124.40
1	B	243	TRP	CA-C-O	5.30	127.53	121.28
1	A	575	ASP	N-CA-C	-5.29	106.88	113.38
1	B	218	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	A	105	VAL	CA-C-N	5.28	128.13	120.79
1	A	105	VAL	C-N-CA	5.28	128.13	120.79
1	A	366	SER	CA-C-O	5.27	125.94	120.40
1	A	352	ASN	CA-CB-CG	-5.25	107.35	112.60
1	A	273	VAL	CA-C-N	-5.24	115.61	123.00
1	A	273	VAL	C-N-CA	-5.24	115.61	123.00
1	A	253	ALA	CA-C-N	5.24	126.34	120.42
1	A	253	ALA	C-N-CA	5.24	126.34	120.42
1	B	317	ARG	O-C-N	5.24	128.08	121.95
1	B	401	ILE	CA-C-N	-5.24	115.62	122.74
1	B	401	ILE	C-N-CA	-5.24	115.62	122.74
1	A	229	PRO	CB-CA-C	-5.23	104.53	111.23
1	B	220	SER	CB-CA-C	-5.23	99.64	111.30
1	A	354	MET	N-CA-CB	-5.23	102.41	110.20
1	B	562	LYS	CB-CA-C	-5.22	100.04	110.42
1	A	236	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	296	LYS	CA-C-O	5.20	126.60	120.98
1	A	601	ILE	CB-CA-C	-5.20	102.73	110.33
1	A	586	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	A	608	GLU	CA-C-O	5.18	125.73	119.31
1	B	45	ASP	CA-CB-CG	-5.17	107.42	112.60
1	A	45	ASP	CA-C-O	-5.15	115.11	119.59
1	B	467	LYS	CA-C-O	-5.15	115.25	120.71
1	A	193	ASP	CA-C-N	-5.15	116.31	122.90
1	A	193	ASP	C-N-CA	-5.15	116.31	122.90
1	B	360	ASN	CA-C-O	-5.14	113.52	119.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	PHE	CA-C-O	-5.14	115.40	120.80
1	B	412	GLU	CB-CG-CD	-5.14	103.86	112.60
1	A	510	ASN	CB-CA-C	5.14	115.26	110.17
1	A	550	TYR	CA-C-O	-5.14	115.43	121.44
1	B	386	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	A	190	HIS	N-CA-CB	5.13	118.79	110.32
1	B	16	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	197	VAL	O-C-N	5.11	125.45	121.46
1	A	553	TRP	CA-CB-CG	5.11	123.31	113.60
1	A	218	GLN	CG-CD-NE2	5.11	124.06	116.40
1	A	71	ALA	CA-C-N	-5.10	116.38	122.90
1	A	71	ALA	C-N-CA	-5.10	116.38	122.90
1	A	486	THR	N-CA-C	5.10	117.04	108.73
1	A	446	TYR	CA-C-O	-5.09	115.20	120.70
1	A	437	SER	N-CA-C	5.08	116.67	108.34
1	B	220	SER	CA-CB-OG	5.08	121.25	111.10
1	A	193	ASP	N-CA-CB	-5.07	101.95	111.13
1	A	299	PHE	N-CA-CB	5.07	119.72	110.60
1	A	157	ASP	OD1-CG-OD2	-5.07	110.74	122.90
1	B	94	ILE	O-C-N	5.06	128.29	122.93
1	B	203	THR	N-CA-C	-5.06	107.79	114.31
1	A	276	LYS	CA-C-O	-5.05	114.32	120.54
1	B	536	THR	O-C-N	-5.05	116.90	122.86
1	B	640	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	B	173	THR	CA-CB-CG2	5.05	119.08	110.50
1	A	36	LEU	N-CA-C	5.04	116.63	108.41
1	A	630	ARG	CA-C-O	-5.04	115.91	121.31
1	B	559	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	A	218	GLN	CB-CG-CD	5.04	121.17	112.60
1	B	542	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	540	TYR	O-C-N	5.04	124.96	120.48
1	B	165	VAL	N-CA-C	-5.04	107.01	112.80
1	B	95	HIS	CA-CB-CG	-5.04	108.77	113.80
1	B	593	ILE	O-C-N	-5.04	117.68	122.97
1	B	519	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	222	THR	CB-CA-C	5.03	120.73	109.56
1	A	502	ALA	CB-CA-C	-5.03	103.14	110.03
1	A	68	PHE	CA-CB-CG	5.03	118.83	113.80
1	A	261	SER	CB-CA-C	-5.03	99.40	109.35
1	B	452	PHE	CA-C-O	-5.02	114.75	120.58
1	A	260	ALA	CA-C-N	5.02	130.86	122.73
1	A	260	ALA	C-N-CA	5.02	130.86	122.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	LYS	CA-C-O	-5.02	113.51	121.94
1	B	414	LYS	O-C-N	-5.02	117.37	123.29
1	A	272	ARG	O-C-N	5.01	129.00	122.89
1	B	141	THR	CA-CB-OG1	-5.01	102.09	109.60
1	B	300	ASP	CA-C-N	-5.01	112.02	120.58
1	B	300	ASP	C-N-CA	-5.01	112.02	120.58
1	B	50	HIS	O-C-N	5.00	127.86	122.15
1	B	349	GLN	CG-CD-NE2	-5.00	108.89	116.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5168	0	5085	124	1
1	B	5168	0	5086	107	1
2	C	28	0	26	20	0
2	D	28	0	25	2	0
3	A	14	0	13	14	0
3	B	14	0	13	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	272	0	0	7	0
6	B	299	0	0	7	0
All	All	10995	0	10248	235	1

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 12.

All (235) 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:558:ASN:HD21	3:A:701:NAG:C1	1.07	1.58
1:B:558:ASN:HD21	3:B:701:NAG:C1	1.27	1.45
1:A:558:ASN:ND2	3:A:701:NAG:C2	1.82	1.42
1:A:558:ASN:HD21	3:A:701:NAG:C2	1.34	1.41
1:A:558:ASN:ND2	3:A:701:NAG:H2	1.40	1.36
1:B:558:ASN:HD21	3:B:701:NAG:C2	1.47	1.25
2:C:1:NAG:C3	2:C:2:NAG:H82	1.69	1.21
2:C:1:NAG:C4	2:C:2:NAG:H82	1.73	1.17
2:C:1:NAG:C2	2:C:2:NAG:H82	1.79	1.12
2:C:1:NAG:H4	2:C:2:NAG:H82	1.37	1.04
2:C:1:NAG:H4	2:C:2:NAG:C8	1.87	1.04
1:B:558:ASN:ND2	3:B:701:NAG:C2	2.18	1.03
2:C:1:NAG:H4	2:C:2:NAG:C7	1.89	1.03
1:B:558:ASN:ND2	3:B:701:NAG:H2	1.77	1.00
2:C:1:NAG:H2	2:C:2:NAG:H82	1.49	0.93
2:C:1:NAG:H2	2:C:2:NAG:C8	1.99	0.92
2:C:1:NAG:O4	2:C:2:NAG:N2	2.03	0.91
1:B:558:ASN:HB3	1:B:561:GLU:HG3	1.51	0.90
2:C:1:NAG:HO4	2:C:2:NAG:C1	1.78	0.90
1:A:558:ASN:ND2	3:A:701:NAG:H4	1.92	0.84
2:C:1:NAG:C4	2:C:2:NAG:C8	2.50	0.83
1:B:151:VAL:HG23	1:B:153:THR:HG23	1.65	0.79
1:B:558:ASN:ND2	3:B:701:NAG:H4	1.96	0.79
1:A:499:ILE:HG22	1:A:530:PRO:HG3	1.65	0.78
1:A:28:LYS:HG2	1:A:29:TYR:CE2	2.20	0.77
1:B:132:LEU:HA	1:B:135:ILE:HD12	1.66	0.76
1:A:558:ASN:ND2	3:A:701:NAG:C4	2.50	0.75
1:A:424:ILE:HG12	1:A:428:LEU:HD11	1.70	0.74
1:B:28:LYS:HG2	1:B:29:TYR:CE1	2.24	0.73
1:A:558:ASN:ND2	3:A:701:NAG:C3	2.52	0.73
2:C:1:NAG:C3	2:C:2:NAG:C8	2.60	0.72
1:B:161:LYS:O	1:B:161:LYS:HG2	1.91	0.71
1:A:558:ASN:HD22	3:A:701:NAG:H2	1.49	0.71
2:C:1:NAG:C4	2:C:2:NAG:C7	2.66	0.71
1:A:59:THR:C	1:A:60:LEU:HG	2.16	0.70
1:B:131:ASN:ND2	2:D:1:NAG:C2	2.55	0.69
1:B:272:ARG:NH2	1:B:453:ASP:OD2	2.26	0.69
1:B:644:TRP:CH2	1:B:646:GLY:HA2	2.29	0.67
1:B:630:ARG:HD2	6:B:893:HOH:O	1.94	0.67
2:C:1:NAG:O4	2:C:2:NAG:C2	2.43	0.67
2:C:1:NAG:C2	2:C:2:NAG:C8	2.60	0.67
1:B:122:ILE:O	1:B:126:LYS:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:TRP:CZ3	1:B:646:GLY:HA2	2.30	0.66
1:A:458:HIS:HB3	1:A:590:ASN:OD1	1.97	0.65
1:A:470:ARG:HH22	1:B:538:ASP:CG	2.04	0.65
1:A:510:ASN:HD21	1:A:512:ASN:HD22	1.45	0.65
1:B:558:ASN:CB	1:B:561:GLU:HG3	2.27	0.65
1:A:161:LYS:HG2	1:A:161:LYS:O	1.98	0.63
1:A:558:ASN:HD22	3:A:701:NAG:H4	1.64	0.63
1:B:233:ILE:HG12	1:B:238:VAL:HG22	1.81	0.63
1:A:6:VAL:HG11	1:A:65:ARG:NH2	2.12	0.63
2:C:1:NAG:O4	2:C:2:NAG:O5	2.17	0.62
1:B:558:ASN:CG	3:B:701:NAG:C1	2.73	0.62
1:A:119:PRO:N	1:A:120:PRO:CD	2.62	0.62
1:B:359:GLU:HB3	1:B:367:ILE:HB	1.81	0.62
1:A:558:ASN:HD22	3:A:701:NAG:C2	2.01	0.61
1:A:86:ILE:HG13	1:A:88:SER:HB3	1.81	0.61
1:A:534:LEU:HB2	1:B:482:TRP:CD1	2.35	0.61
1:B:127:LYS:HD2	1:B:194:ILE:HD11	1.83	0.61
1:A:272:ARG:NH2	1:A:453:ASP:OD2	2.32	0.60
1:B:100:PHE:HB3	1:B:101:PRO:HD2	1.83	0.60
1:B:575:ASP:OD1	6:B:801:HOH:O	2.16	0.60
2:C:1:NAG:C4	2:C:2:NAG:N2	2.64	0.60
1:A:45:ASP:O	1:A:559:ARG:NH1	2.34	0.59
1:B:558:ASN:ND2	3:B:701:NAG:C4	2.65	0.59
1:B:119:PRO:HB2	1:B:120:PRO:HD3	1.85	0.59
1:A:467:LYS:HD3	1:A:485:GLU:OE1	2.03	0.58
1:B:408:SER:HB2	1:B:615:LEU:HD12	1.84	0.58
1:B:352:ASN:HB2	6:B:849:HOH:O	2.04	0.58
1:B:490:LYS:HA	1:B:589:VAL:CG2	2.34	0.58
1:A:316:ASN:ND2	1:A:321:PRO:HA	2.19	0.57
1:A:630:ARG:HA	1:B:607:GLN:O	2.04	0.57
1:A:316:ASN:HD22	1:A:321:PRO:HA	1.70	0.57
1:B:497:ILE:HB	1:B:552:VAL:HB	1.87	0.56
1:B:104:SER:OG	1:B:107:GLU:HG2	2.06	0.56
1:A:499:ILE:CG2	1:A:530:PRO:HG3	2.36	0.56
1:A:452:PHE:HZ	1:A:622:LEU:HD22	1.71	0.56
1:B:64:PRO:HB3	1:B:85:ARG:HD3	1.89	0.55
1:A:510:ASN:ND2	1:A:512:ASN:H	2.04	0.54
1:A:296:LYS:HE2	6:A:963:HOH:O	2.06	0.54
1:A:104:SER:O	1:A:108:GLN:HG3	2.08	0.54
1:A:558:ASN:CG	3:A:701:NAG:C1	2.73	0.54
1:A:201:GLU:HA	1:A:201:GLU:OE1	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ASN:HD22	1:A:512:ASN:H	1.56	0.53
1:B:491:THR:O	1:B:494:ASP:HB2	2.08	0.53
1:B:131:ASN:ND2	2:D:1:NAG:O5	2.40	0.53
1:B:52:LEU:O	1:B:55:GLU:HB2	2.09	0.52
1:A:322:HIS:HB3	6:A:1065:HOH:O	2.10	0.52
1:B:217:LYS:HG3	1:B:218:GLN:N	2.25	0.52
1:B:340:LEU:HG	1:B:343:ALA:HB2	1.92	0.52
1:A:558:ASN:HD22	3:A:701:NAG:C3	2.20	0.52
1:A:328:THR:HG22	6:A:837:HOH:O	2.10	0.52
1:B:59:THR:O	1:B:60:LEU:HD13	2.10	0.52
1:A:558:ASN:HD22	3:A:701:NAG:C4	2.20	0.52
1:A:148:GLU:OE1	1:A:148:GLU:HA	2.10	0.51
1:B:499:ILE:HG22	1:B:530:PRO:HG3	1.92	0.51
1:B:151:VAL:CG2	1:B:153:THR:HG23	2.39	0.51
1:A:188:GLU:OE2	1:A:190:HIS:HE1	1.93	0.51
1:A:206:GLN:NE2	1:B:367:ILE:HG23	2.26	0.51
1:A:48:LYS:HE2	1:A:453:ASP:OD2	2.11	0.51
1:A:507:VAL:HG22	1:A:524:ARG:HB2	1.92	0.51
1:A:118:TYR:CD2	1:A:120:PRO:HD2	2.46	0.50
1:A:296:LYS:HE3	1:A:298:PHE:CZ	2.46	0.50
2:C:1:NAG:O3	2:C:2:NAG:C8	2.59	0.50
1:A:322:HIS:HD2	6:A:1029:HOH:O	1.94	0.50
1:B:57:HIS:O	1:B:61:VAL:HG23	2.11	0.50
1:A:408:SER:HB2	1:A:615:LEU:HD12	1.94	0.50
1:A:28:LYS:HG2	1:A:29:TYR:CD2	2.46	0.50
1:A:495:ALA:HB1	1:A:554:VAL:HB	1.94	0.50
1:B:407:LEU:HD21	1:B:446:TYR:OH	2.12	0.49
1:B:39:HIS:HB3	1:B:101:PRO:HB2	1.93	0.49
1:A:510:ASN:HD22	1:A:510:ASN:C	2.19	0.49
1:B:316:ASN:HD22	1:B:321:PRO:HA	1.78	0.49
1:A:540:TYR:HB2	1:A:541:PRO:HD3	1.94	0.48
1:B:621:GLU:OE2	1:B:623:ARG:HD2	2.12	0.48
1:A:141:THR:HG21	1:A:303:GLU:HB3	1.94	0.48
1:B:57:HIS:HB3	1:B:60:LEU:HD23	1.96	0.48
1:B:418:ILE:HA	1:B:423:GLU:OE1	2.14	0.48
1:A:78:HIS:CE1	1:A:94:ILE:HD11	2.49	0.48
1:A:288:ASP:HB3	1:A:293:PHE:HB2	1.95	0.48
1:B:561:GLU:HB3	1:B:581:TRP:CZ3	2.48	0.48
1:A:471:ILE:HD13	1:A:476:SER:HB3	1.95	0.48
1:B:490:LYS:HA	1:B:589:VAL:HG23	1.95	0.48
1:B:490:LYS:HD3	1:B:589:VAL:HG21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LYS:HE3	1:A:194:ILE:HD11	1.95	0.48
1:B:458:HIS:HB3	1:B:590:ASN:OD1	2.13	0.48
1:A:538:ASP:OD2	1:B:470:ARG:NH2	2.46	0.48
1:A:24:ILE:HG13	1:A:87:ARG:HH21	1.79	0.47
1:B:16:GLU:CD	1:B:16:GLU:H	2.23	0.47
1:A:119:PRO:N	1:A:120:PRO:HD3	2.30	0.47
1:B:28:LYS:HG2	1:B:29:TYR:CD1	2.49	0.47
1:A:66:LYS:C	1:A:67:ILE:HD13	2.39	0.47
1:B:644:TRP:HA	1:B:645:PRO:HD2	1.73	0.47
1:B:6:VAL:HG11	1:B:65:ARG:NH2	2.30	0.47
1:A:36:LEU:CD1	1:A:73:ILE:HG12	2.45	0.47
1:B:8:HIS:CG	1:B:9:PRO:HD2	2.50	0.47
1:B:119:PRO:N	1:B:120:PRO:CD	2.77	0.47
1:A:31:ILE:HG12	6:A:1049:HOH:O	2.15	0.47
1:A:491:THR:O	1:A:492:GLU:C	2.58	0.46
1:B:354:MET:HB2	1:B:373:GLU:HB3	1.97	0.46
1:B:142:MET:HG2	1:B:155:ARG:HG2	1.96	0.46
2:C:1:NAG:C1	2:C:2:NAG:H82	2.45	0.46
1:A:359:GLU:OE1	1:B:168:TYR:HE2	1.97	0.46
1:B:316:ASN:ND2	1:B:321:PRO:HA	2.30	0.46
1:A:340:LEU:HG	1:A:343:ALA:HB2	1.96	0.46
1:A:221:LEU:HG	1:A:222:THR:N	2.31	0.46
1:A:281:GLU:HG3	1:A:282:LEU:O	2.16	0.46
1:A:352:ASN:HB2	6:A:812:HOH:O	2.16	0.46
1:A:626:ASN:OD1	1:B:607:GLN:HG3	2.15	0.46
1:A:538:ASP:OD1	1:B:470:ARG:NH2	2.49	0.46
1:A:458:HIS:HD2	1:A:590:ASN:O	1.99	0.45
1:A:8:HIS:CG	1:A:9:PRO:HD2	2.52	0.45
1:B:558:ASN:HD22	3:B:701:NAG:H4	1.78	0.45
2:C:1:NAG:O3	2:C:2:NAG:H82	2.08	0.45
1:B:540:TYR:HB2	1:B:541:PRO:HD3	1.98	0.45
1:A:613:MET:HE3	6:B:939:HOH:O	2.17	0.45
1:A:375:ASN:OD1	1:A:396:LYS:HG2	2.17	0.44
1:A:510:ASN:HD22	1:A:511:PRO:HD2	1.82	0.44
1:B:491:THR:O	1:B:494:ASP:N	2.44	0.44
1:A:562:LYS:HE2	1:A:563:TRP:CZ2	2.52	0.44
1:B:252:ARG:O	1:B:306:PHE:HB2	2.17	0.44
1:A:286:TYR:OH	1:A:387:TPQ:O5	2.36	0.44
1:B:282:LEU:HD11	1:B:306:PHE:CZ	2.52	0.44
1:B:613:MET:HE3	6:B:904:HOH:O	2.17	0.44
1:B:465:SER:HA	1:B:504:ALA:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HB2	1:A:115:PRO:HD3	2.00	0.44
1:A:296:LYS:HE3	1:A:298:PHE:CE1	2.52	0.44
1:A:467:LYS:N	1:A:483:THR:O	2.48	0.44
1:A:482:TRP:CH2	1:B:441:TYR:HB3	2.52	0.44
1:B:13:LEU:HA	1:B:17:GLU:OE1	2.18	0.44
1:B:41:ILE:H	1:B:331:HIS:CE1	2.35	0.44
1:B:458:HIS:C	1:B:459:ASN:HD22	2.25	0.44
1:B:339:LEU:HD21	1:B:341:LYS:HD3	1.99	0.43
1:A:174:GLY:O	1:A:192:ARG:HB2	2.17	0.43
1:B:211:SER:HB2	1:B:212:PRO:HD2	2.00	0.43
1:B:328:THR:HG22	6:B:869:HOH:O	2.18	0.43
1:A:185:LYS:O	1:A:187:VAL:HG13	2.18	0.43
1:A:607:GLN:HB3	1:B:629:GLU:O	2.18	0.43
1:A:102:ILE:HD13	1:A:102:ILE:HG21	1.79	0.43
1:A:125:VAL:HG13	1:A:130:LEU:HB2	2.00	0.43
1:A:587:GLU:O	1:A:591:LYS:HD3	2.17	0.43
1:B:418:ILE:HG23	1:B:423:GLU:HB2	2.00	0.43
1:A:441:TYR:HB3	1:B:482:TRP:CH2	2.54	0.43
1:A:331:HIS:HA	1:A:336:THR:O	2.19	0.43
1:B:141:THR:HG21	1:B:303:GLU:HB3	2.01	0.43
1:A:13:LEU:HD12	1:A:18:PHE:CE1	2.54	0.43
1:A:561:GLU:HB3	1:A:581:TRP:CZ3	2.54	0.42
1:A:131:ASN:OD1	1:A:133:SER:HB2	2.18	0.42
1:A:558:ASN:OD1	1:A:558:ASN:C	2.60	0.42
1:A:402:LYS:HE3	6:A:1052:HOH:O	2.19	0.42
1:A:510:ASN:HD22	1:A:511:PRO:CD	2.32	0.42
1:A:644:TRP:HA	1:A:645:PRO:HD2	1.81	0.42
1:A:67:ILE:O	1:A:81:LEU:HD12	2.19	0.42
1:A:418:ILE:HA	1:A:423:GLU:OE1	2.19	0.42
1:B:119:PRO:CB	1:B:120:PRO:HD3	2.47	0.42
1:A:220:SER:HB2	1:B:640:ARG:O	2.20	0.41
1:A:359:GLU:HB3	1:A:367:ILE:HB	2.02	0.41
1:B:191:ASP:C	1:B:191:ASP:OD1	2.63	0.41
1:B:507:VAL:HG22	1:B:524:ARG:HB2	2.02	0.41
1:A:102:ILE:HG22	1:A:103:LEU:O	2.21	0.41
1:A:137:CYS:HA	1:A:158:CYS:HA	2.02	0.41
1:A:165:VAL:HG21	1:B:367:ILE:HG21	2.02	0.41
1:A:314:ILE:HA	1:A:315:PRO:HD3	1.92	0.41
1:B:421:LYS:NZ	6:B:821:HOH:O	2.52	0.41
1:A:57:HIS:O	1:A:61:VAL:HG23	2.20	0.41
1:B:535:LEU:HD12	1:B:542:GLN:HE21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ALA:CB	1:A:554:VAL:HB	2.50	0.41
1:A:134:GLU:OE1	1:A:134:GLU:HA	2.21	0.41
1:B:464:THR:O	1:B:504:ALA:HA	2.20	0.41
1:B:507:VAL:HG22	1:B:524:ARG:CB	2.50	0.41
1:B:558:ASN:HD21	3:B:701:NAG:C4	2.30	0.41
1:B:635:LYS:HE2	1:B:635:LYS:HB3	1.90	0.41
1:A:288:ASP:OD2	1:A:414:LYS:NZ	2.51	0.41
1:A:538:ASP:CG	1:B:470:ARG:HH22	2.28	0.41
1:B:161:LYS:HE3	1:B:161:LYS:HB3	1.59	0.41
1:A:74:ASN:O	1:A:75:SER:HB2	2.19	0.41
1:A:462:GLU:OE2	1:A:520:GLU:OE1	2.39	0.41
1:A:293:PHE:HE1	1:A:412:GLU:OE2	2.03	0.41
1:A:48:LYS:NZ	1:A:592:ASP:OD2	2.51	0.41
1:A:353:ILE:O	1:B:615:LEU:HD22	2.20	0.41
1:A:466:LEU:HD22	1:A:484:THR:HG22	2.02	0.41
1:A:538:ASP:CG	1:B:470:ARG:NH2	2.79	0.41
1:A:584:GLN:NE2	3:A:701:NAG:O4	2.48	0.41
1:B:99:GLY:HA2	1:B:570:ASP:O	2.21	0.41
1:B:177:ILE:HD13	1:B:177:ILE:HG21	1.90	0.41
1:B:534:LEU:HD12	1:B:602:HIS:CE1	2.56	0.41
1:A:15:LYS:O	1:A:16:GLU:C	2.63	0.40
1:A:78:HIS:HA	1:A:93:ASN:O	2.20	0.40
1:A:345:CYS:SG	1:A:379:ARG:HB3	2.61	0.40
1:B:501:LEU:O	1:B:502:ALA:HB2	2.21	0.40
1:B:613:MET:HA	1:B:614:PRO:HD3	1.84	0.40
1:A:425:LYS:HD3	1:A:425:LYS:HA	1.60	0.40
1:A:510:ASN:HA	1:A:511:PRO:HD3	1.96	0.40
1:B:558:ASN:OD1	3:B:701:NAG:C1	2.69	0.40
1:B:536:THR:OG1	1:B:538:ASP:OD1	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:NE2	1:B:640:ARG:NH1[4_455]	1.95	0.25

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	640/642 (100%)	612 (96%)	28 (4%)	0	100	100
1	B	640/642 (100%)	605 (94%)	33 (5%)	2 (0%)	36	42
All	All	1280/1284 (100%)	1217 (95%)	61 (5%)	2 (0%)	43	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	473	ASP
1	B	502	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	576/575 (100%)	546 (95%)	30 (5%)	21	26
1	B	576/575 (100%)	540 (94%)	36 (6%)	16	19
All	All	1152/1150 (100%)	1086 (94%)	66 (6%)	18	23

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ILE
1	A	47	GLU
1	A	49	ASP
1	A	56	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	LEU
1	A	88	SER
1	A	113	LYS
1	A	126	LYS
1	A	138	SER
1	A	139	SER
1	A	163	SER
1	A	193	ASP
1	A	198	PRO
1	A	239	SER
1	A	261	SER
1	A	269	LYS
1	A	280	SER
1	A	306	PHE
1	A	338	ILE
1	A	340	LEU
1	A	349	GLN
1	A	400	SER
1	A	418	ILE
1	A	425	LYS
1	A	455	ASP
1	A	463	LYS
1	A	524	ARG
1	A	537	GLU
1	A	613	MET
1	A	615	LEU
1	B	6	VAL
1	B	31	ILE
1	B	47	GLU
1	B	49	ASP
1	B	56	THR
1	B	60	LEU
1	B	62	SER
1	B	86	ILE
1	B	90	VAL
1	B	91	SER
1	B	106	ASP
1	B	127	LYS
1	B	138	SER
1	B	139	SER
1	B	151	VAL
1	B	161	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	SER
1	B	193	ASP
1	B	194	ILE
1	B	201	GLU
1	B	213	PRO
1	B	220	SER
1	B	232	GLN
1	B	239	SER
1	B	261	SER
1	B	291	GLU
1	B	306	PHE
1	B	340	LEU
1	B	363	PRO
1	B	425	LYS
1	B	463	LYS
1	B	465	SER
1	B	524	ARG
1	B	629	GLU
1	B	640	ARG
1	B	641	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	93	ASN
1	A	150	ASN
1	A	190	HIS
1	A	206	GLN
1	A	232	GLN
1	A	234	ASN
1	A	268	HIS
1	A	316	ASN
1	A	360	ASN
1	A	458	HIS
1	A	510	ASN
1	A	549	ASN
1	A	558	ASN
1	B	33	ASN
1	B	76	GLN
1	B	202	ASN
1	B	224	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	227	GLN
1	B	232	GLN
1	B	316	ASN
1	B	331	HIS
1	B	542	GLN
1	B	549	ASN
1	B	558	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TPQ	A	387	1	13,14,15	2.48	5 (38%)	13,19,21	1.57	6 (46%)
1	TPQ	B	387	1	13,14,15	2.58	6 (46%)	13,19,21	1.38	2 (15%)

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
1	TPQ	A	387	1	-	3/5/22/24	0/1/1/1
1	TPQ	B	387	1	-	3/5/22/24	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	TPQ	C1-C2	-5.84	1.41	1.49
1	A	387	TPQ	C1-C2	-5.12	1.42	1.49
1	B	387	TPQ	O5-C5	3.84	1.34	1.24
1	B	387	TPQ	O2-C2	3.76	1.34	1.24
1	A	387	TPQ	O5-C5	3.72	1.34	1.24
1	A	387	TPQ	O2-C2	3.71	1.34	1.24
1	A	387	TPQ	C6-C1	2.48	1.40	1.34
1	B	387	TPQ	C6-C1	2.48	1.40	1.34
1	A	387	TPQ	C3-C4	2.25	1.40	1.36
1	B	387	TPQ	C3-C4	2.14	1.39	1.36
1	B	387	TPQ	C4-C5	-2.10	1.41	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	TPQ	C6-C5-C4	2.51	121.19	116.80
1	A	387	TPQ	C4-C3-C2	-2.45	117.66	120.30
1	A	387	TPQ	O5-C5-C4	-2.45	115.57	119.43
1	A	387	TPQ	C6-C5-C4	2.43	121.05	116.80
1	B	387	TPQ	C1-C6-C5	-2.38	118.58	122.59
1	A	387	TPQ	O2-C2-C3	-2.14	116.97	121.83
1	A	387	TPQ	C1-C6-C5	-2.08	119.09	122.59
1	A	387	TPQ	C3-C2-C1	2.02	122.50	118.36

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	387	TPQ	C2-C1-CB-CA
1	A	387	TPQ	C6-C1-CB-CA
1	B	387	TPQ	N-CA-CB-C1
1	B	387	TPQ	C2-C1-CB-CA
1	B	387	TPQ	C6-C1-CB-CA
1	A	387	TPQ	N-CA-CB-C1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	387	TPQ	1	0

5.5 Carbohydrates

4 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	C	1	2,1	14,14,15	1.37	2 (14%)	17,19,21	2.20	6 (35%)
2	NAG	C	2	2	14,14,15	1.37	2 (14%)	17,19,21	2.21	6 (35%)
2	NAG	D	1	2,1	14,14,15	1.53	3 (21%)	17,19,21	6.14	3 (17%)
2	NAG	D	2	2	14,14,15	1.14	2 (14%)	17,19,21	1.47	2 (11%)

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	C	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	NAG	C8-C7	3.53	1.57	1.50
2	D	1	NAG	C1-C2	3.41	1.57	1.52
2	D	2	NAG	C8-C7	3.36	1.57	1.50
2	C	2	NAG	O7-C7	-3.30	1.15	1.23
2	C	1	NAG	O7-C7	-3.30	1.15	1.23
2	D	1	NAG	O5-C1	2.82	1.48	1.43
2	C	1	NAG	C1-C2	2.07	1.55	1.52
2	C	2	NAG	C1-C2	2.05	1.55	1.52
2	D	2	NAG	O5-C1	-2.01	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-C2-N2	24.67	149.31	110.43
2	C	2	NAG	C1-O5-C5	4.34	118.00	112.19
2	C	1	NAG	C1-O5-C5	4.33	117.98	112.19
2	D	2	NAG	C1-C2-N2	-4.16	103.88	110.43
2	C	2	NAG	C4-C3-C2	-4.09	105.02	111.02
2	C	1	NAG	C4-C3-C2	-4.07	105.05	111.02
2	C	1	NAG	C1-C2-N2	-4.06	104.03	110.43
2	C	2	NAG	C1-C2-N2	-4.03	104.09	110.43
2	C	2	NAG	C3-C4-C5	-3.58	103.74	110.23
2	C	1	NAG	C3-C4-C5	-3.57	103.77	110.23
2	D	1	NAG	C1-O5-C5	3.43	116.78	112.19
2	C	2	NAG	O3-C3-C2	2.86	115.35	109.40
2	C	1	NAG	O3-C3-C2	2.85	115.32	109.40
2	D	1	NAG	O5-C1-C2	-2.53	107.38	111.29
2	D	2	NAG	C1-O5-C5	2.34	115.33	112.19
2	C	1	NAG	O4-C4-C5	2.09	114.47	109.32
2	C	2	NAG	O4-C4-C5	2.08	114.44	109.32

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	NAG	C1
2	D	1	NAG	C2

All (8) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 22 short contacts:

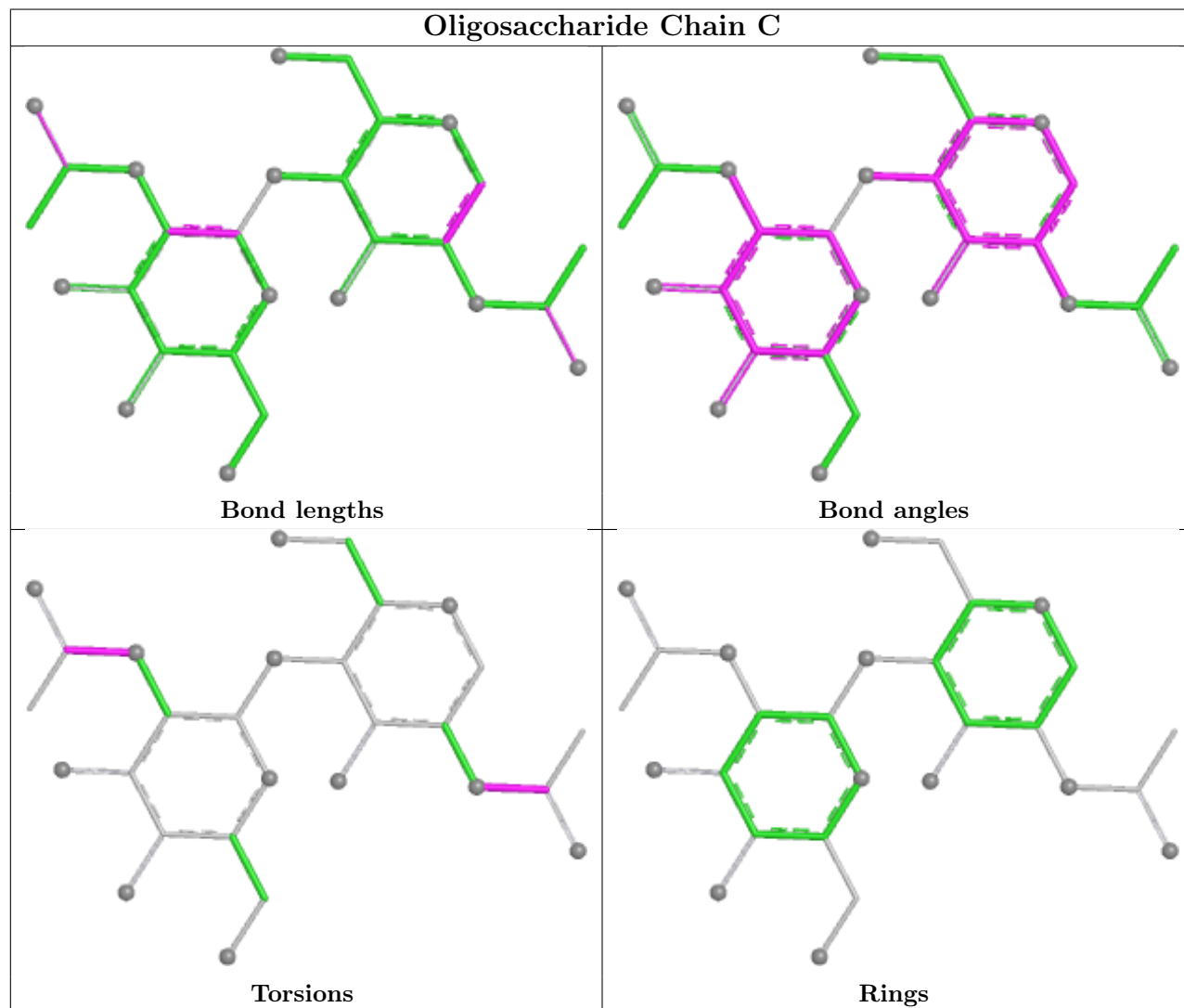
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	2	0

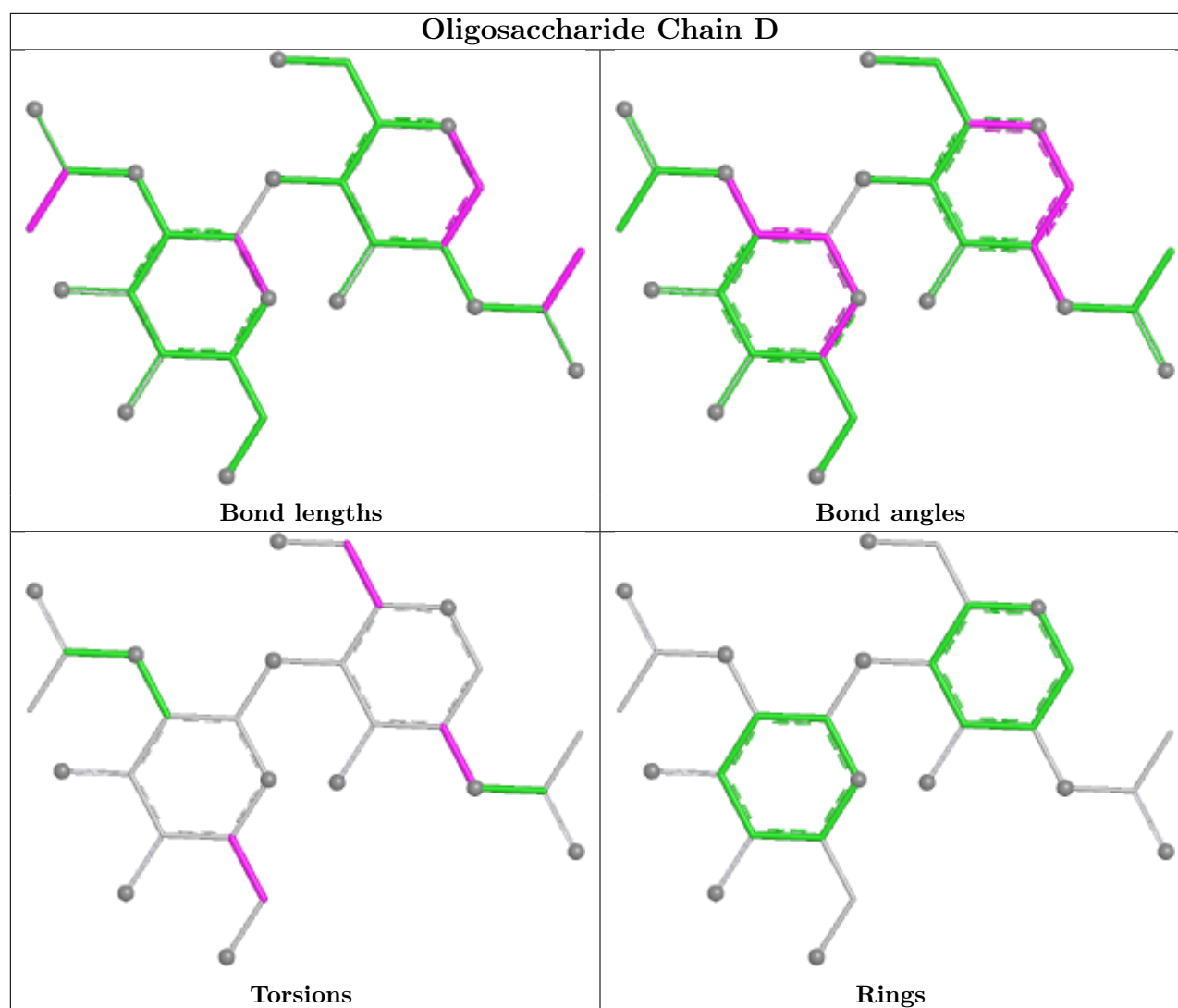
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	20	0
2	C	2	NAG	20	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 6 ligands modelled in this entry, 4 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	$\# Z > 2$
3	NAG	B	701	1	14,14,15	1.36	2 (14%)	17,19,21	2.20	6 (35%)
3	NAG	A	701	1	14,14,15	1.37	2 (14%)	17,19,21	2.20	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	701	1	-	2/6/23/26	0/1/1/1
3	NAG	A	701	1	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	NAG	O7-C7	-3.30	1.15	1.23
3	B	701	NAG	O7-C7	-3.30	1.15	1.23
3	A	701	NAG	C1-C2	2.08	1.55	1.52
3	B	701	NAG	C1-C2	2.05	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	701	NAG	C1-O5-C5	4.32	117.98	112.19
3	A	701	NAG	C1-O5-C5	4.31	117.97	112.19
3	B	701	NAG	C4-C3-C2	-4.08	105.04	111.02
3	A	701	NAG	C4-C3-C2	-4.07	105.06	111.02
3	B	701	NAG	C1-C2-N2	-4.06	104.04	110.43
3	A	701	NAG	C1-C2-N2	-4.04	104.06	110.43
3	A	701	NAG	C3-C4-C5	-3.58	103.74	110.23
3	B	701	NAG	C3-C4-C5	-3.56	103.77	110.23
3	B	701	NAG	O3-C3-C2	2.83	115.28	109.40
3	A	701	NAG	O3-C3-C2	2.83	115.27	109.40
3	A	701	NAG	O4-C4-C5	2.09	114.47	109.32
3	B	701	NAG	O4-C4-C5	2.07	114.43	109.32

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	NAG	O7-C7-N2-C2
3	B	701	NAG	O7-C7-N2-C2
3	A	701	NAG	C8-C7-N2-C2
3	B	701	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	NAG	10	0
3	A	701	NAG	14	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.