



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:28 AM BST

PDB ID : 2C6N
Title : Structure of human somatic angiotensin-I converting enzyme N domain with lisinopril
Authors : Corradi, H.R.; Schwager, S.L.U.; Nichinda, A.; Sturrock, E.D.; Acharya, K.R.
Deposited on : 2005-11-10
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

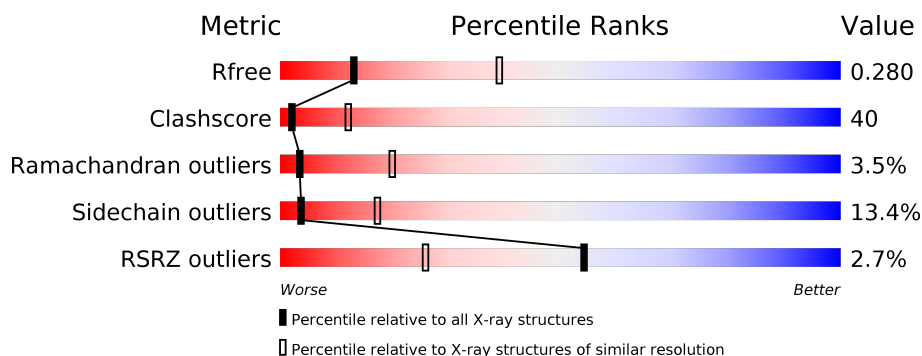
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	612	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>41%</div> <div>9%</div> </div> <div>.</div> </div>
1	B	612	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>38%</div> <div>9%</div> </div> <div>.</div> </div>
2	C	2	<div> <div></div> <div>100%</div> </div>
2	D	2	<div> <div></div> <div>50%</div> <div>50%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	2	X	-	-	-
3	NAG	B	693	X	-	X	X
3	NAG	B	695	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9621 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 ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	7	0	0
			4747	3057	811	861	18			
1	B	609	Total	C	N	O	S	9	0	0
			4665	3005	797	845	18			

- 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 (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

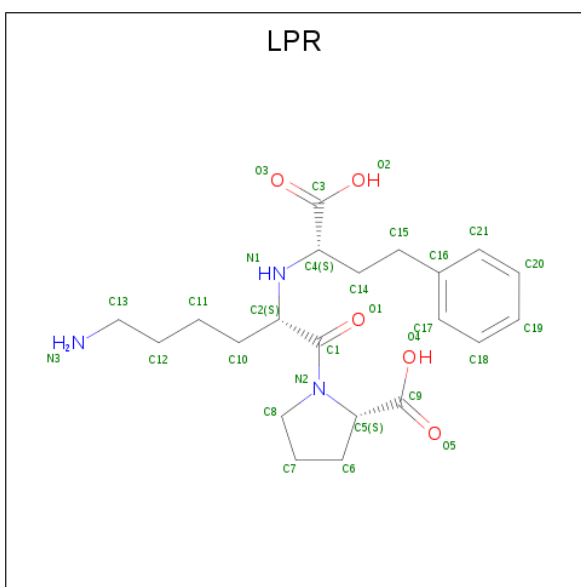
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 6 is [N2-[(S)-1-CARBOXY-3-PHENYLPROPYL]-L-LYSYL-L-PROLINE (three-letter code: LPR) (formula: C₂₁H₃₁N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			29	21	3	5		
6	B	1	Total	C	N	O	0	0
			29	21	3	5		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

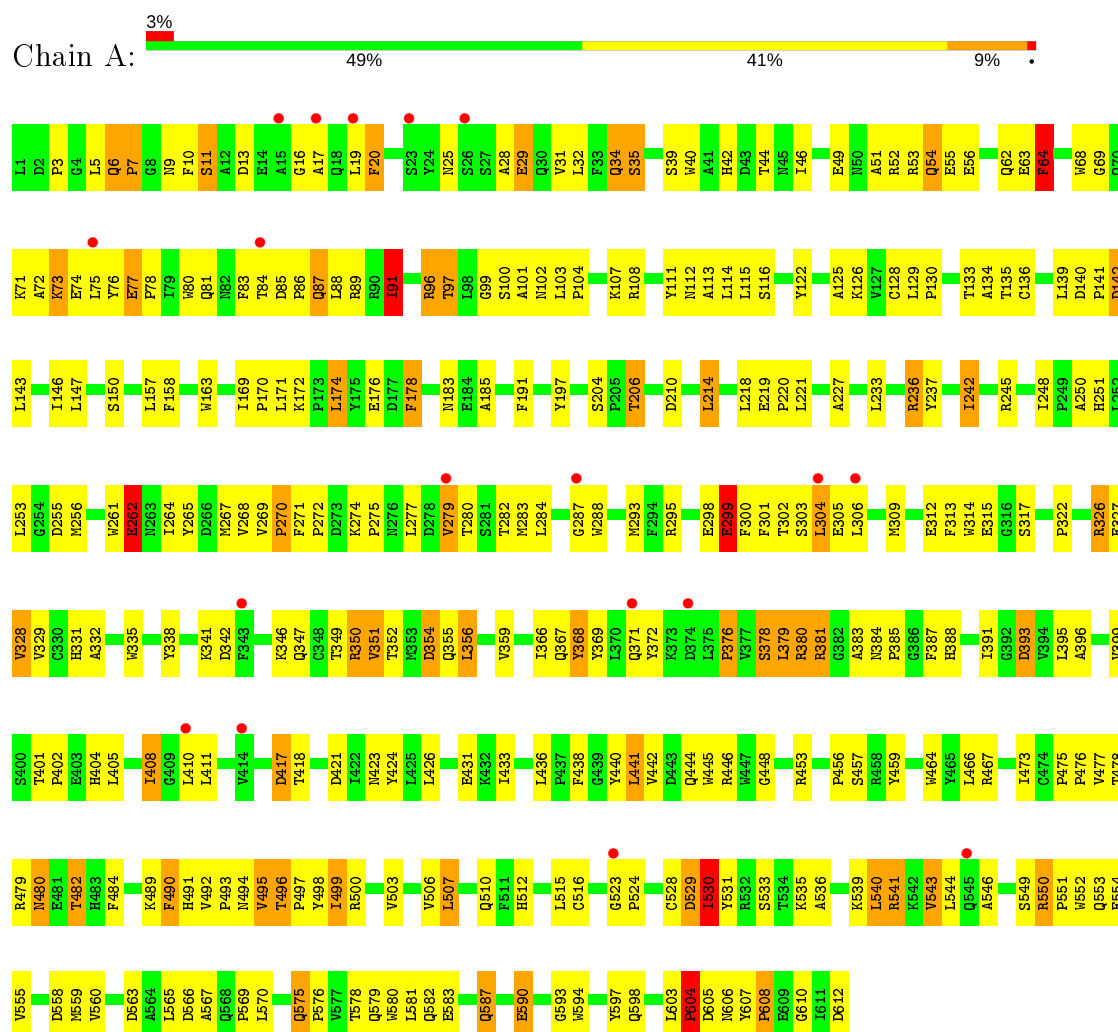
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	8	Total	O	0	0
			8	8		
9	B	11	Total	O	0	0
			11	11		

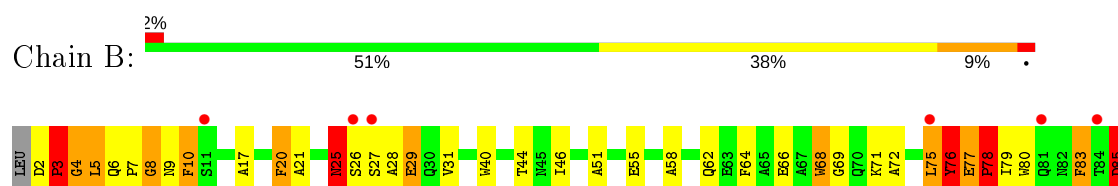
3 Residue-property plots

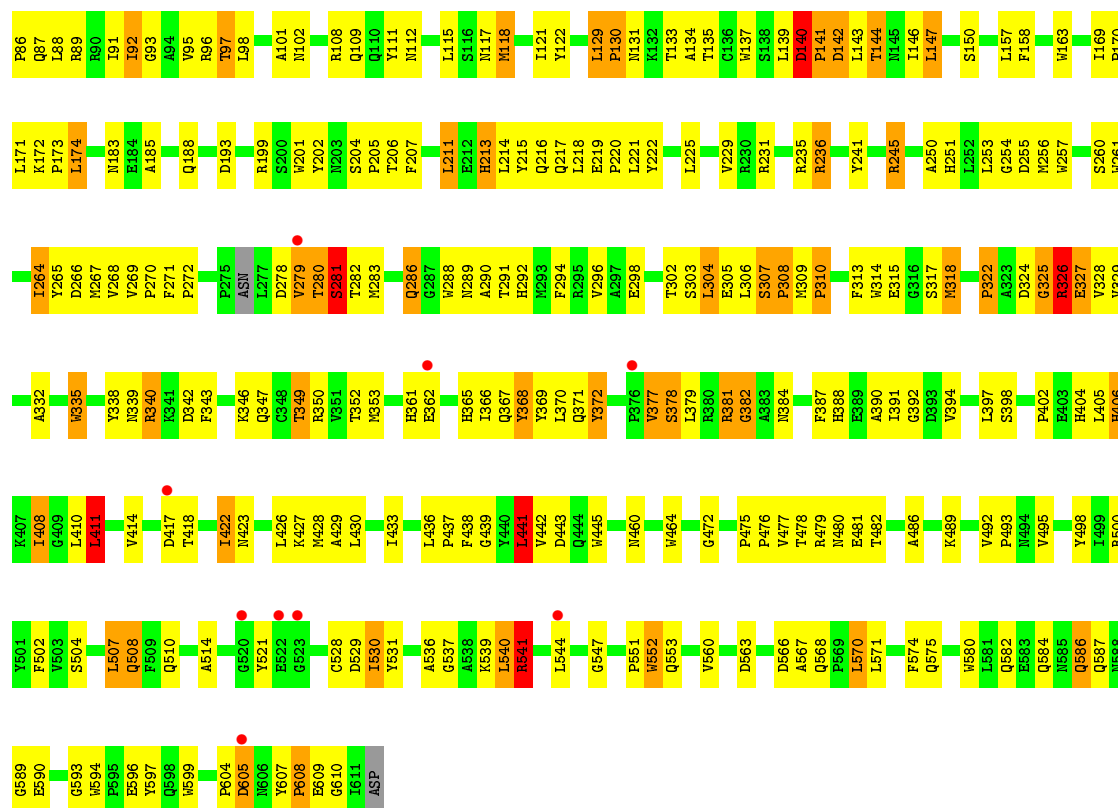
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM



• Molecule 1: ANGIOTENSIN-CONVERTING ENZYME, SOMATIC ISOFORM





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

Chain C: 100%

MAG1
MAG2

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

Chain D: 50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.30Å 210.90Å 171.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 3.00 89.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (28.76-3.00) 95.0 (89.76-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.294 , 0.308 0.275 , 0.280	Depositor DCC
R_{free} test set	1088 reflections (3.09%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	9621	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, NAG, CL, LPR, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	4/4901 (0.1%)	0.89	23/6707 (0.3%)
1	B	0.58	3/4819 (0.1%)	0.92	26/6608 (0.4%)
All	All	0.59	7/9720 (0.1%)	0.90	49/13315 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	8
All	All	1	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	ARG	CB-CG	8.17	1.74	1.52
1	B	25	ASN	CB-CG	-6.37	1.36	1.51
1	B	541	ARG	CB-CG	6.19	1.69	1.52
1	A	381	ARG	CG-CD	6.03	1.67	1.51
1	A	351	VAL	CB-CG1	-5.53	1.41	1.52
1	B	350	ARG	CA-CB	5.24	1.65	1.53
1	A	350	ARG	CB-CG	5.18	1.66	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	SER	C-N-CD	-10.95	96.50	120.60
1	B	305	GLU	N-CA-C	9.82	137.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	GLU	C-N-CD	-8.88	101.06	120.60
1	A	523	GLY	N-CA-C	-8.38	92.16	113.10
1	B	76	TYR	N-CA-C	8.24	133.24	111.00
1	B	3	PRO	N-CA-C	8.04	133.02	112.10
1	A	351	VAL	N-CA-CB	-7.77	94.41	111.50
1	B	349	THR	C-N-CA	-7.49	102.99	121.70
1	B	441	LEU	CA-CB-CG	7.18	131.82	115.30
1	A	280	THR	N-CA-C	-6.80	92.64	111.00
1	A	380	ARG	N-CA-C	-6.79	92.67	111.00
1	A	62	GLN	C-N-CA	-6.77	104.78	121.70
1	B	540	LEU	C-N-CA	-6.75	104.82	121.70
1	A	381	ARG	CB-CA-C	6.37	123.13	110.40
1	A	380	ARG	CA-C-N	-6.24	103.48	117.20
1	A	349	THR	N-CA-C	6.23	127.83	111.00
1	B	5	LEU	N-CA-C	-6.21	94.24	111.00
1	A	174	LEU	CA-CB-CG	6.19	129.54	115.30
1	A	550	ARG	CA-CB-CG	6.12	126.87	113.40
1	B	326	ARG	N-CA-C	5.77	126.57	111.00
1	B	9	ASN	N-CA-C	5.68	126.35	111.00
1	B	417	ASP	N-CA-C	-5.61	95.85	111.00
1	A	64	PHE	N-CA-C	-5.60	95.87	111.00
1	B	305	GLU	C-N-CA	-5.58	107.76	121.70
1	B	4	GLY	N-CA-C	-5.52	99.29	113.10
1	A	606	ASN	N-CA-C	-5.51	96.11	111.00
1	B	29	GLU	OE1-CD-OE2	-5.48	116.72	123.30
1	B	75	LEU	N-CA-C	-5.45	96.29	111.00
1	A	381	ARG	N-CA-C	-5.42	96.37	111.00
1	A	550	ARG	CB-CG-CD	-5.37	97.64	111.60
1	A	91	ILE	N-CA-C	-5.37	96.51	111.00
1	A	288	TRP	N-CA-C	5.36	125.47	111.00
1	B	78	PRO	N-CA-C	-5.34	98.20	112.10
1	B	610	GLY	C-N-CA	5.31	134.97	121.70
1	B	135	THR	N-CA-C	-5.30	96.70	111.00
1	A	350	ARG	N-CA-CB	5.28	120.10	110.60
1	A	142	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	335	TRP	N-CA-C	5.26	125.21	111.00
1	B	85	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	140	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	529	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	549	SER	C-N-CA	-5.23	108.63	121.70
1	A	417	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	605	ASP	CB-CG-OD2	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	325	GLY	N-CA-C	5.18	126.06	113.10
1	A	279	VAL	N-CA-C	-5.17	97.04	111.00
1	A	350	ARG	CA-C-N	-5.16	105.85	117.20
1	B	8	GLY	N-CA-C	-5.05	100.48	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	530	ILE	CB

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	380	ARG	Mainchain
1	B	140	ASP	Peptide
1	B	215	TYR	Sidechain
1	B	541	ARG	Mainchain
1	B	609	GLU	Peptide
1	B	76	TYR	Sidechain
1	B	83	PHE	Peptide
1	B	85	ASP	Peptide
1	B	86	PRO	Peptide

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	4747	0	4318	390	0
1	B	4665	0	4155	332	0
2	C	28	0	25	2	0
2	D	28	0	25	6	0
3	A	28	0	26	7	0
3	B	28	0	26	11	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	1	0
6	A	29	0	27	2	0
6	B	29	0	27	0	0
7	A	12	0	14	5	0
8	B	4	0	3	1	0
9	A	8	0	0	1	0
9	B	11	0	0	1	0
All	All	9621	0	8646	730	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 40.

All (730) 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:381:ARG:CG	1:A:381:ARG:CB	1.74	1.63
1:B:482:THR:CG2	2:D:1:NAG:H82	1.56	1.33
1:A:6:GLN:HG3	1:A:7:PRO:CD	1.78	1.11
3:B:693:NAG:O3	3:B:693:NAG:H83	1.50	1.11
3:A:693:NAG:O7	3:A:693:NAG:H3	1.48	1.10
3:B:693:NAG:C3	3:B:693:NAG:C8	2.30	1.10
1:B:98:LEU:HB2	1:B:102:ASN:ND2	1.66	1.09
1:B:236:ARG:HE	1:B:267:MET:HE2	1.11	1.09
1:B:482:THR:HG21	2:D:1:NAG:H82	1.12	1.08
1:B:174:LEU:H	1:B:174:LEU:HD23	1.16	1.08
1:B:482:THR:HG21	2:D:1:NAG:C8	1.83	1.07
3:B:693:NAG:H3	3:B:693:NAG:H82	1.17	1.06
3:B:693:NAG:H3	3:B:693:NAG:C8	1.79	1.06
1:A:279:VAL:CG1	1:A:282:THR:HG22	1.85	1.05
1:A:279:VAL:HG13	1:A:282:THR:HG22	1.12	1.05
1:A:99:GLY:O	1:A:185:ALA:HB1	1.57	1.05
1:B:586:GLN:HG3	1:B:587:GLN:N	1.74	1.00
1:A:20:PHE:C	1:A:20:PHE:HD2	1.65	1.00
1:B:98:LEU:HB2	1:B:102:ASN:HD21	1.17	1.00
1:A:279:VAL:HG11	1:A:410:LEU:CB	1.91	1.00
1:A:6:GLN:CG	1:A:7:PRO:HD2	1.93	0.99
1:B:58:ALA:O	1:B:62:GLN:HG3	1.61	0.99
1:A:352:THR:HG22	1:A:354:ASP:OD2	1.63	0.99
1:B:306:LEU:H	1:B:541:ARG:HH11	0.99	0.98
1:B:369:TYR:HA	1:B:372:TYR:HE2	1.29	0.97
1:B:102:ASN:HB3	1:B:188:GLN:NE2	1.79	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HE	1:B:267:MET:CE	1.76	0.97
1:A:6:GLN:HG3	1:A:7:PRO:HD2	0.99	0.96
1:A:356:LEU:O	1:A:356:LEU:HD12	1.65	0.96
1:B:306:LEU:H	1:B:541:ARG:NH1	1.63	0.96
1:B:406:HIS:HB2	1:B:411:LEU:O	1.64	0.95
1:A:17:ALA:HA	1:A:76:TYR:CZ	2.02	0.94
1:B:26:SER:HA	3:B:693:NAG:O6	1.68	0.94
1:B:202:TYR:O	1:B:552:TRP:CZ2	2.21	0.93
1:A:530:ILE:HG23	1:A:530:ILE:O	1.67	0.92
1:A:279:VAL:HG13	1:A:282:THR:CG2	2.00	0.92
1:B:129:LEU:N	1:B:129:LEU:HD12	1.83	0.92
1:B:4:GLY:O	1:B:6:GLN:N	2.03	0.92
1:B:552:TRP:CD1	1:B:553:GLN:N	2.37	0.91
1:A:91:ILE:HG23	1:A:378:SER:OG	1.71	0.91
1:A:72:ALA:O	1:A:76:TYR:HB2	1.70	0.90
1:A:84:THR:O	1:A:86:PRO:HD3	1.69	0.90
1:A:31:VAL:HG21	1:A:64:PHE:HD1	1.37	0.90
1:B:118:MET:HG2	1:B:171:LEU:HD11	1.53	0.90
1:A:300:PHE:CE2	1:A:304:LEU:CD1	2.55	0.89
1:B:384:ASN:ND2	1:B:552:TRP:HE3	1.68	0.89
1:B:20:PHE:HD2	1:B:20:PHE:C	1.75	0.89
1:A:369:TYR:HD2	1:A:372:TYR:OH	1.54	0.89
1:B:236:ARG:NE	1:B:267:MET:CE	2.34	0.89
1:A:550:ARG:HB3	1:A:551:PRO:HD3	1.54	0.88
1:A:86:PRO:C	1:A:88:LEU:H	1.74	0.88
7:A:2433:GOL:O1	1:B:593:GLY:HA3	1.73	0.88
1:B:129:LEU:C	1:B:131:ASN:H	1.76	0.87
1:A:20:PHE:C	1:A:20:PHE:CD2	2.42	0.87
1:A:369:TYR:CD2	1:A:372:TYR:OH	2.27	0.87
1:B:482:THR:HG22	2:D:1:NAG:H82	1.52	0.87
1:B:129:LEU:O	1:B:131:ASN:N	2.08	0.87
1:B:27:SER:HG	1:B:68:TRP:HH2	1.23	0.87
1:B:306:LEU:N	1:B:541:ARG:HH11	1.73	0.87
1:B:279:VAL:HG13	1:B:279:VAL:O	1.72	0.86
1:B:326:ARG:O	1:B:328:VAL:HG13	1.75	0.86
1:A:147:LEU:HD23	1:A:256:MET:N	1.88	0.86
1:B:174:LEU:N	1:B:174:LEU:HD23	1.90	0.85
1:A:350:ARG:HG3	1:A:351:VAL:HB	1.59	0.85
1:A:191:PHE:CE1	1:A:197:TYR:HD1	1.95	0.85
1:A:352:THR:CG2	1:A:354:ASP:OD2	2.23	0.85
1:B:129:LEU:H	1:B:129:LEU:HD12	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:C	1:A:530:ILE:HD11	1.97	0.84
1:A:300:PHE:CE2	1:A:304:LEU:HD13	2.11	0.84
1:A:191:PHE:CE1	1:A:197:TYR:CD1	2.66	0.84
1:B:309:MET:HE1	1:B:370:LEU:HD11	1.60	0.84
1:A:550:ARG:HB3	1:A:551:PRO:CD	2.06	0.84
1:A:20:PHE:HD2	1:A:20:PHE:O	1.60	0.83
1:B:213:HIS:O	1:B:216:GLN:HB2	1.77	0.83
1:A:402:PRO:HA	1:A:411:LEU:HD12	1.62	0.82
1:A:399:VAL:O	1:A:405:LEU:HD21	1.79	0.82
1:B:279:VAL:CG1	1:B:279:VAL:O	2.27	0.82
1:A:270:PRO:HD3	1:A:426:LEU:HD22	1.62	0.82
1:B:552:TRP:N	1:B:552:TRP:CD1	2.45	0.81
1:B:202:TYR:O	1:B:552:TRP:CH2	2.34	0.81
1:B:20:PHE:CD2	1:B:20:PHE:C	2.52	0.81
1:A:139:LEU:HD22	1:A:163:TRP:CZ2	2.16	0.81
3:B:695:NAG:C1	3:B:695:NAG:O7	2.30	0.80
1:A:31:VAL:CG2	1:A:64:PHE:HD1	1.95	0.79
1:A:20:PHE:CB	1:A:76:TYR:HE1	1.94	0.79
1:A:507:LEU:HG	1:A:507:LEU:O	1.80	0.79
1:A:16:GLY:O	1:A:76:TYR:OH	1.99	0.79
1:A:550:ARG:CB	1:A:551:PRO:CD	2.59	0.79
1:A:49:GLU:O	1:A:53:ARG:HG3	1.83	0.79
1:B:147:LEU:HD22	1:B:256:MET:HA	1.63	0.79
1:B:280:THR:C	1:B:282:THR:H	1.84	0.79
3:B:693:NAG:H83	3:B:693:NAG:C3	2.05	0.78
1:A:332:ALA:CB	1:A:347:GLN:HG3	2.14	0.78
1:B:236:ARG:NE	1:B:267:MET:HE2	1.90	0.78
1:A:441:LEU:O	1:A:444:GLN:HB2	1.83	0.78
1:A:46:ILE:HG22	1:A:327:GLU:O	1.84	0.78
1:A:96:ARG:HG2	1:A:96:ARG:O	1.82	0.78
1:B:174:LEU:CD2	1:B:174:LEU:H	1.95	0.78
1:A:402:PRO:CA	1:A:411:LEU:HD12	2.14	0.78
1:A:597:TYR:O	1:A:598:GLN:HB3	1.84	0.78
1:A:262:GLU:HG2	1:A:431:GLU:HB2	1.66	0.77
1:A:535:LYS:HD2	1:A:535:LYS:H	1.49	0.77
1:B:369:TYR:HA	1:B:372:TYR:CE2	2.18	0.77
1:B:482:THR:CG2	2:D:1:NAG:C8	2.47	0.76
1:B:280:THR:O	1:B:283:MET:N	2.18	0.76
1:B:384:ASN:HD22	1:B:552:TRP:HE3	0.88	0.76
1:A:86:PRO:C	1:A:88:LEU:N	2.35	0.76
1:A:20:PHE:HE1	1:A:72:ALA:CA	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ALA:HB2	1:A:347:GLN:HG3	1.67	0.75
1:B:2:ASP:CB	1:B:3:PRO:O	2.34	0.75
1:B:289:ASN:HB3	1:B:292:HIS:H	1.52	0.75
1:A:125:ALA:C	1:A:126:LYS:HG3	2.06	0.75
1:B:507:LEU:HA	1:B:510:GLN:HG3	1.69	0.75
1:B:304:LEU:N	1:B:304:LEU:HD23	2.00	0.75
1:A:221:LEU:HD23	1:A:433:ILE:HD12	1.69	0.75
1:A:441:LEU:HD23	1:A:442:VAL:N	2.01	0.75
1:A:530:ILE:CG2	1:A:530:ILE:O	2.33	0.75
1:B:216:GLN:HE21	1:B:216:GLN:HA	1.51	0.75
1:B:44:THR:O	1:B:328:VAL:HG12	1.87	0.75
1:B:464:TRP:CE3	1:B:475:PRO:HD3	2.22	0.75
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.69	0.74
1:A:64:PHE:CE2	1:A:68:TRP:CD1	2.75	0.74
1:B:77:GLU:O	1:B:77:GLU:HG3	1.87	0.74
1:B:391:ILE:HD12	1:B:544:LEU:HD21	1.70	0.74
1:A:351:VAL:HG12	1:A:351:VAL:O	1.88	0.74
1:B:235:ARG:NH1	9:B:2004:HOH:O	2.10	0.74
1:B:174:LEU:CD2	1:B:174:LEU:N	2.51	0.73
1:B:102:ASN:HB3	1:B:188:GLN:HE22	1.49	0.73
1:A:9:ASN:OD1	1:A:10:PHE:N	2.22	0.73
1:B:291:THR:CG2	1:B:314:TRP:HZ3	2.02	0.73
1:B:540:LEU:O	1:B:540:LEU:HD23	1.88	0.73
1:A:395:LEU:O	1:A:399:VAL:HG23	1.89	0.72
1:B:530:ILE:O	1:B:530:ILE:HG23	1.88	0.72
1:A:178:PHE:CE1	1:A:495:VAL:HG21	2.24	0.72
3:A:693:NAG:O7	3:A:693:NAG:C3	2.30	0.72
1:A:332:ALA:HB3	6:A:705:LPR:H101	1.72	0.72
1:B:310:PRO:O	1:B:313:PHE:HB3	1.90	0.72
1:A:453:ARG:HD3	8:B:710:ACT:O	1.90	0.72
1:A:368:TYR:O	1:A:372:TYR:CD2	2.43	0.72
1:B:10:PHE:CD1	1:B:10:PHE:N	2.56	0.72
1:A:440:TYR:O	1:A:444:GLN:HG2	1.88	0.72
1:A:381:ARG:CD	1:A:381:ARG:CB	2.67	0.71
1:A:515:LEU:CB	1:A:530:ILE:HD13	2.20	0.71
1:A:31:VAL:O	1:A:34:GLN:HG3	1.89	0.71
1:B:271:PHE:CE1	1:B:422:ILE:HG21	2.25	0.71
1:A:300:PHE:CD2	1:A:304:LEU:HD13	2.26	0.71
1:A:20:PHE:HE1	1:A:72:ALA:HA	1.55	0.71
1:A:446:ARG:NH2	1:A:496:THR:O	2.23	0.71
1:B:29:GLU:HG3	1:B:338:TYR:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:PHE:CD1	1:A:197:TYR:HB2	2.26	0.70
1:B:171:LEU:HD21	1:B:493:PRO:HB3	1.73	0.70
1:A:456:PRO:HA	1:A:459:TYR:CD2	2.26	0.70
1:A:31:VAL:HG21	1:A:64:PHE:CD1	2.24	0.70
1:B:4:GLY:C	1:B:6:GLN:N	2.40	0.70
1:A:20:PHE:HB2	1:A:76:TYR:HE1	1.56	0.70
1:A:146:ILE:O	1:A:150:SER:HB3	1.92	0.70
1:B:280:THR:C	1:B:282:THR:N	2.42	0.70
1:A:147:LEU:CD2	1:A:256:MET:HA	2.21	0.70
1:A:350:ARG:HG3	1:A:351:VAL:CB	2.22	0.70
1:A:91:ILE:HG12	1:A:379:LEU:HD21	1.74	0.70
1:B:142:ASP:O	1:B:146:ILE:HG13	1.92	0.69
1:B:265:TYR:CE1	1:B:427:LYS:HB2	2.26	0.69
1:B:366:ILE:O	1:B:369:TYR:N	2.25	0.69
1:B:280:THR:HG22	1:B:281:SER:N	2.07	0.69
1:B:332:ALA:HB2	1:B:347:GLN:HG3	1.74	0.69
1:A:63:GLU:HB2	1:A:108:ARG:HH12	1.57	0.69
1:B:7:PRO:HG3	1:B:68:TRP:CD2	2.28	0.69
7:A:2433:GOL:O1	1:B:593:GLY:CA	2.40	0.69
1:A:593:GLY:HA3	7:A:2434:GOL:O1	1.93	0.69
1:B:118:MET:HG2	1:B:171:LEU:CD1	2.23	0.69
1:A:69:GLY:O	1:A:73:LYS:HG3	1.93	0.69
1:A:75:LEU:HD23	1:A:75:LEU:H	1.57	0.69
1:B:173:PRO:HG2	1:B:174:LEU:CD2	2.24	0.68
1:A:20:PHE:CD2	1:A:20:PHE:O	2.43	0.68
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.74	0.68
1:A:404:HIS:ND1	1:A:529:ASP:OD2	2.24	0.68
1:A:75:LEU:N	1:A:75:LEU:HD23	2.09	0.68
1:B:384:ASN:ND2	1:B:552:TRP:CE3	2.48	0.68
1:B:406:HIS:CA	1:B:411:LEU:HB3	2.23	0.68
1:B:552:TRP:HD1	1:B:552:TRP:N	1.90	0.67
1:B:29:GLU:OE1	3:B:693:NAG:H62	1.93	0.67
1:B:62:GLN:NE2	1:B:108:ARG:HD3	2.09	0.67
1:B:118:MET:CG	1:B:171:LEU:HD11	2.25	0.67
1:B:402:PRO:O	1:B:411:LEU:HD12	1.95	0.67
1:A:129:LEU:N	1:A:129:LEU:HD12	2.10	0.67
1:A:253:LEU:HD22	1:A:253:LEU:N	2.10	0.66
1:B:563:ASP:OD1	1:B:563:ASP:O	2.13	0.66
1:A:20:PHE:CE1	1:A:72:ALA:HA	2.30	0.66
1:B:221:LEU:HD12	1:B:433:ILE:HD13	1.78	0.66
1:A:515:LEU:CB	1:A:530:ILE:CD1	2.74	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:PHE:O	1:B:211:LEU:HD12	1.96	0.66
1:B:406:HIS:CB	1:B:411:LEU:HB3	2.25	0.66
1:A:492:VAL:N	1:A:493:PRO:HD2	2.10	0.66
1:B:278:ASP:OD2	1:B:353:MET:CB	2.44	0.66
1:A:147:LEU:CD2	1:A:256:MET:N	2.59	0.66
1:B:25:ASN:OD1	3:B:693:NAG:H5	1.95	0.66
1:A:529:ASP:OD1	1:A:529:ASP:C	2.34	0.65
1:B:26:SER:HA	3:B:693:NAG:C6	2.26	0.65
1:A:279:VAL:CG1	1:A:282:THR:CG2	2.68	0.65
1:A:480:ASN:OD1	1:A:482:THR:HG23	1.97	0.65
1:A:46:ILE:HG23	1:A:46:ILE:O	1.96	0.65
1:B:133:THR:O	1:B:134:ALA:HB3	1.96	0.65
1:B:216:GLN:NE2	1:B:216:GLN:HA	2.11	0.65
1:B:76:TYR:O	1:B:80:TRP:HB3	1.95	0.65
1:A:236:ARG:HG2	1:A:267:MET:CE	2.27	0.65
1:B:140:ASP:OD1	1:B:140:ASP:C	2.35	0.65
1:B:406:HIS:CB	1:B:411:LEU:O	2.43	0.65
1:A:515:LEU:O	1:A:530:ILE:HD11	1.97	0.64
1:A:529:ASP:OD1	1:A:531:TYR:HB2	1.98	0.64
1:A:87:GLN:O	1:A:87:GLN:HG2	1.97	0.64
1:A:91:ILE:CG2	1:A:378:SER:OG	2.44	0.64
1:A:34:GLN:HG3	1:A:35:SER:H	1.63	0.64
1:A:122:TYR:CD1	1:A:493:PRO:HG3	2.33	0.64
1:B:279:VAL:O	1:B:283:MET:HG3	1.97	0.64
1:B:329:VAL:O	1:B:346:LYS:CE	2.46	0.63
1:A:17:ALA:HA	1:A:76:TYR:CE1	2.32	0.63
1:A:206:THR:CG2	1:A:210:ASP:OD2	2.46	0.63
1:B:464:TRP:CZ3	1:B:475:PRO:HD3	2.34	0.63
1:B:306:LEU:CB	1:B:541:ARG:HG3	2.28	0.63
1:A:147:LEU:HD21	1:A:256:MET:HA	1.80	0.63
1:B:279:VAL:HG22	1:B:410:LEU:O	1.99	0.63
1:B:64:PHE:CE1	1:B:68:TRP:NE1	2.66	0.63
1:A:300:PHE:CE2	1:A:304:LEU:HD11	2.32	0.63
1:A:31:VAL:CB	1:A:64:PHE:HD1	2.11	0.63
1:B:329:VAL:O	1:B:346:LYS:HE3	1.98	0.63
1:A:283:MET:HE1	1:A:356:LEU:HB2	1.81	0.63
1:B:139:LEU:HD22	1:B:163:TRP:CZ2	2.34	0.63
1:B:280:THR:O	1:B:282:THR:N	2.32	0.63
1:B:489:LYS:O	1:B:493:PRO:HD2	1.98	0.63
1:A:399:VAL:O	1:A:405:LEU:CD2	2.46	0.62
1:B:29:GLU:CG	1:B:338:TYR:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:THR:O	1:A:405:LEU:HG	2.00	0.62
1:B:183:ASN:HD21	1:B:193:ASP:HB2	1.65	0.62
1:B:570:LEU:HD23	1:B:574:PHE:HD1	1.63	0.62
1:A:312:GLU:CD	1:A:341:LYS:O	2.38	0.62
1:A:125:ALA:O	1:A:126:LYS:HG3	2.00	0.61
1:A:402:PRO:HA	1:A:411:LEU:CD1	2.28	0.61
1:A:236:ARG:HG2	1:A:267:MET:HE3	1.81	0.61
1:B:77:GLU:OE2	1:B:96:ARG:NH2	2.32	0.61
1:A:251:HIS:CE1	1:A:476:PRO:HB3	2.35	0.61
1:A:369:TYR:HA	1:A:372:TYR:CZ	2.35	0.61
1:A:122:TYR:CD2	1:A:122:TYR:C	2.74	0.61
1:A:20:PHE:CE1	1:A:72:ALA:HB2	2.36	0.61
1:B:286:GLN:CG	1:B:286:GLN:O	2.48	0.61
1:A:530:ILE:HG12	1:A:536:ALA:CB	2.31	0.61
1:B:146:ILE:O	1:B:150:SER:HB3	2.00	0.61
1:A:489:LYS:O	1:A:493:PRO:HD2	2.01	0.61
1:A:86:PRO:HA	1:A:89:ARG:H	1.65	0.61
1:B:29:GLU:OE2	1:B:339:ASN:HA	2.01	0.61
1:A:402:PRO:O	1:A:411:LEU:HD12	2.01	0.60
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.82	0.60
1:B:372:TYR:HD2	1:B:372:TYR:H	1.49	0.60
1:B:264:ILE:HG23	1:B:264:ILE:O	1.99	0.60
1:A:31:VAL:CB	1:A:64:PHE:CD1	2.84	0.60
1:A:31:VAL:HB	1:A:64:PHE:CD1	2.36	0.60
1:B:441:LEU:HD23	1:B:442:VAL:N	2.16	0.60
1:B:97:THR:HG22	1:B:97:THR:O	2.01	0.60
1:A:270:PRO:HD3	1:A:426:LEU:CD2	2.30	0.60
1:A:16:GLY:HA2	1:A:19:LEU:HB2	1.84	0.60
1:B:404:HIS:HB2	1:B:529:ASP:OD2	2.01	0.60
1:B:62:GLN:OE1	1:B:112:ASN:ND2	2.35	0.60
1:A:236:ARG:HE	1:A:267:MET:CE	2.14	0.60
1:A:51:ALA:O	1:A:55:GLU:HG3	2.00	0.60
1:B:315:GLU:C	1:B:317:SER:H	2.04	0.60
1:A:261:TRP:O	1:A:264:ILE:HG12	2.02	0.60
1:A:20:PHE:HB2	1:A:76:TYR:CE1	2.37	0.60
1:A:86:PRO:O	1:A:88:LEU:N	2.33	0.60
1:A:279:VAL:CG1	1:A:410:LEU:CB	2.76	0.59
1:A:29:GLU:OE1	3:A:693:NAG:C2	2.50	0.59
1:B:279:VAL:CG2	1:B:410:LEU:O	2.50	0.59
1:B:97:THR:O	1:B:97:THR:CG2	2.50	0.59
2:C:1:NAG:H62	2:C:2:NAG:O5	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:CD1	1:A:424:TYR:HA	2.33	0.59
1:A:139:LEU:HD22	1:A:163:TRP:CH2	2.38	0.59
1:A:100:SER:O	1:A:103:LEU:N	2.35	0.59
1:A:147:LEU:CD2	1:A:256:MET:CA	2.81	0.59
1:B:309:MET:CE	1:B:370:LEU:HD11	2.30	0.59
1:A:304:LEU:O	1:A:306:LEU:HG	2.02	0.59
1:A:283:MET:HE1	1:A:356:LEU:CD2	2.32	0.59
1:A:478:THR:O	1:A:479:ARG:HD2	2.03	0.59
1:A:69:GLY:O	1:A:73:LYS:CG	2.50	0.59
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.37	0.59
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.83	0.58
1:B:83:PHE:CB	1:B:85:ASP:H	2.16	0.58
1:A:551:PRO:O	1:A:555:VAL:HG23	2.04	0.58
1:A:64:PHE:CE2	1:A:68:TRP:NE1	2.72	0.58
1:A:368:TYR:C	1:A:372:TYR:CE2	2.76	0.58
1:B:17:ALA:HA	1:B:76:TYR:CE1	2.37	0.58
1:B:251:HIS:CE1	1:B:476:PRO:HB3	2.37	0.58
1:B:7:PRO:HG3	1:B:68:TRP:CG	2.37	0.58
1:A:11:SER:O	1:A:76:TYR:HE2	1.86	0.58
1:B:291:THR:CG2	1:B:314:TRP:CZ3	2.86	0.58
1:A:248:ILE:O	1:A:473:ILE:HA	2.03	0.58
1:A:515:LEU:C	1:A:530:ILE:CD1	2.70	0.58
1:B:580:TRP:O	1:B:584:GLN:HG2	2.04	0.58
1:A:206:THR:HG23	1:A:210:ASP:CG	2.25	0.58
1:A:40:TRP:O	1:A:44:THR:HG23	2.04	0.57
1:B:173:PRO:HG2	1:B:174:LEU:HD23	1.86	0.57
1:B:75:LEU:HB3	1:B:76:TYR:CD2	2.40	0.57
1:A:99:GLY:C	1:A:185:ALA:HB1	2.22	0.57
1:A:178:PHE:CD2	1:A:178:PHE:C	2.77	0.57
1:B:504:SER:O	1:B:508:GLN:HB3	2.05	0.57
1:A:100:SER:O	1:A:103:LEU:HB2	2.04	0.57
1:A:17:ALA:HA	1:A:76:TYR:OH	2.04	0.57
1:A:402:PRO:CA	1:A:411:LEU:CD1	2.83	0.57
1:B:426:LEU:O	1:B:429:ALA:HB3	2.05	0.57
1:A:64:PHE:HE2	1:A:68:TRP:CD1	2.21	0.56
1:B:288:TRP:CH2	1:B:296:VAL:HG21	2.40	0.56
1:B:291:THR:HG22	1:B:314:TRP:HZ3	1.69	0.56
1:B:379:LEU:C	1:B:381:ARG:H	2.08	0.56
1:B:379:LEU:O	1:B:381:ARG:N	2.30	0.56
1:B:291:THR:HG22	1:B:314:TRP:CZ3	2.41	0.56
1:A:147:LEU:HD23	1:A:255:ASP:C	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ALA:HA	1:A:64:PHE:CE1	2.39	0.56
1:B:552:TRP:CG	1:B:553:GLN:N	2.72	0.56
1:A:261:TRP:N	1:A:261:TRP:CD1	2.73	0.56
1:A:493:PRO:HG2	1:A:494:ASN:HD22	1.69	0.56
1:A:108:ARG:O	1:A:112:ASN:ND2	2.39	0.56
1:A:399:VAL:HA	1:A:404:HIS:CD2	2.41	0.56
1:B:318:MET:SD	1:B:322:PRO:HD3	2.46	0.56
1:B:17:ALA:O	1:B:20:PHE:HB3	2.05	0.56
1:A:253:LEU:N	1:A:253:LEU:CD2	2.69	0.55
1:A:464:TRP:CE3	1:A:475:PRO:HD3	2.41	0.55
1:A:11:SER:O	1:A:76:TYR:CE2	2.59	0.55
1:A:31:VAL:HA	1:A:34:GLN:HG2	1.89	0.55
1:A:326:ARG:O	1:A:328:VAL:HG12	2.06	0.55
1:A:29:GLU:OE1	3:A:693:NAG:N2	2.39	0.55
1:B:98:LEU:CB	1:B:102:ASN:HD21	2.05	0.55
1:A:139:LEU:HA	1:A:143:LEU:HB2	1.88	0.55
1:B:438:PHE:HA	1:B:441:LEU:HD13	1.88	0.55
1:A:236:ARG:HE	1:A:267:MET:HE2	1.72	0.55
1:A:32:LEU:HD13	1:A:338:TYR:CD2	2.41	0.55
1:A:299:GLU:HG3	1:A:299:GLU:O	2.05	0.55
1:A:350:ARG:HG3	1:A:351:VAL:CG2	2.37	0.55
1:A:283:MET:CE	1:A:356:LEU:CD2	2.84	0.55
1:A:368:TYR:O	1:A:372:TYR:CE2	2.60	0.55
1:A:383:ALA:HB1	1:A:552:TRP:CB	2.37	0.55
1:B:289:ASN:HB3	1:B:292:HIS:CB	2.37	0.55
1:B:530:ILE:CG2	1:B:530:ILE:O	2.55	0.55
1:B:478:THR:O	1:B:479:ARG:HD2	2.06	0.55
1:A:383:ALA:HB1	1:A:552:TRP:HB3	1.88	0.54
1:A:381:ARG:CG	1:A:381:ARG:CA	2.80	0.54
1:A:140:ASP:OD2	1:A:141:PRO:CA	2.54	0.54
1:A:206:THR:HG23	1:A:210:ASP:OD2	2.08	0.54
1:B:27:SER:CB	1:B:68:TRP:CZ2	2.90	0.54
1:B:92:ILE:HG13	1:B:92:ILE:O	2.07	0.54
1:A:87:GLN:CG	1:A:87:GLN:O	2.56	0.54
1:A:3:PRO:C	1:A:5:LEU:H	2.10	0.54
1:B:26:SER:HA	3:B:693:NAG:HO6	1.69	0.54
1:A:393:ASP:O	1:A:396:ALA:HB3	2.08	0.54
1:A:490:PHE:C	1:A:490:PHE:CD2	2.80	0.54
1:B:225:LEU:O	1:B:229:VAL:HG23	2.07	0.54
1:A:283:MET:CE	1:A:356:LEU:HD23	2.38	0.54
1:A:367:GLN:O	1:A:371:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:HD2	1:A:64:PHE:C	2.11	0.54
1:B:540:LEU:CD2	1:B:544:LEU:HG	2.39	0.53
1:A:206:THR:HG23	1:A:210:ASP:OD1	2.09	0.53
1:A:550:ARG:NH1	1:A:554:GLU:HB3	2.23	0.53
1:B:379:LEU:C	1:B:381:ARG:N	2.61	0.53
1:B:406:HIS:HB2	1:B:411:LEU:HB3	1.89	0.53
1:B:271:PHE:HE1	1:B:422:ILE:HG21	1.70	0.53
1:B:27:SER:OG	1:B:68:TRP:CH2	2.61	0.53
1:B:27:SER:OG	1:B:68:TRP:HH2	1.89	0.53
1:A:593:GLY:HA3	7:A:2434:GOL:HO1	1.73	0.53
1:B:253:LEU:HD12	1:B:261:TRP:CD2	2.43	0.53
1:B:270:PRO:O	1:B:272:PRO:HD3	2.08	0.53
1:B:326:ARG:O	1:B:327:GLU:C	2.47	0.53
1:B:77:GLU:N	1:B:78:PRO:CD	2.71	0.53
1:A:233:LEU:HB3	1:A:242:ILE:CD1	2.37	0.53
1:A:550:ARG:CB	1:A:551:PRO:HD3	2.24	0.53
1:A:99:GLY:O	1:A:185:ALA:CB	2.45	0.53
1:A:80:TRP:HA	1:A:83:PHE:CE1	2.44	0.53
1:B:143:LEU:O	1:B:146:ILE:N	2.41	0.53
1:B:270:PRO:HD3	1:B:426:LEU:HD22	1.91	0.53
1:B:147:LEU:HD22	1:B:256:MET:CA	2.36	0.53
1:B:405:LEU:O	1:B:408:ILE:HG12	2.08	0.53
1:A:384:ASN:HB2	1:A:385:PRO:HD2	1.91	0.53
1:A:402:PRO:C	1:A:411:LEU:HD12	2.29	0.53
1:A:499:ILE:HG13	1:A:499:ILE:O	2.09	0.53
1:B:372:TYR:HD1	1:B:547:GLY:CA	2.21	0.53
1:A:122:TYR:O	1:A:122:TYR:CD2	2.63	0.52
1:A:53:ARG:O	1:A:56:GLU:N	2.38	0.52
1:A:306:LEU:HD21	1:A:541:ARG:HB2	1.91	0.52
1:A:64:PHE:CD2	1:A:64:PHE:C	2.82	0.52
1:B:540:LEU:O	1:B:540:LEU:CD2	2.56	0.52
1:B:306:LEU:H	1:B:541:ARG:CZ	2.18	0.52
1:B:44:THR:O	1:B:328:VAL:CG1	2.57	0.52
1:A:417:ASP:O	1:A:421:ASP:HB2	2.09	0.52
1:A:29:GLU:OE1	3:A:693:NAG:H2	2.10	0.52
1:A:302:THR:OG1	1:A:303:SER:N	2.42	0.52
1:B:306:LEU:N	1:B:541:ARG:HE	2.08	0.52
1:A:214:LEU:HD21	1:A:506:VAL:HG11	1.92	0.52
1:B:329:VAL:HB	1:B:346:LYS:HE3	1.91	0.52
1:A:265:TYR:CZ	1:A:269:VAL:HG23	2.45	0.52
1:B:495:VAL:O	1:B:495:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:O	1:A:269:VAL:C	2.48	0.52
1:B:514:ALA:HB2	1:B:560:VAL:HG22	1.91	0.52
1:B:27:SER:HB2	1:B:68:TRP:CZ2	2.45	0.51
1:A:63:GLU:O	1:A:63:GLU:HG2	2.10	0.51
1:B:68:TRP:O	1:B:71:LYS:N	2.42	0.51
1:A:271:PHE:HB2	1:A:423:ASN:HD21	1.75	0.51
1:B:329:VAL:O	1:B:346:LYS:HE2	2.10	0.51
1:A:331:HIS:CD2	1:A:490:PHE:CE2	2.98	0.51
1:A:510:GLN:OE1	1:A:566:ASP:N	2.41	0.51
1:A:6:GLN:CG	1:A:7:PRO:CD	2.70	0.51
1:A:233:LEU:HB3	1:A:242:ILE:HD12	1.91	0.51
1:A:25:ASN:O	1:A:29:GLU:HG3	2.10	0.51
1:B:332:ALA:CB	1:B:347:GLN:HG3	2.41	0.51
1:B:372:TYR:HD1	1:B:547:GLY:HA2	1.76	0.51
1:A:269:VAL:HG13	1:A:269:VAL:O	2.09	0.51
1:A:283:MET:HE1	1:A:356:LEU:HD23	1.92	0.51
1:B:44:THR:C	1:B:328:VAL:HG12	2.31	0.51
1:A:104:PRO:HG2	1:A:107:LYS:HD2	1.92	0.51
1:A:20:PHE:CE1	1:A:72:ALA:CB	2.93	0.51
1:A:100:SER:O	1:A:102:ASN:N	2.44	0.51
1:A:140:ASP:OD2	1:A:141:PRO:HA	2.10	0.51
1:A:46:ILE:CG2	1:A:46:ILE:O	2.59	0.50
1:A:583:GLU:O	1:A:587:GLN:HG3	2.11	0.50
1:A:597:TYR:O	1:A:598:GLN:CB	2.54	0.50
1:A:80:TRP:O	1:A:81:GLN:CB	2.59	0.50
1:B:398:SER:HB3	1:B:529:ASP:HA	1.92	0.50
1:A:541:ARG:HG3	1:A:541:ARG:O	2.10	0.50
1:B:482:THR:HG21	2:D:1:NAG:C7	2.40	0.50
1:B:202:TYR:HB3	1:B:552:TRP:CH2	2.45	0.50
1:B:302:THR:CG2	1:B:308:PRO:HB3	2.41	0.50
1:B:307:SER:HB3	1:B:367:GLN:OE1	2.11	0.50
1:A:328:VAL:CG2	1:A:329:VAL:N	2.75	0.50
1:A:441:LEU:CD1	1:A:467:ARG:HA	2.42	0.50
1:A:20:PHE:HB3	1:A:76:TYR:HE1	1.73	0.50
1:B:372:TYR:CD1	1:B:547:GLY:HA2	2.46	0.50
1:B:387:PHE:O	1:B:391:ILE:HG12	2.12	0.50
1:A:20:PHE:CE2	1:A:68:TRP:HE3	2.29	0.50
1:A:531:TYR:O	1:A:533:SER:N	2.45	0.50
1:B:10:PHE:HD1	1:B:10:PHE:H	1.57	0.50
1:B:339:ASN:C	1:B:340:ARG:HG3	2.32	0.50
1:A:279:VAL:HG21	1:A:410:LEU:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:CD1	1:B:129:LEU:N	2.56	0.50
1:B:264:ILE:CG2	1:B:264:ILE:O	2.59	0.50
1:A:206:THR:HG22	1:A:210:ASP:OD2	2.10	0.50
1:B:20:PHE:HD2	1:B:20:PHE:O	1.95	0.50
1:B:313:PHE:CD2	1:B:313:PHE:C	2.85	0.50
1:A:29:GLU:HB3	1:A:338:TYR:O	2.11	0.50
1:A:366:ILE:HA	1:A:369:TYR:CD1	2.46	0.50
1:B:294:PHE:HE1	1:B:349:THR:HG1	1.60	0.50
1:A:408:ILE:O	1:A:408:ILE:CG1	2.59	0.49
1:A:309:MET:SD	1:A:366:ILE:HG21	2.52	0.49
1:B:111:TYR:CE2	1:B:115:LEU:HD11	2.48	0.49
1:B:172:LYS:N	1:B:173:PRO:HD2	2.26	0.49
1:A:77:GLU:N	1:A:78:PRO:HD2	2.27	0.49
1:B:236:ARG:NE	1:B:267:MET:HE1	2.25	0.49
1:A:302:THR:O	1:A:305:GLU:N	2.46	0.49
1:A:575:GLN:HB3	1:A:576:PRO:HD3	1.93	0.49
1:B:147:LEU:O	1:B:254:GLY:HA2	2.12	0.49
1:B:265:TYR:OH	1:B:423:ASN:HB3	2.13	0.49
1:A:313:PHE:O	1:A:317:SER:HB2	2.13	0.49
1:A:20:PHE:HE1	1:A:72:ALA:CB	2.26	0.49
1:B:500:ARG:HB3	5:B:702:CL:CL	2.49	0.49
1:B:89:ARG:HA	1:B:92:ILE:HG23	1.94	0.49
1:A:495:VAL:O	1:A:495:VAL:HG12	2.12	0.49
1:B:309:MET:CE	1:B:366:ILE:HG21	2.43	0.49
1:B:507:LEU:O	1:B:507:LEU:HG	2.13	0.49
1:B:536:ALA:O	1:B:539:LYS:N	2.46	0.49
1:B:570:LEU:HD23	1:B:574:PHE:CD1	2.45	0.49
1:B:72:ALA:O	1:B:76:TYR:HB2	2.13	0.49
1:A:100:SER:C	1:A:102:ASN:H	2.17	0.49
1:A:315:GLU:C	1:A:317:SER:H	2.16	0.49
1:B:270:PRO:HD3	1:B:426:LEU:CD2	2.43	0.49
1:A:122:TYR:CE1	1:A:490:PHE:HA	2.48	0.48
1:B:118:MET:CG	1:B:171:LEU:CD1	2.89	0.48
1:B:302:THR:HG22	1:B:308:PRO:HB3	1.94	0.48
1:B:92:ILE:O	1:B:96:ARG:HG2	2.12	0.48
1:A:456:PRO:HA	1:A:459:TYR:CE2	2.48	0.48
1:A:448:GLY:HA3	1:A:453:ARG:NH1	2.29	0.48
1:B:308:PRO:O	1:B:310:PRO:HD3	2.12	0.48
1:A:13:ASP:O	1:A:17:ALA:N	2.47	0.48
1:A:204:SER:C	1:A:206:THR:H	2.15	0.48
1:A:300:PHE:CD2	1:A:395:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:HIS:HD2	1:A:46:ILE:HA	1.79	0.48
1:A:84:THR:O	1:A:86:PRO:CD	2.52	0.48
1:A:284:LEU:HD23	1:A:351:VAL:HG11	1.96	0.48
1:A:539:LYS:HE3	1:A:559:MET:O	2.14	0.48
1:B:362:GLU:O	1:B:365:HIS:HB2	2.14	0.48
1:A:408:ILE:O	1:A:408:ILE:HG12	2.13	0.48
1:A:445:TRP:HB2	1:A:466:LEU:HD12	1.96	0.48
1:B:218:LEU:O	1:B:221:LEU:HB2	2.14	0.48
1:A:178:PHE:CZ	1:A:495:VAL:HG21	2.48	0.47
1:B:439:GLY:O	1:B:502:PHE:HB2	2.14	0.47
1:A:331:HIS:CD2	1:A:490:PHE:CD2	3.02	0.47
1:A:218:LEU:HD13	1:A:436:LEU:HD13	1.97	0.47
1:B:241:TYR:O	1:B:599:TRP:HH2	1.96	0.47
1:B:286:GLN:O	1:B:286:GLN:HG3	2.14	0.47
1:B:40:TRP:HZ3	1:B:335:TRP:HD1	1.62	0.47
1:A:550:ARG:CB	1:A:551:PRO:HD2	2.42	0.47
1:A:11:SER:C	1:A:13:ASP:H	2.17	0.47
1:B:303:SER:C	1:B:304:LEU:HD23	2.35	0.47
1:B:372:TYR:CD2	1:B:372:TYR:N	2.78	0.47
1:B:68:TRP:O	1:B:69:GLY:C	2.51	0.47
1:A:401:THR:OG1	1:A:404:HIS:HB2	2.15	0.47
1:A:583:GLU:O	1:A:587:GLN:CG	2.63	0.47
1:B:25:ASN:ND2	1:B:26:SER:N	2.63	0.47
1:A:20:PHE:CE1	1:A:72:ALA:CA	2.87	0.47
1:A:25:ASN:O	1:A:29:GLU:CG	2.63	0.47
1:B:129:LEU:HD21	1:B:137:TRP:CZ2	2.50	0.47
1:A:304:LEU:O	1:A:306:LEU:N	2.48	0.47
1:A:64:PHE:CD2	1:A:68:TRP:CD1	3.02	0.47
1:B:199:ARG:C	1:B:201:TRP:H	2.18	0.47
1:A:510:GLN:HE21	1:A:560:VAL:HG11	1.80	0.46
1:A:191:PHE:HE1	1:A:197:TYR:CD1	2.30	0.46
1:B:202:TYR:HD2	1:B:552:TRP:HZ3	1.63	0.46
1:B:315:GLU:C	1:B:317:SER:N	2.69	0.46
1:B:98:LEU:HB3	1:B:101:ALA:HB3	1.98	0.46
1:A:329:VAL:O	1:A:346:LYS:HE3	2.15	0.46
1:A:544:LEU:C	1:A:546:ALA:H	2.19	0.46
1:B:292:HIS:O	1:B:296:VAL:HG23	2.15	0.46
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.72	0.46
1:A:298:GLU:O	1:A:301:PHE:N	2.48	0.46
1:A:39:SER:OG	1:A:54:GLN:NE2	2.41	0.46
1:B:158:PHE:HA	1:B:607:TYR:OH	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LEU:N	1:B:304:LEU:CD2	2.71	0.46
1:A:129:LEU:N	1:A:129:LEU:CD1	2.77	0.46
1:B:406:HIS:N	1:B:411:LEU:HB3	2.31	0.46
1:A:100:SER:C	1:A:102:ASN:N	2.69	0.46
1:A:529:ASP:OD1	1:A:531:TYR:N	2.46	0.46
1:B:80:TRP:CE3	1:B:92:ILE:HG12	2.51	0.46
1:A:441:LEU:C	1:A:441:LEU:HD23	2.36	0.46
1:A:441:LEU:HD11	1:A:467:ARG:HA	1.96	0.46
1:A:498:TYR:C	1:A:500:ARG:H	2.19	0.46
1:B:171:LEU:HD21	1:B:493:PRO:CB	2.45	0.46
1:B:217:GLN:O	1:B:220:PRO:HD2	2.16	0.46
1:B:377:VAL:C	1:B:379:LEU:H	2.19	0.46
1:A:115:LEU:HD21	1:A:178:PHE:CD1	2.51	0.46
1:B:326:ARG:H	1:B:326:ARG:HG3	1.16	0.46
1:B:85:ASP:OD1	1:B:87:GLN:N	2.31	0.46
1:A:218:LEU:O	1:A:221:LEU:HB2	2.16	0.46
1:A:494:ASN:HD22	1:A:494:ASN:N	2.14	0.46
1:B:441:LEU:CD2	1:B:442:VAL:N	2.78	0.46
1:B:510:GLN:OE1	1:B:566:ASP:N	2.49	0.46
1:A:567:ALA:O	1:A:570:LEU:HB3	2.16	0.45
1:B:219:GLU:N	1:B:220:PRO:CD	2.80	0.45
1:A:143:LEU:HD13	1:A:163:TRP:HB2	1.98	0.45
1:A:329:VAL:O	1:A:346:LYS:CE	2.63	0.45
1:A:100:SER:O	1:A:103:LEU:CB	2.64	0.45
1:A:507:LEU:HB2	1:A:565:LEU:HD23	1.98	0.45
1:B:122:TYR:CE1	1:B:163:TRP:HZ2	2.34	0.45
1:B:51:ALA:O	1:B:55:GLU:HG3	2.17	0.45
1:B:62:GLN:OE1	1:B:112:ASN:OD1	2.34	0.45
1:A:498:TYR:O	1:A:500:ARG:N	2.50	0.45
1:B:486:ALA:O	1:B:492:VAL:HG21	2.17	0.45
1:A:91:ILE:HD11	1:A:376:PRO:HG2	1.98	0.45
1:A:300:PHE:HD2	1:A:395:LEU:HD23	1.80	0.45
1:A:404:HIS:O	1:A:408:ILE:HG23	2.16	0.45
1:A:507:LEU:HB2	1:A:565:LEU:CD2	2.46	0.45
1:A:610:GLY:C	1:A:612:ASP:H	2.01	0.45
1:A:73:LYS:HE3	1:A:73:LYS:HB3	1.73	0.45
1:B:199:ARG:O	1:B:201:TRP:N	2.50	0.45
1:B:406:HIS:O	1:B:408:ILE:O	2.33	0.45
1:B:133:THR:O	1:B:134:ALA:CB	2.62	0.45
1:B:442:VAL:O	1:B:445:TRP:HB3	2.16	0.45
1:B:381:ARG:O	1:B:382:GLY:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ALA:O	1:B:391:ILE:C	2.54	0.45
1:A:492:VAL:N	1:A:493:PRO:CD	2.79	0.45
1:B:20:PHE:HE1	1:B:72:ALA:HA	1.82	0.45
1:B:307:SER:HA	1:B:308:PRO:HD3	1.60	0.45
1:A:114:LEU:HG	3:A:695:NAG:H82	1.98	0.45
1:A:142:ASP:O	1:A:146:ILE:HG13	2.17	0.45
1:A:491:HIS:CE1	6:A:705:LPR:O1	2.70	0.45
1:B:411:LEU:HA	1:B:411:LEU:HD23	1.63	0.45
1:A:262:GLU:HG3	1:A:262:GLU:H	1.43	0.44
1:A:482:THR:HG21	2:C:1:NAG:HN2	1.82	0.44
1:A:459:TYR:CD1	1:A:484:PHE:CE1	3.05	0.44
1:A:603:LEU:O	1:A:604:PRO:O	2.35	0.44
1:A:277:LEU:HD11	1:A:424:TYR:HB2	1.98	0.44
1:A:438:PHE:CE1	1:A:467:ARG:NH2	2.85	0.44
1:A:9:ASN:OD1	1:A:10:PHE:O	2.36	0.44
1:B:169:ILE:N	1:B:170:PRO:HD2	2.33	0.44
1:A:607:TYR:HA	1:A:608:PRO:HA	1.59	0.44
1:A:579:GLN:OE1	1:B:571:LEU:HD22	2.18	0.44
1:B:77:GLU:HA	1:B:80:TRP:CD1	2.52	0.44
1:A:580:TRP:CZ3	1:A:581:LEU:HD23	2.53	0.44
1:B:253:LEU:HG	1:B:261:TRP:CE2	2.52	0.44
1:B:279:VAL:CG1	1:B:283:MET:HG3	2.48	0.44
1:B:289:ASN:O	1:B:290:ALA:C	2.55	0.44
1:A:214:LEU:CD2	1:A:506:VAL:HG11	2.48	0.44
1:B:306:LEU:O	1:B:307:SER:HB2	2.17	0.44
1:B:568:GLN:HA	1:B:571:LEU:HD12	1.99	0.44
1:B:472:GLY:HA3	1:B:594:TRP:CH2	2.53	0.44
1:B:245:ARG:HB3	1:B:596:GLU:HG3	2.00	0.44
1:B:604:PRO:O	1:B:605:ASP:C	2.55	0.44
1:A:270:PRO:O	1:A:272:PRO:HD3	2.18	0.44
1:B:80:TRP:CZ3	1:B:93:GLY:CA	3.00	0.44
1:A:236:ARG:HE	1:A:267:MET:HE3	1.83	0.44
1:A:269:VAL:O	1:A:269:VAL:CG1	2.65	0.44
1:A:283:MET:CE	1:A:356:LEU:HD22	2.47	0.44
1:A:298:GLU:O	1:A:301:PHE:HB2	2.18	0.44
1:A:158:PHE:HA	1:A:607:TYR:OH	2.18	0.44
1:A:75:LEU:CD2	1:A:75:LEU:N	2.76	0.44
1:B:140:ASP:HA	1:B:141:PRO:HA	1.80	0.44
1:B:460:ASN:N	1:B:481:GLU:OE2	2.30	0.44
1:A:100:SER:HA	1:A:185:ALA:HB1	1.99	0.43
1:A:233:LEU:HD22	1:A:237:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:SER:HA	1:B:205:PRO:HD3	1.86	0.43
1:B:586:GLN:O	1:B:589:GLY:N	2.47	0.43
1:B:6:GLN:HA	1:B:7:PRO:HD3	1.72	0.43
1:A:34:GLN:HG3	1:A:35:SER:N	2.32	0.43
1:A:96:ARG:NH2	1:A:97:THR:OG1	2.51	0.43
1:B:207:PHE:CZ	1:B:211:LEU:HD11	2.54	0.43
1:A:368:TYR:CE2	1:A:544:LEU:HA	2.53	0.43
1:B:147:LEU:HD13	1:B:256:MET:CE	2.49	0.43
1:B:2:ASP:CB	1:B:3:PRO:C	2.86	0.43
1:B:551:PRO:C	1:B:552:TRP:HD1	2.21	0.43
1:B:183:ASN:HD21	1:B:193:ASP:CB	2.30	0.43
1:A:293:MET:HG2	1:A:356:LEU:HD22	2.00	0.43
1:A:369:TYR:HD2	1:A:372:TYR:HH	0.70	0.43
1:B:117:ASN:O	1:B:121:ILE:HG13	2.19	0.43
1:B:377:VAL:C	1:B:379:LEU:N	2.72	0.43
1:A:570:LEU:HD12	1:A:570:LEU:O	2.19	0.43
1:B:204:SER:C	1:B:206:THR:H	2.21	0.43
1:B:280:THR:C	1:B:283:MET:H	2.16	0.43
1:B:492:VAL:HB	1:B:493:PRO:CD	2.49	0.43
1:A:221:LEU:HD23	1:A:433:ILE:CD1	2.42	0.43
1:B:537:GLY:O	1:B:541:ARG:HG2	2.17	0.43
1:A:31:VAL:HB	1:A:64:PHE:CE1	2.52	0.43
1:A:510:GLN:HG2	1:A:569:PRO:HG3	2.00	0.43
1:A:512:HIS:O	1:A:516:CYS:SG	2.77	0.43
1:B:255:ASP:OD1	1:B:257:TRP:N	2.45	0.43
1:B:265:TYR:HE1	1:B:427:LYS:HB2	1.81	0.43
1:B:436:LEU:HB2	1:B:437:PRO:CD	2.48	0.43
1:B:77:GLU:CD	1:B:96:ARG:NH2	2.72	0.43
1:A:503:VAL:HG13	1:A:565:LEU:HD11	2.00	0.43
1:B:256:MET:HB3	1:B:257:TRP:CE3	2.54	0.43
1:B:89:ARG:HA	1:B:92:ILE:CG2	2.49	0.43
1:A:528:CYS:SG	1:A:529:ASP:N	2.92	0.43
1:A:597:TYR:CD1	1:A:597:TYR:C	2.92	0.43
1:A:31:VAL:HG11	1:A:64:PHE:CD1	2.54	0.42
1:A:366:ILE:HA	1:A:369:TYR:HD1	1.84	0.42
1:A:524:PRO:HA	9:A:2008:HOH:O	2.18	0.42
1:A:113:ALA:HB1	3:A:695:NAG:HN2	1.84	0.42
1:B:261:TRP:N	1:B:261:TRP:CD1	2.86	0.42
1:B:607:TYR:HA	1:B:608:PRO:HA	1.64	0.42
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.58	0.42
1:A:418:THR:O	1:A:421:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:LEU:CG	1:A:507:LEU:O	2.57	0.42
1:B:207:PHE:CE1	1:B:211:LEU:HD11	2.54	0.42
1:B:324:ASP:OD1	1:B:325:GLY:N	2.52	0.42
1:A:402:PRO:HB3	1:A:411:LEU:CD1	2.49	0.42
1:A:550:ARG:HB3	1:A:551:PRO:HD2	1.92	0.42
1:A:610:GLY:C	1:A:612:ASP:N	2.67	0.42
1:B:75:LEU:HB3	1:B:76:TYR:CE2	2.54	0.42
1:A:129:LEU:HD12	1:A:129:LEU:H	1.82	0.42
1:B:143:LEU:O	1:B:144:THR:C	2.57	0.42
1:B:368:TYR:O	1:B:372:TYR:CD2	2.72	0.42
1:B:441:LEU:HD23	1:B:441:LEU:C	2.39	0.42
1:B:71:LYS:O	1:B:72:ALA:C	2.56	0.42
1:A:140:ASP:HA	1:A:141:PRO:HA	1.75	0.42
1:A:441:LEU:HD23	1:A:442:VAL:CA	2.48	0.42
1:A:510:GLN:HB3	1:A:510:GLN:HE21	1.61	0.42
1:B:335:TRP:O	1:B:343:PHE:HA	2.19	0.42
1:B:567:ALA:O	1:B:568:GLN:C	2.58	0.42
1:B:85:ASP:HB3	1:B:88:LEU:CB	2.49	0.42
1:A:227:ALA:HB1	1:A:590:GLU:HG2	2.01	0.42
1:A:64:PHE:HD2	1:A:64:PHE:O	2.03	0.42
1:B:268:VAL:O	1:B:269:VAL:C	2.58	0.42
1:A:253:LEU:HD12	1:A:261:TRP:CD2	2.55	0.42
1:A:71:LYS:O	1:A:74:GLU:N	2.52	0.42
1:B:529:ASP:OD1	1:B:531:TYR:HB2	2.20	0.42
1:A:128:CYS:CB	1:A:136:CYS:HG	2.26	0.42
1:A:219:GLU:HB3	1:A:220:PRO:HD3	2.02	0.42
1:A:300:PHE:CD2	1:A:304:LEU:CD1	2.96	0.42
1:B:20:PHE:CD2	1:B:21:ALA:N	2.87	0.42
1:B:367:GLN:O	1:B:371:GLN:HG2	2.19	0.42
1:B:361:HIS:HA	1:B:392:GLY:HA3	2.02	0.42
1:A:54:GLN:HE21	1:A:54:GLN:HB2	1.73	0.42
1:B:139:LEU:HD13	1:B:163:TRP:CD2	2.55	0.42
1:A:103:LEU:O	1:A:108:ARG:HG3	2.20	0.42
1:B:251:HIS:CE1	1:B:476:PRO:CB	3.02	0.41
1:B:265:TYR:O	1:B:267:MET:N	2.53	0.41
7:A:2433:GOL:HO1	1:B:593:GLY:CA	2.32	0.41
1:A:328:VAL:HG23	1:A:329:VAL:N	2.34	0.41
1:A:603:LEU:C	1:A:604:PRO:O	2.57	0.41
1:B:406:HIS:N	1:B:411:LEU:CB	2.84	0.41
1:B:521:TYR:CE2	1:B:528:CYS:HB2	2.55	0.41
1:A:335:TRP:N	1:A:335:TRP:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:HG22	1:A:479:ARG:N	2.35	0.41
1:B:222:TYR:HH	1:B:261:TRP:HZ2	1.67	0.41
1:B:268:VAL:HG21	1:B:430:LEU:HD11	2.02	0.41
1:A:274:LYS:HB3	1:A:275:PRO:CD	2.46	0.41
1:A:369:TYR:HA	1:A:372:TYR:CE2	2.56	0.41
1:B:147:LEU:CD2	1:B:256:MET:HA	2.42	0.41
1:B:394:VAL:O	1:B:397:LEU:HB2	2.21	0.41
1:B:438:PHE:HE2	1:B:498:TYR:HH	1.67	0.41
1:A:125:ALA:O	1:A:126:LYS:CG	2.67	0.41
1:A:540:LEU:O	1:A:543:VAL:HG22	2.21	0.41
1:B:137:TRP:HB3	1:B:142:ASP:HB2	2.02	0.41
1:B:384:ASN:OD1	1:B:387:PHE:HD1	2.04	0.41
1:A:191:PHE:CZ	1:A:197:TYR:HD1	2.37	0.41
1:A:236:ARG:NE	1:A:267:MET:HE3	2.36	0.41
1:A:575:GLN:O	1:A:578:THR:HB	2.21	0.41
1:B:129:LEU:HB3	1:B:130:PRO:HD2	2.03	0.41
1:B:265:TYR:CE1	1:B:427:LYS:CB	3.00	0.41
1:B:279:VAL:HG12	1:B:283:MET:HG3	2.02	0.41
1:A:100:SER:HA	1:A:185:ALA:CB	2.51	0.41
1:A:355:GLN:O	1:A:359:VAL:HG23	2.21	0.41
1:A:369:TYR:CE2	1:A:372:TYR:OH	2.73	0.41
1:A:529:ASP:C	1:A:531:TYR:H	2.22	0.41
1:B:498:TYR:C	1:B:500:ARG:N	2.73	0.41
1:B:586:GLN:HG3	1:B:587:GLN:H	1.74	0.41
1:B:77:GLU:N	1:B:78:PRO:HD2	2.36	0.41
1:A:331:HIS:CD2	1:A:490:PHE:CZ	3.08	0.41
1:A:492:VAL:H	1:A:493:PRO:HD2	1.84	0.41
1:B:7:PRO:O	1:B:8:GLY:C	2.59	0.41
1:A:141:PRO:O	1:A:142:ASP:C	2.59	0.41
1:A:169:ILE:N	1:A:170:PRO:HD2	2.36	0.41
1:A:401:THR:HA	1:A:402:PRO:HD3	1.65	0.41
1:A:172:LYS:O	1:A:176:GLU:HG3	2.21	0.40
1:A:204:SER:C	1:A:206:THR:N	2.73	0.40
1:A:387:PHE:CE1	1:A:552:TRP:HB2	2.56	0.40
1:A:277:LEU:CD1	1:A:424:TYR:CA	2.99	0.40
1:A:332:ALA:CA	1:A:347:GLN:HG3	2.51	0.40
1:A:277:LEU:HD12	1:A:424:TYR:HA	2.03	0.40
1:B:28:ALA:HA	1:B:31:VAL:HG12	2.03	0.40
1:B:265:TYR:CD1	1:B:427:LYS:HG3	2.55	0.40
1:A:134:ALA:O	1:A:135:THR:C	2.60	0.40
1:A:496:THR:HA	1:A:497:PRO:HD3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HE	1:B:340:ARG:HB2	1.50	0.40
1:B:377:VAL:O	1:B:379:LEU:N	2.54	0.40
1:B:46:ILE:H	1:B:46:ILE:HG13	1.65	0.40
1:A:350:ARG:HG3	1:A:351:VAL:N	2.33	0.40
1:A:73:LYS:HB3	1:A:77:GLU:HG3	2.02	0.40
1:B:140:ASP:OD1	1:B:140:ASP:O	2.39	0.40
1:B:352:THR:HG22	1:B:353:MET:N	2.36	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	610/612 (100%)	506 (83%)	83 (14%)	21 (3%)	3	20
1	B	605/612 (99%)	514 (85%)	70 (12%)	21 (4%)	3	20
All	All	1215/1224 (99%)	1020 (84%)	153 (13%)	42 (4%)	3	20

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	PRO
1	A	85	ASP
1	B	3	PRO
1	B	130	PRO
1	B	308	PRO
1	B	608	PRO
1	A	287	GLY
1	A	299	GLU
1	A	604	PRO
1	B	141	PRO
1	A	101	ALA

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Mol	Chain	Res	Type
1	A	130	PRO
1	A	262	GLU
1	A	490	PHE
1	A	499	ILE
1	A	530	ILE
1	B	144	THR
1	B	266	ASP
1	B	281	SER
1	A	133	THR
1	A	322	PRO
1	A	608	PRO
1	B	5	LEU
1	B	382	GLY
1	B	411	LEU
1	A	111	TYR
1	A	250	ALA
1	A	376	PRO
1	A	391	ILE
1	B	185	ALA
1	B	250	ALA
1	B	378	SER
1	A	87	GLN
1	B	597	TYR
1	B	279	VAL
1	A	495	VAL
1	B	310	PRO
1	B	377	VAL
1	B	78	PRO
1	B	530	ILE
1	B	79	ILE
1	A	270	PRO

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/526 (87%)	398 (87%)	60 (13%)	4	18
1	B	437/526 (83%)	377 (86%)	60 (14%)	3	17
All	All	895/1052 (85%)	775 (87%)	120 (13%)	4	17

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	11	SER
1	A	20	PHE
1	A	29	GLU
1	A	34	GLN
1	A	35	SER
1	A	52	ARG
1	A	54	GLN
1	A	64	PHE
1	A	73	LYS
1	A	77	GLU
1	A	91	ILE
1	A	96	ARG
1	A	97	THR
1	A	116	SER
1	A	171	LEU
1	A	174	LEU
1	A	178	PHE
1	A	183	ASN
1	A	206	THR
1	A	214	LEU
1	A	236	ARG
1	A	242	ILE
1	A	245	ARG
1	A	262	GLU
1	A	295	ARG
1	A	299	GLU
1	A	304	LEU
1	A	314	TRP
1	A	326	ARG
1	A	328	VAL
1	A	342	ASP

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Mol	Chain	Res	Type
1	A	354	ASP
1	A	356	LEU
1	A	368	TYR
1	A	378	SER
1	A	379	LEU
1	A	388	HIS
1	A	393	ASP
1	A	408	ILE
1	A	441	LEU
1	A	457	SER
1	A	480	ASN
1	A	482	THR
1	A	496	THR
1	A	507	LEU
1	A	530	ILE
1	A	540	LEU
1	A	541	ARG
1	A	543	VAL
1	A	553	GLN
1	A	558	ASP
1	A	563	ASP
1	A	575	GLN
1	A	582	GLN
1	A	587	GLN
1	A	590	GLU
1	A	594	TRP
1	A	604	PRO
1	A	605	ASP
1	B	3	PRO
1	B	10	PHE
1	B	20	PHE
1	B	25	ASN
1	B	66	GLU
1	B	68	TRP
1	B	78	PRO
1	B	85	ASP
1	B	91	ILE
1	B	92	ILE
1	B	95	VAL
1	B	97	THR
1	B	109	GLN
1	B	118	MET

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Mol	Chain	Res	Type
1	B	129	LEU
1	B	147	LEU
1	B	174	LEU
1	B	211	LEU
1	B	213	HIS
1	B	214	LEU
1	B	231	ARG
1	B	236	ARG
1	B	245	ARG
1	B	260	SER
1	B	264	ILE
1	B	280	THR
1	B	281	SER
1	B	286	GLN
1	B	298	GLU
1	B	304	LEU
1	B	318	MET
1	B	322	PRO
1	B	326	ARG
1	B	327	GLU
1	B	340	ARG
1	B	342	ASP
1	B	368	TYR
1	B	372	TYR
1	B	378	SER
1	B	381	ARG
1	B	388	HIS
1	B	406	HIS
1	B	408	ILE
1	B	411	LEU
1	B	414	VAL
1	B	418	THR
1	B	422	ILE
1	B	428	MET
1	B	441	LEU
1	B	443	ASP
1	B	477	VAL
1	B	480	ASN
1	B	507	LEU
1	B	508	GLN
1	B	552	TRP
1	B	570	LEU

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Mol	Chain	Res	Type
1	B	575	GLN
1	B	582	GLN
1	B	586	GLN
1	B	590	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	42	HIS
1	A	50	ASN
1	A	54	GLN
1	A	87	GLN
1	A	331	HIS
1	A	406	HIS
1	A	491	HIS
1	A	494	ASN
1	A	575	GLN
1	A	598	GLN
1	B	50	ASN
1	B	102	ASN
1	B	109	GLN
1	B	112	ASN
1	B	131	ASN
1	B	183	ASN
1	B	188	GLN
1	B	216	GLN
1	B	286	GLN
1	B	331	HIS
1	B	347	GLN
1	B	406	HIS
1	B	416	ASN
1	B	494	ASN
1	B	575	GLN
1	B	579	GLN
1	B	582	GLN
1	B	587	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	1,2	14,14,15	2.66	3 (21%)	17,19,21	1.41	3 (17%)
2	NAG	C	2	2	14,14,15	2.24	1 (7%)	17,19,21	1.30	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.26	0	17,19,21	1.02	1 (5%)
2	NAG	D	2	2	14,14,15	2.34	1 (7%)	17,19,21	1.04	1 (5%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C8-C7	-8.69	1.32	1.50
2	C	1	NAG	C8-C7	-8.62	1.32	1.50
2	C	2	NAG	C8-C7	-8.17	1.33	1.50
2	C	1	NAG	C4-C3	-2.44	1.46	1.52
2	C	1	NAG	C1-C2	2.43	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-C2-N2	-3.23	104.98	110.49
2	D	2	NAG	C1-C2-N2	-3.22	104.99	110.49
2	C	1	NAG	C6-C5-C4	-3.06	105.84	113.00
2	C	2	NAG	C1-C2-N2	-2.81	105.69	110.49
2	C	2	NAG	C1-O5-C5	-2.61	108.66	112.19
2	C	1	NAG	O5-C5-C6	2.61	111.29	107.20
2	C	2	NAG	C4-C3-C2	-2.27	107.69	111.02
2	C	1	NAG	C2-N2-C7	2.22	126.06	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2	NAG	C2

All (2) torsion outliers are listed below:

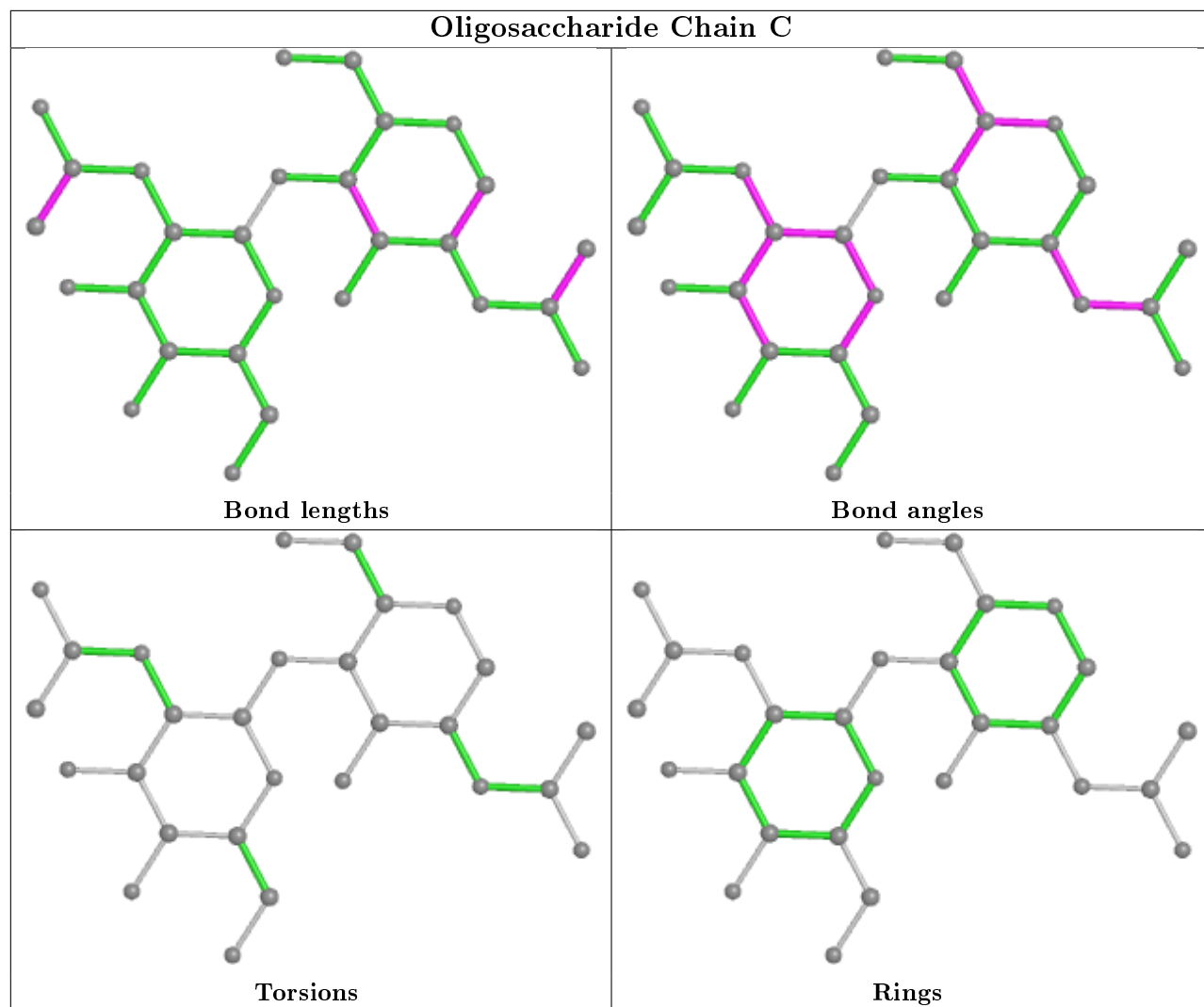
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

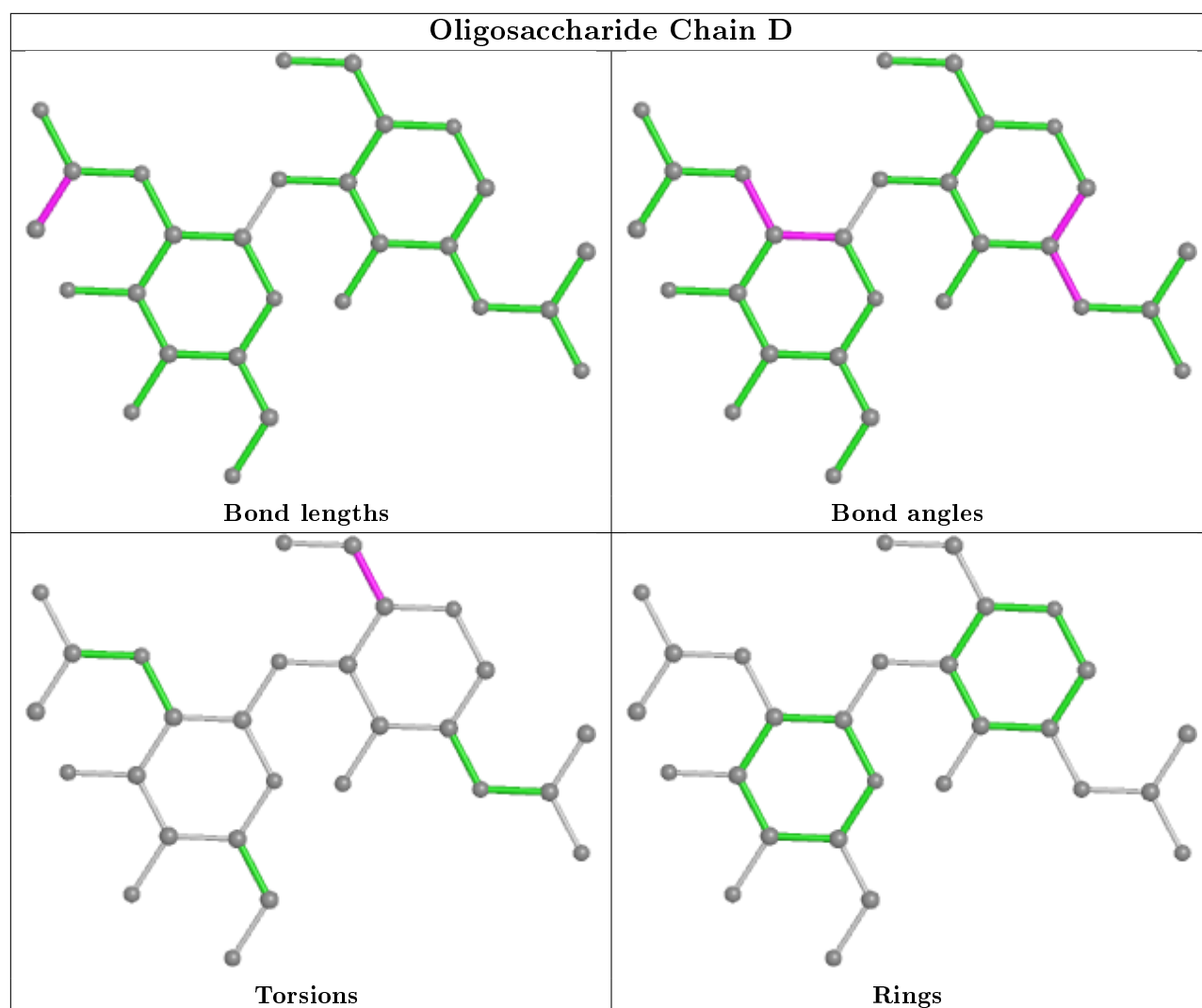
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	2	0
2	C	2	NAG	1	0
2	D	1	NAG	6	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 ⓘ

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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
7	GOL	A	2434	-	5,5,5	3.52	3 (60%)	5,5,5	1.49	1 (20%)
8	ACT	B	710	-	1,3,3	3.78	1 (100%)	0,3,3	0.00	-
3	NAG	A	693	1	14,14,15	0.26	0	17,19,21	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	695	1	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
3	NAG	A	695	1	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
3	NAG	B	693	1	14,14,15	0.25	0	17,19,21	1.17	2 (11%)
6	LPR	A	705	4	24,30,30	5.17	14 (58%)	29,39,39	1.99	8 (27%)
6	LPR	B	705	4	24,30,30	5.45	13 (54%)	29,39,39	1.80	6 (20%)
7	GOL	A	2433	-	5,5,5	3.37	3 (60%)	5,5,5	2.06	1 (20%)

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
7	GOL	A	2434	-	-	0/4/4/4	-
3	NAG	A	693	1	-	2/6/23/26	0/1/1/1
3	NAG	B	695	1	-	2/6/23/26	0/1/1/1
3	NAG	A	695	1	-	0/6/23/26	0/1/1/1
6	LPR	B	705	4	-	2/22/40/40	0/2/2/2
6	LPR	A	705	4	-	5/22/40/40	0/2/2/2
3	NAG	B	693	1	1/1/5/7	5/6/23/26	0/1/1/1
7	GOL	A	2433	-	-	0/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	705	LPR	C4-N1	-23.28	1.17	1.47
6	A	705	LPR	C4-N1	-21.82	1.19	1.47
7	A	2434	GOL	O2-C2	-6.51	1.24	1.43
6	B	705	LPR	C14-C4	-6.32	1.45	1.53
7	A	2433	GOL	O2-C2	-4.63	1.29	1.43
6	A	705	LPR	C17-C16	4.33	1.48	1.38
6	A	705	LPR	C14-C4	-4.14	1.48	1.53
7	A	2433	GOL	O3-C3	4.13	1.59	1.42
7	A	2433	GOL	C3-C2	3.81	1.67	1.51
6	A	705	LPR	C7-C6	-3.79	1.36	1.51
8	B	710	ACT	CH3-C	3.78	1.53	1.48
6	B	705	LPR	C17-C16	3.74	1.46	1.38
6	A	705	LPR	C2-C1	3.70	1.60	1.53
6	A	705	LPR	C5-N2	3.63	1.53	1.47
6	B	705	LPR	C21-C16	3.62	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	705	LPR	C20-C19	3.62	1.47	1.38
6	A	705	LPR	C19-C18	3.60	1.47	1.38
6	A	705	LPR	C21-C16	3.59	1.46	1.38
6	B	705	LPR	O1-C1	3.51	1.28	1.22
6	B	705	LPR	C7-C6	-3.47	1.37	1.51
7	A	2434	GOL	C3-C2	3.43	1.65	1.51
6	A	705	LPR	C20-C19	3.43	1.47	1.38
6	B	705	LPR	C2-C1	3.41	1.59	1.53
6	B	705	LPR	C19-C18	3.41	1.47	1.38
6	A	705	LPR	C20-C21	3.26	1.45	1.38
6	B	705	LPR	C20-C21	3.20	1.45	1.38
6	A	705	LPR	O1-C1	3.14	1.27	1.22
6	B	705	LPR	C5-N2	2.93	1.52	1.47
6	A	705	LPR	C18-C17	2.81	1.44	1.38
6	B	705	LPR	C18-C17	2.59	1.44	1.38
7	A	2434	GOL	O3-C3	2.36	1.52	1.42
6	A	705	LPR	C12-C13	-2.28	1.40	1.51
6	B	705	LPR	C12-C13	-2.04	1.41	1.51
6	A	705	LPR	C1-N2	2.02	1.39	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	705	LPR	C4-N1-C2	6.62	129.54	115.52
6	A	705	LPR	C4-N1-C2	6.43	129.13	115.52
6	A	705	LPR	C15-C14-C4	4.10	121.32	113.04
7	A	2433	GOL	O3-C3-C2	-4.05	90.80	110.20
6	A	705	LPR	C11-C10-C2	3.49	124.69	113.92
3	B	693	NAG	C1-C2-N2	-3.31	104.84	110.49
3	A	693	NAG	C1-C2-N2	-3.23	104.96	110.49
3	B	695	NAG	C1-C2-N2	-3.20	105.02	110.49
3	A	695	NAG	C1-C2-N2	-3.20	105.02	110.49
7	A	2434	GOL	O3-C3-C2	-3.09	95.39	110.20
6	A	705	LPR	C6-C7-C8	3.03	113.57	104.98
6	A	705	LPR	C14-C15-C16	2.98	123.53	113.18
6	B	705	LPR	C15-C14-C4	2.92	118.94	113.04
6	B	705	LPR	C6-C7-C8	2.82	112.97	104.98
6	B	705	LPR	C11-C10-C2	2.74	122.36	113.92
6	B	705	LPR	C14-C15-C16	2.71	122.61	113.18
6	A	705	LPR	C6-C5-C9	-2.60	107.05	113.98
6	A	705	LPR	C7-C6-C5	2.53	110.86	104.26
6	B	705	LPR	C7-C6-C5	2.52	110.84	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	693	NAG	C2-N2-C7	2.23	126.08	122.90
6	A	705	LPR	C14-C4-N1	2.23	128.32	112.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	693	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	693	NAG	C3-C2-N2-C7
6	A	705	LPR	C15-C14-C4-C3
6	A	705	LPR	C15-C14-C4-N1
3	B	693	NAG	C3-C2-N2-C7
6	B	705	LPR	C15-C14-C4-C3
3	B	695	NAG	C1-C2-N2-C7
6	B	705	LPR	C15-C14-C4-N1
3	B	693	NAG	C8-C7-N2-C2
3	B	693	NAG	O7-C7-N2-C2
3	B	693	NAG	C4-C5-C6-O6
3	B	695	NAG	O5-C5-C6-O6
6	A	705	LPR	C2-C10-C11-C12
3	A	693	NAG	C4-C5-C6-O6
6	A	705	LPR	C14-C15-C16-C17
6	A	705	LPR	C14-C15-C16-C21
3	B	693	NAG	O5-C5-C6-O6

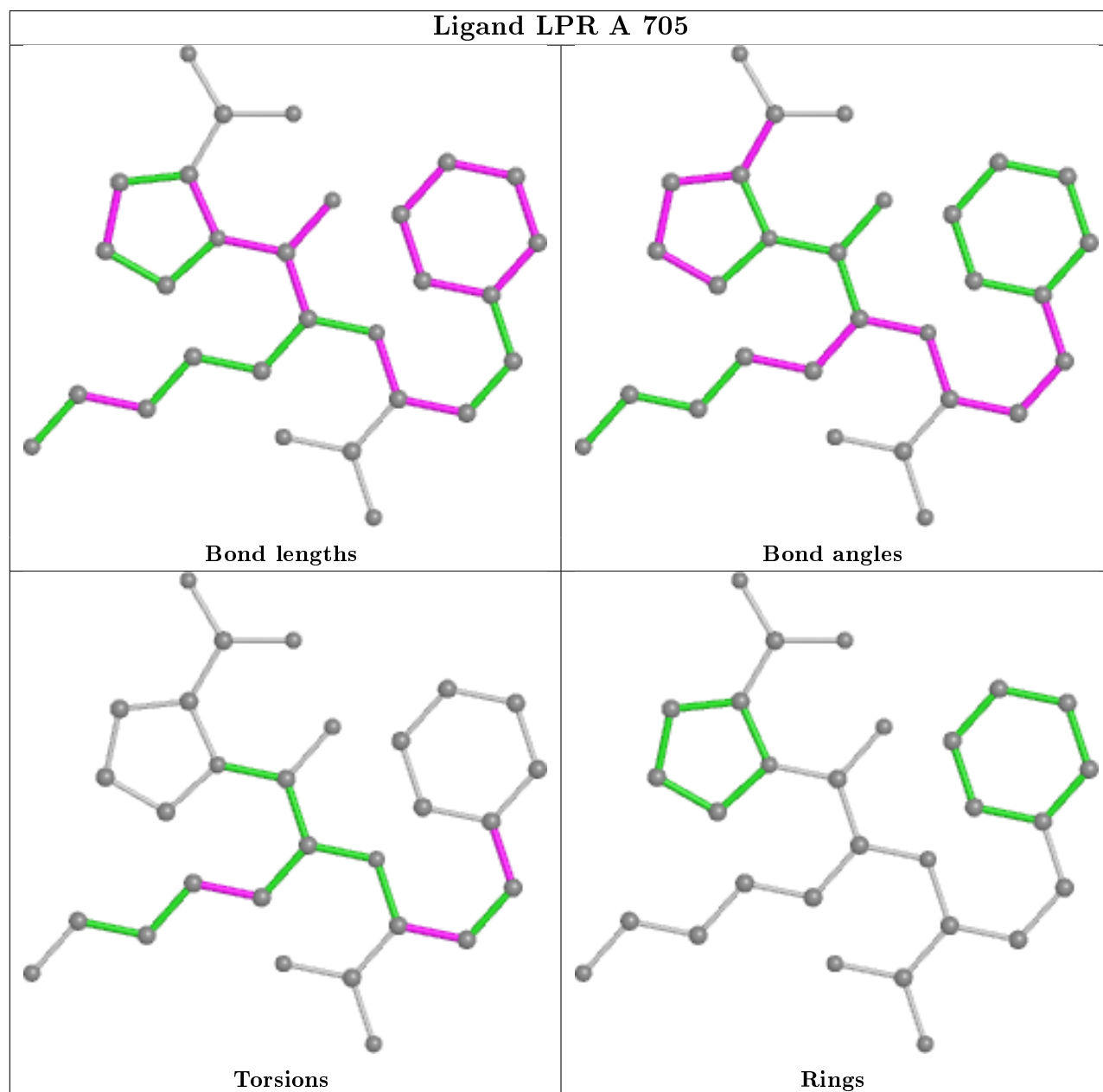
There are no ring outliers.

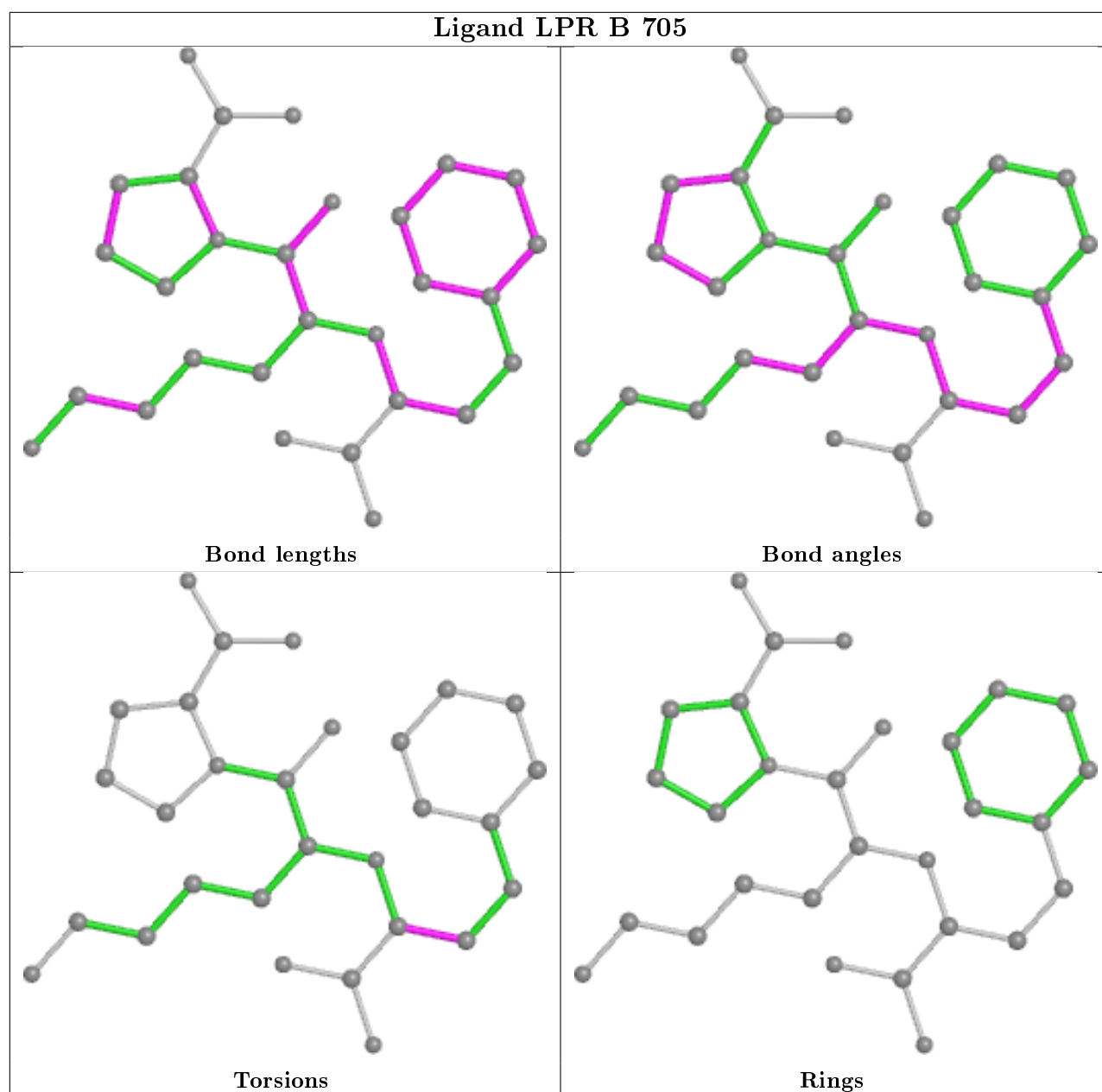
8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2434	GOL	2	0
8	B	710	ACT	1	0
3	A	693	NAG	5	0
3	B	695	NAG	1	0
3	A	695	NAG	2	0
3	B	693	NAG	10	0
6	A	705	LPR	2	0
7	A	2433	GOL	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	612/612 (100%)	0.27	18 (2%)	51 23	5, 39, 64, 72	4 (0%)
1	B	609/612 (99%)	0.25	15 (2%)	57 29	4, 41, 67, 81	4 (0%)
All	All	1221/1224 (99%)	0.26	33 (2%)	54 26	4, 40, 66, 81	8 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	GLY	3.2
1	A	15	ALA	3.1
1	B	417	ASP	3.1
1	B	376	PRO	3.0
1	B	544	LEU	2.9
1	A	17	ALA	2.8
1	A	19	LEU	2.8
1	B	26	SER	2.7
1	B	523	GLY	2.7
1	B	11	SER	2.6
1	B	362	GLU	2.5
1	A	23	SER	2.4
1	B	81	GLN	2.4
1	A	306	LEU	2.3
1	A	304	LEU	2.3
1	A	279	VAL	2.3
1	B	27	SER	2.2
1	B	84	THR	2.2
1	B	75	LEU	2.1
1	A	26	SER	2.1
1	A	414	VAL	2.1
1	A	374	ASP	2.1
1	B	605	ASP	2.1
1	A	545	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	279	VAL	2.1
1	A	410	LEU	2.1
1	B	522	GLU	2.0
1	A	523	GLY	2.0
1	A	84	THR	2.0
1	A	287	GLY	2.0
1	A	343	PHE	2.0
1	A	371	GLN	2.0
1	A	75	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

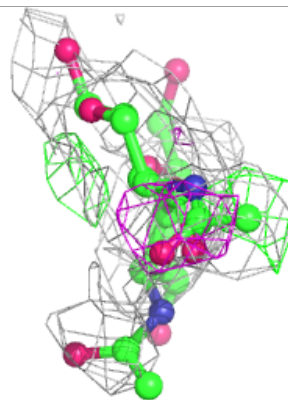
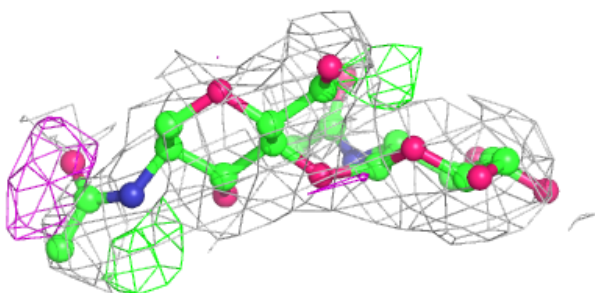
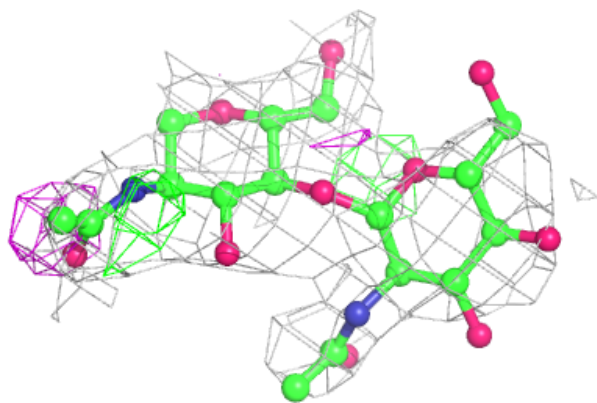
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	D	2	14/15	0.68	0.38	90,92,93,94	0
2	NAG	C	2	14/15	0.70	0.37	100,101,103,103	0
2	NAG	C	1	14/15	0.76	0.31	29,32,35,37	0
2	NAG	D	1	14/15	0.89	0.25	32,35,37,38	0

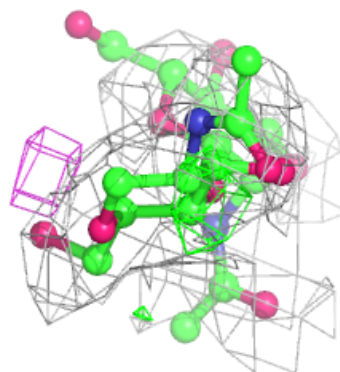
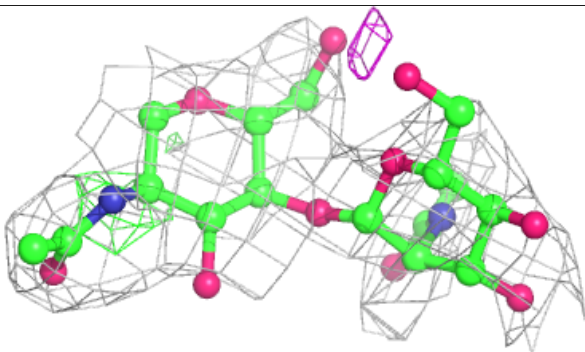
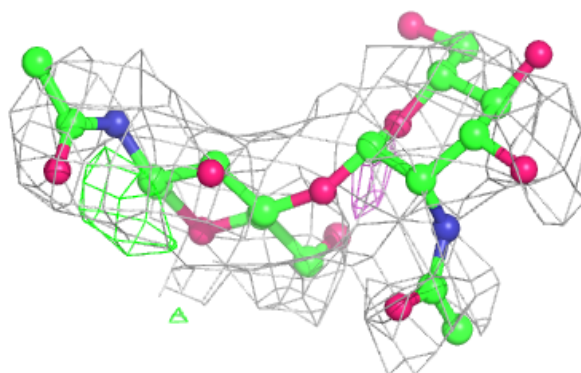
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands ⓘ

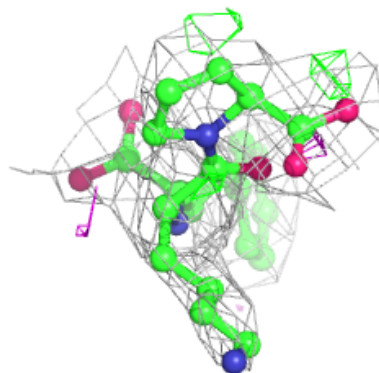
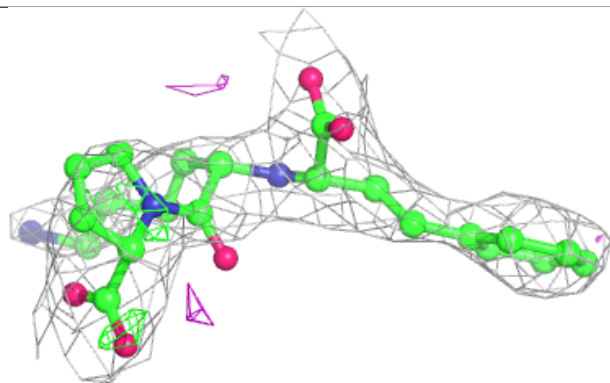
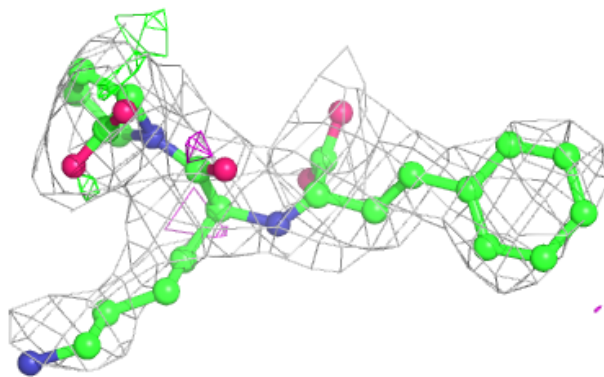
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	693	14/15	0.56	0.54	66,69,70,70	0
3	NAG	B	695	14/15	0.66	0.53	77,78,81,83	0
3	NAG	A	693	14/15	0.73	0.31	69,72,74,75	0
3	NAG	A	695	14/15	0.81	0.33	73,74,75,76	0
8	ACT	B	710	4/4	0.83	0.28	29,30,30,32	0
5	CL	A	703	1/1	0.84	0.15	31,31,31,31	0
7	GOL	A	2434	6/6	0.87	0.34	28,29,30,31	0
6	LPR	A	705	29/29	0.87	0.38	43,47,49,49	0
7	GOL	A	2433	6/6	0.87	0.31	25,27,27,27	0
6	LPR	B	705	29/29	0.92	0.30	35,40,43,45	0
4	ZN	B	701	1/1	0.97	0.09	31,31,31,31	0
5	CL	B	702	1/1	0.97	0.14	25,25,25,25	0
4	ZN	A	701	1/1	0.98	0.08	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

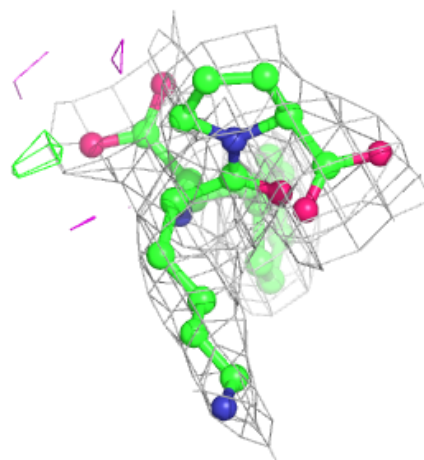
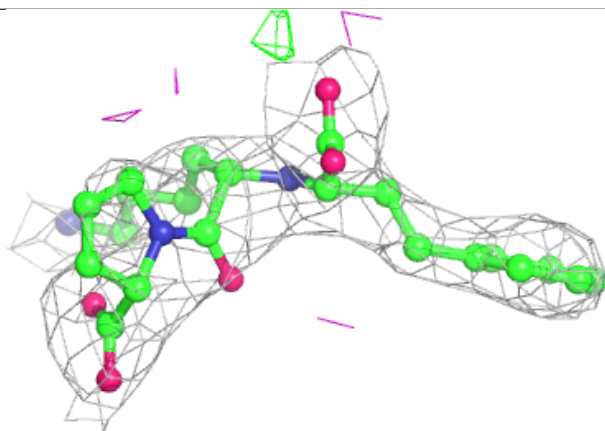
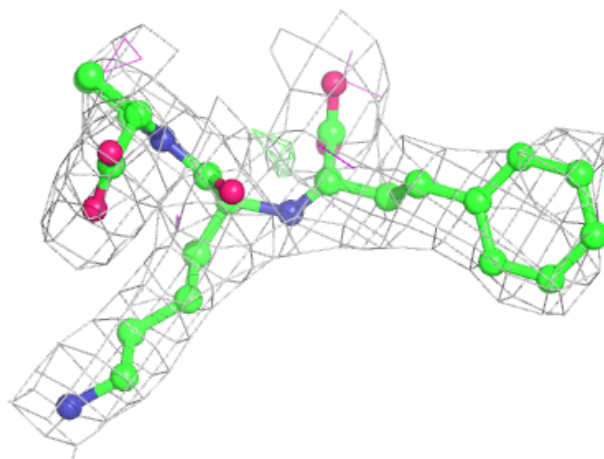
Electron density around LPR A 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LPR B 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.