



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:37 AM UTC

PDB ID : 2C6N / pdb_00002c6n
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 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

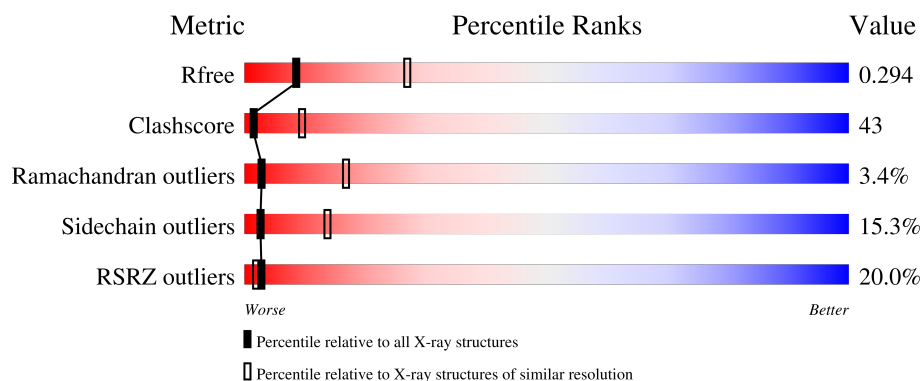
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

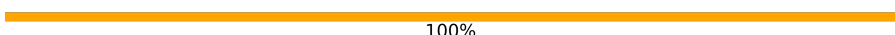
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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	
1	B	612	
2	C	2	
2	D	2	

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	D	2	X	-	-	-
3	NAG	B	693	X	-	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.

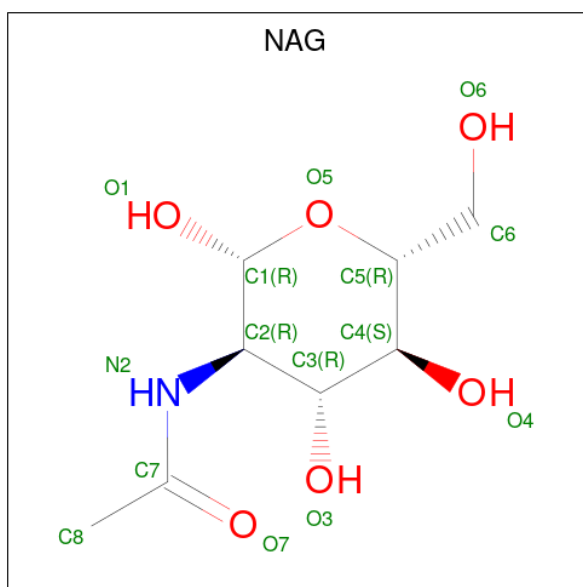
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	7	0	0
			4747	3057	811	861	18			
1	B	609	Total	C	N	O	S	9	0	0
			4665	3005	797	845	18			

- 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 (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	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		

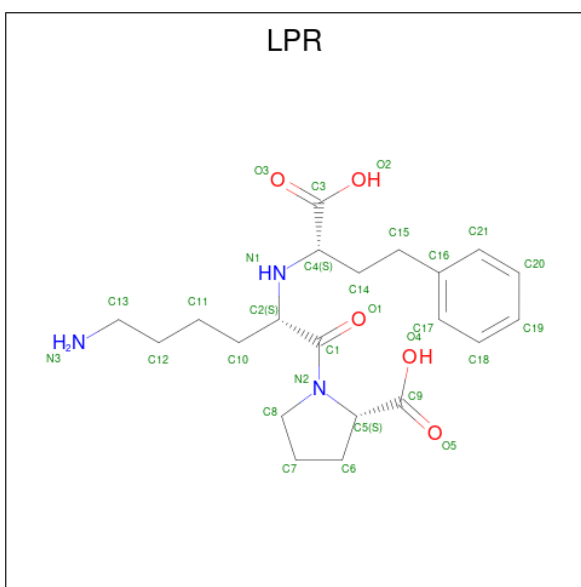
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

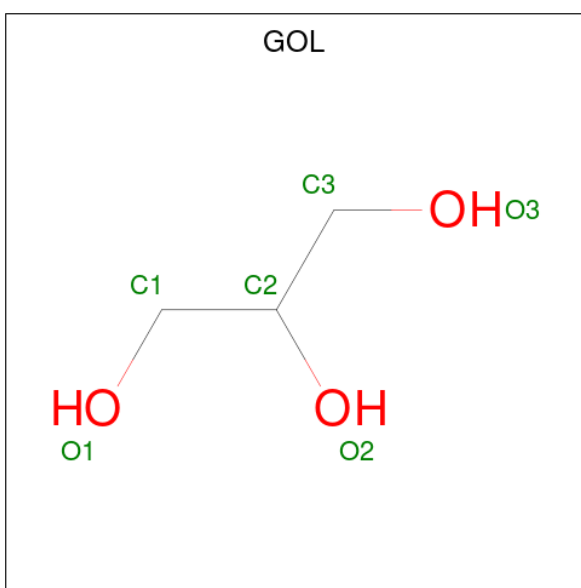
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

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



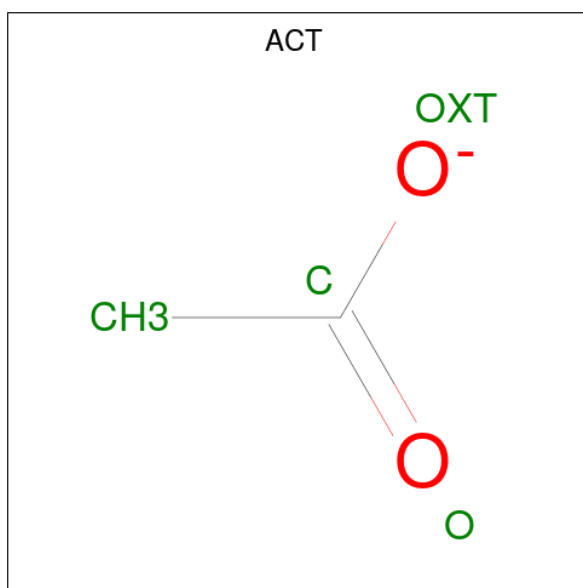
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			29	21	3	5		
6	B	1	Total	C	N	O	0	0
			29	21	3	5		

- Molecule 7 is GLYCEROL (CCD ID: 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 (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

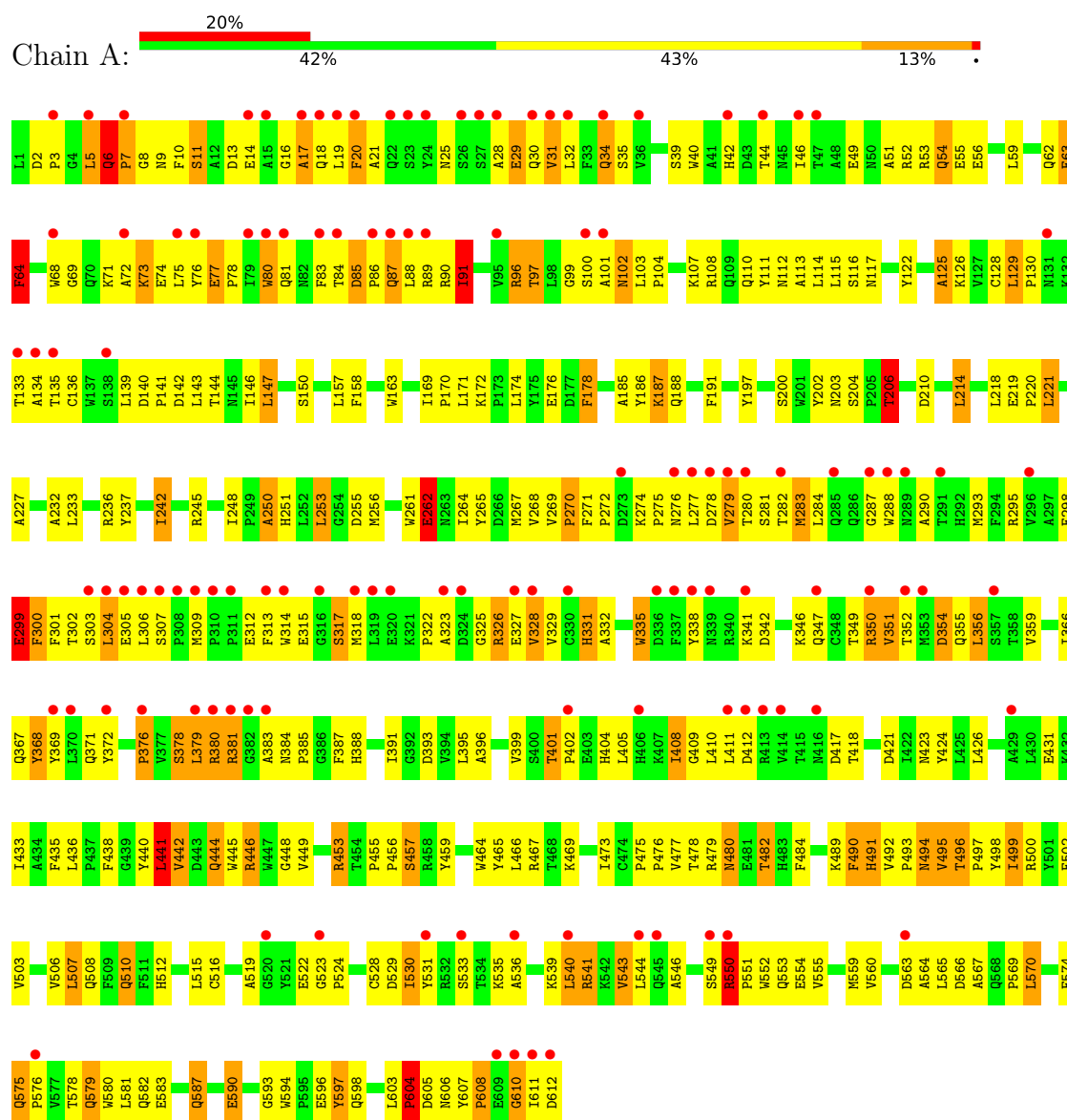
- Molecule 9 is water.

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

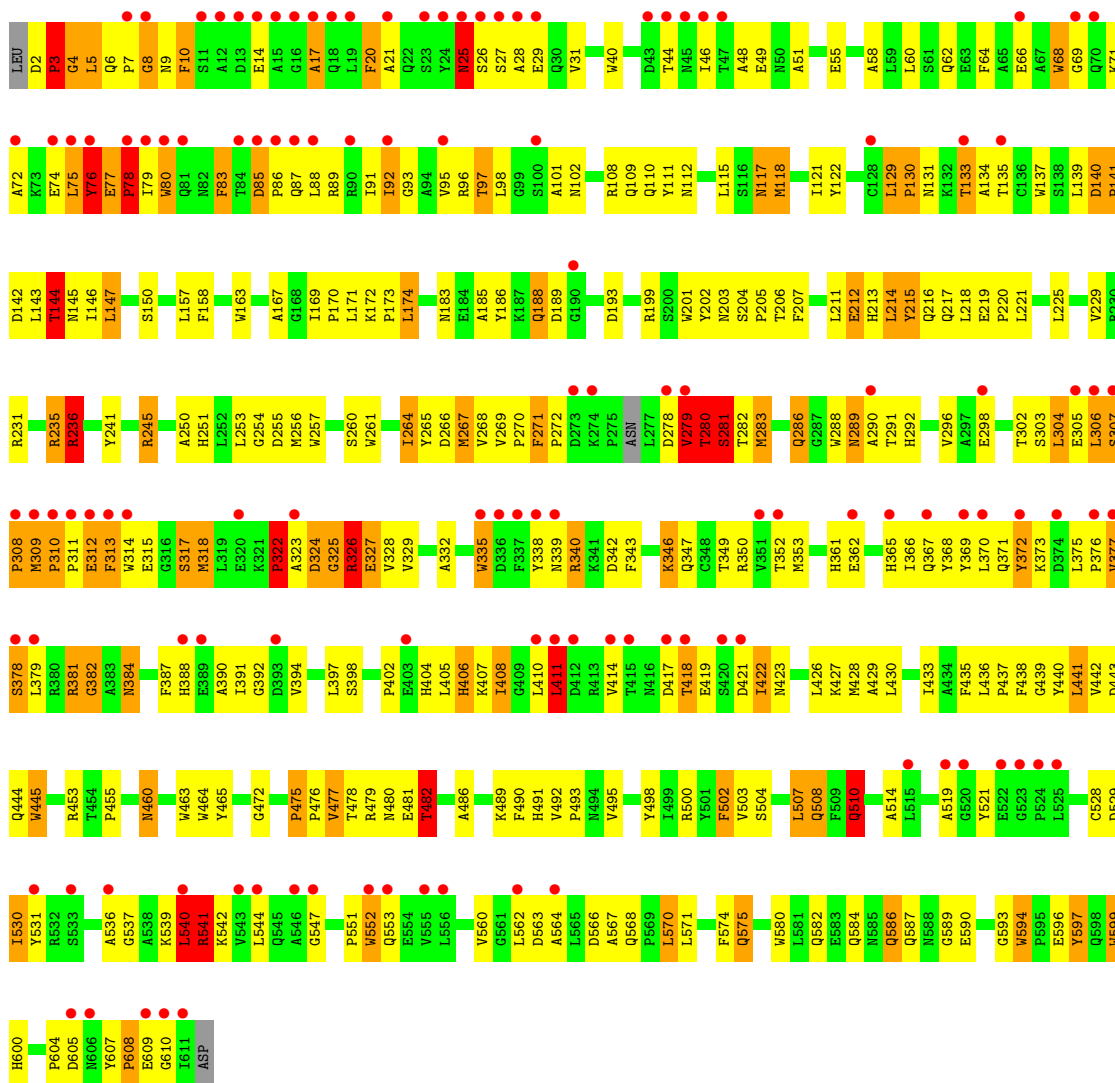
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 28.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (28.76-3.00) 95.0 (28.76-3.00)	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 0.287 , 0.294	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 , 63.4	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.76	8/4901 (0.2%)	1.40	91/6707 (1.4%)
1	B	0.75	9/4819 (0.2%)	1.41	96/6608 (1.5%)
All	All	0.76	17/9720 (0.2%)	1.41	187/13315 (1.4%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	ARG	N-CA	-7.90	1.36	1.46
1	B	267	MET	SD-CE	-7.86	1.59	1.79
1	B	350	ARG	CA-C	7.81	1.63	1.52
1	A	381	ARG	CB-CG	7.39	1.74	1.52
1	B	350	ARG	CA-CB	7.11	1.65	1.53
1	B	540	LEU	C-O	-6.91	1.15	1.24
1	A	351	VAL	CA-CB	-6.86	1.45	1.54
1	A	351	VAL	N-CA	-6.59	1.38	1.46
1	B	117	ASN	CA-C	-6.35	1.44	1.52
1	B	25	ASN	CB-CG	-6.26	1.36	1.52
1	B	25	ASN	N-CA	-6.12	1.39	1.46
1	B	610	GLY	C-N	5.66	1.41	1.33
1	B	541	ARG	CB-CG	5.60	1.69	1.52
1	A	549	SER	C-O	-5.47	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	ARG	C-O	5.37	1.30	1.24
1	A	280	THR	CA-C	-5.26	1.45	1.52
1	A	283	MET	SD-CE	-5.24	1.66	1.79

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	ARG	N-CA-C	-17.52	92.67	114.75
1	A	91	ILE	N-CA-C	-17.50	96.51	111.56
1	B	305	GLU	N-CA-C	16.41	137.53	113.40
1	B	76	TYR	N-CA-C	15.89	133.24	112.26
1	A	280	THR	N-CA-C	-15.45	92.64	114.12
1	A	64	PHE	N-CA-C	-14.20	95.87	111.07
1	A	611	ILE	N-CA-C	-13.12	97.71	112.80
1	A	349	THR	N-CA-C	12.97	127.83	109.15
1	A	62	GLN	CA-C-N	-11.42	104.78	122.49
1	A	62	GLN	C-N-CA	-11.42	104.78	122.49
1	B	75	LEU	N-CA-C	-10.94	96.29	112.04
1	B	9	ASN	N-CA-C	10.86	126.35	110.28
1	A	401	THR	CA-C-N	10.67	131.48	119.32
1	A	401	THR	C-N-CA	10.67	131.48	119.32
1	B	326	ARG	N-CA-C	10.66	126.57	108.23
1	B	323	ALA	N-CA-C	10.41	122.38	111.14
1	B	335	TRP	N-CA-C	10.24	125.21	108.52
1	A	351	VAL	N-CA-CB	-10.19	94.41	111.23
1	B	133	THR	N-CA-C	-10.04	101.15	113.50
1	A	523	GLY	N-CA-C	-9.89	92.16	112.34
1	A	6	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	B	349	THR	CA-C-N	-9.71	102.99	121.54
1	B	349	THR	C-N-CA	-9.71	102.99	121.54
1	A	550	ARG	CA-C-N	9.46	130.05	119.93
1	A	550	ARG	C-N-CA	9.46	130.05	119.93
1	B	418	THR	N-CA-C	-9.38	102.64	114.56
1	B	519	ALA	N-CA-C	-9.32	101.60	113.16
1	A	380	ARG	CA-C-O	9.27	129.04	118.47
1	B	312	GLU	N-CA-C	-9.10	100.19	111.11
1	A	288	TRP	N-CA-C	9.06	125.47	107.62
1	B	417	ASP	N-CA-C	-9.04	95.85	109.86
1	A	350	ARG	N-CA-C	8.96	123.19	107.61
1	A	597	TYR	N-CA-C	-8.73	99.07	110.33
1	B	305	GLU	CA-C-N	-8.61	107.76	122.14
1	B	305	GLU	C-N-CA	-8.61	107.76	122.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	540	LEU	CA-C-N	-8.60	104.82	121.58
1	B	540	LEU	C-N-CA	-8.60	104.82	121.58
1	B	48	ALA	N-CA-C	-8.54	103.30	114.31
1	A	102	ASN	N-CA-C	-8.53	103.00	112.72
1	A	21	ALA	N-CA-C	8.49	122.14	111.69
1	A	283	MET	N-CA-C	-8.48	101.26	111.69
1	B	322	PRO	CA-C-N	8.36	131.81	120.44
1	B	322	PRO	C-N-CA	8.36	131.81	120.44
1	B	465	TYR	N-CA-C	-8.30	102.19	111.07
1	B	77	GLU	CA-C-N	8.30	130.22	119.84
1	B	77	GLU	C-N-CA	8.30	130.22	119.84
1	A	605	ASP	N-CA-C	8.29	122.68	112.23
1	B	384	ASN	N-CA-C	-8.20	97.54	108.11
1	B	236	ARG	N-CA-C	8.06	120.14	111.36
1	B	541	ARG	N-CA-C	-8.06	103.43	113.18
1	B	3	PRO	N-CA-C	8.04	133.02	112.10
1	A	368	TYR	N-CA-C	-8.02	102.48	111.14
1	A	381	ARG	N-CA-C	-7.92	96.37	108.96
1	A	8	GLY	N-CA-C	-7.90	102.37	111.85
1	B	564	ALA	N-CA-C	7.89	118.30	107.73
1	B	444	GLN	N-CA-C	-7.80	103.76	113.28
1	A	200	SER	N-CA-C	-7.79	103.77	113.28
1	B	5	LEU	N-CA-C	-7.78	94.24	110.80
1	A	465	TYR	N-CA-C	-7.75	102.77	111.14
1	A	381	ARG	CB-CA-C	7.73	123.13	110.22
1	A	17	ALA	N-CA-C	-7.72	104.01	113.50
1	B	135	THR	N-CA-C	-7.71	96.70	108.96
1	A	18	GLN	N-CA-C	-7.66	102.87	112.90
1	B	324	ASP	N-CA-C	-7.62	102.98	111.28
1	B	419	GLU	N-CA-C	-7.60	103.07	111.36
1	B	317	SER	N-CA-C	7.56	121.67	108.75
1	B	435	PHE	N-CA-C	7.44	119.03	111.07
1	A	187	LYS	N-CA-C	-7.38	104.27	113.20
1	B	280	THR	N-CA-C	7.37	120.75	111.24
1	B	610	GLY	CA-C-N	7.37	134.97	121.70
1	B	610	GLY	C-N-CA	7.37	134.97	121.70
1	A	523	GLY	CA-C-N	7.33	128.41	120.13
1	A	523	GLY	C-N-CA	7.33	128.41	120.13
1	B	502	PHE	N-CA-C	-7.30	102.92	111.03
1	B	455	PRO	CA-C-N	-7.26	112.15	119.56
1	B	455	PRO	C-N-CA	-7.26	112.15	119.56
1	A	349	THR	CB-CA-C	-7.25	99.65	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASN	N-CA-C	7.24	119.25	111.36
1	A	91	ILE	CB-CA-C	-7.22	104.58	111.44
1	A	300	PHE	N-CA-C	-7.12	103.44	111.14
1	A	6	GLN	CG-CD-NE2	7.08	127.01	116.40
1	B	323	ALA	CA-C-N	7.05	129.73	120.28
1	B	323	ALA	C-N-CA	7.05	129.73	120.28
1	A	444	GLN	N-CA-C	-7.02	103.56	111.14
1	A	349	THR	CA-C-N	-6.98	111.22	121.76
1	A	349	THR	C-N-CA	-6.98	111.22	121.76
1	A	85	ASP	CA-C-N	-6.96	113.00	119.82
1	A	85	ASP	C-N-CA	-6.96	113.00	119.82
1	B	307	SER	C-N-CD	-6.95	96.50	125.00
1	B	78	PRO	N-CA-C	-6.93	98.20	112.47
1	A	491	HIS	N-CA-C	6.90	119.83	111.82
1	A	117	ASN	N-CA-C	6.89	118.67	111.03
1	B	491	HIS	N-CA-C	6.88	120.77	112.38
1	A	380	ARG	CB-CA-C	-6.79	100.41	109.16
1	A	125	ALA	N-CA-C	6.78	119.31	110.43
1	B	110	GLN	N-CA-C	-6.69	103.92	111.14
1	A	441	LEU	N-CA-C	6.68	119.12	111.11
1	A	610	GLY	N-CA-C	6.67	121.37	110.77
1	A	5	LEU	N-CA-C	-6.65	106.37	114.75
1	A	611	ILE	CA-C-N	6.63	133.63	121.70
1	A	611	ILE	C-N-CA	6.63	133.63	121.70
1	B	610	GLY	O-C-N	-6.61	117.55	122.71
1	B	482	THR	N-CA-C	-6.60	104.97	113.16
1	B	74	GLU	N-CA-C	6.56	121.14	113.20
1	B	307	SER	CA-C-N	6.53	128.01	119.84
1	B	307	SER	C-N-CA	6.53	128.01	119.84
1	A	606	ASN	N-CA-C	-6.52	96.11	107.20
1	A	18	GLN	CA-C-N	-6.47	109.82	121.14
1	A	18	GLN	C-N-CA	-6.47	109.82	121.14
1	A	564	ALA	N-CA-C	6.46	116.77	108.24
1	B	271	PHE	CA-C-N	6.41	126.33	119.28
1	B	271	PHE	C-N-CA	6.41	126.33	119.28
1	B	540	LEU	N-CA-C	-6.39	105.61	113.41
1	A	550	ARG	CA-CB-CG	6.39	126.87	114.10
1	B	445	TRP	N-CA-C	-6.36	103.64	111.40
1	B	80	TRP	N-CA-C	-6.29	105.92	113.97
1	A	110	GLN	N-CA-C	-6.28	104.35	111.07
1	A	510	GLN	N-CA-C	-6.26	104.45	111.28
1	A	206	THR	N-CA-CB	-6.23	101.51	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	HIS	CA-C-N	-6.22	113.97	120.38
1	B	600	HIS	C-N-CA	-6.22	113.97	120.38
1	B	373	LYS	N-CA-C	-6.21	104.96	112.54
1	B	212	GLU	N-CA-C	-6.18	103.27	111.24
1	B	283	MET	N-CA-C	-6.16	103.30	111.24
1	B	289	ASN	N-CA-C	6.15	118.97	109.07
1	A	350	ARG	N-CA-CB	6.14	120.10	110.71
1	B	14	GLU	N-CA-C	-6.08	104.59	112.68
1	A	446	ARG	N-CA-C	6.08	117.58	111.07
1	A	30	GLN	N-CA-C	-6.02	102.34	111.56
1	B	599	TRP	N-CA-C	6.00	118.70	110.24
1	A	442	VAL	N-CA-C	5.95	116.42	110.23
1	A	550	ARG	CB-CG-CD	-5.94	97.64	111.30
1	A	611	ILE	O-C-N	5.92	128.58	122.07
1	A	279	VAL	N-CA-C	-5.92	97.04	109.34
1	A	281	SER	N-CA-C	5.91	120.51	113.12
1	B	117	ASN	CA-CB-CG	-5.90	106.70	112.60
1	B	4	GLY	N-CA-C	-5.86	99.29	113.18
1	B	463	TRP	N-CA-C	-5.85	104.54	111.03
1	B	77	GLU	C-N-CD	-5.84	101.06	125.00
1	A	2	ASP	N-CA-C	-5.81	101.77	109.84
1	B	421	ASP	N-CA-C	-5.80	104.92	112.23
1	B	440	TYR	N-CA-C	-5.77	106.78	113.88
1	A	63	GLU	CB-CG-CD	-5.75	102.83	112.60
1	A	317	SER	N-CA-C	5.71	118.78	109.24
1	A	508	GLN	N-CA-C	-5.71	106.16	113.23
1	A	290	ALA	N-CA-C	-5.70	105.58	112.54
1	B	309	MET	CA-C-N	5.64	126.19	120.38
1	B	309	MET	C-N-CA	5.64	126.19	120.38
1	A	453	ARG	N-CA-C	-5.63	105.14	111.28
1	B	375	LEU	N-CA-C	5.63	117.07	110.31
1	B	594	TRP	CA-C-N	5.63	125.47	119.28
1	B	594	TRP	C-N-CA	5.63	125.47	119.28
1	A	519	ALA	N-CA-C	-5.59	105.28	111.71
1	A	469	LYS	N-CA-C	5.55	118.05	111.33
1	B	510	GLN	N-CA-C	-5.53	105.33	111.36
1	A	250	ALA	N-CA-C	5.52	122.56	110.80
1	A	335	TRP	N-CA-C	5.51	117.95	109.07
1	B	186	TYR	N-CA-C	5.49	119.08	112.38
1	B	349	THR	N-CA-C	5.48	118.30	110.24
1	B	313	PHE	N-CA-C	5.45	117.92	111.33
1	B	167	ALA	N-CA-C	5.45	120.02	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	PHE	N-CA-C	-5.45	104.22	111.24
1	B	325	GLY	N-CA-C	5.43	126.06	113.18
1	A	549	SER	CA-C-N	-5.40	108.63	121.80
1	A	549	SER	C-N-CA	-5.40	108.63	121.80
1	A	80	TRP	N-CA-C	-5.39	103.38	110.43
1	B	8	GLY	N-CA-C	-5.36	100.48	113.18
1	B	17	ALA	N-CA-C	-5.35	105.62	111.82
1	B	349	THR	CB-CA-C	-5.33	101.85	109.84
1	A	232	ALA	N-CA-C	-5.29	105.52	111.28
1	B	475	PRO	CA-C-N	5.25	126.19	120.83
1	B	475	PRO	C-N-CA	5.25	126.19	120.83
1	B	562	LEU	N-CA-C	5.25	118.37	109.76
1	B	214	LEU	N-CA-C	5.23	117.72	111.71
1	A	409	GLY	N-CA-C	5.21	122.62	115.27
1	A	91	ILE	N-CA-CB	5.19	117.12	111.41
1	A	307	SER	N-CA-C	5.19	116.23	109.64
1	B	309	MET	N-CA-C	5.18	121.26	109.81
1	A	351	VAL	N-CA-C	5.16	120.07	109.34
1	A	449	VAL	N-CA-C	-5.15	105.83	110.82
1	B	306	LEU	N-CA-C	5.12	119.27	112.30
1	A	350	ARG	CB-CG-CD	5.11	123.05	111.30
1	A	409	GLY	CA-C-N	-5.09	114.60	122.49
1	A	409	GLY	C-N-CA	-5.09	114.60	122.49
1	B	215	TYR	N-CA-C	-5.07	105.84	112.23
1	B	189	ASP	N-CA-C	-5.06	106.79	113.17
1	B	575	GLN	N-CA-C	5.03	120.93	109.81

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	85	ASP	Peptide
1	B	86	PRO	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4747	0	4318	414	0
1	B	4665	0	4155	359	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	12	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	1	0
6	A	29	0	27	2	0
6	B	29	0	27	0	0
7	A	12	0	14	4	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	781	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 43.

All (781) 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:B:552:TRP:CD1	1:B:553:GLN:H	1.59	1.19
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:693:NAG:O7	3:A:693:NAG:H3	1.48	1.10
3:B:693:NAG:C8	3:B:693:NAG:C3	2.30	1.10
1:B:98:LEU:HB2	1:B:102:ASN:ND2	1.66	1.09
1:B:174:LEU:H	1:B:174:LEU:HD23	1.16	1.08
1:B:482:THR:HG21	2:D:1:NAG:H82	1.12	1.08
1:B:482:THR:HG21	2:D:1:NAG:C8	1.83	1.07
1:B:236:ARG:HE	1:B:267:MET:HE2	1.13	1.07
3:B:693:NAG:C8	3:B:693:NAG:H3	1.79	1.06
3:B:693:NAG:H3	3:B:693:NAG:H82	1.17	1.06
1:A:236:ARG:HE	1:A:267:MET:HE3	1.20	1.06
1:A:279:VAL:CG1	1:A:282:THR:HG22	1.85	1.05
1:A:20:PHE:HD2	1:A:20:PHE:C	1.65	1.05
1:A:99:GLY:O	1:A:185:ALA:HB1	1.57	1.05
1:A:279:VAL:HG13	1:A:282:THR:HG22	1.12	1.05
1:B:586:GLN:HG3	1:B:587:GLN:N	1.74	1.00
1:A:279:VAL:HG11	1:A:410:LEU:CB	1.91	1.00
1:B:98:LEU:HB2	1:B:102:ASN:HD21	1.17	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
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:HD12	1:A:356:LEU:O	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:B:20:PHE:HD2	1:B:20:PHE:C	1.75	0.94
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:20:PHE:C	1:A:20:PHE:CD2	2.42	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:A:86:PRO:C	1:A:88:LEU:H	1.74	0.92
1:B:129:LEU:HD12	1:B:129:LEU:N	1.83	0.92
1:B:4:GLY:O	1:B:6:GLN:N	2.03	0.92
1:B:129:LEU:C	1:B:131:ASN:H	1.76	0.91
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:515:LEU:C	1:A:530:ILE:HD11	1.97	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
7:A:2433:GOL:O1	1:B:593:GLY:HA3	1.73	0.88
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:O	1:B:279:VAL:HG13	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:HD23	1:B:174:LEU:N	1.90	0.85
1:B:20:PHE:C	1:B:20:PHE:CD2	2.52	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:HD12	1:B:129:LEU:H	1.40	0.85
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: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:B:280:THR:C	1:B:282:THR:H	1.84	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:O	1:B:279:VAL:CG1	2.27	0.82
1:A:270:PRO:HD3	1:A:426:LEU:HD22	1.62	0.82
1:B:552:TRP:CD1	1:B:552:TRP:N	2.45	0.81
1:B:202:TYR:O	1:B:552:TRP:CH2	2.34	0.81
1:A:125:ALA:C	1:A:126:LYS:HG3	2.06	0.81
1:A:139:LEU:HD22	1:A:163:TRP:CZ2	2.16	0.81
1:A:86:PRO:C	1:A:88:LEU:N	2.35	0.80
3:B:695:NAG:C1	3:B:695:NAG:O7	2.30	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:PHE:CB	1:A:76:TYR:HE1	1.94	0.79
1:A:31:VAL:CG2	1:A:64:PHE:HD1	1.95	0.79
1:A:507:LEU:O	1:A:507:LEU:HG	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
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: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:H	1:B:174:LEU:CD2	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:236:ARG:NE	1:A:267:MET:HE3	1.99	0.77
1:A:262:GLU:HG2	1:A:431:GLU:HB2	1.66	0.77
1:A:535:LYS:H	1:A:535:LYS:HD2	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:B:309:MET:HE1	1:B:366:ILE:CG2	2.15	0.76
1:A:20:PHE:HE1	1:A:72:ALA:CA	1.99	0.76
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: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:O	1:A:530:ILE:CG2	2.33	0.75
1:B:4:GLY:C	1:B:6:GLN:N	2.40	0.75
1:B:216:GLN:HA	1:B:216:GLN:HE21	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:280:THR:C	1:B:282:THR:N	2.42	0.74
1:A:283:MET:HE3	1:A:356:LEU:HD23	1.69	0.74
1:B:77:GLU:O	1:B:77:GLU:HG3	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:174:LEU:CD2	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:129:LEU:C	1:B:131:ASN:N	2.45	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:HG23	1:B:530:ILE:O	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:A:453:ARG:HD3	8:B:710:ACT:O	1.90	0.72
1:B:310:PRO:O	1:B:313:PHE:HB3	1.90	0.72
1:A:368:TYR:O	1:A:372:TYR:CD2	2.43	0.72
1:B:10:PHE:N	1:B:10:PHE:CD1	2.56	0.72
1:A:440:TYR:O	1:A:444:GLN:HG2	1.88	0.72
1:A:381:ARG:CB	1:A:381:ARG:CD	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
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:31:VAL:HG21	1:A:64:PHE:CD1	2.24	0.70
1:A:456:PRO:HA	1:A:459:TYR:CD2	2.26	0.70
1:A:529:ASP:OD1	1:A:529:ASP:C	2.34	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:A:91:ILE:HG12	1:A:379:LEU:HD21	1.74	0.70
1:A:147:LEU:CD2	1:A:256:MET:HA	2.21	0.70
1:A:236:ARG:HG2	1:A:267:MET:HE1	1.73	0.70
1:A:350:ARG:HG3	1:A:351:VAL:CB	2.22	0.70
1:B:142:ASP:O	1:B:146:ILE:HG13	1.92	0.69
1:B:140:ASP:OD1	1:B:140:ASP:C	2.35	0.69
1:B:265:TYR:CE1	1:B:427:LYS:HB2	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:309:MET:HE1	1:B:366:ILE:HG21	1.74	0.69
1:A:593:GLY:HA3	7:A:2434:GOL:O1	1.93	0.69
7:A:2433:GOL:O1	1:B:593:GLY:CA	2.40	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:H	1:A:75:LEU:HD23	1.57	0.69
1:B:173:PRO:HG2	1:B:174:LEU:CD2	2.24	0.68
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.74	0.68
1:A:75:LEU:HD23	1:A:75:LEU:N	2.09	0.68
1:A:404:HIS:ND1	1:A:529:ASP:OD2	2.24	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:N	1:B:552:TRP:HD1	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:A:20:PHE:CD2	1:A:20:PHE:O	2.43	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:HD12	1:A:129:LEU:N	2.10	0.67
1:A:312:GLU:CD	1:A:341:LYS:O	2.38	0.66
1:A:253:LEU:N	1:A:253:LEU:HD22	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
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:A:122:TYR:C	1:A:122:TYR:CD2	2.74	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:TYR:O	1:B:80:TRP:HB3	1.95	0.65
1:B:133:THR:O	1:B:134:ALA:HB3	1.96	0.65
1:B:216:GLN:HA	1:B:216:GLN:NE2	2.11	0.65
1:A:236:ARG:HG2	1:A:267:MET:CE	2.27	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:B:315:GLU:C	1:B:317:SER:H	2.04	0.64
1:B:236:ARG:NE	1:B:267:MET:HE2	1.94	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:306:LEU:CB	1:B:541:ARG:HG3	2.28	0.63
1:B:464:TRP:CZ3	1:B:475:PRO:HD3	2.34	0.63
1:A:147:LEU:HD21	1:A:256:MET:HA	1.80	0.63
1:B:64:PHE:CE1	1:B:68:TRP:NE1	2.66	0.63
1:B:279:VAL:HG22	1:B:410:LEU:O	1.99	0.63
1:A:31:VAL:CB	1:A:64:PHE:HD1	2.11	0.63
1:A:300:PHE:CE2	1:A:304:LEU:HD11	2.32	0.63
1:A:368:TYR:C	1:A:372:TYR:CE2	2.76	0.63
1:B:329:VAL:O	1:B:346:LYS:HE3	1.98	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:206:THR:HG23	1:A:210:ASP:CG	2.25	0.62
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
1:A:99:GLY:C	1:A:185:ALA:HB1	2.22	0.62
1:A:178:PHE:C	1:A:178:PHE:CD2	2.77	0.62
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:283:MET:HE1	1:A:356:LEU:HB2	1.82	0.62
1:A:402:PRO:HA	1:A:411:LEU:CD1	2.28	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TYR:HA	1:A:372:TYR:CZ	2.35	0.61
1:B:379:LEU:C	1:B:381:ARG:H	2.08	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:86:PRO:HA	1:A:89:ARG:H	1.65	0.61
1:A:147:LEU:HD23	1:A:255:ASP:C	2.25	0.61
1:A:489:LYS:O	1:A:493:PRO:HD2	2.01	0.61
1:B:29:GLU:OE2	1:B:339:ASN:HA	2.01	0.61
1:B:309:MET:CE	1:B:370:LEU:HD11	2.30	0.61
1:A:125:ALA:O	1:A:126:LYS:HG3	2.00	0.60
1:A:157:LEU:HD13	1:A:476:PRO:HB2	1.82	0.60
1:A:402:PRO:O	1:A:411:LEU:HD12	2.01	0.60
1:B:372:TYR:H	1:B:372:TYR:HD2	1.49	0.60
1:A:515:LEU:C	1:A:530:ILE:CD1	2.70	0.60
1:B:264:ILE:O	1:B:264:ILE:HG23	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:97:THR:O	1:B:97:THR:HG22	2.01	0.60
1:B:441:LEU:HD23	1:B:442:VAL:N	2.16	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:62:GLN:OE1	1:B:112:ASN:ND2	2.35	0.60
1:B:404:HIS:HB2	1:B:529:ASP:OD2	2.01	0.60
1:A:51:ALA:O	1:A:55:GLU:HG3	2.00	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:261:TRP:O	1:A:264:ILE:HG12	2.02	0.60
1:A:29:GLU:OE1	3:A:693:NAG:C2	2.50	0.59
1:A:279:VAL:CG1	1:A:410:LEU:CB	2.76	0.59
1:B:97:THR:O	1:B:97:THR:CG2	2.50	0.59
1:B:279:VAL:CG2	1:B:410:LEU:O	2.50	0.59
1:B:309:MET:HE1	1:B:366:ILE:HG22	1.84	0.59
2:C:1:NAG:H62	2:C:2:NAG:O5	2.02	0.59
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:A:69:GLY:O	1:A:73:LYS:CG	2.50	0.59
1:A:304:LEU:O	1:A:306:LEU:HG	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:THR:O	1:A:479:ARG:HD2	2.03	0.59
1:B:335:TRP:CE3	1:B:335:TRP:HA	2.37	0.59
1:A:610:GLY:C	1:A:612:ASP:H	2.01	0.59
1:B:157:LEU:HD13	1:B:476:PRO:HB2	1.83	0.58
1:A:283:MET:HE3	1:A:356:LEU:CD2	2.33	0.58
1:A:3:PRO:C	1:A:5:LEU:H	2.10	0.58
1:A:490:PHE:C	1:A:490:PHE:CD2	2.80	0.58
1:B:83:PHE:CB	1:B:85:ASP:H	2.16	0.58
1:A:64:PHE:CE2	1:A:68:TRP:NE1	2.72	0.58
1:A:64:PHE:HD2	1:A:64:PHE:C	2.11	0.58
1:A:551:PRO:O	1:A:555:VAL:HG23	2.04	0.58
1:B:7:PRO:HG3	1:B:68:TRP:CG	2.37	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: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:B:326:ARG:O	1:B:327:GLU:C	2.47	0.58
1:B:379:LEU:C	1:B:381:ARG:N	2.61	0.58
1:A:248:ILE:O	1:A:473:ILE:HA	2.03	0.58
1:B:580:TRP:O	1:B:584:GLN:HG2	2.04	0.58
1:A:40:TRP:O	1:A:44:THR:HG23	2.04	0.57
1:B:75:LEU:HB3	1:B:76:TYR:CD2	2.40	0.57
1:B:173:PRO:HG2	1:B:174:LEU:HD23	1.86	0.57
1:A:402:PRO:C	1:A:411:LEU:HD12	2.29	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:A:64:PHE:C	1:A:64:PHE:CD2	2.82	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:O	1:B:381:ARG:N	2.30	0.56
1:A:268:VAL:O	1:A:269:VAL:C	2.48	0.56
1:B:291:THR:HG22	1:B:314:TRP:CZ3	2.41	0.56
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:CD1	1:A:261:TRP:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:VAL:HA	1:A:404:HIS:CD2	2.41	0.56
1:B:68:TRP:CD1	1:B:68:TRP:H	2.24	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:B:44:THR:C	1:B:328:VAL:HG12	2.31	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:26:SER:HA	3:B:693:NAG:HO6	1.68	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:236:ARG:NE	1:B:267:MET:HE1	2.19	0.55
1:B:438:PHE:HA	1:B:441:LEU:HD13	1.88	0.55
1:A:32:LEU:HD13	1:A:338:TYR:CD2	2.41	0.55
1:A:283:MET:CE	1:A:356:LEU:CD2	2.84	0.55
1:A:299:GLU:O	1:A:299:GLU:HG3	2.05	0.55
1:A:350:ARG:HG3	1:A:351:VAL:CG2	2.37	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:O	1:B:530:ILE:CG2	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:B:313:PHE:C	1:B:313:PHE:CD2	2.85	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:O	1:B:92:ILE:HG13	2.07	0.54
1:A:87:GLN:O	1:A:87:GLN:CG	2.56	0.54
1:A:393:ASP:O	1:A:396:ALA:HB3	2.08	0.54
1:B:225:LEU:O	1:B:229:VAL:HG23	2.07	0.54
1:A:367:GLN:O	1:A:371:GLN:HG2	2.07	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:315:GLU:C	1:A:317:SER:H	2.16	0.53
1:A:550:ARG:NH1	1:A:554:GLU:HB3	2.23	0.53
1:B:27:SER:OG	1:B:68:TRP:CH2	2.61	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:SER:OG	1:B:68:TRP:HH2	1.89	0.53
1:B:271:PHE:HE1	1:B:422:ILE:HG21	1.70	0.53
1:B:406:HIS:HB2	1:B:411:LEU:HB3	1.89	0.53
1:A:100:SER:C	1:A:102:ASN:H	2.17	0.53
1:A:593:GLY:HA3	7:A:2434:GOL:HO1	1.73	0.53
1:B:77:GLU:N	1:B:78:PRO:CD	2.71	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:339:ASN:C	1:B:340:ARG:HG3	2.32	0.53
1:A:99:GLY:O	1:A:185:ALA:CB	2.45	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: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:499:ILE:HG13	1:A:499:ILE:O	2.09	0.53
1:B:280:THR:C	1:B:283:MET:H	2.16	0.53
1:B:372:TYR:HD1	1:B:547:GLY:CA	2.21	0.53
1:A:53:ARG:O	1:A:56:GLU:N	2.38	0.52
1:A:122:TYR:CD2	1:A:122:TYR:O	2.63	0.52
1:A:306:LEU:HD21	1:A:541:ARG:HB2	1.91	0.52
1:B:540:LEU:O	1:B:540:LEU:CD2	2.56	0.52
1:A:204:SER:C	1:A:206:THR:H	2.15	0.52
1:B:44:THR:O	1:B:328:VAL:CG1	2.57	0.52
1:B:306:LEU:H	1:B:541:ARG:CZ	2.18	0.52
1:B:552:TRP:CG	1:B:553:GLN:H	2.21	0.52
1:A:29:GLU:OE1	3:A:693:NAG:H2	2.10	0.52
1:A:417:ASP:O	1:A:421:ASP:HB2	2.09	0.52
1:A:302:THR:OG1	1:A:303:SER:N	2.42	0.52
1:A:11:SER:C	1:A:13:ASP:H	2.17	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:68:TRP:O	1:B:69:GLY:C	2.51	0.52
1:B:303:SER:C	1:B:304:LEU:HD23	2.35	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:O	1:A:63:GLU:HG2	2.10	0.51
1:A:283:MET:CE	1:A:356:LEU:HD23	2.38	0.51
1:B:68:TRP:O	1:B:71:LYS:N	2.42	0.51
1:B:495:VAL:HG12	1:B:495:VAL:O	2.09	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:B:199:ARG:C	1:B:201:TRP:H	2.18	0.51
1:B:377:VAL:C	1:B:379:LEU:H	2.19	0.51
1:A:6:GLN:CG	1:A:7:PRO:CD	2.70	0.51
1:A:510:GLN:OE1	1:A:566:ASP:N	2.41	0.51
1:A:25:ASN:O	1:A:29:GLU:HG3	2.10	0.51
1:A:233:LEU:HB3	1:A:242:ILE:HD12	1.91	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:O	1:A:269:VAL:HG13	2.09	0.51
1:A:20:PHE:CE1	1:A:72:ALA:CB	2.93	0.51
1:A:104:PRO:HG2	1:A:107:LYS:HD2	1.92	0.51
1:A:544:LEU:C	1:A:546:ALA:H	2.19	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:O	1:A:46:ILE:CG2	2.59	0.50
1:A:80:TRP:O	1:A:81:GLN:CB	2.59	0.50
1:A:441:LEU:HD23	1:A:441:LEU:C	2.36	0.50
1:A:498:TYR:C	1:A:500:ARG:H	2.19	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:B:398:SER:HB3	1:B:529:ASP:HA	1.92	0.50
1:A:100:SER:C	1:A:102:ASN:N	2.69	0.50
1:A:541:ARG:O	1:A:541:ARG:HG3	2.10	0.50
1:B:202:TYR:HB3	1:B:552:TRP:CH2	2.45	0.50
1:B:482:THR:HG21	2:D:1:NAG:C7	2.40	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:20:PHE:HB3	1:A:76:TYR:HE1	1.73	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:PHE:HD1	1:B:10:PHE:H	1.57	0.50
1:A:279:VAL:HG21	1:A:410:LEU:CB	2.42	0.50
1:B:129:LEU:N	1:B:129:LEU:CD1	2.56	0.50
1:A:206:THR:HG22	1:A:210:ASP:OD2	2.10	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: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:381:ARG:O	1:B:382:GLY:C	2.54	0.49
1:B:390:ALA:O	1:B:391:ILE:C	2.54	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: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:A:128:CYS:CB	1:A:136:CYS:HG	2.20	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:HG12	1:A:495:VAL:O	2.12	0.49
1:B:72:ALA:O	1:B:76:TYR:HB2	2.13	0.49
1:B:289:ASN:O	1:B:290:ALA:C	2.55	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:264:ILE:O	1:B:264:ILE:CG2	2.59	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:309:MET:HE1	1:B:370:LEU:HD11	1.94	0.48
1:B:604:PRO:O	1:B:605:ASP:C	2.55	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:PHE:CD2	1:A:395:LEU:HD23	2.48	0.48
1:B:2:ASP:CB	1:B:3:PRO:C	2.86	0.48
1:B:551:PRO:C	1:B:552:TRP:HD1	2.21	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:445:TRP:HB2	1:A:466:LEU:HD12	1.96	0.48
1:B:77:GLU:CD	1:B:96:ARG:NH2	2.72	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:309:MET:HE2	1:B:309:MET:HA	1.96	0.47
1:B:309:MET:HE2	1:B:370:LEU:HD11	1.94	0.47
1:B:439:GLY:O	1:B:502:PHE:HB2	2.14	0.47
1:A:218:LEU:HD13	1:A:436:LEU:HD13	1.97	0.47
1:A:331:HIS:CD2	1:A:490:PHE:CD2	3.02	0.47
1:B:241:TYR:O	1:B:599:TRP:HH2	1.96	0.47
1:A:597:TYR:CD1	1:A:597:TYR:C	2.92	0.47
1:B:40:TRP:HZ3	1:B:335:TRP:HD1	1.62	0.47
1:B:286:GLN:O	1:B:286:GLN:HG3	2.14	0.47
1:B:507:LEU:HG	1:B:507:LEU:O	2.13	0.47
1:A:17:ALA:HA	1:A:76:TYR:HH	1.80	0.47
1:A:550:ARG:CB	1:A:551:PRO:HD2	2.42	0.47
1:B:204:SER:C	1:B:206:THR:H	2.21	0.47
1:B:377:VAL:C	1:B:379:LEU:N	2.72	0.47
1:B:372:TYR:N	1:B:372:TYR:CD2	2.78	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:71:LYS:O	1:B:72:ALA:C	2.56	0.47
1:B:143:LEU:O	1:B:144:THR:C	2.57	0.47
1:B:283:MET:HE2	1:B:288:TRP:CE3	2.50	0.47
1:B:441:LEU:HD23	1:B:441:LEU:C	2.39	0.47
1:B:567:ALA:O	1:B:568:GLN:C	2.58	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:A:610:GLY:C	1:A:612:ASP:N	2.67	0.47
1:B:129:LEU:HD21	1:B:137:TRP:CZ2	2.50	0.47
1:A:64:PHE:CD2	1:A:68:TRP:CD1	3.02	0.47
1:A:304:LEU:O	1:A:306:LEU:N	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HB3	1:B:101:ALA:HB3	1.98	0.46
1:B:202:TYR:HD2	1:B:552:TRP:HZ3	1.63	0.46
1:A:329:VAL:O	1:A:346:LYS:HE3	2.15	0.46
1:A:603:LEU:C	1:A:604:PRO:O	2.57	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:39:SER:OG	1:A:54:GLN:NE2	2.41	0.46
1:A:298:GLU:O	1:A:301:PHE:N	2.48	0.46
1:B:158:PHE:HA	1:B:607:TYR:OH	2.14	0.46
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: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:B:315:GLU:C	1:B:317:SER:N	2.69	0.46
1:A:441:LEU:HD11	1:A:467:ARG:HA	1.96	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:A:115:LEU:HD21	1:A:178:PHE:CD1	2.51	0.46
1:A:293:MET:HE3	1:A:356:LEU:HA	1.98	0.46
1:A:529:ASP:C	1:A:531:TYR:H	2.22	0.46
1:B:85:ASP:OD1	1:B:87:GLN:N	2.31	0.46
1:B:326:ARG:H	1:B:326:ARG:HG3	1.16	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:268:VAL:O	1:B:269:VAL:C	2.58	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:B:7:PRO:O	1:B:8:GLY:C	2.59	0.45
1:A:100:SER:O	1:A:103:LEU:CB	2.64	0.45
1:A:141:PRO:O	1:A:142:ASP:C	2.59	0.45
1:A:507:LEU:HB2	1:A:565:LEU:HD23	1.98	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:B:122:TYR:CE1	1:B:163:TRP:HZ2	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:TYR:C	1:B:500:ARG:N	2.73	0.45
1:A:91:ILE:HD11	1:A:376:PRO:HG2	1.98	0.45
1:A:204:SER:C	1:A:206:THR:N	2.73	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:73:LYS:HB3	1:A:73:LYS:HE3	1.73	0.45
1:A:134:ALA:O	1:A:135:THR:C	2.60	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:A:125:ALA:C	1:A:126:LYS:CG	2.85	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:A:326:ARG:O	1:A:327:GLU:C	2.59	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:309:MET:CE	1:B:366:ILE:HG21	2.43	0.45
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.63	0.45
1:B:489:LYS:O	1:B:490:PHE:C	2.59	0.45
1:A:262:GLU:H	1:A:262:GLU:HG3	1.43	0.44
1:A:459:TYR:CD1	1:A:484:PHE:CE1	3.05	0.44
1:A:482:THR:HG21	2:C:1:NAG:HN2	1.82	0.44
1:A:603:LEU:O	1:A:604:PRO:O	2.35	0.44
1:B:199:ARG:C	1:B:201:TRP:N	2.75	0.44
1:A:9:ASN:OD1	1:A:10:PHE:O	2.36	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:B:169:ILE:N	1:B:170:PRO:HD2	2.33	0.44
1:B:236:ARG:CD	1:B:267:MET:HE1	2.47	0.44
1:B:255:ASP:OD1	1:B:255:ASP:C	2.60	0.44
1:A:103:LEU:O	1:A:104:PRO:C	2.58	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:20:PHE:HD2	1:B:20:PHE:O	1.95	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:VAL:CG1	1:B:283:MET:HG3	2.48	0.44
1:A:214:LEU:CD2	1:A:506:VAL:HG11	2.48	0.44
1:B:147:LEU:HD13	1:B:256:MET:HE2	1.99	0.44
1:B:306:LEU:O	1:B:307:SER:HB2	2.17	0.44
1:B:472:GLY:HA3	1:B:594:TRP:CH2	2.53	0.44
1:B:568:GLN:HA	1:B:571:LEU:HD12	1.99	0.44
1:B:597:TYR:CD1	1:B:597:TYR:C	2.96	0.44
1:A:83:PHE:O	1:A:84:THR:C	2.60	0.44
1:A:408:ILE:O	1:A:408:ILE:HG12	2.13	0.44
1:B:245:ARG:HB3	1:B:596:GLU:HG3	2.00	0.44
1:B:507:LEU:C	1:B:507:LEU:HD23	2.42	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:75:LEU:N	1:A:75:LEU:CD2	2.76	0.44
1:A:88:LEU:C	1:A:90:ARG:N	2.75	0.44
1:A:158:PHE:HA	1:A:607:TYR:OH	2.18	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: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
1:B:6:GLN:HA	1:B:7:PRO:HD3	1.72	0.43
1:B:204:SER:HA	1:B:205:PRO:HD3	1.86	0.43
1:B:406:HIS:O	1:B:407:LYS:C	2.60	0.43
1:B:586:GLN:O	1:B:589:GLY:N	2.47	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:B:265:TYR:C	1:B:267:MET:H	2.26	0.43
1:A:304:LEU:O	1:A:305:GLU:C	2.61	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:311:PRO:O	1:B:312:GLU:C	2.62	0.43
1:A:202:TYR:O	1:A:203:ASN:C	2.61	0.43
1:B:183:ASN:HD21	1:B:193:ASP:CB	2.30	0.43
1:B:202:TYR:O	1:B:203:ASN:C	2.61	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:PRO:O	1:B:377:VAL:C	2.61	0.43
1:A:570:LEU:O	1:A:570:LEU:HD12	2.19	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:A:596:GLU:C	1:A:597:TYR:O	2.59	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:53:ARG:O	1:A:54:GLN:C	2.61	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:A:503:VAL:HG13	1:A:565:LEU:HD11	2.00	0.43
1:B:89:ARG:HA	1:B:92:ILE:CG2	2.49	0.43
1:B:256:MET:HB3	1:B:257:TRP:CE3	2.54	0.43
1:A:528:CYS:SG	1:A:529:ASP:N	2.92	0.43
1:A:31:VAL:HG11	1:A:64:PHE:CD1	2.54	0.42
1:A:113:ALA:HB1	3:A:695:NAG:HN2	1.84	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:B:261:TRP:CD1	1:B:261:TRP:N	2.86	0.42
1:B:475:PRO:C	1:B:477:VAL:H	2.27	0.42
1:B:607:TYR:HA	1:B:608:PRO:HA	1.64	0.42
1:A:14:GLU:C	1:A:16:GLY:H	2.25	0.42
1:A:411:LEU:HA	1:A:411:LEU:HD23	1.58	0.42
1:A:418:THR:O	1:A:421:ASP:N	2.52	0.42
1:A:507:LEU:O	1:A:507:LEU:CG	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: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:368:TYR:O	1:B:372:TYR:CD2	2.72	0.42
1:B:498:TYR:C	1:B:500:ARG:H	2.26	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:HE21	1:A:510:GLN:HB3	1.61	0.42
1:B:85:ASP:HB3	1:B:88:LEU:CB	2.49	0.42
1:B:335:TRP:O	1:B:343:PHE:HA	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:PHE:O	1:B:503:VAL:C	2.62	0.42
1:A:64:PHE:HD2	1:A:64:PHE:O	2.03	0.42
1:A:227:ALA:HB1	1:A:590:GLU:HG2	2.01	0.42
1:A:318:MET:HE2	1:A:346:LYS:HG2	2.02	0.42
1:A:71:LYS:O	1:A:74:GLU:N	2.52	0.42
1:A:253:LEU:HD12	1:A:261:TRP:CD2	2.55	0.42
1:A:498:TYR:C	1:A:500:ARG:N	2.77	0.42
1:B:529:ASP:OD1	1:B:531:TYR:HB2	2.20	0.42
1:A:186:TYR:C	1:A:188:GLN:H	2.23	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:361:HIS:HA	1:B:392:GLY:HA3	2.02	0.42
1:B:367:GLN:O	1:B:371:GLN:HG2	2.19	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:A:435:PHE:O	1:A:436:LEU:C	2.63	0.41
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
1:A:328:VAL:HG23	1:A:329:VAL:N	2.34	0.41
1:B:25:ASN:CG	3:B:693:NAG:H5	2.40	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:CD1	1:A:335:TRP:N	2.87	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:276:ASN:C	1:A:278:ASP:H	2.29	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:552:TRP:O	1:B:553:GLN:C	2.64	0.41
1:A:3:PRO:C	1:A:5:LEU:N	2.78	0.41
1:A:125:ALA:O	1:A:126:LYS:CG	2.67	0.41
1:A:411:LEU:O	1:A:412:ASP:C	2.61	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:478:THR:HG22	1:A:479:ARG:N	2.35	0.41
1:A:575:GLN:O	1:A:578:THR:HB	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:315:GLU:C	1:A:317:SER:N	2.78	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:331:HIS:CD2	1:A:490:PHE:CZ	3.08	0.41
1:A:455:PRO:C	1:A:457:SER:N	2.78	0.41
1:A:492:VAL:H	1:A:493:PRO:HD2	1.84	0.41
1:A:494:ASN:O	1:A:495:VAL:C	2.64	0.41
1:A:531:TYR:C	1:A:533:SER:N	2.77	0.41
1:B:77:GLU:N	1:B:78:PRO:HD2	2.36	0.41
1:B:586:GLN:HG3	1:B:587:GLN:H	1.74	0.41
1:B:586:GLN:O	1:B:587:GLN:C	2.64	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:B:143:LEU:C	1:B:145:ASN:N	2.79	0.41
1:A:172:LYS:O	1:A:176:GLU:HG3	2.21	0.40
1:A:384:ASN:O	1:A:385:PRO:C	2.63	0.40
1:A:387:PHE:CE1	1:A:552:TRP:HB2	2.56	0.40
1:A:574:PHE:O	1:A:575:GLN:C	2.62	0.40
1:A:277:LEU:CD1	1:A:424:TYR:CA	2.99	0.40
1:A:277:LEU:HD12	1:A:424:TYR:HA	2.03	0.40
1:A:332:ALA:CA	1:A:347:GLN:HG3	2.51	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:B:529:ASP:OD1	1:B:529:ASP:C	2.63	0.40
1:A:323:ALA:C	1:A:325:GLY:H	2.29	0.40
1:A:496:THR:HA	1:A:497:PRO:HD3	1.92	0.40
1:B:46:ILE:H	1:B:46:ILE:HG13	1.65	0.40
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:384:ASN:OD1	1:B:384:ASN:C	2.64	0.40
1:A:73:LYS:HB3	1:A:77:GLU:HG3	2.02	0.40
1:A:350:ARG:HG3	1:A:351:VAL:N	2.33	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

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	595/612 (97%)	494 (83%)	81 (14%)	20 (3%)	3	17
1	B	597/612 (98%)	506 (85%)	70 (12%)	21 (4%)	3	16
All	All	1192/1224 (97%)	1000 (84%)	151 (13%)	41 (3%)	3	17

All (41) 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
1	A	130	PRO
1	A	262	GLU
1	A	490	PHE
1	A	499	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/526 (87%)	391 (85%)	67 (15%)	3	15
1	B	437/526 (83%)	367 (84%)	70 (16%)	2	12
All	All	895/1052 (85%)	758 (85%)	137 (15%)	3	14

All (137) 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	31	VAL
1	A	34	GLN
1	A	52	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	54	GLN
1	A	59	LEU
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	129	LEU
1	A	144	THR
1	A	147	LEU
1	A	171	LEU
1	A	174	LEU
1	A	178	PHE
1	A	187	LYS
1	A	206	THR
1	A	214	LEU
1	A	221	LEU
1	A	242	ILE
1	A	245	ARG
1	A	253	LEU
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	331	HIS
1	A	342	ASP
1	A	354	ASP
1	A	356	LEU
1	A	378	SER
1	A	379	LEU
1	A	388	HIS
1	A	408	ILE
1	A	441	LEU
1	A	457	SER
1	A	480	ASN
1	A	482	THR
1	A	494	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	496	THR
1	A	507	LEU
1	A	522	GLU
1	A	530	ILE
1	A	540	LEU
1	A	541	ARG
1	A	543	VAL
1	A	550	ARG
1	A	553	GLN
1	A	563	ASP
1	A	570	LEU
1	A	575	GLN
1	A	579	GLN
1	A	582	GLN
1	A	587	GLN
1	A	590	GLU
1	A	594	TRP
1	A	604	PRO
1	B	3	PRO
1	B	10	PHE
1	B	20	PHE
1	B	25	ASN
1	B	49	GLU
1	B	60	LEU
1	B	66	GLU
1	B	68	TRP
1	B	78	PRO
1	B	91	ILE
1	B	92	ILE
1	B	95	VAL
1	B	97	THR
1	B	109	GLN
1	B	118	MET
1	B	129	LEU
1	B	144	THR
1	B	147	LEU
1	B	174	LEU
1	B	188	GLN
1	B	212	GLU
1	B	214	LEU
1	B	231	ARG
1	B	235	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	236	ARG
1	B	245	ARG
1	B	260	SER
1	B	264	ILE
1	B	279	VAL
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	346	LYS
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	453	ARG
1	B	460	ASN
1	B	477	VAL
1	B	480	ASN
1	B	482	THR
1	B	507	LEU
1	B	508	GLN
1	B	510	GLN
1	B	540	LEU
1	B	542	LYS
1	B	552	TRP
1	B	570	LEU

Continued on next page...

Continued from previous page...

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) 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	286	GLN
1	A	331	HIS
1	A	347	GLN
1	A	406	HIS
1	A	471	GLN
1	A	491	HIS
1	A	494	ASN
1	A	512	HIS
1	A	575	GLN
1	A	582	GLN
1	A	598	GLN
1	A	600	HIS
1	B	102	ASN
1	B	109	GLN
1	B	131	ASN
1	B	183	ASN
1	B	188	GLN
1	B	216	GLN
1	B	224	ASN
1	B	286	GLN
1	B	331	HIS
1	B	347	GLN
1	B	371	GLN
1	B	575	GLN
1	B	579	GLN
1	B	582	GLN
1	B	585	ASN
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	2.68	3 (21%)	17,19,21	1.33	2 (11%)
2	NAG	C	2	2	14,14,15	2.25	1 (7%)	17,19,21	1.29	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.26	0	17,19,21	1.03	1 (5%)
2	NAG	D	2	2	14,14,15	2.34	1 (7%)	17,19,21	1.06	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	-8.71	1.32	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C8-C7	-8.64	1.32	1.50
2	C	2	NAG	C8-C7	-8.19	1.33	1.50
2	C	1	NAG	C1-C2	2.66	1.56	1.52
2	C	1	NAG	C4-C3	-2.39	1.46	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-C2-N2	-3.46	104.98	110.43
2	D	2	NAG	C1-C2-N2	-3.45	104.99	110.43
2	C	2	NAG	C1-C2-N2	-3.01	105.69	110.43
2	C	1	NAG	C6-C5-C4	-2.92	105.84	113.02
2	C	2	NAG	C1-O5-C5	-2.63	108.66	112.19
2	C	1	NAG	C2-N2-C7	2.36	126.06	122.90
2	C	2	NAG	C4-C3-C2	-2.27	107.69	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2	NAG	C2

All (2) torsion outliers are listed below:

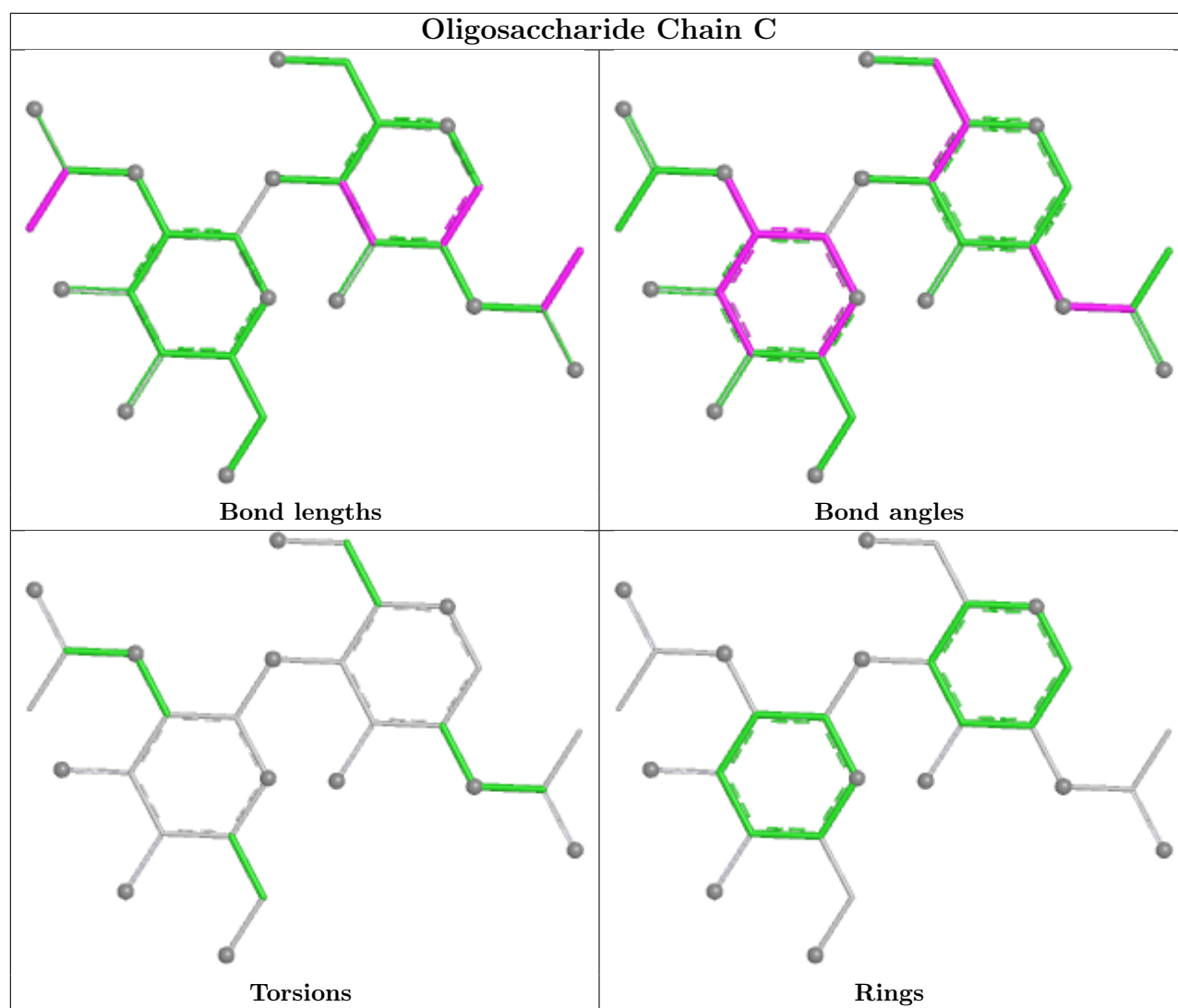
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

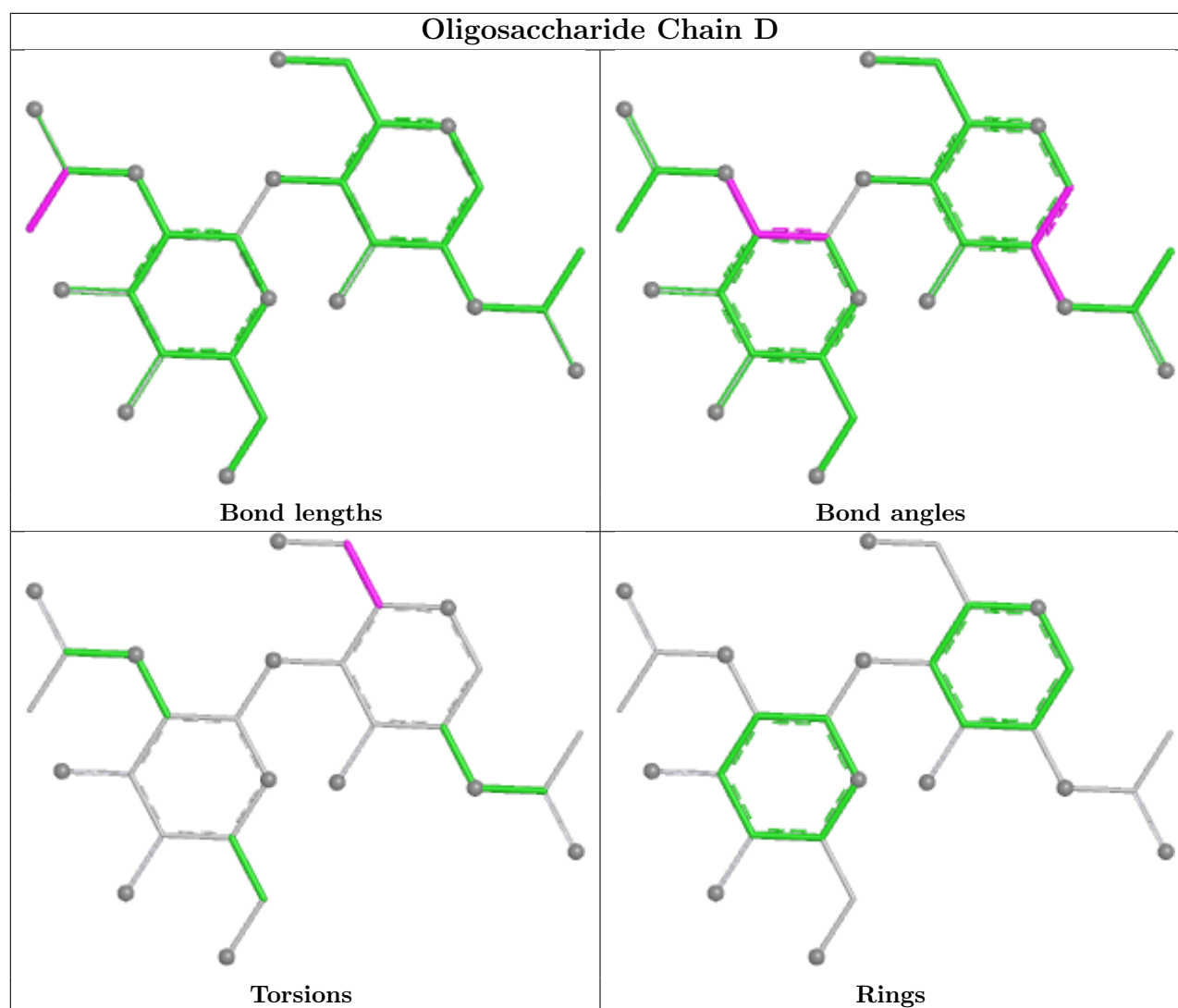
There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0
2	C	1	NAG	2	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 [i](#)

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	$\# Z > 2$
3	NAG	A	693	1	14,14,15	0.26	0	17,19,21	1.04	1 (5%)
3	NAG	B	695	1	14,14,15	0.26	0	17,19,21	1.03	1 (5%)
3	NAG	B	693	1	14,14,15	0.25	0	17,19,21	1.20	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	2434	-	5,5,5	3.64	3 (60%)	5,5,5	1.61	1 (20%)
6	LPR	A	705	4	30,30,30	3.27	15 (50%)	38,39,39	1.91	8 (21%)
7	GOL	A	2433	-	5,5,5	3.48	3 (60%)	5,5,5	2.21	1 (20%)
3	NAG	A	695	1	14,14,15	0.26	0	17,19,21	1.03	1 (5%)
6	LPR	B	705	4	30,30,30	3.34	14 (46%)	38,39,39	1.76	9 (23%)
8	ACT	B	710	-	3,3,3	1.60	1 (33%)	3,3,3	0.73	0

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	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	B	693	1	1/1/5/7	5/6/23/26	0/1/1/1
7	GOL	A	2434	-	-	0/4/4/4	-
6	LPR	A	705	4	-	7/30/40/40	0/2/2/2
7	GOL	A	2433	-	-	0/4/4/4	-
3	NAG	A	695	1	-	0/6/23/26	0/1/1/1
6	LPR	B	705	4	-	2/30/40/40	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	705	LPR	C4-N1	-12.30	1.17	1.47
6	A	705	LPR	C4-N1	-11.52	1.19	1.47
7	A	2434	GOL	O2-C2	-6.68	1.24	1.43
7	A	2433	GOL	O2-C2	-4.75	1.29	1.43
6	A	705	LPR	C17-C16	4.70	1.48	1.38
6	B	705	LPR	C20-C19	4.26	1.47	1.38
6	A	705	LPR	C19-C18	4.24	1.47	1.38
7	A	2433	GOL	O3-C3	4.15	1.59	1.42
7	A	2433	GOL	C3-C2	4.09	1.67	1.51
6	B	705	LPR	C17-C16	4.04	1.46	1.38
6	A	705	LPR	C20-C19	4.03	1.47	1.38
6	A	705	LPR	C20-C21	4.02	1.45	1.38
6	B	705	LPR	C19-C18	4.00	1.47	1.38
6	B	705	LPR	C20-C21	3.95	1.45	1.38
6	B	705	LPR	C21-C16	3.91	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705	LPR	C7-C6	-3.91	1.36	1.51
6	A	705	LPR	C21-C16	3.89	1.46	1.38
6	B	705	LPR	C5-C9	3.81	1.59	1.52
6	A	705	LPR	C2-C1	3.70	1.60	1.53
7	A	2434	GOL	C3-C2	3.68	1.65	1.51
6	B	705	LPR	C7-C6	-3.58	1.37	1.51
6	B	705	LPR	C14-C4	-3.52	1.45	1.53
6	B	705	LPR	O1-C1	3.49	1.28	1.22
6	A	705	LPR	C18-C17	3.48	1.44	1.38
6	A	705	LPR	C5-N2	3.44	1.53	1.47
6	B	705	LPR	C2-C1	3.41	1.59	1.53
6	B	705	LPR	C18-C17	3.20	1.44	1.38
6	A	705	LPR	O1-C1	3.12	1.27	1.22
6	B	705	LPR	C5-N2	2.87	1.52	1.47
6	A	705	LPR	C5-C9	2.47	1.57	1.52
7	A	2434	GOL	O3-C3	2.37	1.52	1.42
6	A	705	LPR	C12-C13	-2.35	1.40	1.51
6	A	705	LPR	C14-C4	-2.32	1.48	1.53
8	B	710	ACT	OXT-C	2.28	1.41	1.30
6	B	705	LPR	C12-C13	-2.11	1.41	1.51
6	A	705	LPR	C1-N2	2.05	1.39	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	705	LPR	C2-N1-C4	6.21	129.54	115.67
6	A	705	LPR	C2-N1-C4	6.03	129.13	115.67
7	A	2433	GOL	O3-C3-C2	-4.35	90.80	110.38
6	A	705	LPR	C14-C4-C3	-4.23	100.31	110.35
6	A	705	LPR	C15-C14-C4	4.00	121.32	113.21
6	B	705	LPR	C14-C4-C3	-3.70	101.58	110.35
3	B	693	NAG	C1-C2-N2	-3.55	104.84	110.43
6	A	705	LPR	C11-C10-C2	3.54	124.69	113.80
3	A	693	NAG	C1-C2-N2	-3.47	104.96	110.43
3	B	695	NAG	C1-C2-N2	-3.43	105.02	110.43
3	A	695	NAG	C1-C2-N2	-3.43	105.02	110.43
7	A	2434	GOL	O3-C3-C2	-3.33	95.39	110.38
6	A	705	LPR	C7-C6-C5	3.22	110.86	104.14
6	B	705	LPR	C7-C6-C5	3.21	110.84	104.14
6	A	705	LPR	C14-C15-C16	3.13	123.53	113.22
6	A	705	LPR	C6-C7-C8	3.12	113.57	104.90
6	B	705	LPR	C6-C7-C8	2.90	112.97	104.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	705	LPR	C14-C15-C16	2.85	122.61	113.22
6	B	705	LPR	C15-C14-C4	2.83	118.94	113.21
6	B	705	LPR	C11-C10-C2	2.78	122.36	113.80
3	B	693	NAG	C2-N2-C7	2.38	126.08	122.90
6	A	705	LPR	C14-C4-N1	2.29	128.32	112.17
6	B	705	LPR	O2-C3-C4	2.06	120.48	113.51
6	B	705	LPR	C14-C4-N1	2.00	126.28	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	693	NAG	C1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	693	NAG	C3-C2-N2-C7
3	B	693	NAG	C3-C2-N2-C7
3	B	695	NAG	C1-C2-N2-C7
6	A	705	LPR	C15-C14-C4-N1
6	B	705	LPR	C15-C14-C4-N1
3	B	693	NAG	C8-C7-N2-C2
3	B	693	NAG	O7-C7-N2-C2
6	A	705	LPR	C15-C14-C4-C3
6	B	705	LPR	C15-C14-C4-C3
3	B	693	NAG	C4-C5-C6-O6
3	B	695	NAG	O5-C5-C6-O6
3	A	693	NAG	C4-C5-C6-O6
6	A	705	LPR	C6-C5-C9-O4
6	A	705	LPR	C14-C15-C16-C17
3	B	693	NAG	O5-C5-C6-O6
6	A	705	LPR	C14-C15-C16-C21
6	A	705	LPR	N2-C5-C9-O4
6	A	705	LPR	C2-C10-C11-C12

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	693	NAG	5	0
3	B	695	NAG	1	0

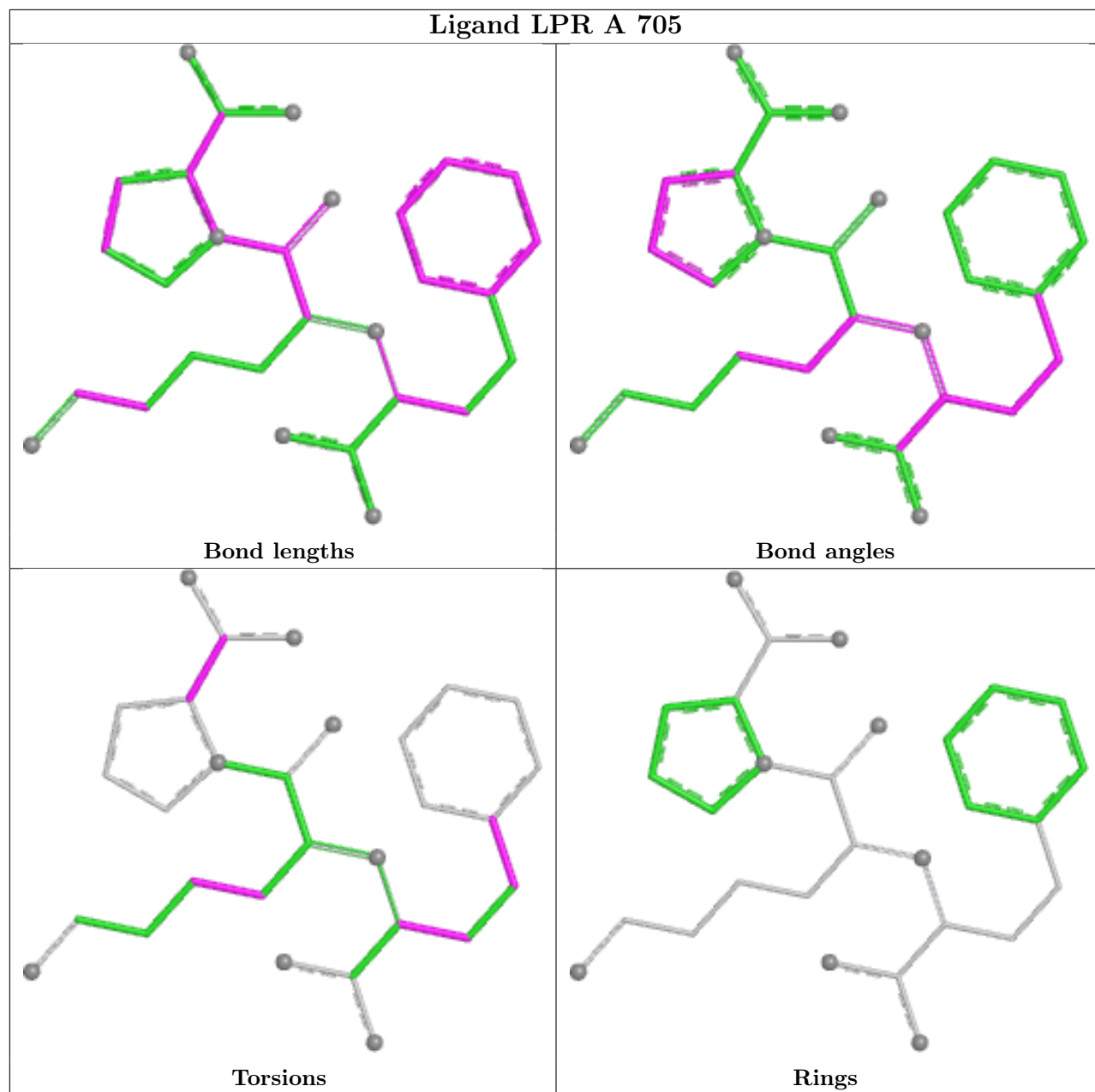
Continued on next page...

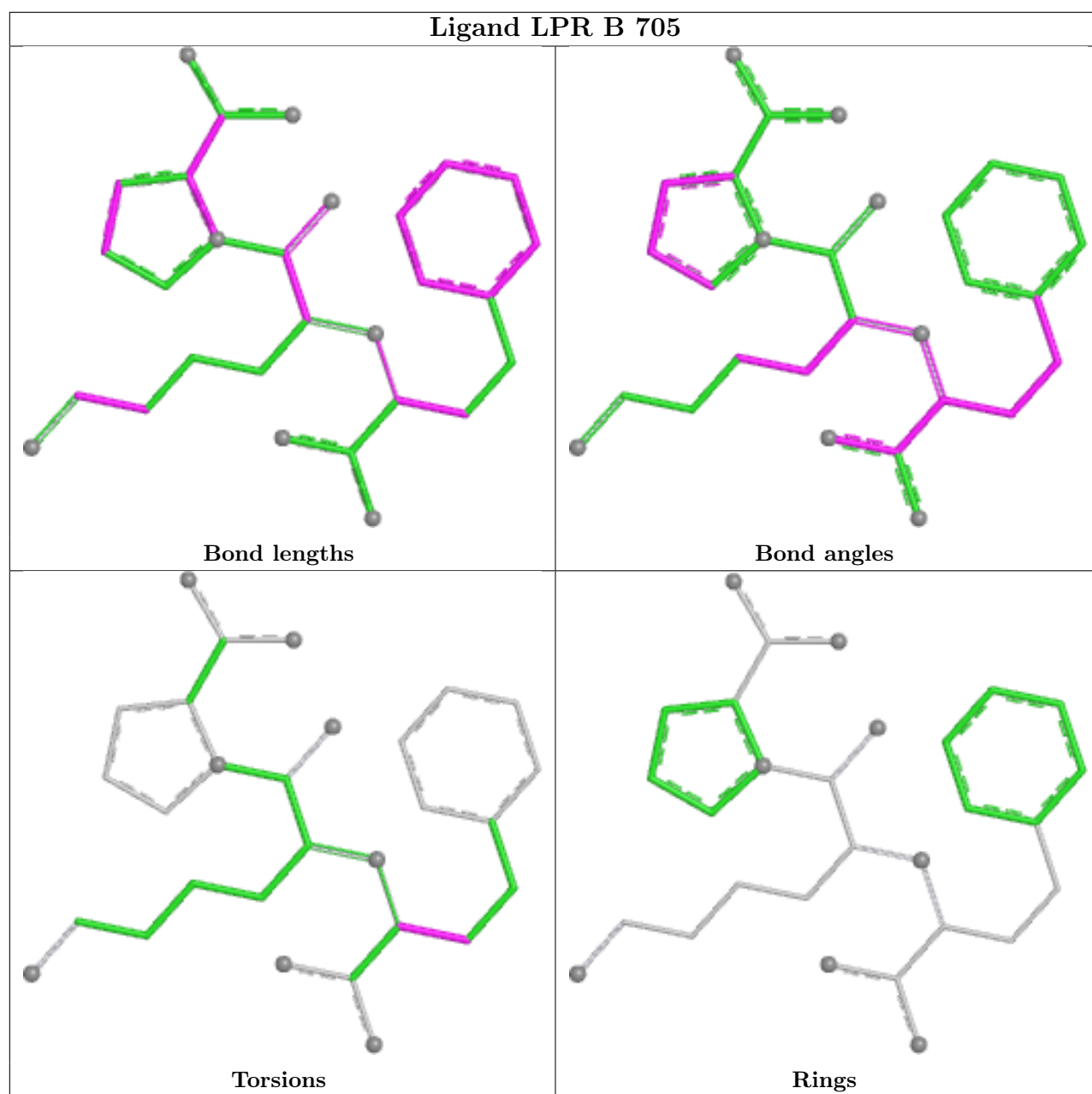
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	693	NAG	11	0
7	A	2434	GOL	2	0
6	A	705	LPR	2	0
7	A	2433	GOL	2	0
3	A	695	NAG	2	0
8	B	710	ACT	1	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.

Ligand LPR A 705





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%)	1.03	121 (19%) 3 2	5, 39, 64, 72	4 (0%)
1	B	609/612 (99%)	1.04	123 (20%) 3 2	4, 41, 67, 81	4 (0%)
All	All	1221/1224 (99%)	1.04	244 (19%) 3 2	4, 40, 66, 81	8 (0%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	SER	6.0
1	A	412	ASP	5.5
1	B	520	GLY	5.5
1	A	81	GLN	4.8
1	A	26	SER	4.8
1	A	304	LEU	4.7
1	A	307	SER	4.7
1	B	81	GLN	4.7
1	B	279	VAL	4.6
1	A	310	PRO	4.5
1	B	85	ASP	4.4
1	B	11	SER	4.4
1	B	84	THR	4.3
1	B	605	ASP	4.3
1	B	26	SER	4.2
1	A	19	LEU	4.2
1	B	376	PRO	4.2
1	A	30	GLN	4.1
1	A	27	SER	4.1
1	B	417	ASP	4.0
1	A	22	GLN	4.0
1	B	352	THR	3.9
1	A	330	CYS	3.9
1	A	352	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	547	GLY	3.8
1	B	309	MET	3.7
1	B	410	LEU	3.7
1	B	86	PRO	3.7
1	B	290	ALA	3.7
1	A	291	THR	3.7
1	B	88	LEU	3.7
1	B	12	ALA	3.6
1	B	609	GLU	3.6
1	B	133	THR	3.6
1	A	316	GLY	3.6
1	A	369	TYR	3.6
1	A	357	SER	3.6
1	B	370	LEU	3.5
1	A	135	THR	3.5
1	A	28	ALA	3.5
1	A	276	ASN	3.4
1	A	17	ALA	3.4
1	B	87	GLN	3.4
1	B	78	PRO	3.4
1	B	13	ASP	3.4
1	B	552	TRP	3.4
1	B	70	GLN	3.4
1	B	362	GLU	3.3
1	B	611	ILE	3.3
1	B	544	LEU	3.3
1	A	383	ALA	3.3
1	A	80	TRP	3.3
1	B	312	GLU	3.3
1	A	372	TYR	3.2
1	B	372	TYR	3.2
1	A	612	ASP	3.2
1	B	543	VAL	3.2
1	B	412	ASP	3.2
1	B	27	SER	3.2
1	B	47	THR	3.2
1	B	45	ASN	3.1
1	A	327	GLU	3.1
1	A	303	SER	3.1
1	B	310	PRO	3.1
1	B	546	ALA	3.1
1	B	540	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	280	THR	3.1
1	A	86	PRO	3.1
1	A	296	VAL	3.0
1	B	14	GLU	3.0
1	B	7	PRO	3.0
1	B	75	LEU	3.0
1	A	289	ASN	3.0
1	B	76	TYR	3.0
1	A	306	LEU	3.0
1	B	72	ALA	3.0
1	A	34	GLN	3.0
1	A	609	GLU	3.0
1	A	413	ARG	3.0
1	B	378	SER	3.0
1	A	309	MET	3.0
1	B	536	ALA	2.9
1	B	44	THR	2.9
1	A	305	GLU	2.9
1	B	25	ASN	2.9
1	A	68	TRP	2.9
1	B	8	GLY	2.9
1	A	20	PHE	2.9
1	A	411	LEU	2.9
1	B	421	ASP	2.9
1	B	74	GLU	2.9
1	A	523	GLY	2.9
1	B	135	THR	2.9
1	B	95	VAL	2.9
1	B	365	HIS	2.8
1	A	134	ALA	2.8
1	A	314	TRP	2.8
1	B	18	GLN	2.8
1	A	88	LEU	2.8
1	A	549	SER	2.8
1	A	79	ILE	2.7
1	B	338	TYR	2.7
1	A	308	PRO	2.7
1	B	90	ARG	2.7
1	A	544	LEU	2.7
1	B	606	ASN	2.7
1	B	306	LEU	2.6
1	B	393	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	523	GLY	2.6
1	A	319	LEU	2.6
1	B	307	SER	2.6
1	A	287	GLY	2.6
1	A	320	GLU	2.6
1	A	75	LEU	2.6
1	A	338	TYR	2.6
1	A	376	PRO	2.6
1	B	16	GLY	2.6
1	B	305	GLU	2.6
1	B	388	HIS	2.6
1	B	531	TYR	2.6
1	B	411	LEU	2.6
1	B	525	LEU	2.6
1	B	403	GLU	2.6
1	A	313	PHE	2.5
1	A	95	VAL	2.5
1	A	273	ASP	2.5
1	A	336	ASP	2.5
1	A	414	VAL	2.5
1	B	79	ILE	2.5
1	B	415	THR	2.5
1	A	42	HIS	2.5
1	A	370	LEU	2.5
1	A	84	THR	2.5
1	B	377	VAL	2.5
1	A	46	ILE	2.5
1	B	339	ASN	2.5
1	A	402	PRO	2.5
1	A	5	LEU	2.5
1	B	23	SER	2.5
1	A	131	ASN	2.5
1	A	44	THR	2.5
1	A	3	PRO	2.5
1	A	36	VAL	2.5
1	A	545	GLN	2.5
1	B	553	GLN	2.5
1	B	335	TRP	2.4
1	B	369	TYR	2.4
1	A	533	SER	2.4
1	A	339	ASN	2.4
1	A	382	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	531	TYR	2.4
1	B	24	TYR	2.4
1	A	15	ALA	2.4
1	A	318	MET	2.4
1	B	274	LYS	2.4
1	A	416	ASN	2.4
1	B	524	PRO	2.4
1	A	31	VAL	2.4
1	B	69	GLY	2.4
1	B	610	GLY	2.4
1	B	15	ALA	2.4
1	B	28	ALA	2.4
1	A	341	LYS	2.4
1	B	308	PRO	2.4
1	A	277	LEU	2.4
1	A	14	GLU	2.4
1	A	279	VAL	2.4
1	B	519	ALA	2.3
1	B	80	TRP	2.3
1	B	337	PHE	2.3
1	B	17	ALA	2.3
1	B	278	ASP	2.3
1	B	522	GLU	2.3
1	A	89	ARG	2.3
1	A	550	ARG	2.3
1	B	190	GLY	2.3
1	B	313	PHE	2.3
1	B	336	ASP	2.3
1	A	611	ILE	2.3
1	B	92	ILE	2.3
1	B	311	PRO	2.3
1	A	288	TRP	2.3
1	A	100	SER	2.3
1	A	350	ARG	2.3
1	A	380	ARG	2.3
1	A	278	ASP	2.3
1	A	328	VAL	2.3
1	B	43	ASP	2.3
1	B	29	GLU	2.2
1	B	298	GLU	2.2
1	A	520	GLY	2.2
1	A	536	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	610	GLY	2.2
1	A	18	GLN	2.2
1	A	76	TYR	2.2
1	A	285	GLN	2.2
1	B	273	ASP	2.2
1	A	347	GLN	2.2
1	B	562	LEU	2.2
1	A	324	ASP	2.2
1	A	83	PHE	2.2
1	A	24	TYR	2.2
1	A	540	LEU	2.2
1	B	379	LEU	2.2
1	A	101	ALA	2.2
1	B	374	ASP	2.2
1	A	282	THR	2.1
1	B	100	SER	2.1
1	A	563	ASP	2.1
1	B	128	CYS	2.1
1	B	351	VAL	2.1
1	A	32	LEU	2.1
1	B	420	SER	2.1
1	B	533	SER	2.1
1	B	314	TRP	2.1
1	B	555	VAL	2.1
1	A	406	HIS	2.1
1	B	19	LEU	2.1
1	B	46	ILE	2.1
1	B	418	THR	2.1
1	B	323	ALA	2.1
1	B	389	GLU	2.1
1	A	138	SER	2.1
1	B	515	LEU	2.1
1	A	47	THR	2.1
1	A	381	ARG	2.1
1	B	66	GLU	2.1
1	A	379	LEU	2.1
1	A	323	ALA	2.1
1	A	429	ALA	2.1
1	A	87	GLN	2.1
1	A	311	PRO	2.1
1	B	320	GLU	2.1
1	A	72	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	564	ALA	2.0
1	A	7	PRO	2.0
1	A	337	PHE	2.0
1	B	414	VAL	2.0
1	B	556	LEU	2.0
1	A	353	MET	2.0
1	A	133	THR	2.0
1	B	21	ALA	2.0
1	A	576	PRO	2.0
1	B	367	GLN	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](#)

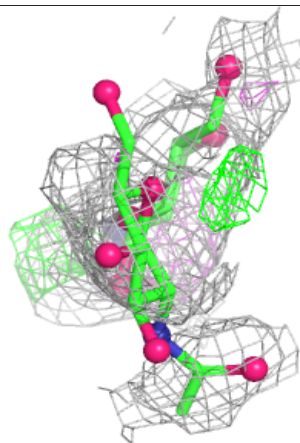
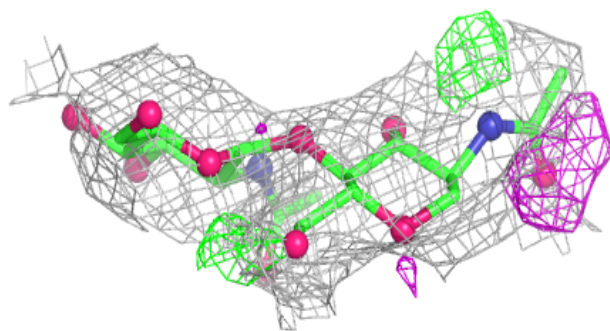
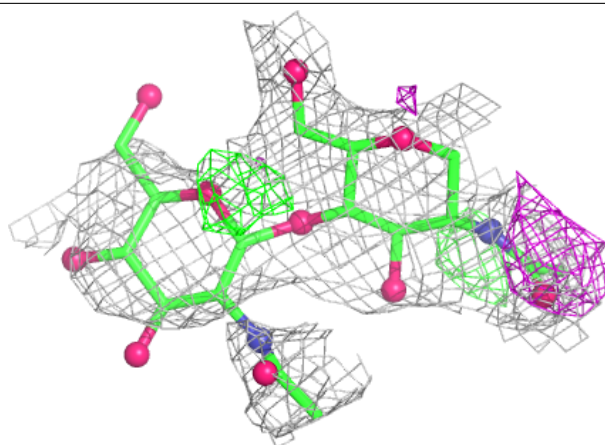
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

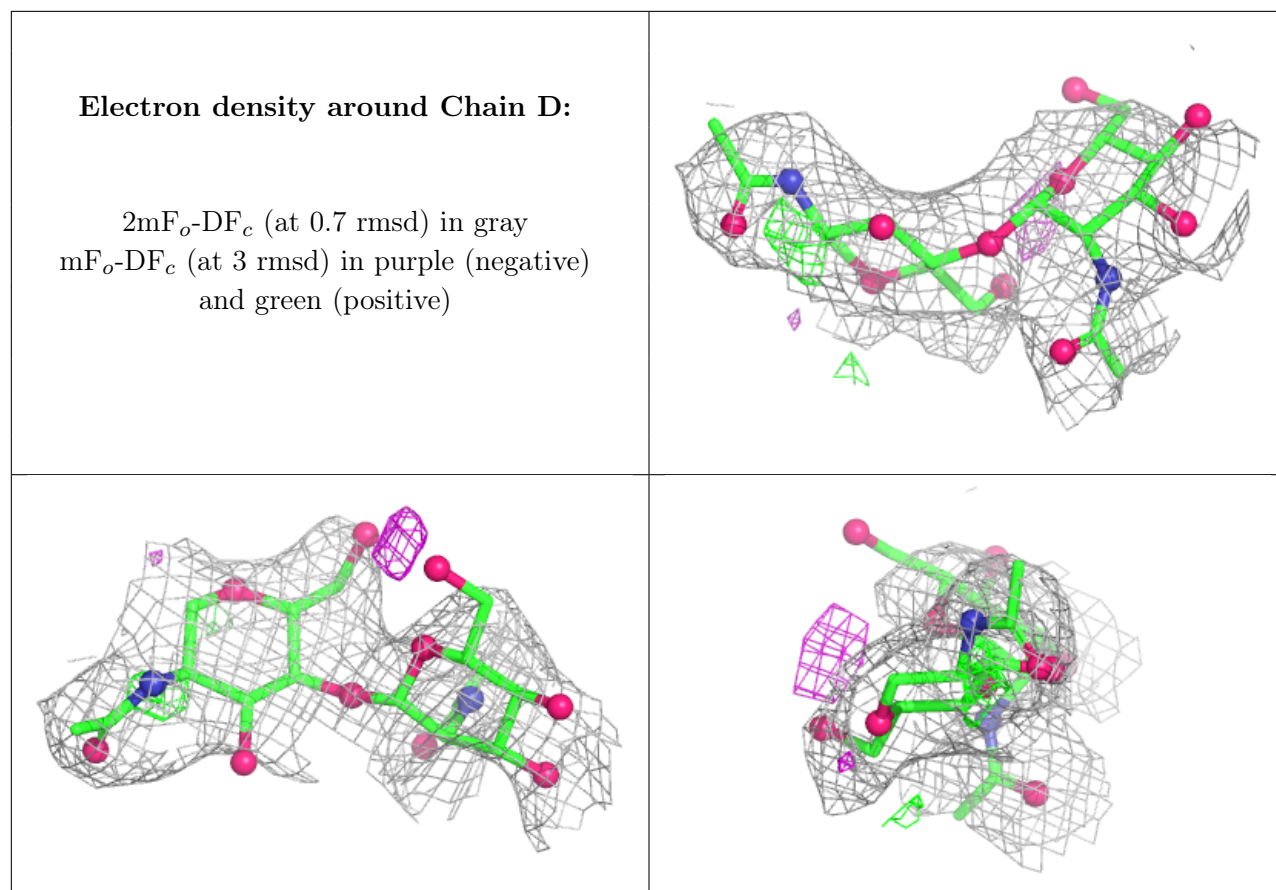
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	C	2	14/15	0.41	0.29	100,101,103,103	0
2	NAG	C	1	14/15	0.59	0.23	29,32,35,37	0
2	NAG	D	2	14/15	0.59	0.22	90,92,93,94	0
2	NAG	D	1	14/15	0.79	0.18	32,35,37,38	0

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)





6.4 Ligands ⓘ

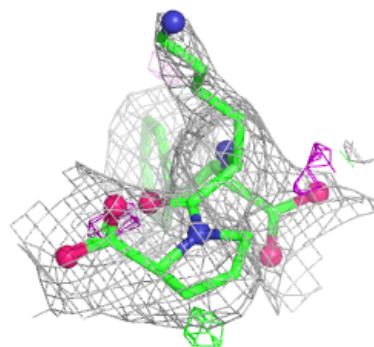
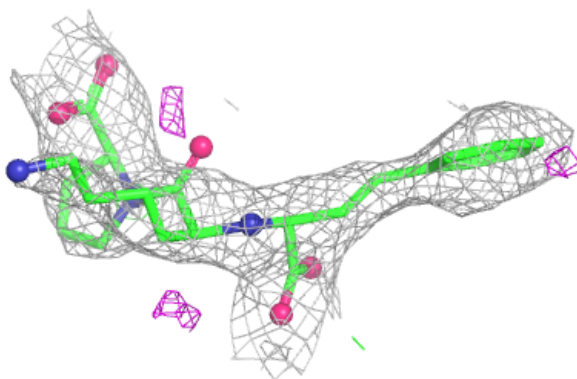
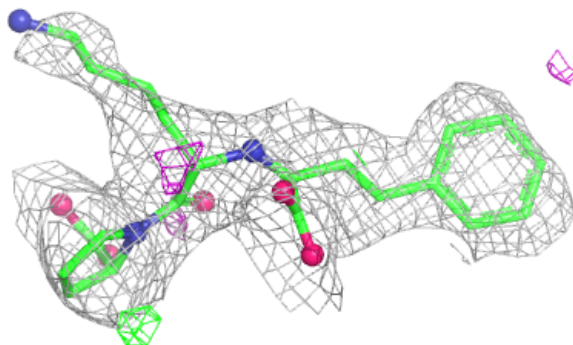
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.11	0.23	66,69,70,70	0
3	NAG	A	693	14/15	0.56	0.19	69,72,74,75	0
3	NAG	B	695	14/15	0.62	0.29	77,78,81,83	0
5	CL	A	703	1/1	0.73	0.13	31,31,31,31	0
3	NAG	A	695	14/15	0.76	0.21	73,74,75,76	0
8	ACT	B	710	4/4	0.79	0.19	29,30,30,32	0
7	GOL	A	2433	6/6	0.85	0.23	25,27,27,27	0
6	LPR	A	705	29/29	0.85	0.19	43,47,49,49	0
7	GOL	A	2434	6/6	0.86	0.23	28,29,30,31	0
6	LPR	B	705	29/29	0.88	0.16	35,40,43,45	0
5	CL	B	702	1/1	0.96	0.04	25,25,25,25	0
4	ZN	B	701	1/1	0.98	0.03	31,31,31,31	0
4	ZN	A	701	1/1	0.99	0.04	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.

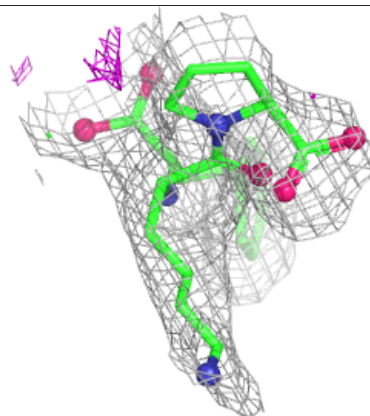
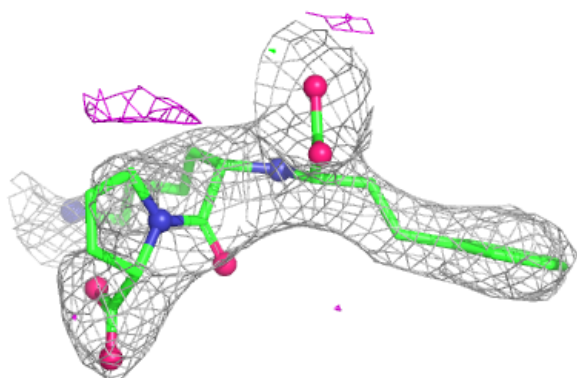
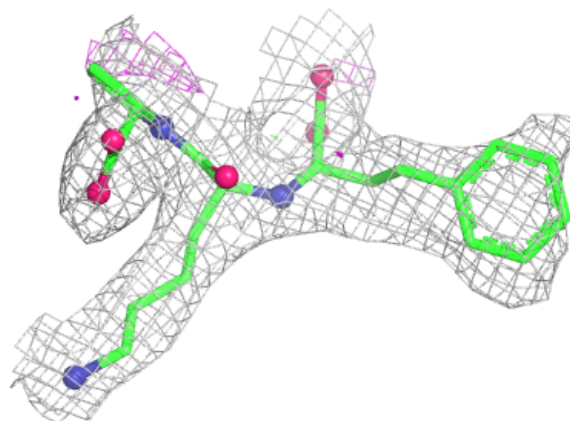
Electron density around LPR A 705:

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.