



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:40 PM UTC

PDB ID : 2C8N / pdb_00002c8n
Title : The Structure of a family 51 arabinofuranosidase, Araf51, from *Clostridium thermocellum* in complex with 1,3-linked arabinoside of xylobiose.
Authors : Taylor, E.J.; Smith, N.L.; Turkenburg, J.P.; D'Souza, S.; Gilbert, H.J.; Davies, G.J.
Deposited on : 2005-12-06
Resolution : 2.90 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:

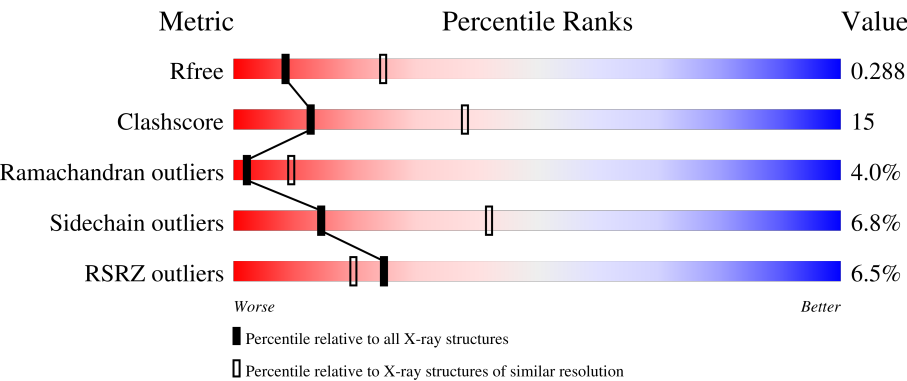
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



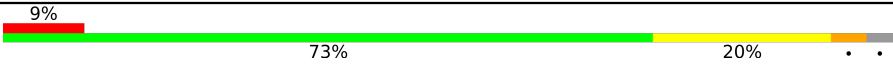
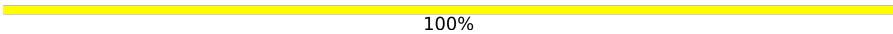
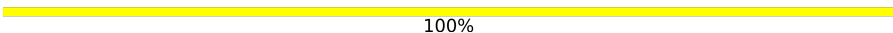
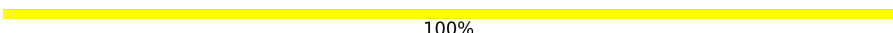
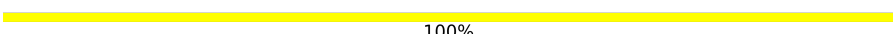
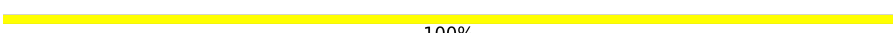
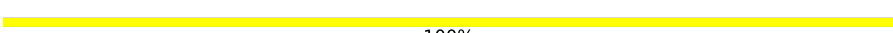
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	513	5% 76%17%...
1	B	513	5% 69%23%...
1	C	513	7% 70%21%5%..
1	D	513	4% 70%21%5%..
1	E	513	8% 72%19%6%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	513	
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24200 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 ALPHA-L-ARABINOFURANOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			4017	2552	683	760	22			
1	B	500	Total	C	N	O	S	0	0	0
			4013	2545	686	760	22			
1	C	499	Total	C	N	O	S	0	1	0
			3989	2533	681	753	22			
1	D	498	Total	C	N	O	S	0	0	0
			3933	2487	672	753	21			
1	E	497	Total	C	N	O	S	0	0	0
			3927	2496	670	741	20			
1	F	500	Total	C	N	O	S	0	0	0
			3966	2518	679	748	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	173	ALA	GLU	engineered mutation	UNP Q4CJG5
B	173	ALA	GLU	engineered mutation	UNP Q4CJG5
C	173	ALA	GLU	engineered mutation	UNP Q4CJG5
D	173	ALA	GLU	engineered mutation	UNP Q4CJG5
E	173	ALA	GLU	engineered mutation	UNP Q4CJG5
F	173	ALA	GLU	engineered mutation	UNP Q4CJG5

- Molecule 2 is an oligosaccharide called alpha-L-arabinofuranose-(1-3)-alpha-D-xylopyranose.



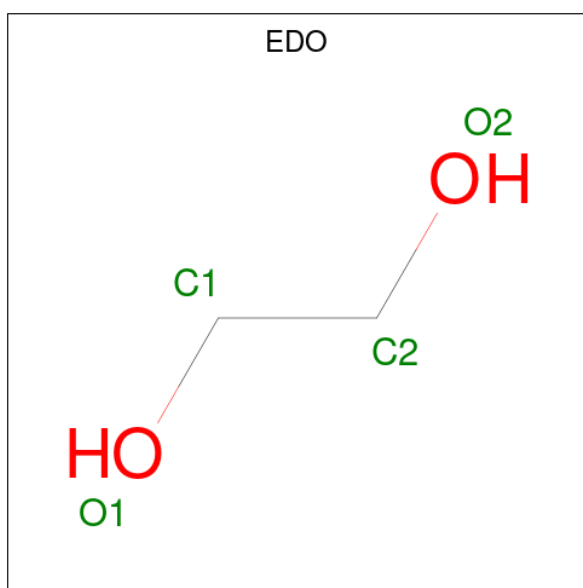
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			18	10	8			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	H	2	Total	C	O	0	0	0
			18	10	8			
2	I	2	Total	C	O	0	0	0
			18	10	8			
2	J	2	Total	C	O	0	0	0
			18	10	8			
2	K	2	Total	C	O	0	0	0
			18	10	8			
2	L	2	Total	C	O	0	0	0
			18	10	8			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

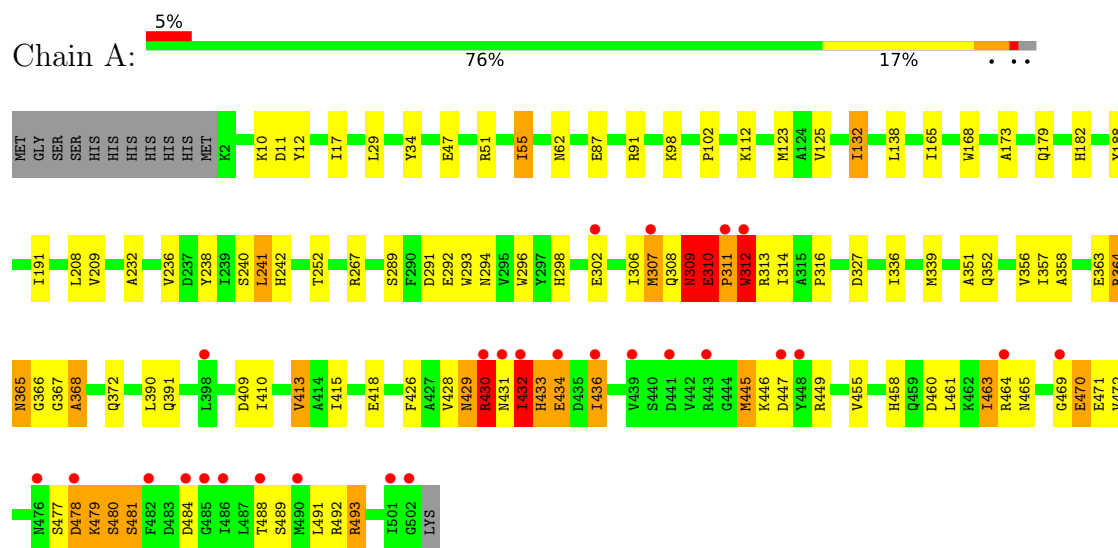
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	35	Total	O	0	0
			35	35		
4	B	37	Total	O	0	0
			37	37		
4	C	36	Total	O	0	0
			36	36		
4	D	31	Total	O	0	0
			31	31		
4	E	40	Total	O	0	0
			40	40		
4	F	32	Total	O	0	0
			32	32		

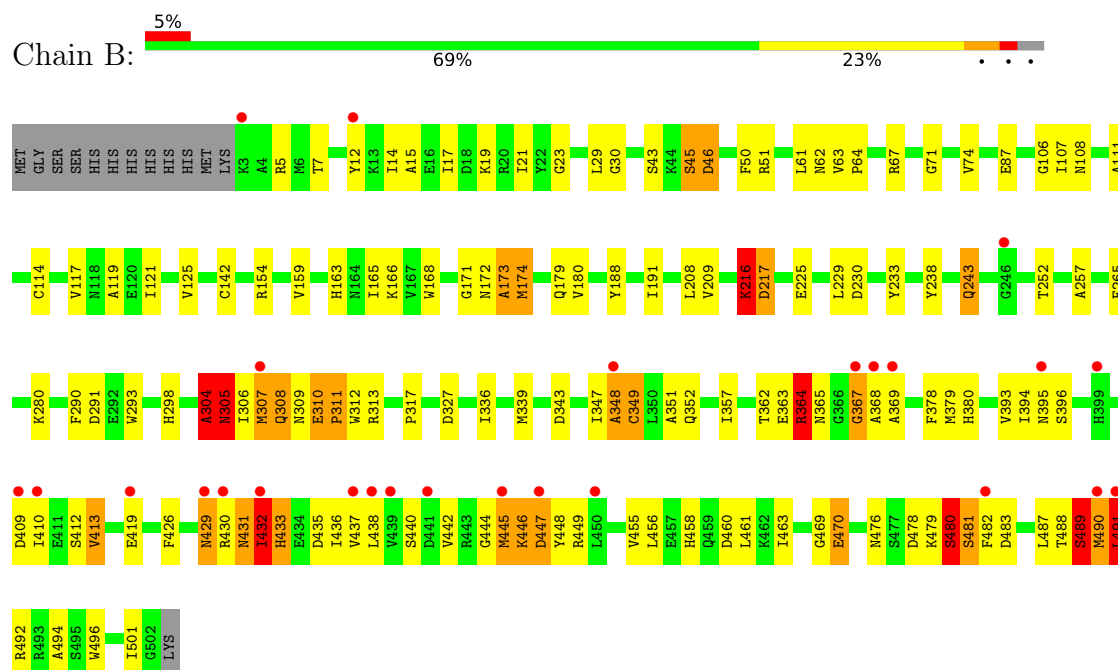
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: ALPHA-L-ARABINOFURANOSIDASE



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE



Chain C:

7% 70% 21% 5%

Chain C: MET GLY SER SER HIS HIS HIS HIS HIS MET LYS LYS A4 R5 M6 T7 K10 D11 Y12 K13 I14 A15 E16 I17 K19 G23 E27 H28 L29 G30 R31 S43 K44 E47 R51 E56 V63 P64 P69 G70 G71 N72 G82 V83 G84 E87 K98 G106 K112 W113 C114 V117 E120 M126 P145 K149 Y150 H157 K160 F161 P162 W168 N172 A173 Q179 V180 D203 I206 E207 L208 S214 M218 P219 L229 Y233 Y238 I239 L241 H242 N250 A253 L262 Y287 L288 S289 F290 D291 E292 W293 N294 Y297 H298 R301 E302 K307 Q308 N309 E310 P311 D327 L333 K334 K339 K340 D343 A348 C349 I354 N355 V356 I357 E363 R364 N365 G366 G367 A368 H380 G385 R386 L390 S391 P392 N395 L398 H399 V407 I410 I415 Y416 N417 E418 E419 K420 E421 F426 R430 N431 I432 H433 E434 D435 I436 V437 L438 V439 S440 R443 G444 M445 K446 Y447 Y448 L451 E452 E457 H458 Q459 D460 L461 K462 L463 N468 N476 S477 D478 K479 S480 S481 F482 D483 D484 G485 L486 L487 W488

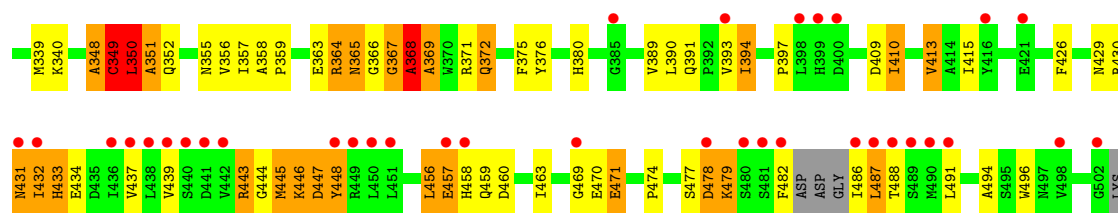
Chain D:

4% 70% 21% 5%

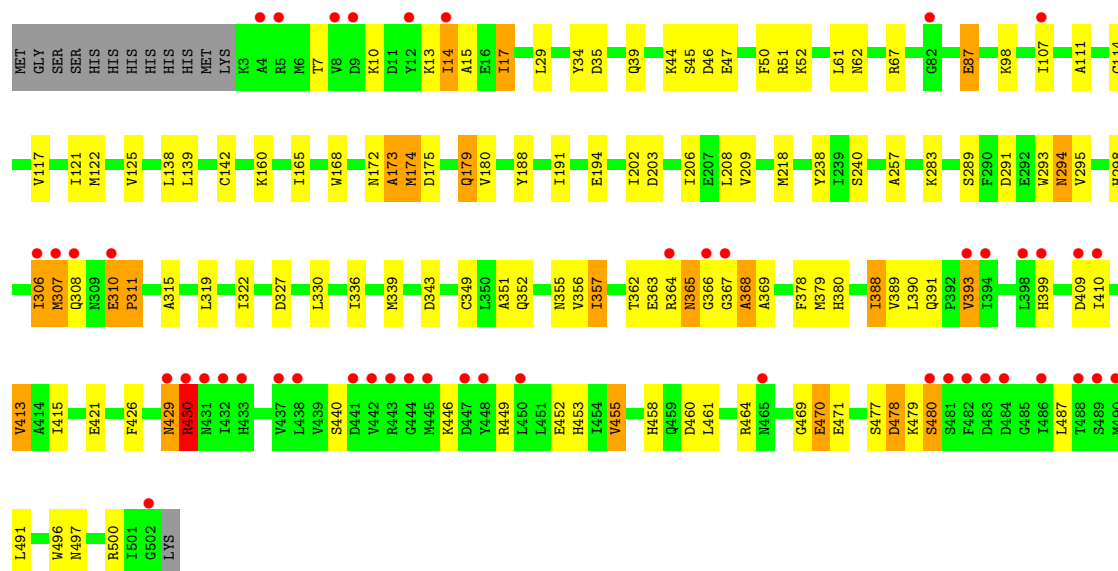
Amino Acid	Frequency (%)
MET	4%
GLY	70%
SER	21%
HIS	5%
LYS	5%

Chain E:

8% 72% 19% 6% 5%



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE



• Molecule 2: alpha-L-arabinofuranose-(1-3)-alpha-D-xylopyranose



• Molecule 2: alpha-L-arabinofuranose-(1-3)-alpha-D-xylopyranose



• Molecule 2: alpha-L-arabinofuranose-(1-3)-alpha-D-xylopyranose



• Molecule 2: alpha-L-arabinofuranose-(1-3)-alpha-D-xylopyranose

Chain J:  100%

YSIS
AHR2

- Molecule 2: α -L-arabinofuranose-(1-3)- α -D-xylopyranose

Chain K:  100%

YSIS
AHR2

- Molecule 2: α -L-arabinofuranose-(1-3)- α -D-xylopyranose

Chain L:  100%

YSIS
AHR2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.45Å 173.45Å 272.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.86 – 2.90 145.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (145.86-2.90) 98.8 (145.86-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.255 0.249 , 0.288	Depositor DCC
R_{free} test set	7173 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24200	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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: XYS, AHR, EDO

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	0.49	0/4110	0.86	6/5566 (0.1%)
1	B	0.49	0/4105	0.86	5/5558 (0.1%)
1	C	0.49	0/4082	0.88	7/5531 (0.1%)
1	D	0.50	0/4021	0.87	9/5447 (0.2%)
1	E	0.50	0/4019	0.88	7/5447 (0.1%)
1	F	0.47	0/4058	0.83	4/5496 (0.1%)
All	All	0.49	0/24395	0.86	38/33045 (0.1%)

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	5
1	B	0	6
1	C	0	2
1	D	0	4
1	E	0	3
All	All	0	20

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	GLN	N-CA-C	-6.73	104.04	113.20
1	E	460	ASP	N-CA-C	-6.63	105.48	113.97
1	D	363	GLU	N-CA-C	6.55	118.11	110.97
1	A	429	ASN	CA-C-N	6.31	133.05	121.70
1	A	429	ASN	C-N-CA	6.31	133.05	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	ILE	N-CA-C	-6.12	106.78	111.62
1	B	216	LYS	N-CA-C	6.12	118.58	108.49
1	D	432	ILE	N-CA-C	6.06	121.95	109.34
1	A	310	GLU	C-N-CD	-5.98	100.47	125.00
1	A	132	ILE	N-CA-C	5.96	116.61	110.36
1	C	448	TYR	N-CA-C	5.93	119.38	109.95
1	B	45	SER	CA-C-N	5.91	132.33	121.70
1	B	45	SER	C-N-CA	5.91	132.33	121.70
1	E	39	GLN	CA-C-N	5.81	127.11	119.84
1	E	39	GLN	C-N-CA	5.81	127.11	119.84
1	C	457	GLU	N-CA-C	5.76	116.98	108.86
1	C	348	ALA	CA-C-N	5.58	131.74	121.70
1	C	348	ALA	C-N-CA	5.58	131.74	121.70
1	E	350	LEU	CA-C-N	5.48	131.57	121.70
1	E	350	LEU	C-N-CA	5.48	131.57	121.70
1	D	429	ASN	CA-C-N	5.38	131.39	121.70
1	D	429	ASN	C-N-CA	5.38	131.39	121.70
1	A	312	TRP	N-CA-C	5.36	118.78	111.39
1	F	39	GLN	CA-C-N	5.35	124.80	119.24
1	F	39	GLN	C-N-CA	5.35	124.80	119.24
1	A	429	ASN	N-CA-C	-5.33	99.45	110.80
1	F	429	ASN	CA-C-N	5.31	131.26	121.70
1	F	429	ASN	C-N-CA	5.31	131.26	121.70
1	D	350	LEU	CA-C-N	5.29	131.22	121.70
1	D	350	LEU	C-N-CA	5.29	131.22	121.70
1	D	309	ASN	CA-C-N	5.24	131.14	121.70
1	D	309	ASN	C-N-CA	5.24	131.14	121.70
1	D	428	VAL	N-CA-C	5.17	115.72	108.17
1	C	15	ALA	N-CA-C	5.12	115.09	107.88
1	E	368	ALA	CA-C-N	5.07	130.82	121.70
1	E	368	ALA	C-N-CA	5.07	130.82	121.70
1	C	460	ASP	CA-C-N	5.06	130.81	121.70
1	C	460	ASP	C-N-CA	5.06	130.81	121.70

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	309	ASN	Peptide
1	A	310	GLU	Peptide
1	A	312	TRP	Peptide
1	A	432	ILE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	433	HIS	Peptide
1	B	216	LYS	Peptide
1	B	304	ALA	Peptide
1	B	347	ILE	Peptide
1	B	348	ALA	Peptide
1	B	45	SER	Peptide
1	B	491	LEU	Peptide
1	C	419	GLU	Peptide
1	C	458	HIS	Peptide
1	D	312	TRP	Peptide
1	D	431	ASN	Peptide
1	D	471	GLU	Peptide
1	D	485	GLY	Peptide
1	E	308	GLN	Peptide
1	E	348	ALA	Peptide
1	E	459	GLN	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	4017	0	3920	121	0
1	B	4013	0	3908	162	0
1	C	3989	0	3870	113	0
1	D	3933	0	3767	117	0
1	E	3927	0	3786	113	0
1	F	3966	0	3845	96	0
2	G	18	0	7	0	0
2	H	18	0	7	0	0
2	I	18	0	7	0	0
2	J	18	0	7	0	0
2	K	18	0	7	0	0
2	L	18	0	7	0	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
3	C	8	0	12	0	0
3	D	4	0	6	0	0
3	E	8	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	4	0	6	0	0
4	A	35	0	0	1	0
4	B	37	0	0	1	0
4	C	36	0	0	0	0
4	D	31	0	0	0	0
4	E	40	0	0	1	0
4	F	32	0	0	1	0
All	All	24200	0	23192	719	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 15.

All (719) 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:B:431:ASN:CB	1:B:432:ILE:HG22	1.11	1.56
1:D:431:ASN:HB3	1:D:432:ILE:C	1.38	1.45
1:B:431:ASN:CB	1:B:432:ILE:CG2	2.05	1.32
1:A:310:GLU:HB3	1:A:311:PRO:CB	1.73	1.18
1:E:478:ASP:HA	1:E:479:LYS:HB2	1.22	1.18
1:B:431:ASN:HA	1:B:432:ILE:HB	1.18	1.17
1:F:469:GLY:HA2	1:F:470:GLU:HB2	1.17	1.16
1:A:310:GLU:HB3	1:A:311:PRO:HB3	1.20	1.12
1:C:410:ILE:HD11	1:C:436:ILE:HG13	1.32	1.11
1:C:478:ASP:HB3	1:C:479:LYS:HA	1.23	1.11
1:B:480:SER:HA	1:B:481:SER:HB2	1.33	1.10
1:A:469:GLY:HA2	1:A:470:GLU:HB2	1.20	1.10
1:D:480:SER:HB3	1:D:481:SER:HA	1.24	1.09
1:B:429:ASN:CG	1:B:491:LEU:HD12	1.76	1.09
1:A:433:HIS:H	1:A:434:GLU:HB3	1.15	1.09
1:E:367:GLY:HA2	1:E:368:ALA:CB	1.81	1.08
1:F:367:GLY:HA3	1:F:368:ALA:HB2	1.35	1.08
1:B:307:MET:HG3	1:B:308:GLN:H	1.11	1.07
1:E:447:ASP:HB2	1:E:448:TYR:HA	1.08	1.07
1:E:447:ASP:CB	1:E:448:TYR:HA	1.85	1.07
1:E:348:ALA:HA	1:E:349:CYS:HB2	1.32	1.06
1:A:367:GLY:HA3	1:A:368:ALA:CB	1.83	1.06
1:B:431:ASN:HB2	1:B:432:ILE:CG2	1.74	1.06
1:D:469:GLY:HA2	1:D:470:GLU:HB3	1.36	1.06
1:A:480:SER:HA	1:A:481:SER:HB2	1.08	1.05
1:A:310:GLU:H	1:A:311:PRO:HD3	1.21	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:ASN:HA	1:F:430:ARG:O	1.57	1.03
1:C:420:LYS:N	1:C:421:GLU:HA	1.70	1.03
1:E:445:MET:HA	1:E:446:LYS:HB3	1.36	1.03
1:D:431:ASN:HB3	1:D:432:ILE:O	1.58	1.02
1:A:433:HIS:H	1:A:434:GLU:CB	1.74	1.01
1:B:431:ASN:HB3	1:B:432:ILE:CG2	1.76	1.01
1:D:431:ASN:CB	1:D:432:ILE:C	2.34	1.01
1:D:350:LEU:HA	1:D:351:ALA:HB3	1.42	1.00
1:B:431:ASN:HB3	1:B:432:ILE:HG22	1.00	0.99
1:B:304:ALA:HB3	1:B:305:ASN:HB2	1.41	0.99
1:D:430:ARG:HA	1:D:431:ASN:O	1.61	0.99
1:D:311:PRO:HG2	1:D:312:TRP:NE1	1.77	0.99
1:A:410:ILE:HD11	1:A:436:ILE:HD11	1.45	0.99
1:B:431:ASN:HA	1:B:432:ILE:CB	1.91	0.99
1:F:367:GLY:CA	1:F:368:ALA:HB2	1.93	0.99
1:A:367:GLY:HA3	1:A:368:ALA:HB2	0.99	0.99
1:A:367:GLY:CA	1:A:368:ALA:HB2	1.92	0.98
1:A:310:GLU:N	1:A:311:PRO:HD3	1.74	0.98
1:F:469:GLY:CA	1:F:470:GLU:HB2	1.93	0.98
1:B:431:ASN:HB2	1:B:432:ILE:HG22	0.97	0.96
1:A:364:ARG:C	1:A:366:GLY:HA3	1.91	0.96
1:C:348:ALA:HA	1:C:349:CYS:HB2	1.47	0.96
1:B:432:ILE:HG23	1:B:432:ILE:O	1.64	0.95
1:C:431:ASN:HA	1:C:432:ILE:O	1.65	0.95
1:C:363:GLU:HB2	1:C:368:ALA:HB3	1.47	0.95
1:B:348:ALA:CA	1:B:349:CYS:HB2	1.98	0.94
1:E:367:GLY:HA2	1:E:368:ALA:HB2	1.47	0.94
1:A:469:GLY:CA	1:A:470:GLU:HB2	1.97	0.94
1:D:480:SER:CB	1:D:481:SER:HA	1.97	0.94
1:E:350:LEU:HA	1:E:351:ALA:HB3	1.51	0.93
1:E:368:ALA:HA	1:E:369:ALA:HB2	1.50	0.93
1:D:471:GLU:O	1:D:472:VAL:HG23	1.69	0.91
1:A:363:GLU:H	1:A:368:ALA:HB1	1.36	0.90
1:C:363:GLU:HB2	1:C:368:ALA:CB	2.01	0.90
1:B:431:ASN:CA	1:B:432:ILE:HB	1.99	0.90
1:D:351:ALA:H	1:D:352:GLN:HA	1.37	0.90
1:E:447:ASP:HB2	1:E:448:TYR:CA	2.00	0.89
1:B:348:ALA:CB	1:B:349:CYS:HB2	2.03	0.89
1:B:429:ASN:CG	1:B:491:LEU:CD1	2.45	0.89
1:A:477:SER:HB3	1:A:478:ASP:HA	1.53	0.88
1:E:351:ALA:H	1:E:352:GLN:HA	1.38	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ASN:CA	1:B:432:ILE:CB	2.51	0.88
1:A:310:GLU:CB	1:A:311:PRO:HB3	2.03	0.88
1:A:480:SER:HA	1:A:481:SER:CB	1.96	0.88
1:B:469:GLY:HA2	1:B:470:GLU:CB	2.04	0.87
1:D:312:TRP:N	1:D:313:ARG:HB2	1.89	0.87
1:A:477:SER:HB3	1:A:478:ASP:CA	2.05	0.87
1:C:419:GLU:HB3	1:C:420:LYS:HB3	1.54	0.87
1:D:311:PRO:HG2	1:D:312:TRP:CD1	2.09	0.87
1:B:307:MET:CG	1:B:308:GLN:H	1.87	0.87
1:E:478:ASP:CA	1:E:479:LYS:HB2	2.04	0.86
1:A:309:ASN:CB	1:A:310:GLU:HA	2.05	0.86
1:B:491:LEU:HB3	1:B:492:ARG:O	1.73	0.86
1:B:348:ALA:HB1	1:B:349:CYS:HB2	1.58	0.85
1:E:291:ASP:HA	1:E:349:CYS:HB3	1.58	0.85
1:E:310:GLU:H	1:E:311:PRO:HA	1.41	0.85
1:E:457:GLU:HB3	1:E:458:HIS:HB2	1.57	0.85
1:F:469:GLY:HA2	1:F:470:GLU:CB	2.04	0.85
1:C:460:ASP:HA	1:C:461:LEU:CB	2.05	0.85
1:D:469:GLY:HA2	1:D:470:GLU:CB	2.07	0.85
1:E:367:GLY:HA2	1:E:368:ALA:HB3	1.58	0.85
1:B:216:LYS:N	1:B:217:ASP:HB2	1.92	0.83
1:B:304:ALA:CB	1:B:305:ASN:HB2	2.08	0.83
1:E:457:GLU:HB3	1:E:458:HIS:CA	2.08	0.83
1:B:348:ALA:HA	1:B:349:CYS:HB2	1.61	0.83
1:B:429:ASN:OD1	1:B:491:LEU:HD12	1.78	0.83
1:A:469:GLY:HA2	1:A:470:GLU:CB	2.07	0.83
1:E:350:LEU:HA	1:E:351:ALA:CB	2.09	0.83
1:E:308:GLN:N	1:E:309:ASN:O	2.11	0.83
1:D:350:LEU:HA	1:D:351:ALA:CB	2.08	0.83
1:C:291:ASP:HA	1:C:349:CYS:HB3	1.61	0.82
1:A:309:ASN:HB2	1:A:310:GLU:HA	1.60	0.82
1:A:465:ASN:HD21	1:A:472:VAL:H	1.28	0.81
1:A:433:HIS:N	1:A:434:GLU:HB3	1.96	0.81
1:E:348:ALA:CA	1:E:349:CYS:HB2	2.11	0.81
1:C:410:ILE:HD11	1:C:436:ILE:CG1	2.10	0.81
1:B:431:ASN:HB2	1:B:432:ILE:C	2.06	0.81
1:A:312:TRP:N	1:A:313:ARG:HB2	1.94	0.81
1:E:308:GLN:CB	1:E:309:ASN:HB2	2.10	0.81
1:B:367:GLY:N	1:B:368:ALA:HB2	1.96	0.80
1:C:478:ASP:CB	1:C:479:LYS:HA	2.04	0.80
1:C:420:LYS:H	1:C:421:GLU:HA	1.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ASN:CA	1:B:432:ILE:HG22	2.11	0.79
1:C:410:ILE:CD1	1:C:436:ILE:HG13	2.12	0.79
1:A:363:GLU:H	1:A:368:ALA:CB	1.95	0.79
1:E:457:GLU:HB3	1:E:458:HIS:CB	2.11	0.79
1:B:482:PHE:HB2	1:B:487:LEU:HD12	1.63	0.79
1:C:432:ILE:HG22	1:C:494:ALA:HB2	1.65	0.79
1:D:366:GLY:HA3	1:D:367:GLY:O	1.82	0.79
1:B:348:ALA:HB1	1:B:349:CYS:CB	2.13	0.78
1:E:470:GLU:CB	1:E:471:GLU:HB2	2.14	0.78
1:E:363:GLU:O	1:E:364:ARG:HB2	1.84	0.78
1:B:469:GLY:HA2	1:B:470:GLU:HB3	1.65	0.78
1:B:409:ASP:O	1:B:430:ARG:HB3	1.82	0.78
1:F:188:TYR:HA	1:F:191:ILE:HG22	1.64	0.78
1:C:418:GLU:H	1:C:419:GLU:C	1.91	0.77
1:B:367:GLY:CA	1:B:368:ALA:HB2	2.15	0.77
1:D:480:SER:HB3	1:D:481:SER:CA	2.11	0.77
1:B:432:ILE:CG2	1:B:432:ILE:O	2.31	0.76
1:D:429:ASN:HA	1:D:430:ARG:O	1.85	0.76
1:F:478:ASP:HA	1:F:479:LYS:HG2	1.67	0.76
1:F:310:GLU:CB	1:F:311:PRO:HA	2.16	0.76
1:C:291:ASP:HA	1:C:349:CYS:CB	2.16	0.76
1:E:366:GLY:HA2	1:E:367:GLY:O	1.85	0.76
1:D:472:VAL:O	1:D:473:TYR:HB3	1.86	0.76
1:F:380:HIS:HD2	1:F:496:TRP:HE1	1.32	0.75
1:E:367:GLY:CA	1:E:368:ALA:CB	2.64	0.75
1:B:216:LYS:H	1:B:217:ASP:HB2	1.51	0.74
1:C:431:ASN:HA	1:C:432:ILE:C	2.13	0.74
1:E:445:MET:HA	1:E:446:LYS:CB	2.17	0.74
1:A:310:GLU:HB3	1:A:311:PRO:CG	2.17	0.74
1:B:291:ASP:HA	1:B:349:CYS:CB	2.18	0.74
1:B:458:HIS:HD2	1:B:460:ASP:H	1.35	0.73
1:C:432:ILE:O	1:C:432:ILE:HG13	1.86	0.73
1:D:431:ASN:HB3	1:D:432:ILE:CA	2.18	0.73
1:B:431:ASN:CA	1:B:432:ILE:CG2	2.66	0.73
1:C:478:ASP:HB3	1:C:479:LYS:CA	2.11	0.73
1:C:420:LYS:N	1:C:421:GLU:CA	2.50	0.73
1:A:480:SER:CA	1:A:481:SER:HB2	2.02	0.73
1:F:367:GLY:CA	1:F:368:ALA:CB	2.65	0.73
1:B:310:GLU:HG2	1:B:313:ARG:HD2	1.70	0.72
1:A:410:ILE:HD13	1:A:429:ASN:HB2	1.71	0.72
1:B:491:LEU:CB	1:B:492:ARG:CA	2.66	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:ASN:H	1:E:431:ASN:HD22	1.38	0.72
1:A:433:HIS:N	1:A:434:GLU:CB	2.51	0.72
1:E:351:ALA:N	1:E:352:GLN:HA	2.00	0.72
1:C:460:ASP:HA	1:C:461:LEU:HB2	1.70	0.72
1:D:309:ASN:N	1:D:310:GLU:HB2	2.05	0.72
1:B:478:ASP:HA	1:B:479:LYS:HB2	1.71	0.71
1:B:307:MET:HG3	1:B:308:GLN:N	1.96	0.71
1:B:310:GLU:HB3	1:B:311:PRO:HA	1.72	0.70
1:C:418:GLU:N	1:C:419:GLU:C	2.49	0.70
1:E:291:ASP:HA	1:E:349:CYS:CB	2.20	0.70
1:B:46:ASP:HB3	1:B:50:PHE:O	1.90	0.70
1:E:340:LYS:HG3	1:E:413:VAL:HG11	1.73	0.70
1:B:431:ASN:H	1:B:431:ASN:ND2	1.89	0.70
1:B:446:LYS:H	1:B:446:LYS:HD3	1.57	0.70
1:E:447:ASP:CB	1:E:448:TYR:CA	2.63	0.70
1:A:312:TRP:CA	1:A:313:ARG:HB2	2.22	0.69
1:D:312:TRP:H	1:D:313:ARG:HB2	1.54	0.69
1:E:363:GLU:H	1:E:368:ALA:H	1.38	0.69
1:A:309:ASN:HB2	1:A:310:GLU:CA	2.22	0.69
1:F:51:ARG:HH22	1:F:368:ALA:HB3	1.56	0.69
1:A:460:ASP:HB3	1:A:463:ILE:HB	1.74	0.69
1:B:304:ALA:CA	1:B:305:ASN:HB2	2.22	0.69
1:B:291:ASP:HA	1:B:349:CYS:HB3	1.74	0.69
1:C:363:GLU:O	1:C:364:ARG:HB3	1.93	0.69
1:C:435:ASP:OD1	1:C:493:ARG:HG3	1.93	0.69
1:B:436:ILE:O	1:B:491:LEU:HG	1.93	0.68
1:C:15:ALA:HB2	1:C:343:ASP:HB3	1.74	0.68
1:D:307:MET:C	1:D:308:GLN:HG3	2.18	0.68
1:F:364:ARG:C	1:F:366:GLY:HA3	2.19	0.68
1:A:460:ASP:O	1:A:461:LEU:HB2	1.94	0.68
1:D:351:ALA:N	1:D:352:GLN:HA	1.99	0.68
1:C:333:LEU:HD22	1:C:430:ARG:HH11	1.59	0.67
1:E:457:GLU:HB3	1:E:458:HIS:HA	1.75	0.67
1:B:216:LYS:CE	1:B:216:LYS:O	2.41	0.67
1:F:339:MET:HE1	1:F:426:PHE:CD2	2.30	0.67
1:B:23:GLY:HA2	1:B:63:VAL:HG13	1.76	0.67
1:B:310:GLU:CB	1:B:311:PRO:HA	2.24	0.67
1:B:432:ILE:O	1:B:433:HIS:ND1	2.29	0.66
1:A:298:HIS:HE1	1:A:327:ASP:OD2	1.77	0.66
1:B:491:LEU:HB2	1:B:492:ARG:HA	1.78	0.66
1:D:431:ASN:CB	1:D:432:ILE:O	2.39	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:GLN:CB	1:E:309:ASN:CB	2.73	0.66
1:A:312:TRP:HA	1:A:313:ARG:HB2	1.77	0.66
1:A:477:SER:HB3	1:A:478:ASP:CB	2.26	0.66
1:C:460:ASP:HA	1:C:461:LEU:HB3	1.78	0.66
1:D:15:ALA:HB2	1:D:343:ASP:HB3	1.77	0.66
1:B:480:SER:HA	1:B:481:SER:CB	2.14	0.66
1:C:348:ALA:CA	1:C:349:CYS:HB2	2.24	0.66
1:D:29:LEU:HD13	1:D:356:VAL:HG11	1.78	0.66
1:D:478:ASP:HA	1:D:479:LYS:CB	2.26	0.66
1:C:172:ASN:HD22	1:C:179:GLN:HE22	1.40	0.66
1:F:363:GLU:OE1	1:F:363:GLU:HA	1.96	0.65
1:F:478:ASP:HA	1:F:479:LYS:CG	2.26	0.65
1:A:310:GLU:HB3	1:A:311:PRO:CD	2.25	0.65
1:A:364:ARG:O	1:A:366:GLY:HA3	1.96	0.65
1:F:310:GLU:HB3	1:F:311:PRO:HA	1.78	0.65
1:F:458:HIS:HD2	1:F:460:ASP:H	1.41	0.65
1:A:410:ILE:CD1	1:A:436:ILE:HD11	2.24	0.64
1:A:363:GLU:O	1:A:364:ARG:HG2	1.97	0.64
1:B:230:ASP:O	1:B:280:LYS:NZ	2.28	0.64
1:B:491:LEU:CB	1:B:492:ARG:HA	2.28	0.64
1:C:31:ARG:NH1	1:C:364:ARG:HB2	2.13	0.64
1:A:365:ASN:N	1:A:366:GLY:HA3	2.10	0.64
1:B:480:SER:CA	1:B:481:SER:HB2	2.20	0.63
1:D:482:PHE:HA	1:D:486:ILE:O	1.98	0.63
1:F:380:HIS:CD2	1:F:496:TRP:HE1	2.14	0.63
1:B:310:GLU:HB3	1:B:311:PRO:CA	2.29	0.63
1:B:431:ASN:CB	1:B:432:ILE:CB	2.74	0.63
1:E:445:MET:CA	1:E:446:LYS:HB3	2.19	0.63
1:F:293:TRP:O	1:F:294:ASN:HB2	1.95	0.63
1:B:432:ILE:O	1:B:433:HIS:CG	2.51	0.63
1:C:477:SER:O	1:C:478:ASP:HB2	1.97	0.63
1:E:311:PRO:O	1:E:313:ARG:HB2	1.98	0.63
1:B:479:LYS:O	1:B:480:SER:HB3	1.98	0.63
1:D:209:VAL:HG22	1:D:238:TYR:HB2	1.81	0.63
1:A:479:LYS:N	1:A:479:LYS:HD2	2.14	0.63
1:B:363:GLU:H	1:B:368:ALA:HA	1.64	0.63
1:D:460:ASP:O	1:D:462:LYS:N	2.30	0.62
1:D:311:PRO:CG	1:D:312:TRP:CD1	2.81	0.62
1:D:478:ASP:HA	1:D:479:LYS:HB3	1.81	0.62
1:B:469:GLY:HA2	1:B:470:GLU:HB2	1.80	0.62
1:C:485:GLY:HA2	1:C:486:ILE:C	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:458:HIS:HE1	1:F:471:GLU:HG2	1.65	0.62
1:B:67:ARG:HD2	1:B:291:ASP:HB2	1.82	0.62
1:B:216:LYS:O	1:B:216:LYS:HE3	1.99	0.62
1:B:491:LEU:HB3	1:B:492:ARG:C	2.25	0.62
1:E:293:TRP:O	1:E:351:ALA:HB3	2.00	0.62
1:A:310:GLU:HB3	1:A:311:PRO:CA	2.30	0.62
1:C:485:GLY:HA2	1:C:486:ILE:O	1.99	0.62
1:A:311:PRO:HA	1:A:313:ARG:HG3	1.81	0.62
1:C:419:GLU:CB	1:C:420:LYS:HB3	2.29	0.61
1:D:469:GLY:CA	1:D:470:GLU:HB3	2.21	0.61
1:B:487:LEU:HD13	1:B:501:ILE:HD11	1.83	0.61
1:B:490:MET:HE3	1:B:490:MET:HA	1.82	0.61
1:E:367:GLY:CA	1:E:368:ALA:HB2	2.25	0.61
1:C:145:PRO:HA	1:C:162:PRO:HG3	1.81	0.61
1:D:478:ASP:CB	1:D:479:LYS:HB3	2.31	0.61
1:E:340:LYS:HG3	1:E:413:VAL:CG1	2.30	0.61
1:F:367:GLY:N	1:F:368:ALA:HB2	2.15	0.61
1:C:363:GLU:CB	1:C:368:ALA:HB3	2.27	0.61
1:F:46:ASP:HB3	1:F:52:LYS:HE3	1.82	0.61
1:E:308:GLN:H	1:E:309:ASN:C	2.09	0.61
1:B:362:THR:HA	1:B:369:ALA:H	1.66	0.60
1:D:442:VAL:HG12	1:D:485:GLY:O	2.00	0.60
1:C:457:GLU:O	1:C:458:HIS:HB2	2.00	0.60
1:F:298:HIS:HE1	1:F:327:ASP:OD2	1.85	0.60
1:F:310:GLU:HB2	1:F:311:PRO:HA	1.84	0.60
1:F:364:ARG:O	1:F:366:GLY:HA3	2.02	0.60
1:A:339:MET:HE1	1:A:426:PHE:CD2	2.37	0.60
1:B:491:LEU:HB3	1:B:492:ARG:CA	2.30	0.60
1:F:453:HIS:HD2	1:F:480:SER:HB2	1.66	0.60
1:F:478:ASP:HA	1:F:479:LYS:CB	2.31	0.60
1:D:477:SER:O	1:D:478:ASP:HB2	2.01	0.60
1:C:420:LYS:H	1:C:421:GLU:CA	2.15	0.59
1:E:477:SER:O	1:E:478:ASP:HB2	2.01	0.59
1:E:312:TRP:HA	1:E:313:ARG:HB2	1.83	0.59
1:C:452:GLU:OE2	1:C:476:ASN:ND2	2.35	0.59
1:D:298:HIS:HE1	1:D:327:ASP:OD2	1.84	0.59
1:A:307:MET:HA	1:A:308:GLN:C	2.27	0.59
1:D:172:ASN:O	1:D:173:ALA:C	2.46	0.59
1:A:363:GLU:N	1:A:368:ALA:HB1	2.13	0.59
1:B:317:PRO:HG3	1:B:364:ARG:HH21	1.67	0.58
1:D:309:ASN:CA	1:D:310:GLU:HB2	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TYR:HA	1:B:191:ILE:HG22	1.84	0.58
1:F:17:ILE:HD12	1:F:389:VAL:HG23	1.85	0.58
1:C:458:HIS:HA	1:C:459:GLN:CB	2.33	0.58
1:E:380:HIS:CD2	1:E:496:TRP:HE1	2.20	0.58
1:A:310:GLU:CB	1:A:311:PRO:CD	2.81	0.58
1:B:367:GLY:HA3	1:B:368:ALA:HB2	1.85	0.58
1:F:7:THR:HG23	1:F:393:VAL:HG23	1.85	0.58
1:F:429:ASN:CA	1:F:430:ARG:O	2.43	0.58
1:C:432:ILE:CG2	1:C:494:ALA:HB2	2.32	0.58
1:C:385:GLY:HA2	1:C:415:ILE:HG12	1.86	0.57
1:D:363:GLU:O	1:D:364:ARG:HB2	2.04	0.57
1:F:310:GLU:HB3	1:F:311:PRO:CA	2.34	0.57
1:A:458:HIS:HD2	1:A:460:ASP:H	1.52	0.57
1:A:311:PRO:C	1:A:312:TRP:CD1	2.82	0.57
1:B:336:ILE:HG23	1:B:413:VAL:HG22	1.85	0.57
1:E:380:HIS:HD2	1:E:496:TRP:HE1	1.51	0.57
1:D:482:PHE:CD1	1:D:486:ILE:O	2.57	0.57
1:A:241:LEU:C	1:A:242:HIS:HD2	2.13	0.57
1:A:312:TRP:H	1:A:313:ARG:HB2	1.68	0.57
1:D:307:MET:N	1:D:309:ASN:HB2	2.19	0.57
1:B:431:ASN:HA	1:B:432:ILE:CG2	2.30	0.57
1:B:51:ARG:HH22	1:B:368:ALA:CB	2.17	0.57
1:B:225:GLU:N	1:B:225:GLU:OE1	2.38	0.57
1:A:410:ILE:HD12	1:A:491:LEU:HD12	1.87	0.56
1:A:431:ASN:CA	1:A:432:ILE:O	2.53	0.56
1:B:348:ALA:HB1	1:B:349:CYS:CA	2.35	0.56
1:D:114:CYS:HA	1:D:117:VAL:HG22	1.86	0.56
1:B:429:ASN:ND2	1:B:491:LEU:CD1	2.68	0.56
1:A:209:VAL:HG22	1:A:238:TYR:HB2	1.88	0.56
1:F:257:ALA:HA	1:F:430:ARG:HH21	1.71	0.56
1:F:362:THR:HB	1:F:368:ALA:HB1	1.88	0.56
1:D:478:ASP:CA	1:D:479:LYS:HB3	2.36	0.56
1:E:240:SER:HA	1:E:289:SER:O	2.05	0.56
1:D:453:HIS:HE1	1:D:497:ASN:HD22	1.53	0.55
1:A:309:ASN:CB	1:A:310:GLU:CA	2.80	0.55
1:E:482:PHE:HD1	1:E:487:LEU:HB2	1.69	0.55
1:A:182:HIS:HB3	1:F:194:GLU:OE1	2.06	0.55
1:E:365:ASN:N	1:E:366:GLY:HA3	2.20	0.55
1:F:310:GLU:CB	1:F:311:PRO:CA	2.83	0.55
1:F:14:ILE:HG13	1:F:391:GLN:HG2	1.89	0.55
1:D:430:ARG:HA	1:D:431:ASN:C	2.16	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:ILE:O	1:E:433:HIS:HB2	2.07	0.55
1:F:15:ALA:HB2	1:F:343:ASP:HB3	1.88	0.55
1:B:15:ALA:HB2	1:B:343:ASP:HB3	1.88	0.55
1:B:307:MET:C	1:B:309:ASN:H	2.15	0.55
1:B:448:TYR:HD2	1:B:501:ILE:HG22	1.71	0.55
1:F:172:ASN:O	1:F:173:ALA:C	2.50	0.55
1:B:437:VAL:HA	1:B:490:MET:H	1.72	0.55
1:F:470:GLU:HG3	4:F:2030:HOH:O	2.06	0.54
1:A:125:VAL:HG12	1:A:138:LEU:HD23	1.88	0.54
1:B:469:GLY:CA	1:B:470:GLU:CB	2.81	0.54
1:C:82:GLY:O	1:C:106:GLY:HA3	2.07	0.54
1:B:290:PHE:O	1:B:348:ALA:CB	2.55	0.54
1:B:431:ASN:H	1:B:431:ASN:HD22	1.55	0.54
1:E:312:TRP:CD1	1:E:312:TRP:H	2.25	0.54
1:F:175:ASP:OD2	1:F:218:MET:HG3	2.07	0.54
1:B:21:ILE:HA	1:B:348:ALA:H	1.73	0.54
1:B:348:ALA:CA	1:B:349:CYS:CB	2.77	0.54
1:C:12:TYR:CE1	1:C:391:GLN:HG3	2.43	0.54
1:E:429:ASN:O	1:E:494:ALA:HA	2.08	0.54
1:E:67:ARG:NH2	1:E:172:ASN:OD1	2.41	0.54
1:A:311:PRO:HA	1:A:313:ARG:CG	2.38	0.54
1:B:396:SER:HB2	1:B:410:ILE:HG22	1.90	0.53
1:C:339:MET:HE1	1:C:426:PHE:CD1	2.43	0.53
1:F:168:TRP:HB2	1:F:208:LEU:HD23	1.91	0.53
1:C:27:GLU:HG2	1:C:29:LEU:HB2	1.90	0.53
1:D:67:ARG:HD2	1:D:291:ASP:HB2	1.90	0.53
1:F:440:SER:HB2	1:F:487:LEU:HB3	1.90	0.53
1:E:431:ASN:H	1:E:431:ASN:ND2	2.06	0.53
1:E:431:ASN:HD22	1:E:431:ASN:N	2.01	0.53
1:B:12:TYR:CE2	1:C:12:TYR:CE2	2.97	0.53
1:B:438:LEU:N	1:B:489:SER:O	2.42	0.53
1:C:419:GLU:C	1:C:421:GLU:HA	2.33	0.53
1:E:393:VAL:HG13	1:E:394:ILE:H	1.73	0.53
1:E:339:MET:HE1	1:E:426:PHE:CD1	2.43	0.53
1:C:47:GLU:CD	1:C:47:GLU:H	2.15	0.52
1:A:168:TRP:HB2	1:A:208:LEU:HD23	1.90	0.52
1:A:312:TRP:N	1:A:313:ARG:CB	2.71	0.52
1:A:310:GLU:CB	1:A:311:PRO:CB	2.66	0.52
1:D:350:LEU:CA	1:D:351:ALA:CB	2.85	0.52
1:F:61:LEU:HD22	1:F:378:PHE:CD1	2.45	0.52
1:B:456:LEU:HB3	1:B:496:TRP:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:ASP:CA	1:C:461:LEU:CB	2.85	0.52
1:B:380:HIS:CD2	1:B:496:TRP:HE1	2.27	0.52
1:F:336:ILE:HG23	1:F:413:VAL:HG22	1.91	0.52
1:B:172:ASN:O	1:B:173:ALA:C	2.52	0.52
1:B:216:LYS:O	1:B:216:LYS:HE2	2.10	0.52
1:D:478:ASP:CA	1:D:479:LYS:CB	2.88	0.52
1:E:310:GLU:H	1:E:311:PRO:CA	2.16	0.52
1:B:174:MET:HG3	1:B:179:GLN:HE22	1.75	0.52
1:B:469:GLY:CA	1:B:470:GLU:HB3	2.37	0.52
1:C:410:ILE:HD11	1:C:436:ILE:CD1	2.40	0.52
1:D:336:ILE:HG23	1:D:413:VAL:CG2	2.39	0.52
1:D:431:ASN:HB3	1:D:433:HIS:N	2.13	0.52
1:F:209:VAL:HG22	1:F:238:TYR:HB2	1.92	0.52
1:C:458:HIS:HD2	1:C:459:GLN:O	1.93	0.51
1:D:482:PHE:HD1	1:D:486:ILE:O	1.93	0.51
1:F:363:GLU:HB2	1:F:368:ALA:HA	1.92	0.51
1:B:51:ARG:HH22	1:B:368:ALA:HB3	1.75	0.51
1:E:188:TYR:HA	1:E:191:ILE:HG22	1.91	0.51
1:E:443:ARG:HB3	1:E:443:ARG:NH1	2.25	0.51
1:D:311:PRO:HG2	1:D:312:TRP:HE1	1.72	0.51
1:E:478:ASP:HA	1:E:479:LYS:CB	2.14	0.51
1:F:362:THR:HA	1:F:369:ALA:H	1.75	0.51
1:A:12:TYR:OH	1:D:391:GLN:HG2	2.10	0.51
1:B:19:LYS:O	1:B:64:PRO:HG2	2.11	0.51
1:D:480:SER:CB	1:D:481:SER:CA	2.79	0.51
1:F:478:ASP:HB3	1:F:479:LYS:C	2.36	0.51
1:E:312:TRP:HA	1:E:313:ARG:CB	2.40	0.51
1:F:453:HIS:CD2	1:F:480:SER:HB2	2.45	0.51
1:A:293:TRP:O	1:A:294:ASN:HB2	2.10	0.51
1:C:172:ASN:O	1:C:173:ALA:C	2.53	0.51
1:C:460:ASP:CA	1:C:461:LEU:HB2	2.39	0.51
1:F:322:ILE:HG22	1:F:464:ARG:HD2	1.93	0.51
1:A:311:PRO:CA	1:A:313:ARG:HG3	2.41	0.51
1:D:471:GLU:O	1:D:472:VAL:CG2	2.53	0.51
1:E:209:VAL:HG22	1:E:238:TYR:HB2	1.91	0.51
1:A:173:ALA:O	1:A:179:GLN:NE2	2.44	0.50
1:B:429:ASN:O	1:B:494:ALA:HA	2.12	0.50
1:D:478:ASP:CG	1:D:479:LYS:HB3	2.37	0.50
1:F:13:LYS:HG2	1:F:388:ILE:HG21	1.93	0.50
1:F:429:ASN:HA	1:F:430:ARG:C	2.35	0.50
1:A:308:GLN:O	1:A:309:ASN:C	2.53	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:460:ASP:O	1:C:463:ILE:HB	2.11	0.50
1:E:7:THR:H	1:E:393:VAL:HG12	1.77	0.50
1:E:389:VAL:HA	1:E:415:ILE:HG22	1.92	0.50
1:A:313:ARG:HD3	1:A:316:PRO:HB3	1.93	0.50
1:A:465:ASN:ND2	1:A:471:GLU:H	2.09	0.50
1:B:243:GLN:O	1:B:293:TRP:HA	2.12	0.50
1:C:51:ARG:HH12	1:C:367:GLY:H	1.60	0.50
1:E:51:ARG:HH22	1:E:368:ALA:HA	1.76	0.50
1:A:309:ASN:HB3	1:A:310:GLU:HA	1.91	0.50
1:C:5:ARG:HB2	1:C:395:ASN:HB3	1.94	0.50
1:D:293:TRP:O	1:D:351:ALA:HB3	2.11	0.50
1:E:203:ASP:O	1:E:206:ILE:HG12	2.12	0.50
1:F:240:SER:HA	1:F:289:SER:O	2.11	0.50
1:A:240:SER:HA	1:A:289:SER:O	2.11	0.50
1:C:114:CYS:HA	1:C:117:VAL:HG22	1.94	0.50
1:C:380:HIS:HD2	1:C:496:TRP:HE1	1.60	0.50
1:D:262:LEU:HD11	1:D:290:PHE:CZ	2.47	0.50
1:A:409:ASP:O	1:A:430:ARG:O	2.29	0.49
1:F:356:VAL:O	1:F:357:ILE:C	2.55	0.49
1:F:399:HIS:HD2	1:F:409:ASP:OD1	1.95	0.49
1:A:463:ILE:HD13	1:A:464:ARG:H	1.77	0.49
1:F:17:ILE:HD12	1:F:389:VAL:CG2	2.42	0.49
1:B:444:GLY:HA2	1:B:445:MET:CB	2.41	0.49
1:D:409:ASP:O	1:D:430:ARG:O	2.29	0.49
1:A:47:GLU:H	1:A:47:GLU:CD	2.20	0.49
1:E:99:SER:HA	1:E:312:TRP:HB3	1.94	0.49
1:A:306:ILE:HG22	1:A:307:MET:HG3	1.94	0.49
1:B:71:GLY:O	1:B:74:VAL:HG12	2.12	0.49
1:D:188:TYR:HA	1:D:191:ILE:HG22	1.95	0.49
1:D:311:PRO:HA	1:D:313:ARG:HG3	1.94	0.49
1:D:363:GLU:O	1:D:364:ARG:CB	2.60	0.49
1:D:24:SER:OG	1:D:353:LEU:HB2	2.13	0.49
1:B:363:GLU:OE1	1:B:363:GLU:HA	2.13	0.49
1:A:267:ARG:HD3	4:A:2027:HOH:O	2.13	0.49
1:E:29:LEU:HD13	1:E:356:VAL:HG11	1.95	0.49
1:E:214:SER:O	1:E:242:HIS:HB2	2.13	0.49
1:B:488:THR:O	1:B:488:THR:N	2.46	0.48
1:C:168:TRP:HB2	1:C:208:LEU:HD23	1.95	0.48
1:E:350:LEU:CA	1:E:351:ALA:HB3	2.34	0.48
1:A:291:ASP:O	1:A:292:GLU:HG3	2.13	0.48
1:A:478:ASP:CG	1:A:479:LYS:H	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:CB	1:B:311:PRO:CA	2.91	0.48
1:B:482:PHE:HD1	1:B:487:LEU:HB2	1.78	0.48
1:D:350:LEU:CA	1:D:351:ALA:HB3	2.29	0.48
1:A:232:ALA:O	1:A:236:VAL:HG22	2.13	0.48
1:B:432:ILE:O	1:B:433:HIS:CB	2.60	0.48
1:D:175:ASP:OD2	1:D:213:SER:HA	2.12	0.48
1:E:409:ASP:HA	1:E:430:ARG:O	2.12	0.48
1:E:410:ILE:HD11	1:E:491:LEU:HD12	1.96	0.48
1:A:123:MET:HE2	1:A:165:ILE:HD13	1.94	0.48
1:B:367:GLY:CA	1:B:368:ALA:CB	2.86	0.48
1:C:293:TRP:O	1:C:294:ASN:HB2	2.13	0.48
1:D:472:VAL:O	1:D:473:TYR:CB	2.57	0.48
1:D:478:ASP:HB3	1:D:479:LYS:C	2.37	0.48
1:E:323:TYR:H	1:E:372:GLN:HE22	1.60	0.48
1:B:106:GLY:O	1:B:108:ASN:N	2.47	0.48
1:B:339:MET:HE1	1:B:426:PHE:CD1	2.48	0.48
1:F:114:CYS:HA	1:F:117:VAL:HG22	1.95	0.48
1:B:166:LYS:HE3	4:B:2019:HOH:O	2.13	0.48
1:B:444:GLY:CA	1:B:445:MET:HB2	2.44	0.48
1:D:15:ALA:HB2	1:D:343:ASP:CB	2.44	0.48
1:D:330:LEU:HA	1:D:333:LEU:HD12	1.95	0.48
1:D:471:GLU:HA	1:D:473:TYR:CD1	2.49	0.48
1:C:29:LEU:HD13	1:C:356:VAL:HG11	1.96	0.48
1:D:6:MET:HB2	1:D:394:ILE:HD12	1.95	0.48
1:A:309:ASN:HB2	1:A:310:GLU:CB	2.44	0.47
1:D:173:ALA:O	1:D:179:GLN:NE2	2.47	0.47
1:D:492:ARG:O	1:D:493:ARG:C	2.57	0.47
1:F:410:ILE:HD12	1:F:491:LEU:CD1	2.44	0.47
1:B:114:CYS:HA	1:B:117:VAL:HG22	1.96	0.47
1:B:479:LYS:HG3	1:B:490:MET:HG3	1.96	0.47
1:F:380:HIS:HD2	1:F:496:TRP:NE1	2.08	0.47
1:A:492:ARG:HG3	1:A:493:ARG:N	2.29	0.47
1:D:154:ARG:HG2	1:D:159:VAL:HB	1.96	0.47
1:D:399:HIS:HD2	1:D:409:ASP:OD1	1.98	0.47
1:F:458:HIS:CE1	1:F:471:GLU:HG2	2.47	0.47
1:D:311:PRO:HD2	1:D:312:TRP:HD1	1.79	0.47
1:F:477:SER:O	1:F:478:ASP:HB2	2.15	0.47
1:B:432:ILE:HD13	1:B:432:ILE:HA	1.68	0.47
1:C:238:TYR:HA	1:C:287:TYR:O	2.15	0.47
1:C:380:HIS:CD2	1:C:496:TRP:HE1	2.33	0.47
1:E:45:SER:HA	1:E:50:PHE:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:GLU:H	1:F:368:ALA:CB	2.28	0.47
1:B:229:LEU:O	1:B:233:TYR:HB2	2.15	0.47
1:B:290:PHE:O	1:B:348:ALA:HB1	2.15	0.47
1:A:336:ILE:HG23	1:A:413:VAL:HG22	1.96	0.47
1:C:229:LEU:O	1:C:233:TYR:HB2	2.14	0.47
1:C:291:ASP:CA	1:C:349:CYS:HB3	2.41	0.47
1:B:209:VAL:HG22	1:B:238:TYR:HB2	1.96	0.47
1:C:291:ASP:O	1:C:292:GLU:HG3	2.14	0.47
1:E:241:LEU:C	1:E:242:HIS:HD2	2.23	0.47
1:A:29:LEU:HD13	1:A:356:VAL:HG11	1.95	0.46
1:F:172:ASN:ND2	1:F:179:GLN:OE1	2.46	0.46
1:F:455:VAL:HG23	1:F:497:ASN:ND2	2.31	0.46
1:A:241:LEU:C	1:A:242:HIS:CD2	2.93	0.46
1:A:460:ASP:O	1:A:461:LEU:CB	2.63	0.46
1:B:61:LEU:HD22	1:B:378:PHE:HD2	1.79	0.46
1:C:241:LEU:HD22	1:C:290:PHE:CE2	2.51	0.46
1:D:473:TYR:O	1:D:473:TYR:CD2	2.68	0.46
1:E:443:ARG:HA	1:E:444:GLY:O	2.14	0.46
1:F:142:CYS:HB3	1:F:165:ILE:HD12	1.97	0.46
1:A:351:ALA:HA	1:A:352:GLN:HA	1.70	0.46
1:B:431:ASN:HB2	1:B:432:ILE:CB	2.42	0.46
1:C:72:ASN:ND2	1:C:179:GLN:OE1	2.48	0.46
1:D:311:PRO:HD2	1:D:312:TRP:CD1	2.51	0.46
1:D:453:HIS:CE1	1:D:497:ASN:HD22	2.32	0.46
1:E:358:ALA:O	1:E:372:GLN:HG3	2.16	0.46
1:E:366:GLY:CA	1:E:367:GLY:O	2.62	0.46
1:F:365:ASN:N	1:F:366:GLY:HA3	2.28	0.46
1:B:380:HIS:HD2	1:B:496:TRP:HE1	1.64	0.46
1:C:241:LEU:C	1:C:242:HIS:HD2	2.24	0.46
1:C:340:LYS:HD2	1:C:392:PRO:HG3	1.97	0.46
1:E:432:ILE:O	1:E:433:HIS:CB	2.63	0.46
1:B:351:ALA:HA	1:B:352:GLN:HA	1.67	0.46
1:E:393:VAL:HG13	1:E:394:ILE:N	2.31	0.46
1:A:428:VAL:HG12	1:A:429:ASN:N	2.31	0.46
1:A:492:ARG:HG3	1:A:493:ARG:H	1.81	0.46
1:B:168:TRP:HB2	1:B:208:LEU:HD23	1.97	0.46
1:B:431:ASN:HB2	1:B:432:ILE:CA	2.46	0.46
1:D:167:VAL:HG22	1:D:207:GLU:HB2	1.98	0.46
1:B:290:PHE:O	1:B:348:ALA:HB2	2.16	0.46
1:E:368:ALA:HA	1:E:369:ALA:CB	2.31	0.46
1:C:15:ALA:HB2	1:C:343:ASP:CB	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:SER:O	1:C:242:HIS:HB2	2.16	0.45
1:D:309:ASN:N	1:D:310:GLU:CB	2.76	0.45
1:E:308:GLN:CB	1:E:309:ASN:CG	2.89	0.45
1:E:348:ALA:HA	1:E:349:CYS:CB	2.23	0.45
1:F:29:LEU:HD21	1:F:319:LEU:HD13	1.97	0.45
1:A:310:GLU:CB	1:A:311:PRO:CA	2.93	0.45
1:B:445:MET:HE3	1:B:445:MET:HA	1.98	0.45
1:C:354:ILE:O	1:C:356:VAL:N	2.46	0.45
1:C:432:ILE:HA	1:C:433:HIS:HA	1.69	0.45
1:F:478:ASP:HA	1:F:479:LYS:HB2	1.96	0.45
1:C:126:ASN:OD1	1:C:126:ASN:C	2.59	0.45
1:E:323:TYR:H	1:E:372:GLN:NE2	2.14	0.45
1:E:478:ASP:CA	1:E:479:LYS:CB	2.83	0.45
1:C:262:LEU:HD22	1:C:334:MET:HG2	1.98	0.45
1:D:313:ARG:HB3	1:D:316:PRO:HG3	1.99	0.45
1:E:298:HIS:HE1	1:E:327:ASP:OD2	2.00	0.45
1:E:365:ASN:C	1:E:365:ASN:HD22	2.24	0.45
1:F:365:ASN:N	1:F:366:GLY:CA	2.80	0.45
1:A:91:ARG:HH22	1:A:314:ILE:HD11	1.81	0.45
1:C:367:GLY:CA	1:C:368:ALA:HB3	2.46	0.45
1:F:125:VAL:HG12	1:F:138:LEU:HD23	1.99	0.45
1:A:12:TYR:CE1	1:A:391:GLN:HG3	2.51	0.45
1:B:431:ASN:ND2	1:B:431:ASN:N	2.63	0.45
1:E:371:ARG:HD3	1:E:375:PHE:CD1	2.52	0.45
1:F:203:ASP:O	1:F:206:ILE:HG12	2.17	0.45
1:F:307:MET:HA	1:F:308:GLN:HA	1.69	0.45
1:D:61:LEU:HD22	1:D:378:PHE:HD1	1.82	0.45
1:D:214:SER:O	1:D:242:HIS:HB2	2.17	0.45
1:D:229:LEU:O	1:D:233:TYR:HB2	2.17	0.45
1:A:445:MET:HE3	1:A:445:MET:HA	1.97	0.45
1:C:419:GLU:HB3	1:C:420:LYS:CB	2.38	0.45
1:F:61:LEU:HD22	1:F:378:PHE:HD1	1.82	0.45
1:B:111:ALA:HA	1:B:121:ILE:HD11	1.99	0.44
1:C:203:ASP:O	1:C:206:ILE:HG12	2.17	0.44
1:D:38:TYR:CZ	1:D:40:PRO:HG3	2.52	0.44
1:E:9:ASP:HB3	1:E:12:TYR:HB3	1.97	0.44
1:E:106:GLY:O	1:E:108:ASN:N	2.50	0.44
1:C:364:ARG:HA	1:C:365:ASN:HA	1.66	0.44
1:C:430:ARG:O	1:C:431:ASN:HB3	2.18	0.44
1:D:67:ARG:HB2	1:D:122:MET:HE3	1.99	0.44
1:B:412:SER:HA	1:B:426:PHE:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:ALA:HA	1:F:352:GLN:HA	1.60	0.44
1:D:100:ILE:HG12	1:D:312:TRP:O	2.18	0.44
1:D:339:MET:HE1	1:D:426:PHE:CD1	2.53	0.44
1:D:431:ASN:C	1:D:432:ILE:HG13	2.42	0.44
1:F:478:ASP:CB	1:F:479:LYS:HB2	2.47	0.44
1:A:188:TYR:HA	1:A:191:ILE:HG22	1.99	0.44
1:E:351:ALA:N	1:E:352:GLN:CA	2.77	0.44
1:B:125:VAL:O	1:B:171:GLY:HA2	2.18	0.44
1:C:356:VAL:O	1:C:357:ILE:C	2.61	0.44
1:C:459:GLN:O	1:C:460:ASP:HB3	2.18	0.44
1:B:429:ASN:HD21	1:B:436:ILE:HD11	1.83	0.44
1:B:458:HIS:CD2	1:B:460:ASP:H	2.24	0.44
1:F:452:GLU:HG2	1:F:500:ARG:HH11	1.82	0.44
1:A:432:ILE:HA	1:A:433:HIS:HA	1.70	0.44
1:B:440:SER:HB2	1:B:487:LEU:HB3	2.00	0.44
1:D:371:ARG:HD3	1:D:375:PHE:CE1	2.53	0.44
1:E:23:GLY:N	1:E:348:ALA:O	2.48	0.44
1:F:174:MET:HE3	1:F:174:MET:HB2	1.88	0.44
1:D:471:GLU:HA	1:D:473:TYR:HD1	1.82	0.43
1:A:311:PRO:C	1:A:312:TRP:HD1	2.23	0.43
1:A:431:ASN:CA	1:A:432:ILE:HG13	2.46	0.43
1:B:304:ALA:CA	1:B:305:ASN:CB	2.95	0.43
1:E:175:ASP:OD1	1:E:214:SER:OG	2.29	0.43
1:F:34:TYR:HB2	1:F:315:ALA:HB2	2.00	0.43
1:B:429:ASN:ND2	1:B:491:LEU:HD11	2.33	0.43
1:D:431:ASN:CB	1:D:432:ILE:CA	2.89	0.43
1:E:153:MET:HG2	1:E:157:HIS:CE1	2.53	0.43
1:F:14:ILE:HG22	1:F:389:VAL:HB	2.00	0.43
1:F:295:VAL:HG22	1:F:330:LEU:HD23	2.00	0.43
1:F:306:ILE:H	1:F:306:ILE:HG12	1.46	0.43
1:B:154:ARG:HG2	1:B:159:VAL:HB	2.00	0.43
1:D:410:ILE:HD12	1:D:491:LEU:HD12	2.01	0.43
1:E:312:TRP:CA	1:E:313:ARG:HB2	2.48	0.43
1:C:333:LEU:HD22	1:C:430:ARG:NH1	2.31	0.43
1:D:121:ILE:HD11	1:D:123:MET:SD	2.57	0.43
1:D:246:GLY:HA2	1:D:297:TYR:CD1	2.53	0.43
1:F:363:GLU:H	1:F:368:ALA:HB1	1.83	0.43
1:B:216:LYS:HB3	1:B:265:PHE:CE1	2.53	0.43
1:B:257:ALA:HA	1:B:430:ARG:HH21	1.83	0.43
1:A:51:ARG:O	1:A:55:ILE:HD12	2.19	0.43
1:A:242:HIS:CD2	1:A:242:HIS:N	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:O	1:B:119:ALA:HB2	2.19	0.43
1:B:290:PHE:C	1:B:348:ALA:HB2	2.44	0.43
1:C:84:GLY:HA2	1:C:157:HIS:CD2	2.54	0.43
1:C:218:MET:HE2	1:C:219:PRO:HD2	2.00	0.43
1:B:159:VAL:HG11	1:B:163:HIS:CE1	2.54	0.43
1:D:102:PRO:HG3	1:D:314:ILE:HD12	2.00	0.43
1:A:410:ILE:CD1	1:A:491:LEU:HD12	2.48	0.43
1:C:149:LYS:HD3	1:C:150:TYR:CE2	2.54	0.43
1:C:433:HIS:ND1	1:C:433:HIS:N	2.67	0.43
1:C:444:GLY:HA3	1:C:445:MET:HA	1.53	0.43
1:D:125:VAL:HG12	1:D:138:LEU:HD23	2.00	0.43
1:D:432:ILE:HB	1:D:433:HIS:CD2	2.53	0.43
1:E:296:TRP:CD1	1:E:296:TRP:C	2.97	0.43
1:E:443:ARG:HB3	1:E:443:ARG:HH11	1.81	0.43
1:C:298:HIS:HE1	1:C:327:ASP:OD2	2.02	0.43
1:D:336:ILE:HG23	1:D:413:VAL:HG22	2.01	0.43
1:E:445:MET:CA	1:E:446:LYS:CB	2.88	0.43
1:C:308:GLN:O	1:C:309:ASN:CB	2.67	0.42
1:F:45:SER:HA	1:F:50:PHE:O	2.19	0.42
1:A:367:GLY:CA	1:A:368:ALA:CB	2.62	0.42
1:B:29:LEU:O	1:B:30:GLY:C	2.61	0.42
1:D:106:GLY:O	1:D:108:ASN:N	2.52	0.42
1:A:431:ASN:O	1:A:493:ARG:O	2.36	0.42
1:C:458:HIS:HD2	1:C:459:GLN:C	2.28	0.42
1:D:100:ILE:CG1	1:D:312:TRP:O	2.68	0.42
1:E:359:PRO:HA	1:E:372:GLN:HB2	2.01	0.42
1:B:429:ASN:HB2	1:B:491:LEU:HD13	2.01	0.42
1:F:179:GLN:HE21	1:F:179:GLN:HB3	1.49	0.42
1:B:446:LYS:HA	1:B:447:ASP:HA	1.82	0.42
1:B:491:LEU:CB	1:B:492:ARG:C	2.92	0.42
1:C:407:VAL:HG13	1:C:430:ARG:HH21	1.85	0.42
1:E:376:TYR:CG	1:E:474:PRO:HD3	2.55	0.42
1:A:433:HIS:H	1:A:434:GLU:HB2	1.73	0.42
1:B:23:GLY:HA3	1:B:348:ALA:O	2.20	0.42
1:D:484:ASP:HA	1:D:485:GLY:HA2	1.45	0.42
1:A:310:GLU:CB	1:A:311:PRO:HD3	2.36	0.42
1:C:448:TYR:HD1	1:C:501:ILE:HG22	1.85	0.42
1:D:291:ASP:O	1:D:292:GLU:HG3	2.19	0.42
1:D:433:HIS:N	1:D:433:HIS:ND1	2.68	0.42
1:E:312:TRP:CD1	1:E:312:TRP:N	2.88	0.42
1:E:457:GLU:CB	1:E:458:HIS:HA	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:ASP:HA	1:F:349:CYS:HB2	2.02	0.42
1:A:312:TRP:N	1:A:312:TRP:CD1	2.88	0.42
1:B:174:MET:HB2	1:B:174:MET:HE3	1.57	0.42
1:F:429:ASN:CA	1:F:430:ARG:C	2.92	0.42
1:A:312:TRP:CA	1:A:313:ARG:CB	2.96	0.42
1:B:5:ARG:HB2	1:B:395:ASN:HB3	2.02	0.42
1:B:311:PRO:HB2	1:B:312:TRP:H	1.63	0.42
1:D:17:ILE:HG13	1:D:389:VAL:HG23	2.01	0.42
1:E:456:LEU:HB2	1:E:496:TRP:HD1	1.85	0.42
1:F:35:ASP:OD1	1:F:364:ARG:O	2.36	0.42
1:B:142:CYS:HB3	1:B:165:ILE:HD12	2.01	0.42
1:C:440:SER:HB2	1:C:487:LEU:HB3	2.01	0.42
1:E:172:ASN:O	1:E:173:ALA:C	2.62	0.42
1:A:460:ASP:CB	1:A:463:ILE:HB	2.47	0.41
1:B:252:THR:HG21	1:B:461:LEU:HD13	2.02	0.41
1:C:240:SER:HA	1:C:289:SER:O	2.20	0.41
1:C:386:ARG:O	1:C:417:ASN:HB2	2.20	0.41
1:E:114:CYS:HA	1:E:117:VAL:HG22	2.01	0.41
1:B:7:THR:HG23	1:B:393:VAL:HB	2.02	0.41
1:B:291:ASP:HA	1:B:349:CYS:HB2	1.98	0.41
1:C:19:LYS:O	1:C:64:PRO:HG2	2.21	0.41
1:C:367:GLY:HA3	1:C:368:ALA:O	2.19	0.41
1:D:122:MET:HE1	1:D:349:CYS:SG	2.61	0.41
1:D:432:ILE:HA	1:D:433:HIS:HA	1.62	0.41
1:E:482:PHE:CD1	1:E:487:LEU:HB2	2.54	0.41
1:D:293:TRP:O	1:D:294:ASN:HB2	2.20	0.41
1:A:477:SER:CB	1:A:478:ASP:CA	2.87	0.41
1:C:172:ASN:HD22	1:C:179:GLN:NE2	2.12	0.41
1:C:206:ILE:HD12	1:C:208:LEU:HD21	2.01	0.41
1:E:4:ALA:HB2	1:E:397:PRO:HD2	2.02	0.41
1:E:336:ILE:HG23	1:E:413:VAL:HG22	2.01	0.41
1:F:10:LYS:H	1:F:10:LYS:HG2	1.69	0.41
1:F:17:ILE:CD1	1:F:389:VAL:CG2	2.98	0.41
1:F:67:ARG:HB2	1:F:122:MET:HE3	2.03	0.41
1:A:34:TYR:CZ	1:A:102:PRO:HG2	2.55	0.41
1:A:428:VAL:CG1	1:A:429:ASN:N	2.83	0.41
1:C:419:GLU:O	1:C:421:GLU:HG3	2.21	0.41
1:D:174:MET:HE3	1:D:174:MET:HB2	1.90	0.41
1:D:309:ASN:CB	1:D:310:GLU:HB2	2.51	0.41
1:A:311:PRO:O	1:A:312:TRP:HD1	2.03	0.41
1:A:366:GLY:HA2	1:A:367:GLY:HA2	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:TRP:HB2	1:D:208:LEU:HD23	2.02	0.41
1:E:67:ARG:HD2	1:E:291:ASP:HB2	2.02	0.41
1:F:478:ASP:CA	1:F:479:LYS:CB	2.96	0.41
1:A:308:GLN:HB3	1:A:309:ASN:H	1.63	0.41
1:A:310:GLU:CG	1:A:311:PRO:HB3	2.49	0.41
1:C:447:ASP:OD1	1:C:447:ASP:N	2.54	0.41
1:D:238:TYR:HA	1:D:287:TYR:O	2.21	0.41
1:A:480:SER:HB3	1:A:489:SER:HA	2.03	0.41
1:C:23:GLY:HA2	1:C:63:VAL:HG13	2.03	0.41
1:C:70:GLY:HA2	1:C:71:GLY:HA3	1.88	0.41
1:C:448:TYR:CD1	1:C:501:ILE:HG22	2.56	0.41
1:F:455:VAL:HG23	1:F:497:ASN:HD22	1.85	0.41
1:A:410:ILE:HD11	1:A:436:ILE:CD1	2.32	0.41
1:C:483:ASP:HA	1:C:484:ASP:HA	1.87	0.41
1:E:166:LYS:HB3	4:E:2020:HOH:O	2.21	0.41
1:F:139:LEU:HD23	1:F:202:ILE:HB	2.01	0.41
1:B:304:ALA:N	1:B:305:ASN:HB2	2.36	0.40
1:B:431:ASN:HD22	1:B:431:ASN:N	2.19	0.40
1:C:448:TYR:HB2	1:C:502:GLY:C	2.46	0.40
1:D:416:TYR:HD1	1:D:423:VAL:HG22	1.86	0.40
1:E:125:VAL:O	1:E:171:GLY:HA2	2.21	0.40
1:C:27:GLU:HA	1:C:69:PRO:O	2.21	0.40
1:E:439:VAL:HG12	1:E:488:THR:HG22	2.02	0.40
1:B:348:ALA:HA	1:B:349:CYS:CB	2.43	0.40
1:B:479:LYS:HG3	1:B:490:MET:HB3	2.03	0.40
1:C:339:MET:HE3	1:C:415:ILE:HG21	2.03	0.40
1:F:111:ALA:HA	1:F:121:ILE:HD11	2.04	0.40
1:A:252:THR:HG21	1:A:461:LEU:HD13	2.03	0.40
1:A:296:TRP:CD1	1:A:296:TRP:C	2.99	0.40
1:B:51:ARG:HH22	1:B:368:ALA:HB1	1.85	0.40
1:B:298:HIS:HE1	1:B:327:ASP:OD2	2.04	0.40
1:C:241:LEU:HD11	1:C:288:LEU:HD23	2.03	0.40
1:A:358:ALA:O	1:A:372:GLN:HG3	2.22	0.40
1:A:409:ASP:HA	1:A:430:ARG:O	2.22	0.40
1:D:371:ARG:HD3	1:D:375:PHE:CD1	2.57	0.40
1:E:291:ASP:CA	1:E:349:CYS:HB3	2.38	0.40
1:F:87:GLU:CD	1:F:87:GLU:H	2.29	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	499/513 (97%)	445 (89%)	37 (7%)	17 (3%)	3	12
1	B	497/513 (97%)	435 (88%)	40 (8%)	22 (4%)	2	8
1	C	498/513 (97%)	446 (90%)	32 (6%)	20 (4%)	2	9
1	D	492/513 (96%)	428 (87%)	42 (8%)	22 (4%)	2	8
1	E	493/513 (96%)	436 (88%)	32 (6%)	25 (5%)	1	6
1	F	498/513 (97%)	445 (89%)	40 (8%)	13 (3%)	4	17
All	All	2977/3078 (97%)	2635 (88%)	223 (8%)	119 (4%)	2	9

All (119) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	309	ASN
1	A	310	GLU
1	A	311	PRO
1	A	364	ARG
1	A	368	ALA
1	A	432	ILE
1	A	434	GLU
1	A	470	GLU
1	A	493	ARG
1	B	217	ASP
1	B	304	ALA
1	B	307	MET
1	B	310	GLU
1	B	311	PRO
1	B	349	CYS
1	B	481	SER
1	C	309	ASN
1	C	310	GLU
1	C	349	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	458	HIS
1	C	461	LEU
1	C	478	ASP
1	C	481	SER
1	D	351	ALA
1	D	364	ARG
1	D	431	ASN
1	D	432	ILE
1	D	446	LYS
1	D	447	ASP
1	D	473	TYR
1	D	478	ASP
1	D	493	ARG
1	E	62	ASN
1	E	107	ILE
1	E	309	ASN
1	E	311	PRO
1	E	349	CYS
1	E	351	ALA
1	E	364	ARG
1	E	368	ALA
1	E	369	ALA
1	E	433	HIS
1	E	434	GLU
1	F	310	GLU
1	F	430	ARG
1	F	470	GLU
1	A	445	MET
1	A	478	ASP
1	A	480	SER
1	A	481	SER
1	B	62	ASN
1	B	107	ILE
1	B	173	ALA
1	B	364	ARG
1	B	433	HIS
1	B	470	GLU
1	C	418	GLU
1	C	432	ILE
1	C	486	ILE
1	D	107	ILE
1	D	309	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	367	GLY
1	D	430	ARG
1	D	434	GLU
1	D	470	GLU
1	E	367	GLY
1	E	445	MET
1	E	478	ASP
1	E	479	LYS
1	F	294	ASN
1	F	368	ALA
1	A	430	ARG
1	A	484	ASP
1	C	297	TYR
1	C	355	ASN
1	C	493	ARG
1	D	173	ALA
1	D	472	VAL
1	D	479	LYS
1	E	471	GLU
1	F	357	ILE
1	F	478	ASP
1	B	305	ASN
1	B	432	ILE
1	B	491	LEU
1	C	308	GLN
1	C	311	PRO
1	E	394	ILE
1	E	432	ILE
1	E	447	ASP
1	A	357	ILE
1	B	46	ASP
1	B	357	ILE
1	B	489	SER
1	C	431	ASN
1	C	460	ASP
1	D	357	ILE
1	D	461	LEU
1	E	297	TYR
1	E	310	GLU
1	E	355	ASN
1	F	355	ASN
1	F	449	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	480	SER
1	C	307	MET
1	C	357	ILE
1	C	419	GLU
1	D	310	GLU
1	E	469	GLY
1	F	62	ASN
1	F	173	ALA
1	F	307	MET
1	B	367	GLY
1	B	306	ILE
1	E	317	PRO
1	E	357	ILE
1	D	311	PRO
1	F	311	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	434/450 (96%)	407 (94%)	27 (6%)	16	46
1	B	434/450 (96%)	403 (93%)	31 (7%)	13	40
1	C	428/450 (95%)	392 (92%)	36 (8%)	10	31
1	D	420/450 (93%)	394 (94%)	26 (6%)	16	46
1	E	417/450 (93%)	389 (93%)	28 (7%)	15	43
1	F	423/450 (94%)	397 (94%)	26 (6%)	17	46
All	All	2556/2700 (95%)	2382 (93%)	174 (7%)	14	42

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	11	ASP
1	A	17	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	55	ILE
1	A	87	GLU
1	A	98	LYS
1	A	112	LYS
1	A	132	ILE
1	A	241	LEU
1	A	302	GLU
1	A	307	MET
1	A	312	TRP
1	A	365	ASN
1	A	390	LEU
1	A	413	VAL
1	A	415	ILE
1	A	418	GLU
1	A	430	ARG
1	A	432	ILE
1	A	436	ILE
1	A	446	LYS
1	A	447	ASP
1	A	449	ARG
1	A	455	VAL
1	A	463	ILE
1	A	479	LYS
1	A	488	THR
1	B	17	ILE
1	B	43	SER
1	B	87	GLU
1	B	174	MET
1	B	180	VAL
1	B	216	LYS
1	B	243	GLN
1	B	305	ASN
1	B	364	ARG
1	B	365	ASN
1	B	379	MET
1	B	394	ILE
1	B	413	VAL
1	B	419	GLU
1	B	429	ASN
1	B	431	ASN
1	B	432	ILE
1	B	435	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	442	VAL
1	B	445	MET
1	B	446	LYS
1	B	447	ASP
1	B	449	ARG
1	B	455	VAL
1	B	463	ILE
1	B	476	ASN
1	B	480	SER
1	B	483	ASP
1	B	489	SER
1	B	490	MET
1	B	491	LEU
1	C	7	THR
1	C	13	LYS
1	C	16	GLU
1	C	17	ILE
1	C	43	SER
1	C	44	LYS
1	C	47	GLU
1	C	56	GLU
1	C	87	GLU
1	C	98	LYS
1	C	112	LYS
1	C	160	LYS
1	C	180	VAL
1	C	218	MET
1	C	241	LEU
1	C	250	ASN
1	C	302	GLU
1	C	307	MET
1	C	364	ARG
1	C	365	ASN
1	C	390	LEU
1	C	415	ILE
1	C	430	ARG
1	C	432	ILE
1	C	433	HIS
1	C	435	ASP
1	C	436	ILE
1	C	458	HIS
1	C	460	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	463	ILE
1	C	468	ASN
1	C	479	LYS
1	C	480	SER
1	C	483	ASP
1	C	486	ILE
1	C	487	LEU
1	D	16	GLU
1	D	17	ILE
1	D	121	ILE
1	D	160	LYS
1	D	220	THR
1	D	248	LYS
1	D	308	GLN
1	D	314	ILE
1	D	350	LEU
1	D	393	VAL
1	D	394	ILE
1	D	413	VAL
1	D	415	ILE
1	D	418	GLU
1	D	430	ARG
1	D	432	ILE
1	D	433	HIS
1	D	436	ILE
1	D	440	SER
1	D	455	VAL
1	D	459	GLN
1	D	463	ILE
1	D	468	ASN
1	D	488	THR
1	D	490	MET
1	D	501	ILE
1	E	44	LYS
1	E	47	GLU
1	E	87	GLU
1	E	98	LYS
1	E	107	ILE
1	E	160	LYS
1	E	179	GLN
1	E	180	VAL
1	E	305	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	312	TRP
1	E	349	CYS
1	E	350	LEU
1	E	365	ASN
1	E	372	GLN
1	E	390	LEU
1	E	391	GLN
1	E	410	ILE
1	E	413	VAL
1	E	431	ASN
1	E	437	VAL
1	E	443	ARG
1	E	446	LYS
1	E	448	TYR
1	E	456	LEU
1	E	457	GLU
1	E	463	ILE
1	E	486	ILE
1	E	487	LEU
1	F	14	ILE
1	F	17	ILE
1	F	44	LYS
1	F	47	GLU
1	F	87	GLU
1	F	98	LYS
1	F	107	ILE
1	F	160	LYS
1	F	174	MET
1	F	179	GLN
1	F	180	VAL
1	F	283	LYS
1	F	306	ILE
1	F	365	ASN
1	F	379	MET
1	F	388	ILE
1	F	390	LEU
1	F	393	VAL
1	F	413	VAL
1	F	415	ILE
1	F	421	GLU
1	F	430	ARG
1	F	446	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	455	VAL
1	F	461	LEU
1	F	480	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	144	HIS
1	A	242	HIS
1	A	298	HIS
1	A	429	ASN
1	A	433	HIS
1	A	458	HIS
1	A	465	ASN
1	A	468	ASN
1	A	476	ASN
1	B	72	ASN
1	B	104	GLN
1	B	163	HIS
1	B	243	GLN
1	B	298	HIS
1	B	365	ASN
1	B	380	HIS
1	B	399	HIS
1	B	429	ASN
1	B	458	HIS
1	C	72	ASN
1	C	104	GLN
1	C	179	GLN
1	C	298	HIS
1	C	309	ASN
1	C	341	HIS
1	C	380	HIS
1	C	429	ASN
1	C	458	HIS
1	D	72	ASN
1	D	104	GLN
1	D	223	GLN
1	D	242	HIS
1	D	298	HIS
1	D	305	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	308	GLN
1	D	365	ASN
1	D	399	HIS
1	D	429	ASN
1	D	459	GLN
1	D	468	ASN
1	D	497	ASN
1	E	72	ASN
1	E	104	GLN
1	E	298	HIS
1	E	365	ASN
1	E	380	HIS
1	E	429	ASN
1	E	459	GLN
1	E	476	ASN
1	F	72	ASN
1	F	137	ASN
1	F	182	HIS
1	F	298	HIS
1	F	380	HIS
1	F	399	HIS
1	F	453	HIS
1	F	458	HIS
1	F	497	ASN

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 ⓘ

12 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	XYS	G	1	2	9,9,10	0.83	0	10,12,14	1.78	2 (20%)
2	AHR	G	2	2	9,9,10	0.49	0	11,12,14	1.46	2 (18%)
2	XYS	H	1	2	9,9,10	0.88	0	10,12,14	1.85	3 (30%)
2	AHR	H	2	2	9,9,10	0.53	0	11,12,14	2.00	3 (27%)
2	XYS	I	1	2	9,9,10	0.79	0	10,12,14	2.00	3 (30%)
2	AHR	I	2	2	9,9,10	0.42	0	11,12,14	0.97	1 (9%)
2	XYS	J	1	2	9,9,10	0.93	0	10,12,14	2.02	3 (30%)
2	AHR	J	2	2	9,9,10	0.51	0	11,12,14	1.29	2 (18%)
2	XYS	K	1	2	9,9,10	0.86	0	10,12,14	1.52	2 (20%)
2	AHR	K	2	2	9,9,10	0.54	0	11,12,14	1.32	2 (18%)
2	XYS	L	1	2	9,9,10	0.87	0	10,12,14	1.48	2 (20%)
2	AHR	L	2	2	9,9,10	0.49	0	11,12,14	1.18	2 (18%)

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	XYS	G	1	2	-	-	1/1/1/1
2	AHR	G	2	2	-	2/2/15/18	0/1/1/1
2	XYS	H	1	2	-	-	1/1/1/1
2	AHR	H	2	2	-	2/2/15/18	0/1/1/1
2	XYS	I	1	2	-	-	0/1/1/1
2	AHR	I	2	2	-	0/2/15/18	0/1/1/1
2	XYS	J	1	2	-	-	1/1/1/1
2	AHR	J	2	2	-	0/2/15/18	0/1/1/1
2	XYS	K	1	2	-	-	0/1/1/1
2	AHR	K	2	2	-	0/2/15/18	0/1/1/1
2	XYS	L	1	2	-	-	0/1/1/1
2	AHR	L	2	2	-	0/2/15/18	0/1/1/1

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	XYS	O3-C3-C4	4.68	119.60	110.05
2	H	2	AHR	O4-C4-C3	4.53	108.82	104.63
2	H	1	XYS	O3-C3-C4	4.29	118.80	110.05
2	J	1	XYS	O3-C3-C4	4.11	118.44	110.05
2	L	1	XYS	O3-C3-C4	3.53	117.26	110.05
2	H	2	AHR	C1-C2-C3	3.47	107.18	101.63
2	K	1	XYS	O3-C3-C4	3.45	117.09	110.05
2	G	1	XYS	C5-O5-C1	3.41	116.92	111.42
2	J	1	XYS	C5-O5-C1	3.35	116.83	111.42
2	G	1	XYS	O3-C3-C4	3.28	116.75	110.05
2	I	1	XYS	C5-O5-C1	3.23	116.62	111.42
2	J	2	AHR	C1-C2-C3	3.00	106.43	101.63
2	G	2	AHR	C1-C2-C3	2.96	106.36	101.63
2	G	2	AHR	O4-C4-C3	2.85	107.27	104.63
2	H	1	XYS	C5-O5-C1	2.83	115.98	111.42
2	I	2	AHR	C1-C2-C3	2.64	105.84	101.63
2	I	1	XYS	C4-C3-C2	-2.51	107.94	110.92
2	J	1	XYS	C4-C3-C2	-2.51	107.94	110.92
2	K	2	AHR	C1-C2-C3	2.50	105.63	101.63
2	L	2	AHR	C1-C2-C3	2.47	105.57	101.63
2	H	2	AHR	C5-C4-C3	-2.44	109.34	115.10
2	L	1	XYS	C5-O5-C1	2.31	115.14	111.42
2	K	2	AHR	O4-C4-C3	2.13	106.60	104.63
2	J	2	AHR	O4-C4-C3	2.12	106.59	104.63
2	H	1	XYS	C4-C3-C2	-2.10	108.42	110.92
2	K	1	XYS	O4-C4-C5	-2.04	104.55	109.22
2	L	2	AHR	O4-C4-C3	2.02	106.50	104.63

There are no chirality outliers.

All (4) torsion outliers are listed below:

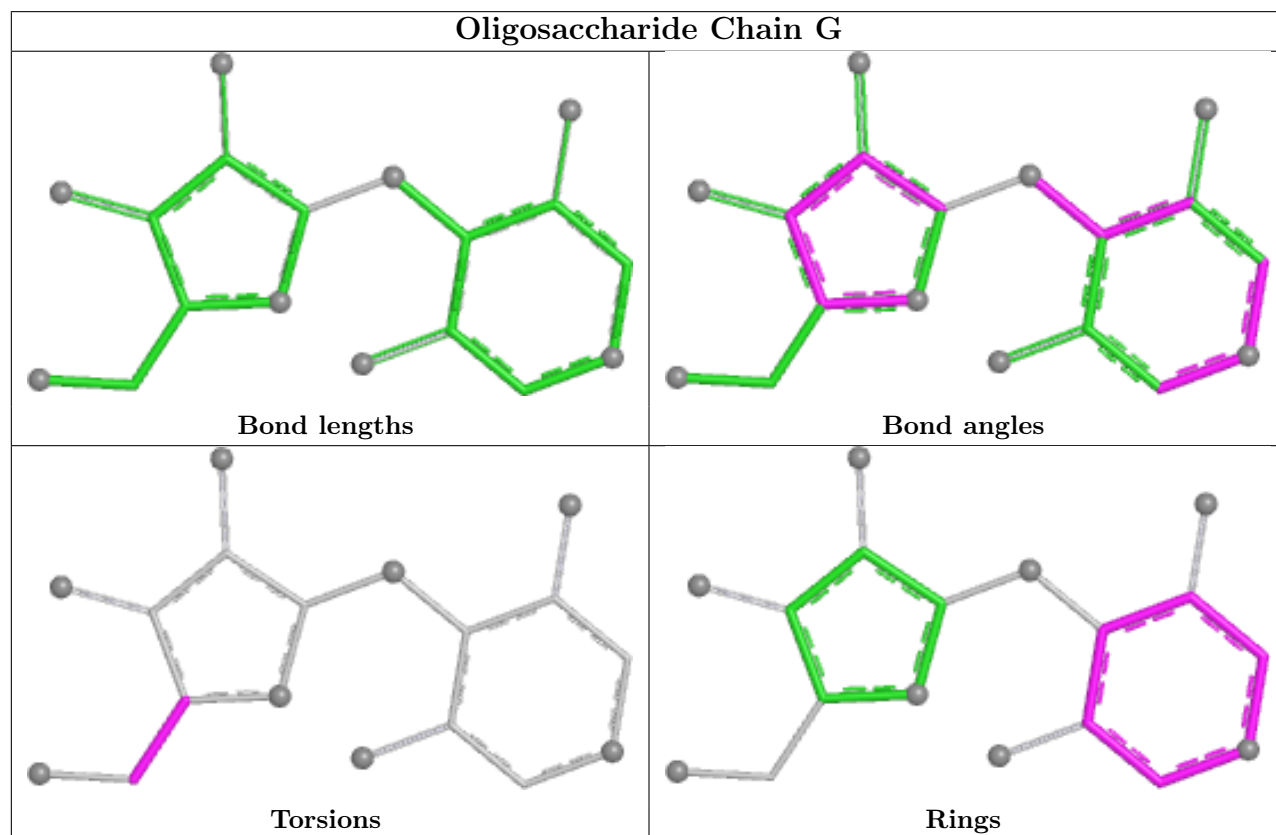
Mol	Chain	Res	Type	Atoms
2	G	2	AHR	O4-C4-C5-O5
2	H	2	AHR	C3-C4-C5-O5
2	G	2	AHR	C3-C4-C5-O5
2	H	2	AHR	O4-C4-C5-O5

All (3) ring outliers are listed below:

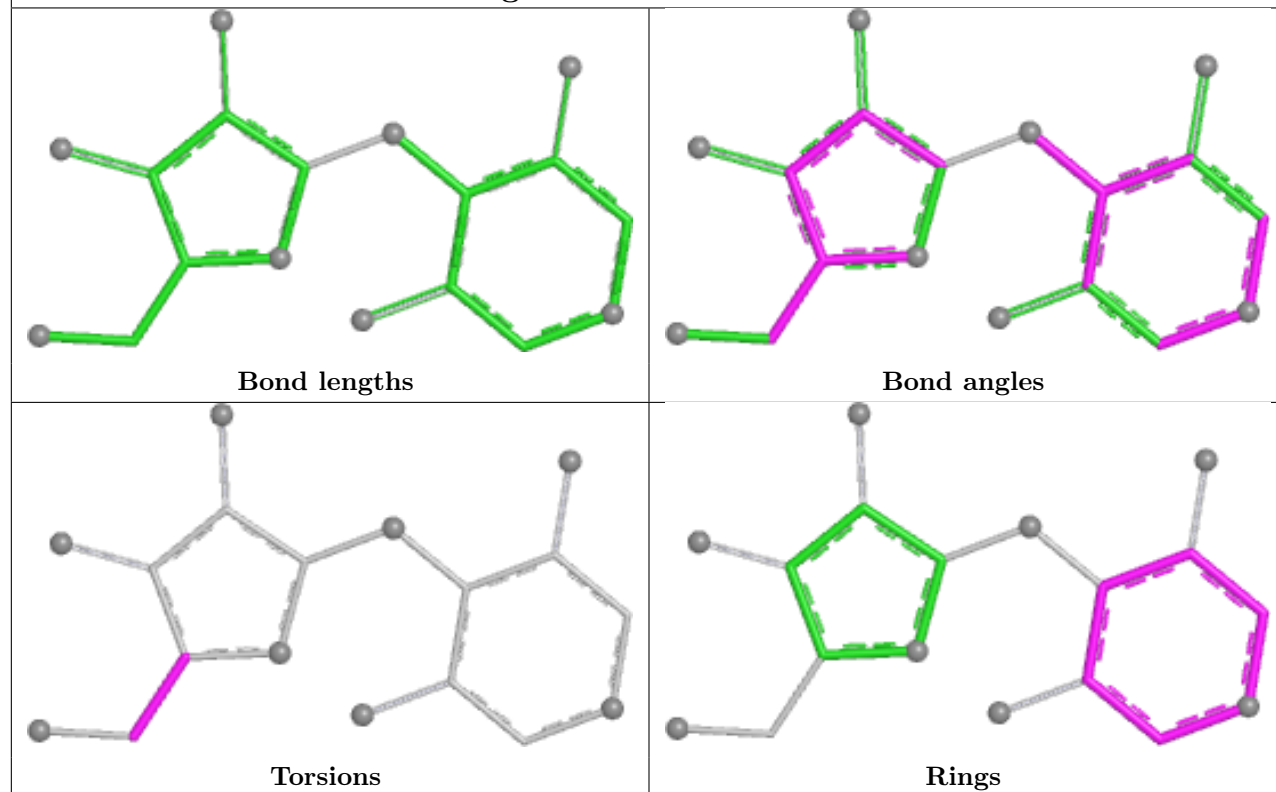
Mol	Chain	Res	Type	Atoms
2	H	1	XYS	C1-C2-C3-C4-C5-O5
2	G	1	XYS	C1-C2-C3-C4-C5-O5
2	J	1	XYS	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

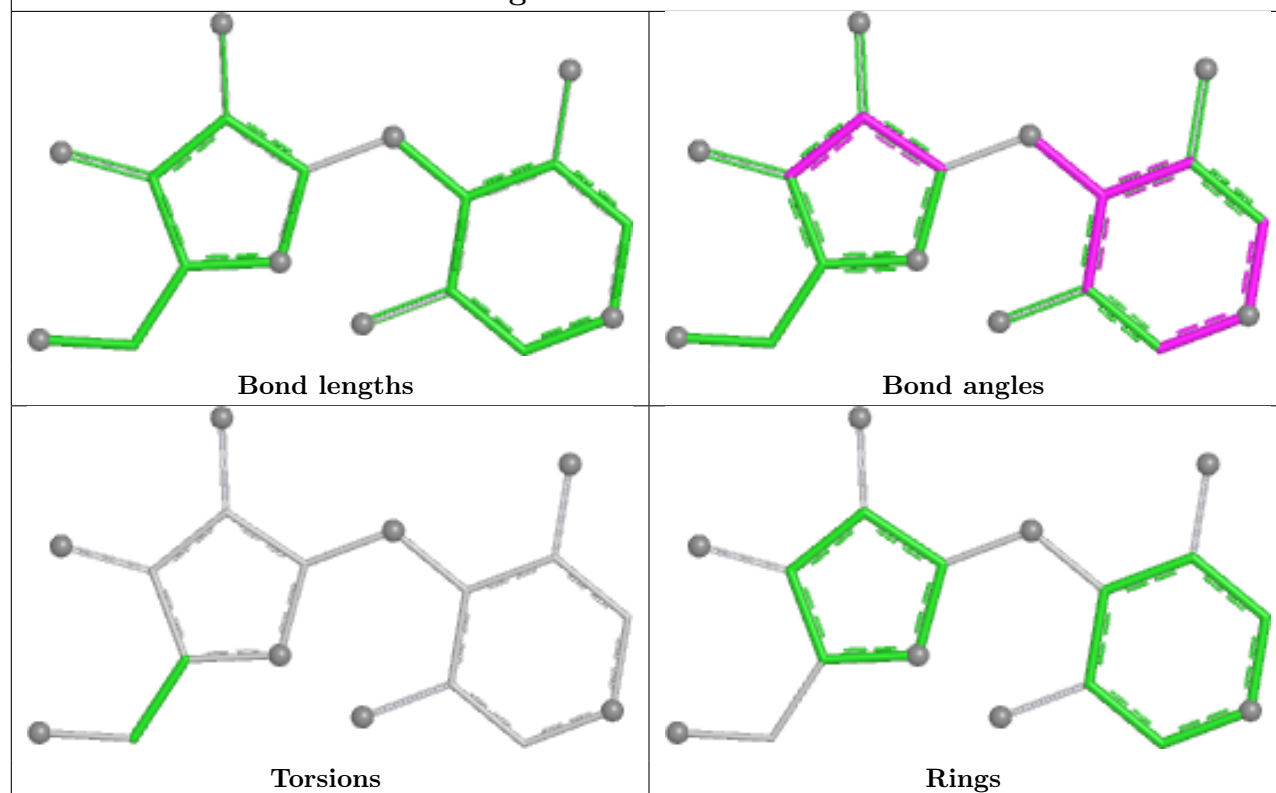
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

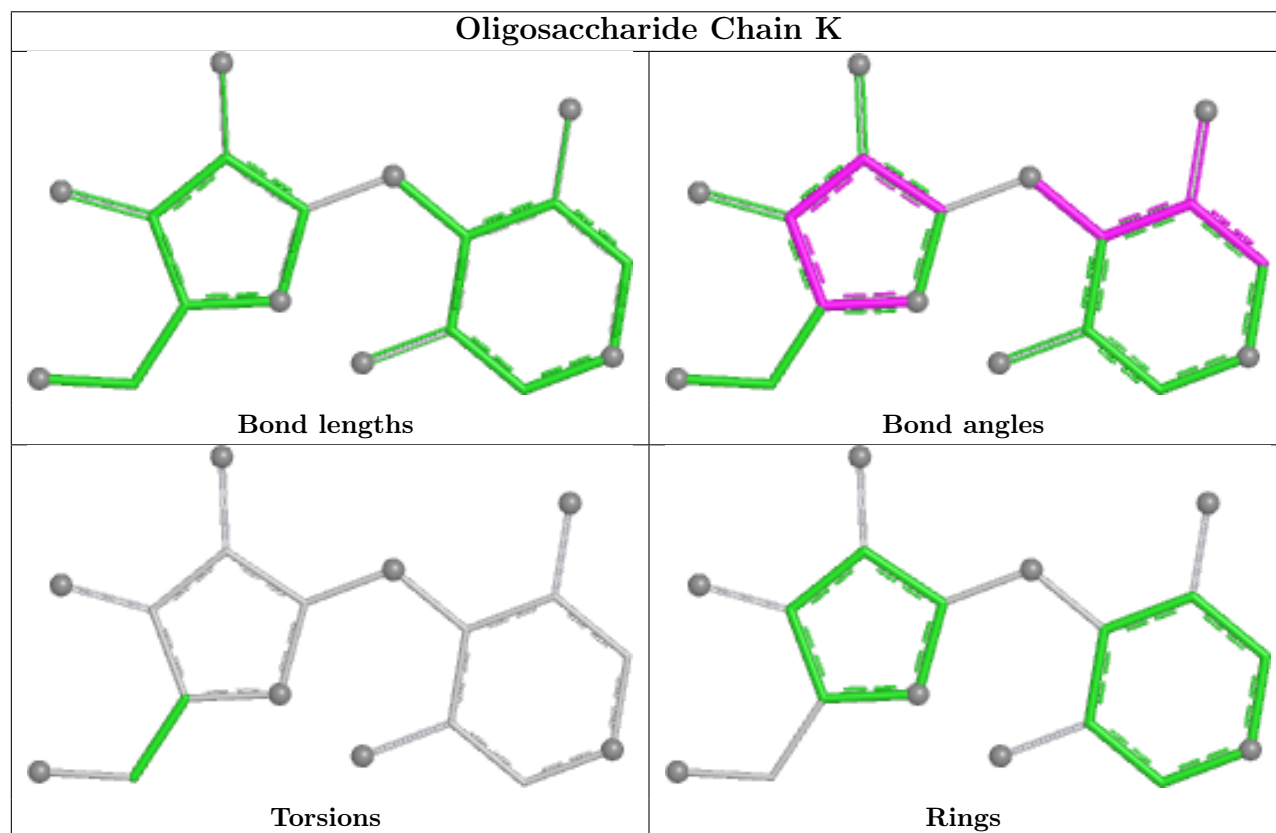
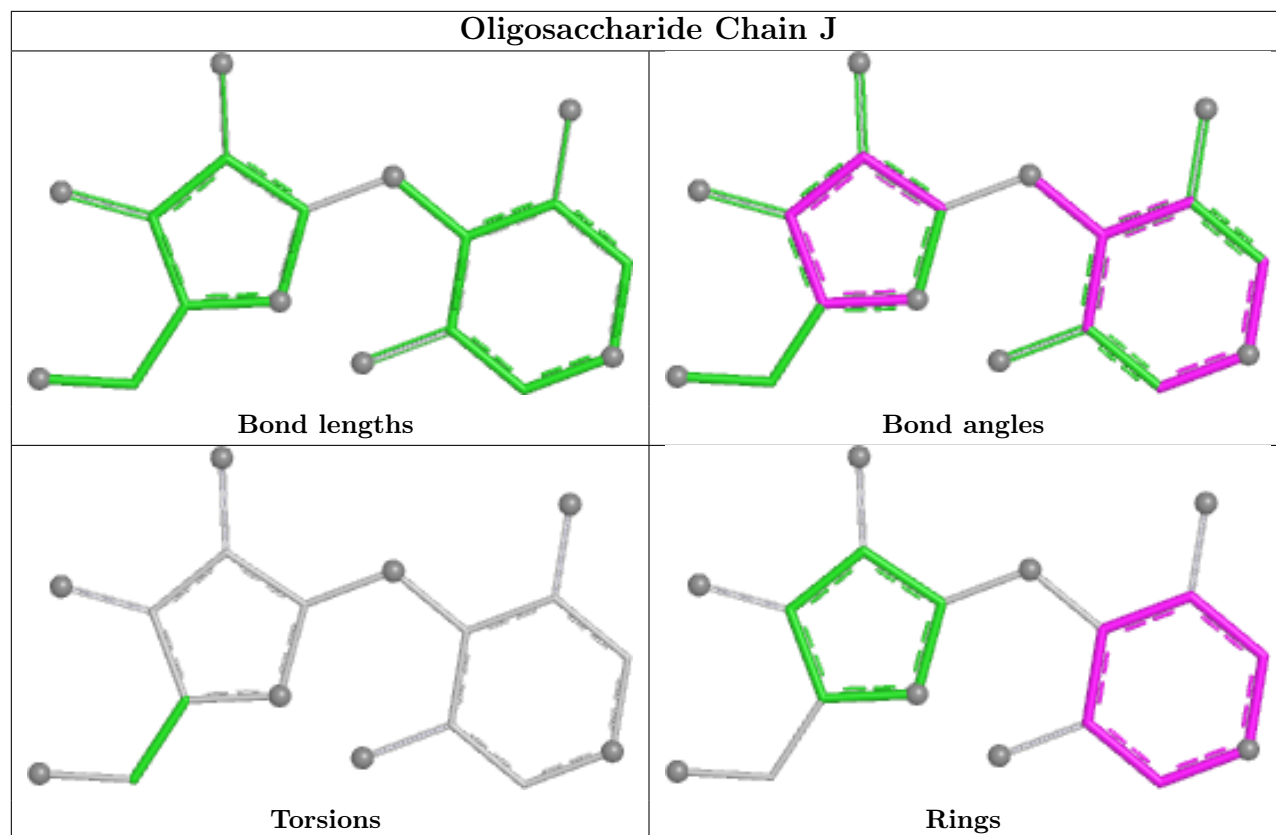


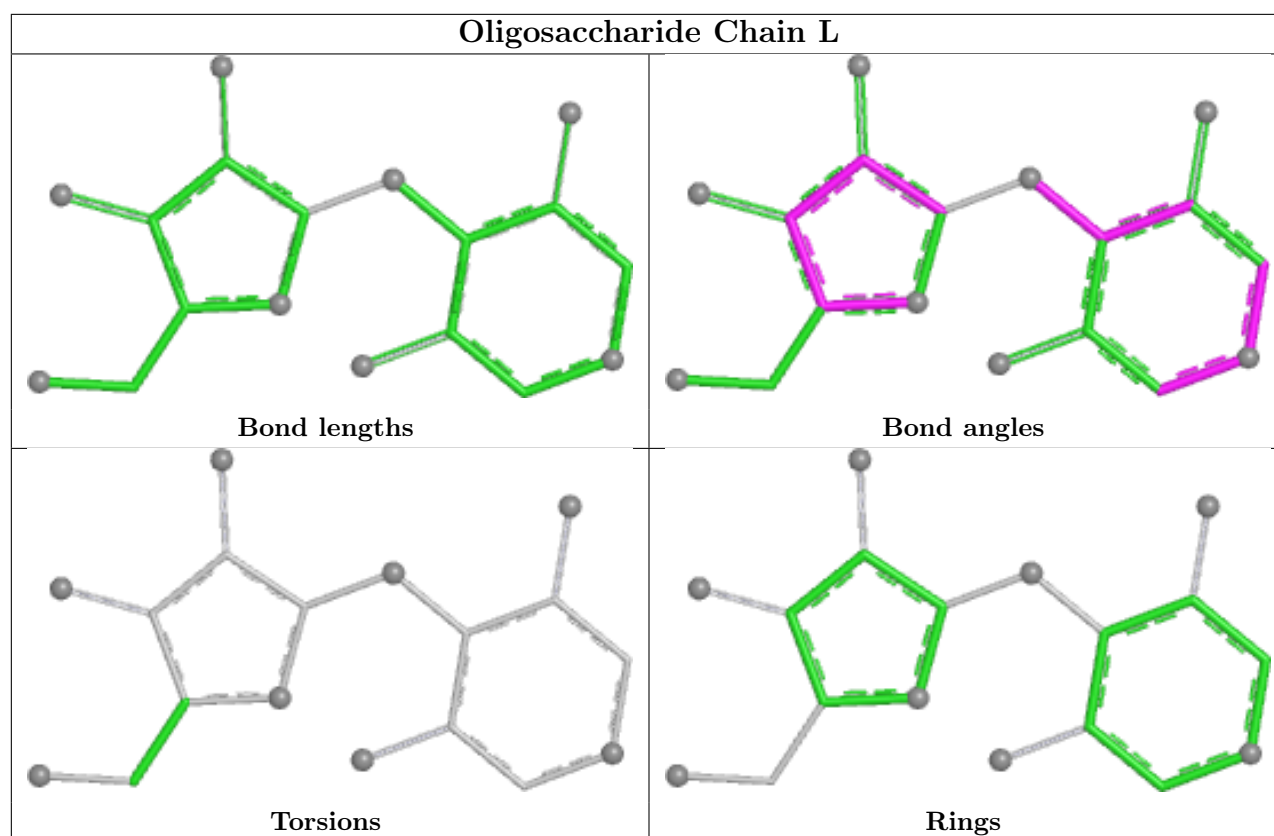
Oligosaccharide Chain H



Oligosaccharide Chain I







5.6 Ligand geometry [i](#)

9 ligands 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	$\# Z > 2$
3	EDO	C	1503	-	3,3,3	0.51	0	2,2,2	0.25	0
3	EDO	B	1503	-	3,3,3	0.54	0	2,2,2	0.15	0
3	EDO	F	1503	-	3,3,3	0.44	0	2,2,2	0.28	0
3	EDO	E	1504	-	3,3,3	0.40	0	2,2,2	0.52	0
3	EDO	D	1503	-	3,3,3	0.44	0	2,2,2	0.34	0
3	EDO	A	1504	-	3,3,3	0.50	0	2,2,2	0.23	0
3	EDO	C	1504	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	E	1503	-	3,3,3	0.61	0	2,2,2	0.24	0
3	EDO	A	1503	-	3,3,3	0.52	0	2,2,2	0.19	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	EDO	C	1503	-	-	1/1/1/1	-
3	EDO	B	1503	-	-	1/1/1/1	-
3	EDO	F	1503	-	-	0/1/1/1	-
3	EDO	E	1504	-	-	0/1/1/1	-
3	EDO	D	1503	-	-	1/1/1/1	-
3	EDO	A	1504	-	-	1/1/1/1	-
3	EDO	C	1504	-	-	0/1/1/1	-
3	EDO	E	1503	-	-	0/1/1/1	-
3	EDO	A	1503	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1504	EDO	O1-C1-C2-O2
3	D	1503	EDO	O1-C1-C2-O2
3	A	1503	EDO	O1-C1-C2-O2
3	C	1503	EDO	O1-C1-C2-O2
3	B	1503	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	501/513 (97%)	0.63	27 (5%)	31	24	49, 53, 56, 64	0
1	B	500/513 (97%)	0.62	26 (5%)	33	26	49, 53, 57, 64	0
1	C	499/513 (97%)	0.64	34 (6%)	23	18	27, 53, 57, 64	1 (0%)
1	D	498/513 (97%)	0.66	19 (3%)	44	36	49, 53, 56, 64	0
1	E	497/513 (96%)	0.76	43 (8%)	16	13	49, 53, 56, 62	0
1	F	500/513 (97%)	0.71	47 (9%)	14	12	49, 53, 57, 64	0
All	All	2995/3078 (97%)	0.67	196 (6%)	25	20	27, 53, 56, 64	1 (0%)

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	ASN	5.2
1	F	367	GLY	4.7
1	E	431	ASN	4.7
1	B	348	ALA	4.3
1	E	398	LEU	4.0
1	D	437	VAL	3.9
1	A	302	GLU	3.8
1	C	120[A]	GLU	3.7
1	B	432	ILE	3.6
1	E	439	VAL	3.5
1	E	9	ASP	3.5
1	D	490	MET	3.5
1	B	429	ASN	3.4
1	C	484	ASP	3.4
1	E	416	TYR	3.4
1	E	478	ASP	3.4
1	A	476	ASN	3.4
1	F	445	MET	3.4
1	F	310	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	447	ASP	3.3
1	D	429	ASN	3.3
1	E	502	GLY	3.3
1	D	433	HIS	3.2
1	A	398	LEU	3.2
1	A	485	GLY	3.2
1	B	445	MET	3.2
1	A	484	ASP	3.2
1	A	469	GLY	3.2
1	B	437	VAL	3.1
1	E	480	SER	3.1
1	F	431	ASN	3.1
1	A	502	GLY	3.1
1	C	367	GLY	3.1
1	C	437	VAL	3.1
1	A	441	ASP	3.1
1	E	490	MET	3.1
1	E	4	ALA	3.0
1	E	482	PHE	3.0
1	D	488	THR	3.0
1	A	436	ILE	3.0
1	F	12	TYR	3.0
1	F	484	ASP	3.0
1	C	445	MET	3.0
1	E	432	ILE	3.0
1	F	489	SER	3.0
1	E	448	TYR	2.9
1	B	367	GLY	2.9
1	F	481	SER	2.9
1	B	490	MET	2.9
1	E	437	VAL	2.9
1	F	438	LEU	2.9
1	E	440	SER	2.9
1	D	432	ILE	2.9
1	B	441	ASP	2.9
1	C	478	ASP	2.9
1	B	491	LEU	2.9
1	D	366	GLY	2.8
1	F	308	GLN	2.8
1	D	430	ARG	2.8
1	E	488	THR	2.8
1	F	450	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	385	GLY	2.8
1	D	12	TYR	2.8
1	C	11	ASP	2.8
1	F	441	ASP	2.8
1	F	430	ARG	2.8
1	C	502	GLY	2.8
1	E	457	GLU	2.8
1	F	437	VAL	2.8
1	F	429	ASN	2.8
1	C	307	MET	2.8
1	E	310	GLU	2.7
1	A	447	ASP	2.7
1	E	400	ASP	2.7
1	F	502	GLY	2.7
1	E	436	ILE	2.7
1	C	485	GLY	2.7
1	A	478	ASP	2.7
1	F	409	ASP	2.7
1	F	482	PHE	2.7
1	E	12	TYR	2.7
1	C	439	VAL	2.7
1	C	239	ILE	2.6
1	C	482	PHE	2.6
1	E	491	LEU	2.6
1	E	486	ILE	2.6
1	B	3	LYS	2.6
1	F	488	THR	2.6
1	A	432	ILE	2.6
1	A	430	ARG	2.6
1	A	490	MET	2.6
1	E	441	ASP	2.6
1	B	430	ARG	2.6
1	B	409	ASP	2.6
1	C	486	ILE	2.5
1	E	449	ARG	2.5
1	E	304	ALA	2.5
1	C	446	LYS	2.5
1	F	364	ARG	2.5
1	E	399	HIS	2.5
1	D	502	GLY	2.5
1	F	486	ILE	2.5
1	F	9	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	501	ILE	2.4
1	A	482	PHE	2.4
1	F	490	MET	2.4
1	D	409	ASP	2.4
1	F	483	ASP	2.4
1	F	5	ARG	2.4
1	A	312	TRP	2.4
1	C	398	LEU	2.4
1	E	438	LEU	2.4
1	C	480	SER	2.4
1	D	312	TRP	2.4
1	D	416	TYR	2.4
1	F	448	TYR	2.4
1	D	485	GLY	2.4
1	B	419	GLU	2.4
1	A	307	MET	2.4
1	F	398	LEU	2.4
1	C	364	ARG	2.3
1	D	369	ALA	2.3
1	A	448	TYR	2.3
1	B	438	LEU	2.3
1	E	450	LEU	2.3
1	F	14	ILE	2.3
1	A	311	PRO	2.3
1	C	253	ALA	2.3
1	F	4	ALA	2.3
1	A	501	ILE	2.3
1	C	436	ILE	2.3
1	C	448	TYR	2.3
1	F	82	GLY	2.3
1	B	368	ALA	2.3
1	B	369	ALA	2.3
1	C	490	MET	2.3
1	E	469	GLY	2.3
1	B	395	ASN	2.3
1	E	487	LEU	2.3
1	C	458	HIS	2.3
1	F	107	ILE	2.3
1	C	416	TYR	2.3
1	E	6	MET	2.2
1	E	393	VAL	2.2
1	B	12	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	301	ASN	2.2
1	F	410	ILE	2.2
1	A	464	ARG	2.2
1	F	447	ASP	2.2
1	A	439	VAL	2.2
1	B	439	VAL	2.2
1	E	481	SER	2.2
1	C	4	ALA	2.2
1	C	459	GLN	2.2
1	A	434	GLU	2.2
1	C	443	ARG	2.2
1	E	458	HIS	2.2
1	D	483	ASP	2.2
1	B	307	MET	2.2
1	D	482	PHE	2.2
1	A	486	ILE	2.1
1	A	431	ASN	2.1
1	F	442	VAL	2.1
1	B	482	PHE	2.1
1	C	399	HIS	2.1
1	C	395	ASN	2.1
1	E	451	LEU	2.1
1	B	410	ILE	2.1
1	F	306	ILE	2.1
1	F	394	ILE	2.1
1	F	433	HIS	2.1
1	D	180	VAL	2.1
1	F	465	ASN	2.1
1	C	451	LEU	2.1
1	A	488	THR	2.1
1	E	220	THR	2.1
1	F	443	ARG	2.1
1	F	307	MET	2.1
1	F	393	VAL	2.1
1	F	366	GLY	2.1
1	F	444	GLY	2.1
1	E	178	TRP	2.1
1	E	489	SER	2.0
1	F	399	HIS	2.0
1	A	443	ARG	2.0
1	B	246	GLY	2.0
1	F	432	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	302	GLU	2.0
1	B	399	HIS	2.0
1	F	8	VAL	2.0
1	F	480	SER	2.0
1	B	450	LEU	2.0
1	C	10	LYS	2.0
1	E	421	GLU	2.0
1	E	442	VAL	2.0
1	E	498	VAL	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](#)

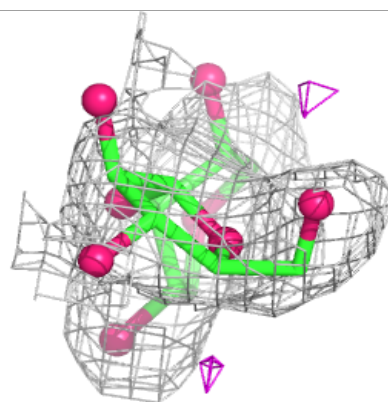
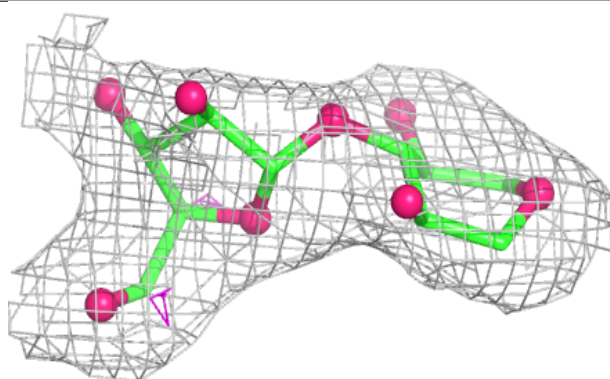
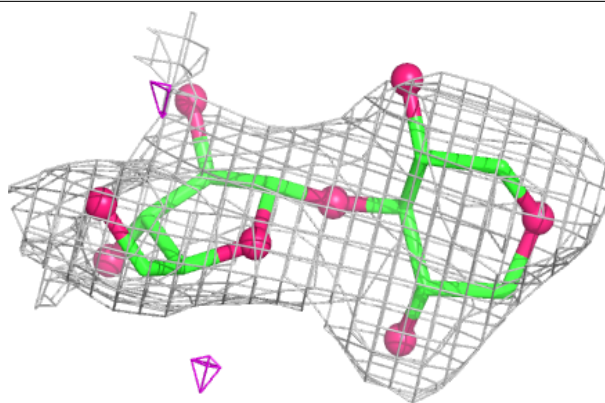
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	XYS	G	1	9/10	0.79	0.18	58,60,61,61	0
2	XYS	K	1	9/10	0.82	0.14	58,60,61,61	0
2	XYS	J	1	9/10	0.83	0.15	58,60,61,61	0
2	XYS	I	1	9/10	0.85	0.12	58,60,61,61	0
2	XYS	H	1	9/10	0.89	0.11	58,60,61,61	0
2	XYS	L	1	9/10	0.90	0.12	58,60,61,61	0
2	AHR	L	2	9/10	0.90	0.11	54,55,56,57	0
2	AHR	J	2	9/10	0.91	0.12	54,55,57,57	0
2	AHR	G	2	9/10	0.91	0.14	54,56,57,57	0
2	AHR	H	2	9/10	0.93	0.11	54,55,57,57	0
2	AHR	I	2	9/10	0.94	0.12	54,56,57,57	0
2	AHR	K	2	9/10	0.96	0.10	54,55,57,57	0

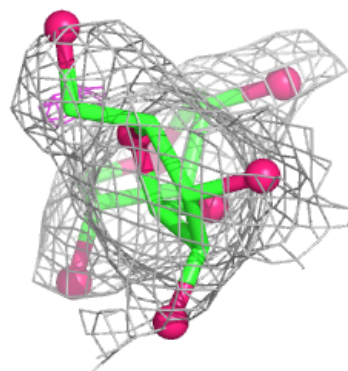
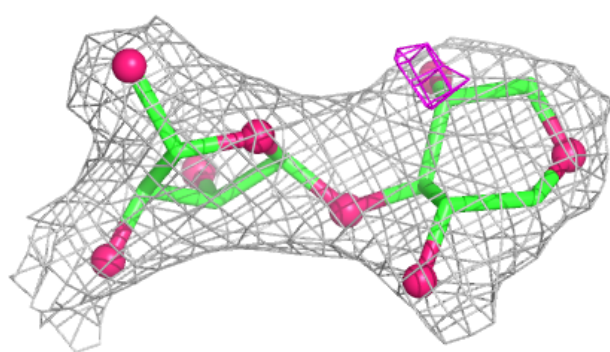
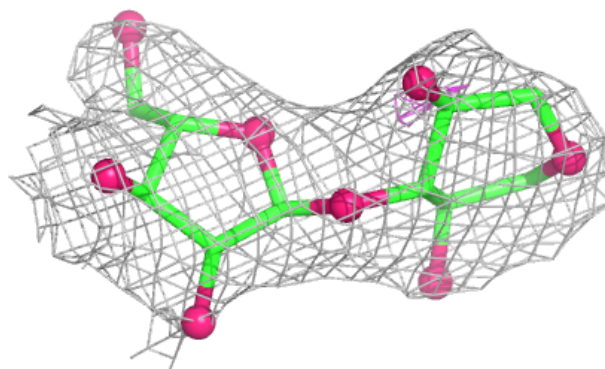
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

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

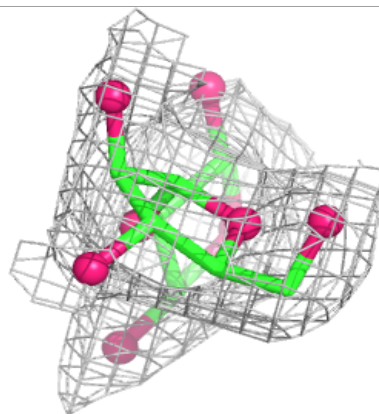
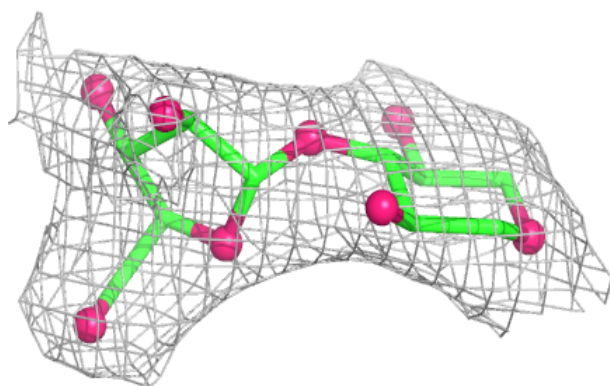
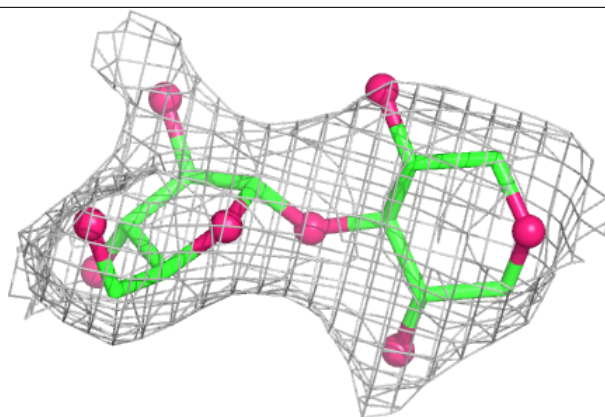
**Electron density around Chain H:**

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

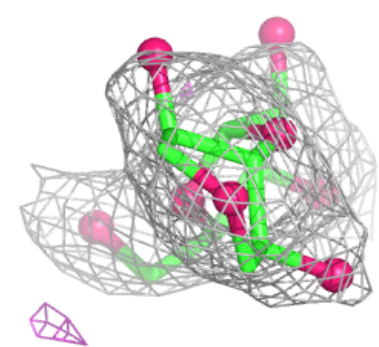
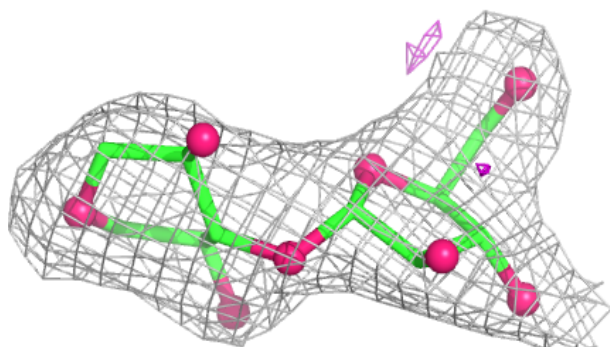
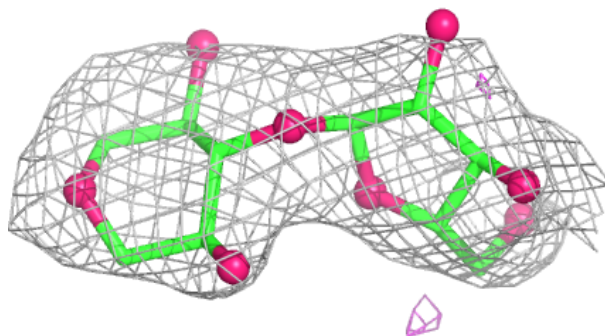


Electron density around Chain I:

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

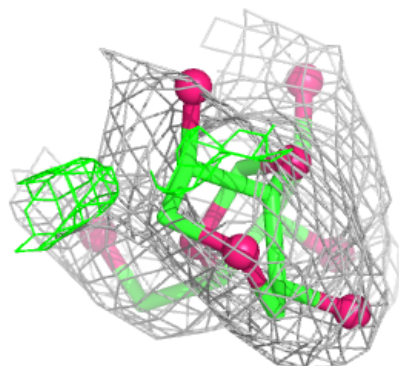
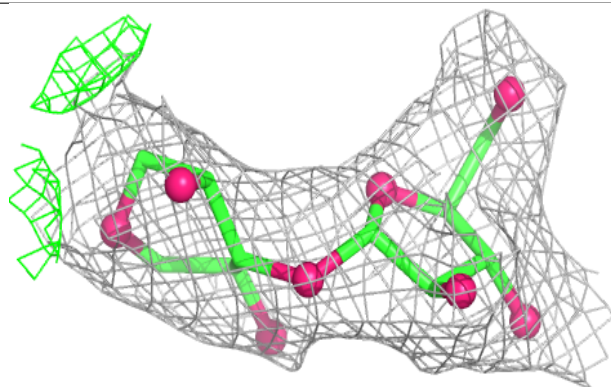
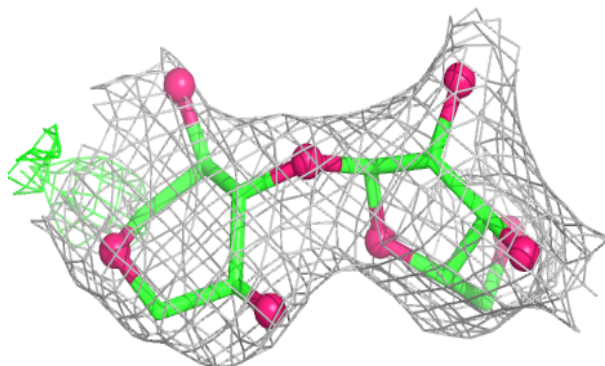
**Electron density around Chain J:**

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

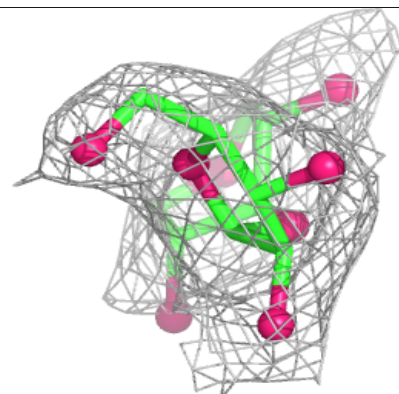
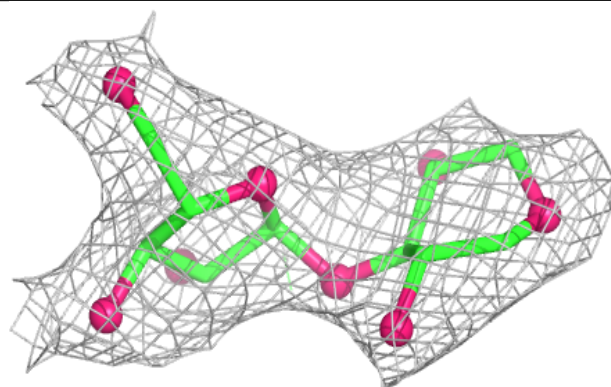
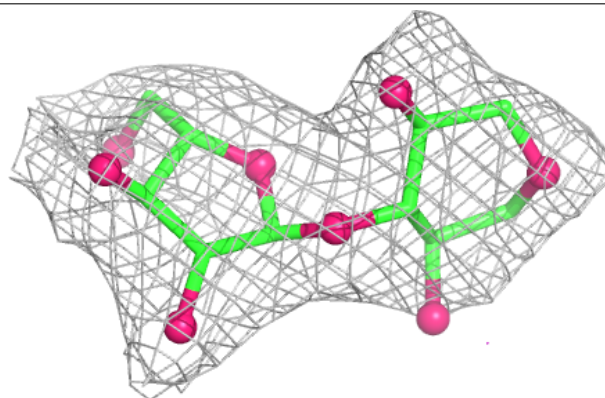


Electron density around Chain K:

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

**Electron density around Chain L:**

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



6.4 Ligands [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
3	EDO	F	1503	4/4	0.73	0.17	56,56,56,57	0
3	EDO	B	1503	4/4	0.75	0.20	56,57,58,58	0
3	EDO	C	1504	4/4	0.82	0.18	52,53,55,56	0
3	EDO	D	1503	4/4	0.82	0.16	57,57,57,58	0
3	EDO	E	1504	4/4	0.82	0.17	57,58,59,60	0
3	EDO	A	1504	4/4	0.82	0.14	53,54,54,54	0
3	EDO	A	1503	4/4	0.83	0.23	55,55,55,56	0
3	EDO	C	1503	4/4	0.89	0.17	57,59,59,60	0
3	EDO	E	1503	4/4	0.89	0.18	55,56,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.