



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:12 AM UTC

PDB ID : 7Z1I / pdb_00007z1i
Title : Plant myrosinase TGG1 from Arabidopsis thaliana
Authors : Gao, Y.; Farmer, E.; Jimenez-Sandoval, P.; Santiago, J.
Deposited on : 2022-02-24
Resolution : 3.09 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

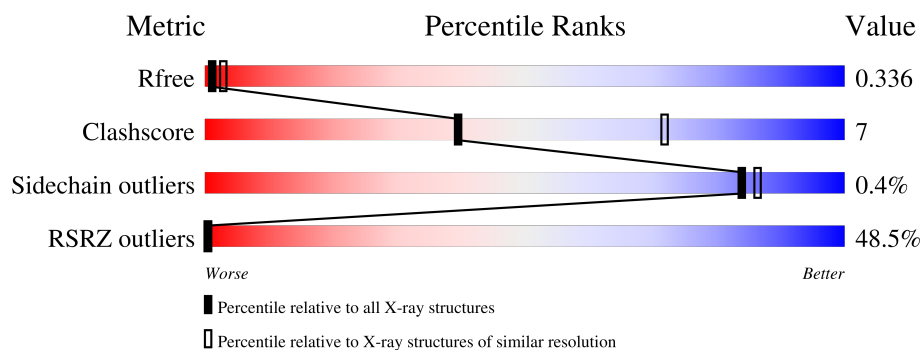
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	536	
1	B	536	
1	C	536	
1	D	536	
2	E	2	
2	F	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15094 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 Myrosinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3850	2467	638	728	17			
1	B	493	Total	C	N	O	S	0	0	0
			3845	2464	637	727	17			
1	C	493	Total	C	N	O	S	0	0	0
			3601	2281	600	705	15			
1	D	492	Total	C	N	O	S	0	0	0
			3390	2107	584	688	11			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	expression tag	UNP P37702
A	17	THR	-	expression tag	UNP P37702
A	18	MET	-	expression tag	UNP P37702
A	542	LEU	-	expression tag	UNP P37702
A	543	GLU	-	expression tag	UNP P37702
A	544	GLY	-	expression tag	UNP P37702
A	545	SER	-	expression tag	UNP P37702
A	546	GLU	-	expression tag	UNP P37702
A	547	ASN	-	expression tag	UNP P37702
A	548	LEU	-	expression tag	UNP P37702
A	549	TYR	-	expression tag	UNP P37702
A	550	PHE	-	expression tag	UNP P37702
A	551	GLN	-	expression tag	UNP P37702
B	16	ALA	-	expression tag	UNP P37702
B	17	THR	-	expression tag	UNP P37702
B	18	MET	-	expression tag	UNP P37702
B	542	LEU	-	expression tag	UNP P37702
B	543	GLU	-	expression tag	UNP P37702
B	544	GLY	-	expression tag	UNP P37702
B	545	SER	-	expression tag	UNP P37702
B	546	GLU	-	expression tag	UNP P37702

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Chain	Residue	Modelled	Actual	Comment	Reference
B	547	ASN	-	expression tag	UNP P37702
B	548	LEU	-	expression tag	UNP P37702
B	549	TYR	-	expression tag	UNP P37702
B	550	PHE	-	expression tag	UNP P37702
B	551	GLN	-	expression tag	UNP P37702
C	16	ALA	-	expression tag	UNP P37702
C	17	THR	-	expression tag	UNP P37702
C	18	MET	-	expression tag	UNP P37702
C	542	LEU	-	expression tag	UNP P37702
C	543	GLU	-	expression tag	UNP P37702
C	544	GLY	-	expression tag	UNP P37702
C	545	SER	-	expression tag	UNP P37702
C	546	GLU	-	expression tag	UNP P37702
C	547	ASN	-	expression tag	UNP P37702
C	548	LEU	-	expression tag	UNP P37702
C	549	TYR	-	expression tag	UNP P37702
C	550	PHE	-	expression tag	UNP P37702
C	551	GLN	-	expression tag	UNP P37702
D	16	ALA	-	expression tag	UNP P37702
D	17	THR	-	expression tag	UNP P37702
D	18	MET	-	expression tag	UNP P37702
D	542	LEU	-	expression tag	UNP P37702
D	543	GLU	-	expression tag	UNP P37702
D	544	GLY	-	expression tag	UNP P37702
D	545	SER	-	expression tag	UNP P37702
D	546	GLU	-	expression tag	UNP P37702
D	547	ASN	-	expression tag	UNP P37702
D	548	LEU	-	expression tag	UNP P37702
D	549	TYR	-	expression tag	UNP P37702
D	550	PHE	-	expression tag	UNP P37702
D	551	GLN	-	expression tag	UNP P37702

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	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: $C_8H_{15}NO_6$).



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	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	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		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

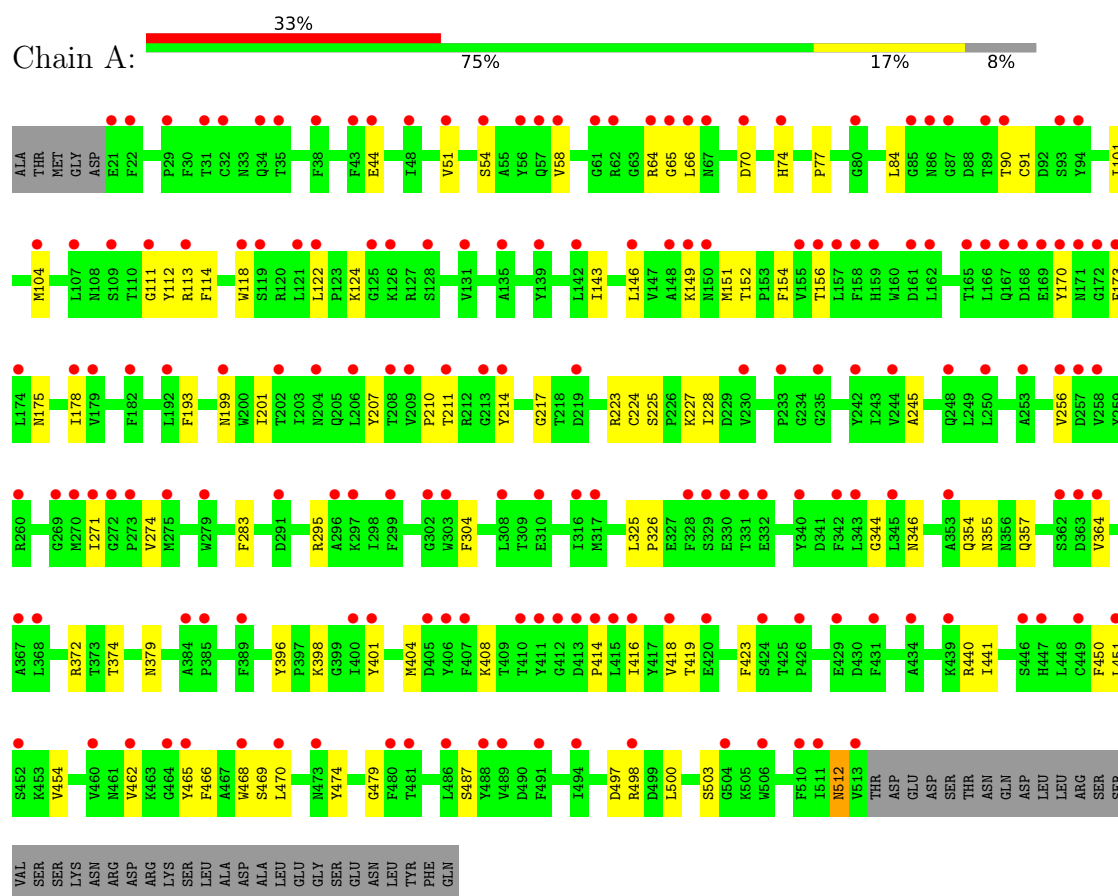
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

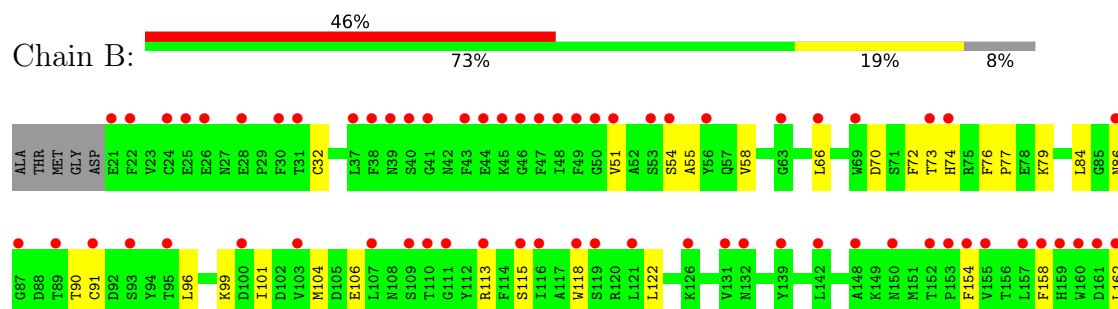
3 Residue-property plots

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: Myrosinase 1

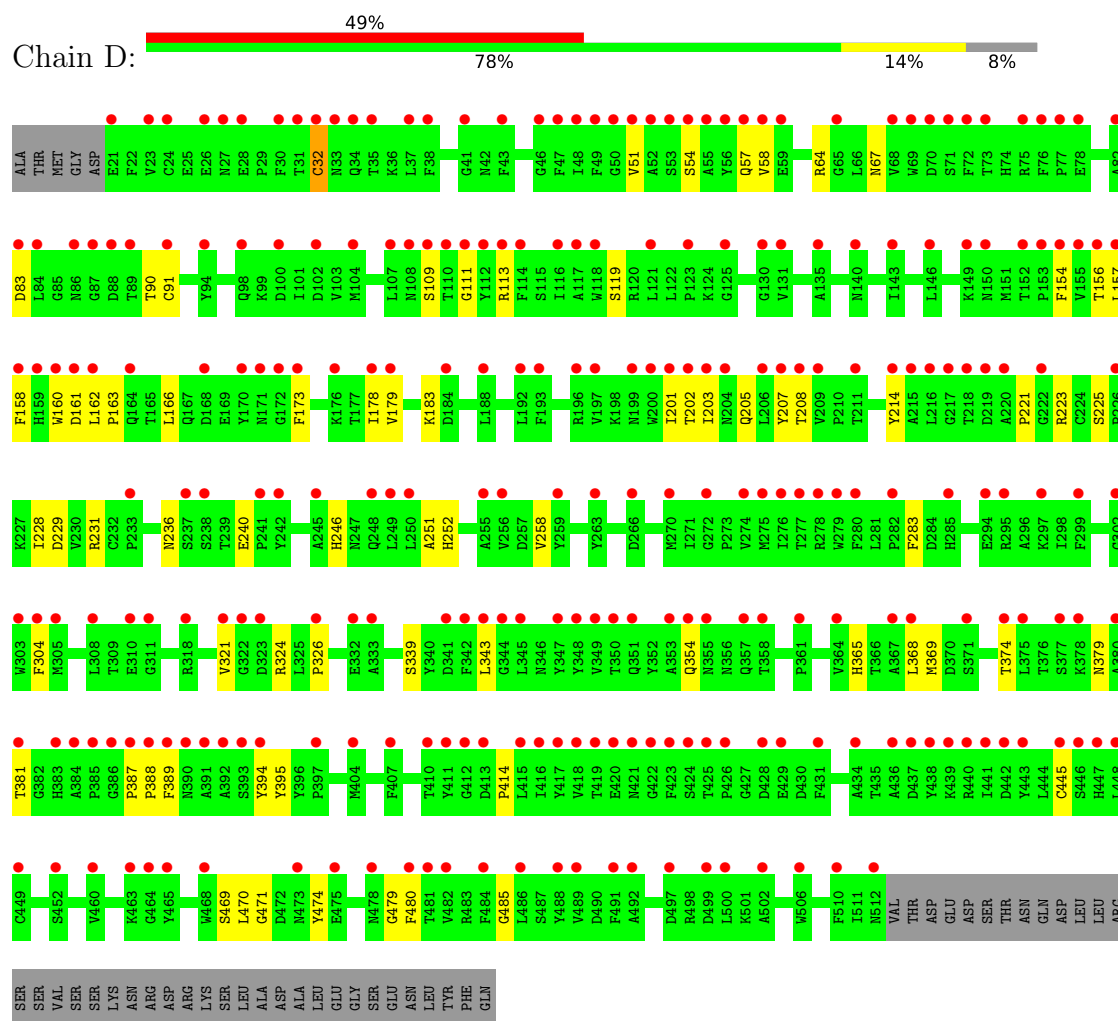


• Molecule 1: Myrosinase 1

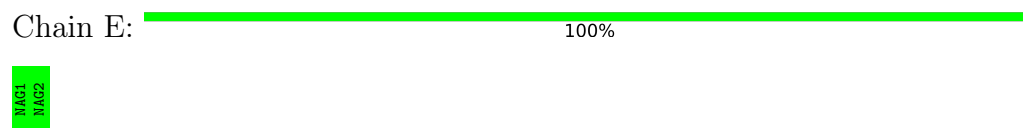




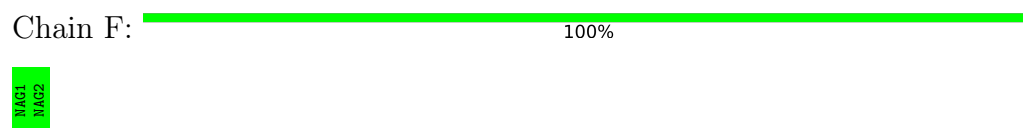
- Molecule 1: Myrosinase 1



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.99Å 88.99Å 120.98Å 108.79° 92.87° 102.97°	Depositor
Resolution (Å)	55.52 – 3.09 55.52 – 3.09	Depositor EDS
% Data completeness (in resolution range)	98.0 (55.52-3.09) 84.2 (55.52-3.09)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.317 , 0.341 0.313 , 0.336	Depositor DCC
R_{free} test set	2398 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	60.6	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 110.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15094	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.45% 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: CA, NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.10	0/3963	0.26	0/5398
1	B	0.10	0/3957	0.25	0/5391
1	C	0.08	0/3702	0.23	0/5073
1	D	0.08	0/3473	0.23	0/4778
All	All	0.09	0/15095	0.24	0/20640

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3850	0	3542	55	0
1	B	3845	0	3545	61	0
1	C	3601	0	3073	31	0
1	D	3390	0	2712	44	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
3	A	98	0	91	1	0
3	B	112	0	104	1	0
3	C	70	0	65	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	70	0	65	2	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
All	All	15094	0	13247	190	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 7.

All (190) 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:C:274:VAL:HG22	1:C:344:GLY:HA3	1.68	0.75
1:A:66:LEU:HD13	1:B:66:LEU:HD13	1.68	0.74
1:A:170:TYR:HB2	1:A:175:ASN:HD22	1.53	0.72
1:B:389:PHE:HD2	1:B:390:ASN:HD22	1.40	0.69
1:B:500:LEU:HD22	1:B:504:GLY:HA3	1.72	0.69
1:B:99:LYS:NZ	1:B:496:GLY:O	2.27	0.68
1:D:283:PHE:HA	1:D:379:ASN:HB2	1.76	0.68
1:A:51:VAL:HG21	1:A:470:LEU:HD13	1.79	0.64
1:A:295:ARG:NH2	1:A:355:ASN:OD1	2.30	0.64
1:B:77:PRO:HB2	1:B:84:LEU:HD22	1.81	0.63
1:D:67:ASN:HD22	1:D:161:ASP:HB2	1.65	0.62
1:B:91:CYS:O	1:B:498:ARG:NH2	2.34	0.61
1:A:487:SER:HB3	1:A:500:LEU:HD23	1.81	0.60
1:B:51:VAL:HG21	1:B:470:LEU:HD13	1.84	0.60
1:B:257:ASP:HB2	1:B:335:LEU:HD11	1.83	0.60
1:C:404:MET:HB3	1:C:460:VAL:HG11	1.81	0.60
1:A:346:ASN:OD1	1:A:419:THR:OG1	2.16	0.59
1:B:404:MET:HB3	1:B:460:VAL:HG11	1.84	0.59
1:B:253:ALA:HB1	1:B:335:LEU:HG	1.85	0.59
1:A:146:LEU:HB3	1:A:151:MET:HB2	1.84	0.58
1:B:380:ALA:HB3	3:B:603:NAG:H82	1.85	0.58
1:A:418:VAL:HB	1:A:465:TYR:HA	1.84	0.58
1:A:225:SER:HB2	1:A:228:ILE:HG12	1.85	0.58
1:A:357:GLN:HG3	1:A:372:ARG:HD3	1.86	0.57
1:B:187:ASP:OD1	1:B:263:TYR:OH	2.18	0.57
1:D:388:PRO:HA	1:D:394:TYR:HA	1.87	0.57
1:D:51:VAL:HG21	1:D:470:LEU:HD13	1.87	0.56
1:D:90:THR:OG1	1:D:91:CYS:N	2.39	0.56
1:A:154:PHE:HA	1:A:199:ASN:HB2	1.87	0.56
1:B:173:PHE:HA	1:B:178:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:VAL:HG22	1:B:344:GLY:HA3	1.87	0.55
1:C:408:LYS:HA	1:C:413:ASP:HA	1.89	0.55
1:D:156:THR:HA	1:D:201:ILE:HB	1.88	0.55
1:B:361:PRO:HG2	1:B:364:VAL:HG22	1.88	0.55
3:D:601:NAG:H83	3:D:601:NAG:H3	1.88	0.55
1:C:208:THR:HG23	1:C:212:ARG:HD3	1.89	0.54
1:C:418:VAL:HB	1:C:465:TYR:HA	1.89	0.54
1:B:421:ASN:HD22	1:B:465:TYR:HE2	1.55	0.54
1:B:101:ILE:HA	1:B:104:MET:HE3	1.90	0.54
1:B:225:SER:HB2	1:B:228:ILE:HG12	1.90	0.54
1:C:346:ASN:OD1	1:C:419:THR:OG1	2.23	0.54
1:A:364:VAL:O	1:A:364:VAL:HG12	2.07	0.53
1:A:497:ASP:OD1	3:A:606:NAG:O6	2.26	0.53
1:C:293:THR:HG22	1:C:297:LYS:HE3	1.90	0.53
1:A:245:ALA:HB1	1:A:304:PHE:HE1	1.73	0.53
1:B:379:ASN:OD1	1:B:382:GLY:N	2.42	0.53
1:D:236:ASN:HB3	1:D:240:GLU:HG3	1.89	0.53
1:B:325:LEU:HD12	1:B:326:PRO:HD2	1.91	0.53
1:D:113:ARG:HA	1:D:154:PHE:HB2	1.90	0.53
1:C:435:THR:HA	1:C:501:LYS:HG2	1.91	0.52
1:A:111:GLY:HA2	1:A:152:THR:H	1.75	0.52
1:B:497:ASP:N	1:B:497:ASP:OD1	2.42	0.52
1:D:469:SER:H	1:D:485:GLY:HA2	1.75	0.52
1:C:221:PRO:HG2	1:C:223:ARG:HG3	1.92	0.52
1:A:274:VAL:HG22	1:A:344:GLY:HA3	1.90	0.52
1:B:379:ASN:OD1	1:B:383:HIS:N	2.38	0.52
1:B:72:PHE:CZ	1:B:79:LYS:HD3	2.45	0.52
1:C:325:LEU:HD12	1:C:326:PRO:HD2	1.91	0.51
1:B:90:THR:OG1	1:B:91:CYS:N	2.43	0.51
1:B:451:LEU:HD11	1:B:462:VAL:HG11	1.92	0.51
1:A:77:PRO:HB2	1:A:84:LEU:HD22	1.93	0.51
1:A:91:CYS:O	1:A:498:ARG:NH2	2.43	0.51
1:D:321:VAL:HG12	1:D:324:ARG:HB2	1.93	0.51
1:D:389:PHE:H	1:D:394:TYR:HA	1.76	0.51
1:A:170:TYR:O	1:A:175:ASN:HB2	2.10	0.51
1:B:390:ASN:HD21	1:B:393:SER:HB3	1.75	0.51
1:A:90:THR:OG1	1:A:91:CYS:N	2.43	0.50
1:A:214:TYR:CE2	1:A:223:ARG:HD3	2.47	0.50
1:A:408:LYS:HA	1:A:414:PRO:HB3	1.93	0.49
1:A:325:LEU:HD12	1:A:326:PRO:HD2	1.93	0.49
1:A:70:ASP:O	1:A:74:HIS:ND1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:GLN:N	1:D:374:THR:O	2.46	0.49
1:A:451:LEU:HD11	1:A:462:VAL:HG11	1.95	0.49
1:C:225:SER:HB2	1:C:228:ILE:HG12	1.94	0.49
1:A:64:ARG:NH1	1:A:65:GLY:O	2.42	0.49
1:B:118:TRP:HE1	1:B:122:LEU:HD12	1.78	0.49
1:D:54:SER:HB2	1:D:57:GLN:HG3	1.95	0.48
1:A:416:ILE:HB	1:A:462:VAL:HG22	1.95	0.48
1:B:418:VAL:HB	1:B:465:TYR:HA	1.95	0.48
1:D:54:SER:O	1:D:58:VAL:HG22	2.13	0.48
1:A:156:THR:HA	1:A:201:ILE:HB	1.95	0.48
1:B:352:TYR:HE1	1:B:385:PRO:HD3	1.76	0.48
1:D:221:PRO:HG2	1:D:223:ARG:HG3	1.95	0.48
1:D:343:LEU:HD12	1:D:414:PRO:HG3	1.94	0.48
1:A:396:TYR:CZ	1:A:398:LYS:HB3	2.49	0.48
1:D:162:LEU:HD11	1:D:178:ILE:HD11	1.94	0.48
1:D:160:TRP:HZ2	1:D:205:GLN:HB2	1.78	0.48
1:C:67:ASN:HD22	1:C:161:ASP:HB2	1.79	0.47
1:B:73:THR:HG21	1:B:86:ASN:HB3	1.96	0.47
1:B:207:TYR:CZ	1:B:211:THR:HG21	2.48	0.47
1:D:109:SER:OG	1:D:111:GLY:O	2.31	0.47
1:D:158:PHE:HD2	1:D:203:ILE:HG23	1.79	0.47
1:D:225:SER:HB2	1:D:228:ILE:HG12	1.95	0.47
1:D:381:THR:HG21	3:D:604:NAG:H4	1.97	0.47
1:D:183:LYS:HG3	1:D:258:VAL:HG21	1.97	0.47
1:B:273:PRO:HD2	1:B:340:TYR:HB2	1.97	0.47
1:D:207:TYR:HD1	1:D:304:PHE:HE1	1.63	0.47
1:B:355:ASN:OD1	1:B:357:GLN:NE2	2.41	0.47
1:A:113:ARG:HA	1:A:154:PHE:O	2.15	0.46
1:C:471:GLY:C	1:C:485:GLY:HA3	2.41	0.46
1:C:497:ASP:N	1:C:497:ASP:OD1	2.48	0.46
1:D:158:PHE:HB3	1:D:203:ILE:HG12	1.96	0.46
1:D:179:VAL:HG13	1:D:251:ALA:HA	1.98	0.46
1:D:368:LEU:HD12	1:D:368:LEU:H	1.81	0.46
1:C:429:GLU:OE2	1:C:439:LYS:NZ	2.47	0.46
1:D:474:TYR:CE2	1:D:479:GLY:HA2	2.51	0.46
1:A:143:ILE:HD13	1:A:193:PHE:HB3	1.97	0.46
1:A:207:TYR:CZ	1:A:211:THR:HG21	2.51	0.46
1:A:401:TYR:HB2	1:A:450:PHE:HB3	1.97	0.46
1:A:468:TRP:HA	1:A:469:SER:HA	1.55	0.46
1:C:173:PHE:HA	1:C:178:ILE:HG21	1.98	0.46
1:B:54:SER:O	1:B:58:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASP:O	1:C:74:HIS:ND1	2.39	0.45
1:B:32:CYS:HB2	1:B:445:CYS:HB2	1.59	0.45
1:A:149:LYS:HB3	1:A:151:MET:HE2	1.98	0.45
1:B:390:ASN:ND2	1:B:393:SER:HB3	2.31	0.45
1:B:158:PHE:HD2	1:B:203:ILE:HG23	1.81	0.45
1:C:204:ASN:OD1	1:C:205:GLN:HG3	2.16	0.45
1:A:54:SER:O	1:A:58:VAL:HG22	2.17	0.45
1:B:225:SER:OG	1:B:236:ASN:O	2.35	0.45
1:D:365:HIS:CE1	1:D:369:MET:HB2	2.52	0.45
1:D:387:PRO:HB2	1:D:395:TYR:CE2	2.52	0.45
1:A:210:PRO:HG2	1:A:245:ALA:HB2	1.99	0.44
1:B:441:ILE:HG12	1:B:503:SER:HA	1.98	0.44
1:C:179:VAL:HG13	1:C:251:ALA:HA	1.99	0.44
1:C:460:VAL:HG12	1:C:462:VAL:HG23	2.00	0.44
1:D:64:ARG:NH1	1:D:119:SER:OG	2.46	0.44
1:A:173:PHE:HA	1:A:178:ILE:HG21	2.00	0.44
1:A:217:GLY:HA3	1:A:224:CYS:HB3	1.98	0.44
1:C:335:LEU:O	1:C:339:SER:HB3	2.16	0.44
1:B:460:VAL:HG12	1:B:462:VAL:HG23	2.00	0.44
1:D:387:PRO:HB2	1:D:395:TYR:CZ	2.52	0.44
1:A:354:GLN:HG2	1:A:374:THR:HB	2.00	0.44
1:C:64:ARG:HD3	1:C:120:ARG:NH2	2.33	0.44
1:C:346:ASN:CG	1:C:420:GLU:HB2	2.43	0.43
1:D:157:LEU:HD12	1:D:202:THR:HA	2.00	0.43
1:B:217:GLY:HA3	1:B:224:CYS:HB3	2.00	0.43
1:B:487:SER:HB3	1:B:500:LEU:HD23	2.00	0.43
1:A:118:TRP:HE1	1:A:122:LEU:HD12	1.84	0.43
1:A:256:VAL:HA	1:A:271:ILE:HD13	2.00	0.43
1:A:112:TYR:CE2	1:A:114:PHE:HB3	2.53	0.43
1:D:173:PHE:HA	1:D:178:ILE:HG21	1.99	0.43
1:D:246:HIS:ND1	1:D:326:PRO:HB2	2.33	0.43
1:D:321:VAL:HA	1:D:324:ARG:HH21	1.82	0.43
1:A:283:PHE:O	1:A:379:ASN:HB2	2.19	0.43
1:B:214:TYR:CE2	1:B:223:ARG:HD3	2.53	0.43
1:B:113:ARG:HA	1:B:154:PHE:O	2.18	0.43
1:D:32:CYS:HB2	1:D:445:CYS:HB2	1.40	0.43
1:B:195:ASP:OD1	1:B:195:ASP:N	2.51	0.42
1:A:44:GLU:H	1:A:44:GLU:CD	2.27	0.42
1:B:106:GLU:CD	1:B:500:LEU:HD12	2.45	0.42
1:B:346:ASN:OD1	1:B:419:THR:OG1	2.30	0.42
1:D:214:TYR:CE1	1:D:223:ARG:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ILE:HG12	1:A:503:SER:HA	2.01	0.42
1:B:55:ALA:H	1:B:115:SER:HB3	1.83	0.42
1:C:158:PHE:HB3	1:C:203:ILE:HG12	2.02	0.42
1:C:420:GLU:HG2	1:C:468:TRP:CE3	2.54	0.42
1:A:418:VAL:O	1:A:466:PHE:N	2.49	0.42
1:B:96:LEU:HB3	1:B:99:LYS:HD3	2.02	0.42
1:B:437:ASP:O	1:B:441:ILE:HG13	2.20	0.42
1:D:229:ASP:CG	1:D:231:ARG:HE	2.28	0.42
1:C:455:ILE:HD11	1:C:462:VAL:HB	2.02	0.42
1:B:174:LEU:HD12	1:B:174:LEU:HA	1.91	0.42
1:B:203:ILE:HB	1:B:206:LEU:CD2	2.50	0.42
1:A:423:PHE:O	1:A:440:ARG:NH2	2.52	0.42
1:B:70:ASP:O	1:B:74:HIS:ND1	2.43	0.42
1:A:227:LYS:CB	1:A:364:VAL:HG22	2.50	0.41
1:C:468:TRP:HA	1:C:469:SER:HA	1.59	0.41
1:C:274:VAL:HG13	1:C:344:GLY:O	2.20	0.41
1:D:205:GLN:HB3	1:D:208:THR:OG1	2.21	0.41
1:B:162:LEU:HD12	1:B:163:PRO:HD2	2.02	0.41
1:A:404:MET:SD	1:A:416:ILE:HG21	2.61	0.41
1:B:179:VAL:HG13	1:B:251:ALA:HA	2.03	0.41
1:A:474:TYR:CE1	1:A:479:GLY:HA2	2.55	0.41
1:D:471:GLY:C	1:D:485:GLY:HA3	2.45	0.41
1:A:101:ILE:HA	1:A:104:MET:HE3	2.01	0.41
1:B:468:TRP:HA	1:B:469:SER:HA	1.55	0.41
1:B:76:PHE:HB2	1:B:79:LYS:HB2	2.03	0.41
1:B:424:SER:HB3	1:B:484:PHE:CZ	2.56	0.41
1:A:124:LYS:HD2	1:B:168:ASP:HA	2.01	0.41
1:D:252:HIS:NE2	1:D:339:SER:O	2.54	0.41
1:C:51:VAL:HG21	1:C:470:LEU:HD13	2.03	0.40
1:C:205:GLN:NE2	1:C:420:GLU:OE1	2.54	0.40
1:A:404:MET:HB2	1:A:454:VAL:HG21	2.03	0.40
1:D:163:PRO:HD2	1:D:166:LEU:HD12	2.03	0.40
1:B:395:TYR:CD2	1:B:447:HIS:HE1	2.40	0.40
1:A:512:ASN:HD22	1:A:512:ASN:HA	1.52	0.40
1:B:262:LYS:HE3	1:B:263:TYR:CE2	2.56	0.40
1:C:61:GLY:N	1:C:88:ASP:O	2.53	0.40
1:D:83:ASP:OD2	1:D:480:PHE:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	385/458 (84%)	384 (100%)	1 (0%)	86	87
1	B	395/458 (86%)	394 (100%)	1 (0%)	86	87
1	C	336/458 (73%)	334 (99%)	2 (1%)	78	83
1	D	285/458 (62%)	284 (100%)	1 (0%)	84	86
All	All	1401/1832 (76%)	1396 (100%)	5 (0%)	84	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	512	ASN
1	B	512	ASN
1	C	32	CYS
1	C	236	ASN
1	D	32	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	ASN
1	B	390	ASN
1	C	42	ASN
1	C	248	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	E	1	1,2	14,14,15	0.37	0	17,19,21	0.60	0
2	NAG	E	2	2	14,14,15	0.37	0	17,19,21	0.41	0
2	NAG	F	1	1,2	14,14,15	0.33	0	17,19,21	0.51	0
2	NAG	F	2	2	14,14,15	0.35	0	17,19,21	0.37	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
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

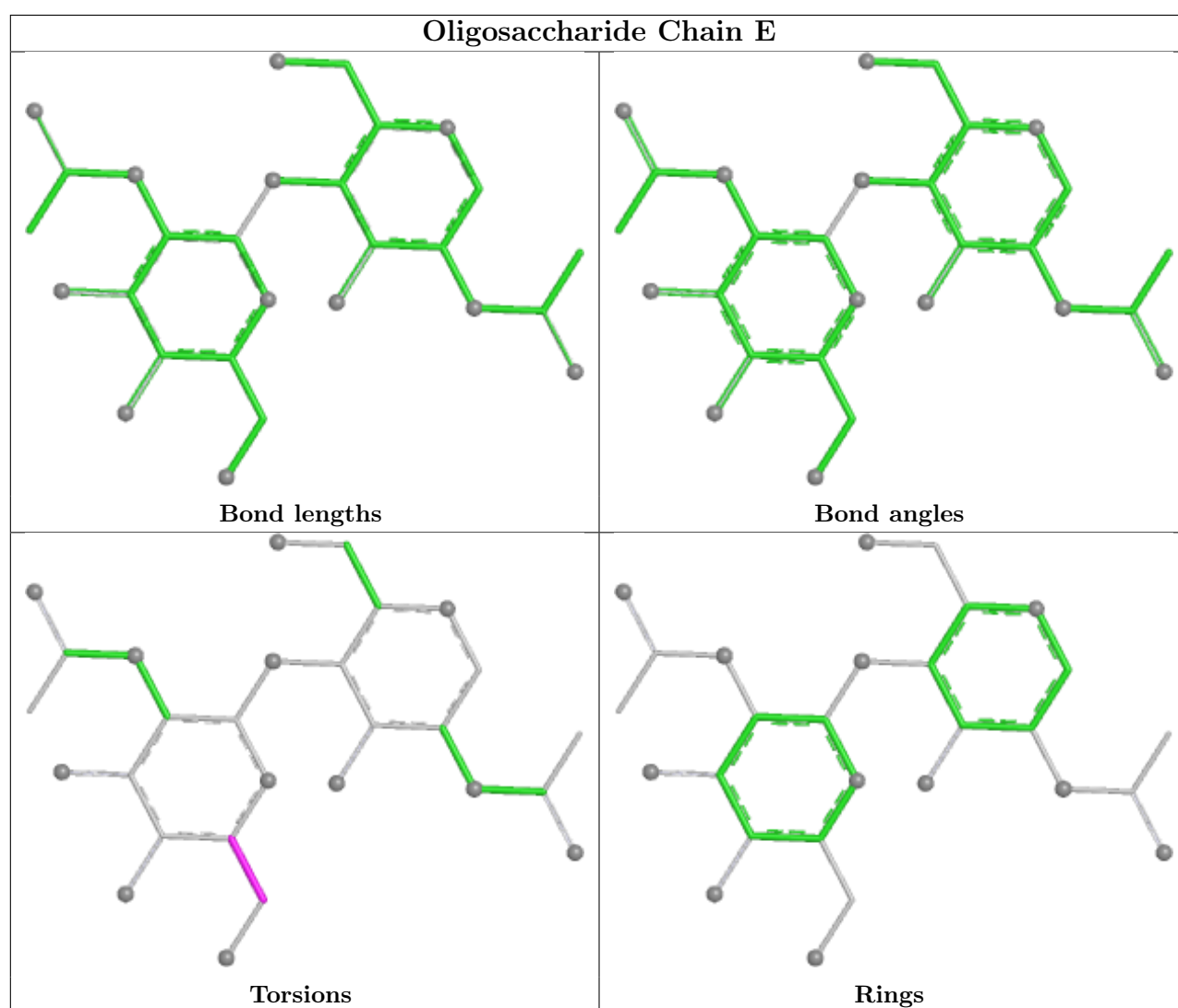
All (6) torsion outliers are listed below:

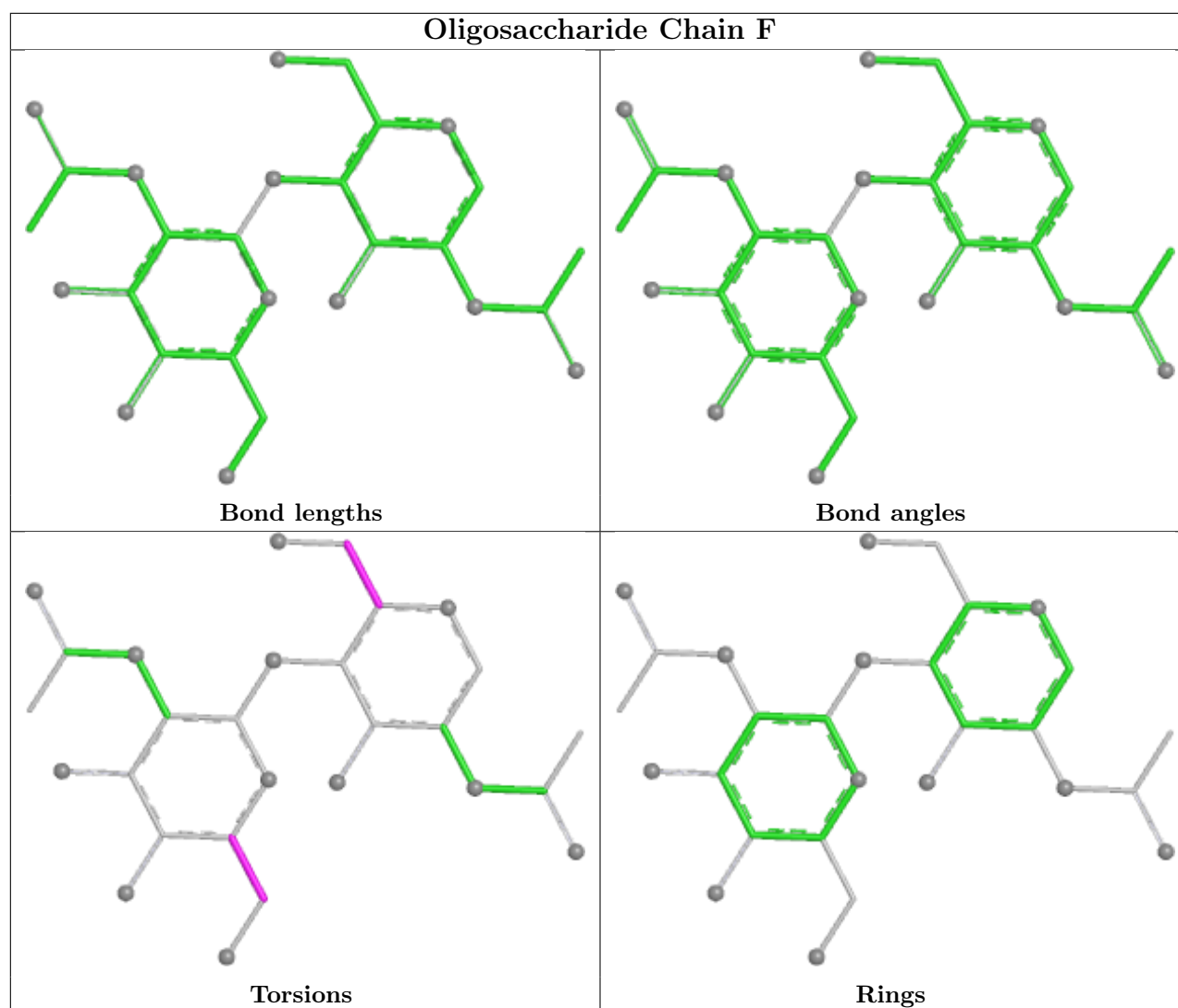
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6

There are no ring outliers.

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.





5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	604	1	14,14,15	0.25	0	17,19,21	0.44	0
3	NAG	A	606	1	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	B	604	1	14,14,15	0.23	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	601	1	14,14,15	0.22	0	17,19,21	0.55	0
3	NAG	D	602	1	14,14,15	0.30	0	17,19,21	0.54	0
3	NAG	A	605	1	14,14,15	1.42	1 (7%)	17,19,21	1.26	2 (11%)
3	NAG	D	604	1	14,14,15	0.32	0	17,19,21	0.51	0
3	NAG	A	603	1	14,14,15	0.35	0	17,19,21	0.46	0
3	NAG	C	605	1	14,14,15	0.35	0	17,19,21	0.53	0
3	NAG	B	607	1	14,14,15	0.32	0	17,19,21	0.49	0
3	NAG	B	608	1	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	A	602	1	14,14,15	0.19	0	17,19,21	0.54	0
3	NAG	D	605	1	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	A	607	1	14,14,15	0.26	0	17,19,21	0.55	0
3	NAG	C	602	1	14,14,15	0.31	0	17,19,21	0.46	0
3	NAG	C	604	1	14,14,15	0.21	0	17,19,21	0.46	0
3	NAG	B	606	1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	D	603	1	14,14,15	0.25	0	17,19,21	0.42	0
3	NAG	B	601	1	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	C	603	1	14,14,15	0.60	0	17,19,21	1.29	1 (5%)
3	NAG	B	603	1	14,14,15	0.34	0	17,19,21	0.36	0
3	NAG	D	601	1	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
3	NAG	B	605	1	14,14,15	1.24	1 (7%)	17,19,21	2.56	2 (11%)
3	NAG	C	601	1	14,14,15	0.33	0	17,19,21	0.49	0
3	NAG	B	602	1	14,14,15	0.35	0	17,19,21	0.59	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	604	1	-	2/6/23/26	0/1/1/1
3	NAG	A	606	1	-	2/6/23/26	0/1/1/1
3	NAG	B	604	1	-	2/6/23/26	0/1/1/1
3	NAG	A	601	1	-	2/6/23/26	0/1/1/1
3	NAG	D	602	1	-	3/6/23/26	0/1/1/1
3	NAG	A	605	1	-	2/6/23/26	0/1/1/1
3	NAG	D	604	1	-	4/6/23/26	0/1/1/1
3	NAG	A	603	1	-	4/6/23/26	0/1/1/1
3	NAG	C	605	1	-	2/6/23/26	0/1/1/1
3	NAG	B	607	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	608	1	-	0/6/23/26	0/1/1/1
3	NAG	A	602	1	-	4/6/23/26	0/1/1/1
3	NAG	D	605	1	-	2/6/23/26	0/1/1/1
3	NAG	A	607	1	-	3/6/23/26	0/1/1/1
3	NAG	C	602	1	-	4/6/23/26	0/1/1/1
3	NAG	C	604	1	-	2/6/23/26	0/1/1/1
3	NAG	B	606	1	-	3/6/23/26	0/1/1/1
3	NAG	D	603	1	-	2/6/23/26	0/1/1/1
3	NAG	B	601	1	-	2/6/23/26	0/1/1/1
3	NAG	C	603	1	-	3/6/23/26	0/1/1/1
3	NAG	B	603	1	-	2/6/23/26	0/1/1/1
3	NAG	D	601	1	-	6/6/23/26	0/1/1/1
3	NAG	B	605	1	-	1/6/23/26	0/1/1/1
3	NAG	C	601	1	-	0/6/23/26	0/1/1/1
3	NAG	B	602	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	NAG	O5-C1	-5.07	1.35	1.43
3	B	605	NAG	O5-C1	4.44	1.51	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	NAG	C1-O5-C5	10.12	125.75	112.19
3	C	603	NAG	C1-O5-C5	5.00	118.88	112.19
3	D	601	NAG	C2-N2-C7	4.57	129.02	122.90
3	A	605	NAG	C3-C4-C5	4.16	117.77	110.23
3	A	605	NAG	C4-C3-C2	2.38	114.51	111.02
3	D	601	NAG	C1-C2-N2	2.19	113.88	110.43
3	B	605	NAG	O5-C5-C4	2.11	115.96	110.83

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	607	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	604	NAG	O5-C5-C6-O6
3	B	607	NAG	O5-C5-C6-O6
3	B	603	NAG	O5-C5-C6-O6
3	B	602	NAG	O5-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	B	601	NAG	O5-C5-C6-O6
3	D	604	NAG	O5-C5-C6-O6
3	A	603	NAG	O5-C5-C6-O6
3	C	603	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	A	603	NAG	C4-C5-C6-O6
3	A	604	NAG	C4-C5-C6-O6
3	B	603	NAG	C4-C5-C6-O6
3	B	604	NAG	O5-C5-C6-O6
3	B	601	NAG	C4-C5-C6-O6
3	C	602	NAG	C4-C5-C6-O6
3	C	604	NAG	O5-C5-C6-O6
3	C	603	NAG	C4-C5-C6-O6
3	A	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O7-C7-N2-C2
3	A	603	NAG	C8-C7-N2-C2
3	A	603	NAG	O7-C7-N2-C2
3	C	602	NAG	C8-C7-N2-C2
3	C	602	NAG	O7-C7-N2-C2
3	D	601	NAG	C8-C7-N2-C2
3	D	601	NAG	O7-C7-N2-C2
3	C	602	NAG	O5-C5-C6-O6
3	A	605	NAG	C4-C5-C6-O6
3	B	602	NAG	C4-C5-C6-O6
3	B	606	NAG	O5-C5-C6-O6
3	C	604	NAG	C4-C5-C6-O6
3	D	603	NAG	C4-C5-C6-O6
3	C	605	NAG	C4-C5-C6-O6
3	A	606	NAG	O5-C5-C6-O6
3	D	604	NAG	C4-C5-C6-O6
3	A	606	NAG	C4-C5-C6-O6
3	A	601	NAG	C4-C5-C6-O6
3	D	601	NAG	C4-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	A	607	NAG	O5-C5-C6-O6
3	D	601	NAG	O5-C5-C6-O6
3	D	602	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	605	NAG	O5-C5-C6-O6
3	B	604	NAG	C4-C5-C6-O6
3	D	603	NAG	O5-C5-C6-O6
3	A	605	NAG	O5-C5-C6-O6
3	C	605	NAG	O5-C5-C6-O6
3	A	607	NAG	C1-C2-N2-C7
3	D	602	NAG	C1-C2-N2-C7
3	D	605	NAG	C1-C2-N2-C7
3	D	604	NAG	C3-C2-N2-C7
3	D	605	NAG	C3-C2-N2-C7
3	B	606	NAG	C4-C5-C6-O6
3	B	606	NAG	C1-C2-N2-C7
3	C	603	NAG	C1-C2-N2-C7
3	D	601	NAG	C1-C2-N2-C7
3	D	604	NAG	C1-C2-N2-C7
3	A	607	NAG	C3-C2-N2-C7
3	D	601	NAG	C3-C2-N2-C7
3	D	602	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	606	NAG	1	0
3	D	604	NAG	1	0
3	B	603	NAG	1	0
3	D	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	493/536 (91%)	1.80	175 (35%) 1 0	60, 95, 129, 156	0
1	B	493/536 (91%)	2.12	247 (50%) 0 0	80, 121, 154, 182	0
1	C	493/536 (91%)	2.22	270 (54%) 0 0	101, 148, 218, 234	0
1	D	492/536 (91%)	2.23	264 (53%) 0 0	100, 149, 198, 226	0
All	All	1971/2144 (91%)	2.09	956 (48%) 0 0	60, 127, 199, 234	0

All (956) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	272	GLY	7.9
1	D	419	THR	6.7
1	B	269	GLY	6.7
1	A	161	ASP	6.4
1	D	350	THR	6.3
1	C	421	ASN	5.7
1	D	351	GLN	5.7
1	D	53	SER	5.5
1	C	481	THR	5.3
1	C	470	LEU	5.2
1	B	276	ILE	5.1
1	B	87	GLY	5.1
1	C	87	GLY	5.0
1	C	100	ASP	5.0
1	C	272	GLY	5.0
1	D	506	TRP	5.0
1	D	161	ASP	4.9
1	A	272	GLY	4.9
1	D	157	LEU	4.8
1	D	303	TRP	4.7
1	B	161	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	46	GLY	4.7
1	D	418	VAL	4.7
1	B	206	LEU	4.7
1	D	275	MET	4.7
1	C	269	GLY	4.6
1	B	467	ALA	4.6
1	A	158	PHE	4.6
1	C	350	THR	4.6
1	D	349	VAL	4.6
1	C	110	THR	4.5
1	B	109	SER	4.5
1	D	199	ASN	4.5
1	D	89	THR	4.4
1	B	464	GLY	4.4
1	D	484	PHE	4.4
1	C	498	ARG	4.4
1	D	214	TYR	4.3
1	D	384	ALA	4.3
1	D	206	LEU	4.3
1	C	56	TYR	4.3
1	C	513	VAL	4.3
1	D	207	TYR	4.3
1	C	276	ILE	4.3
1	C	279	TRP	4.3
1	C	345	LEU	4.3
1	A	85	GLY	4.2
1	D	91	CYS	4.2
1	C	161	ASP	4.2
1	A	414	PRO	4.2
1	B	303	TRP	4.1
1	B	465	TYR	4.1
1	C	411	TYR	4.1
1	D	411	TYR	4.1
1	D	385	PRO	4.1
1	D	464	GLY	4.1
1	C	277	THR	4.1
1	D	465	TYR	4.1
1	A	21	GLU	4.1
1	D	270	MET	4.1
1	B	328	PHE	4.1
1	C	299	PHE	4.1
1	C	143	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	150	ASN	4.1
1	A	109	SER	4.1
1	C	51	VAL	4.1
1	B	401	TYR	4.1
1	B	351	GLN	4.1
1	D	112	TYR	4.1
1	B	327	GLU	4.1
1	C	152	THR	4.0
1	C	67	ASN	4.0
1	C	478	ASN	4.0
1	B	410	THR	4.0
1	C	484	PHE	4.0
1	C	160	TRP	4.0
1	C	278	ARG	4.0
1	C	465	TYR	4.0
1	D	54	SER	4.0
1	D	153	PRO	4.0
1	A	214	TYR	4.0
1	B	53	SER	4.0
1	B	350	THR	4.0
1	B	51	VAL	3.9
1	B	131	VAL	3.9
1	B	204	ASN	3.9
1	C	486	LEU	3.9
1	B	315	ASP	3.9
1	B	160	TRP	3.9
1	B	345	LEU	3.9
1	B	279	TRP	3.9
1	D	155	VAL	3.9
1	C	125	GLY	3.9
1	A	511	ILE	3.9
1	B	416	ILE	3.9
1	C	69	TRP	3.9
1	D	299	PHE	3.8
1	C	302	GLY	3.8
1	C	173	PHE	3.8
1	D	280	PHE	3.8
1	C	174	LEU	3.8
1	B	219	ASP	3.8
1	C	68	VAL	3.8
1	B	257	ASP	3.8
1	D	255	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	51	VAL	3.8
1	D	256	VAL	3.8
1	B	50	GLY	3.8
1	B	385	PRO	3.8
1	C	431	PHE	3.8
1	C	480	PHE	3.8
1	D	218	THR	3.8
1	B	270	MET	3.7
1	D	56	TYR	3.7
1	B	100	ASP	3.7
1	B	166	LEU	3.7
1	D	26	GLU	3.7
1	D	203	ILE	3.7
1	D	201	ILE	3.7
1	C	97	TRP	3.7
1	D	512	ASN	3.7
1	B	471	GLY	3.7
1	D	49	PHE	3.7
1	B	242	TYR	3.6
1	B	253	ALA	3.6
1	D	209	VAL	3.6
1	D	73	THR	3.6
1	C	206	LEU	3.6
1	D	84	LEU	3.6
1	D	150	ASN	3.6
1	D	358	THR	3.6
1	C	389	PHE	3.6
1	B	412	GLY	3.6
1	D	468	TRP	3.6
1	C	351	GLN	3.6
1	D	348	TYR	3.6
1	D	439	LYS	3.5
1	D	121	LEU	3.5
1	D	452	SER	3.5
1	B	248	GLN	3.5
1	D	497	ASP	3.5
1	B	103	VAL	3.5
1	C	52	ALA	3.5
1	C	101	ILE	3.5
1	D	48	ILE	3.5
1	C	83	ASP	3.5
1	C	159	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	497	ASP	3.5
1	D	308	LEU	3.5
1	C	298	ILE	3.5
1	A	169	GLU	3.5
1	C	417	TYR	3.5
1	A	413	ASP	3.5
1	C	391	ALA	3.5
1	D	113	ARG	3.5
1	D	425	THR	3.5
1	A	32	CYS	3.5
1	D	383	HIS	3.5
1	B	413	ASP	3.5
1	D	69	TRP	3.5
1	D	438	TYR	3.4
1	C	346	ASN	3.4
1	C	489	VAL	3.4
1	A	157	LEU	3.4
1	B	298	ILE	3.4
1	B	397	PRO	3.4
1	A	257	ASP	3.4
1	C	122	LEU	3.4
1	D	272	GLY	3.4
1	D	421	ASN	3.4
1	D	297	LYS	3.4
1	C	488	TYR	3.4
1	C	367	ALA	3.4
1	C	203	ILE	3.4
1	A	206	LEU	3.4
1	A	480	PHE	3.4
1	C	53	SER	3.4
1	C	393	SER	3.4
1	B	249	LEU	3.4
1	A	233	PRO	3.4
1	C	202	THR	3.4
1	D	71	SER	3.3
1	D	499	ASP	3.3
1	A	87	GLY	3.3
1	A	401	TYR	3.3
1	D	52	ALA	3.3
1	A	35	THR	3.3
1	C	211	THR	3.3
1	B	66	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	344	GLY	3.3
1	C	275	MET	3.3
1	D	94	TYR	3.3
1	D	242	TYR	3.3
1	D	159	HIS	3.3
1	B	278	ARG	3.3
1	A	328	PHE	3.3
1	C	459	ASN	3.3
1	B	178	ILE	3.3
1	D	55	ALA	3.3
1	C	428	ASP	3.3
1	D	156	THR	3.3
1	C	493	ASN	3.3
1	D	82	ALA	3.3
1	B	415	LEU	3.3
1	C	301	HIS	3.3
1	B	86	ASN	3.3
1	A	111	GLY	3.3
1	C	348	TYR	3.2
1	D	440	ARG	3.2
1	B	115	SER	3.2
1	B	500	LEU	3.2
1	D	486	LEU	3.2
1	A	202	THR	3.2
1	C	418	VAL	3.2
1	D	118	TRP	3.2
1	B	255	ALA	3.2
1	C	135	ALA	3.2
1	D	28	GLU	3.2
1	C	371	SER	3.2
1	A	407	PHE	3.2
1	A	489	VAL	3.2
1	B	287	GLN	3.2
1	D	98	GLN	3.2
1	A	89	THR	3.2
1	D	116	ILE	3.2
1	D	249	LEU	3.2
1	C	314	PRO	3.2
1	D	23	VAL	3.2
1	D	238	SER	3.2
1	C	70	ASP	3.2
1	D	83	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	108	ASN	3.2
1	B	139	TYR	3.2
1	D	417	TYR	3.2
1	B	273	PRO	3.2
1	C	29	PRO	3.2
1	C	300	PHE	3.2
1	D	387	PRO	3.2
1	D	426	PRO	3.2
1	D	460	VAL	3.2
1	A	248	GLN	3.2
1	C	377	SER	3.2
1	C	265	ASP	3.2
1	C	220	ALA	3.2
1	B	335	LEU	3.2
1	D	429	GLU	3.2
1	A	173	PHE	3.2
1	B	38	PHE	3.2
1	C	158	PHE	3.2
1	C	104	MET	3.2
1	C	416	ILE	3.2
1	D	295	ARG	3.2
1	D	31	THR	3.2
1	A	405	ASP	3.1
1	C	219	ASP	3.1
1	B	118	TRP	3.1
1	D	343	LEU	3.1
1	D	179	VAL	3.1
1	A	178	ILE	3.1
1	B	157	LEU	3.1
1	D	100	ASP	3.1
1	D	160	TRP	3.1
1	D	390	ASN	3.1
1	D	447	HIS	3.1
1	A	415	LEU	3.1
1	D	188	LEU	3.1
1	A	172	GLY	3.1
1	C	472	ASP	3.1
1	A	44	GLU	3.1
1	D	310	GLU	3.1
1	B	189	CYS	3.1
1	C	47	PHE	3.1
1	C	210	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	199	ASN	3.1
1	B	74	HIS	3.1
1	D	216	LEU	3.1
1	D	211	THR	3.1
1	A	22	PHE	3.1
1	B	244	VAL	3.1
1	B	462	VAL	3.1
1	B	506	TRP	3.1
1	C	113	ARG	3.1
1	B	414	PRO	3.1
1	A	48	ILE	3.1
1	B	220	ALA	3.1
1	B	296	ALA	3.1
1	D	391	ALA	3.1
1	B	331	THR	3.1
1	C	95	THR	3.1
1	D	222	GLY	3.1
1	D	481	THR	3.1
1	C	72	PHE	3.1
1	D	47	PHE	3.1
1	B	198	LYS	3.1
1	C	45	LYS	3.1
1	B	291	ASP	3.1
1	C	181	ASP	3.1
1	B	56	TYR	3.1
1	B	348	TYR	3.1
1	A	296	ALA	3.0
1	D	171	ASN	3.0
1	D	278	ARG	3.0
1	B	152	THR	3.0
1	C	482	VAL	3.0
1	B	476	PHE	3.0
1	C	280	PHE	3.0
1	A	330	GLU	3.0
1	C	468	TRP	3.0
1	D	326	PRO	3.0
1	C	406	TYR	3.0
1	C	107	LEU	3.0
1	A	159	HIS	3.0
1	B	473	ASN	3.0
1	C	98	GLN	3.0
1	C	89	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	21	GLU	3.0
1	D	75	ARG	3.0
1	A	74	HIS	3.0
1	A	86	ASN	3.0
1	A	269	GLY	3.0
1	B	409	THR	3.0
1	C	410	THR	3.0
1	D	35	THR	3.0
1	A	66	LEU	3.0
1	A	128	SER	3.0
1	B	107	LEU	3.0
1	C	157	LEU	3.0
1	C	285	HIS	3.0
1	B	46	GLY	3.0
1	A	256	VAL	3.0
1	A	460	VAL	3.0
1	B	349	VAL	3.0
1	B	150	ASN	3.0
1	B	239	THR	3.0
1	C	48	ILE	3.0
1	A	118	TRP	3.0
1	B	148	ALA	3.0
1	B	384	ALA	3.0
1	B	418	VAL	3.0
1	C	205	GLN	3.0
1	B	330	GLU	2.9
1	C	153	PRO	2.9
1	C	330	GLU	2.9
1	C	506	TRP	2.9
1	B	119	SER	2.9
1	A	219	ASP	2.9
1	D	46	GLY	2.9
1	D	154	PHE	2.9
1	B	48	ILE	2.9
1	A	449	CYS	2.9
1	D	473	ASN	2.9
1	D	200	TRP	2.9
1	B	207	TYR	2.9
1	B	424	SER	2.9
1	A	61	GLY	2.9
1	B	41	GLY	2.9
1	B	172	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	311	GLY	2.9
1	B	510	PHE	2.9
1	C	375	LEU	2.9
1	C	118	TRP	2.9
1	B	49	PHE	2.9
1	C	503	SER	2.9
1	D	237	SER	2.9
1	D	377	SER	2.9
1	B	159	HIS	2.9
1	D	491	PHE	2.9
1	B	375	LEU	2.9
1	A	156	THR	2.9
1	D	152	THR	2.9
1	B	391	ALA	2.9
1	D	294	GLU	2.9
1	B	300	PHE	2.9
1	C	407	PHE	2.9
1	D	76	PHE	2.9
1	D	111	GLY	2.9
1	C	415	LEU	2.9
1	D	448	LEU	2.9
1	B	326	PRO	2.9
1	D	489	VAL	2.9
1	D	488	TYR	2.9
1	D	510	PHE	2.9
1	B	290	LYS	2.9
1	C	142	LEU	2.9
1	C	162	LEU	2.9
1	B	246	HIS	2.8
1	B	362	SER	2.8
1	C	424	SER	2.8
1	B	245	ALA	2.8
1	B	44	GLU	2.8
1	A	279	TRP	2.8
1	B	407	PHE	2.8
1	D	192	LEU	2.8
1	D	217	GLY	2.8
1	D	423	PHE	2.8
1	B	396	TYR	2.8
1	C	170	TYR	2.8
1	C	394	TYR	2.8
1	C	132	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	158	PHE	2.8
1	B	299	PHE	2.8
1	D	32	CYS	2.8
1	B	377	SER	2.8
1	C	82	ALA	2.8
1	C	392	ALA	2.8
1	D	215	ALA	2.8
1	D	393	SER	2.8
1	D	131	VAL	2.8
1	B	444	LEU	2.8
1	B	512	ASN	2.8
1	D	412	GLY	2.8
1	B	170	TYR	2.8
1	C	384	ALA	2.8
1	B	426	PRO	2.8
1	C	238	SER	2.8
1	C	426	PRO	2.8
1	C	487	SER	2.8
1	B	202	THR	2.8
1	D	375	LEU	2.8
1	B	431	PHE	2.8
1	C	499	ASP	2.8
1	D	114	PHE	2.8
1	D	204	ASN	2.8
1	B	438	TYR	2.8
1	C	207	TYR	2.8
1	C	402	TYR	2.8
1	A	148	ALA	2.8
1	C	103	VAL	2.8
1	C	221	PRO	2.8
1	D	123	PRO	2.8
1	D	420	GLU	2.8
1	A	270	MET	2.7
1	A	340	TYR	2.7
1	A	58	VAL	2.7
1	D	357	GLN	2.7
1	D	162	LEU	2.7
1	B	240	GLU	2.7
1	D	279	TRP	2.7
1	B	320	TYR	2.7
1	B	461	ASN	2.7
1	A	209	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	155	VAL	2.7
1	A	29	PRO	2.7
1	C	444	LEU	2.7
1	B	271	ILE	2.7
1	C	328	PHE	2.7
1	C	494	ILE	2.7
1	A	412	GLY	2.7
1	B	358	THR	2.7
1	C	382	GLY	2.7
1	A	64	ARG	2.7
1	B	126	LYS	2.7
1	B	406	TYR	2.7
1	C	395	TYR	2.7
1	A	447	HIS	2.7
1	C	355	ASN	2.7
1	D	392	ALA	2.7
1	D	492	ALA	2.7
1	B	489	VAL	2.7
1	C	256	VAL	2.7
1	C	349	VAL	2.7
1	D	68	VAL	2.7
1	C	343	LEU	2.7
1	A	273	PRO	2.7
1	B	22	PHE	2.7
1	B	43	PHE	2.7
1	B	455	ILE	2.7
1	C	466	PHE	2.7
1	D	389	PHE	2.7
1	B	475	GLU	2.7
1	A	54	SER	2.7
1	B	93	SER	2.7
1	C	54	SER	2.7
1	C	115	SER	2.7
1	A	56	TYR	2.7
1	C	168	ASP	2.7
1	B	336	VAL	2.7
1	D	415	LEU	2.7
1	C	354	GLN	2.7
1	D	276	ILE	2.7
1	B	154	PHE	2.7
1	B	280	PHE	2.7
1	D	173	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	193	PHE	2.7
1	B	21	GLU	2.7
1	B	308	LEU	2.7
1	A	316	ILE	2.6
1	B	511	ILE	2.6
1	C	248	GLN	2.6
1	D	178	ILE	2.6
1	B	193	PHE	2.6
1	C	305	MET	2.6
1	D	378	LYS	2.6
1	B	457	GLU	2.6
1	C	222	GLY	2.6
1	D	422	GLY	2.6
1	A	155	VAL	2.6
1	A	162	LEU	2.6
1	B	121	LEU	2.6
1	B	368	LEU	2.6
1	B	470	LEU	2.6
1	B	185	TYR	2.6
1	C	94	TYR	2.6
1	D	285	HIS	2.6
1	D	88	ASP	2.6
1	A	473	ASN	2.6
1	B	304	PHE	2.6
1	A	65	GLY	2.6
1	D	475	GLU	2.6
1	C	358	THR	2.6
1	B	343	LEU	2.6
1	D	345	LEU	2.6
1	A	43	PHE	2.6
1	D	480	PHE	2.6
1	C	357	GLN	2.6
1	D	355	ASN	2.6
1	B	25	GLU	2.6
1	B	110	THR	2.6
1	C	131	VAL	2.6
1	C	245	ALA	2.6
1	B	340	TYR	2.6
1	C	404	MET	2.6
1	D	305	MET	2.6
1	C	273	PRO	2.6
1	D	397	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	354	GLN	2.6
1	D	428	ASP	2.6
1	A	504	GLY	2.6
1	C	217	GLY	2.6
1	B	162	LEU	2.6
1	A	253	ALA	2.6
1	B	353	ALA	2.6
1	C	55	ALA	2.6
1	C	492	ALA	2.6
1	D	482	VAL	2.6
1	B	501	LYS	2.6
1	B	411	TYR	2.6
1	B	447	HIS	2.6
1	C	38	PHE	2.6
1	C	112	TYR	2.6
1	C	185	TYR	2.6
1	C	77	PRO	2.6
1	D	424	SER	2.6
1	A	291	ASP	2.6
1	C	102	ASP	2.6
1	B	250	LEU	2.6
1	C	169	GLU	2.6
1	B	260	ARG	2.6
1	D	434	ALA	2.6
1	A	165	THR	2.6
1	B	69	TRP	2.5
1	B	200	TRP	2.5
1	B	468	TRP	2.5
1	C	73	THR	2.6
1	A	299	PHE	2.5
1	C	507	PHE	2.5
1	A	411	TYR	2.5
1	C	383	HIS	2.5
1	D	443	TYR	2.5
1	C	109	SER	2.5
1	D	344	GLY	2.5
1	A	166	LEU	2.5
1	D	146	LEU	2.5
1	A	168	ASP	2.5
1	A	171	ASN	2.5
1	A	513	VAL	2.5
1	B	513	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	384	ALA	2.5
1	D	502	ALA	2.5
1	A	416	ILE	2.5
1	B	309	THR	2.5
1	C	151	MET	2.5
1	A	385	PRO	2.5
1	C	60	GLY	2.5
1	C	63	GLY	2.5
1	D	37	LEU	2.5
1	C	64	ARG	2.5
1	C	297	LYS	2.5
1	A	353	ALA	2.5
1	B	132	ASN	2.5
1	C	390	ASN	2.5
1	B	47	PHE	2.5
1	A	242	TYR	2.5
1	A	107	LEU	2.5
1	A	345	LEU	2.5
1	C	249	LEU	2.5
1	D	368	LEU	2.5
1	B	54	SER	2.5
1	B	292	ALA	2.5
1	C	467	ALA	2.5
1	B	288	GLU	2.5
1	B	459	ASN	2.5
1	C	512	ASN	2.5
1	D	266	ASP	2.5
1	D	104	MET	2.5
1	C	177	THR	2.5
1	C	208	THR	2.5
1	C	376	THR	2.5
1	D	38	PHE	2.5
1	D	208	THR	2.5
1	D	361	PRO	2.5
1	A	192	LEU	2.5
1	D	87	GLY	2.5
1	A	34	GLN	2.5
1	A	244	VAL	2.5
1	A	93	SER	2.5
1	A	310	GLU	2.5
1	B	26	GLU	2.5
1	B	28	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	203	ILE	2.5
1	C	21	GLU	2.5
1	B	341	ASP	2.5
1	B	389	PHE	2.5
1	D	27	ASN	2.5
1	D	33	ASN	2.5
1	B	419	THR	2.5
1	A	174	LEU	2.5
1	B	113	ARG	2.5
1	B	314	PRO	2.5
1	C	66	LEU	2.5
1	C	80	GLY	2.5
1	B	454	VAL	2.5
1	B	460	VAL	2.5
1	D	367	ALA	2.4
1	D	441	ILE	2.4
1	C	475	GLU	2.4
1	A	342	PHE	2.4
1	A	389	PHE	2.4
1	A	67	ASN	2.4
1	C	108	ASN	2.4
1	A	31	THR	2.4
1	A	303	TRP	2.4
1	B	73	THR	2.4
1	C	200	TRP	2.4
1	D	219	ASP	2.4
1	C	166	LEU	2.4
1	A	170	TYR	2.4
1	D	322	GLY	2.4
1	C	502	ALA	2.4
1	B	310	GLU	2.4
1	A	439	LYS	2.4
1	B	480	PHE	2.4
1	C	114	PHE	2.4
1	A	90	THR	2.4
1	B	421	ASN	2.4
1	B	265	ASP	2.4
1	C	218	THR	2.4
1	C	323	ASP	2.4
1	A	426	PRO	2.4
1	A	434	ALA	2.4
1	C	164	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	416	ILE	2.4
1	B	173	PHE	2.4
1	C	332	GLU	2.4
1	C	491	PHE	2.4
1	B	188	LEU	2.4
1	D	24	CYS	2.4
1	D	107	LEU	2.4
1	A	410	THR	2.4
1	C	27	ASN	2.4
1	C	204	ASN	2.4
1	C	388	PRO	2.4
1	C	495	THR	2.4
1	A	364	VAL	2.4
1	A	418	VAL	2.4
1	C	403	VAL	2.4
1	D	102	ASP	2.4
1	B	316	ILE	2.4
1	D	143	ILE	2.4
1	C	270	MET	2.4
1	C	182	PHE	2.4
1	D	431	PHE	2.4
1	B	216	LEU	2.4
1	C	281	LEU	2.4
1	A	329	SER	2.4
1	C	303	TRP	2.4
1	A	462	VAL	2.4
1	B	209	VAL	2.4
1	C	209	VAL	2.4
1	C	419	THR	2.4
1	D	277	THR	2.4
1	D	388	PRO	2.4
1	C	236	ASN	2.4
1	C	338	GLY	2.4
1	D	172	GLY	2.4
1	D	478	ASN	2.4
1	C	116	ILE	2.4
1	C	255	ALA	2.4
1	C	340	TYR	2.4
1	D	347	TYR	2.4
1	D	442	ASP	2.4
1	C	49	PHE	2.4
1	C	76	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	109	SER	2.4
1	B	31	THR	2.3
1	C	91	CYS	2.4
1	B	235	GLY	2.3
1	C	165	THR	2.3
1	A	139	TYR	2.3
1	D	196	ARG	2.3
1	D	353	ALA	2.3
1	A	275	MET	2.3
1	B	37	LEU	2.3
1	D	500	LEU	2.3
1	B	319	GLU	2.3
1	D	332	GLU	2.3
1	A	258	VAL	2.3
1	C	336	VAL	2.3
1	A	80	GLY	2.3
1	B	425	THR	2.3
1	B	504	GLY	2.3
1	C	172	GLY	2.3
1	D	449	CYS	2.3
1	B	214	TYR	2.3
1	D	184	ASP	2.3
1	D	323	ASP	2.3
1	A	343	LEU	2.3
1	A	470	LEU	2.3
1	B	342	PHE	2.3
1	C	304	PHE	2.3
1	C	500	LEU	2.3
1	B	420	GLU	2.3
1	B	153	PRO	2.3
1	B	388	PRO	2.3
1	D	65	GLY	2.3
1	D	130	GLY	2.3
1	A	481	THR	2.3
1	D	404	MET	2.3
1	C	214	TYR	2.3
1	C	171	ASN	2.3
1	A	70	ASP	2.3
1	D	57	GLN	2.3
1	D	164	GLN	2.3
1	D	58	VAL	2.3
1	B	282	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	414	PRO	2.3
1	C	130	GLY	2.3
1	B	367	ALA	2.3
1	B	392	ALA	2.3
1	C	148	ALA	2.3
1	D	380	ALA	2.3
1	A	362	SER	2.3
1	B	495	THR	2.3
1	B	503	SER	2.3
1	C	425	THR	2.3
1	D	202	THR	2.3
1	D	374	THR	2.3
1	A	142	LEU	2.3
1	A	250	LEU	2.3
1	A	488	TYR	2.3
1	B	24	CYS	2.3
1	B	205	GLN	2.3
1	D	34	GLN	2.3
1	D	197	VAL	2.3
1	D	77	PRO	2.3
1	B	218	THR	2.3
1	C	335	LEU	2.3
1	A	491	PHE	2.3
1	B	40	SER	2.3
1	C	43	PHE	2.3
1	C	154	PHE	2.3
1	C	342	PHE	2.3
1	D	176	LYS	2.3
1	A	179	VAL	2.3
1	B	258	VAL	2.3
1	C	258	VAL	2.3
1	D	341	ASP	2.3
1	D	59	GLU	2.2
1	A	208	THR	2.2
1	B	208	THR	2.2
1	D	304	PHE	2.2
1	D	394	TYR	2.2
1	A	113	ARG	2.2
1	A	498	ARG	2.2
1	C	62	ARG	2.2
1	D	318	ARG	2.2
1	A	230	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	497	ASP	2.2
1	C	310	GLU	2.2
1	C	420	GLU	2.2
1	A	271	ILE	2.2
1	C	316	ILE	2.2
1	A	135	ALA	2.2
1	A	235	GLY	2.2
1	B	241	PRO	2.2
1	C	385	PRO	2.2
1	C	96	LEU	2.2
1	C	412	GLY	2.2
1	C	193	PHE	2.2
1	A	260	ARG	2.2
1	B	402	TYR	2.2
1	B	488	TYR	2.2
1	A	424	SER	2.2
1	B	274	VAL	2.2
1	C	244	VAL	2.2
1	A	204	ASN	2.2
1	C	42	ASN	2.2
1	D	437	ASP	2.2
1	B	111	GLY	2.2
1	C	361	PRO	2.2
1	D	436	ALA	2.2
1	A	126	LYS	2.2
1	B	474	TYR	2.2
1	C	396	TYR	2.2
1	A	121	LEU	2.2
1	D	282	PRO	2.2
1	D	445	CYS	2.2
1	C	398	LYS	2.2
1	D	70	ASP	2.2
1	A	38	PHE	2.2
1	B	498	ARG	2.2
1	B	383	HIS	2.2
1	C	90	THR	2.2
1	B	394	TYR	2.2
1	D	170	TYR	2.2
1	B	446	SER	2.2
1	C	136	ILE	2.2
1	C	362	SER	2.2
1	A	146	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	142	LEU	2.2
1	C	146	LEU	2.2
1	A	199	ASN	2.2
1	A	420	GLU	2.2
1	D	78	GLU	2.2
1	B	439	LYS	2.2
1	A	510	PHE	2.2
1	C	105	ASP	2.2
1	D	72	PHE	2.2
1	D	407	PHE	2.2
1	D	413	ASP	2.2
1	A	131	VAL	2.1
1	B	155	VAL	2.1
1	B	177	THR	2.1
1	D	110	THR	2.1
1	C	139	TYR	2.1
1	C	347	TYR	2.1
1	B	116	ILE	2.1
1	A	486	LEU	2.1
1	A	119	SER	2.1
1	B	286	SER	2.1
1	A	62	ARG	2.1
1	A	429	GLU	2.1
1	D	245	ALA	2.1
1	A	125	GLY	2.1
1	B	63	GLY	2.1
1	A	150	ASN	2.1
1	B	361	PRO	2.1
1	A	431	PHE	2.1
1	A	363	ASP	2.1
1	C	74	HIS	2.1
1	C	179	VAL	2.1
1	D	364	VAL	2.1
1	A	494	ILE	2.1
1	B	400	ILE	2.1
1	A	149	LYS	2.1
1	A	297	LYS	2.1
1	B	451	LEU	2.1
1	C	509	LYS	2.1
1	A	167	GLN	2.1
1	B	164	GLN	2.1
1	D	248	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	135	ALA	2.1
1	C	422	GLY	2.1
1	D	371	SER	2.1
1	D	30	PHE	2.1
1	A	51	VAL	2.1
1	A	468	TRP	2.1
1	B	403	VAL	2.1
1	B	472	ASP	2.1
1	B	482	VAL	2.1
1	C	88	ASP	2.1
1	C	490	ASP	2.1
1	D	274	VAL	2.1
1	A	122	LEU	2.1
1	C	138	TYR	2.1
1	C	216	LEU	2.1
1	C	308	LEU	2.1
1	D	149	LYS	2.1
1	D	410	THR	2.1
1	B	313	TYR	2.1
1	A	57	GLN	2.1
1	B	267	GLN	2.1
1	D	117	ALA	2.1
1	A	302	GLY	2.1
1	D	241	PRO	2.1
1	D	158	PHE	2.1
1	B	171	ASN	2.1
1	D	140	ASN	2.1
1	A	506	TRP	2.1
1	B	91	CYS	2.1
1	A	94	TYR	2.1
1	B	259	TYR	2.1
1	D	259	TYR	2.1
1	D	220	ALA	2.1
1	D	41	GLY	2.1
1	D	50	GLY	2.1
1	D	302	GLY	2.1
1	A	446	SER	2.1
1	A	452	SER	2.1
1	A	308	LEU	2.1
1	B	486	LEU	2.1
1	C	260	ARG	2.1
1	D	250	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	104	MET	2.1
1	A	331	THR	2.1
1	A	465	TYR	2.1
1	B	293	THR	2.1
1	C	189	CYS	2.1
1	C	313	TYR	2.1
1	C	366	THR	2.1
1	C	474	TYR	2.1
1	D	263	TYR	2.1
1	D	381	THR	2.1
1	D	333	ALA	2.1
1	A	464	GLY	2.1
1	D	386	GLY	2.1
1	A	332	GLU	2.1
1	B	30	PHE	2.1
1	C	450	PHE	2.1
1	B	176	LYS	2.0
1	B	463	LYS	2.0
1	D	321	VAL	2.0
1	C	75	ARG	2.0
1	C	127	ARG	2.0
1	A	211	THR	2.0
1	C	380	ALA	2.0
1	C	401	TYR	2.0
1	B	311	GLY	2.0
1	C	85	GLY	2.0
1	D	125	GLY	2.0
1	D	226	PRO	2.0
1	A	368	LEU	2.0
1	A	451	LEU	2.0
1	D	446	SER	2.0
1	A	317	MET	2.0
1	B	39	ASN	2.0
1	C	86	ASN	2.0
1	D	86	ASN	2.0
1	A	367	ALA	2.0
1	A	406	TYR	2.0
1	B	89	THR	2.0
1	B	95	THR	2.0
1	C	430	ASP	2.0
1	D	168	ASP	2.0
1	A	182	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	213	GLY	2.0
1	B	479	GLY	2.0
1	D	43	PHE	2.0
1	D	342	PHE	2.0
1	B	45	LYS	2.0
1	C	226	PRO	2.0
1	C	282	PRO	2.0
1	D	233	PRO	2.0
1	D	463	LYS	2.0
1	C	319	GLU	2.0
1	A	400	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

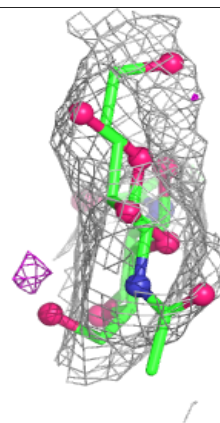
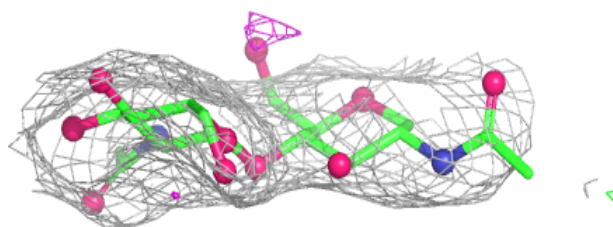
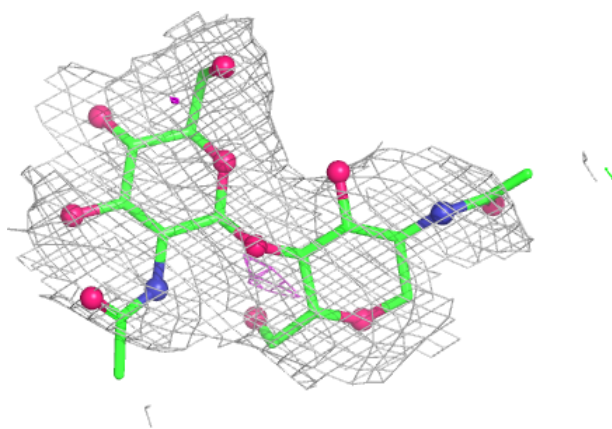
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

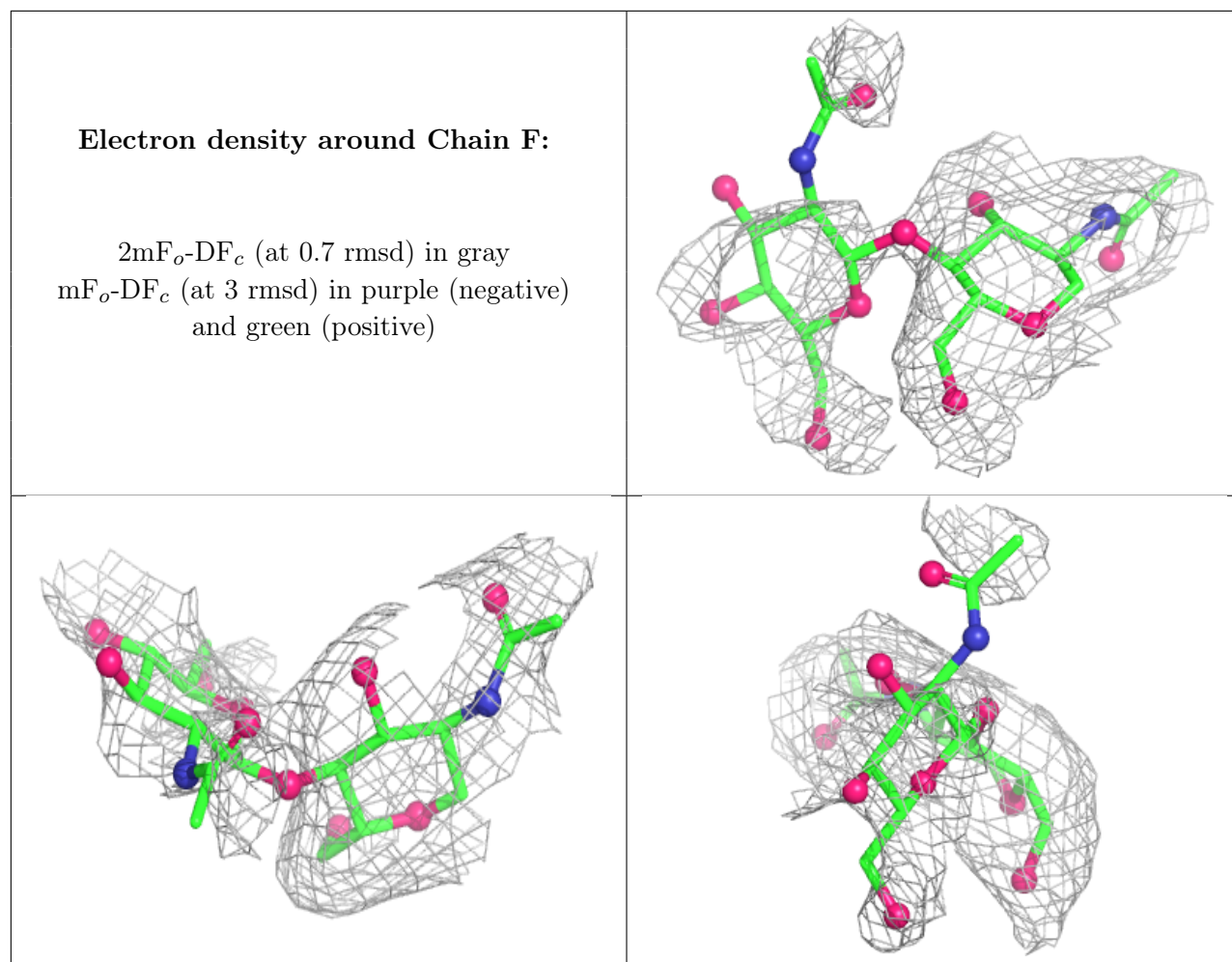
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	2	14/15	0.30	0.23	157,164,176,179	0
2	NAG	E	2	14/15	0.53	0.17	128,128,128,128	0
2	NAG	E	1	14/15	0.69	0.21	120,120,120,120	0
2	NAG	F	1	14/15	0.70	0.20	127,136,142,164	0

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 E:

$2mF_o - DF_c$ (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(Å ²)	Q<0.9
3	NAG	C	605	14/15	0.06	0.24	204,204,204,204	0
3	NAG	C	603	14/15	0.25	0.23	181,181,181,181	0
3	NAG	D	604	14/15	0.28	0.29	203,203,203,203	0
3	NAG	C	602	14/15	0.46	0.28	149,149,149,149	0
3	NAG	D	605	14/15	0.46	0.23	168,168,168,168	0
3	NAG	B	607	14/15	0.47	0.25	155,155,155,155	0
3	NAG	A	607	14/15	0.47	0.18	142,142,142,142	0
3	NAG	B	603	14/15	0.49	0.27	128,128,128,128	0
3	NAG	B	604	14/15	0.49	0.20	148,148,148,148	0
3	NAG	C	601	14/15	0.50	0.20	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	C	604	14/15	0.51	0.21	211,211,211,211	0
3	NAG	A	605	14/15	0.52	0.20	147,147,147,147	0
3	NAG	B	608	14/15	0.52	0.22	155,155,155,155	0
3	NAG	B	606	14/15	0.52	0.20	138,138,138,138	0
3	NAG	A	604	14/15	0.53	0.22	124,124,124,124	0
3	NAG	B	605	14/15	0.56	0.20	159,159,159,159	0
3	NAG	A	606	14/15	0.60	0.20	140,140,140,140	0
3	NAG	D	602	14/15	0.64	0.19	144,144,144,144	0
3	NAG	D	601	14/15	0.65	0.23	168,168,168,168	0
3	NAG	B	602	14/15	0.71	0.17	132,132,132,132	0
3	NAG	A	603	14/15	0.71	0.18	102,116,151,160	0
3	NAG	D	603	14/15	0.72	0.18	120,120,120,120	0
3	NAG	B	601	14/15	0.77	0.17	96,101,105,107	0
3	NAG	A	602	14/15	0.80	0.19	90,101,111,116	0
3	NAG	A	601	14/15	0.84	0.14	78,84,93,98	0
4	CA	D	606	1/1	0.86	0.16	124,124,124,124	0
4	CA	A	608	1/1	0.97	0.09	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.