



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:10 PM UTC

PDB ID : 2V53 / pdb\_00002v53  
Title : Crystal structure of a SPARC-collagen complex  
Authors : Hohenester, E.; Sasaki, T.; Giudici, C.; Farndale, R.W.; Bachinger, H.P.  
Deposited on : 2008-10-01  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

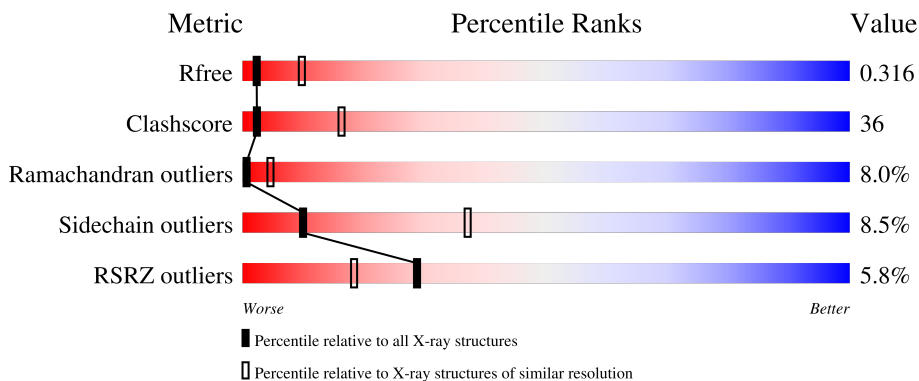
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	230	
2	B	33	
2	C	33	
2	D	33	
3	E	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	HYP	B	33	-	-	X	-

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 2300 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 SPARC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1639	1034	272	315	18	0	0	1

- Molecule 2 is a protein called COLLAGEN ALPHA-1(III) CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	33	205	128	34	42	1	0	0	0
2	C	33	211	131	37	42	1	0	0	0
2	D	33	211	131	37	42	1	0	0	0

- Molecule 3 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
			Total	C	N	O			
3	E	2	28	16	2	10	0	0	0

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

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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).

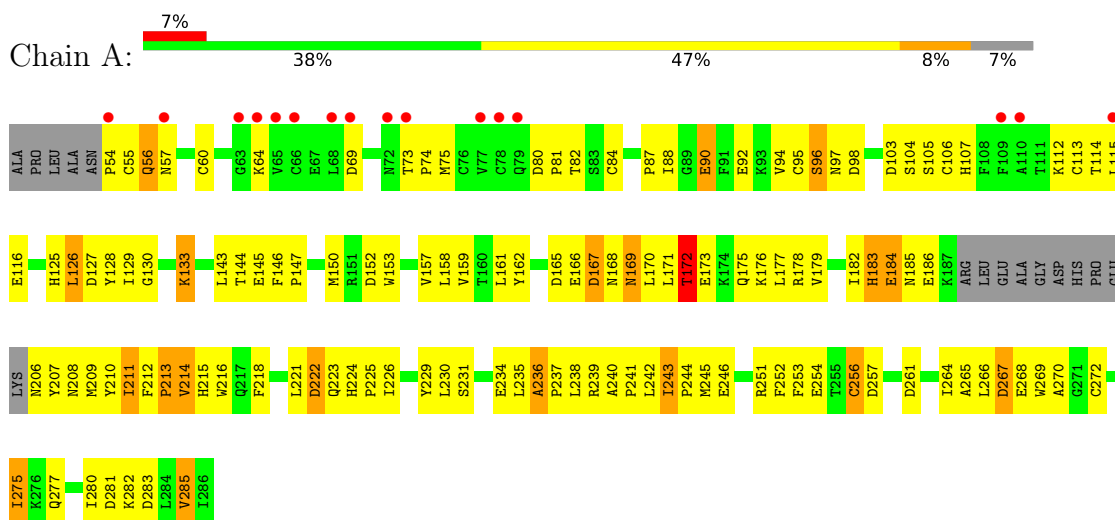


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		

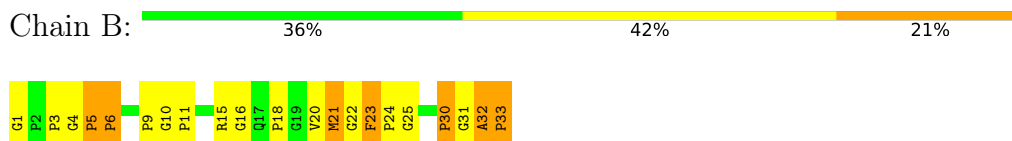
### 3 Residue-property plots [i](#)

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.

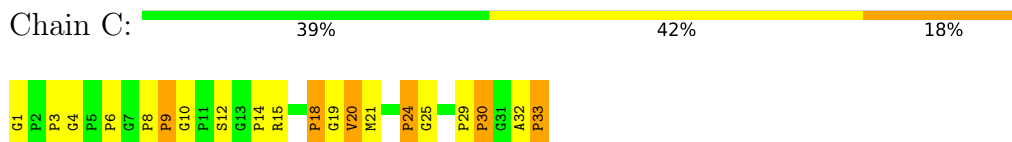
- Molecule 1: SPARC



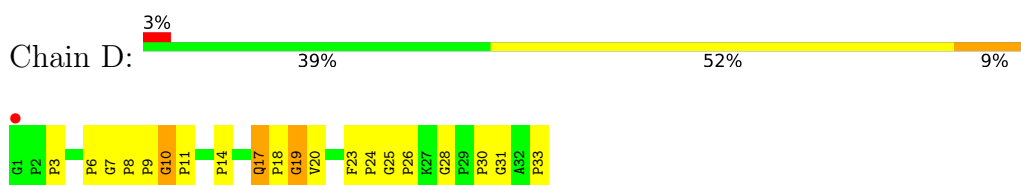
- Molecule 2: COLLAGEN ALPHA-1(III) CHAIN



- Molecule 2: COLLAGEN ALPHA-1(III) CHAIN



- Molecule 2: COLLAGEN ALPHA-1(III) CHAIN



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



MAG1  
MAG2

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.79Å 89.79Å 127.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 3.20 19.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.84-3.20) 99.3 (19.84-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.45 (at 3.22Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.254 , 0.320 0.247 , 0.316	Depositor DCC
$R_{free}$ test set	950 reflections (10.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.2	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, HYP, NAG, SO4

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	0.62	1/1682 (0.1%)	0.97	7/2300 (0.3%)
2	B	0.58	0/150	0.98	2/195 (1.0%)
2	C	0.55	0/156	0.96	2/202 (1.0%)
2	D	0.51	0/156	1.17	4/202 (2.0%)
All	All	0.60	1/2144 (0.0%)	0.98	15/2899 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	VAL	C-N	-6.89	1.23	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	CYS	N-CA-C	-7.51	104.08	113.55
2	D	10	GLY	CA-C-N	7.40	127.98	119.99
2	D	10	GLY	C-N-CA	7.40	127.98	119.99
1	A	54	PRO	N-CA-CB	6.86	110.55	103.00
2	C	25	GLY	CA-C-N	6.02	126.49	119.99
2	C	25	GLY	C-N-CA	6.02	126.49	119.99
1	A	186	GLU	N-CA-C	-5.64	107.00	112.97
1	A	243	ILE	CA-C-N	-5.62	115.09	120.83
1	A	243	ILE	C-N-CA	-5.62	115.09	120.83
1	A	152	ASP	N-CA-C	-5.59	105.10	111.14
2	D	25	GLY	CA-C-N	5.59	126.82	119.84
2	D	25	GLY	C-N-CA	5.59	126.82	119.84
1	A	178	ARG	N-CA-C	-5.55	105.63	112.90
2	B	10	GLY	CA-C-N	5.48	125.38	119.85
2	B	10	GLY	C-N-CA	5.48	125.38	119.85

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1639	0	1442	118	0
2	B	205	0	182	22	0
2	C	211	0	193	25	0
2	D	211	0	193	17	0
3	E	28	0	25	1	0
4	A	1	0	0	0	0
5	D	5	0	0	0	0
All	All	2300	0	2035	154	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 36.

All (154) 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)
2:B:33:HYP:HA	2:C:32:ALA:HB3	1.38	1.06
1:A:87:PRO:HG3	1:A:103:ASP:O	1.70	0.92
1:A:158:LEU:HD11	1:A:213:PRO:HA	1.57	0.87
1:A:209:MET:HG3	1:A:210:TYR:H	1.41	0.84
1:A:126:LEU:C	1:A:126:LEU:HD12	2.04	0.83
1:A:231:SER:OG	1:A:234:GLU:HG3	1.79	0.83
1:A:277:GLN:HA	1:A:280:ILE:HG13	1.62	0.81
2:C:12:SER:HA	2:D:11:PRO:HD2	1.64	0.78
1:A:239:ARG:O	1:A:243:ILE:HG13	1.86	0.75
1:A:144:THR:C	1:A:146:PHE:H	1.96	0.74
1:A:128:TYR:HB3	1:A:243:ILE:HD12	1.69	0.73
2:B:33:HYP:CA	2:C:32:ALA:HB3	2.19	0.71
1:A:144:THR:O	1:A:147:PRO:HD2	1.90	0.70
2:B:15:ARG:HA	2:C:14:PRO:HD2	1.74	0.70
1:A:153:TRP:O	1:A:157:VAL:HG23	1.92	0.70
1:A:236:ALA:HB3	1:A:237:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:THR:HG23	1:A:175:GLN:OE1	1.94	0.68
1:A:229:TYR:CE2	1:A:265:ALA:HB2	2.28	0.68
2:D:17:GLN:HE21	2:D:17:GLN:HA	1.57	0.68
2:B:32:ALA:HB1	2:B:33:HYP:HD22	1.76	0.68
1:A:209:MET:HG3	1:A:210:TYR:N	2.09	0.66
1:A:147:PRO:HG3	1:A:252:PHE:HE1	1.61	0.65
1:A:157:VAL:HG22	2:D:20:VAL:HG11	1.77	0.65
1:A:170:LEU:O	1:A:171:LEU:HD23	1.98	0.63
2:C:10:GLY:O	2:D:10:GLY:HA3	1.98	0.63
1:A:166:GLU:O	1:A:167:ASP:HB2	1.97	0.62
2:C:15:ARG:HA	2:D:14:PRO:HD2	1.82	0.62
2:B:4:GLY:O	2:C:4:GLY:HA3	2.00	0.60
1:A:206:ASN:O	1:A:209:MET:HG2	2.01	0.60
2:B:25:GLY:HA3	2:D:23:PHE:O	2.01	0.60
1:A:146:PHE:HB3	1:A:147:PRO:HD3	1.83	0.59
1:A:212:PHE:O	1:A:213:PRO:C	2.45	0.59
2:B:31:GLY:HA3	2:D:28:GLY:O	2.02	0.59
2:B:30:HYP:OD1	2:C:29:PRO:HD2	2.02	0.59
1:A:158:LEU:CD1	1:A:213:PRO:HA	2.30	0.59
1:A:242:LEU:C	1:A:244:PRO:HD2	2.28	0.58
1:A:235:LEU:O	1:A:236:ALA:C	2.46	0.58
1:A:183:HIS:O	1:A:185:ASN:N	2.37	0.58
1:A:147:PRO:HG3	1:A:252:PHE:CE1	2.39	0.57
1:A:129:ILE:HG22	1:A:241:PRO:HA	1.85	0.57
1:A:158:LEU:O	1:A:161:LEU:HB2	2.05	0.56
1:A:144:THR:C	1:A:146:PHE:N	2.60	0.55
1:A:133:LYS:HA	3:E:2:NAG:H83	1.87	0.55
1:A:239:ARG:HG2	1:A:243:ILE:HD11	1.88	0.54
1:A:144:THR:O	1:A:146:PHE:N	2.41	0.54
1:A:126:LEU:C	1:A:126:LEU:CD1	2.77	0.52
2:B:11:PRO:O	2:C:10:GLY:HA3	2.09	0.52
1:A:245:MET:C	1:A:246:GLU:HG2	2.35	0.52
1:A:158:LEU:HD12	1:A:213:PRO:HG3	1.92	0.52
1:A:166:GLU:C	1:A:169:ASN:HD21	2.18	0.52
1:A:168:ASN:HD22	1:A:168:ASN:N	2.06	0.52
1:A:257:ASP:OD1	1:A:261:ASP:OD1	2.26	0.52
1:A:213:PRO:O	1:A:214:VAL:C	2.52	0.52
1:A:229:TYR:CD2	1:A:265:ALA:HB2	2.44	0.52
2:B:32:ALA:O	2:B:33:HYP:C	2.58	0.51
2:B:32:ALA:CB	2:B:33:HYP:HD22	2.36	0.51
1:A:175:GLN:C	1:A:177:LEU:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:H	1:A:230:LEU:HD21	1.75	0.51
1:A:168:ASN:HD22	1:A:168:ASN:H	1.58	0.51
1:A:238:LEU:C	1:A:241:PRO:HD2	2.36	0.51
1:A:112:LYS:O	1:A:115:LEU:HB2	2.11	0.51
1:A:105:SER:O	1:A:106:CYS:C	2.53	0.51
1:A:212:PHE:HB3	1:A:213:PRO:HD3	1.92	0.51
1:A:128:TYR:HD1	1:A:129:ILE:O	1.94	0.50
1:A:88:ILE:HG13	1:A:92:GLU:OE1	2.11	0.50
1:A:169:ASN:H	1:A:169:ASN:ND2	2.08	0.50
1:A:129:ILE:HG13	1:A:130:GLY:H	1.76	0.50
1:A:60:CYS:HB3	1:A:64:LYS:HB2	1.94	0.50
1:A:238:LEU:O	1:A:242:LEU:HB2	2.12	0.49
1:A:168:ASN:HA	1:A:171:LEU:O	2.12	0.49
2:B:30:HYP:HA	2:C:29:PRO:O	2.12	0.49
1:A:96:SER:O	1:A:97:ASN:C	2.56	0.49
1:A:212:PHE:CE1	1:A:216:TRP:HB2	2.48	0.49
2:B:4:GLY:O	2:C:4:GLY:CA	2.61	0.48
1:A:113:CYS:C	1:A:115:LEU:H	2.22	0.48
1:A:242:LEU:HD13	2:C:21:MET:HE1	1.95	0.48
2:B:20:VAL:HG12	2:B:21:MET:N	2.28	0.48
2:C:8:PRO:O	2:D:7:GLY:HA3	2.13	0.48
1:A:211:ILE:HA	1:A:275:ILE:CD1	2.44	0.47
2:B:1:GLY:O	2:C:1:GLY:HA2	2.14	0.47
1:A:88:ILE:O	1:A:88:ILE:HG22	2.13	0.47
1:A:87:PRO:HD3	1:A:103:ASP:HB3	1.96	0.47
1:A:222:ASP:OD1	1:A:226:ILE:HA	2.14	0.47
1:A:253:PHE:O	1:A:264:ILE:HD11	2.14	0.47
1:A:55:CYS:O	1:A:56:GLN:C	2.58	0.47
1:A:223:GLN:N	1:A:234:GLU:OE2	2.36	0.47
2:B:22:GLY:O	2:B:23:PHE:C	2.58	0.47
1:A:126:LEU:HD12	1:A:127:ASP:N	2.30	0.46
2:C:9:HYP:HA	2:D:8:PRO:HD2	1.96	0.46
1:A:281:ASP:C	1:A:283:ASP:H	2.24	0.46
1:A:171:LEU:C	1:A:172:THR:O	2.59	0.46
1:A:183:HIS:O	1:A:184:GLU:C	2.58	0.46
1:A:257:ASP:OD1	1:A:257:ASP:C	2.58	0.46
1:A:84:CYS:HB2	1:A:107:HIS:CE1	2.50	0.46
1:A:162:TYR:HB2	1:A:179:VAL:HG11	1.98	0.46
2:C:15:ARG:CA	2:D:14:PRO:HD2	2.43	0.46
2:C:20:VAL:O	2:D:19:GLY:HA3	2.15	0.46
1:A:175:GLN:C	1:A:177:LEU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:CYS:SG	1:A:96:SER:N	2.88	0.46
1:A:211:ILE:HA	1:A:275:ILE:HD11	1.97	0.46
1:A:215:HIS:O	1:A:216:TRP:C	2.59	0.45
1:A:168:ASN:N	1:A:168:ASN:ND2	2.65	0.45
1:A:128:TYR:HA	1:A:240:ALA:HB1	1.97	0.45
1:A:175:GLN:O	1:A:177:LEU:N	2.50	0.45
1:A:80:ASP:O	1:A:81:PRO:C	2.60	0.45
1:A:158:LEU:HD21	1:A:216:TRP:CD2	2.51	0.45
1:A:143:LEU:HD22	1:A:251:ARG:NH1	2.31	0.45
1:A:251:ARG:O	1:A:254:GLU:HG2	2.16	0.45
1:A:90:GLU:HA	1:A:90:GLU:OE1	2.17	0.44
1:A:153:TRP:CE3	2:D:23:PHE:HE1	2.35	0.44
1:A:212:PHE:HB3	1:A:213:PRO:CD	2.48	0.44
2:B:4:GLY:O	2:B:5:PRO:O	2.35	0.44
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.73	0.44
2:C:20:VAL:HG12	2:C:21:MET:N	2.33	0.44
1:A:165:ASP:HA	1:A:170:LEU:HD12	1.99	0.44
1:A:218:PHE:HD1	1:A:269:TRP:CG	2.36	0.43
1:A:246:GLU:OE2	2:C:24:HYP:OD1	2.31	0.43
1:A:55:CYS:O	1:A:57:ASN:N	2.51	0.43
1:A:128:TYR:HB2	1:A:240:ALA:O	2.19	0.43
1:A:281:ASP:O	1:A:283:ASP:N	2.51	0.43
2:C:19:GLY:O	2:D:19:GLY:CA	2.67	0.43
1:A:96:SER:O	1:A:98:ASP:N	2.52	0.43
1:A:240:ALA:N	1:A:241:PRO:HD2	2.34	0.43
1:A:159:VAL:C	1:A:161:LEU:H	2.27	0.42
1:A:173:GLU:O	1:A:177:LEU:HD13	2.19	0.42
2:B:33:HYP:HA	2:C:32:ALA:CB	2.27	0.42
1:A:270:ALA:HB1	1:A:275:ILE:HG22	2.00	0.42
1:A:69:ASP:HB3	1:A:75:MET:SD	2.60	0.42
1:A:245:MET:O	1:A:246:GLU:HG2	2.19	0.42
1:A:240:ALA:C	1:A:242:LEU:H	2.27	0.42
1:A:242:LEU:C	1:A:244:PRO:CD	2.92	0.42
1:A:281:ASP:C	1:A:281:ASP:OD1	2.63	0.42
1:A:92:GLU:O	1:A:104:SER:HA	2.19	0.42
1:A:165:ASP:CA	1:A:170:LEU:HD12	2.50	0.42
1:A:209:MET:CG	1:A:210:TYR:H	2.23	0.42
1:A:143:LEU:HD13	1:A:251:ARG:HG2	2.01	0.41
1:A:161:LEU:O	1:A:162:TYR:C	2.63	0.41
1:A:265:ALA:O	1:A:266:LEU:C	2.63	0.41
2:C:12:SER:CA	2:D:11:PRO:HD2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:MET:HE3	2:B:21:MET:HB2	1.73	0.41
1:A:146:PHE:CE2	1:A:150:MET:HE3	2.56	0.41
1:A:275:ILE:HG22	1:A:275:ILE:O	2.20	0.41
1:A:221:LEU:O	1:A:222:ASP:C	2.63	0.41
2:C:18:HYP:HA	2:D:17:GLN:O	2.20	0.41
1:A:73:THR:HA	1:A:74:PRO:HD3	1.96	0.40
1:A:267:ASP:O	1:A:268:GLU:C	2.63	0.40
2:C:29:PRO:HA	2:C:30:HYP:HD23	1.84	0.40
1:A:222:ASP:HA	1:A:234:GLU:OE2	2.22	0.40
2:C:32:ALA:HA	2:C:33:HYP:HD23	1.69	0.40
2:B:5:PRO:HA	2:B:6:HYP:HD23	1.83	0.40
2:B:16:GLY:HA3	2:D:14:PRO:O	2.21	0.40
2:B:32:ALA:HB1	2:B:33:HYP:CD	2.47	0.40
1:A:153:TRP:CE3	2:D:23:PHE:CE1	3.10	0.40
1:A:224:HIS:HA	1:A:225:PRO:HA	1.72	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/230 (92%)	156 (74%)	39 (18%)	16 (8%)	1	5
2	B	25/33 (76%)	18 (72%)	4 (16%)	3 (12%)	0	1
2	C	25/33 (76%)	17 (68%)	7 (28%)	1 (4%)	2	17
2	D	25/33 (76%)	21 (84%)	1 (4%)	3 (12%)	0	1
All	All	286/329 (87%)	212 (74%)	51 (18%)	23 (8%)	1	4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	167	ASP
1	A	172	THR
1	A	184	GLU
2	B	5	PRO
1	A	116	GLU
1	A	176	LYS
1	A	183	HIS
1	A	207	TYR
1	A	282	LYS
2	B	32	ALA
2	D	26	PRO
2	D	31	GLY
1	A	82	THR
1	A	213	PRO
1	A	222	ASP
2	C	20	VAL
2	D	19	GLY
1	A	56	GLN
1	A	208	ASN
2	B	21	MET
1	A	236	ALA
1	A	214	VAL

### 5.3.2 Protein sidechains [i](#)

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	173/211 (82%)	157 (91%)	16 (9%)	8	33
2	B	12/14 (86%)	11 (92%)	1 (8%)	10	38
2	C	13/14 (93%)	13 (100%)	0	100	100
2	D	13/14 (93%)	12 (92%)	1 (8%)	12	41
All	All	211/253 (83%)	193 (92%)	18 (8%)	10	37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	94	VAL
1	A	96	SER
1	A	114	THR
1	A	125	HIS
1	A	126	LEU
1	A	133	LYS
1	A	169	ASN
1	A	172	THR
1	A	182	ILE
1	A	211	ILE
1	A	256	CYS
1	A	267	ASP
1	A	272	CYS
1	A	275	ILE
1	A	285	VAL
2	B	23	PHE
2	D	17	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	97	ASN
1	A	168	ASN
1	A	169	ASN
1	A	206	ASN
1	A	217	GLN
1	A	260	ASN
2	D	17	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

21 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HYP	D	6	2	7,8,9	1.14	1 (14%)	5,10,12	1.44	1 (20%)
2	HYP	D	3	2	7,8,9	1.04	1 (14%)	5,10,12	1.79	1 (20%)
2	HYP	C	24	2	7,8,9	1.20	1 (14%)	5,10,12	1.70	2 (40%)
2	HYP	C	33	2	7,8,9	0.81	0	5,10,12	2.42	2 (40%)
2	HYP	D	18	2	7,8,9	1.12	1 (14%)	5,10,12	1.61	0
2	HYP	C	6	2	7,8,9	0.95	0	5,10,12	2.36	2 (40%)
2	HYP	B	30	2	7,8,9	0.75	0	5,10,12	2.01	2 (40%)
2	HYP	B	3	2	7,8,9	0.67	0	5,10,12	2.50	2 (40%)
2	HYP	B	33	2	7,8,9	0.76	0	5,10,12	1.92	2 (40%)
2	HYP	D	30	2	7,8,9	0.81	0	5,10,12	2.15	2 (40%)
2	HYP	D	33	2	7,8,9	0.83	0	5,10,12	2.46	2 (40%)
2	HYP	C	18	2	7,8,9	1.25	1 (14%)	5,10,12	1.45	0
2	HYP	C	3	2	7,8,9	0.95	0	5,10,12	2.27	2 (40%)
2	HYP	B	9	2	7,8,9	0.91	0	5,10,12	1.92	2 (40%)
2	HYP	B	18	2	7,8,9	0.86	0	5,10,12	2.41	2 (40%)
2	HYP	D	9	2	7,8,9	0.98	0	5,10,12	2.04	2 (40%)
2	HYP	B	24	2	7,8,9	1.25	1 (14%)	5,10,12	2.12	2 (40%)
2	HYP	C	30	2	7,8,9	0.83	0	5,10,12	1.73	2 (40%)
2	HYP	D	24	2	7,8,9	1.09	1 (14%)	5,10,12	1.81	3 (60%)
2	HYP	C	9	2	7,8,9	0.99	0	5,10,12	1.60	1 (20%)
2	HYP	B	6	2	7,8,9	1.03	1 (14%)	5,10,12	2.03	2 (40%)

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. <sup>1-2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	D	6	2	-	0/0/11/13	0/1/1/1
2	HYP	D	3	2	-	0/0/11/13	0/1/1/1
2	HYP	C	24	2	-	0/0/11/13	0/1/1/1
2	HYP	C	33	2	-	0/0/11/13	0/1/1/1
2	HYP	D	18	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	C	6	2	-	0/0/11/13	0/1/1/1
2	HYP	B	30	2	-	0/0/11/13	0/1/1/1
2	HYP	B	3	2	-	0/0/11/13	0/1/1/1
2	HYP	B	33	2	-	0/0/11/13	0/1/1/1
2	HYP	D	30	2	-	0/0/11/13	0/1/1/1
2	HYP	D	33	2	-	0/0/11/13	0/1/1/1
2	HYP	C	18	2	-	0/0/11/13	0/1/1/1
2	HYP	C	3	2	-	0/0/11/13	0/1/1/1
2	HYP	B	9	2	-	0/0/11/13	0/1/1/1
2	HYP	B	18	2	-	0/0/11/13	0/1/1/1
2	HYP	D	9	2	-	0/0/11/13	0/1/1/1
2	HYP	B	24	2	-	0/0/11/13	0/1/1/1
2	HYP	C	30	2	-	0/0/11/13	0/1/1/1
2	HYP	D	24	2	-	0/0/11/13	0/1/1/1
2	HYP	C	9	2	-	0/0/11/13	0/1/1/1
2	HYP	B	6	2	-	0/0/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	24	HYP	CA-N	-2.55	1.44	1.48
2	D	24	HYP	CA-N	-2.42	1.44	1.48
2	C	18	HYP	CA-N	-2.35	1.44	1.48
2	D	6	HYP	CA-N	-2.28	1.44	1.48
2	D	18	HYP	CA-N	-2.18	1.44	1.48
2	B	6	HYP	CA-N	-2.17	1.44	1.48
2	D	3	HYP	CA-N	-2.17	1.44	1.48
2	B	24	HYP	CA-N	-2.15	1.45	1.48

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	33	HYP	CG-CB-CA	4.39	108.83	103.75
2	C	6	HYP	CB-CG-CD	4.35	108.00	103.16
2	B	3	HYP	CG-CB-CA	3.93	108.29	103.75
2	C	3	HYP	CG-CB-CA	3.90	108.26	103.75
2	B	18	HYP	CB-CG-CD	3.87	107.47	103.16
2	D	33	HYP	CB-CG-CD	3.84	107.43	103.16
2	D	30	HYP	CB-CG-CD	3.74	107.33	103.16
2	B	3	HYP	CB-CG-CD	3.70	107.27	103.16
2	B	18	HYP	CG-CB-CA	3.60	107.91	103.75
2	B	24	HYP	CB-CG-CD	3.48	107.03	103.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	33	HYP	CG-CB-CA	3.34	107.62	103.75
2	B	30	HYP	CB-CG-CD	3.34	106.87	103.16
2	B	6	HYP	CG-CB-CA	3.25	107.50	103.75
2	B	9	HYP	CG-CB-CA	3.23	107.49	103.75
2	D	3	HYP	CB-CG-CD	3.20	106.72	103.16
2	C	33	HYP	CB-CG-CD	3.12	106.63	103.16
2	D	9	HYP	CG-CB-CA	2.97	107.18	103.75
2	C	9	HYP	CB-CG-CD	2.94	106.43	103.16
2	B	33	HYP	CB-CG-CD	2.84	106.32	103.16
2	C	3	HYP	CB-CG-CD	2.77	106.24	103.16
2	B	6	HYP	CB-CG-CD	2.69	106.16	103.16
2	D	24	HYP	CG-CB-CA	2.67	106.84	103.75
2	D	9	HYP	CB-CG-CD	2.66	106.11	103.16
2	C	6	HYP	CG-CB-CA	2.61	106.78	103.75
2	C	24	HYP	CB-CG-CD	2.59	106.03	103.16
2	B	33	HYP	CG-CB-CA	2.51	106.66	103.75
2	C	24	HYP	CG-CB-CA	2.42	106.56	103.75
2	B	30	HYP	CG-CB-CA	2.41	106.53	103.75
2	D	30	HYP	CG-CB-CA	2.33	106.45	103.75
2	D	6	HYP	CB-CG-CD	2.24	105.64	103.16
2	C	30	HYP	CB-CG-CD	2.20	105.60	103.16
2	B	24	HYP	OD1-CG-CD	-2.19	105.83	110.30
2	D	24	HYP	O-C-CA	-2.14	119.26	124.77
2	D	24	HYP	CB-CG-CD	2.13	105.53	103.16
2	C	30	HYP	CG-CB-CA	2.07	106.14	103.75
2	B	9	HYP	O-C-CA	-2.05	119.49	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	24	HYP	1	0
2	C	33	HYP	1	0
2	B	30	HYP	2	0
2	B	33	HYP	7	0
2	C	18	HYP	1	0
2	C	30	HYP	1	0
2	C	9	HYP	1	0
2	B	6	HYP	1	0

## 5.5 Carbohydrates i

2 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
3	NAG	E	1	3,1	14,14,15	0.49	0	17,19,21	1.30	4 (23%)
3	NAG	E	2	3	14,14,15	0.51	0	17,19,21	1.32	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2	NAG	C4-C3-C2	-3.74	105.53	111.02
3	E	1	NAG	C1-C2-N2	-2.40	106.65	110.43
3	E	1	NAG	O5-C5-C6	2.40	112.33	107.66
3	E	1	NAG	O4-C4-C3	-2.33	104.87	110.38
3	E	1	NAG	C4-C3-C2	2.27	114.34	111.02
3	E	2	NAG	C1-C2-N2	2.26	113.99	110.43

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2

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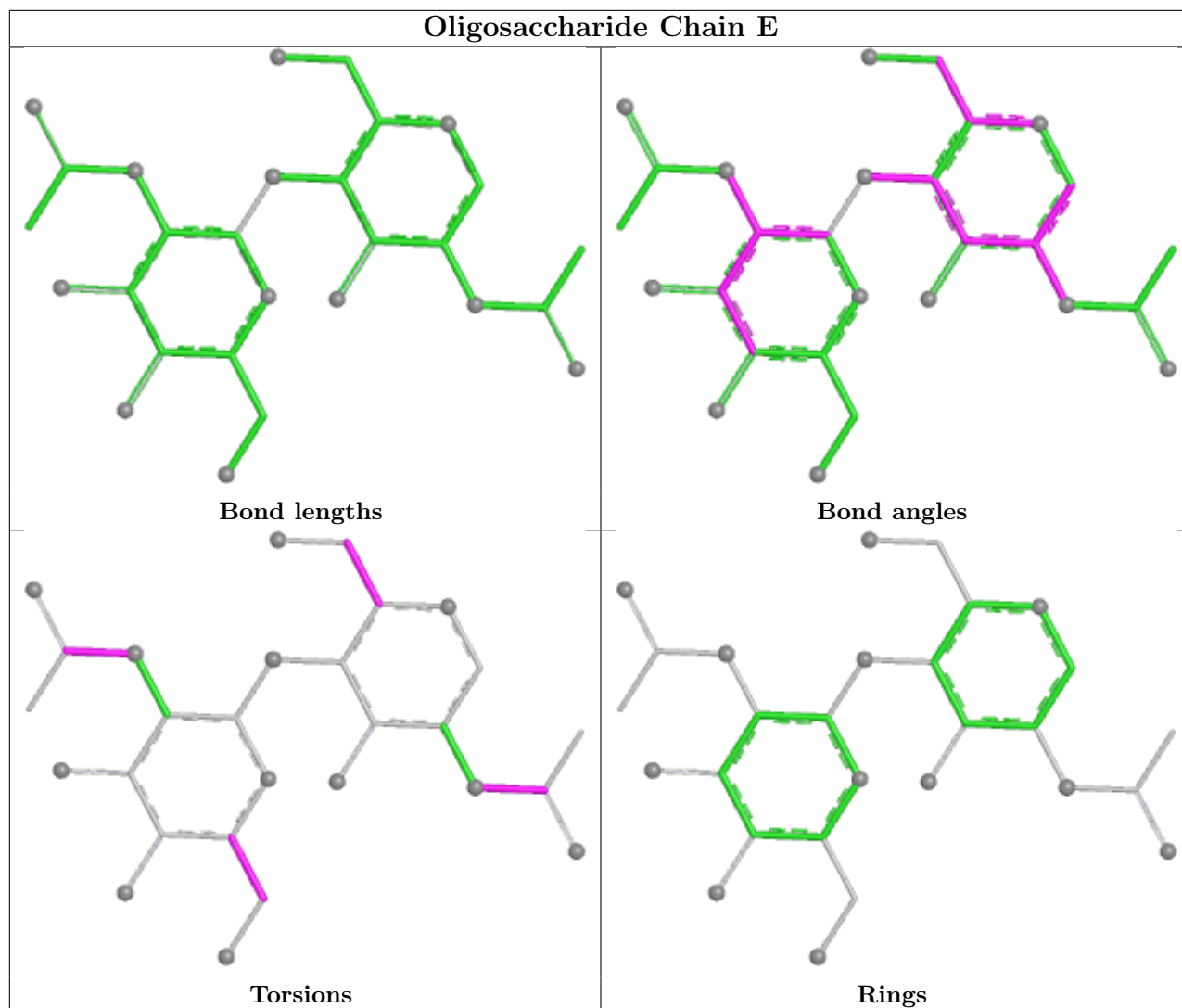
Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	NAG	1	0

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



## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
5	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.24	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/230 (93%)	0.20	16 (7%) 20 13	43, 84, 138, 163	0
2	B	26/33 (78%)	-0.10	0 100 100	59, 78, 123, 162	0
2	C	26/33 (78%)	-0.14	0 100 100	57, 79, 126, 127	0
2	D	26/33 (78%)	0.11	1 (3%) 44 27	59, 79, 122, 170	0
All	All	293/329 (89%)	0.14	17 (5%) 29 18	43, 83, 138, 170	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	VAL	5.7
1	A	63	GLY	5.5
2	D	1	GLY	5.0
1	A	64	LYS	4.7
1	A	79	GLN	4.3
1	A	77	VAL	3.4
1	A	69	ASP	2.9
1	A	57	ASN	2.8
1	A	110	ALA	2.6
1	A	78	CYS	2.6
1	A	66	CYS	2.5
1	A	68	LEU	2.5
1	A	54	PRO	2.4
1	A	109	PHE	2.3
1	A	115	LEU	2.3
1	A	72	ASN	2.1
1	A	73	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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.

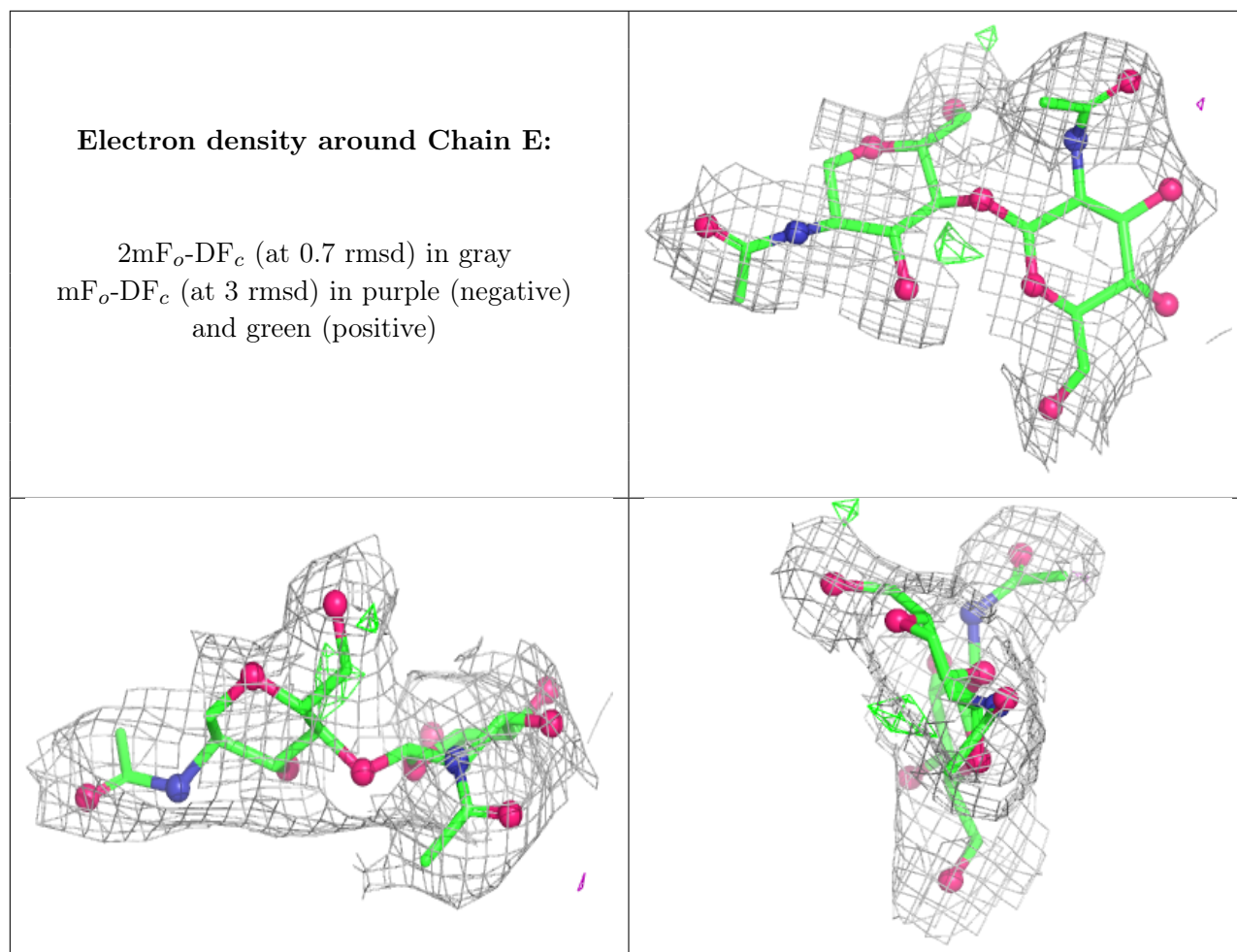
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HYP	D	30	8/9	0.68	0.13	138,141,152,152	0
2	HYP	C	33	8/9	0.77	0.14	115,125,128,129	0
2	HYP	B	33	8/9	0.79	0.10	108,119,122,125	0
2	HYP	B	30	8/9	0.80	0.10	112,115,120,122	0
2	HYP	D	33	8/9	0.83	0.20	156,161,163,165	0
2	HYP	B	6	8/9	0.87	0.09	97,99,100,100	0
2	HYP	B	3	8/9	0.87	0.10	134,138,144,145	0
2	HYP	D	6	8/9	0.90	0.10	93,95,98,99	0
2	HYP	D	3	8/9	0.91	0.12	93,96,99,102	0
2	HYP	B	9	8/9	0.91	0.08	74,83,85,86	0
2	HYP	C	30	8/9	0.92	0.08	87,93,96,101	0
2	HYP	C	9	8/9	0.93	0.08	80,84,87,90	0
2	HYP	D	24	8/9	0.93	0.12	70,75,78,80	0
2	HYP	D	9	8/9	0.94	0.10	76,79,84,87	0
2	HYP	C	18	8/9	0.94	0.09	57,61,65,67	0
2	HYP	C	6	8/9	0.95	0.06	98,100,102,103	0
2	HYP	D	18	8/9	0.95	0.09	57,61,71,73	0
2	HYP	B	18	8/9	0.95	0.08	56,64,65,66	0
2	HYP	C	3	8/9	0.95	0.09	112,115,117,119	0
2	HYP	C	24	8/9	0.95	0.09	58,59,59,59	0
2	HYP	B	24	8/9	0.96	0.10	58,58,59,96	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	E	2	14/15	0.70	0.12	90,99,108,114	0
3	NAG	E	1	14/15	0.88	0.12	80,89,94,95	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.



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	SO4	D	401	5/5	0.78	0.21	109,116,117,119	0
4	CA	A	301	1/1	0.99	0.06	83,83,83,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.