



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2024 – 12:10 AM EDT

PDB ID : 7UKO  
Title : Integrin alpha IIB beta3 complex with sibrifiban (Mn)  
Authors : Lin, F.-Y.; Zhu, J.; Zhu, J.; Springer, T.A.  
Deposited on : 2022-04-01  
Resolution : 2.60 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:

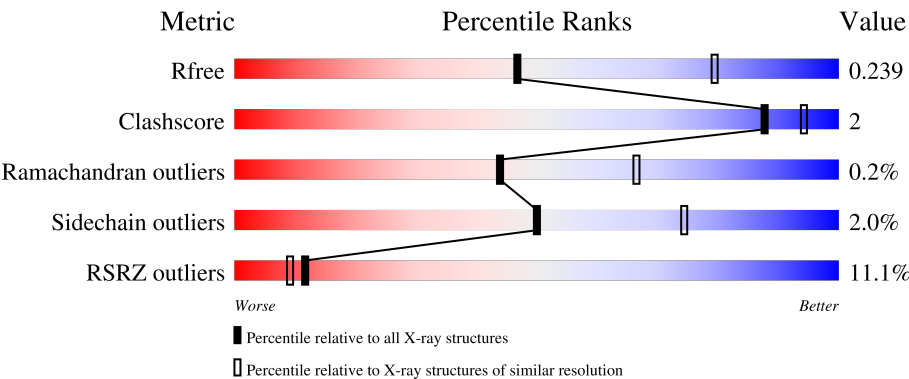
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.002 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.38.3

# 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 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	457	<div><div>2%</div><div>94%</div><div>5%</div><div>.</div></div>
1	C	457	<div><div>2%</div><div>93%</div><div>7%</div><div>.</div></div>
2	B	472	<div><div>8%</div><div>90%</div><div>8%</div><div>..</div></div>
2	D	472	<div><div>9%</div><div>91%</div><div>8%</div><div>.</div></div>
3	E	221	<div><div>38%</div><div>88%</div><div>9%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
3	H	221	
4	F	214	
4	L	214	
5	G	5	
6	I	2	
6	K	2	
7	J	4	

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 21809 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 Integrin alpha-IIb heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	5	0
			3508	2230	605	665	8			
1	C	453	Total	C	N	O	S	0	3	0
			3495	2219	602	666	8			

- Molecule 2 is a protein called Isoform Beta-3C of Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	466	Total	C	N	O	S	4	3	0
			3610	2248	616	713	33			
2	D	471	Total	C	N	O	S	3	1	0
			3631	2260	620	716	35			

- Molecule 3 is a protein called 10E5 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1631	1035	264	326	6			
3	H	216	Total	C	N	O	S	0	0	0
			1642	1041	266	329	6			

- Molecule 4 is a protein called 10E5 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			
4	L	214	Total	C	N	O	S	0	0	0
			1637	1019	268	341	9			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 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
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	K	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	J	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	4	Total	Ca	0	0
			4	4		
9	C	4	Total	Ca	0	0
			4	4		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

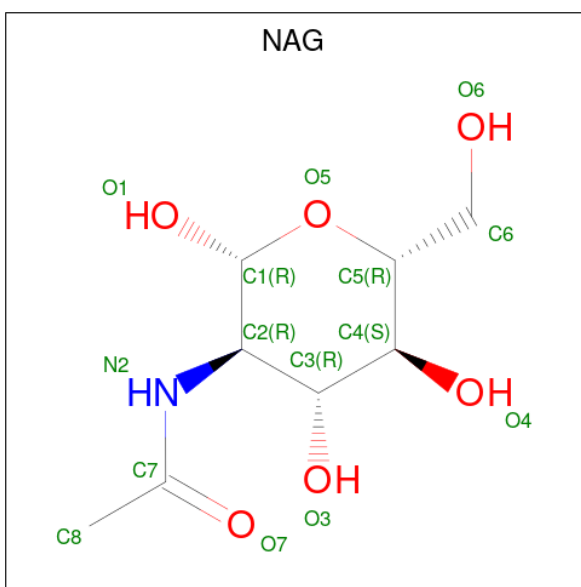


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			6	3	3		
10	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

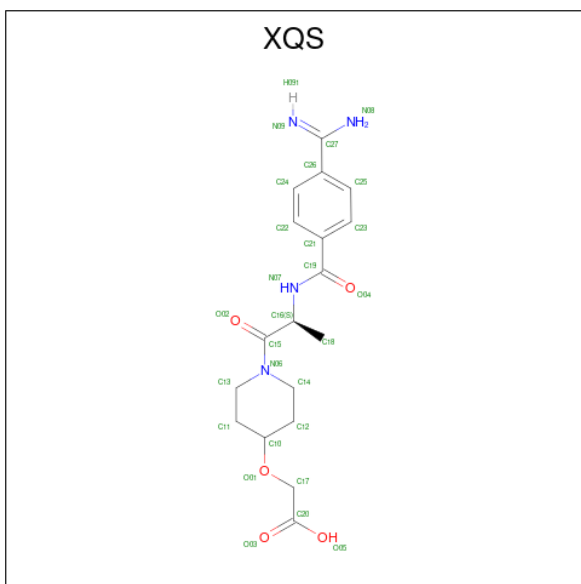
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	3	Total	Mn	0	0
			3	3		
11	D	3	Total	Mn	0	0
			3	3		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 13 is sibrifiban (active form) (three-letter code: XQS) (formula:  $C_{18}H_{24}N_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	N	O	0	0
			27	18	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	D	1	Total	C	N	O	0	0
			27	18	4	5		

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	1	Total	Cl	0	0
			1	1		

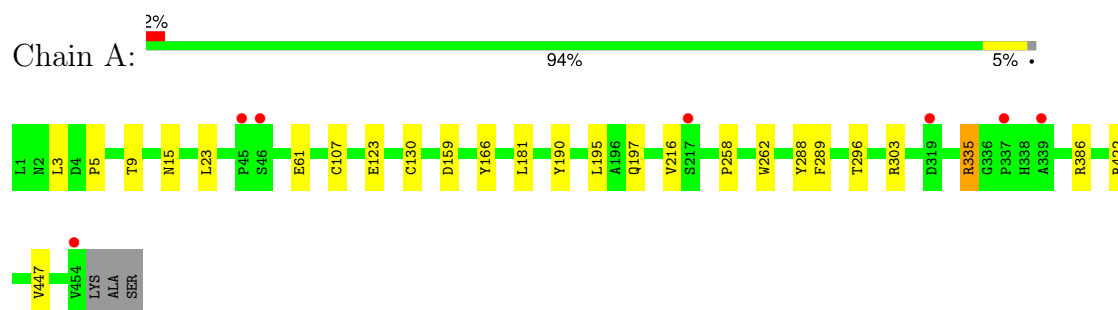
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	299	Total	O	0	0
			299	299		
15	B	150	Total	O	0	0
			150	150		
15	C	92	Total	O	0	0
			92	92		
15	D	85	Total	O	0	0
			85	85		
15	E	11	Total	O	0	0
			11	11		
15	F	18	Total	O	0	0
			18	18		
15	H	24	Total	O	0	0
			24	24		
15	L	38	Total	O	0	0
			38	38		

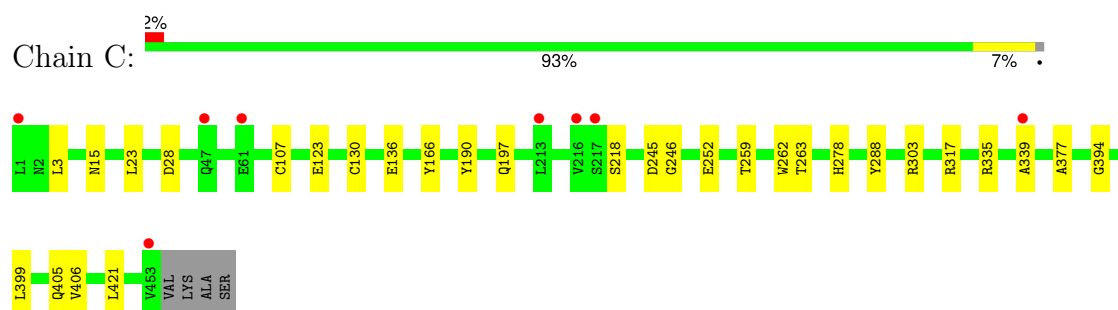
### 3 Residue-property plots [i](#)

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.

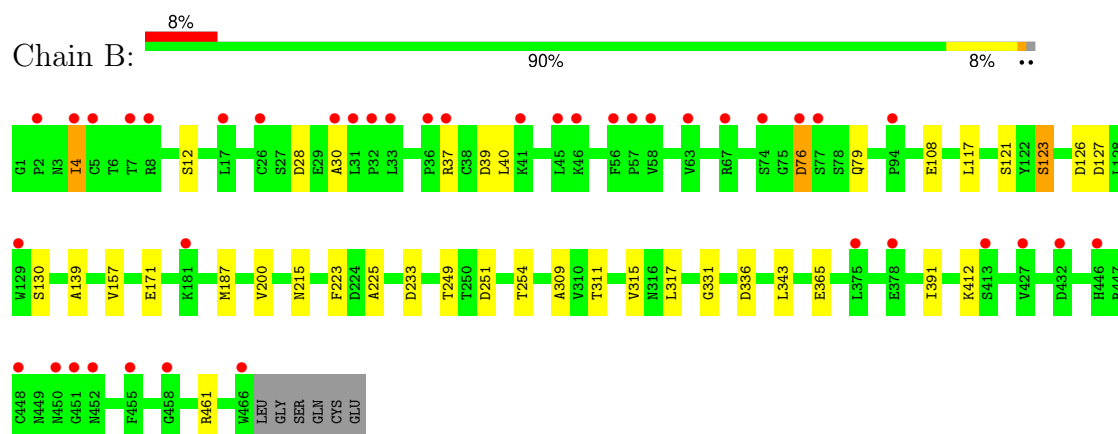
- Molecule 1: Integrin alpha-IIb heavy chain



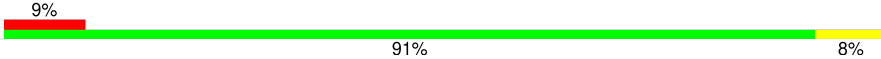
- Molecule 1: Integrin alpha-IIb heavy chain

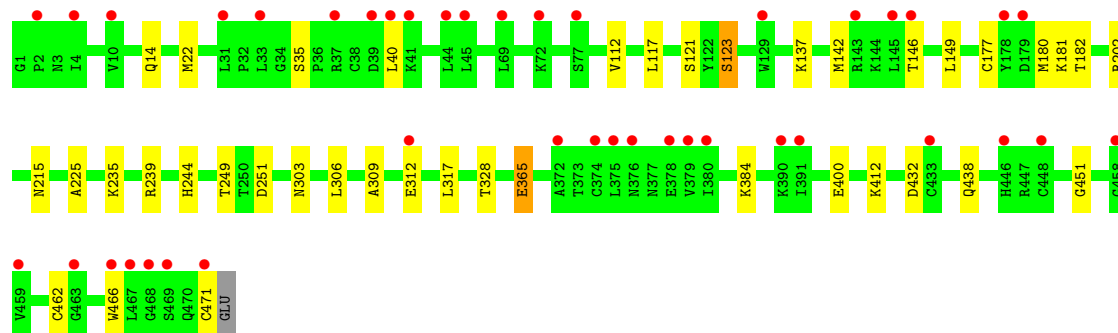


- Molecule 2: Isoform Beta-3C of Integrin beta-3




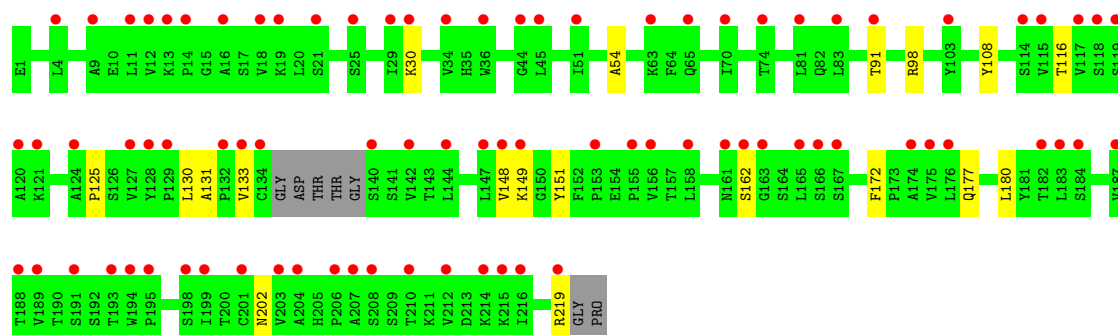
- Molecule 2: Isoform Beta-3C of Integrin beta-3

Chain D: 



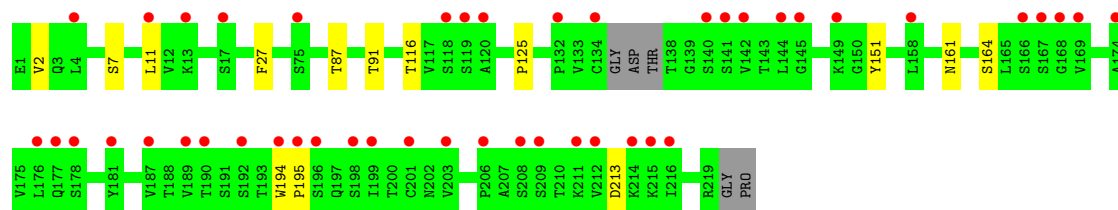
• Molecule 3: 10E5 Fab heavy chain

Chain E: 



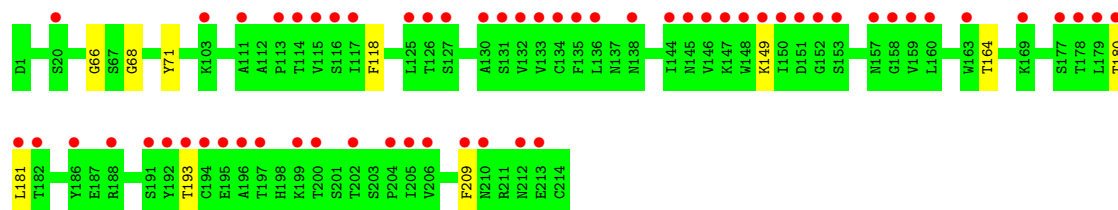
• Molecule 3: 10E5 Fab heavy chain

Chain H: 

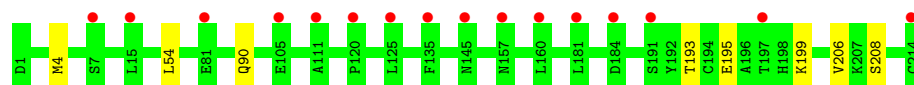


• Molecule 4: 10E5 Fab light chain

Chain F: 



• Molecule 4: 10E5 Fab light chain



- Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-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 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	258.39Å 144.60Å 104.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.60 49.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.29-2.60) 88.8 (49.29-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.84 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, $R_{free}$	0.214 , 0.239 0.214 , 0.239	Depositor DCC
$R_{free}$ test set	118716 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: BMA, GOL, NAG, SO4, MN, MAN, CL, XQS, CA

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	0.27	0/3620	0.49	0/4933
1	C	0.26	0/3594	0.47	0/4897
2	B	0.26	0/3680	0.46	0/4991
2	D	0.25	0/3698	0.45	0/5013
3	E	0.25	0/1673	0.45	0/2290
3	H	0.25	0/1684	0.46	0/2305
4	F	0.25	0/1673	0.46	0/2269
4	L	0.25	0/1673	0.45	0/2269
All	All	0.26	0/21295	0.46	0/28967

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	3508	0	3355	11	0
1	C	3495	0	3327	11	0
2	B	3610	0	3526	20	0
2	D	3631	0	3548	16	0
3	E	1631	0	1590	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1642	0	1600	5	0
4	F	1637	0	1553	7	0
4	L	1637	0	1553	4	0
5	G	61	0	52	0	0
6	I	28	0	25	0	0
6	K	28	0	25	1	0
7	J	50	0	43	0	0
8	A	10	0	0	0	0
8	C	10	0	0	0	0
8	L	5	0	0	0	0
9	A	4	0	0	0	0
9	C	4	0	0	0	0
10	A	12	0	16	2	0
11	B	3	0	0	0	0
11	D	3	0	0	0	0
12	B	14	0	13	0	0
12	D	14	0	13	0	0
13	B	27	0	0	1	0
13	D	27	0	0	1	0
14	C	1	0	0	0	0
15	A	299	0	0	1	0
15	B	150	0	0	0	0
15	C	92	0	0	0	0
15	D	85	0	0	0	0
15	E	11	0	0	0	0
15	F	18	0	0	0	0
15	H	24	0	0	0	0
15	L	38	0	0	1	0
All	All	21809	0	20239	79	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 2.

All (79) 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)
3:E:149:LYS:NZ	4:F:180:THR:HG21	2.02	0.74
1:C:245:ASP:OD1	1:C:246:GLY:N	2.26	0.68
1:A:386:ARG:HH11	10:A:507:GOL:H31	1.58	0.67
2:B:121:SER:HB2	13:B:2005:XQS:O03	1.94	0.67
2:B:39:ASP:OD1	2:B:40:LEU:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:121:SER:HB2	13:D:2005:XQS:O03	1.98	0.63
1:A:15[B]:ASN:ND2	15:A:602:HOH:O	2.32	0.61
2:D:123:SER:HB2	2:D:251:ASP:OD2	2.01	0.61
1:A:9:THR:HB	1:A:447:VAL:HB	1.85	0.56
2:B:130:SER:OG	2:B:336:ASP:O	2.19	0.55
2:B:28:ASP:OD1	2:B:30:ALA:N	2.40	0.55
2:D:400:GLU:HB2	6:K:1:NAG:H83	1.90	0.53
3:E:177:GLN:N	3:E:180:LEU:O	2.39	0.53
2:D:365:GLU:OE2	2:D:412:LYS:NZ	2.42	0.52
2:B:28:ASP:O	2:B:37:ARG:NH2	2.42	0.52
2:B:123:SER:HB2	2:B:251:ASP:OD2	2.09	0.52
1:A:262:TRP:HB3	2:B:317:LEU:HD13	1.92	0.51
1:A:296:THR:OG1	10:A:508:GOL:H12	2.10	0.51
2:B:76:ASP:HB3	2:B:79:GLN:H	1.75	0.51
2:D:177:CYS:HB3	2:D:182:THR:HG23	1.91	0.51
1:C:107:CYS:HA	1:C:130:CYS:HA	1.93	0.50
2:B:139:ALA:HB2	2:B:200:VAL:HG11	1.93	0.50
2:B:331:GLY:HA3	2:B:343:LEU:HD21	1.94	0.50
1:C:3:LEU:O	1:C:405:GLN:NE2	2.36	0.50
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.94	0.49
2:B:108:GLU:HG3	2:B:391:ILE:HG22	1.95	0.48
2:B:365:GLU:OE2	2:B:412:LYS:NZ	2.36	0.48
2:D:117:LEU:HD11	2:D:225:ALA:HB1	1.95	0.48
1:C:377:ALA:HB2	1:C:421:LEU:HD11	1.95	0.48
1:C:262:TRP:HB3	2:D:317:LEU:HD13	1.96	0.48
3:E:131:ALA:HB3	3:E:219:ARG:HG3	1.96	0.48
1:C:394:GLY:HA2	1:C:399:LEU:HD23	1.96	0.47
3:E:30:LYS:HG3	3:E:54:ALA:HA	1.96	0.47
2:B:233:ASP:N	2:B:233:ASP:OD1	2.43	0.47
2:D:112:VAL:HG23	2:D:146:THR:HG21	1.95	0.47
2:D:239:ARG:O	2:D:244:HIS:NE2	2.44	0.47
2:B:12:SER:HB3	2:B:461:ARG:HD3	1.98	0.47
1:A:303:ARG:NH1	1:A:335:ARG:HG3	2.29	0.46
4:L:193:THR:HG23	4:L:208:SER:HB3	1.97	0.46
3:E:125:PRO:HB3	3:E:151:TYR:HB3	1.97	0.46
1:C:303:ARG:NH1	1:C:335:ARG:HD3	2.30	0.46
3:E:91:THR:HG23	3:E:116:THR:HA	1.97	0.46
1:A:258:PRO:HA	1:A:289:PHE:O	2.16	0.46
2:D:14:GLN:HB2	2:D:438:GLN:HE22	1.80	0.46
2:B:4:ILE:H	2:B:4:ILE:HD13	1.81	0.45
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:162:SER:N	3:E:202:ASN:OD1	2.50	0.45
3:E:172:PHE:CD2	4:F:164:THR:HG23	2.52	0.45
1:A:159:ASP:CG	2:D:137:LYS:HG2	2.37	0.45
3:H:161:ASN:HB2	3:H:164:SER:HB3	1.99	0.44
2:D:142:MET:HB2	2:D:149:LEU:HD22	1.99	0.44
1:A:181:LEU:O	1:A:197:GLN:HA	2.19	0.43
1:C:28:ASP:HB2	1:C:136:GLU:OE2	2.19	0.43
1:C:278:HIS:CE1	1:C:339:ALA:HB1	2.54	0.42
3:E:133:VAL:HG21	4:F:209:PHE:HB3	2.00	0.42
3:E:98:ARG:HG3	3:E:108:TYR:HB2	2.02	0.42
3:H:194:TRP:CG	3:H:195:PRO:HA	2.54	0.42
3:E:149:LYS:HZ3	4:F:180:THR:HG21	1.80	0.42
1:A:3:LEU:O	1:A:5:PRO:HD3	2.20	0.42
4:F:66:GLY:HA3	4:F:71:TYR:HA	2.00	0.42
2:B:117:LEU:HD11	2:B:225:ALA:HB1	2.02	0.42
2:B:223:PHE:CZ	2:B:254:THR:HG21	2.55	0.42
2:B:249:THR:HA	2:B:309:ALA:O	2.20	0.41
3:E:130:LEU:HB3	4:F:118:PHE:HB3	2.01	0.41
3:H:2:VAL:HG13	3:H:27:PHE:CE1	2.54	0.41
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.02	0.41
2:D:22:MET:HG2	2:D:40:LEU:HD22	2.03	0.41
2:D:306:LEU:HB3	2:D:328:THR:HG22	2.02	0.41
4:F:149:LYS:HB2	4:F:193:THR:HB	2.03	0.41
2:D:249:THR:HG22	2:D:309:ALA:HB3	2.02	0.41
4:L:195:GLU:HG2	4:L:206:VAL:HG22	2.03	0.41
1:C:259:THR:HA	1:C:263:THR:HA	2.02	0.41
3:E:125:PRO:HB2	3:E:148:VAL:HG13	2.02	0.41
1:A:107:CYS:HA	1:A:130:CYS:HA	2.02	0.41
4:L:199:LYS:NZ	15:L:406:HOH:O	2.54	0.40
1:C:303:ARG:HH12	1:C:335:ARG:NE	2.19	0.40
2:B:311:THR:O	2:B:315[B]:VAL:HG23	2.21	0.40
2:D:466:TRP:HB3	2:D:471:CYS:SG	2.61	0.40
3:H:91:THR:HG23	3:H:116:THR:HA	2.04	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	457/457 (100%)	443 (97%)	13 (3%)	1 (0%)	44	66
1	C	454/457 (99%)	443 (98%)	10 (2%)	1 (0%)	44	66
2	B	467/472 (99%)	445 (95%)	20 (4%)	2 (0%)	30	52
2	D	470/472 (100%)	448 (95%)	21 (4%)	1 (0%)	44	66
3	E	210/221 (95%)	191 (91%)	19 (9%)	0	100	100
3	H	212/221 (96%)	201 (95%)	11 (5%)	0	100	100
4	F	212/214 (99%)	198 (93%)	13 (6%)	1 (0%)	25	47
4	L	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
All	All	2694/2728 (99%)	2574 (96%)	114 (4%)	6 (0%)	44	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	76	ASP
1	C	123	GLU
2	D	451	GLY
2	B	157	VAL
4	F	68	GLY

### 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	367/364 (101%)	358 (98%)	9 (2%)	42	68
1	C	364/364 (100%)	354 (97%)	10 (3%)	40	66
2	B	415/417 (100%)	407 (98%)	8 (2%)	52	75
2	D	417/417 (100%)	404 (97%)	13 (3%)	35	62
3	E	186/190 (98%)	186 (100%)	0	100	100
3	H	187/190 (98%)	183 (98%)	4 (2%)	48	73
4	F	188/188 (100%)	187 (100%)	1 (0%)	86	95
4	L	188/188 (100%)	187 (100%)	1 (0%)	86	95
All	All	2312/2318 (100%)	2266 (98%)	46 (2%)	50	74

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	61	GLU
1	A	166	TYR
1	A	190	TYR
1	A	195	LEU
1	A	216	VAL
1	A	288	TYR
1	A	335	ARG
1	A	422	ARG
2	B	4	ILE
2	B	123	SER
2	B	126[A]	ASP
2	B	126[B]	ASP
2	B	127	ASP
2	B	171	GLU
2	B	187	MET
2	B	215	ASN
1	C	15	ASN
1	C	23	LEU
1	C	166	TYR
1	C	190	TYR
1	C	197	GLN
1	C	218	SER
1	C	252	GLU
1	C	288	TYR
1	C	317	ARG
1	C	406	VAL

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Mol	Chain	Res	Type
2	D	35	SER
2	D	123	SER
2	D	180	MET
2	D	181	LYS
2	D	202	ARG
2	D	215	ASN
2	D	235	LYS
2	D	303	ASN
2	D	312	GLU
2	D	365	GLU
2	D	384	LYS
2	D	432	ASP
2	D	462	CYS
4	F	181	LEU
3	H	7	SER
3	H	11	LEU
3	H	87	THR
3	H	213	ASP
4	L	54	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2	ASN
1	C	333	GLN
2	D	438	GLN
4	F	138	ASN
4	F	156	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 ⓘ

13 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	$\# Z  > 2$
5	NAG	G	1	2,5	14,14,15	0.49	0	17,19,21	0.41	0
5	NAG	G	2	5	14,14,15	0.41	0	17,19,21	0.51	0
5	BMA	G	3	5	11,11,12	1.24	2 (18%)	15,15,17	0.92	1 (6%)
5	MAN	G	4	5	11,11,12	0.76	0	15,15,17	0.89	1 (6%)
5	MAN	G	5	5	11,11,12	1.15	1 (9%)	15,15,17	1.07	1 (6%)
6	NAG	I	1	6,2	14,14,15	0.36	0	17,19,21	0.45	0
6	NAG	I	2	6	14,14,15	0.50	0	17,19,21	0.41	0
7	NAG	J	1	7,2	14,14,15	0.51	0	17,19,21	0.52	0
7	NAG	J	2	7	14,14,15	0.42	0	17,19,21	0.38	0
7	BMA	J	3	7	11,11,12	0.88	0	15,15,17	0.84	1 (6%)
7	MAN	J	4	7	11,11,12	0.75	0	15,15,17	0.87	1 (6%)
6	NAG	K	1	6,2	14,14,15	0.47	0	17,19,21	0.38	0
6	NAG	K	2	6	14,14,15	0.37	0	17,19,21	0.42	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
5	NAG	G	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1
5	BMA	G	3	5	-	0/2/19/22	0/1/1/1
5	MAN	G	4	5	-	0/2/19/22	0/1/1/1
5	MAN	G	5	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	4/6/23/26	0/1/1/1
7	NAG	J	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	J	2	7	-	0/6/23/26	0/1/1/1
7	BMA	J	3	7	-	2/2/19/22	0/1/1/1
7	MAN	J	4	7	-	0/2/19/22	0/1/1/1
6	NAG	K	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	K	2	6	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	5	MAN	C1-C2	2.25	1.57	1.52
5	G	3	BMA	C2-C3	2.16	1.55	1.52
5	G	3	BMA	C4-C5	2.13	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	MAN	C1-C2-C3	2.92	113.90	109.64
7	J	4	MAN	O2-C2-C3	-2.28	105.44	110.15
5	G	4	MAN	O2-C2-C3	-2.25	105.48	110.15
5	G	3	BMA	C2-C3-C4	2.20	114.73	110.86
7	J	3	BMA	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

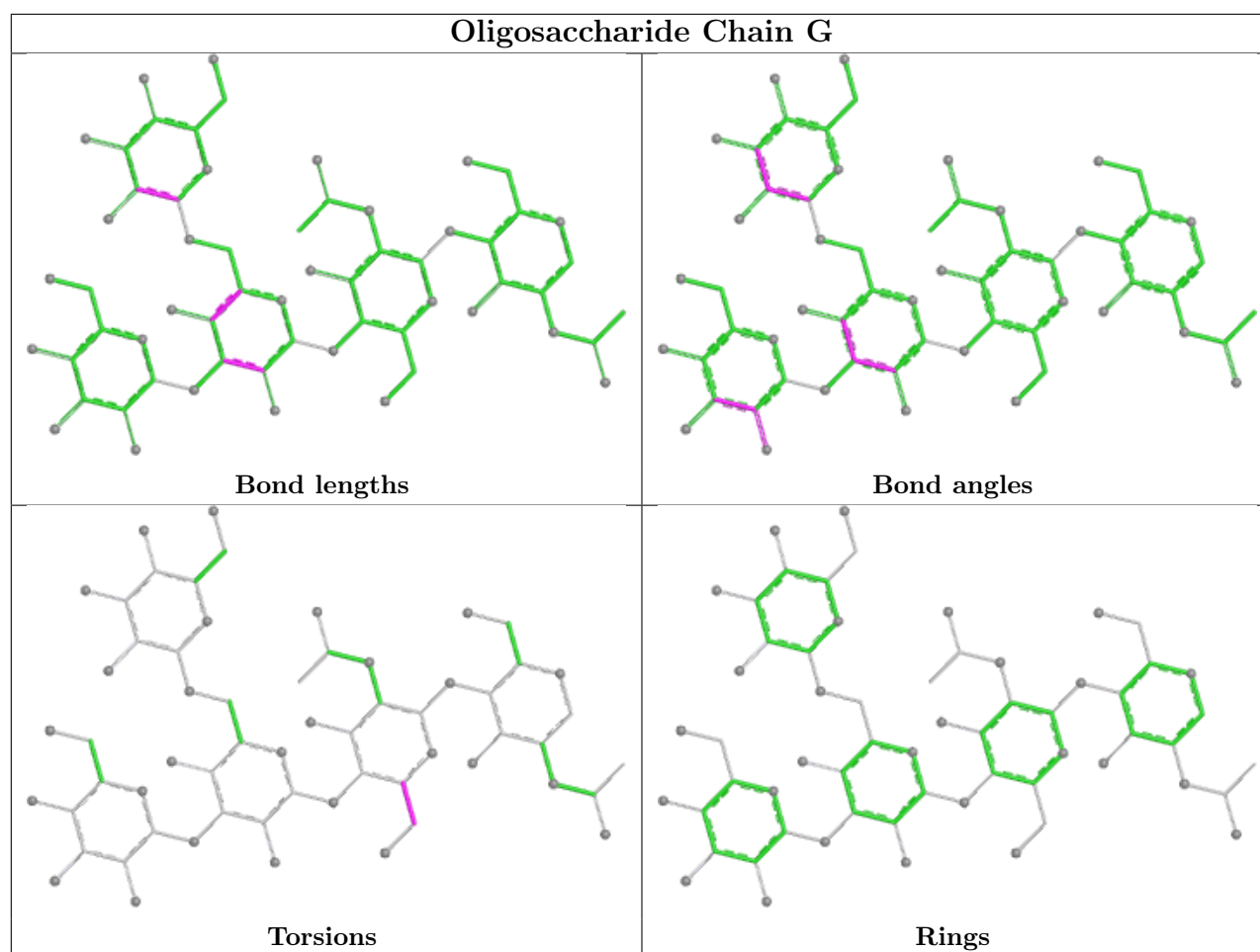
Mol	Chain	Res	Type	Atoms
6	I	2	NAG	C4-C5-C6-O6
6	K	2	NAG	C4-C5-C6-O6
7	J	3	BMA	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C8-C7-N2-C2
6	I	2	NAG	O7-C7-N2-C2
6	K	2	NAG	C8-C7-N2-C2
6	K	2	NAG	O7-C7-N2-C2
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
7	J	3	BMA	C4-C5-C6-O6
7	J	1	NAG	C4-C5-C6-O6
7	J	1	NAG	O5-C5-C6-O6

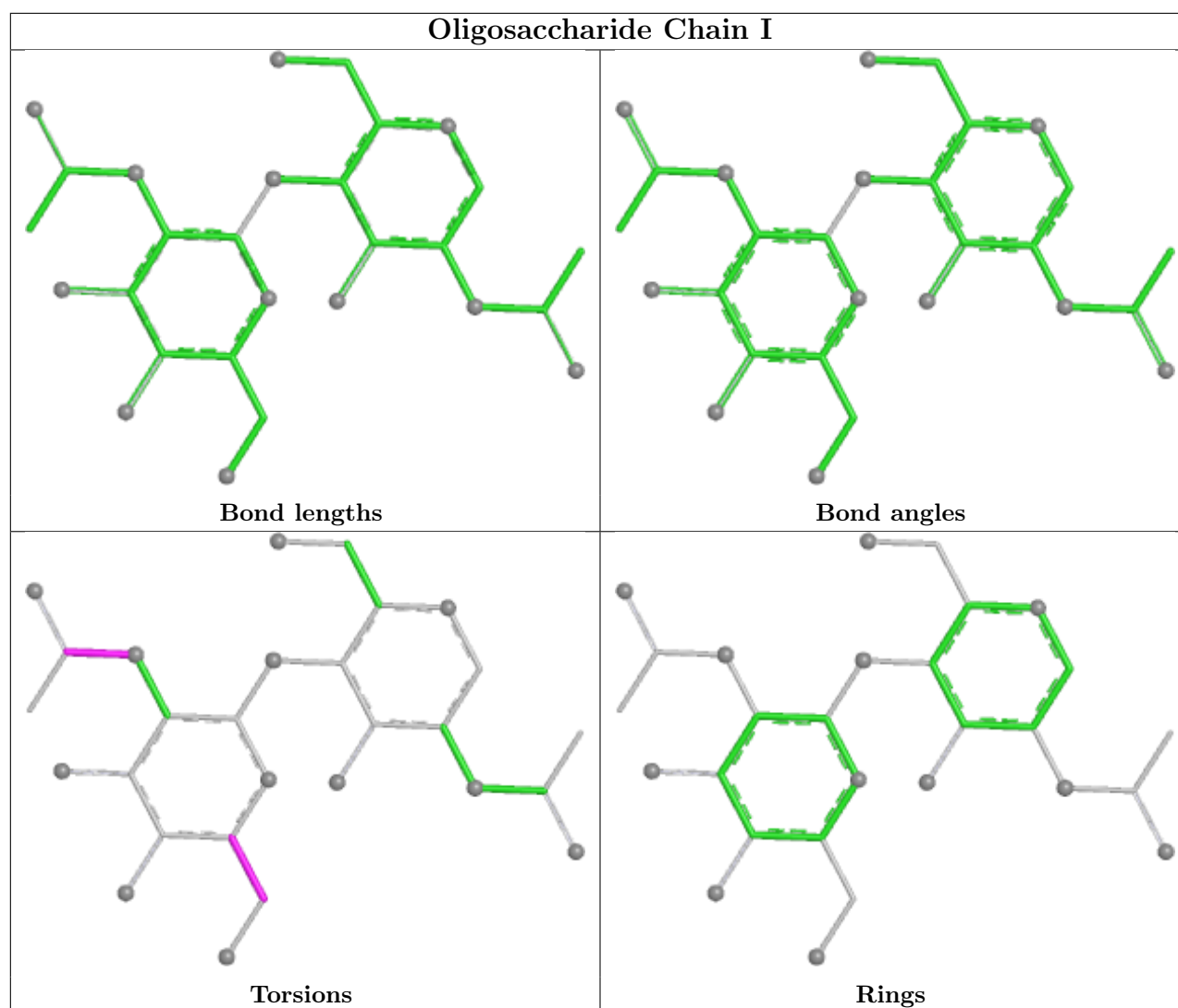
There are no ring outliers.

1 monomer is involved in 1 short contact:

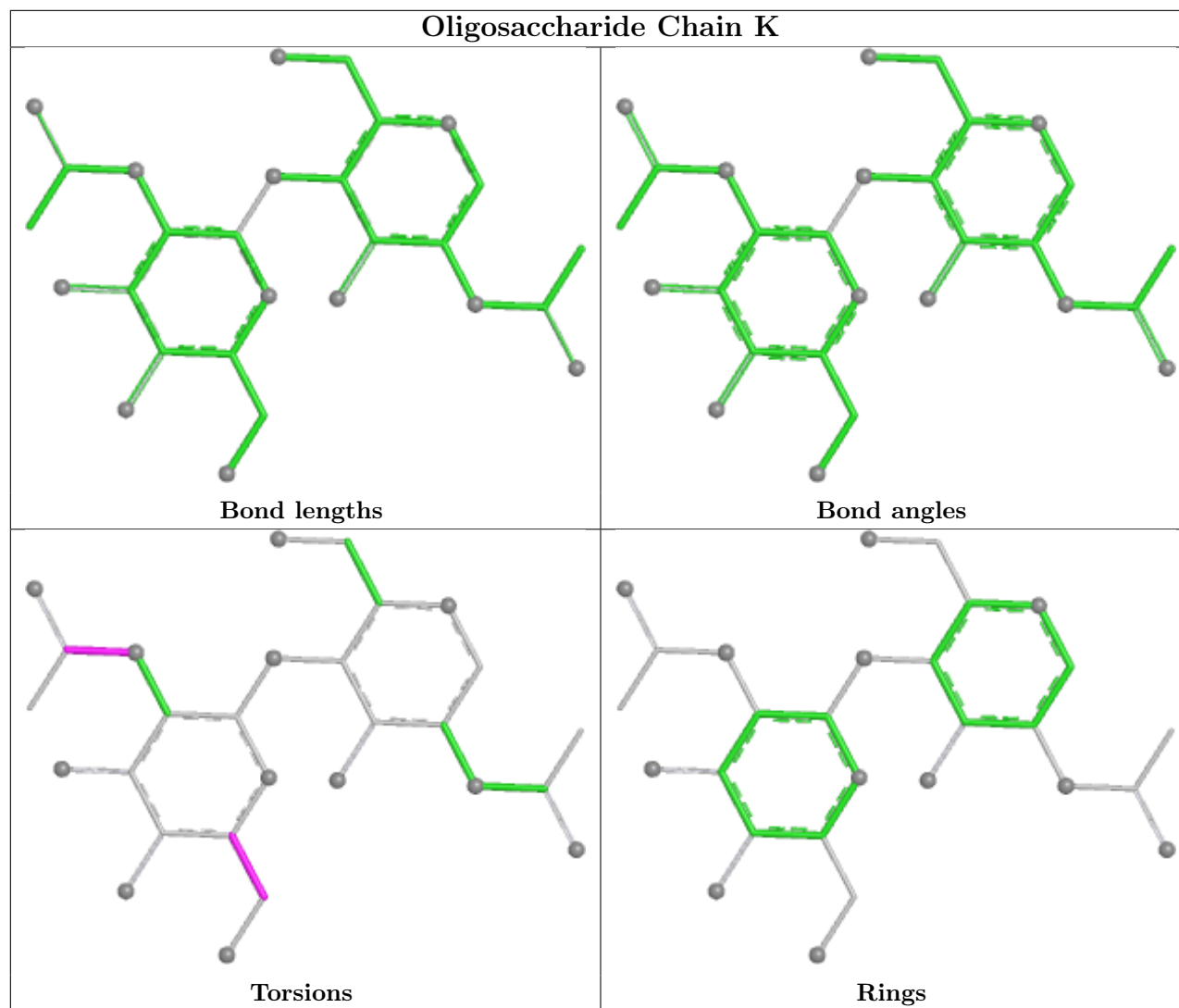
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	1	NAG	1	0

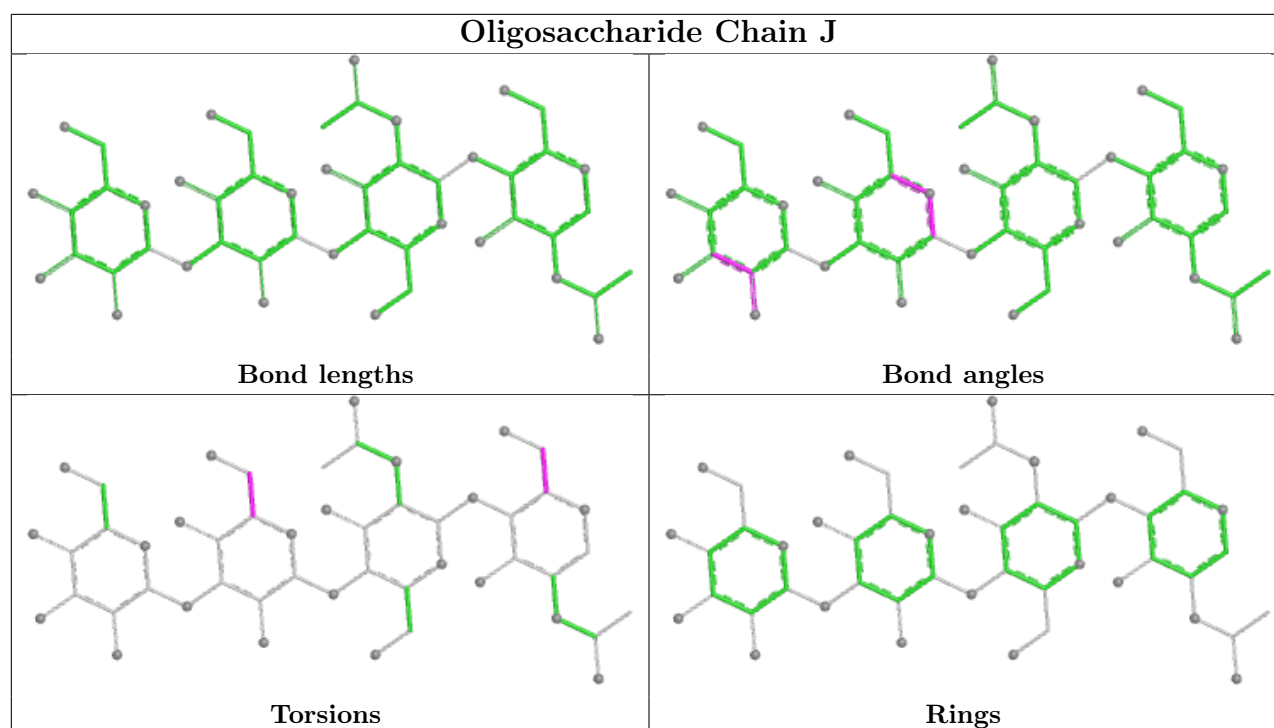
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 15 are monoatomic - leaving 11 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	$\# Z  > 2$
12	NAG	B	2004	2	14,14,15	0.33	0	17,19,21	0.54	0
8	SO4	L	301	-	4,4,4	0.25	0	6,6,6	0.19	0
13	XQS	B	2005	11	28,28,28	3.10	10 (35%)	33,38,38	1.72	5 (15%)
10	GOL	A	508	-	5,5,5	0.37	0	5,5,5	0.66	0
8	SO4	C	507	-	4,4,4	0.25	0	6,6,6	0.07	0
8	SO4	A	501	-	4,4,4	0.22	0	6,6,6	0.24	0
8	SO4	A	506	-	4,4,4	0.26	0	6,6,6	0.48	0
13	XQS	D	2005	11	28,28,28	3.15	11 (39%)	33,38,38	1.61	4 (12%)
8	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.16	0
10	GOL	A	507	-	5,5,5	0.38	0	5,5,5	0.51	0
12	NAG	D	2004	2	14,14,15	0.46	0	17,19,21	0.50	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
12	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
13	XQS	B	2005	11	-	2/25/35/35	0/2/2/2
10	GOL	A	508	-	-	4/4/4/4	-
13	XQS	D	2005	11	-	3/25/35/35	0/2/2/2
10	GOL	A	507	-	-	0/4/4/4	-
12	NAG	D	2004	2	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	D	2005	XQS	C22-C21	8.03	1.51	1.39
13	D	2005	XQS	C25-C23	7.97	1.51	1.38
13	D	2005	XQS	C24-C26	7.94	1.51	1.39
13	B	2005	XQS	C25-C23	7.81	1.51	1.38
13	B	2005	XQS	C22-C21	7.73	1.51	1.39
13	B	2005	XQS	C24-C26	7.61	1.50	1.39
13	D	2005	XQS	C15-N06	4.91	1.42	1.35
13	B	2005	XQS	C15-N06	4.56	1.41	1.35
13	D	2005	XQS	C19-N07	3.59	1.42	1.34
13	B	2005	XQS	C19-N07	3.49	1.42	1.34
13	B	2005	XQS	C23-C21	-2.97	1.34	1.39
13	B	2005	XQS	C25-C26	-2.95	1.34	1.39
13	D	2005	XQS	C23-C21	-2.87	1.35	1.39
13	D	2005	XQS	C25-C26	-2.82	1.35	1.39
13	B	2005	XQS	C24-C22	-2.77	1.34	1.38
13	B	2005	XQS	C14-N06	-2.41	1.42	1.47
13	D	2005	XQS	C14-N06	-2.40	1.42	1.47
13	D	2005	XQS	C24-C22	-2.39	1.34	1.38
13	B	2005	XQS	C13-N06	-2.21	1.43	1.47
13	D	2005	XQS	C26-C27	2.20	1.51	1.47
13	D	2005	XQS	C13-N06	-2.18	1.43	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	2005	XQS	C14-N06-C13	5.44	123.78	112.68
13	D	2005	XQS	C14-N06-C13	4.97	122.82	112.68
13	B	2005	XQS	C14-C12-C10	-4.11	105.88	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	D	2005	XQS	C11-C13-N06	4.09	118.68	110.66
13	B	2005	XQS	C11-C13-N06	3.64	117.79	110.66
13	D	2005	XQS	C14-C12-C10	-3.33	106.72	110.32
13	B	2005	XQS	C13-C11-C10	-2.94	107.14	110.32
13	B	2005	XQS	C12-C14-N06	2.92	116.39	110.66
13	D	2005	XQS	C12-C14-N06	2.90	116.35	110.66

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	508	GOL	C1-C2-C3-O3
10	A	508	GOL	O2-C2-C3-O3
13	B	2005	XQS	C24-C26-C27-N08
13	D	2005	XQS	C24-C26-C27-N08
10	A	508	GOL	O1-C1-C2-C3
13	D	2005	XQS	C11-C10-O01-C17
13	B	2005	XQS	C25-C26-C27-N08
13	D	2005	XQS	C25-C26-C27-N08
10	A	508	GOL	O1-C1-C2-O2
12	B	2004	NAG	C4-C5-C6-O6
12	B	2004	NAG	O5-C5-C6-O6

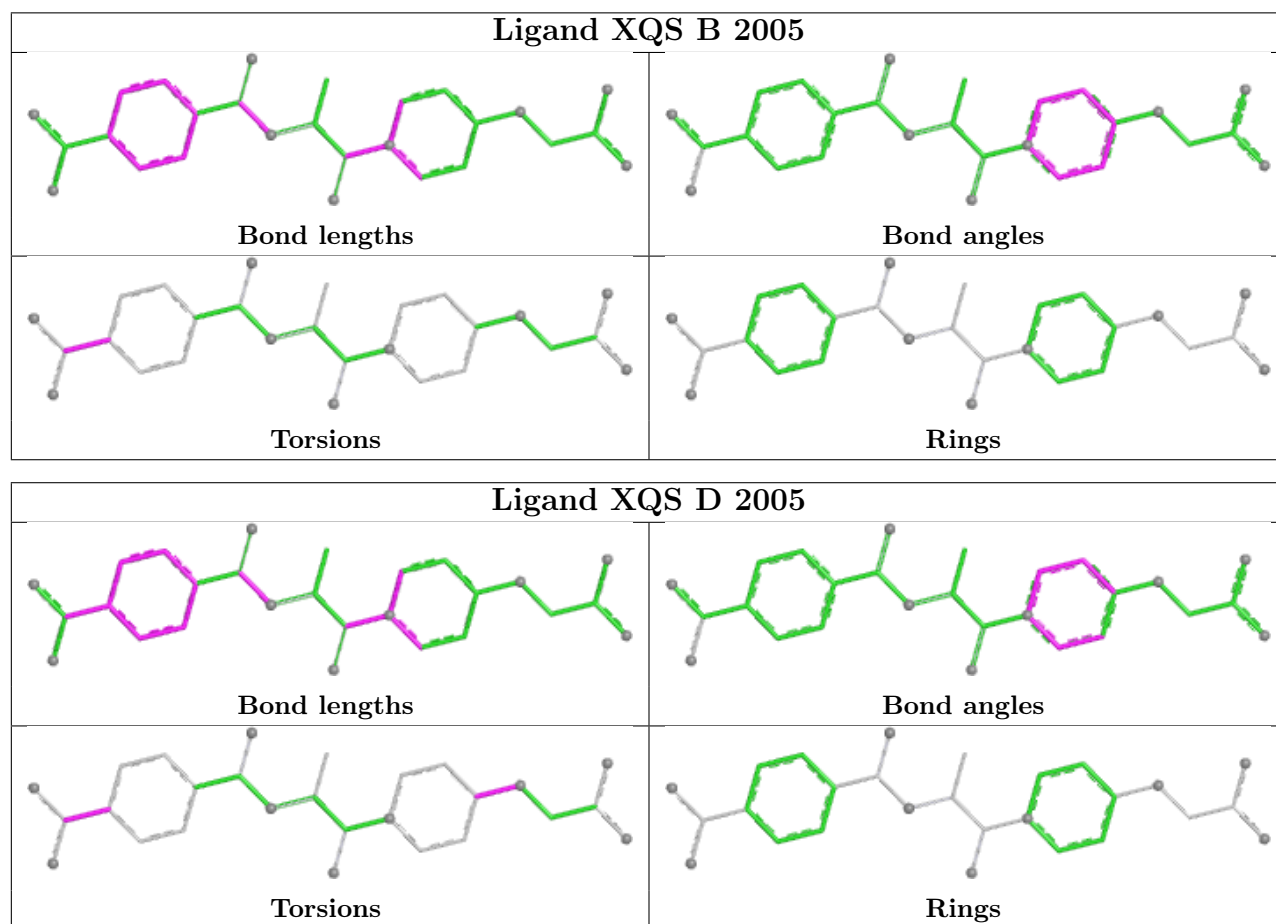
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	2005	XQS	1	0
10	A	508	GOL	1	0
13	D	2005	XQS	1	0
10	A	507	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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, 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	454/457 (99%)	-0.22	7 (1%) 71 67	21, 35, 52, 72	5 (1%)
1	C	453/457 (99%)	0.23	8 (1%) 67 62	21, 49, 69, 91	3 (0%)
2	B	466/472 (98%)	0.51	40 (8%) 18 15	20, 57, 120, 136	4 (0%)
2	D	471/472 (99%)	0.81	41 (8%) 17 14	24, 67, 111, 128	2 (0%)
3	E	214/221 (96%)	1.81	83 (38%) 1 1	67, 112, 153, 163	0
3	H	216/221 (97%)	1.23	45 (20%) 3 2	47, 84, 118, 126	0
4	F	214/214 (100%)	1.65	60 (28%) 2 1	69, 111, 156, 175	0
4	L	214/214 (100%)	0.91	16 (7%) 22 17	51, 74, 89, 115	0
All	All	2702/2728 (99%)	0.67	300 (11%) 12 9	20, 63, 133, 175	14 (0%)

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	147	LEU	5.8
3	E	165	LEU	5.6
2	D	471	CYS	4.9
3	E	212	VAL	4.8
2	D	375	LEU	4.7
4	F	130	ALA	4.7
4	F	204	PRO	4.5
1	A	454	VAL	4.3
4	F	125	LEU	4.2
3	H	189	VAL	4.2
2	D	2	PRO	4.1
4	F	193	THR	4.1
1	A	217	SER	4.1
4	F	152	GLY	4.1
4	F	135	PHE	4.1
4	F	181	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
4	F	136	LEU	4.0
2	D	469	SER	3.9
4	F	182	THR	3.9
4	F	180	THR	3.9
3	E	203	VAL	3.8
4	F	134	CYS	3.8
2	D	376	ASN	3.8
3	E	214	LYS	3.8
4	F	179	LEU	3.8
3	E	199	ILE	3.8
3	E	174	ALA	3.7
2	B	451	GLY	3.7
3	E	176	LEU	3.7
4	F	209	PHE	3.7
2	B	33	LEU	3.7
1	C	217	SER	3.7
2	B	129	TRP	3.6
3	E	189	VAL	3.6
4	F	195	GLU	3.6
2	B	57	PRO	3.6
4	F	132	VAL	3.5
4	F	205	ILE	3.5
4	L	157	ASN	3.5
2	B	458	GLY	3.5
3	E	144	LEU	3.5
2	B	4	ILE	3.4
4	F	148	TRP	3.4
1	A	46	SER	3.4
1	C	453	VAL	3.4
3	E	216	ILE	3.4
4	L	145	ASN	3.4
4	F	126	THR	3.4
3	E	149	LYS	3.3
2	B	77	SER	3.3
3	H	212	VAL	3.3
3	H	134	CYS	3.2
2	D	467	LEU	3.2
2	B	74	SER	3.2
4	F	117	ILE	3.2
1	C	1	LEU	3.2
2	D	145	LEU	3.2
3	H	206	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	115	VAL	3.2
4	F	197	THR	3.2
3	H	198	SER	3.2
4	F	131	SER	3.2
4	F	150	ILE	3.2
3	E	81	LEU	3.2
4	F	157	ASN	3.1
4	F	160	LEU	3.1
2	B	181	LYS	3.1
3	E	120	ALA	3.1
3	H	177	GLN	3.1
2	D	468	GLY	3.1
3	E	194	TRP	3.1
4	F	149	LYS	3.1
3	E	83	LEU	3.0
3	E	182	THR	3.0
4	F	178	THR	3.0
3	E	132	PRO	3.0
2	D	466	TRP	3.0
3	E	11	LEU	3.0
4	F	159	VAL	3.0
2	B	466	TRP	3.0
2	D	33	LEU	3.0
2	D	178	TYR	3.0
3	H	142	VAL	3.0
3	H	166	SER	3.0
4	F	133	VAL	2.9
2	D	378	GLU	2.9
4	F	186	TYR	2.9
4	F	114	THR	2.9
3	H	195	PRO	2.9
2	B	63	VAL	2.9
1	C	47	GLN	2.9
3	E	129	PRO	2.9
4	F	194	CYS	2.9
4	F	163	TRP	2.9
3	E	115	VAL	2.9
2	D	44	LEU	2.9
4	F	199	LYS	2.8
3	E	114	SER	2.8
3	E	184	SER	2.8
4	L	7	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	128	TYR	2.8
4	F	127	SER	2.8
3	H	158	LEU	2.8
2	D	446	HIS	2.8
3	E	119	SER	2.8
1	A	339	ALA	2.8
2	B	36	PRO	2.8
3	E	14	PRO	2.8
3	H	216	ILE	2.8
4	F	192	TYR	2.8
2	B	37	ARG	2.8
3	E	201	CYS	2.7
4	F	116	SER	2.7
3	E	74	THR	2.7
2	B	375	LEU	2.7
3	E	140	SER	2.7
3	E	204	ALA	2.7
2	B	446	HIS	2.7
2	B	378	GLU	2.7
3	E	153	PRO	2.7
3	H	178	SER	2.7
4	F	177	SER	2.7
2	B	41	LYS	2.7
3	E	133	VAL	2.7
3	E	142	VAL	2.7
1	A	45	PRO	2.7
3	E	36	TRP	2.7
3	E	162	SER	2.7
3	H	174	ALA	2.6
4	F	111	ALA	2.6
4	L	135	PHE	2.6
2	D	374	CYS	2.6
3	E	12	VAL	2.6
4	F	206	VAL	2.6
2	D	31	LEU	2.6
2	D	45	LEU	2.6
3	E	158	LEU	2.6
3	E	127	VAL	2.6
2	D	391	ILE	2.6
4	F	147	LYS	2.5
2	B	31	LEU	2.5
2	B	432	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	18	VAL	2.5
3	H	203	VAL	2.5
4	F	196	ALA	2.5
3	E	30	LYS	2.5
3	H	140	SER	2.5
4	L	125	LEU	2.5
3	E	175	VAL	2.5
4	L	81	GLU	2.5
3	H	196	SER	2.5
2	D	40	LEU	2.5
2	D	69	LEU	2.5
3	E	161	ASN	2.5
2	B	7	THR	2.5
3	H	17	SER	2.5
2	D	10	VAL	2.5
2	B	56	PHE	2.5
3	E	163	GLY	2.5
4	L	105	GLU	2.4
2	D	129	TRP	2.4
3	E	183	LEU	2.4
3	E	148	VAL	2.4
3	E	187	VAL	2.4
3	E	134	CYS	2.4
4	F	169	LYS	2.4
2	D	372	ALA	2.4
3	E	9	ALA	2.4
4	L	111	ALA	2.4
4	F	212	ASN	2.4
4	F	202	THR	2.4
2	B	2	PRO	2.4
2	B	67	ARG	2.4
2	D	37	ARG	2.4
3	E	155	PRO	2.4
3	E	21	SER	2.4
3	E	166	SER	2.4
1	A	319	ASP	2.4
2	B	452	ASN	2.4
3	E	210	THR	2.4
2	B	45	LEU	2.4
3	E	206	PRO	2.4
3	E	167	SER	2.4
3	H	208	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	E	51	ILE	2.4
2	D	41	LYS	2.4
3	H	215	LYS	2.4
2	D	459	VAL	2.4
3	E	198	SER	2.4
2	B	5	CYS	2.4
2	D	463	GLY	2.4
3	H	201	CYS	2.4
4	F	188	ARG	2.3
2	B	46	LYS	2.3
2	D	72	LYS	2.3
3	H	187	VAL	2.3
2	D	4	ILE	2.3
3	E	29	ILE	2.3
3	H	167	SER	2.3
3	H	209	SER	2.3
4	F	158	GLY	2.3
4	F	151	ASP	2.3
4	L	214	CYS	2.3
3	E	195	PRO	2.3
1	C	216	VAL	2.3
1	C	339	ALA	2.3
3	E	45	LEU	2.3
2	D	146	THR	2.3
3	E	188	THR	2.3
3	H	149	LYS	2.3
2	B	32	PRO	2.3
3	H	132	PRO	2.3
4	F	146	VAL	2.3
3	E	124	ALA	2.3
4	F	191	SER	2.3
2	B	17	LEU	2.3
3	E	4	LEU	2.3
3	E	193	THR	2.3
3	E	16	ALA	2.3
3	H	144	LEU	2.3
3	H	176	LEU	2.3
4	F	153	SER	2.3
4	L	160	LEU	2.3
4	L	191	SER	2.3
2	D	312	GLU	2.2
4	F	200	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	380	ILE	2.2
3	H	120	ALA	2.2
3	H	118	SER	2.2
4	F	20	SER	2.2
4	F	213	GLU	2.2
2	B	94	PRO	2.2
4	F	113	PRO	2.2
4	L	197	THR	2.2
3	E	103	TYR	2.2
3	E	44	GLY	2.2
3	H	141	SER	2.2
2	D	39	ASP	2.2
2	D	433	CYS	2.2
2	B	30	ALA	2.2
3	E	219	ARG	2.2
1	C	61	GLU	2.2
3	H	190	THR	2.2
3	E	34	VAL	2.2
3	E	156	VAL	2.2
3	H	11	LEU	2.2
3	E	91	THR	2.1
2	B	76	ASP	2.1
3	E	65	GLN	2.1
2	B	26	CYS	2.1
2	B	8	ARG	2.1
1	A	337	PRO	2.1
4	L	120	PRO	2.1
3	E	19	LYS	2.1
3	E	63	LYS	2.1
4	F	144	ILE	2.1
4	L	184	ASP	2.1
3	E	208	SER	2.1
3	H	13	LYS	2.1
2	B	455	PHE	2.1
2	D	379	VAL	2.1
4	F	210	ASN	2.1
3	H	181	TYR	2.1
3	H	4	LEU	2.1
2	D	143	ARG	2.1
3	H	168	GLY	2.1
3	H	214	LYS	2.1
2	D	77	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	119	SER	2.1
3	H	192	SER	2.1
2	B	58	VAL	2.1
4	F	145	ASN	2.1
4	L	15	LEU	2.1
2	D	179	ASP	2.1
3	E	207	ALA	2.1
3	H	145	GLY	2.1
2	B	448	CYS	2.0
2	D	390	LYS	2.0
2	D	448	CYS	2.0
3	E	121	LYS	2.0
4	F	103	LYS	2.0
3	H	194	TRP	2.0
3	H	199	ILE	2.0
2	B	413	SER	2.0
3	E	25	SER	2.0
3	H	169	VAL	2.0
1	C	213	LEU	2.0
2	D	458	GLY	2.0
3	E	13	LYS	2.0
3	E	215	LYS	2.0
3	H	211	LYS	2.0
3	E	70	ILE	2.0
2	B	427	VAL	2.0
3	E	117	VAL	2.0
4	L	181	LEU	2.0
3	E	118	SER	2.0
3	E	191	SER	2.0
3	H	75	SER	2.0
2	B	450	ASN	2.0
4	F	138	ASN	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](#)

SUGAR-RSR INFOmissingINFO

## 6.4 Ligands ⓘ

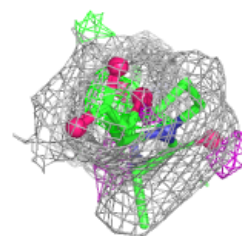
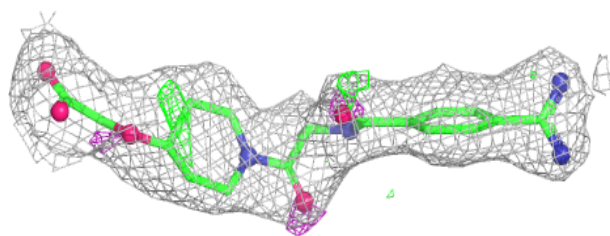
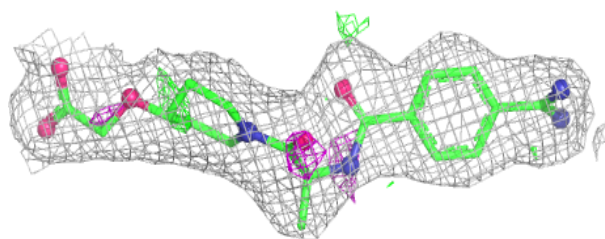
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
12	NAG	B	2004	14/15	0.66	0.17	86,86,86,86	0
12	NAG	D	2004	14/15	0.67	0.16	81,81,81,81	0
11	MN	B	2002	1/1	0.82	0.35	66,66,66,66	0
10	GOL	A	508	6/6	0.83	0.14	39,39,39,39	0
8	SO4	C	507	5/5	0.85	0.20	73,73,73,73	0
8	SO4	A	506	5/5	0.87	0.22	58,58,58,58	0
10	GOL	A	507	6/6	0.88	0.14	35,35,35,35	0
8	SO4	L	301	5/5	0.89	0.23	70,70,70,70	0
8	SO4	A	501	5/5	0.89	0.15	49,49,49,49	0
13	XQS	B	2005	27/27	0.90	0.11	33,33,33,33	0
13	XQS	D	2005	27/27	0.90	0.12	48,48,48,48	0
8	SO4	C	501	5/5	0.91	0.17	69,69,69,69	0
11	MN	D	2002	1/1	0.95	0.18	65,65,65,65	0
14	CL	C	502	1/1	0.95	0.07	53,53,53,53	0
9	CA	A	504	1/1	0.96	0.04	31,31,31,31	0
9	CA	A	503	1/1	0.97	0.05	33,33,33,33	0
9	CA	C	503	1/1	0.97	0.05	67,67,67,67	0
9	CA	C	506	1/1	0.97	0.04	49,49,49,49	0
9	CA	C	504	1/1	0.98	0.06	55,55,55,55	0
11	MN	B	2003	1/1	0.98	0.07	32,32,32,32	0
9	CA	A	502	1/1	0.99	0.03	44,44,44,44	0
9	CA	A	505	1/1	0.99	0.02	31,31,31,31	0
11	MN	D	2001	1/1	0.99	0.04	44,44,44,44	0
9	CA	C	505	1/1	0.99	0.03	50,50,50,50	0
11	MN	D	2003	1/1	0.99	0.08	45,45,45,45	0
11	MN	B	2001	1/1	1.00	0.03	29,29,29,29	0

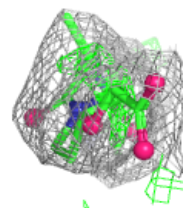
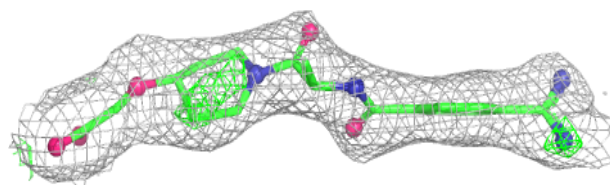
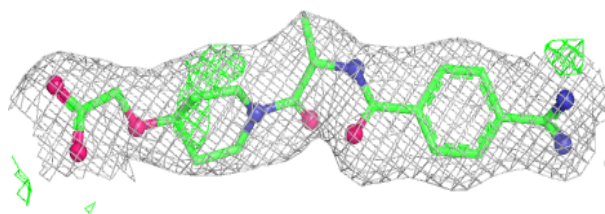
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around XQS B 2005:**

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

**Electron density around XQS D 2005:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.