



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:08 PM BST

PDB ID : 2UWN  
Title : Crystal structure of Human Complement Factor H, SCR domains 6-8 (H402 risk variant), in complex with ligand.  
Authors : Prosser, B.E.; Johnson, S.; Roversi, P.; Herbert, A.P.; Blaum, B.S.; Tyrrell, J.; Jowitt, T.A.; Clark, S.J.; Terelli, E.; Uhrin, D.; Barlow, P.N.; Sim, R.B.; Day, A.J.; Lea, S.M.  
Deposited on : 2007-03-22  
Resolution : 2.35 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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

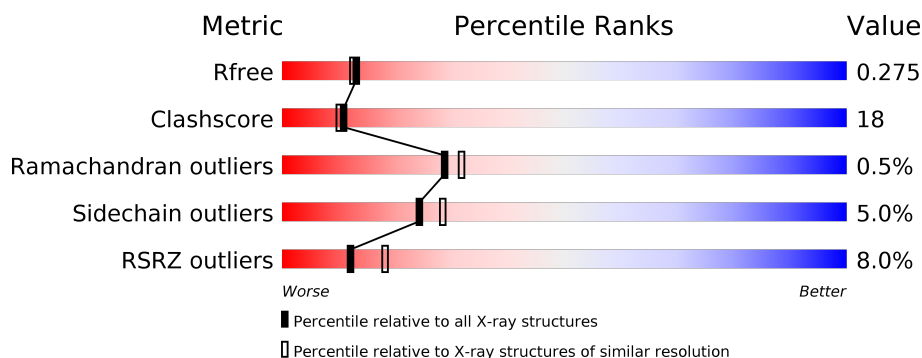
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	187	
2	B	2	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	YYJ	B	2[A]	-	-	X	-

## 2 Entry composition [i](#)

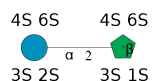
There are 6 unique types of molecules in this entry. The entry contains 1755 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HUMAN COMPLEMENT FACTOR H.

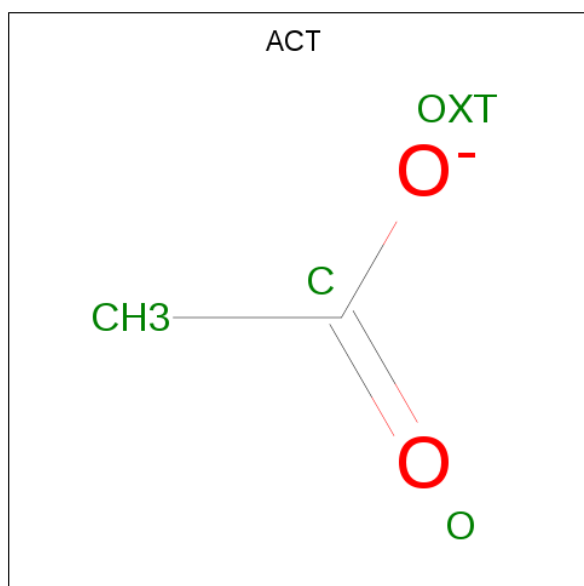
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	2	0
			1489	944	250	281	14			

- Molecule 2 is an oligosaccharide called 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	S	0	2	0
			110	24	70	16			

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

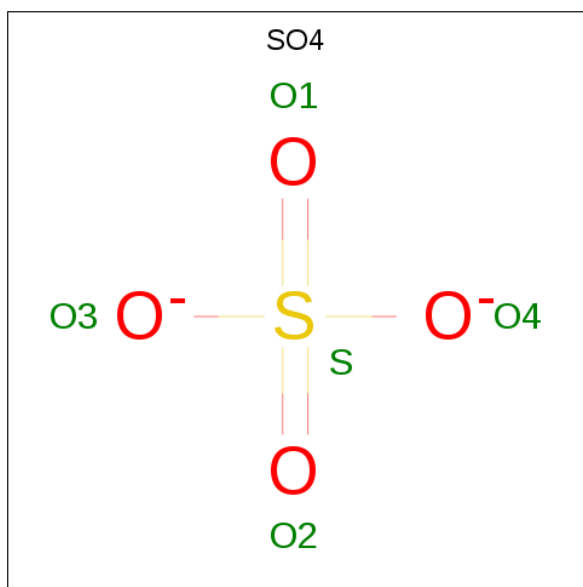


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

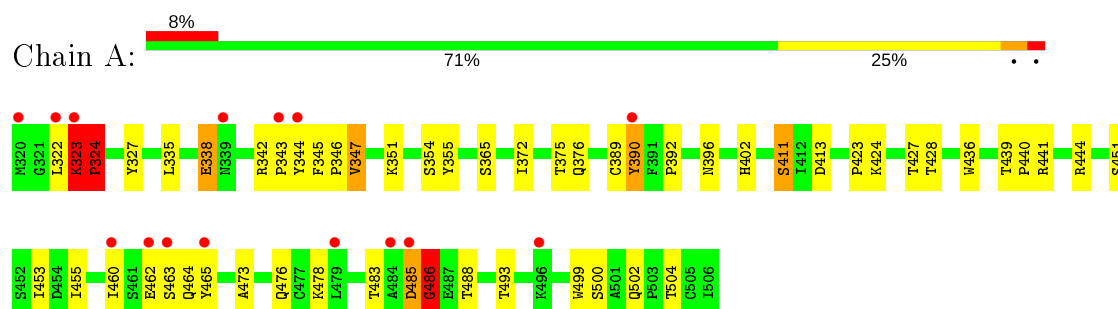
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	135	Total O 135 135	0	0

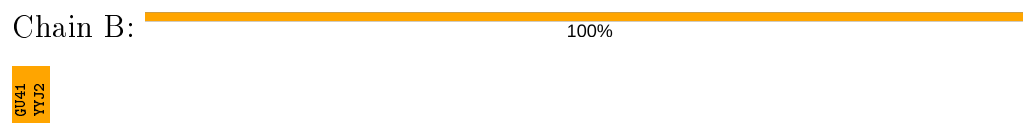
### 3 Residue-property plots

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: HUMAN COMPLEMENT FACTOR H



#### • Molecule 2: 1,3,4,6-tetra-O-sulfo-beta-D-fructofuranose-(2-1)-2,3,4,6-tetra-O-sulfonato-alpha-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.76Å 92.49Å 57.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.35 19.66 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.35) 97.9 (19.66-2.35)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.35Å)	Xtriage
Refinement program		Depositor
R, $R_{free}$	0.214 , 0.246 0.229 , 0.275	Depositor DCC
$R_{free}$ test set	835 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	1755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GU4, ACT, YYJ, SO4, CL

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	0.64	3/1546 (0.2%)	0.64	4/2098 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	486	GLY	C-O	11.69	1.42	1.23
1	A	324	PRO	C-N	7.00	1.50	1.34
1	A	343	PRO	C-N	-6.44	1.19	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	PRO	O-C-N	-8.59	108.95	122.70
1	A	343	PRO	CA-C-N	7.20	133.04	117.20
1	A	486	GLY	C-N-CA	6.13	137.01	121.70
1	A	324	PRO	N-CA-C	-5.03	99.03	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	323	LYS	Mainchain,Peptide
1	A	486	GLY	Mainchain

## 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	1489	0	1379	47	3
2	B	110	0	12	11	3
3	A	4	0	3	1	0
4	A	2	0	0	1	0
5	A	15	0	0	0	0
6	A	135	0	0	15	2
All	All	1755	0	1394	55	5

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 18.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:GLU:HB3	1:A:463:SER:HA	1.30	1.09
1:A:390[A]:TYR:CD1	6:A:2035:HOH:O	2.29	0.84
1:A:453:ILE:HG21	1:A:460:ILE:HD11	1.60	0.83
1:A:485:ASP:H	1:A:486:GLY:HA2	1.45	0.79
1:A:344:TYR:HB2	6:A:2014:HOH:O	1.83	0.77
2:B:2[A]:YYJ:O3S6	2:B:2[A]:YYJ:O5	2.06	0.74
1:A:402:HIS:NE2	2:B:1[A]:GU4:O21	2.19	0.73
1:A:335:LEU:HD21	1:A:372:ILE:HD11	1.72	0.71
1:A:323:LYS:HB3	1:A:324:PRO:CD	2.20	0.70
1:A:453:ILE:CG2	1:A:460:ILE:HD11	2.21	0.70
1:A:392:PRO:HB3	2:B:2[A]:YYJ:O2S4	1.94	0.68
1:A:390[A]:TYR:CE1	6:A:2035:HOH:O	2.46	0.67
1:A:413:ASP:HA	1:A:428:THR:HG22	1.76	0.67
1:A:462:GLU:CB	1:A:463:SER:HA	2.12	0.66
1:A:323:LYS:HB3	1:A:324:PRO:HD3	1.80	0.63
1:A:327:TYR:N	6:A:2005:HOH:O	1.95	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HG13	1:A:351:LYS:HD2	1.80	0.61
1:A:462:GLU:HB3	1:A:463:SER:CA	2.18	0.61
1:A:485:ASP:N	1:A:486:GLY:HA2	2.15	0.61
2:B:1[A]:GU4:O12	2:B:2[A]:YYJ:O3S3	2.21	0.59
1:A:322:LEU:C	1:A:323:LYS:HD3	2.24	0.58
1:A:342:ARG:NE	6:A:2015:HOH:O	2.28	0.58
1:A:323:LYS:N	1:A:323:LYS:HD3	2.19	0.57
2:B:1[A]:GU4:O27	2:B:1[A]:GU4:O2	2.24	0.56
2:B:1[A]:GU4:C1	2:B:2[A]:YYJ:O3	2.52	0.56
1:A:411[B]:SER:OG	6:A:2052:HOH:O	2.18	0.55
2:B:2[A]:YYJ:O3S4	2:B:2[A]:YYJ:O1S3	2.24	0.55
1:A:345:PHE:HA	1:A:346:PRO:C	2.28	0.55
1:A:355:TYR:CE2	1:A:372:ILE:HG23	2.42	0.54
1:A:441:ARG:NH1	3:A:1509:ACT:OXT	2.40	0.53
2:B:1[A]:GU4:O5	2:B:2[A]:YYJ:O3	2.25	0.53
1:A:455:ILE:HG23	4:A:1511:CL:CL	2.45	0.53
1:A:322:LEU:HD11	1:A:376:GLN:HB2	1.92	0.52
1:A:423:PRO:HA	1:A:424:LYS:CG	2.40	0.51
1:A:392:PRO:HB3	2:B:2[B]:YYJ:O3S6	2.10	0.51
1:A:423:PRO:HA	1:A:424:LYS:HG3	1.94	0.50
1:A:478:LYS:NZ	6:A:2112:HOH:O	2.13	0.50
1:A:389:CYS:HB3	1:A:436:TRP:CE2	2.47	0.49
1:A:375:THR:HG22	1:A:376:GLN:N	2.27	0.49
1:A:483:THR:HA	1:A:504:THR:O	2.13	0.49
1:A:424:LYS:HE2	6:A:2135:HOH:O	2.14	0.48
1:A:427:THR:OG1	6:A:2061:HOH:O	2.20	0.48
1:A:464:GLN:HB2	6:A:2093:HOH:O	2.14	0.47
1:A:342:ARG:CG	6:A:2015:HOH:O	2.62	0.47
1:A:396:ASN:ND2	6:A:2043:HOH:O	2.30	0.46
2:B:1[A]:GU4:O12	2:B:2[A]:YYJ:S3	2.73	0.46
1:A:502:GLN:HB2	6:A:2086:HOH:O	2.14	0.46
1:A:327:TYR:HB2	6:A:2005:HOH:O	2.16	0.45
1:A:473:ALA:HB2	1:A:499:TRP:CH2	2.51	0.45
1:A:327:TYR:OH	1:A:338:GLU:HG2	2.18	0.44
1:A:439:THR:HA	1:A:440:PRO:HD3	1.91	0.43
1:A:365:SER:N	6:A:2029:HOH:O	2.39	0.43
1:A:451:SER:HB3	1:A:465:TYR:HE1	1.84	0.41
2:B:1[A]:GU4:O5	2:B:2[A]:YYJ:C3	2.68	0.41
1:A:493:THR:H	1:A:500:SER:HB2	1.86	0.41

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2017:HOH:O	6:A:2116:HOH:O[4_466]	0.35	1.85
6:A:2095:HOH:O	6:A:2105:HOH:O[8_556]	1.83	0.37
1:A:354:SER:OG	2:B:1[A]:GU4:O10[6_455]	2.03	0.17
1:A:444:ARG:NH1	2:B:2[A]:YYJ:O1S3[3_555]	2.08	0.12
1:A:354:SER:OG	2:B:1[B]:GU4:O10[6_455]	2.19	0.01

## 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	187/187 (100%)	173 (92%)	13 (7%)	1 (0%)	29	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	PRO

### 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	162/161 (101%)	152 (94%)	10 (6%)	18	19

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	LYS

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Mol	Chain	Res	Type
1	A	338	GLU
1	A	347	VAL
1	A	390[A]	TYR
1	A	390[B]	TYR
1	A	411[A]	SER
1	A	411[B]	SER
1	A	476	GLN
1	A	485	ASP
1	A	488	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	GU4	B	1[A]	2	27,27,28	1.40	4 (14%)	29,43,45	3.43	15 (51%)
2	GU4	B	1[B]	2	27,27,28	0.92	1 (3%)	29,43,45	2.59	9 (31%)
2	YYJ	B	2[A]	1,2	27,28,28	1.23	2 (7%)	28,46,46	2.16	9 (32%)
2	YYJ	B	2[B]	2	27,28,28	0.94	1 (3%)	28,46,46	1.69	5 (17%)

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	GU4	B	1[A]	2	-	2/21/38/41	0/1/1/1
2	GU4	B	1[B]	2	-	0/21/38/41	0/1/1/1
2	YYJ	B	2[A]	1,2	-	8/23/42/42	0/1/1/1
2	YYJ	B	2[B]	2	-	4/23/42/42	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1[A]	GU4	O5-C1	-3.82	1.37	1.43
2	B	2[A]	YYJ	O2-C2	3.75	1.47	1.40
2	B	2[A]	YYJ	C2-C3	3.12	1.62	1.53
2	B	1[A]	GU4	O2-C2	-2.52	1.43	1.47
2	B	1[A]	GU4	C3-C4	2.38	1.57	1.52
2	B	1[B]	GU4	O2-C2	-2.38	1.43	1.47
2	B	1[A]	GU4	O3-C3	-2.32	1.41	1.46
2	B	2[B]	YYJ	C4-C3	2.02	1.57	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1[A]	GU4	C3-O3-S3	-8.18	103.07	118.88
2	B	1[B]	GU4	C2-O2-S2	-8.00	107.48	117.91
2	B	1[A]	GU4	O2-C2-C3	7.23	114.66	106.65
2	B	1[A]	GU4	C2-O2-S2	-6.56	109.36	117.91
2	B	2[A]	YYJ	C4-O4-S4	-5.58	108.09	118.88
2	B	1[B]	GU4	C3-O3-S3	-5.57	108.12	118.88
2	B	2[B]	YYJ	C4-O4-S4	-5.48	108.28	118.88
2	B	1[B]	GU4	C4-O4-S4	-5.27	108.69	118.88
2	B	1[A]	GU4	O29-S3-O28	5.02	125.95	108.49
2	B	2[A]	YYJ	O6-C6-C5	4.98	116.91	107.62
2	B	1[A]	GU4	O5-C5-C6	-4.63	97.35	107.61
2	B	1[A]	GU4	C4-O4-S4	-3.99	111.16	118.88
2	B	1[A]	GU4	O6-C6-C5	3.87	114.83	107.62
2	B	1[A]	GU4	O5-C1-C2	3.69	116.88	109.41
2	B	1[A]	GU4	O23-S6-O22	3.64	126.85	112.22
2	B	2[A]	YYJ	O2-C2-C3	3.43	120.44	109.74
2	B	1[A]	GU4	O26-S4-O25	3.42	125.94	112.22
2	B	2[B]	YYJ	O3S1-S1-O2S1	3.30	125.48	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2[A]	YYJ	O3S3-S3-O2S3	3.30	125.47	112.22
2	B	1[B]	GU4	O26-S4-O25	3.29	125.42	112.22
2	B	1[B]	GU4	O23-S6-O22	3.29	125.41	112.22
2	B	2[A]	YYJ	O3S1-S1-O2S1	3.28	125.38	112.22
2	B	2[B]	YYJ	O3S6-S6-O2S6	3.28	125.37	112.22
2	B	1[B]	GU4	O27-S3-O28	3.23	125.17	112.22
2	B	2[B]	YYJ	O3S3-S3-O2S3	3.19	125.02	112.22
2	B	1[B]	GU4	O12-S2-O11	3.18	125.00	112.22
2	B	1[A]	GU4	O3-C3-C4	3.18	115.46	108.48
2	B	1[A]	GU4	C3-C4-C5	-3.11	104.07	110.55
2	B	1[A]	GU4	O12-S2-O11	3.08	124.57	112.22
2	B	2[B]	YYJ	O3S4-S4-O2S4	3.06	124.49	112.22
2	B	2[A]	YYJ	O3S4-S4-O2S4	2.93	123.97	112.22
2	B	2[A]	YYJ	O5-C5-C4	2.76	108.09	103.49
2	B	1[A]	GU4	C6-C5-C4	2.60	119.76	113.33
2	B	1[A]	GU4	C4-C3-C2	-2.33	105.69	110.55
2	B	1[B]	GU4	C6-C5-C4	-2.31	107.62	113.33
2	B	2[A]	YYJ	O3-C3-C2	2.21	117.68	111.50
2	B	2[A]	YYJ	O3S6-S6-O2S6	2.08	120.58	112.22
2	B	1[B]	GU4	C1-O5-C5	-2.05	109.41	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

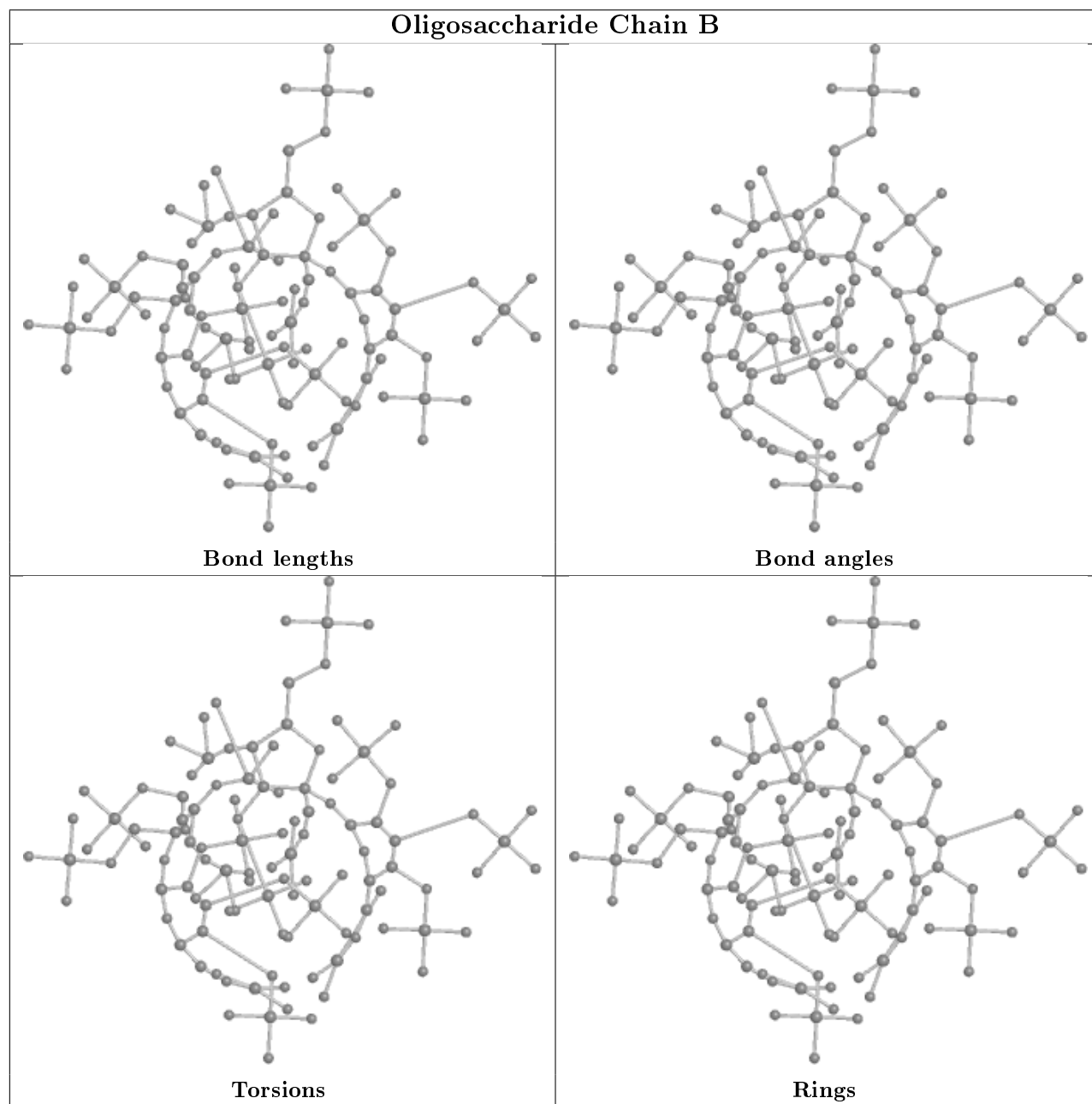
Mol	Chain	Res	Type	Atoms
2	B	2[B]	YYJ	O1-C1-C2-C3
2	B	2[B]	YYJ	O1-C1-C2-O2
2	B	2[B]	YYJ	O1-C1-C2-O5
2	B	2[A]	YYJ	O1-C1-C2-C3
2	B	2[A]	YYJ	O1-C1-C2-O2
2	B	2[A]	YYJ	O1-C1-C2-O5
2	B	2[A]	YYJ	C4-C3-O3-S3
2	B	2[A]	YYJ	C5-C6-O6-S6
2	B	2[A]	YYJ	C1-O1-S1-O1S1
2	B	2[A]	YYJ	C1-O1-S1-O2S1
2	B	2[A]	YYJ	C1-O1-S1-O3S1
2	B	2[B]	YYJ	C1-O1-S1-O2S1
2	B	1[A]	GU4	C6-O6-S6-O22
2	B	1[A]	GU4	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2[B]	YYJ	1	0
2	B	2[A]	YYJ	8	1
2	B	1[B]	GU4	0	1
2	B	1[A]	GU4	7	1

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

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	A	1512	-	4,4,4	0.99	0	6,6,6	1.66	1 (16%)
3	ACT	A	1509	-	1,3,3	1.93	0	0,3,3	0.00	-
5	SO4	A	1513	-	4,4,4	0.99	0	6,6,6	1.66	1 (16%)
5	SO4	A	1514	-	4,4,4	0.98	0	6,6,6	1.66	1 (16%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1513	SO4	O4-S-O3	3.82	125.37	109.06
5	A	1512	SO4	O4-S-O3	3.82	125.35	109.06
5	A	1514	SO4	O4-S-O3	3.81	125.34	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1509	ACT	1	0

## 5.7 Other polymers

There are no such residues in this entry.



## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	343:PRO	C	344:TYR	N	1.19

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	187/187 (100%)	0.42	15 (8%)	12 18	16, 36, 60, 70	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485	ASP	4.7
1	A	344	TYR	4.6
1	A	484	ALA	4.4
1	A	479	LEU	3.9
1	A	390[A]	TYR	3.3
1	A	320	MET	3.2
1	A	465	TYR	2.9
1	A	496	LYS	2.9
1	A	322	LEU	2.7
1	A	323	LYS	2.6
1	A	339	ASN	2.4
1	A	460	ILE	2.3
1	A	343	PRO	2.1
1	A	462	GLU	2.1
1	A	463	SER	2.0

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

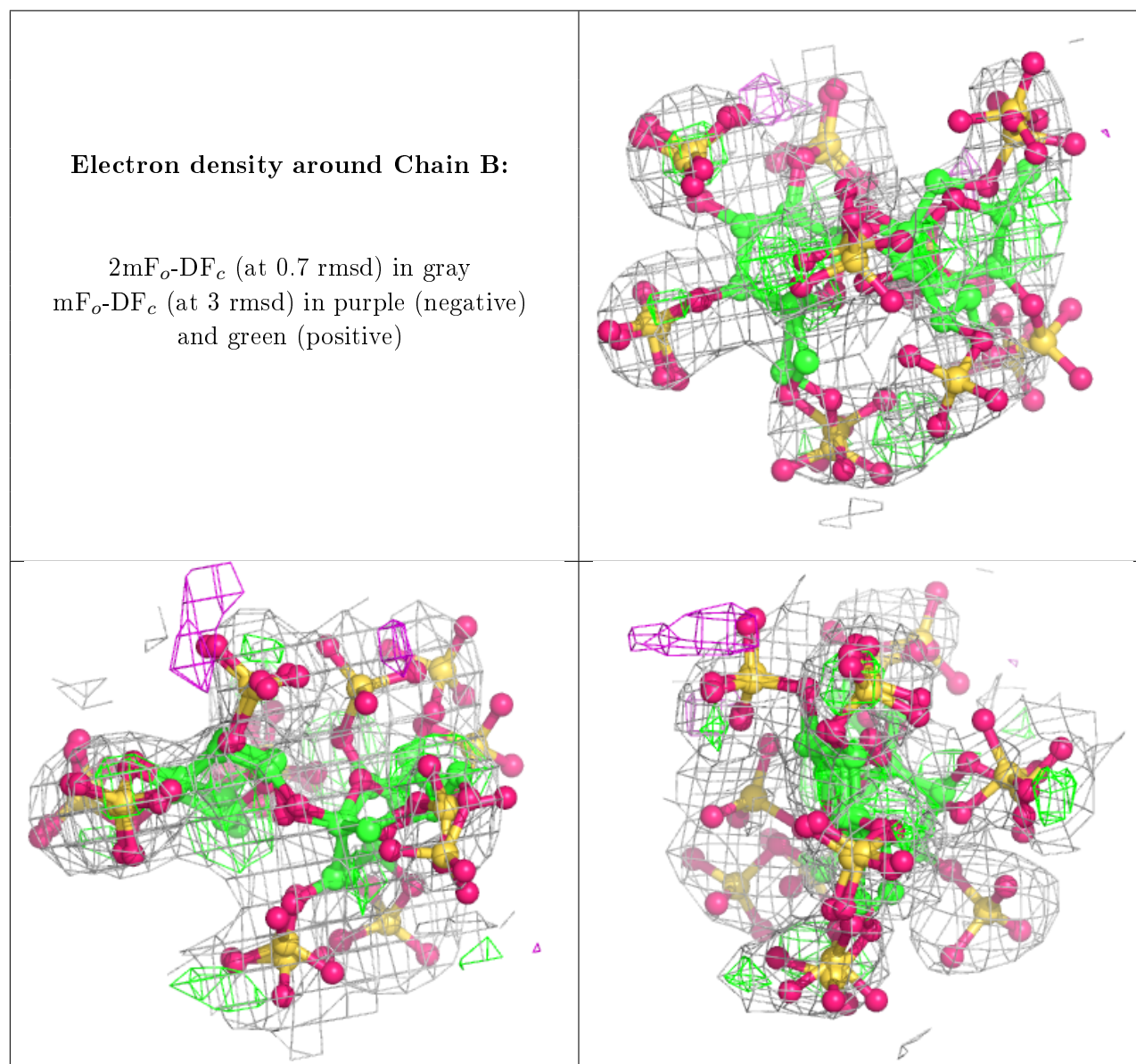
There are no non-standard protein/DNA/RNA residues in this entry.

### 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, 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( $\text{\AA}^2$ )	Q<0.9
2	YYJ	B	2[B]	28/28	0.74	0.30	52,77,81,81	28
2	YYJ	B	2[A]	28/28	0.74	0.30	100,107,110,110	28
2	GU4	B	1[B]	27/28	0.79	0.33	51,70,75,76	27
2	GU4	B	1[A]	27/28	0.79	0.33	70,95,98,99	27

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 ⓘ

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( $\text{\AA}^2$ )	Q<0.9
5	SO4	A	1514	5/5	0.80	0.25	102,103,103,103	0
3	ACT	A	1509	4/4	0.85	0.25	69,69,69,69	4
5	SO4	A	1512	5/5	0.94	0.18	72,72,73,73	0
5	SO4	A	1513	5/5	0.95	0.17	91,91,91,91	0
4	CL	A	1511	1/1	0.95	0.20	58,58,58,58	0
4	CL	A	1510	1/1	0.98	0.13	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.