



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:36 AM BST

PDB ID : 2V8E
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.; Tarelli, E.; Uhrin, D.; Barlow, P.N.; Sim, R.B.; Day, A.J.; Lea, S.M.
Deposited on : 2007-08-07
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

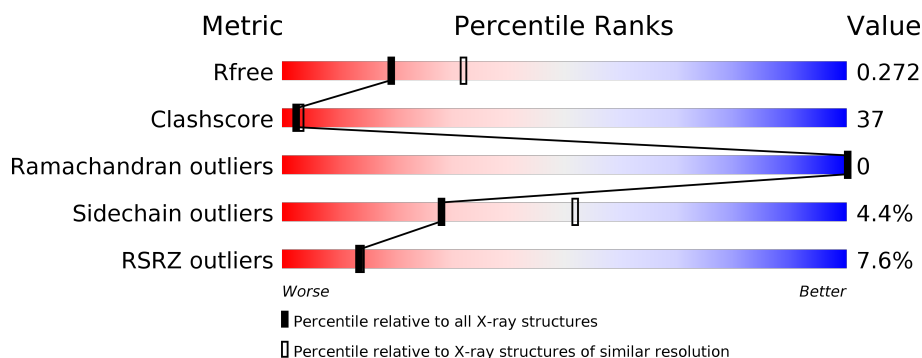
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	<div> <div>7%</div> <div>53%</div> <div>42%</div> <div>• •</div> </div>
2	B	2	<div> <div>50%</div> <div>50%</div> </div>

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	-	-	X	-

2 Entry composition [i](#)

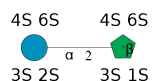
There are 6 unique types of molecules in this entry. The entry contains 1605 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	Se	0	1	0
			1481	937	250	280	12	2			

- 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	0	0
			55	12	35	8			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

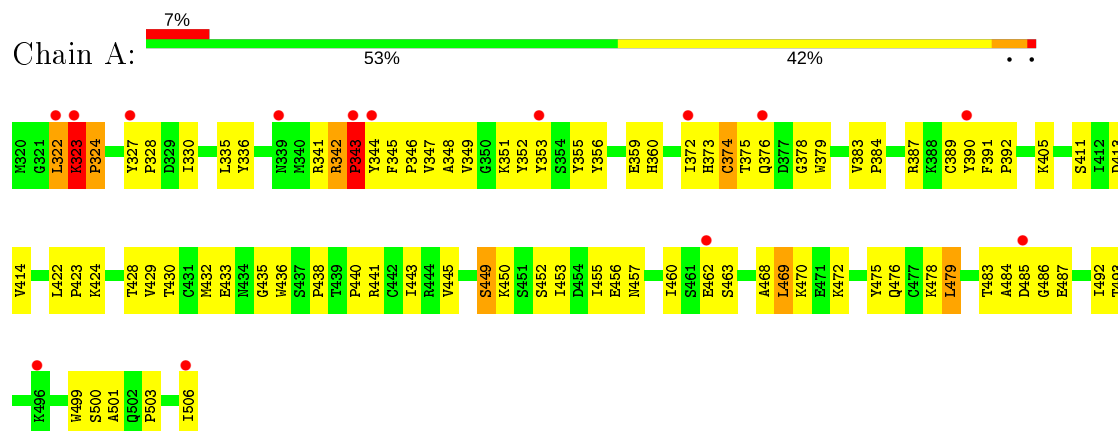
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	46	Total	O	0	0
			46	46		

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: 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, α , β , γ	75.00Å 92.50Å 57.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 35.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 99.0 (35.94-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.51Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.223 , 0.245 0.242 , 0.272	Depositor DCC
R_{free} test set	694 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	1605	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, GU4, 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	0.72	4/1531 (0.3%)	0.82	8/2074 (0.4%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	323	LYS	CB-CG	-12.14	1.19	1.52
1	A	343	PRO	C-N	-11.79	1.06	1.34
1	A	324	PRO	N-CA	-8.80	1.32	1.47
1	A	342	ARG	C-N	7.73	1.49	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	PRO	O-C-N	-15.30	98.22	122.70
1	A	479	LEU	CB-CG-CD1	-14.43	86.47	111.00
1	A	343	PRO	CA-C-N	9.43	137.95	117.20
1	A	324	PRO	CA-N-CD	-7.09	101.57	111.50
1	A	322	LEU	CA-C-N	-5.82	104.39	117.20
1	A	322	LEU	C-N-CA	5.30	134.96	121.70
1	A	324	PRO	CA-C-N	-5.16	105.86	117.20
1	A	323	LYS	N-CA-C	5.04	124.61	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	LYS	Peptide
1	A	343	PRO	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	1481	0	1375	110	0
2	B	55	0	6	10	0
3	A	2	0	0	1	0
4	A	15	0	0	0	0
5	A	6	0	8	0	0
6	A	46	0	0	0	0
All	All	1605	0	1389	110	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 37.

All (110) 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:323:LYS:HE2	1:A:324:PRO:CD	1.54	1.38
1:A:323:LYS:HG2	1:A:324:PRO:CD	1.58	1.33
1:A:323:LYS:CG	1:A:324:PRO:HD3	1.58	1.29
1:A:347:VAL:HG13	1:A:351:LYS:HD2	1.25	1.18
1:A:323:LYS:CE	1:A:324:PRO:HD3	1.75	1.17
1:A:462:GLU:HB3	1:A:463:SER:HA	1.25	1.10
1:A:323:LYS:CD	1:A:324:PRO:HD3	1.81	1.09
1:A:457:ASN:HA	1:A:478:LYS:HE2	1.28	1.07
1:A:423:PRO:HA	1:A:424:LYS:HG3	1.40	1.03
1:A:485:ASP:H	1:A:486:GLY:HA2	1.25	0.98
1:A:323:LYS:HG2	1:A:324:PRO:HD3	1.01	0.96
1:A:323:LYS:HE2	1:A:324:PRO:HD2	1.46	0.95
1:A:390:TYR:HB2	2:B:2:YYJ:O2S4	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:VAL:HG13	1:A:351:LYS:CD	2.05	0.86
1:A:355:TYR:CD2	1:A:372:ILE:HG13	2.12	0.85
1:A:462:GLU:CB	1:A:463:SER:HA	2.06	0.84
1:A:323:LYS:CE	1:A:324:PRO:CD	2.40	0.83
1:A:485:ASP:N	1:A:486:GLY:HA2	1.91	0.82
1:A:390:TYR:HB3	1:A:405:LYS:HZ2	1.44	0.81
1:A:390:TYR:CD2	2:B:2:YYJ:O4	2.35	0.80
1:A:323:LYS:HG2	1:A:324:PRO:N	1.96	0.79
1:A:355:TYR:CE2	1:A:372:ILE:HG13	2.18	0.78
1:A:423:PRO:CA	1:A:424:LYS:HG3	2.14	0.77
1:A:457:ASN:HA	1:A:478:LYS:CE	2.14	0.76
1:A:390:TYR:HB3	1:A:405:LYS:NZ	2.01	0.76
1:A:424:LYS:HE2	1:A:443:ILE:CD1	2.16	0.76
1:A:372:ILE:HG22	1:A:379:TRP:CE3	2.22	0.75
1:A:424:LYS:HE2	1:A:443:ILE:HD13	1.68	0.74
1:A:457:ASN:CA	1:A:478:LYS:HE2	2.13	0.74
1:A:349:VAL:HA	1:A:374:CYS:SG	2.28	0.74
1:A:328:PRO:HG2	1:A:335:LEU:HD11	1.70	0.72
1:A:423:PRO:HA	1:A:424:LYS:CG	2.17	0.72
1:A:390:TYR:CD2	2:B:2:YYJ:S4	2.83	0.71
1:A:413:ASP:HA	1:A:428:THR:HG22	1.74	0.70
1:A:345:PHE:HA	1:A:346:PRO:C	2.12	0.69
1:A:453:ILE:HG21	1:A:460:ILE:HD11	1.77	0.67
1:A:390:TYR:CE2	2:B:2:YYJ:C6	2.78	0.66
1:A:347:VAL:CG1	1:A:351:LYS:HD2	2.15	0.66
1:A:450:LYS:HA	1:A:453:ILE:HD12	1.77	0.66
1:A:375:THR:HG22	1:A:376:GLN:N	2.11	0.65
1:A:387:ARG:HD3	1:A:432:MSE:O	1.96	0.65
1:A:349:VAL:HG23	1:A:374:CYS:O	1.98	0.64
1:A:441:ARG:HG3	1:A:441:ARG:HH21	1.61	0.64
1:A:372:ILE:HG22	1:A:379:TRP:HE3	1.62	0.64
1:A:472:LYS:HE2	1:A:493:THR:OG1	1.98	0.64
1:A:462:GLU:HB3	1:A:463:SER:CA	2.15	0.64
1:A:453:ILE:CG2	1:A:460:ILE:HD11	2.29	0.62
1:A:352:TYR:HB3	1:A:373:HIS:ND1	2.15	0.62
1:A:341:ARG:HA	1:A:344:TYR:CD2	2.38	0.59
1:A:375:THR:HG22	1:A:376:GLN:H	1.67	0.59
1:A:323:LYS:HE2	1:A:324:PRO:CG	2.30	0.59
1:A:347:VAL:CG1	1:A:351:LYS:HB2	2.35	0.57
1:A:323:LYS:HG2	1:A:324:PRO:CG	2.29	0.57
1:A:387:ARG:NE	1:A:435:GLY:HA2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ARG:HA	1:A:344:TYR:CE2	2.39	0.56
1:A:390:TYR:HD2	2:B:2:YYJ:S4	2.25	0.56
1:A:391:PHE:CD2	1:A:392:PRO:HD2	2.42	0.55
1:A:429:VAL:HG22	1:A:436:TRP:CE3	2.41	0.55
1:A:492:ILE:HG13	1:A:499:TRP:CE3	2.43	0.54
1:A:390:TYR:HE2	2:B:2:YYJ:C6	2.21	0.54
1:A:493:THR:HB	1:A:500:SER:OG	2.08	0.53
1:A:441:ARG:NH2	1:A:441:ARG:HG3	2.23	0.53
1:A:475:TYR:CE2	1:A:503:PRO:HB3	2.45	0.52
1:A:355:TYR:CE1	1:A:384:PRO:HB2	2.45	0.52
1:A:390:TYR:CD2	2:B:2:YYJ:O2S4	2.63	0.52
1:A:387:ARG:HE	1:A:435:GLY:HA2	1.75	0.51
1:A:392:PRO:HG3	1:A:440:PRO:HG2	1.91	0.51
1:A:483:THR:HG23	1:A:484:ALA:N	2.24	0.51
1:A:469:LEU:O	1:A:470:LYS:HB2	2.09	0.51
1:A:375:THR:CG2	1:A:376:GLN:H	2.23	0.51
1:A:383:VAL:O	1:A:383:VAL:HG12	2.11	0.50
1:A:483:THR:HG22	1:A:487:GLU:H	1.77	0.50
1:A:375:THR:CG2	1:A:376:GLN:N	2.74	0.49
1:A:348:ALA:HB3	1:A:351:LYS:HE2	1.95	0.48
1:A:390:TYR:CB	2:B:2:YYJ:O2S4	2.53	0.48
1:A:345:PHE:CD2	1:A:347:VAL:HG23	2.47	0.48
1:A:414:VAL:HB	1:A:422:LEU:HD11	1.96	0.48
1:A:390:TYR:CE2	2:B:2:YYJ:C5	2.96	0.48
1:A:322:LEU:HD13	1:A:322:LEU:O	2.13	0.47
1:A:449:SER:O	1:A:452:SER:HB3	2.13	0.47
1:A:330:ILE:HD13	1:A:372:ILE:CD1	2.44	0.47
1:A:429:VAL:HG23	1:A:438:PRO:O	2.15	0.47
1:A:341:ARG:HG2	1:A:353:TYR:CE1	2.50	0.47
1:A:500:SER:O	1:A:501:ALA:HB2	2.15	0.46
1:A:342:ARG:HA	1:A:343:PRO:HA	1.41	0.46
1:A:323:LYS:HE2	1:A:324:PRO:HD3	1.21	0.46
1:A:390:TYR:HD2	2:B:2:YYJ:O2S4	1.99	0.46
1:A:330:ILE:HD13	1:A:372:ILE:HD11	1.98	0.45
1:A:389:CYS:HB3	1:A:436:TRP:CE2	2.51	0.45
1:A:330:ILE:HG23	1:A:384:PRO:HG2	1.98	0.44
1:A:455:ILE:HG23	3:A:1509:CL:CL	2.54	0.44
1:A:475:TYR:CZ	1:A:503:PRO:HB3	2.52	0.44
1:A:387:ARG:HD2	1:A:433:GLU:O	2.18	0.43
1:A:423:PRO:CB	1:A:424:LYS:HG3	2.49	0.43
1:A:391:PHE:HA	1:A:392:PRO:HD3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:TYR:HA	1:A:328:PRO:HD3	1.84	0.42
1:A:344:TYR:O	1:A:346:PRO:O	2.37	0.42
1:A:375:THR:N	1:A:378:GLY:O	2.47	0.41
1:A:390:TYR:O	1:A:390:TYR:CD2	2.73	0.41
1:A:390:TYR:CB	1:A:405:LYS:NZ	2.76	0.41
1:A:336:TYR:CZ	1:A:356:TYR:HB3	2.55	0.41
1:A:430:THR:HB	1:A:432:MSE:HE2	2.01	0.41
1:A:483:THR:HG22	1:A:487:GLU:N	2.35	0.41
1:A:485:ASP:N	1:A:486:GLY:CA	2.71	0.41
1:A:323:LYS:CG	1:A:324:PRO:CD	2.41	0.41
1:A:359:GLU:O	1:A:360:HIS:HB2	2.21	0.41
1:A:445:VAL:HG11	1:A:468:ALA:HB1	2.03	0.41
1:A:479:LEU:HA	1:A:479:LEU:HD12	1.55	0.41
1:A:450:LYS:C	1:A:452:SER:H	2.25	0.40
1:A:456:GLU:O	1:A:457:ASN:HB2	2.20	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	186/187 (100%)	171 (92%)	15 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	161/158 (102%)	153 (95%)	8 (5%)	24	46

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	LYS
1	A	374	CYS
1	A	411[A]	SER
1	A	411[B]	SER
1	A	449	SER
1	A	469	LEU
1	A	476	GLN
1	A	506	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

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
2	GU4	B	1	2	27,27,28	0.84	0	29,43,45	2.55	10 (34%)
2	YYJ	B	2	2	27,28,28	1.07	1 (3%)	28,46,46	1.74	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	2	-	0/21/38/41	0/1/1/1
2	YYJ	B	2	2	-	1/23/42/42	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	YYJ	O6-S6	-2.27	1.50	1.56

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GU4	C2-O2-S2	-7.50	108.13	117.91
2	B	1	GU4	C3-O3-S3	-5.70	107.87	118.88
2	B	2	YYJ	C4-O4-S4	-5.48	108.28	118.88
2	B	1	GU4	C4-O4-S4	-5.19	108.84	118.88
2	B	2	YYJ	O3S3-S3-O2S3	3.46	126.10	112.22
2	B	2	YYJ	O3S1-S1-O2S1	3.38	125.79	112.22
2	B	2	YYJ	O3S6-S6-O2S6	3.26	125.31	112.22
2	B	2	YYJ	O3S4-S4-O2S4	3.21	125.12	112.22
2	B	1	GU4	O12-S2-O11	3.21	125.10	112.22
2	B	1	GU4	O27-S3-O28	3.21	125.09	112.22
2	B	1	GU4	O26-S4-O25	3.18	124.99	112.22
2	B	1	GU4	O23-S6-O22	3.17	124.92	112.22
2	B	1	GU4	C1-O5-C5	-2.73	108.49	112.19
2	B	1	GU4	C6-C5-C4	-2.55	107.02	113.33
2	B	1	GU4	C1-C2-C3	-2.30	105.96	109.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

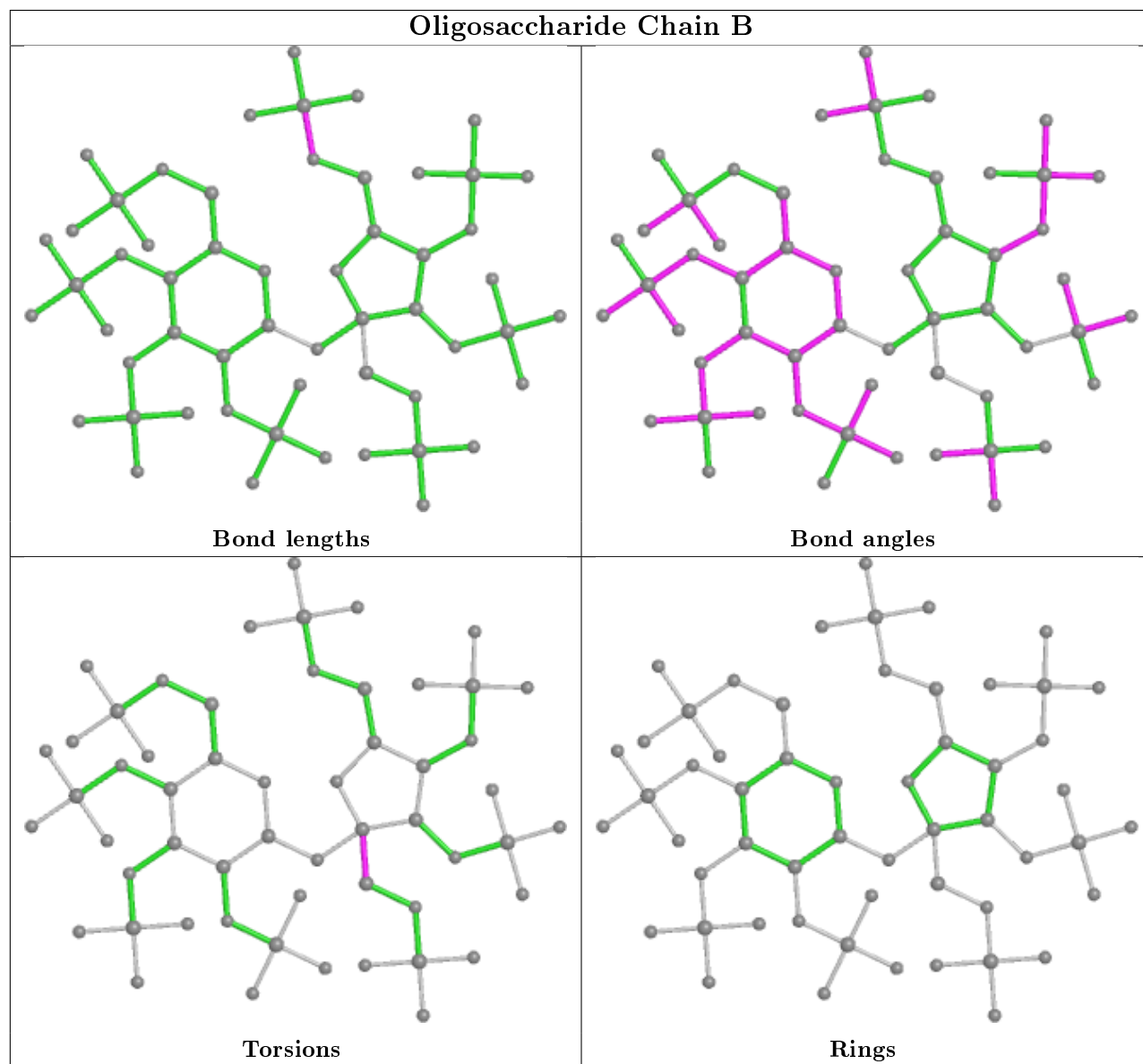
Mol	Chain	Res	Type	Atoms
2	B	2	YYJ	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	YYJ	10	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 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	GOL	A	1513	-	5,5,5	0.31	0	5,5,5	0.29	0
4	SO4	A	1511	-	4,4,4	0.96	0	6,6,6	1.67	1 (16%)
4	SO4	A	1510	-	4,4,4	0.93	0	6,6,6	1.59	1 (16%)
4	SO4	A	1512	-	4,4,4	0.94	0	6,6,6	1.64	1 (16%)

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	GOL	A	1513	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1511	SO4	O4-S-O3	3.85	125.48	109.06
4	A	1512	SO4	O4-S-O3	3.78	125.20	109.06
4	A	1510	SO4	O4-S-O3	3.65	124.66	109.06

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

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	1.06

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	184/187 (98%)	0.46	14 (7%) 13 14	16, 39, 70, 84	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	TYR	8.1
1	A	390	TYR	7.0
1	A	323	LYS	3.7
1	A	372	ILE	3.4
1	A	339	ASN	3.3
1	A	485	ASP	3.1
1	A	353	TYR	2.9
1	A	376	GLN	2.9
1	A	343	PRO	2.9
1	A	462	GLU	2.4
1	A	322	LEU	2.2
1	A	327	TYR	2.1
1	A	506	ILE	2.1
1	A	496	LYS	2.0

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

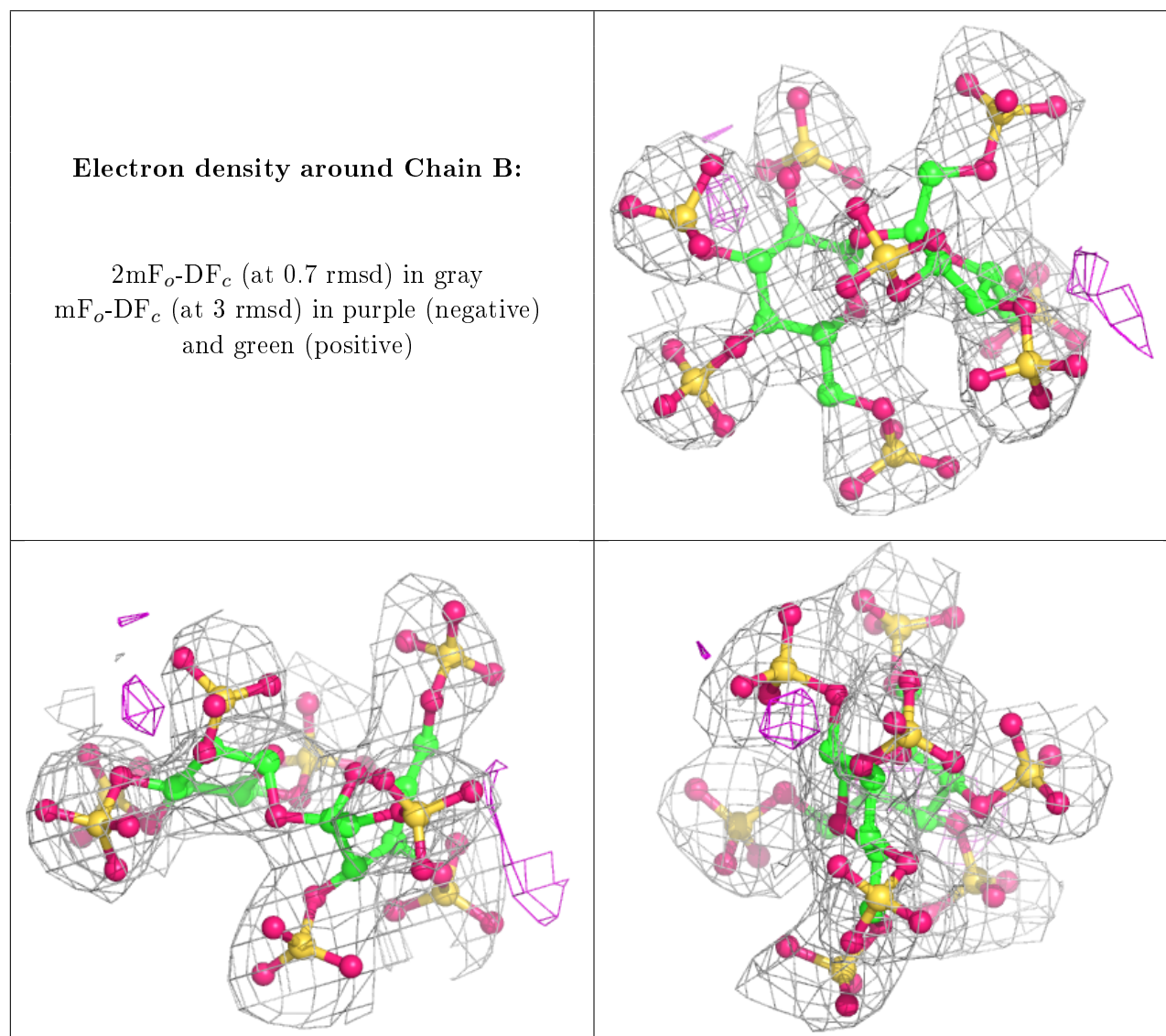
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GU4	B	1	27/28	0.86	0.21	61,75,84,85	0
2	YYJ	B	2	28/28	0.87	0.19	81,90,96,100	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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	1513	6/6	0.76	0.30	53,61,66,68	0
4	SO4	A	1512	5/5	0.84	0.27	105,105,107,108	0
4	SO4	A	1511	5/5	0.92	0.17	72,74,76,78	0
4	SO4	A	1510	5/5	0.95	0.18	45,45,46,49	0
3	CL	A	1509	1/1	0.96	0.15	55,55,55,55	0
3	CL	A	1508	1/1	0.97	0.14	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.