Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2021 – 02:06 pm GMT

PDB ID	:	7PGM
Title	:	HHIP-C in complex with heparin
Authors	:	Griffiths, S.C.; Schwab, R.A.; El Omari, K.; Bishop, B.; Iverson, E.J.; Malinuskas, T.; Dubey, R.; Qian, M.; Covey, D.F.; Gilbert, R.J.C.; Rohatgi, R.; Siebold, C.
Deposited on	:	2021-08-14
Resolution	:	2.70 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:

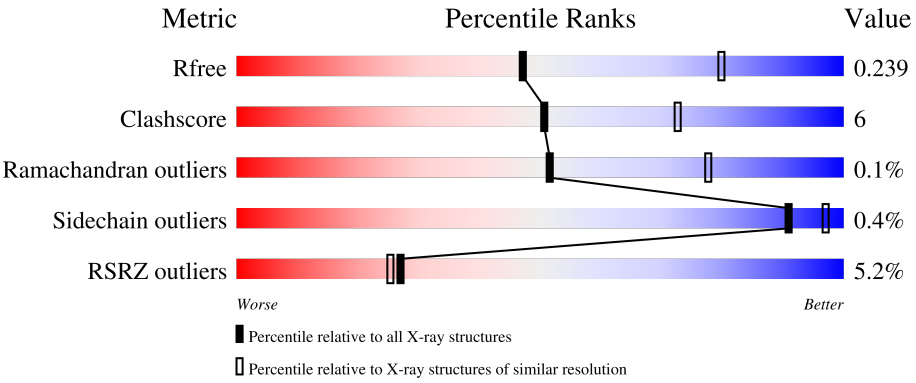
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	470	6% 81% 14% 5%
1	B	470	4% 81% 10% 9%
1	C	470	4% 80% 11% 9%
2	D	8	25% 75%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10309 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 Hedgehog-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3484	2186	614	656	28			
1	B	427	Total	C	N	O	S	0	0	0
			3335	2095	594	619	27			
1	C	429	Total	C	N	O	S	0	0	0
			3349	2105	591	626	27			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	GLU	-	expression tag	UNP Q96QV1
A	211	THR	-	expression tag	UNP Q96QV1
A	212	GLY	-	expression tag	UNP Q96QV1
A	671	GLY	-	expression tag	UNP Q96QV1
A	672	THR	-	expression tag	UNP Q96QV1
A	673	LYS	-	expression tag	UNP Q96QV1
A	674	HIS	-	expression tag	UNP Q96QV1
A	675	HIS	-	expression tag	UNP Q96QV1
A	676	HIS	-	expression tag	UNP Q96QV1
A	677	HIS	-	expression tag	UNP Q96QV1
A	678	HIS	-	expression tag	UNP Q96QV1
A	679	HIS	-	expression tag	UNP Q96QV1
B	210	GLU	-	expression tag	UNP Q96QV1
B	211	THR	-	expression tag	UNP Q96QV1
B	212	GLY	-	expression tag	UNP Q96QV1
B	671	GLY	-	expression tag	UNP Q96QV1
B	672	THR	-	expression tag	UNP Q96QV1
B	673	LYS	-	expression tag	UNP Q96QV1
B	674	HIS	-	expression tag	UNP Q96QV1
B	675	HIS	-	expression tag	UNP Q96QV1
B	676	HIS	-	expression tag	UNP Q96QV1
B	677	HIS	-	expression tag	UNP Q96QV1
B	678	HIS	-	expression tag	UNP Q96QV1

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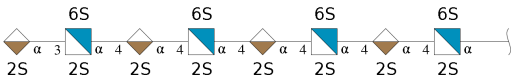
Chain	Residue	Modelled	Actual	Comment	Reference
B	679	HIS	-	expression tag	UNP Q96QV1
C	210	GLU	-	expression tag	UNP Q96QV1
C	211	THR	-	expression tag	UNP Q96QV1
C	212	GLY	-	expression tag	UNP Q96QV1
C	671	GLY	-	expression tag	UNP Q96QV1
C	672	THR	-	expression tag	UNP Q96QV1
C	673	LYS	-	expression tag	UNP Q96QV1
C	674	HIS	-	expression tag	UNP Q96QV1
C	675	HIS	-	expression tag	UNP Q96QV1
C	676	HIS	-	expression tag	UNP Q96QV1
C	677	HIS	-	expression tag	UNP Q96QV1
C	678	HIS	-	expression tag	UNP Q96QV1
C	679	HIS	-	expression tag	UNP Q96QV1

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-3)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



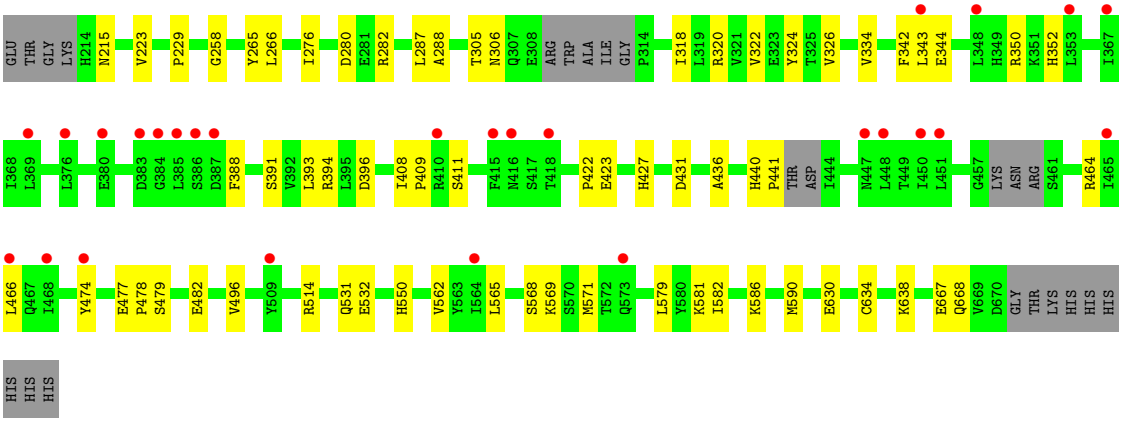
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	8	Total	C	N	O	S	0	0	0
			141	48	4	77	12			

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.

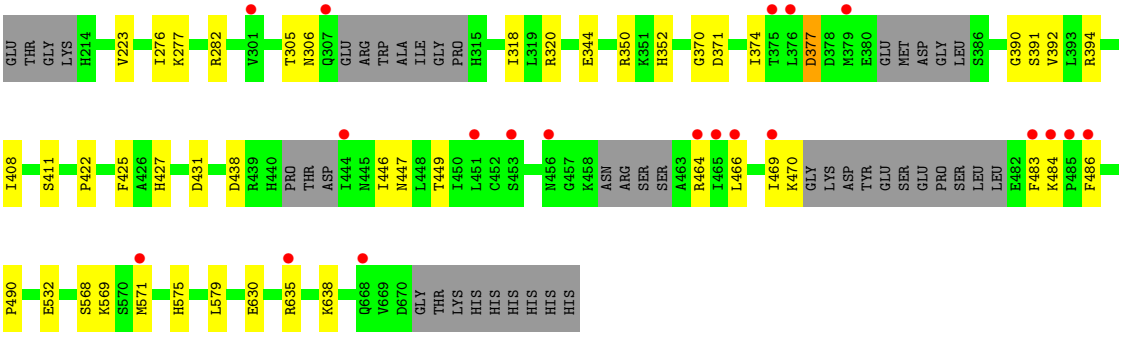
• Molecule 1: Hedgehog-interacting protein

Chain A:



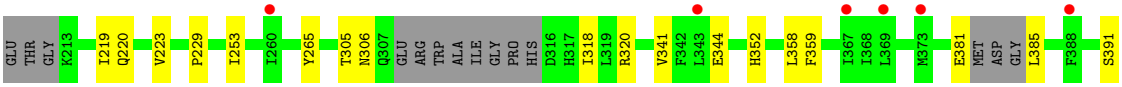
• Molecule 1: Hedgehog-interacting protein

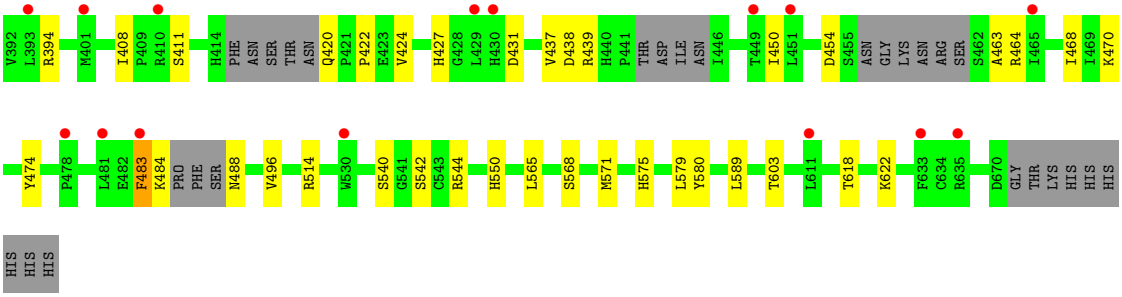
Chain B:



• Molecule 1: Hedgehog-interacting protein

Chain C:





• Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-3)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.64Å 105.25Å 148.43Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	84.86 – 2.70 147.63 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (84.86-2.70) 99.3 (147.63-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX (dev_2645: ???)	Depositor
R, R_{free}	0.216 , 0.240 0.216 , 0.239	Depositor DCC
R_{free} test set	3654 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	73.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10309	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SGN, IDS

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	0.31	0/3563	0.53	0/4812
1	B	0.32	0/3408	0.56	0/4598
1	C	0.29	0/3420	0.52	0/4612
All	All	0.31	0/10391	0.53	0/14022

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

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	3484	0	3384	47	0
1	B	3335	0	3251	33	0
1	C	3349	0	3272	35	0
2	D	141	0	52	8	0
All	All	10309	0	9959	115	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 6.

All (115) 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:318:ILE:HD11	1:A:344:GLU:HB3	1.51	0.90
1:C:394:ARG:HH12	1:C:411:SER:HB2	1.38	0.86
1:B:318:ILE:HD11	1:B:344:GLU:HB3	1.57	0.85
1:C:318:ILE:HD11	1:C:344:GLU:HB3	1.59	0.82
1:B:447:ASN:HB2	1:B:470:LYS:HG3	1.65	0.78
1:B:569:LYS:NZ	2:D:3:SGN:S2	2.60	0.75
1:C:358:LEU:HD13	1:C:437:VAL:HG11	1.69	0.74
1:A:320:ARG:NH1	1:A:344:GLU:OE1	2.24	0.70
1:A:394:ARG:HH12	1:A:411:SER:HB2	1.57	0.70
1:B:575:HIS:ND1	1:B:575:HIS:O	2.25	0.69
1:B:484:LYS:HE2	1:B:532:GLU:HB2	1.75	0.67
1:A:282:ARG:HD2	1:A:350:ARG:HG2	1.75	0.67
1:B:568:SER:H	1:B:571:MET:HB2	1.60	0.67
1:B:394:ARG:HH12	1:B:411:SER:HB2	1.59	0.67
1:A:276:ILE:HG22	1:B:635:ARG:HH22	1.59	0.67
1:A:514:ARG:HG2	1:A:550:HIS:HB3	1.77	0.65
1:A:408:ILE:HD11	1:A:423:GLU:HG3	1.77	0.65
1:B:408:ILE:HG12	1:B:422:PRO:HB2	1.79	0.65
1:B:569:LYS:NZ	2:D:3:SGN:O4S	2.30	0.64
1:C:575:HIS:O	1:C:575:HIS:ND1	2.29	0.64
1:A:265:TYR:O	1:A:334:VAL:HG12	1.98	0.64
1:A:569:LYS:HD2	1:A:569:LYS:H	1.63	0.64
1:C:229:PRO:HB2	1:C:565:LEU:HD22	1.81	0.62
1:A:391:SER:HA	1:A:427:HIS:HA	1.83	0.60
1:C:568:SER:H	1:C:571:MET:HB2	1.66	0.59
1:B:370:GLY:O	1:B:390:GLY:N	2.35	0.59
1:A:568:SER:H	1:A:571:MET:HB2	1.67	0.58
1:C:391:SER:HA	1:C:427:HIS:HA	1.87	0.57
1:B:394:ARG:NH1	1:B:411:SER:HB2	2.19	0.57
1:A:229:PRO:HB2	1:A:565:LEU:HD22	1.85	0.56
1:C:394:ARG:NH1	1:C:411:SER:HB2	2.14	0.56
2:D:7:SGN:O4	2:D:8:IDS:O2S	2.23	0.56
1:A:280:ASP:OD1	1:A:282:ARG:HD3	2.06	0.56
1:C:420:GLN:HG2	1:C:424:VAL:HG11	1.89	0.55
1:C:359:PHE:O	1:C:439:ARG:NH2	2.36	0.55
1:B:276:ILE:HG13	1:B:277:LYS:H	1.72	0.55
1:A:320:ARG:HG3	1:A:344:GLU:HG2	1.89	0.54
1:C:408:ILE:HG12	1:C:422:PRO:HB2	1.90	0.54
1:C:438:ASP:HA	1:C:496:VAL:HG21	1.89	0.54
1:B:446:ILE:HD11	1:B:469:ILE:HG12	1.88	0.53
1:B:464:ARG:NH1	1:B:466:LEU:HD21	2.24	0.53
1:A:266:LEU:HD13	1:A:334:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:HIS:CG	1:B:431:ASP:HB2	2.44	0.53
1:C:306:ASN:OD1	1:C:306:ASN:N	2.42	0.52
1:A:326:VAL:HA	1:A:334:VAL:HA	1.91	0.52
1:C:223:VAL:HG12	1:C:579:LEU:HB3	1.90	0.52
1:A:324:TYR:HB3	1:A:334:VAL:HG21	1.91	0.51
1:A:581:LYS:HD3	1:C:542:SER:OG	2.09	0.51
1:A:408:ILE:HG13	1:A:422:PRO:HB2	1.93	0.51
1:C:468:ILE:HA	1:C:474:TYR:OH	2.10	0.51
1:B:276:ILE:HG13	1:B:277:LYS:N	2.26	0.51
1:B:377:ASP:OD1	1:B:377:ASP:N	2.28	0.51
1:A:215:ASN:OD1	1:A:586:LYS:HE3	2.10	0.50
1:A:306:ASN:N	1:A:306:ASN:OD1	2.44	0.50
2:D:6:IDS:O6B	2:D:6:IDS:O4	2.30	0.50
1:B:484:LYS:HE2	1:B:532:GLU:CB	2.42	0.50
1:C:437:VAL:HG12	1:C:450:ILE:HG12	1.94	0.49
1:A:394:ARG:NH1	1:A:411:SER:HB2	2.24	0.49
1:A:630:GLU:HB3	1:A:638:LYS:HD2	1.93	0.49
1:C:463:ALA:HB3	1:C:483:PHE:HD2	1.78	0.49
1:A:305:THR:HG21	1:A:320:ARG:HH21	1.77	0.49
1:C:305:THR:HG23	1:C:318:ILE:HG23	1.95	0.49
1:A:223:VAL:HG22	1:A:579:LEU:HB3	1.95	0.49
1:A:396:ASP:HB2	1:A:409:PRO:HG3	1.94	0.48
1:A:464:ARG:NH2	1:A:466:LEU:HD21	2.27	0.48
1:B:306:ASN:N	1:B:306:ASN:OD1	2.46	0.48
1:C:381:GLU:HG3	1:C:385:LEU:HD12	1.95	0.48
1:C:484:LYS:NZ	1:C:488:ASN:HB2	2.28	0.47
1:B:223:VAL:HG22	1:B:579:LEU:HB3	1.96	0.47
1:A:320:ARG:HD2	1:A:322:VAL:CG2	2.44	0.47
1:C:463:ALA:HB3	1:C:483:PHE:CD2	2.49	0.47
1:A:590:MET:HB2	1:C:540:SER:HB3	1.96	0.47
1:C:320:ARG:HD3	1:C:341:VAL:HG12	1.96	0.47
1:A:440:HIS:N	1:A:441:PRO:HD3	2.31	0.46
1:A:352:HIS:CG	1:A:431:ASP:HB2	2.51	0.46
1:B:371:ASP:O	1:B:374:ILE:HG12	2.16	0.46
1:C:305:THR:HG21	1:C:320:ARG:NH1	2.31	0.46
1:C:253:ILE:HG13	1:C:265:TYR:HB2	1.97	0.46
1:C:514:ARG:HG2	1:C:550:HIS:HB3	1.98	0.45
1:B:391:SER:HA	1:B:427:HIS:HA	1.98	0.45
1:C:411:SER:O	1:C:470:LYS:HD2	2.16	0.45
2:D:2:IDS:H4	2:D:3:SGN:N2	2.32	0.44
1:B:630:GLU:HB3	1:B:638:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ARG:HH21	1:B:282:ARG:HG3	1.82	0.44
1:B:484:LYS:HD3	1:B:486:PHE:CD2	2.53	0.44
1:C:320:ARG:NH2	1:C:344:GLU:OE1	2.51	0.44
1:B:438:ASP:HB3	1:B:449:THR:HB	2.01	0.43
1:A:479:SER:OG	1:A:482:GLU:OE1	2.35	0.43
1:B:350:ARG:NH2	2:D:6:IDS:O6A	2.46	0.43
1:C:219:ILE:CG2	1:C:580:TYR:HB3	2.49	0.43
1:A:477:GLU:OE1	1:A:478:PRO:HD2	2.19	0.42
2:D:7:SGN:H3	2:D:8:IDS:H2	1.84	0.42
1:A:320:ARG:HD2	1:A:322:VAL:HG22	2.01	0.42
1:A:667:GLU:HG2	1:A:668:GLN:HG3	2.00	0.42
1:A:388:PHE:HB3	1:A:393:LEU:HD11	2.02	0.42
1:A:436:ALA:HB1	1:A:496:VAL:HG23	2.02	0.42
1:A:630:GLU:O	1:A:634:CYS:HA	2.20	0.42
1:A:474:TYR:HA	1:A:477:GLU:HB2	2.01	0.41
1:B:305:THR:HG21	1:B:320:ARG:NH1	2.36	0.41
1:A:305:THR:HG21	1:A:320:ARG:NH2	2.35	0.41
1:C:454:ASP:O	1:C:464:ARG:HB3	2.21	0.41
1:A:280:ASP:OD2	1:A:282:ARG:NH2	2.54	0.41
1:A:287:LEU:HD23	1:A:288:ALA:N	2.35	0.41
1:B:392:VAL:HG23	1:B:425:PHE:HB3	2.02	0.41
1:A:531:GLN:HG2	1:A:532:GLU:N	2.36	0.41
1:C:352:HIS:ND1	1:C:431:ASP:HB2	2.36	0.41
1:A:258:GLY:HA3	1:C:544:ARG:HE	1.85	0.41
1:B:277:LYS:NZ	2:D:5:SGN:H5	2.35	0.41
1:A:342:PHE:C	1:A:343:LEU:HD12	2.42	0.40
1:C:589:LEU:HD23	1:C:589:LEU:HA	1.87	0.40
1:B:352:HIS:ND1	1:B:431:ASP:HB2	2.36	0.40
1:B:484:LYS:NZ	1:B:532:GLU:N	2.69	0.40
1:A:282:ARG:HD2	1:A:350:ARG:CG	2.46	0.40
1:A:562:VAL:HG23	1:A:582:ILE:HD12	2.04	0.40
1:C:618:THR:HG22	1:C:622:LYS:O	2.21	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	439/470 (93%)	430 (98%)	9 (2%)	0	100 100
1	B	415/470 (88%)	406 (98%)	8 (2%)	1 (0%)	47 73
1	C	415/470 (88%)	410 (99%)	5 (1%)	0	100 100
All	All	1269/1410 (90%)	1246 (98%)	22 (2%)	1 (0%)	51 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	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	390/409 (95%)	390 (100%)	0	100 100
1	B	372/409 (91%)	370 (100%)	2 (0%)	88 96
1	C	374/409 (91%)	371 (99%)	3 (1%)	81 93
All	All	1136/1227 (93%)	1131 (100%)	5 (0%)	91 97

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

Mol	Chain	Res	Type
1	B	377	ASP
1	B	483	PHE
1	C	220	GLN
1	C	483	PHE
1	C	603	THR

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

Mol	Chain	Res	Type
1	A	515	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

8 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

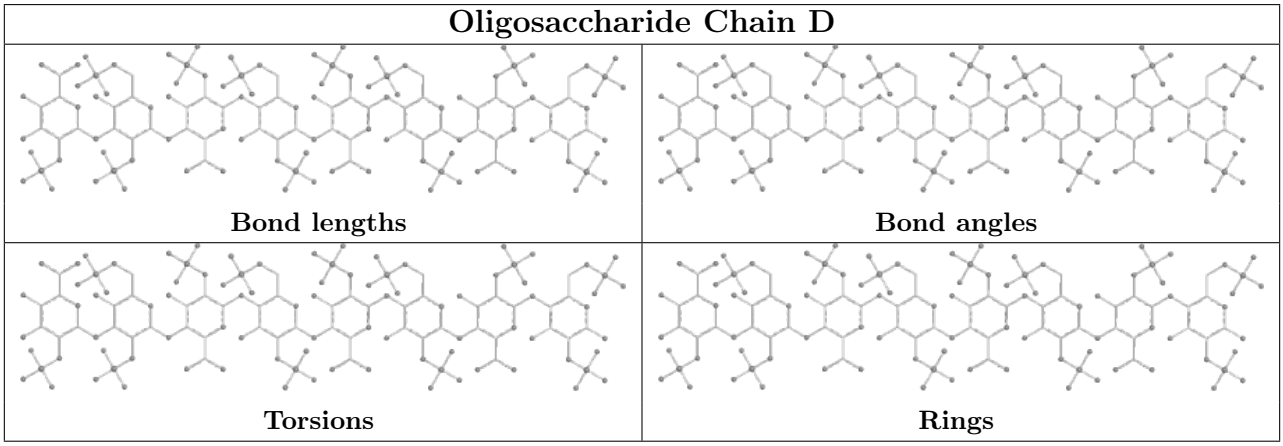
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no ligands in this entry.

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^{th} 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	447/470 (95%)	0.56	27 (6%)	21	20	48, 87, 168, 212	0
1	B	427/470 (90%)	0.62	20 (4%)	31	30	43, 79, 155, 202	0
1	C	429/470 (91%)	0.45	21 (4%)	29	28	53, 97, 166, 230	0
All	All	1303/1410 (92%)	0.54	68 (5%)	27	25	43, 88, 165, 230	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	PHE	8.2
1	B	465	ILE	7.7
1	B	466	LEU	4.9
1	A	384	GLY	4.6
1	A	410	ARG	4.5
1	B	486	PHE	4.4
1	A	448	LEU	4.3
1	A	415	PHE	4.2
1	C	373	MET	4.0
1	A	385	LEU	3.7
1	C	429	LEU	3.7
1	B	379	MET	3.5
1	B	484	LYS	3.5
1	B	464	ARG	3.4
1	B	444	ILE	3.4
1	A	418	THR	3.3
1	A	383	ASP	3.2
1	C	483	PHE	3.2
1	C	369	LEU	3.2
1	A	387	ASP	3.2
1	A	376	LEU	3.0
1	B	307	GLN	3.0
1	C	388	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	633	PHE	3.0
1	B	469	ILE	3.0
1	C	367	ILE	2.9
1	C	478	PRO	2.9
1	C	635	ARG	2.9
1	A	509	TYR	2.8
1	B	451	LEU	2.8
1	A	474	TYR	2.8
1	A	450	ILE	2.7
1	A	343	LEU	2.7
1	A	451	LEU	2.6
1	B	635	ARG	2.6
1	C	611	LEU	2.6
1	B	485	PRO	2.6
1	A	353	LEU	2.5
1	A	348	LEU	2.5
1	A	380	GLU	2.5
1	C	410	ARG	2.5
1	A	468	ILE	2.5
1	A	386	SER	2.4
1	A	416	ASN	2.4
1	C	481	LEU	2.3
1	A	447	ASN	2.3
1	B	456	ASN	2.3
1	A	465	ILE	2.3
1	B	571	MET	2.3
1	A	573	GLN	2.3
1	C	393	LEU	2.3
1	B	375	THR	2.3
1	C	343	LEU	2.2
1	B	453	SER	2.2
1	C	451	LEU	2.2
1	C	401	MET	2.2
1	A	466	LEU	2.2
1	A	367	ILE	2.1
1	B	301	VAL	2.1
1	A	369	LEU	2.1
1	B	376	LEU	2.1
1	C	449	THR	2.1
1	A	564	ILE	2.1
1	C	530	TRP	2.0
1	B	668	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	260	ILE	2.0
1	C	430	HIS	2.0
1	C	465	ILE	2.0

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

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

6.3 Carbohydrates (i)

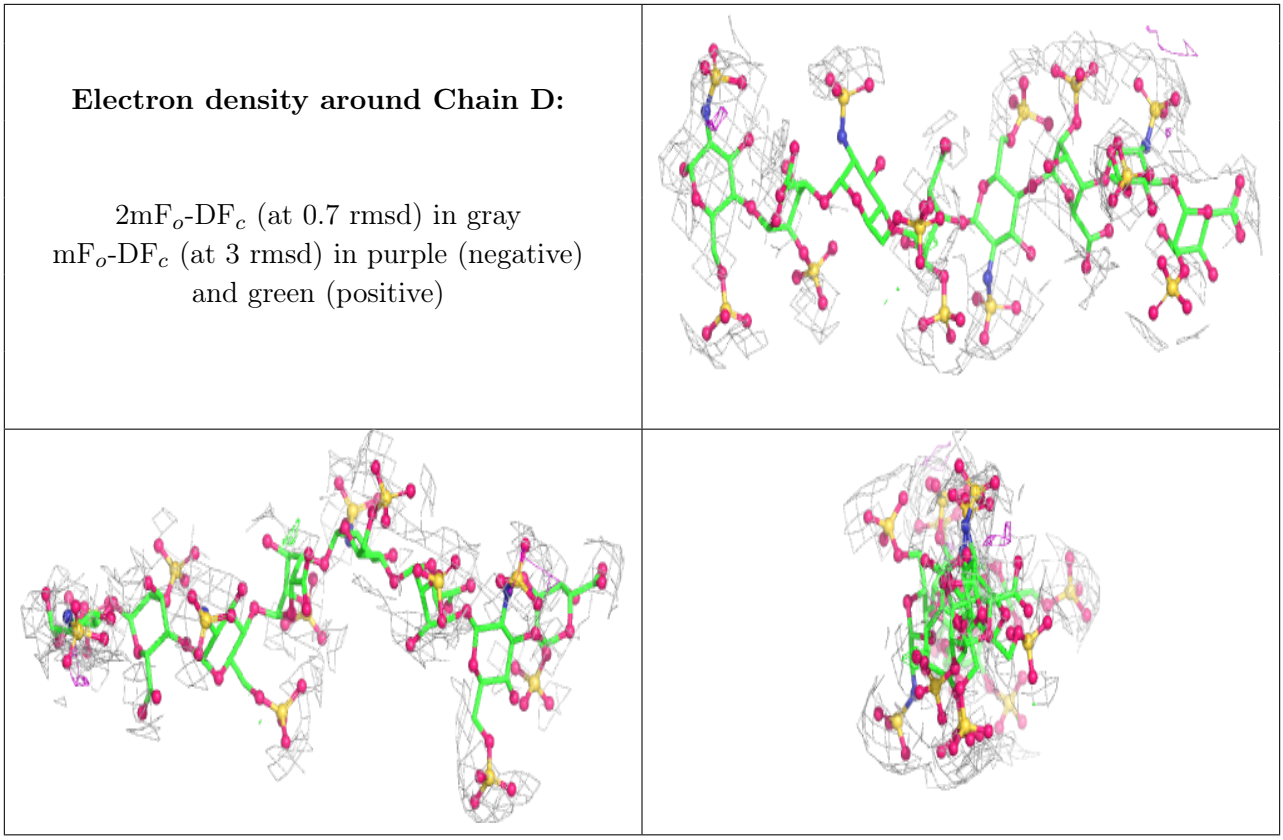
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SGN	D	1	20/20	0.48	0.18	216,225,229,230	0
2	IDS	D	8	16/17	0.70	0.14	192,203,206,208	0
2	IDS	D	2	16/17	0.73	0.12	211,225,230,230	0
2	SGN	D	3	19/20	0.82	0.12	178,196,208,208	0
2	SGN	D	7	19/20	0.83	0.12	176,193,198,199	0
2	IDS	D	4	16/17	0.86	0.13	152,173,184,184	0
2	SGN	D	5	19/20	0.89	0.12	142,164,186,187	0
2	IDS	D	6	16/17	0.89	0.15	154,164,168,171	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain D:

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



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.