



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:30 AM UTC

PDB ID : 2ZCK / pdb_00002zck
Title : Crystal structure of a ternary complex between PSA, a substrat-acyl intermediate and an activating antibody
Authors : Menez, R.; Stura, E.; Jolivet-Reynaud, C.
Deposited on : 2007-11-09
Resolution : 3.10 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

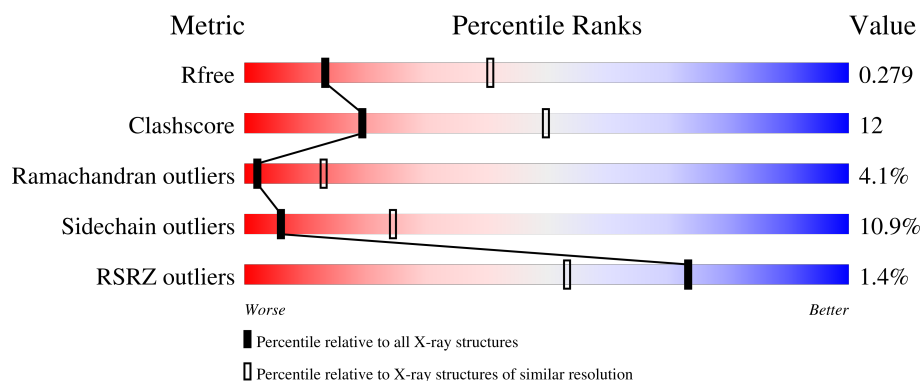
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	P	237	80% 15% • •
2	S	7	29% 43% 43% 14%
3	L	218	% 70% 23% 6% •
4	H	230	2% 63% 28% 7% •
5	A	2	100%

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
5	NAG	A	1	X	-	-	-
5	MAN	A	2	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5329 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 Prostate-specific antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	237	Total	C	N	O	S	0	0	0
			1832	1162	323	333	14			

- Molecule 2 is a protein called KGISSQY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	S	7	Total	C	N	O	0	0	0
			54	34	9	11			

- Molecule 3 is a protein called monoclonal antibody 8G8F5 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	218	Total	C	N	O	S	0	0	0
			1671	1036	279	349	7			

- Molecule 4 is a protein called monoclonal antibody 8G8F5 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	230	Total	C	N	O	S	0	0	0
			1716	1077	280	348	11			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	A	2	Total	C	N	O	0	0	0
			25	14	1	10			

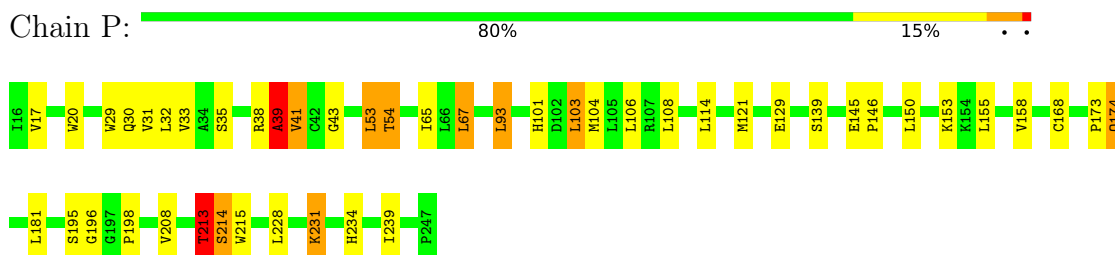
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	11	Total 11	O 11	0	0
6	L	14	Total 14	O 14	0	0
6	H	6	Total 6	O 6	0	0

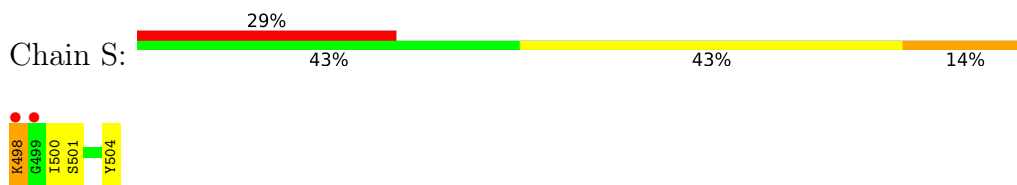
3 Residue-property plots

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.

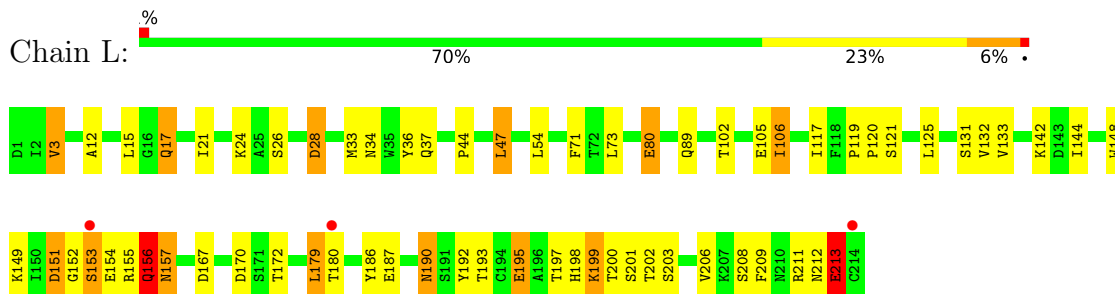
- Molecule 1: Prostate-specific antigen



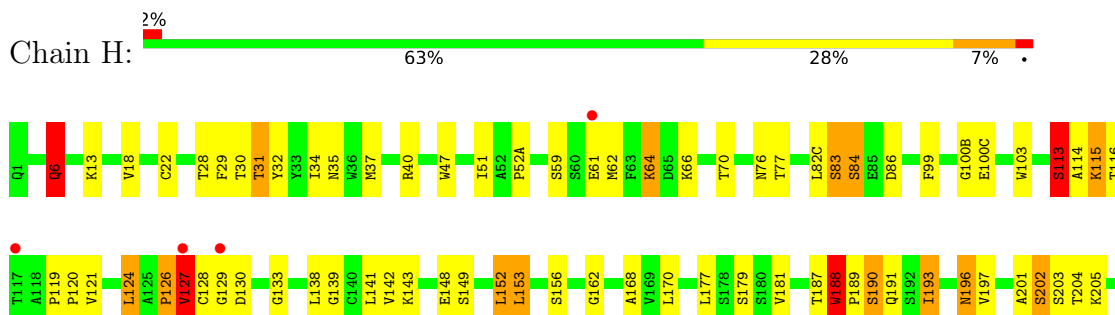
- Molecule 2: KGISSQY

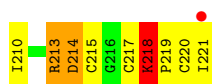


- Molecule 3: monoclonal antibody 8G8F5 Fab



- Molecule 4: monoclonal antibody 8G8F5 Fab





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

Chain A:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	86.77Å 86.77Å 238.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.19 – 3.10 70.19 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (70.19-3.10) 98.7 (70.19-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.221 , 0.275 0.222 , 0.279	Depositor DCC
R_{free} test set	870 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5329	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG

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	P	0.85	0/1883	0.98	5/2564 (0.2%)
2	S	1.20	1/54 (1.9%)	1.01	0/70
3	L	0.84	1/1707 (0.1%)	0.98	4/2319 (0.2%)
4	H	0.89	2/1757 (0.1%)	1.13	6/2398 (0.3%)
All	All	0.86	4/5401 (0.1%)	1.03	15/7351 (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	P	1	2
3	L	1	0
4	H	1	0
All	All	3	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	28	ASP	CA-C	-8.25	1.41	1.52
2	S	498	LYS	C-N	5.88	1.39	1.32
4	H	83	SER	CA-C	5.71	1.61	1.53
4	H	127	VAL	CA-C	5.28	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	67	LEU	N-CA-C	9.80	129.56	110.56
4	H	218	LYS	CA-C-N	9.30	149.33	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	218	LYS	C-N-CA	9.30	149.33	127.00
4	H	218	LYS	C-N-CD	-8.69	101.48	120.60
3	L	156	GLN	N-CA-C	7.63	122.70	113.23
3	L	156	GLN	CA-C-N	6.08	132.64	121.70
3	L	156	GLN	C-N-CA	6.08	132.64	121.70
1	P	39	ALA	CA-C-O	-5.83	114.64	121.46
1	P	213	THR	CA-C-O	-5.81	115.13	121.87
4	H	188	TRP	CB-CA-C	5.66	121.31	110.17
1	P	213	THR	CA-C-N	5.42	131.88	121.54
1	P	213	THR	C-N-CA	5.42	131.88	121.54
4	H	188	TRP	CA-C-N	-5.13	113.43	119.84
4	H	188	TRP	C-N-CA	-5.13	113.43	119.84
3	L	17	GLN	N-CA-C	5.02	116.42	110.19

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	P	67	LEU	CA
3	L	28	ASP	CA
4	H	188	TRP	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	213	THR	Peptide
1	P	39	ALA	Peptide

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	P	1832	0	1803	30	0
2	S	54	0	53	5	0
3	L	1671	0	1588	42	0
4	H	1716	0	1666	52	0
5	A	25	0	22	0	0
6	H	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	14	0	0	0	0
6	P	11	0	0	0	0
All	All	5329	0	5132	121	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 12.

All (121) 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:P:195:SER:O	1:P:213:THR:O	1.85	0.93
4:H:187:THR:O	4:H:188:TRP:O	1.91	0.87
3:L:156:GLN:N	3:L:157:ASN:HB3	1.92	0.85
3:L:156:GLN:H	3:L:157:ASN:HB3	1.43	0.84
1:P:195:SER:OG	2:S:504:TYR:C	2.26	0.78
4:H:127:VAL:HB	4:H:128:CYS:CB	2.20	0.71
4:H:119:PRO:HD2	4:H:204:THR:HG21	1.72	0.71
1:P:215:TRP:CZ2	1:P:228:LEU:HD13	2.29	0.68
4:H:188:TRP:O	4:H:189:PRO:C	2.37	0.67
4:H:127:VAL:HB	4:H:128:CYS:HB2	1.76	0.66
4:H:214:ASP:N	4:H:215:CYS:HA	2.10	0.66
4:H:213:ARG:C	4:H:215:CYS:HA	2.20	0.66
1:P:214:SER:HB3	1:P:228:LEU:O	1.95	0.66
4:H:153:LEU:HD12	4:H:156:SER:HA	1.78	0.65
4:H:83:SER:HB2	4:H:84:SER:O	1.97	0.64
4:H:128:CYS:HB3	4:H:129:GLY:O	1.98	0.63
3:L:12:ALA:HA	3:L:105:GLU:O	1.98	0.63
4:H:83:SER:CB	4:H:84:SER:O	2.47	0.62
1:P:129:GLU:OE1	1:P:231:LYS:HE2	2.00	0.61
4:H:120:PRO:HD2	4:H:143:LYS:O	2.01	0.60
3:L:37:GLN:HB2	3:L:47:LEU:HD21	1.81	0.60
4:H:188:TRP:CD1	4:H:193:ILE:CG2	2.85	0.60
3:L:120:PRO:HB2	3:L:125:LEU:HD11	1.84	0.60
4:H:148:GLU:OE2	4:H:168:ALA:HB3	2.04	0.58
4:H:153:LEU:HG	4:H:196:ASN:HB2	1.87	0.57
4:H:189:PRO:O	4:H:190:SER:C	2.46	0.57
3:L:144:ILE:CG2	3:L:198:HIS:ND1	2.69	0.56
3:L:34:ASN:HD22	3:L:89:GLN:HE22	1.54	0.56
4:H:18:VAL:HG12	4:H:82(C):LEU:HD11	1.89	0.54
1:P:39:ALA:C	1:P:41:VAL:HG23	2.33	0.54
1:P:174:GLN:NE2	2:S:501:SER:OG	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:188:TRP:CD1	4:H:193:ILE:HG21	2.44	0.53
4:H:31:THR:HG23	4:H:32:TYR:CD2	2.44	0.53
1:P:43:GLY:O	1:P:196:GLY:HA3	2.08	0.53
1:P:215:TRP:CZ2	1:P:228:LEU:CD1	2.92	0.53
1:P:93:LEU:HB3	1:P:101:HIS:CD2	2.43	0.52
3:L:198:HIS:O	3:L:200:THR:N	2.42	0.52
1:P:30:GLN:HE22	1:P:198:PRO:HD2	1.76	0.51
4:H:119:PRO:CD	4:H:204:THR:HG21	2.39	0.51
4:H:35:ASN:HD22	4:H:47:TRP:HE1	1.58	0.50
3:L:187:GLU:HA	3:L:211:ARG:NH1	2.26	0.50
4:H:29:PHE:HB2	4:H:76:ASN:HD22	1.77	0.50
1:P:65:ILE:HG22	1:P:67:LEU:HD22	1.94	0.50
3:L:36:TYR:HE2	3:L:89:GLN:HE21	1.58	0.50
3:L:149:LYS:CB	3:L:153:SER:HA	2.42	0.49
4:H:187:THR:HG23	4:H:191:GLN:OE1	2.12	0.49
1:P:39:ALA:CA	1:P:41:VAL:HG23	2.43	0.48
4:H:156:SER:H	4:H:196:ASN:HD21	1.61	0.48
4:H:152:LEU:HD21	4:H:179:SER:CB	2.43	0.48
4:H:100(B):GLY:O	4:H:100(C):GLU:C	2.57	0.47
3:L:120:PRO:CB	3:L:125:LEU:HD11	2.44	0.47
4:H:128:CYS:HB3	4:H:129:GLY:CA	2.45	0.47
3:L:21:ILE:HD12	3:L:102:THR:HG21	1.96	0.47
3:L:149:LYS:HB3	3:L:153:SER:HA	1.96	0.47
4:H:59:SER:HB2	4:H:64:LYS:HD2	1.97	0.47
4:H:142:VAL:HG22	4:H:197:VAL:HG21	1.97	0.47
3:L:15:LEU:HD11	3:L:80:GLU:HG3	1.96	0.46
3:L:202:THR:HA	3:L:203:SER:C	2.40	0.46
1:P:234:HIS:HD2	4:H:99:PHE:N	2.13	0.46
1:P:29:TRP:CE2	1:P:121:MET:HE2	2.50	0.46
3:L:167:ASP:OD1	3:L:167:ASP:C	2.58	0.46
3:L:3:VAL:HG13	3:L:26:SER:HB3	1.99	0.45
4:H:116:THR:HG22	4:H:116:THR:O	2.17	0.45
1:P:33:VAL:O	1:P:41:VAL:HB	2.16	0.45
3:L:156:GLN:HG2	3:L:157:ASN:HB2	1.98	0.45
4:H:28:THR:O	4:H:31:THR:HG22	2.16	0.45
4:H:83:SER:OG	4:H:84:SER:O	2.33	0.45
1:P:145:GLU:HG3	1:P:146:PRO:HD2	2.00	0.44
4:H:113:SER:CB	4:H:114:ALA:HA	2.47	0.44
4:H:113:SER:OG	4:H:114:ALA:HB2	2.17	0.44
1:P:53:LEU:HD22	1:P:103:LEU:HD22	2.00	0.44
3:L:170:ASP:O	3:L:172:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:131:SER:HB3	3:L:180:THR:HG23	1.99	0.44
3:L:132:VAL:HG12	3:L:179:LEU:HG	1.99	0.44
4:H:188:TRP:O	4:H:190:SER:N	2.50	0.44
3:L:151:ASP:CB	3:L:190:ASN:HD21	2.31	0.43
1:P:31:VAL:HG12	1:P:67:LEU:HB3	1.99	0.43
3:L:152:GLY:O	3:L:154:GLU:N	2.51	0.43
4:H:51:ILE:O	4:H:52(A):PRO:HD3	2.18	0.43
1:P:234:HIS:HD2	4:H:99:PHE:H	1.65	0.43
4:H:129:GLY:HA2	4:H:130:ASP:HA	1.75	0.43
4:H:124:LEU:HB2	4:H:139:GLY:C	2.44	0.43
3:L:106:ILE:C	3:L:106:ILE:HD13	2.43	0.43
4:H:30:THR:HA	4:H:52(A):PRO:HB2	2.00	0.43
1:P:195:SER:OG	2:S:504:TYR:HB2	2.19	0.43
1:P:53:LEU:CD2	1:P:103:LEU:HD22	2.48	0.43
1:P:65:ILE:HG13	1:P:108:LEU:CD2	2.49	0.42
4:H:126:PRO:HD2	4:H:188:TRP:CZ3	2.54	0.42
4:H:128:CYS:CB	4:H:129:GLY:HA3	2.49	0.42
3:L:212:ASN:O	3:L:213:GLU:C	2.62	0.42
3:L:151:ASP:HB2	3:L:190:ASN:HD21	1.83	0.42
3:L:121:SER:O	3:L:125:LEU:HD12	2.19	0.42
3:L:195:GLU:HA	3:L:206:VAL:HG12	2.01	0.42
1:P:35:SER:N	1:P:38:ARG:O	2.50	0.42
3:L:148:TRP:CD2	3:L:179:LEU:HD23	2.55	0.42
4:H:6:GLN:HA	4:H:22:CYS:HA	2.01	0.42
4:H:214:ASP:N	4:H:215:CYS:CA	2.80	0.42
3:L:37:GLN:HB2	3:L:47:LEU:CD2	2.46	0.42
3:L:151:ASP:HB2	3:L:190:ASN:ND2	2.35	0.42
3:L:186:TYR:O	3:L:192:TYR:OH	2.37	0.41
3:L:199:LYS:O	3:L:199:LYS:CG	2.67	0.41
1:P:30:GLN:NE2	1:P:139:SER:OG	2.53	0.41
1:P:215:TRP:CH2	1:P:228:LEU:CD1	3.03	0.41
4:H:126:PRO:HD3	4:H:138:LEU:HD12	2.02	0.41
3:L:44:PRO:HG2	4:H:103:TRP:CH2	2.56	0.41
1:P:20:TRP:CZ3	1:P:158:VAL:HA	2.56	0.41
1:P:195:SER:OG	2:S:504:TYR:O	2.38	0.41
3:L:148:TRP:CE3	3:L:179:LEU:HD23	2.56	0.41
3:L:201:SER:O	3:L:202:THR:HG23	2.21	0.41
4:H:113:SER:HB2	4:H:114:ALA:HA	2.02	0.41
4:H:201:ALA:O	4:H:202:SER:CB	2.69	0.41
3:L:119:PRO:HG3	3:L:209:PHE:CD1	2.56	0.40
3:L:193:THR:HB	3:L:208:SER:OG	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:54:THR:O	1:P:104:MET:N	2.54	0.40
3:L:144:ILE:HG22	3:L:198:HIS:ND1	2.37	0.40
1:P:173:PRO:N	2:S:498:LYS:HD2	2.36	0.40
4:H:190:SER:HB3	4:H:191:GLN:HG3	2.04	0.40
3:L:33:MET:HG2	3:L:71:PHE:CG	2.57	0.40
4:H:83:SER:HB2	4:H:84:SER:CB	2.51	0.40
4:H:124:LEU:HD21	4:H:141:LEU:HB2	2.03	0.40
3:L:198:HIS:C	3:L:200:THR:H	2.29	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	P	235/237 (99%)	221 (94%)	12 (5%)	2 (1%)	14	44
2	S	5/7 (71%)	5 (100%)	0	0	100	100
3	L	216/218 (99%)	187 (87%)	22 (10%)	7 (3%)	3	18
4	H	228/230 (99%)	189 (83%)	20 (9%)	19 (8%)	0	4
All	All	684/692 (99%)	602 (88%)	54 (8%)	28 (4%)	2	13

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	41	VAL
1	P	214	SER
3	L	151	ASP
3	L	157	ASN
3	L	199	LYS
3	L	213	GLU
4	H	62	MET

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Mol	Chain	Res	Type
4	H	86	ASP
4	H	115	LYS
4	H	127	VAL
4	H	149	SER
4	H	188	TRP
4	H	202	SER
4	H	217	CYS
4	H	219	PRO
4	H	220	CYS
3	L	153	SER
3	L	155	ARG
4	H	84	SER
3	L	190	ASN
4	H	113	SER
4	H	203	SER
4	H	218	LYS
4	H	162	GLY
4	H	6	GLN
4	H	190	SER
4	H	133	GLY
4	H	126	PRO

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	P	205/205 (100%)	187 (91%)	18 (9%)	9	33
2	S	6/6 (100%)	5 (83%)	1 (17%)	2	10
3	L	189/189 (100%)	172 (91%)	17 (9%)	9	33
4	H	196/196 (100%)	167 (85%)	29 (15%)	3	13
All	All	596/596 (100%)	531 (89%)	65 (11%)	6	24

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	17	VAL
1	P	32	LEU
1	P	53	LEU
1	P	54	THR
1	P	93	LEU
1	P	103	LEU
1	P	106	LEU
1	P	114	LEU
1	P	150	LEU
1	P	153	LYS
1	P	155	LEU
1	P	168	CYS
1	P	174	GLN
1	P	181	LEU
1	P	208	VAL
1	P	213	THR
1	P	231	LYS
1	P	239	ILE
2	S	500	ILE
3	L	3	VAL
3	L	17	GLN
3	L	24	LYS
3	L	28	ASP
3	L	47	LEU
3	L	54	LEU
3	L	73	LEU
3	L	80	GLU
3	L	106	ILE
3	L	117	ILE
3	L	133	VAL
3	L	142	LYS
3	L	156	GLN
3	L	179	LEU
3	L	195	GLU
3	L	197	THR
3	L	213	GLU
4	H	6	GLN
4	H	13	LYS
4	H	31	THR
4	H	34	ILE
4	H	37	MET
4	H	40	ARG
4	H	61	GLU

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Mol	Chain	Res	Type
4	H	64	LYS
4	H	66	LYS
4	H	70	THR
4	H	77	THR
4	H	113	SER
4	H	115	LYS
4	H	121	VAL
4	H	124	LEU
4	H	127	VAL
4	H	152	LEU
4	H	153	LEU
4	H	170	LEU
4	H	177	LEU
4	H	181	VAL
4	H	193	ILE
4	H	196	ASN
4	H	205	LYS
4	H	210	ILE
4	H	213	ARG
4	H	214	ASP
4	H	218	LYS
4	H	221	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	30	GLN
1	P	91	HIS
1	P	95(F)	ASN
1	P	174	GLN
1	P	234	HIS
3	L	6	GLN
3	L	17	GLN
3	L	42	GLN
3	L	53	ASN
3	L	89	GLN
3	L	156	GLN
3	L	161	ASN
3	L	212	ASN
4	H	1	GLN
4	H	35	ASN
4	H	76	ASN

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Mol	Chain	Res	Type
4	H	155	ASN
4	H	191	GLN
4	H	196	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	$\# Z > 2$
5	NAG	A	1	5,1	14,14,15	0.91	0	17,19,21	1.60	3 (17%)
5	MAN	A	2	5	11,11,12	0.71	0	15,15,17	0.91	1 (6%)

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	A	1	5,1	1/1/5/7	5/6/23/26	0/1/1/1
5	MAN	A	2	5	1/1/4/5	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	1	NAG	C3-C4-C5	3.77	117.07	110.23
5	A	1	NAG	C4-C3-C2	2.87	115.22	111.02
5	A	2	MAN	O2-C2-C1	2.70	115.41	109.22
5	A	1	NAG	O5-C1-C2	2.10	114.54	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1	NAG	C1
5	A	2	MAN	C1

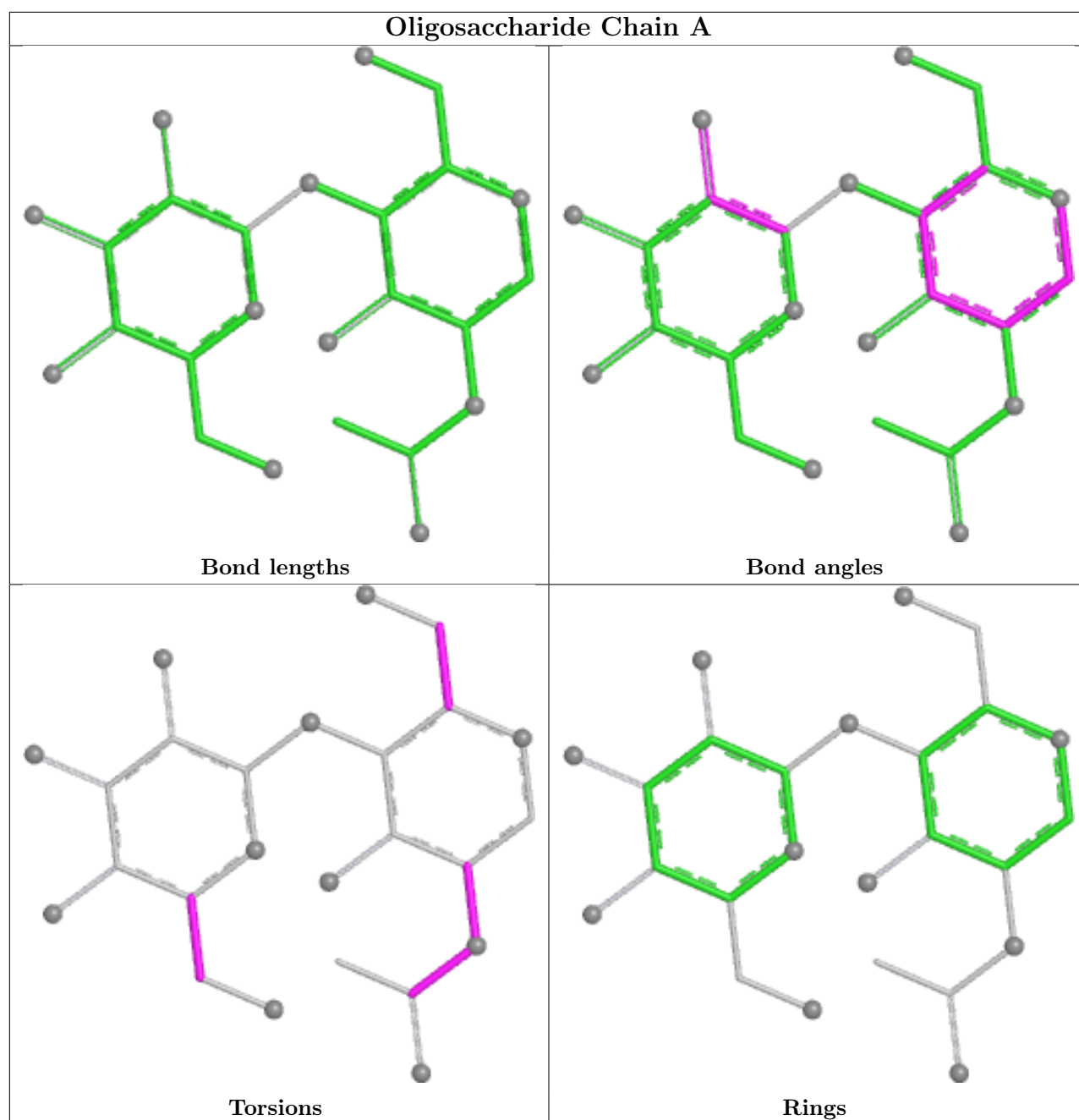
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	NAG	C8-C7-N2-C2
5	A	1	NAG	O7-C7-N2-C2
5	A	1	NAG	O5-C5-C6-O6
5	A	1	NAG	C4-C5-C6-O6
5	A	2	MAN	O5-C5-C6-O6
5	A	1	NAG	C3-C2-N2-C7

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 [i](#)

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 ⓘ

There are no chain breaks in this entry.

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	P	237/237 (100%)	-0.18	0 100 100	43, 53, 68, 75	0
2	S	7/7 (100%)	1.21	2 (28%) 1 1	44, 48, 50, 50	7 (100%)
3	L	218/218 (100%)	0.21	3 (1%) 73 53	43, 74, 104, 122	0
4	H	230/230 (100%)	0.34	5 (2%) 62 41	45, 69, 97, 107	0
All	All	692/692 (100%)	0.13	10 (1%) 73 53	43, 62, 98, 122	7 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	214	CYS	3.6
4	H	221	ILE	3.2
2	S	499	GLY	3.1
4	H	127	VAL	3.1
4	H	61	GLU	2.5
2	S	498	LYS	2.4
3	L	180	THR	2.2
4	H	129	GLY	2.1
3	L	153	SER	2.1
4	H	117	THR	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.

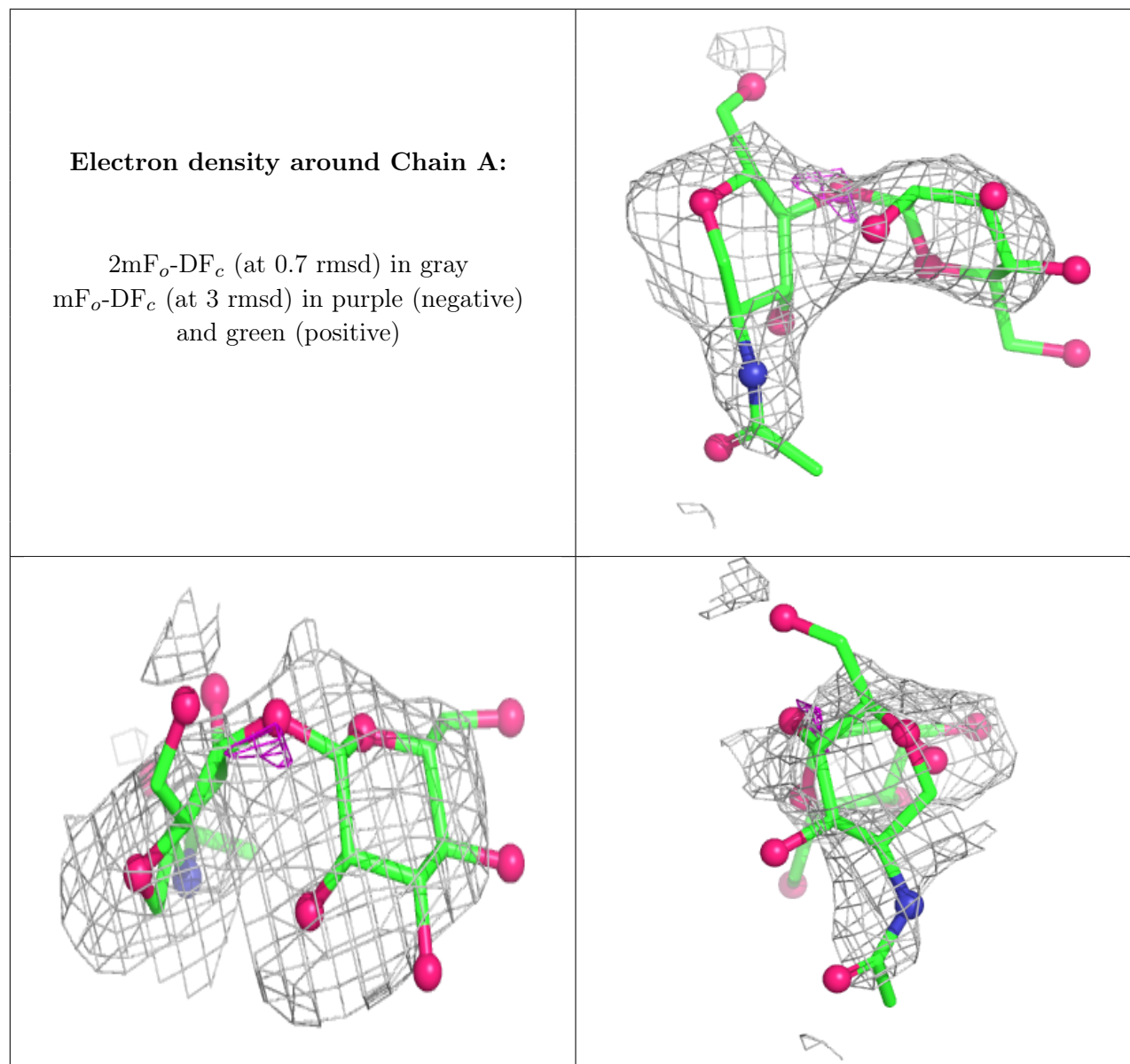
6.3 Carbohydrates [i](#)

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(Å ²)	Q<0.9
5	NAG	A	1	14/15	-	-	89,97,99,101	0
5	MAN	A	2	11/12	-	-	101,102,103,103	0

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.