



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:51 AM UTC

PDB ID : 4DW1 / pdb_00004dw1
Title : Crystal structure of the ATP-gated P2X4 ion channel in the ATP-bound, open state at 2.8 Angstroms
Authors : Hattori, M.; Gouaux, E.
Deposited on : 2012-02-24
Resolution : 2.80 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

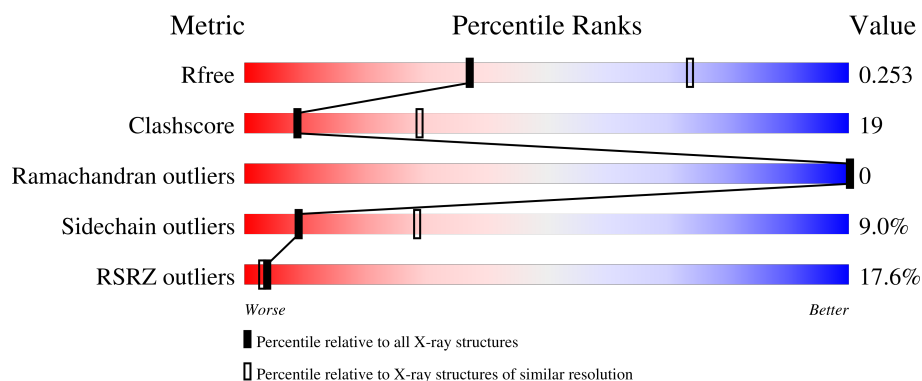
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	A	340	17% 62% 29% 5%
2	B	6	50% 50%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2669 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.

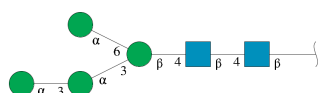
- Molecule 1 is a protein called P2X purinoceptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	324	2448	1551	415	466	16	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

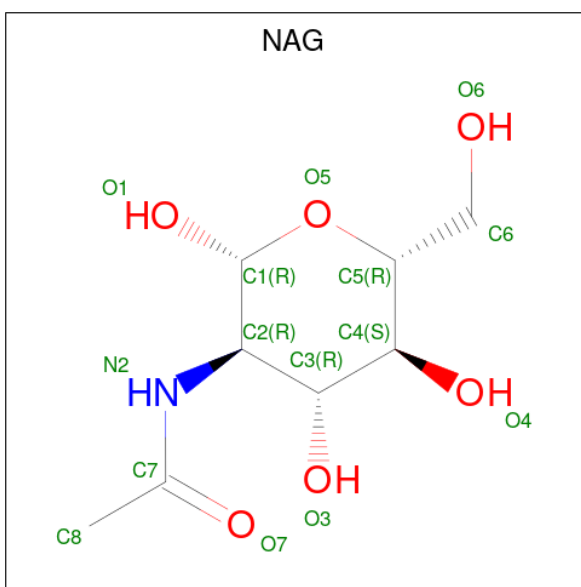
Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP Q6NYR1
A	27	SER	-	expression tag	UNP Q6NYR1
A	78	LYS	ASN	engineered mutation	UNP Q6NYR1
A	187	ARG	ASN	engineered mutation	UNP Q6NYR1
A	252	ARG	HIS	engineered mutation	UNP Q6NYR1

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



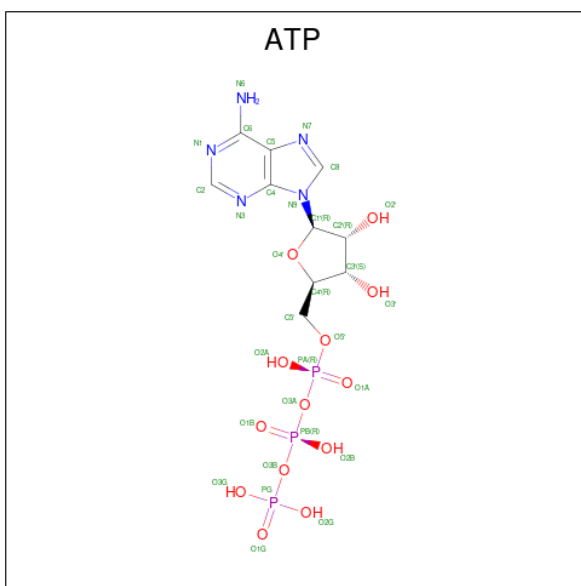
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	72	40	2	30	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

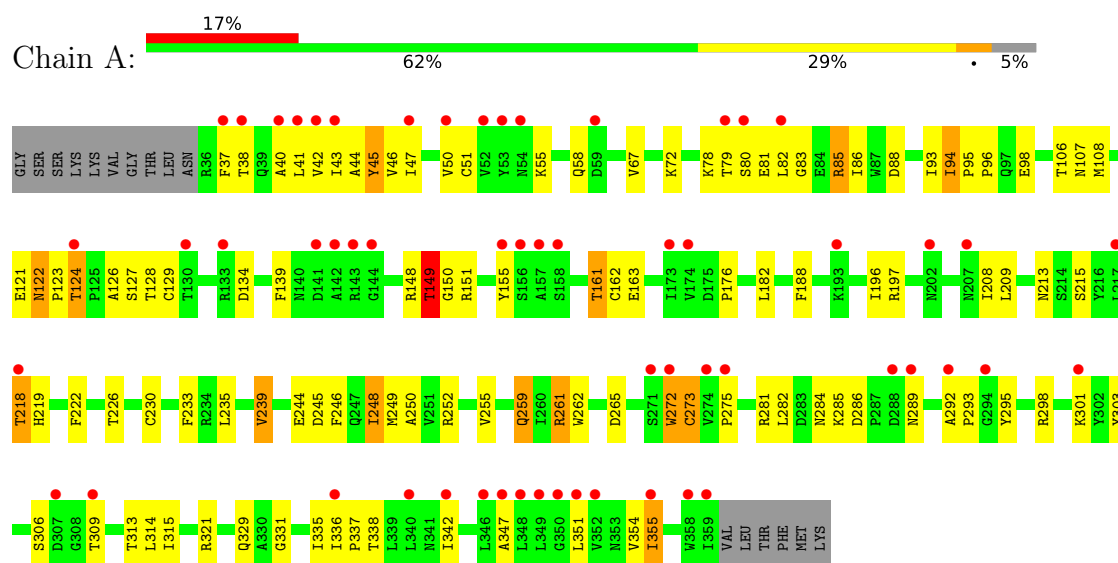
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	92	Total	O	0	0
			92	92		

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: P2X purinoceptor



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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	128.79Å 128.79Å 252.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.94 – 2.80 45.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.94-2.80) 98.8 (45.94-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.208 , 0.254 0.208 , 0.253	Depositor DCC
R_{free} test set	1016 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2669	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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, GOL, NAG, BMA, ATP

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	0.58	0/2502	0.99	11/3414 (0.3%)

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	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	ARG	N-CA-C	-6.62	99.26	109.52
1	A	208	ILE	CB-CA-C	-6.62	103.35	111.88
1	A	272	TRP	N-CA-C	-6.31	99.94	109.60
1	A	273	CYS	N-CA-C	-6.27	103.58	110.91
1	A	149	THR	N-CA-C	6.11	120.47	112.89
1	A	122	ASN	CA-C-N	6.05	126.41	119.93
1	A	122	ASN	C-N-CA	6.05	126.41	119.93
1	A	286	ASP	CA-C-N	5.64	125.31	119.56
1	A	286	ASP	C-N-CA	5.64	125.31	119.56
1	A	226	THR	N-CA-C	5.53	120.09	113.23
1	A	82	LEU	N-CA-C	-5.09	106.76	113.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	THR	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	A	2448	0	2303	88	0
2	B	72	0	61	4	0
3	A	14	0	13	0	0
4	A	31	0	12	3	0
5	A	12	0	16	2	0
6	A	92	0	0	4	0
All	All	2669	0	2405	93	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 19.

All (93) 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:351:LEU:O	1:A:355:ILE:HB	1.61	0.98
1:A:37:PHE:O	1:A:41:LEU:HB2	1.69	0.91
1:A:40:ALA:O	1:A:44:ALA:HB3	1.71	0.90
2:B:2:NAG:O3	2:B:3:BMA:H2	1.73	0.89
1:A:85:ARG:HG2	1:A:85:ARG:HH11	1.42	0.84
1:A:85:ARG:HH11	1:A:85:ARG:CG	1.91	0.83
1:A:124:THR:HG22	1:A:127:SER:H	1.47	0.80
1:A:41:LEU:O	1:A:45:TYR:HB3	1.83	0.79
2:B:2:NAG:H81	2:B:5:MAN:H2	1.68	0.73
1:A:40:ALA:O	1:A:44:ALA:CB	2.35	0.73
1:A:219:HIS:HD2	6:A:656:HOH:O	1.69	0.73
1:A:239:VAL:HG23	1:A:244:GLU:HB2	1.75	0.67
1:A:215:SER:O	1:A:218:THR:HB	1.94	0.67
1:A:123:PRO:HD3	1:A:155:TYR:CE1	2.30	0.67
1:A:249:MET:HE2	1:A:281:ARG:NH1	2.16	0.61
1:A:121:GLU:O	1:A:161:THR:HG21	2.01	0.60
1:A:298:ARG:NH2	4:A:508:ATP:O2G	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:O	1:A:342:ILE:HG13	2.02	0.58
1:A:255:VAL:HG12	1:A:282:LEU:HB2	1.86	0.58
1:A:79:THR:O	1:A:81:GLU:HA	2.05	0.57
1:A:106:THR:O	1:A:182:LEU:HB2	2.05	0.56
1:A:41:LEU:O	1:A:45:TYR:CB	2.52	0.56
1:A:93:ILE:C	1:A:94:ILE:HD13	2.31	0.56
1:A:272:TRP:CG	1:A:273:CYS:H	2.24	0.55
1:A:42:VAL:HG23	1:A:43:ILE:H	1.72	0.55
1:A:106:THR:HB	1:A:250:ALA:HB1	1.90	0.53
1:A:292:ALA:N	1:A:293:PRO:HD3	2.24	0.53
1:A:139:PHE:HD1	1:A:148:ARG:HD2	1.73	0.53
1:A:85:ARG:HG2	1:A:85:ARG:NH1	2.20	0.53
1:A:313:THR:HG22	1:A:315:ILE:CD1	2.40	0.52
1:A:107:ASN:ND2	1:A:176:PRO:HB2	2.26	0.51
1:A:78:LYS:HA	1:A:83:GLY:O	2.11	0.51
1:A:176:PRO:HG2	1:A:252:ARG:HE	1.76	0.51
2:B:2:NAG:C8	2:B:5:MAN:H2	2.39	0.51
1:A:149:THR:N	1:A:150:GLY:HA2	2.24	0.50
1:A:284:ASN:HA	6:A:660:HOH:O	2.10	0.50
1:A:38:THR:O	1:A:42:VAL:HG22	2.11	0.50
1:A:150:GLY:HA2	6:A:682:HOH:O	2.12	0.49
1:A:88:ASP:OD1	1:A:88:ASP:C	2.56	0.49
1:A:245:ASP:HB3	1:A:248:ILE:HG13	1.95	0.49
1:A:124:THR:HG22	1:A:127:SER:N	2.21	0.49
1:A:124:THR:O	1:A:128:THR:HG23	2.13	0.48
1:A:124:THR:CG2	1:A:126:ALA:H	2.27	0.48
1:A:314:LEU:C	1:A:315:ILE:HD12	2.39	0.48
1:A:335:ILE:O	1:A:338:THR:HB	2.13	0.48
1:A:42:VAL:HG23	1:A:43:ILE:N	2.28	0.48
1:A:315:ILE:HD12	1:A:315:ILE:N	2.29	0.48
1:A:149:THR:OG1	1:A:163:GLU:HB3	2.14	0.47
4:A:508:ATP:O2B	5:A:510:GOL:H2	2.14	0.47
1:A:249:MET:HE2	1:A:281:ARG:CZ	2.44	0.47
1:A:121:GLU:HB2	1:A:161:THR:CG2	2.44	0.46
1:A:176:PRO:CG	1:A:252:ARG:HE	2.29	0.46
1:A:239:VAL:HG11	1:A:246:PHE:HD1	1.80	0.46
1:A:301:LYS:HE3	1:A:303:TYR:OH	2.16	0.45
1:A:351:LEU:HA	1:A:354:VAL:CB	2.46	0.45
1:A:249:MET:HE2	1:A:281:ARG:HD2	1.98	0.45
1:A:347:ALA:O	1:A:351:LEU:HG	2.17	0.45
1:A:261:ARG:HE	1:A:261:ARG:HB2	1.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:VAL:HG23	1:A:47:ILE:HD13	2.00	0.44
1:A:58:GLN:OE1	1:A:331:GLY:HA3	2.18	0.44
1:A:272:TRP:O	1:A:273:CYS:HB3	2.18	0.44
1:A:121:GLU:C	1:A:161:THR:HG21	2.42	0.44
1:A:124:THR:HG23	1:A:126:ALA:H	1.83	0.44
1:A:51:CYS:O	1:A:55:LYS:HA	2.19	0.43
1:A:249:MET:CE	1:A:281:ARG:HD2	2.48	0.43
1:A:161:THR:CG2	1:A:162:CYS:N	2.79	0.43
1:A:262:TRP:CH2	1:A:275:PRO:HD3	2.53	0.43
1:A:95:PRO:HB2	1:A:96:PRO:CD	2.49	0.43
1:A:259:GLN:HB2	1:A:261:ARG:NH2	2.34	0.43
1:A:222:PHE:HA	1:A:230:CYS:HB3	2.01	0.42
1:A:272:TRP:O	1:A:273:CYS:CB	2.67	0.42
1:A:107:ASN:O	1:A:108:MET:HG3	2.20	0.42
1:A:85:ARG:CG	1:A:85:ARG:NH1	2.62	0.42
1:A:233:PHE:N	1:A:233:PHE:CD2	2.87	0.42
1:A:121:GLU:N	1:A:161:THR:HG21	2.34	0.42
1:A:265:ASP:CB	1:A:272:TRP:HZ3	2.33	0.42
1:A:188:PHE:HB2	1:A:235:LEU:HD12	2.01	0.42
1:A:108:MET:HE2	1:A:108:MET:HB2	1.85	0.42
1:A:272:TRP:CG	1:A:273:CYS:N	2.88	0.42
1:A:80:SER:HA	1:A:81:GLU:HA	1.63	0.41
1:A:85:ARG:NH1	1:A:86:ILE:O	2.53	0.41
1:A:295:TYR:HD1	5:A:509:GOL:O2	2.03	0.41
1:A:129:CYS:HB2	1:A:134:ASP:HB2	2.02	0.41
1:A:313:THR:HG22	1:A:315:ILE:HD12	2.03	0.41
2:B:2:NAG:O3	2:B:3:BMA:C2	2.57	0.41
1:A:123:PRO:HD3	1:A:155:TYR:CD1	2.55	0.41
1:A:196:ILE:O	1:A:196:ILE:HG13	2.20	0.40
1:A:289:ASN:ND2	6:A:670:HOH:O	2.54	0.40
1:A:94:ILE:HD13	1:A:94:ILE:N	2.36	0.40
1:A:122:ASN:HA	1:A:123:PRO:HD3	1.95	0.40
1:A:222:PHE:HB2	1:A:230:CYS:O	2.21	0.40
1:A:336:ILE:HB	1:A:337:PRO:CD	2.50	0.40
1:A:298:ARG:HH22	4:A:508:ATP:PG	2.45	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/340 (95%)	303 (94%)	19 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/298 (86%)	232 (91%)	23 (9%)	9	28

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	TYR
1	A	50	VAL
1	A	67	VAL
1	A	72	LYS
1	A	85	ARG
1	A	94	ILE
1	A	98	GLU
1	A	124	THR
1	A	161	THR
1	A	197	ARG
1	A	209	LEU
1	A	213	ASN
1	A	218	THR

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Mol	Chain	Res	Type
1	A	239	VAL
1	A	248	ILE
1	A	259	GLN
1	A	261	ARG
1	A	285	LYS
1	A	306	SER
1	A	309	THR
1	A	321	ARG
1	A	329	GLN
1	A	355	ILE

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	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	NAG	B	1	2,1	14,14,15	0.66	0	17,19,21	1.32	2 (11%)
2	NAG	B	2	2	14,14,15	0.59	0	17,19,21	1.57	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BMA	B	3	2	11,11,12	0.64	0	15,15,17	1.74	1 (6%)
2	MAN	B	4	2	11,11,12	0.55	0	15,15,17	2.73	7 (46%)
2	MAN	B	5	2	11,11,12	0.64	0	15,15,17	1.03	1 (6%)
2	MAN	B	6	2	11,11,12	0.64	0	15,15,17	1.29	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
2	NAG	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	MAN	B	4	2	-	2/2/19/22	0/1/1/1
2	MAN	B	5	2	-	0/2/19/22	0/1/1/1
2	MAN	B	6	2	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	MAN	C1-O5-C5	7.57	122.33	112.19
2	B	3	BMA	C2-C3-C4	-5.55	101.10	110.86
2	B	2	NAG	C2-N2-C7	-4.14	117.36	122.90
2	B	6	MAN	C1-C2-C3	-3.65	104.33	109.64
2	B	4	MAN	C2-C3-C4	-3.52	104.68	110.86
2	B	1	NAG	C2-N2-C7	-3.22	118.59	122.90
2	B	1	NAG	C1-O5-C5	3.13	116.38	112.19
2	B	4	MAN	O5-C5-C4	3.12	118.41	110.83
2	B	4	MAN	C6-C5-C4	-2.85	106.03	113.02
2	B	4	MAN	C3-C4-C5	2.78	115.27	110.23
2	B	4	MAN	C1-C2-C3	2.43	113.19	109.64
2	B	4	MAN	O3-C3-C2	2.40	114.96	110.05
2	B	5	MAN	C1-C2-C3	2.29	112.98	109.64
2	B	2	NAG	C3-C4-C5	-2.08	106.46	110.23
2	B	2	NAG	O4-C4-C3	2.06	115.24	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	O5-C5-C6-O6
2	B	4	MAN	C4-C5-C6-O6
2	B	4	MAN	O5-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	2	NAG	C8-C7-N2-C2
2	B	6	MAN	O5-C5-C6-O6
2	B	2	NAG	O7-C7-N2-C2
2	B	6	MAN	C4-C5-C6-O6

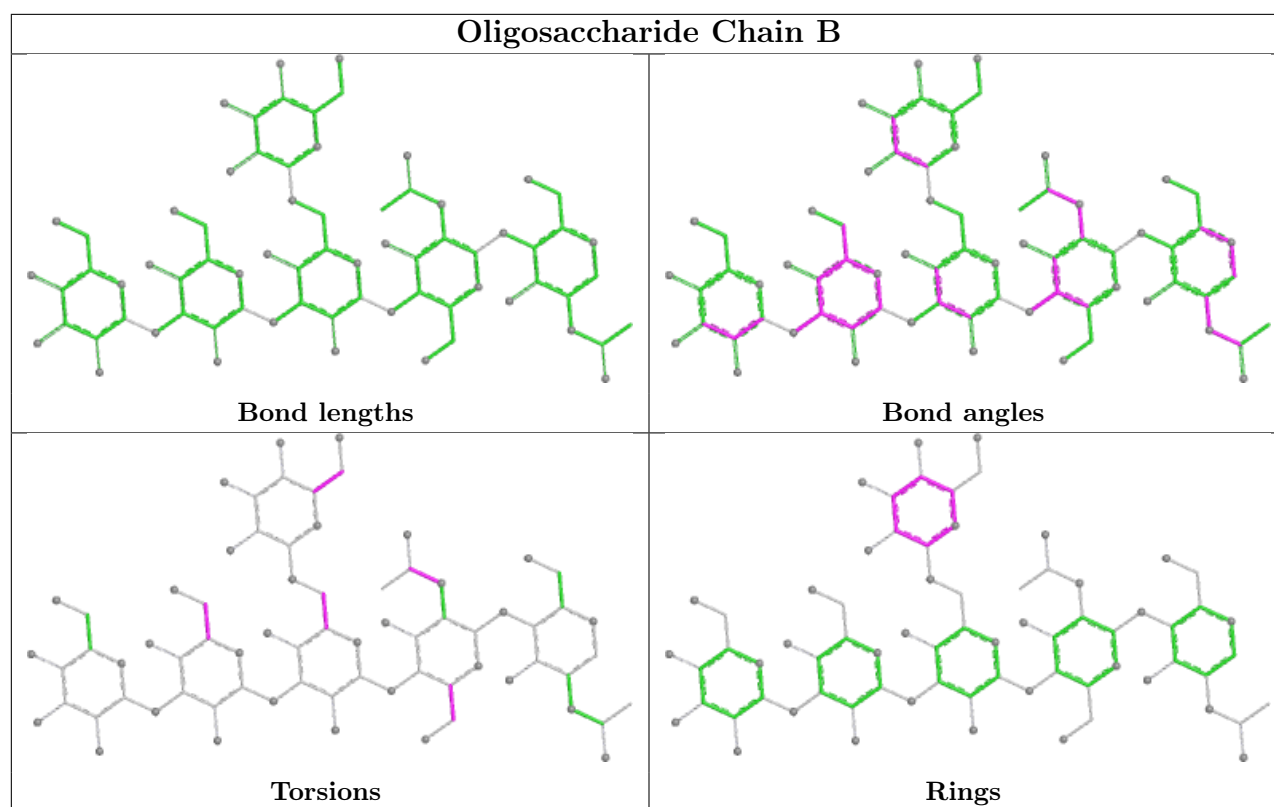
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3	BMA	2	0
2	B	5	MAN	2	0
2	B	2	NAG	4	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](#)

4 ligands 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	GOL	A	509	-	5,5,5	0.33	0	5,5,5	0.72	0
5	GOL	A	510	-	5,5,5	0.39	0	5,5,5	0.41	0
3	NAG	A	507	1	14,14,15	0.65	0	17,19,21	2.03	2 (11%)
4	ATP	A	508	-	32,33,33	1.52	6 (18%)	48,52,52	1.69	10 (20%)

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	509	-	-	2/4/4/4	-
5	GOL	A	510	-	-	2/4/4/4	-
3	NAG	A	507	1	-	4/6/23/26	0/1/1/1
4	ATP	A	508	-	-	2/22/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	508	ATP	C5-C4	5.09	1.48	1.39
4	A	508	ATP	PB-O3A	2.70	1.62	1.59
4	A	508	ATP	C5-C6	2.69	1.48	1.41
4	A	508	ATP	PA-O3A	2.52	1.62	1.59
4	A	508	ATP	C8-N7	2.44	1.36	1.31
4	A	508	ATP	C5-N7	-2.21	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	507	NAG	O5-C1-C2	5.63	120.00	111.29
4	A	508	ATP	C5-C4-N3	-5.53	119.10	126.72
3	A	507	NAG	C1-O5-C5	5.34	119.35	112.19
4	A	508	ATP	N3-C4-N9	4.42	134.69	127.17
4	A	508	ATP	C2-N3-C4	3.69	120.85	111.83
4	A	508	ATP	N3-C2-N1	-3.55	123.21	128.58
4	A	508	ATP	C4-C5-N7	-3.43	106.66	110.58
4	A	508	ATP	C5-N7-C8	2.69	107.68	103.45
4	A	508	ATP	C4-N9-C8	2.65	108.52	105.74
4	A	508	ATP	C6-C5-N7	2.14	136.22	132.09
4	A	508	ATP	C2-N1-C6	2.14	122.24	118.73
4	A	508	ATP	N9-C8-N7	-2.13	110.92	113.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	507	NAG	C8-C7-N2-C2
3	A	507	NAG	O7-C7-N2-C2
4	A	508	ATP	PB-O3B-PG-O3G
5	A	510	GOL	O1-C1-C2-C3
3	A	507	NAG	O5-C5-C6-O6
5	A	509	GOL	O1-C1-C2-C3

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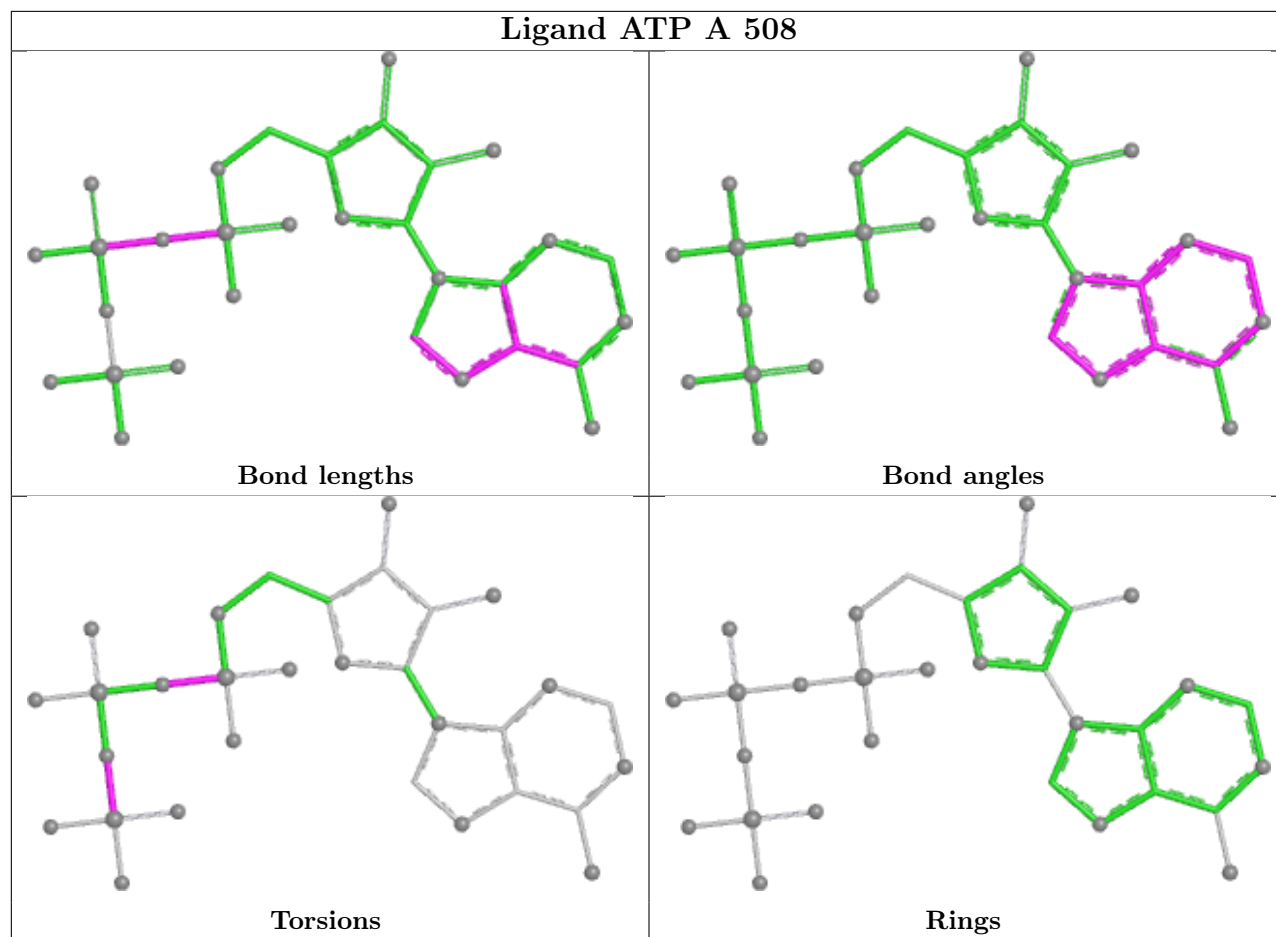
Mol	Chain	Res	Type	Atoms
5	A	509	GOL	O1-C1-C2-O2
5	A	510	GOL	O1-C1-C2-O2
4	A	508	ATP	PB-O3A-PA-O1A
3	A	507	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	GOL	1	0
5	A	510	GOL	1	0
4	A	508	ATP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	324/340 (95%)	0.84	57 (17%) 4 3	56, 77, 181, 204	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	218	THR	5.9
1	A	143	ARG	5.9
1	A	272	TRP	5.8
1	A	348	LEU	5.5
1	A	294	GLY	5.1
1	A	42	VAL	4.8
1	A	43	ILE	4.7
1	A	349	LEU	4.7
1	A	346	LEU	4.4
1	A	130	THR	4.3
1	A	157	ALA	4.1
1	A	351	LEU	4.1
1	A	141	ASP	3.9
1	A	355	ILE	3.8
1	A	359	ILE	3.8
1	A	274	VAL	3.7
1	A	352	VAL	3.7
1	A	173	ILE	3.7
1	A	271	SER	3.6
1	A	59	ASP	3.4
1	A	358	TRP	3.4
1	A	202	ASN	3.3
1	A	155	TYR	3.2
1	A	142	ALA	3.2
1	A	38	THR	3.2
1	A	82	LEU	3.1
1	A	347	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	LEU	3.0
1	A	275	PRO	3.0
1	A	336	ILE	3.0
1	A	54	ASN	3.0
1	A	124	THR	2.9
1	A	174	VAL	2.8
1	A	217	LEU	2.8
1	A	52	VAL	2.7
1	A	37	PHE	2.7
1	A	342	ILE	2.7
1	A	144	GLY	2.6
1	A	289	ASN	2.5
1	A	158	SER	2.4
1	A	53	TYR	2.4
1	A	156	SER	2.3
1	A	133	ARG	2.3
1	A	292	ALA	2.3
1	A	288	ASP	2.3
1	A	350	GLY	2.2
1	A	40	ALA	2.2
1	A	47	ILE	2.2
1	A	309	THR	2.2
1	A	307	ASP	2.1
1	A	80	SER	2.1
1	A	193	LYS	2.1
1	A	301	LYS	2.1
1	A	207	ASN	2.0
1	A	340	LEU	2.0
1	A	79	THR	2.0
1	A	50	VAL	2.0

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

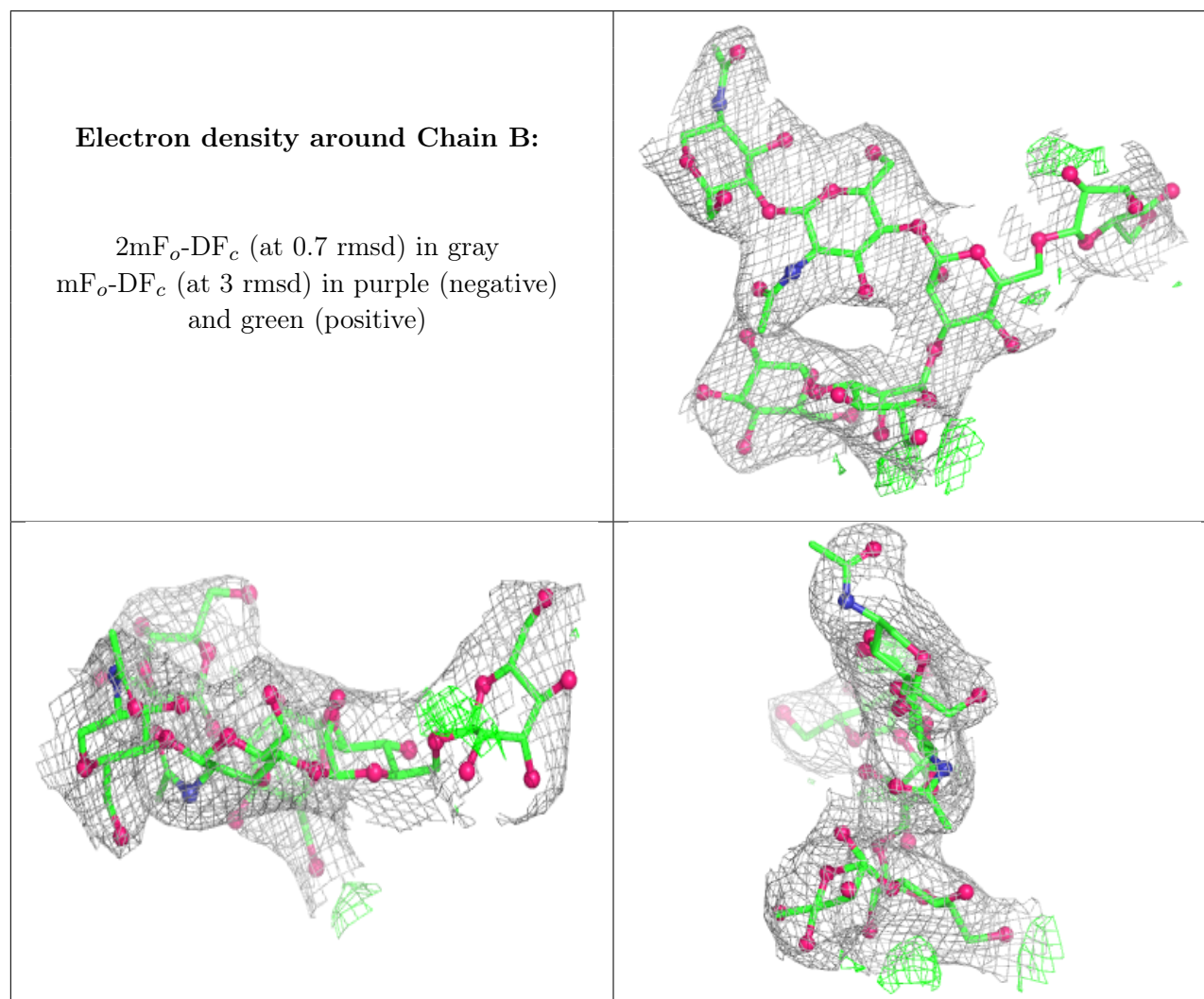
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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($\text{\AA}^2$)	Q<0.9
2	MAN	B	6	11/12	0.53	0.17	121,133,138,143	0
2	BMA	B	3	11/12	0.74	0.14	97,107,117,125	0
2	MAN	B	4	11/12	0.84	0.14	78,89,92,93	0
2	MAN	B	5	11/12	0.93	0.11	73,79,84,84	0
2	NAG	B	2	14/15	0.96	0.08	71,88,92,104	0
2	NAG	B	1	14/15	0.97	0.10	74,83,91,92	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.

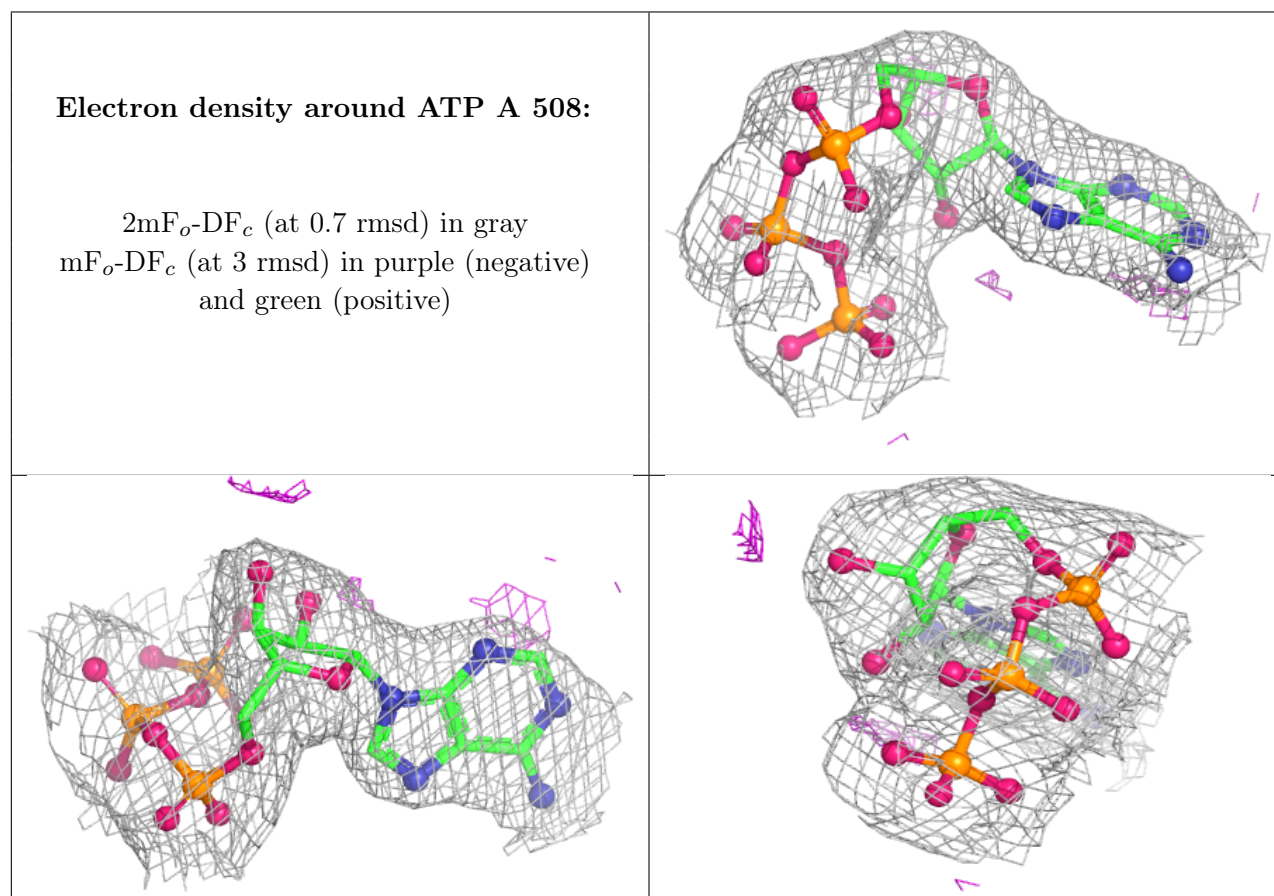


6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	NAG	A	507	14/15	0.29	0.21	107,124,127,127	0
5	GOL	A	510	6/6	0.83	0.19	86,90,95,96	0
5	GOL	A	509	6/6	0.95	0.18	68,71,72,74	0
4	ATP	A	508	31/31	0.98	0.06	58,64,71,74	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.