



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 4MN8 / pdb_00004mn8
Title : Crystal structure of flg22 in complex with the FLS2 and BAK1 ectodomains
Authors : Chai, J.; Sun, Y.; Han, Z.
Deposited on : 2013-09-10
Resolution : 3.06 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

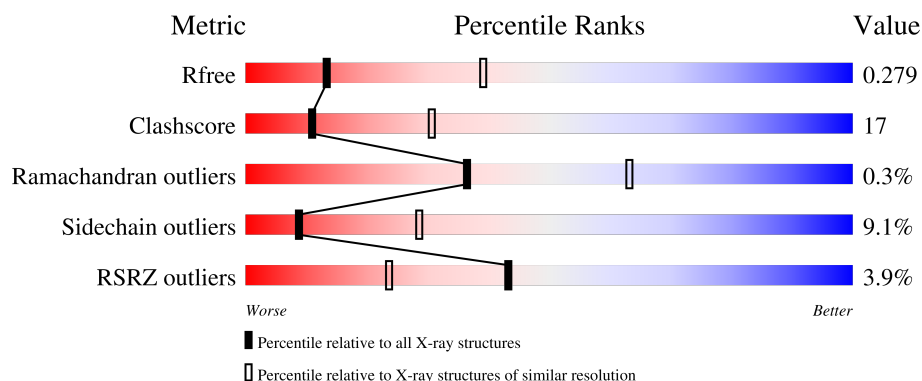
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	782	2% 68% 24% • •
2	B	226	11% 54% 17% 6% 23%
3	C	22	5% 86% 5% 5% 5%
4	D	2	50% 50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7487 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 LRR receptor-like serine/threonine-protein kinase FLS2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	759	Total	C	N	O	S	0	0	0
			5813	3684	969	1138	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	801	HIS	-	expression tag	UNP Q9FL28
A	802	HIS	-	expression tag	UNP Q9FL28
A	803	HIS	-	expression tag	UNP Q9FL28
A	804	HIS	-	expression tag	UNP Q9FL28
A	805	HIS	-	expression tag	UNP Q9FL28
A	806	HIS	-	expression tag	UNP Q9FL28

- Molecule 2 is a protein called BRASSINOSTEROID INSENSITIVE 1-associated receptor kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1287	808	223	253	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	221	HIS	-	expression tag	UNP Q94F62
B	222	HIS	-	expression tag	UNP Q94F62
B	223	HIS	-	expression tag	UNP Q94F62
B	224	HIS	-	expression tag	UNP Q94F62
B	225	HIS	-	expression tag	UNP Q94F62
B	226	HIS	-	expression tag	UNP Q94F62

- Molecule 3 is a protein called flg22.

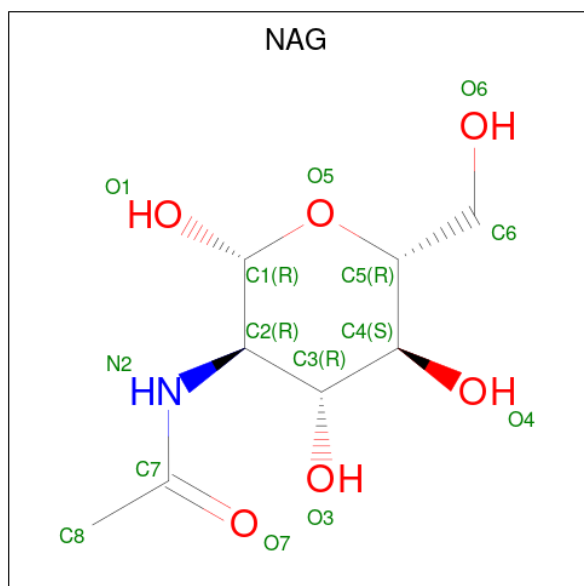
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	0	0	0
			153	90	31	32			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



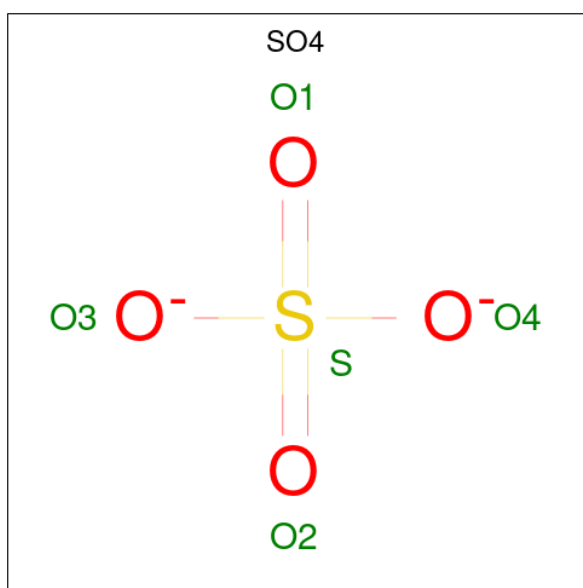
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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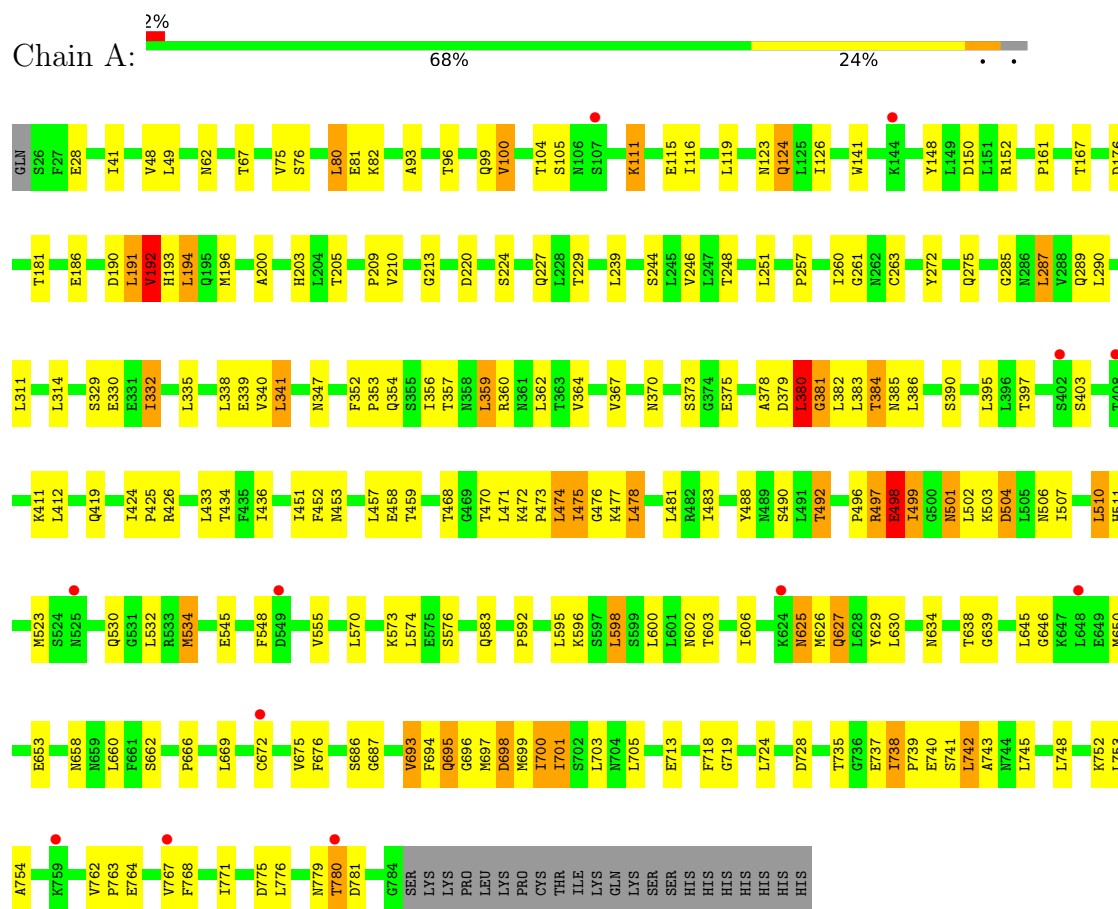
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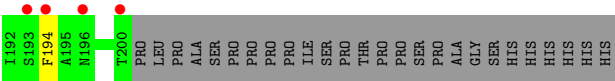
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total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

3 Residue-property plots

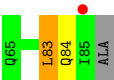
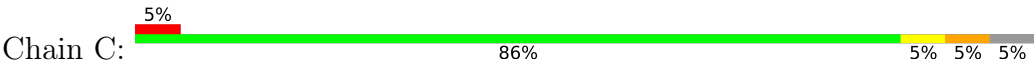
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LRR receptor-like serine/threonine-protein kinase FLS2





● Molecule 3: flg22



● Molecule 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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.86Å 113.68Å 164.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.06 29.96 – 3.06	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.96-3.06) 98.4 (29.96-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.224 , 0.275 0.231 , 0.279	Depositor DCC
R_{free} test set	1932 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	87.7	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7487	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: SO4, 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	A	0.45	1/5910 (0.0%)	0.88	9/8025 (0.1%)
2	B	0.35	0/1307	0.93	6/1789 (0.3%)
3	C	0.28	0/152	0.64	0/202
All	All	0.43	1/7369 (0.0%)	0.89	15/10016 (0.1%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	475	ILE	CA-CB	-5.03	1.47	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	LEU	N-CA-C	-10.03	100.14	112.38
1	A	381	GLY	N-CA-C	-6.96	106.68	114.40
1	A	475	ILE	N-CA-C	-6.42	103.02	111.05
2	B	184	GLY	N-CA-C	6.18	123.19	114.85
1	A	192	VAL	N-CA-C	6.14	116.88	110.62
1	A	475	ILE	CB-CA-C	-5.58	103.51	112.16
1	A	28	GLU	N-CA-C	5.57	120.50	113.25
1	A	695	GLN	N-CA-C	-5.31	105.49	111.28
1	A	498	GLU	N-CA-C	-5.23	106.60	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	THR	CA-C-N	5.21	126.35	119.84
2	B	190	THR	C-N-CA	5.21	126.35	119.84
2	B	177	THR	N-CA-C	5.15	115.62	108.00
2	B	177	THR	CB-CA-C	-5.11	109.19	116.34
2	B	166	LEU	N-CA-C	5.02	118.13	111.30
1	A	780	THR	CB-CA-C	-5.01	110.42	117.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	191	PRO	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	5813	0	5869	219	0
2	B	1287	0	1243	30	0
3	C	153	0	155	1	0
4	D	28	0	25	1	0
5	A	126	0	117	1	0
6	A	60	0	0	2	0
6	B	15	0	0	0	0
6	C	5	0	0	0	0
All	All	7487	0	7409	246	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 17.

All (246) 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:738:ILE:HD13	1:A:738:ILE:C	1.56	1.22
1:A:474:LEU:H	1:A:474:LEU:CD1	1.54	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:N	1:A:474:LEU:HD12	1.52	1.17
1:A:383:LEU:O	1:A:384:THR:HG23	1.45	1.16
1:A:694:PHE:CD1	1:A:718:PHE:HE1	1.63	1.13
1:A:380:LEU:HD13	1:A:380:LEU:O	1.45	1.12
1:A:701:ILE:N	1:A:701:ILE:HD13	1.55	1.10
1:A:700:ILE:C	1:A:701:ILE:HD13	1.79	1.05
1:A:383:LEU:C	1:A:384:THR:HG23	1.83	1.03
1:A:380:LEU:CD1	1:A:380:LEU:C	2.30	1.03
1:A:380:LEU:HD13	1:A:380:LEU:C	1.83	1.02
1:A:694:PHE:HD1	1:A:718:PHE:CE1	1.78	1.02
1:A:738:ILE:C	1:A:738:ILE:CD1	2.30	1.00
1:A:738:ILE:HD13	1:A:738:ILE:O	1.62	0.99
1:A:474:LEU:H	1:A:474:LEU:HD12	0.77	0.92
1:A:694:PHE:CD1	1:A:718:PHE:CE1	2.54	0.89
1:A:738:ILE:HD13	1:A:739:PRO:N	1.88	0.89
1:A:383:LEU:C	1:A:384:THR:CG2	2.42	0.88
1:A:737:GLU:O	1:A:739:PRO:HD3	1.72	0.88
1:A:379:ASP:O	1:A:382:LEU:HB2	1.74	0.87
1:A:699:MET:HG3	2:B:143:ARG:NH1	1.93	0.83
1:A:381:GLY:HA3	1:A:403:SER:O	1.78	0.83
1:A:506:ASN:HD21	1:A:530:GLN:HB2	1.43	0.82
1:A:501:ASN:O	1:A:503:LYS:HG2	1.80	0.81
1:A:699:MET:O	1:A:701:ILE:CD1	2.30	0.79
1:A:473:PRO:HB3	1:A:498:GLU:CG	2.12	0.79
1:A:498:GLU:CA	1:A:498:GLU:OE1	2.30	0.79
1:A:694:PHE:HD1	1:A:718:PHE:HE1	0.86	0.79
1:A:124:GLN:HB3	1:A:148:TYR:HB3	1.65	0.78
1:A:192:VAL:HG12	1:A:193:HIS:ND1	1.98	0.78
1:A:472:LYS:HB3	1:A:474:LEU:CD1	2.14	0.77
1:A:701:ILE:N	1:A:701:ILE:CD1	2.30	0.77
1:A:738:ILE:CD1	1:A:738:ILE:O	2.30	0.77
1:A:506:ASN:ND2	1:A:530:GLN:HB2	2.02	0.74
1:A:360:ARG:O	1:A:385:ASN:ND2	2.21	0.73
1:A:473:PRO:HB3	1:A:498:GLU:HG3	1.67	0.73
1:A:380:LEU:C	1:A:380:LEU:HD12	2.14	0.72
1:A:472:LYS:HB2	1:A:474:LEU:HD13	1.71	0.72
1:A:473:PRO:CB	1:A:498:GLU:HG3	2.19	0.72
1:A:473:PRO:CA	1:A:498:GLU:HG3	2.19	0.72
1:A:603:THR:HG23	1:A:629:TYR:HB3	1.71	0.72
1:A:738:ILE:HD13	1:A:739:PRO:C	2.15	0.72
2:B:161:THR:HG21	2:B:183:ASN:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:LEU:O	1:A:384:THR:CG2	2.30	0.70
1:A:532:LEU:HD11	1:A:534:MET:HE3	1.71	0.70
1:A:700:ILE:HG22	1:A:700:ILE:O	1.91	0.70
1:A:382:LEU:O	1:A:384:THR:HG22	1.92	0.70
1:A:472:LYS:CB	1:A:474:LEU:HD13	2.22	0.69
1:A:433:LEU:HD13	1:A:436:ILE:HD11	1.74	0.69
1:A:697:MET:HB3	1:A:700:ILE:HD12	1.73	0.69
1:A:475:ILE:HG23	1:A:476:GLY:N	2.06	0.69
1:A:380:LEU:O	1:A:380:LEU:CD1	2.29	0.68
1:A:694:PHE:HE1	1:A:703:LEU:HD21	1.58	0.68
1:A:694:PHE:CE1	1:A:703:LEU:HD21	2.29	0.67
2:B:72:ARG:NH2	2:B:74:ASP:OD1	2.27	0.67
1:A:473:PRO:HA	1:A:498:GLU:HG2	1.77	0.66
1:A:669:LEU:HD13	1:A:697:MET:HE1	1.77	0.66
1:A:738:ILE:CD1	1:A:739:PRO:C	2.67	0.66
1:A:473:PRO:HA	1:A:498:GLU:CG	2.26	0.66
1:A:627:GLN:HG2	2:B:72:ARG:HH22	1.60	0.66
1:A:669:LEU:CD1	1:A:697:MET:HE1	2.26	0.66
1:A:472:LYS:CB	1:A:474:LEU:CD1	2.75	0.65
1:A:498:GLU:OE1	1:A:498:GLU:HA	1.97	0.64
1:A:453:ASN:OD1	1:A:477:LYS:NZ	2.30	0.64
1:A:472:LYS:HB3	1:A:474:LEU:HD11	1.78	0.64
1:A:475:ILE:CG2	1:A:476:GLY:N	2.60	0.64
1:A:698:ASP:OD1	1:A:698:ASP:N	2.30	0.64
1:A:498:GLU:OE1	1:A:498:GLU:N	2.30	0.63
1:A:738:ILE:HD13	1:A:739:PRO:CA	2.28	0.63
1:A:473:PRO:CA	1:A:498:GLU:CG	2.76	0.63
2:B:63:THR:HG23	2:B:72:ARG:HB2	1.80	0.63
1:A:458:GLU:HA	1:A:481:LEU:HA	1.81	0.63
1:A:502:LEU:O	1:A:503:LYS:HB2	1.97	0.62
1:A:740:GLU:O	1:A:741:SER:C	2.39	0.62
1:A:340:VAL:HG13	1:A:364:VAL:HB	1.82	0.61
1:A:257:PRO:HG2	1:A:260:ILE:HG12	1.80	0.61
1:A:381:GLY:CA	1:A:403:SER:O	2.48	0.61
2:B:105:THR:HG22	2:B:127:ASN:HB3	1.81	0.61
1:A:473:PRO:CB	1:A:498:GLU:CG	2.79	0.60
1:A:483:ILE:HG22	1:A:507:ILE:HB	1.82	0.60
1:A:666:PRO:HG2	1:A:669:LEU:HD23	1.84	0.60
1:A:676:PHE:HD1	1:A:701:ILE:HD11	1.67	0.59
1:A:359:LEU:HD12	1:A:362:LEU:HD22	1.84	0.59
1:A:196:MET:HG2	1:A:220:ASP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:THR:HA	2:B:185:SER:HB2	1.84	0.59
1:A:397:THR:HG22	1:A:419:GLN:HB2	1.83	0.59
1:A:474:LEU:O	1:A:477:LYS:HB2	2.02	0.59
1:A:699:MET:O	1:A:701:ILE:HD11	2.01	0.58
1:A:100:VAL:HB	1:A:124:GLN:HG3	1.84	0.58
1:A:473:PRO:O	1:A:498:GLU:HG3	2.02	0.58
1:A:364:VAL:HG11	4:D:1:NAG:H82	1.84	0.57
2:B:140:LYS:HD3	2:B:163:VAL:HG12	1.87	0.57
1:A:576:SER:HA	1:A:600:LEU:HD12	1.87	0.56
1:A:693:VAL:HG13	1:A:694:PHE:HD2	1.70	0.56
1:A:693:VAL:HG13	1:A:694:PHE:CD2	2.41	0.55
1:A:426:ARG:NH1	6:A:920:SO4:O4	2.38	0.55
1:A:41:ILE:HD12	1:A:49:LEU:HD11	1.87	0.55
1:A:335:LEU:HD12	1:A:338:LEU:HD22	1.89	0.55
1:A:496:PRO:HB2	1:A:498:GLU:HG2	1.89	0.55
1:A:148:TYR:HE1	1:A:150:ASP:HB2	1.69	0.55
1:A:224:SER:HB3	1:A:246:VAL:HG12	1.89	0.54
1:A:329:SER:O	1:A:332:ILE:HG13	2.06	0.54
1:A:740:GLU:O	1:A:743:ALA:N	2.38	0.54
1:A:694:PHE:CE1	1:A:718:PHE:CE1	2.96	0.54
1:A:754:ALA:N	1:A:775:ASP:O	2.36	0.54
1:A:338:LEU:HD21	1:A:341:LEU:HG	1.90	0.54
1:A:126:ILE:HG23	1:A:150:ASP:HB3	1.90	0.54
1:A:360:ARG:NH2	1:A:382:LEU:HD13	2.22	0.54
1:A:382:LEU:O	1:A:384:THR:CG2	2.56	0.54
1:A:285:GLY:HA2	1:A:311:LEU:HD21	1.89	0.53
1:A:378:ALA:O	1:A:379:ASP:HB2	2.06	0.53
2:B:135:THR:O	2:B:138:ARG:HG2	2.09	0.53
1:A:625:ASN:OD1	1:A:625:ASN:N	2.41	0.53
1:A:379:ASP:C	1:A:381:GLY:N	2.62	0.53
2:B:182:VAL:O	2:B:184:GLY:N	2.42	0.52
1:A:686:SER:OG	1:A:687:GLY:N	2.42	0.52
1:A:699:MET:O	1:A:701:ILE:HD13	2.08	0.52
1:A:474:LEU:O	1:A:477:LYS:N	2.30	0.52
1:A:698:ASP:OD2	2:B:167:GLN:NE2	2.43	0.52
2:B:186:PHE:HD1	2:B:194:PHE:HZ	1.58	0.52
1:A:468:THR:HA	1:A:490:SER:O	2.10	0.51
1:A:473:PRO:HB3	1:A:498:GLU:OE2	2.09	0.51
1:A:452:PHE:HE1	1:A:475:ILE:HD12	1.75	0.51
1:A:638:THR:HG22	1:A:660:LEU:HB2	1.92	0.51
1:A:502:LEU:N	1:A:502:LEU:HD23	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:HD11	3:C:83:LEU:HD21	1.93	0.51
1:A:478:LEU:CD1	1:A:481:LEU:HD22	2.40	0.50
1:A:738:ILE:HD11	1:A:739:PRO:C	2.37	0.50
2:B:32:LEU:HD21	2:B:91:LEU:HD11	1.93	0.50
2:B:109:PRO:HB2	2:B:111:GLN:HG2	1.93	0.50
1:A:287:LEU:O	1:A:311:LEU:HD22	2.12	0.49
1:A:383:LEU:O	1:A:385:ASN:N	2.42	0.49
1:A:696:GLY:O	1:A:698:ASP:OD1	2.30	0.49
1:A:602:ASN:ND2	6:A:911:SO4:O3	2.43	0.49
1:A:498:GLU:N	1:A:498:GLU:CD	2.69	0.49
2:B:85:VAL:HG13	2:B:87:GLN:H	1.77	0.49
1:A:115:GLU:OE2	1:A:115:GLU:N	2.44	0.48
2:B:142:LEU:O	2:B:165:THR:HB	2.13	0.48
1:A:676:PHE:HB3	1:A:701:ILE:HG12	1.94	0.48
2:B:95:GLN:HA	2:B:118:LEU:HA	1.95	0.48
2:B:134:SER:HA	2:B:157:PRO:HB3	1.95	0.48
1:A:473:PRO:C	1:A:498:GLU:HG3	2.39	0.48
1:A:646:GLY:HA2	1:A:669:LEU:HA	1.96	0.48
1:A:93:ALA:HA	1:A:119:LEU:HD21	1.96	0.47
1:A:504:ASP:OD1	1:A:504:ASP:N	2.32	0.47
1:A:548:PHE:HA	1:A:574:LEU:HD21	1.96	0.47
2:B:183:ASN:O	2:B:183:ASN:ND2	2.47	0.47
1:A:738:ILE:HD11	1:A:739:PRO:O	2.14	0.47
1:A:190:ASP:O	1:A:192:VAL:N	2.47	0.47
1:A:186:GLU:HA	1:A:209:PRO:HB3	1.96	0.47
1:A:497:ARG:C	1:A:499:ILE:N	2.72	0.47
1:A:181:THR:HG22	1:A:203:HIS:HB2	1.97	0.47
1:A:475:ILE:HG13	1:A:475:ILE:O	2.14	0.47
1:A:545:GLU:HG2	1:A:570:LEU:HD13	1.97	0.47
1:A:548:PHE:HB3	1:A:573:LYS:HB2	1.96	0.47
1:A:176:ASP:OD1	1:A:200:ALA:N	2.48	0.47
1:A:738:ILE:HD11	1:A:763:PRO:HG2	1.96	0.47
1:A:474:LEU:O	1:A:475:ILE:C	2.58	0.47
1:A:740:GLU:O	1:A:742:LEU:N	2.47	0.47
2:B:61:HIS:HB3	2:B:74:ASP:O	2.15	0.47
1:A:380:LEU:C	1:A:382:LEU:N	2.73	0.46
1:A:697:MET:HB3	1:A:700:ILE:CD1	2.44	0.46
2:B:169:LEU:HD11	2:B:171:LEU:HB3	1.96	0.46
1:A:676:PHE:CD1	1:A:701:ILE:HD11	2.49	0.46
2:B:85:VAL:HG13	2:B:87:GLN:N	2.31	0.46
1:A:357:THR:HA	1:A:383:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:THR:O	1:A:457:LEU:HD12	2.16	0.46
1:A:510:LEU:HD21	1:A:534:MET:HE2	1.97	0.46
1:A:629:TYR:HD1	1:A:653:GLU:HB2	1.81	0.46
1:A:99:GLN:O	1:A:123:ASN:N	2.44	0.46
1:A:474:LEU:C	1:A:476:GLY:N	2.69	0.46
1:A:80:LEU:HD23	1:A:104:THR:HB	1.97	0.46
1:A:738:ILE:CD1	1:A:763:PRO:HG2	2.46	0.45
1:A:205:THR:HG22	1:A:227:GLN:HB2	1.98	0.45
1:A:191:LEU:HD13	1:A:191:LEU:HA	1.37	0.45
1:A:354:GLN:NE2	1:A:375:GLU:O	2.45	0.45
1:A:473:PRO:HB3	1:A:498:GLU:CD	2.42	0.45
1:A:141:TRP:NE1	1:A:161:PRO:HG2	2.32	0.45
1:A:598:LEU:H	1:A:598:LEU:HG	1.69	0.45
1:A:626:MET:HE1	1:A:630:LEU:HB2	1.99	0.45
1:A:719:GLY:HA3	1:A:741:SER:HB3	1.99	0.44
1:A:67:THR:OG1	1:A:76:SER:HB3	2.17	0.44
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.67	0.44
1:A:738:ILE:CD1	1:A:763:PRO:CG	2.95	0.44
1:A:384:THR:OG1	1:A:385:ASN:N	2.49	0.44
1:A:213:GLY:HA2	1:A:239:LEU:HD21	2.00	0.44
2:B:147:LEU:O	2:B:150:ASN:ND2	2.50	0.44
1:A:523:MET:HE3	1:A:523:MET:HB2	1.79	0.44
2:B:94:LEU:HD11	2:B:97:LEU:HD13	2.00	0.44
1:A:728:ASP:HA	1:A:752:LYS:HB2	1.99	0.43
1:A:459:THR:HG23	1:A:483:ILE:HG13	2.00	0.43
1:A:694:PHE:CE1	1:A:703:LEU:CD2	2.99	0.43
1:A:776:LEU:O	1:A:779:ASN:HB2	2.18	0.43
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.92	0.43
1:A:488:TYR:CE2	1:A:511:HIS:HE1	2.36	0.43
1:A:506:ASN:HD21	1:A:530:GLN:CB	2.22	0.43
1:A:196:MET:HE2	1:A:196:MET:HB3	1.82	0.43
2:B:117:GLU:HA	2:B:141:LYS:HG3	2.01	0.43
1:A:452:PHE:CD1	1:A:475:ILE:HA	2.53	0.42
1:A:501:ASN:OD1	1:A:501:ASN:N	2.49	0.42
1:A:627:GLN:HA	1:A:650:MET:O	2.19	0.42
1:A:499:ILE:HG21	1:A:523:MET:HE2	2.01	0.42
1:A:48:VAL:HG21	1:A:82:LYS:HD2	2.01	0.42
1:A:152:ARG:HG2	1:A:176:ASP:H	1.83	0.42
1:A:380:LEU:HD12	1:A:381:GLY:N	2.34	0.42
1:A:738:ILE:HD12	1:A:763:PRO:CG	2.49	0.42
1:A:748:LEU:HB3	1:A:767:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LYS:HB3	1:A:411:LYS:HE2	1.89	0.42
1:A:470:THR:HA	1:A:492:THR:O	2.19	0.42
2:B:71:THR:O	2:B:94:LEU:HD23	2.19	0.42
1:A:380:LEU:C	1:A:382:LEU:H	2.26	0.42
1:A:768:PHE:HA	1:A:771:ILE:HB	2.01	0.42
1:A:497:ARG:C	1:A:499:ILE:H	2.26	0.42
1:A:634:ASN:OD1	1:A:658:ASN:ND2	2.49	0.42
1:A:81:GLU:HG3	1:A:105:SER:HB3	2.01	0.42
1:A:248:THR:HG22	1:A:272:TYR:N	2.35	0.42
1:A:373:SER:HB3	1:A:395:LEU:HB2	2.02	0.42
1:A:645:LEU:HD23	1:A:669:LEU:HD22	2.02	0.42
1:A:111:LYS:HE2	1:A:111:LYS:HB3	1.86	0.41
1:A:148:TYR:CE1	1:A:150:ASP:HB2	2.53	0.41
1:A:152:ARG:HG2	1:A:176:ASP:HB2	2.02	0.41
1:A:352:PHE:CG	1:A:353:PRO:HD2	2.55	0.41
1:A:699:MET:HG3	2:B:143:ARG:HH12	1.79	0.41
1:A:263:CYS:O	1:A:287:LEU:HD22	2.20	0.41
1:A:339:GLU:O	1:A:362:LEU:HD12	2.21	0.41
2:B:132:ILE:HG12	2:B:152:LEU:HD23	2.03	0.41
1:A:48:VAL:HG21	1:A:82:LYS:HB3	2.02	0.41
1:A:229:THR:HG22	1:A:251:LEU:HB2	2.02	0.41
1:A:510:LEU:HD11	1:A:534:MET:HE2	2.01	0.41
1:A:675:VAL:HB	1:A:697:MET:HG2	2.03	0.41
1:A:379:ASP:C	1:A:381:GLY:H	2.29	0.41
1:A:740:GLU:C	1:A:742:LEU:N	2.78	0.41
1:A:311:LEU:HB2	1:A:314:LEU:HG	2.02	0.41
1:A:330:GLU:OE1	1:A:354:GLN:N	2.53	0.41
1:A:367:VAL:O	1:A:370:ASN:ND2	2.52	0.41
1:A:424:ILE:HA	1:A:425:PRO:HD3	1.94	0.41
1:A:506:ASN:ND2	1:A:530:GLN:CB	2.79	0.41
1:A:472:LYS:HA	1:A:473:PRO:HD3	1.94	0.40
1:A:639:GLY:O	1:A:662:SER:N	2.38	0.40
1:A:452:PHE:CE1	1:A:475:ILE:HA	2.56	0.40
1:A:713:GLU:OE2	1:A:713:GLU:N	2.53	0.40
5:A:904:NAG:H83	5:A:904:NAG:H2	1.84	0.40
2:B:124:TYR:HA	2:B:150:ASN:HD21	1.86	0.40
1:A:592:PRO:HG2	1:A:595:LEU:HG	2.02	0.40
2:B:149:ASN:H	2:B:173:ASN:HB2	1.86	0.40
1:A:261:GLY:HA2	1:A:287:LEU:HD21	2.03	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	757/782 (97%)	707 (93%)	50 (7%)	0	100	100
2	B	173/226 (76%)	153 (88%)	17 (10%)	3 (2%)	7	25
3	C	19/22 (86%)	19 (100%)	0	0	100	100
All	All	949/1030 (92%)	879 (93%)	67 (7%)	3 (0%)	36	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	191	PRO
2	B	183	ASN
2	B	190	THR

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	676/699 (97%)	614 (91%)	62 (9%)	8	28
2	B	139/203 (68%)	127 (91%)	12 (9%)	10	31
3	C	16/16 (100%)	14 (88%)	2 (12%)	4	16
All	All	831/918 (90%)	755 (91%)	76 (9%)	9	28

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	75	VAL
1	A	80	LEU
1	A	96	THR
1	A	100	VAL
1	A	111	LYS
1	A	116	ILE
1	A	124	GLN
1	A	167	THR
1	A	191	LEU
1	A	192	VAL
1	A	194	LEU
1	A	210	VAL
1	A	244	SER
1	A	275	GLN
1	A	287	LEU
1	A	289	GLN
1	A	332	ILE
1	A	341	LEU
1	A	347	ASN
1	A	356	ILE
1	A	359	LEU
1	A	380	LEU
1	A	384	THR
1	A	386	LEU
1	A	390	SER
1	A	451	ILE
1	A	471	LEU
1	A	474	LEU
1	A	478	LEU
1	A	492	THR
1	A	497	ARG
1	A	498	GLU
1	A	499	ILE
1	A	501	ASN
1	A	504	ASP
1	A	510	LEU
1	A	534	MET
1	A	555	VAL
1	A	583	GLN
1	A	596	LYS
1	A	598	LEU
1	A	606	ILE

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Mol	Chain	Res	Type
1	A	625	ASN
1	A	627	GLN
1	A	672	CYS
1	A	693	VAL
1	A	695	GLN
1	A	698	ASP
1	A	700	ILE
1	A	701	ILE
1	A	705	LEU
1	A	724	LEU
1	A	735	THR
1	A	738	ILE
1	A	742	LEU
1	A	745	LEU
1	A	753	LEU
1	A	762	VAL
1	A	764	GLU
1	A	780	THR
1	A	781	ASP
2	B	63	THR
2	B	85	VAL
2	B	94	LEU
2	B	111	GLN
2	B	116	THR
2	B	123	LEU
2	B	135	THR
2	B	139	LEU
2	B	142	LEU
2	B	149	ASN
2	B	165	THR
2	B	171	LEU
3	C	83	LEU
3	C	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	286	ASN
1	A	506	ASN
1	A	511	HIS
1	A	530	GLN

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Mol	Chain	Res	Type
1	A	720	ASN
2	B	148	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	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.64	0	17,19,21	0.66	0
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	0.78	0

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
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

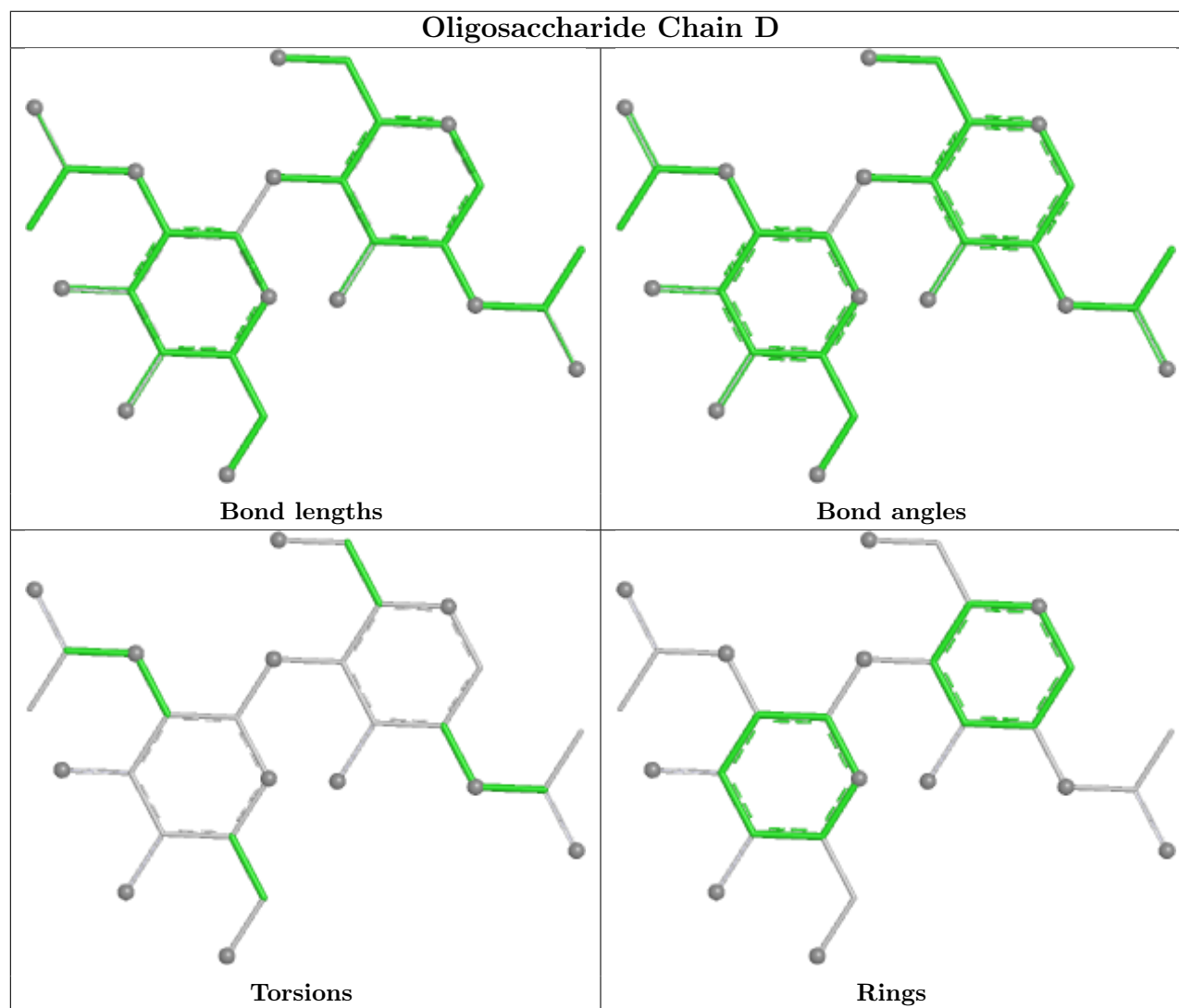
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1	NAG	1	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](#)

25 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	NAG	A	901	1	14,14,15	0.48	0	17,19,21	1.18	1 (5%)
5	NAG	A	904	1	14,14,15	0.41	0	17,19,21	1.92	3 (17%)
6	SO4	B	302	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	A	922	-	4,4,4	0.23	0	6,6,6	0.09	0
5	NAG	A	923	-	14,14,15	0.67	0	19,19,21	1.21	3 (15%)
6	SO4	A	911	-	4,4,4	0.24	0	6,6,6	0.12	0
6	SO4	A	920	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	916	-	4,4,4	0.23	0	6,6,6	0.09	0
6	SO4	A	917	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	A	903	1	14,14,15	0.51	0	17,19,21	0.78	0
6	SO4	A	912	-	4,4,4	0.24	0	6,6,6	0.11	0
6	SO4	A	913	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	A	905	1	14,14,15	0.60	0	17,19,21	0.96	0
6	SO4	B	301	-	4,4,4	0.24	0	6,6,6	0.09	0
6	SO4	A	915	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	919	-	4,4,4	0.22	0	6,6,6	0.12	0
6	SO4	A	914	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	A	921	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	B	303	-	4,4,4	0.23	0	6,6,6	0.08	0
5	NAG	A	902	1	14,14,15	0.46	0	17,19,21	0.89	1 (5%)
5	NAG	A	906	1	14,14,15	0.51	0	17,19,21	0.76	0
6	SO4	A	918	-	4,4,4	0.24	0	6,6,6	0.08	0
5	NAG	A	910	1	14,14,15	0.57	0	17,19,21	1.05	2 (11%)
5	NAG	A	909	-	14,14,15	0.49	0	17,19,21	0.73	0
6	SO4	C	101	-	4,4,4	0.24	0	6,6,6	0.06	0

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	923	-	-	4/6/22/26	0/1/1/1
5	NAG	A	906	1	-	0/6/23/26	0/1/1/1
5	NAG	A	903	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	901	1	-	3/6/23/26	0/1/1/1
5	NAG	A	904	1	-	4/6/23/26	0/1/1/1
5	NAG	A	905	1	-	3/6/23/26	0/1/1/1
5	NAG	A	910	1	-	2/6/23/26	0/1/1/1
5	NAG	A	909	-	-	2/6/23/26	0/1/1/1
5	NAG	A	902	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	904	NAG	C1-O5-C5	6.49	120.88	112.19
5	A	901	NAG	C1-O5-C5	3.75	117.21	112.19
5	A	923	NAG	C3-C4-C5	2.60	115.58	111.19
5	A	923	NAG	O5-C5-C4	2.51	113.97	110.14
5	A	910	NAG	C1-O5-C5	2.50	115.53	112.19
5	A	904	NAG	C4-C3-C2	-2.31	107.63	111.02
5	A	904	NAG	O5-C5-C4	2.27	116.35	110.83
5	A	910	NAG	O5-C1-C2	2.21	114.71	111.29
5	A	923	NAG	C4-C5-C6	-2.06	108.67	112.50
5	A	902	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	NAG	C3-C2-N2-C7
5	A	901	NAG	C8-C7-N2-C2
5	A	901	NAG	O7-C7-N2-C2
5	A	902	NAG	C3-C2-N2-C7
5	A	902	NAG	C8-C7-N2-C2
5	A	902	NAG	O7-C7-N2-C2
5	A	904	NAG	C8-C7-N2-C2
5	A	904	NAG	O7-C7-N2-C2
5	A	905	NAG	C3-C2-N2-C7
5	A	905	NAG	C8-C7-N2-C2
5	A	905	NAG	O7-C7-N2-C2
5	A	909	NAG	C8-C7-N2-C2
5	A	909	NAG	O7-C7-N2-C2
5	A	923	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	923	NAG	O5-C5-C6-O6
5	A	910	NAG	C8-C7-N2-C2
5	A	910	NAG	O7-C7-N2-C2
5	A	904	NAG	O5-C5-C6-O6
5	A	902	NAG	O5-C5-C6-O6
5	A	904	NAG	C4-C5-C6-O6
5	A	903	NAG	C8-C7-N2-C2
5	A	923	NAG	C8-C7-N2-C2
5	A	903	NAG	O7-C7-N2-C2
5	A	923	NAG	O7-C7-N2-C2
5	A	902	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	904	NAG	1	0
6	A	911	SO4	1	0
6	A	920	SO4	1	0

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	759/782 (97%)	0.06	12 (1%) 70 47	53, 87, 141, 187	0
2	B	175/226 (77%)	0.62	24 (13%) 6 4	66, 120, 195, 239	0
3	C	21/22 (95%)	0.81	1 (4%) 35 18	77, 108, 143, 166	0
All	All	955/1030 (92%)	0.18	37 (3%) 43 23	53, 91, 154, 239	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	151	SER	5.3
2	B	200	THR	5.0
2	B	179	ASP	4.8
1	A	549	ASP	4.0
2	B	180	ILE	3.9
2	B	188	LEU	3.7
3	C	85	ILE	3.4
2	B	129	SER	3.3
2	B	174	ASN	3.3
2	B	181	PRO	3.3
2	B	190	THR	3.2
2	B	161	THR	3.1
2	B	150	ASN	3.0
2	B	187	SER	3.0
1	A	780	THR	2.9
2	B	196	ASN	2.8
1	A	144	LYS	2.7
2	B	163	VAL	2.6
2	B	185	SER	2.6
2	B	194	PHE	2.6
1	A	402	SER	2.6
1	A	767	VAL	2.5
1	A	408	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	145	LEU	2.5
2	B	164	LEU	2.5
1	A	648	LEU	2.4
2	B	182	VAL	2.4
1	A	759	LYS	2.3
1	A	525	ASN	2.2
2	B	153	SER	2.1
2	B	193	SER	2.1
1	A	107	SER	2.1
1	A	672	CYS	2.1
2	B	178	GLY	2.1
2	B	167	GLN	2.0
2	B	184	GLY	2.0
1	A	624	LYS	2.0

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

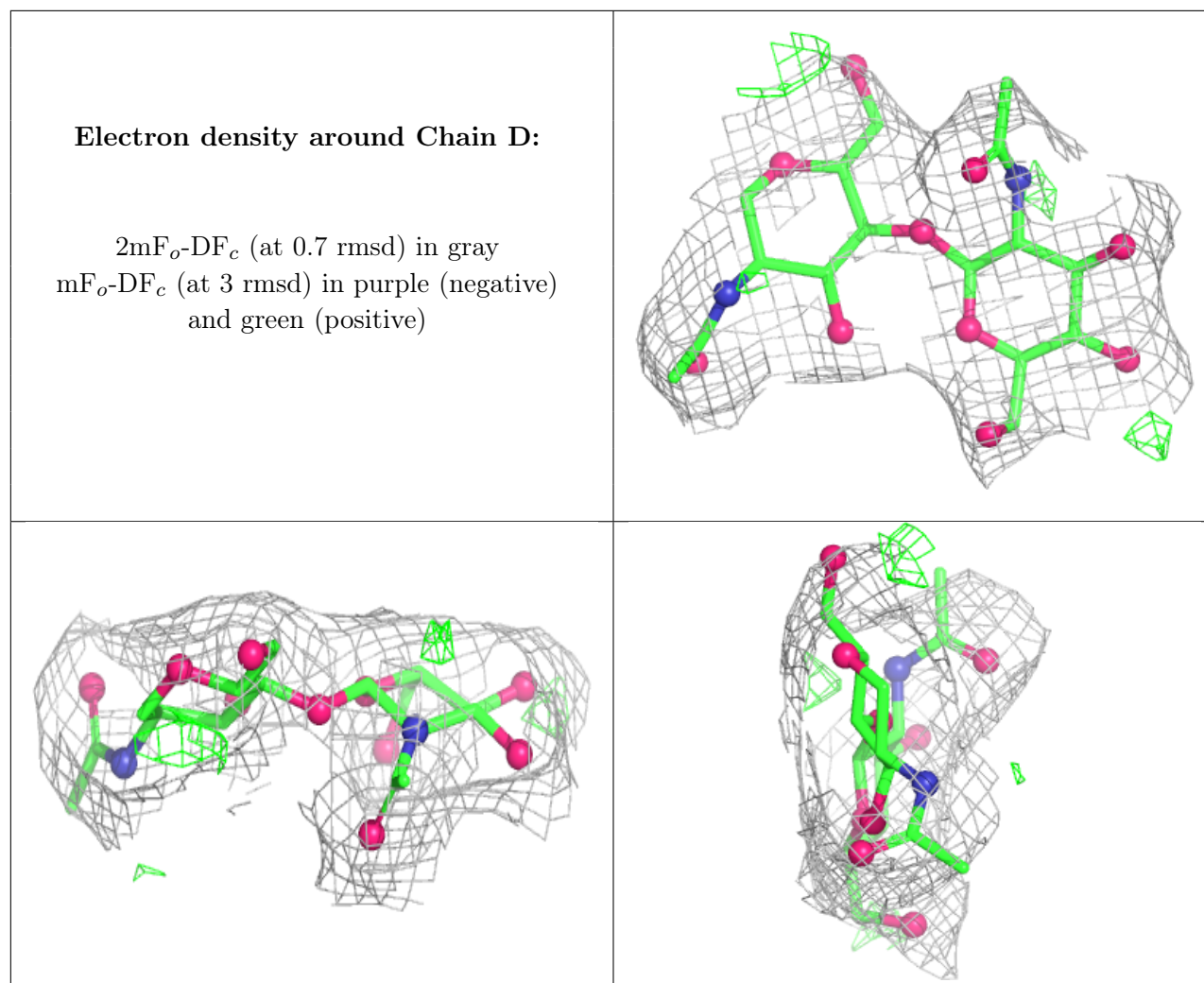
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
4	NAG	D	2	14/15	0.85	0.11	100,119,125,126	0
4	NAG	D	1	14/15	0.97	0.07	65,72,91,96	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](#)

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
5	NAG	A	901	14/15	0.62	0.20	125,136,156,159	0
5	NAG	A	910	14/15	0.64	0.19	91,115,135,141	0
6	SO4	A	918	5/5	0.64	0.12	170,170,172,178	0
6	SO4	B	303	5/5	0.64	0.20	159,164,165,170	0
6	SO4	A	912	5/5	0.69	0.16	94,115,126,139	0
5	NAG	A	923	14/15	0.70	0.15	75,121,129,134	0
6	SO4	A	922	5/5	0.70	0.11	196,202,207,212	0
5	NAG	A	904	14/15	0.70	0.13	73,90,104,111	0
6	SO4	B	301	5/5	0.76	0.14	132,135,139,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	A	919	5/5	0.76	0.16	120,126,135,148	0
6	SO4	A	913	5/5	0.77	0.06	166,172,174,178	0
6	SO4	A	921	5/5	0.78	0.10	173,174,175,179	0
6	SO4	A	917	5/5	0.78	0.08	175,178,179,183	0
6	SO4	A	916	5/5	0.79	0.29	132,138,141,145	0
5	NAG	A	905	14/15	0.79	0.15	101,111,125,130	0
5	NAG	A	906	14/15	0.81	0.31	20,20,20,20	0
5	NAG	A	909	14/15	0.81	0.13	128,135,153,158	0
5	NAG	A	902	14/15	0.85	0.15	111,141,149,157	0
6	SO4	A	914	5/5	0.86	0.12	128,140,141,144	0
6	SO4	B	302	5/5	0.86	0.23	133,153,160,160	0
6	SO4	A	920	5/5	0.86	0.10	146,152,158,160	0
5	NAG	A	903	14/15	0.88	0.15	110,122,136,138	0
6	SO4	C	101	5/5	0.88	0.14	124,131,133,143	0
6	SO4	A	915	5/5	0.91	0.22	111,121,123,125	0
6	SO4	A	911	5/5	0.94	0.12	102,112,115,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.