



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:42 PM UTC

PDB ID : 5GZV / pdb_00005gzv
Title : Crystal Structure of Chitinase ChiW from *Paenibacillus* sp. str. FPU-7 Reveals a Novel Type of Bacterial Cell-Surface-Expressed Multi-Modular Enzyme Machinery
Authors : Itoh, T.; Hibi, T.; Suzuki, F.; Sugimoto, I.; Fujiwara, A.; Inaka, K.; Tanaka, H.; Ohta, K.; Fujii, Y.; Taketo, A.; Kimoto, H.
Deposited on : 2016-10-01
Resolution : 2.61 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

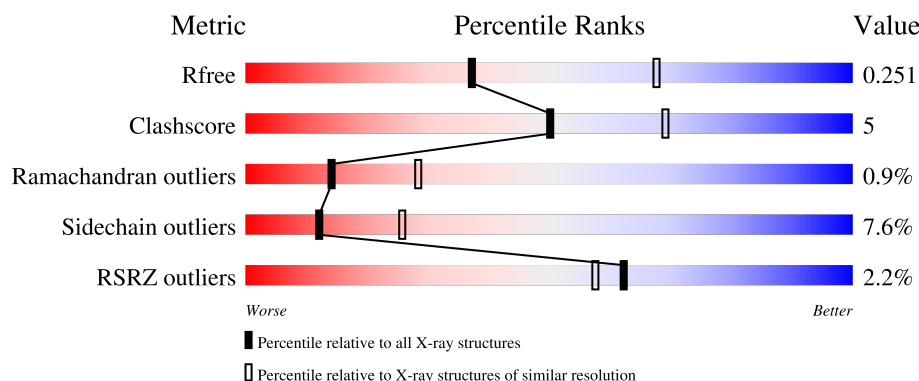
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	885	% 80% 15% ..
1	B	885	3% 77% 17% ..
2	C	2	100%
2	D	2	100%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13773 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 Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	3	0
			6762	4324	1112	1314	12			
1	B	859	Total	C	N	O	S	0	1	0
			6741	4310	1108	1311	12			

There are 46 discrepancies between the modelled and reference sequences:

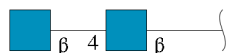
Chain	Residue	Modelled	Actual	Comment	Reference
A	534	MET	-	initiating methionine	UNP K7ZLW6
A	535	ASN	-	expression tag	UNP K7ZLW6
A	536	HIS	-	expression tag	UNP K7ZLW6
A	537	LYS	-	expression tag	UNP K7ZLW6
A	538	VAL	-	expression tag	UNP K7ZLW6
A	539	HIS	-	expression tag	UNP K7ZLW6
A	540	HIS	-	expression tag	UNP K7ZLW6
A	541	HIS	-	expression tag	UNP K7ZLW6
A	542	HIS	-	expression tag	UNP K7ZLW6
A	543	HIS	-	expression tag	UNP K7ZLW6
A	544	HIS	-	expression tag	UNP K7ZLW6
A	545	ILE	-	expression tag	UNP K7ZLW6
A	546	GLU	-	expression tag	UNP K7ZLW6
A	547	GLY	-	expression tag	UNP K7ZLW6
A	548	ARG	-	expression tag	UNP K7ZLW6
A	549	HIS	-	expression tag	UNP K7ZLW6
A	550	MET	-	expression tag	UNP K7ZLW6
A	551	GLU	-	expression tag	UNP K7ZLW6
A	552	LEU	-	expression tag	UNP K7ZLW6
A	553	GLY	-	expression tag	UNP K7ZLW6
A	554	THR	-	expression tag	UNP K7ZLW6
A	555	LEU	-	expression tag	UNP K7ZLW6
A	556	GLU	-	expression tag	UNP K7ZLW6
B	534	MET	-	initiating methionine	UNP K7ZLW6
B	535	ASN	-	expression tag	UNP K7ZLW6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	536	HIS	-	expression tag	UNP K7ZLW6
B	537	LYS	-	expression tag	UNP K7ZLW6
B	538	VAL	-	expression tag	UNP K7ZLW6
B	539	HIS	-	expression tag	UNP K7ZLW6
B	540	HIS	-	expression tag	UNP K7ZLW6
B	541	HIS	-	expression tag	UNP K7ZLW6
B	542	HIS	-	expression tag	UNP K7ZLW6
B	543	HIS	-	expression tag	UNP K7ZLW6
B	544	HIS	-	expression tag	UNP K7ZLW6
B	545	ILE	-	expression tag	UNP K7ZLW6
B	546	GLU	-	expression tag	UNP K7ZLW6
B	547	GLY	-	expression tag	UNP K7ZLW6
B	548	ARG	-	expression tag	UNP K7ZLW6
B	549	HIS	-	expression tag	UNP K7ZLW6
B	550	MET	-	expression tag	UNP K7ZLW6
B	551	GLU	-	expression tag	UNP K7ZLW6
B	552	LEU	-	expression tag	UNP K7ZLW6
B	553	GLY	-	expression tag	UNP K7ZLW6
B	554	THR	-	expression tag	UNP K7ZLW6
B	555	LEU	-	expression tag	UNP K7ZLW6
B	556	GLU	-	expression tag	UNP K7ZLW6

- Molecule 2 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
2	C	2	Total	C	N	O	0	0	0
			29	16	2	11			
2	D	2	Total	C	N	O	0	0	0
			29	16	2	11			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

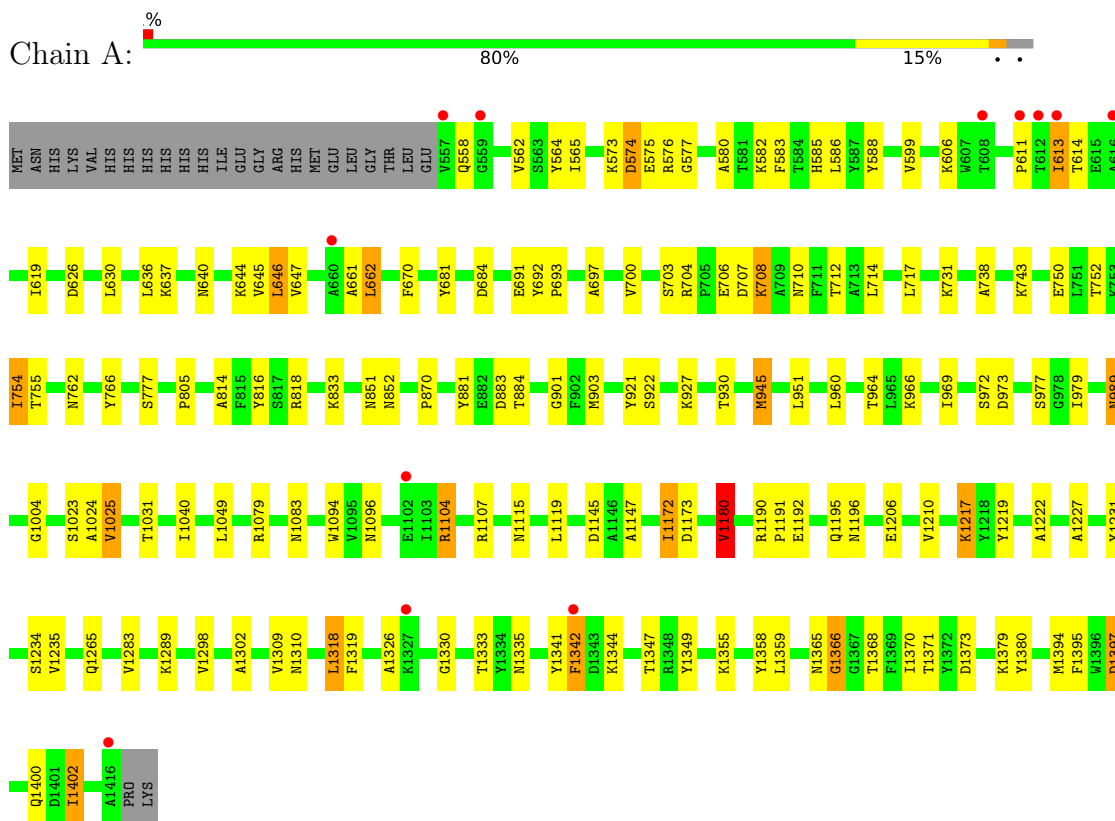
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	85	Total	O	0	0
			85	85		

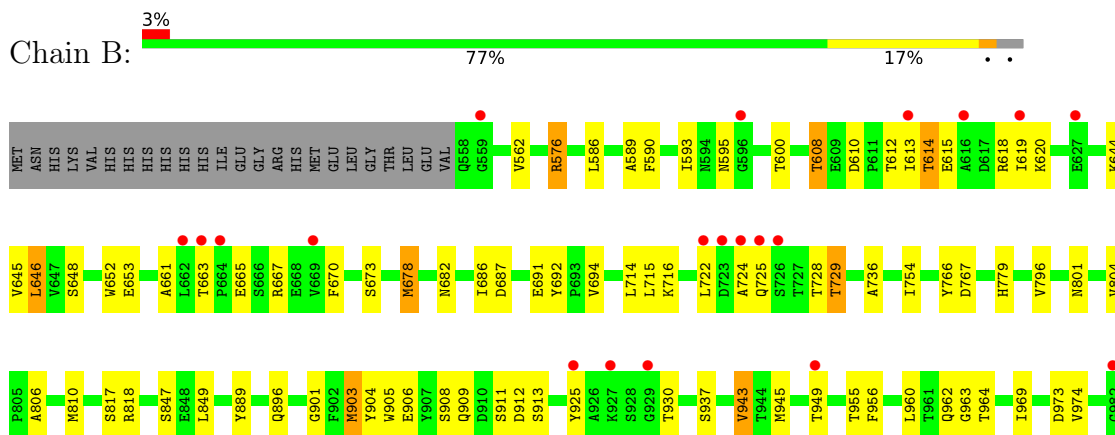
3 Residue-property plots

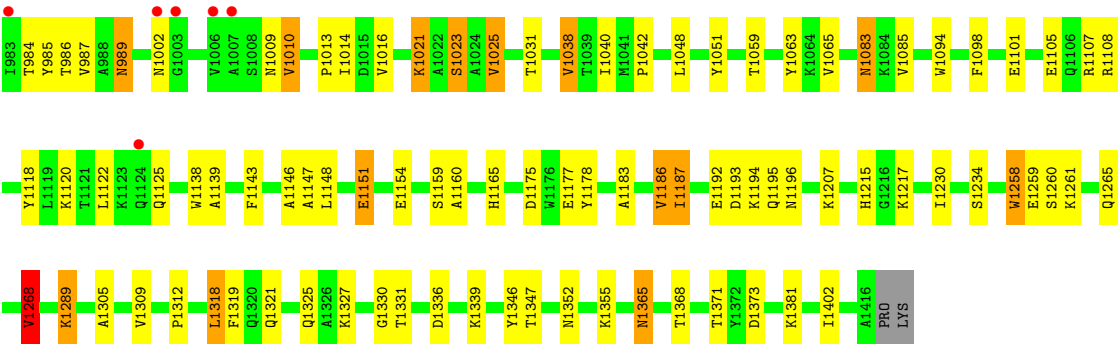
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Chitinase





• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 100%



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.99Å 127.23Å 161.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.61 50.01 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.01-2.61) 99.0 (50.01-2.61)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.203 , 0.253 0.206 , 0.251	Depositor DCC
R_{free} test set	3459 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13773	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8065e-03.*

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: NAG, PO4

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	1.00	2/6945 (0.0%)	1.11	12/9463 (0.1%)
1	B	1.06	4/6918 (0.1%)	1.15	19/9427 (0.2%)
All	All	1.03	6/13863 (0.0%)	1.13	31/18890 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1025	VAL	CA-C	7.40	1.59	1.52
1	B	1051	TYR	C-O	-6.57	1.16	1.23
1	A	693	PRO	C-O	-5.33	1.17	1.23
1	B	1336	ASP	CA-C	-5.19	1.46	1.52
1	A	558	GLN	N-CA	5.11	1.52	1.46
1	B	729	THR	N-CA	5.05	1.50	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1330	GLY	N-CA-C	-8.93	103.45	111.67
1	A	979	ILE	N-CA-C	-8.80	100.32	108.95
1	B	1234	SER	N-CA-C	7.34	121.68	112.87
1	B	989	ASN	N-CA-C	-7.21	97.84	109.96
1	A	1330	GLY	N-CA-C	-6.25	105.92	111.67
1	B	1159	SER	N-CA-C	6.03	117.85	111.28
1	A	1004	GLY	N-CA-C	5.87	119.16	110.42
1	B	1025	VAL	N-CA-CB	-5.75	105.52	112.07
1	A	851	ASN	N-CA-C	5.71	117.96	111.11
1	B	796	VAL	N-CA-C	-5.71	105.28	110.82
1	B	1230	ILE	N-CA-C	5.63	116.37	110.62
1	A	1395	PHE	N-CA-C	5.62	117.51	109.14
1	B	804	VAL	N-CA-C	-5.58	103.83	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	937	SER	N-CA-C	-5.57	101.04	108.34
1	B	1101	GLU	N-CA-C	5.57	118.28	111.82
1	B	1098	PHE	CA-C-N	5.54	126.76	119.84
1	B	1098	PHE	C-N-CA	5.54	126.76	119.84
1	B	901	GLY	N-CA-C	5.47	117.38	110.38
1	B	1040	ILE	N-CA-CB	5.44	116.65	110.72
1	B	904	TYR	N-CA-C	5.39	117.58	109.23
1	A	1172	ILE	N-CA-C	5.39	116.24	108.48
1	A	619	ILE	CB-CA-C	-5.37	105.09	111.97
1	B	889	TYR	N-CA-C	5.34	117.10	111.28
1	A	852	ASN	N-CA-C	5.27	122.03	114.39
1	B	985	TYR	N-CA-C	5.24	117.97	109.06
1	A	818	ARG	N-CA-C	-5.19	100.72	109.07
1	A	901	GLY	N-CA-C	5.13	118.03	110.80
1	A	558	GLN	N-CA-C	5.08	121.63	110.80
1	B	1268	VAL	N-CA-C	-5.08	105.90	110.82
1	B	963	GLY	CA-C-O	-5.03	118.76	122.23
1	A	1366	GLY	N-CA-C	5.01	125.06	113.18

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	6762	0	6539	71	0
1	B	6741	0	6511	71	0
2	C	29	0	27	0	0
2	D	29	0	27	6	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	117	0	0	0	0
4	B	85	0	0	1	0
All	All	13773	0	13104	141	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 5.

All (141) 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:B:906:GLU:OE2	1:B:908:SER:OG	2.07	0.70
1:A:1094:TRP:CZ3	1:A:1107:ARG:HG3	2.26	0.70
1:B:1010:VAL:HG11	1:B:1014:ILE:HD11	1.75	0.69
1:B:909:GLN:HE22	2:D:2:NAG:H81	1.57	0.68
1:A:1310:ASN:HA	1:A:1366:GLY:HA3	1.74	0.68
1:B:1094:TRP:CH2	1:B:1107:ARG:HG2	2.29	0.67
1:A:973:ASP:HB3	1:A:1024:ALA:HB2	1.76	0.66
1:A:588:TYR:OH	1:A:626:ASP:OD2	2.16	0.64
1:B:909:GLN:NE2	2:D:2:NAG:H81	2.11	0.64
1:B:562:VAL:HG23	1:B:810:MET:CE	2.29	0.63
1:A:1206:GLU:O	1:A:1210:VAL:HG23	1.99	0.62
1:A:969:ILE:H	1:A:989:ASN:HD21	1.50	0.60
1:B:905:TRP:HE1	2:D:2:NAG:H83	1.67	0.59
1:B:1186:VAL:HG23	1:B:1187:ILE:HD13	1.85	0.58
1:A:1326:ALA:HB1	1:B:682:ASN:HB3	1.86	0.58
1:A:945:MET:CE	1:A:951:LEU:HD13	2.34	0.57
1:A:564:TYR:CD2	1:A:903[B]:MET:HE3	2.40	0.57
1:A:574:ASP:OD1	1:A:577:GLY:N	2.38	0.56
1:A:712:THR:HA	1:A:754:ILE:CD1	2.36	0.56
1:A:884:THR:OG1	1:A:964:THR:OG1	2.19	0.56
1:B:1373:ASP:OD2	1:B:1381:LYS:NZ	2.39	0.56
1:B:1059:THR:HG22	1:B:1118:TYR:HB2	1.86	0.56
1:A:766:TYR:OH	1:A:903[B]:MET:HE1	2.07	0.55
1:A:1309:VAL:HA	1:A:1368:THR:HG22	1.88	0.55
1:A:644:LYS:HA	1:A:684:ASP:OD2	2.08	0.54
1:A:712:THR:HA	1:A:754:ILE:HD11	1.89	0.54
1:B:645:VAL:O	1:B:645:VAL:HG12	2.07	0.54
1:B:1083:ASN:HD21	1:B:1146:ALA:HA	1.73	0.54
2:D:1:NAG:H82	2:D:1:NAG:H1	1.90	0.54
1:B:562:VAL:HG23	1:B:810:MET:HE2	1.88	0.54
1:B:687:ASP:HA	1:B:736:ALA:O	2.08	0.53
1:B:613:ILE:HG23	1:B:613:ILE:O	2.08	0.53
1:B:1289:LYS:HE3	1:B:1289:LYS:HA	1.90	0.53
1:A:1335:ASN:HD21	1:A:1402:ILE:H	1.57	0.53
1:A:637:LYS:HA	1:A:640:ASN:O	2.08	0.53
1:A:1049:LEU:C	1:A:1049:LEU:HD23	2.34	0.53
1:B:1318:LEU:HD22	1:B:1319:PHE:CE2	2.43	0.53
1:A:1355:LYS:HE3	1:A:1380:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:TRP:CD2	2:D:1:NAG:H83	2.44	0.52
1:A:750:GLU:O	1:A:754:ILE:HB	2.09	0.52
1:B:974:VAL:HG12	1:B:987:VAL:HG21	1.92	0.52
1:B:1260:SER:OG	1:B:1321:GLN:NE2	2.41	0.52
1:B:576:ARG:HD3	1:B:912:ASP:HA	1.92	0.51
1:B:969:ILE:H	1:B:989:ASN:HD21	1.57	0.51
1:A:945:MET:HE2	1:A:951:LEU:HD13	1.92	0.51
1:A:564:TYR:CE2	1:A:903[B]:MET:HE3	2.46	0.51
1:B:1177:GLU:HA	1:B:1178:TYR:CD1	2.46	0.51
1:A:1180:VAL:HG22	1:A:1234:SER:HB3	1.92	0.51
1:B:1177:GLU:HG2	1:B:1178:TYR:CE1	2.46	0.51
1:B:1183:ALA:HB3	1:B:1186:VAL:HG22	1.92	0.51
1:B:1085:VAL:HG21	1:B:1160:ALA:HB2	1.91	0.51
1:B:661:ALA:HB2	1:B:714:LEU:HD22	1.92	0.51
1:B:608:THR:O	1:B:618:ARG:HD2	2.11	0.50
1:B:610:ASP:HB3	1:B:613:ILE:HG22	1.94	0.50
1:A:1318:LEU:HD22	1:A:1319:PHE:CD2	2.47	0.50
1:A:755:THR:HG21	1:A:805:PRO:HD2	1.94	0.50
1:B:1151:GLU:O	1:B:1154:GLU:HB3	2.12	0.50
1:A:646:LEU:HD23	1:A:646:LEU:N	2.27	0.49
1:A:1173:ASP:HA	1:A:1222:ALA:O	2.12	0.49
1:B:1138:TRP:O	1:B:1139:ALA:HB3	2.11	0.49
1:A:1309:VAL:HG12	1:A:1368:THR:CG2	2.43	0.49
1:B:1258:TRP:CD1	1:B:1259:GLU:HG3	2.47	0.49
1:A:814:ALA:HB1	1:A:816:TYR:CE1	2.47	0.49
1:B:715:LEU:HD13	1:B:754:ILE:HG23	1.94	0.49
1:A:1096:ASN:HA	1:A:1104:ARG:HD2	1.95	0.49
1:B:1193:ASP:O	1:B:1194:LYS:C	2.55	0.48
1:B:943:VAL:HG23	1:B:956:PHE:CZ	2.48	0.48
1:B:1346:TYR:HE2	1:B:1368:THR:HG23	1.77	0.48
1:A:964:THR:H	1:A:1025:VAL:HG22	1.78	0.47
1:B:767:ASP:CG	1:B:818:ARG:HH11	2.21	0.47
1:B:663:THR:O	1:B:667:ARG:HG3	2.14	0.47
1:B:1309:VAL:HG11	1:B:1327:LYS:O	2.15	0.47
1:B:1013:PRO:HA	1:B:1042:PRO:HD3	1.96	0.47
1:A:1217:LYS:HE2	1:A:1219:TYR:CE1	2.50	0.47
1:A:580:ALA:HB2	1:A:636:LEU:HD13	1.97	0.47
1:B:973:ASP:O	1:B:1021:LYS:HG3	2.16	0.46
1:B:1346:TYR:CE2	1:B:1368:THR:HG23	2.51	0.46
1:B:1165:HIS:CE1	1:B:1215:HIS:CE1	3.04	0.46
1:B:1105:GLU:OE1	1:B:1108:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:PHE:CD2	1:A:714:LEU:HD11	2.51	0.45
1:A:1397:ASP:C	1:A:1397:ASP:OD1	2.59	0.45
1:B:925:TYR:HB3	4:B:1644:HOH:O	2.16	0.45
1:B:1309:VAL:HG12	1:B:1368:THR:HB	1.98	0.45
1:B:1154:GLU:OE1	1:B:1207:LYS:NZ	2.40	0.45
1:A:630:LEU:HD13	1:A:681:TYR:CG	2.52	0.45
1:A:989:ASN:H	1:A:989:ASN:HD22	1.64	0.44
1:A:611:PRO:HA	1:A:614:THR:CG2	2.47	0.44
1:A:1227:ALA:HB1	1:A:1283:VAL:HG21	1.99	0.44
1:A:562:VAL:HG22	1:A:585:HIS:HB2	1.99	0.44
1:A:1079:ARG:HA	1:A:1079:ARG:HD3	1.85	0.44
1:A:697:ALA:HB3	1:A:700:VAL:HB	1.98	0.44
1:B:1365:ASN:OD1	1:B:1365:ASN:N	2.50	0.44
1:B:648:SER:HA	1:B:687:ASP:HB3	2.00	0.44
1:B:987:VAL:O	1:B:987:VAL:HG23	2.17	0.44
1:A:647:VAL:O	1:A:647:VAL:HG13	2.18	0.43
1:A:881:TYR:CE2	1:A:883:ASP:HB3	2.53	0.43
1:A:582:LYS:HA	1:A:921:TYR:CD1	2.53	0.43
1:A:707:ASP:O	1:A:708:LYS:C	2.59	0.43
1:A:945:MET:HE1	1:A:951:LEU:HD13	1.99	0.43
1:A:966:LYS:HE2	1:A:1023:SER:O	2.18	0.43
1:A:1302:ALA:O	1:A:1373:ASP:HB2	2.19	0.43
1:B:1147:ALA:HB1	1:B:1196:ASN:HB3	2.00	0.43
1:A:1231:TYR:CE1	1:A:1235:VAL:HG21	2.53	0.43
1:B:817:SER:HB3	1:B:849:LEU:HD11	2.01	0.43
1:A:1349:TYR:HB2	1:A:1358:TYR:CE1	2.53	0.43
1:B:847:SER:HB3	1:B:911:SER:HA	2.01	0.42
1:B:646:LEU:HD23	1:B:646:LEU:H	1.83	0.42
1:A:583:PHE:CE1	1:A:586:LEU:HD12	2.55	0.42
1:A:1333:THR:HB	1:A:1400:GLN:HB3	2.01	0.42
1:B:589:ALA:HA	1:B:590:PHE:HA	1.82	0.42
1:B:767:ASP:OD2	2:D:1:NAG:O6	2.35	0.42
1:B:586:LEU:C	1:B:586:LEU:HD23	2.44	0.42
1:B:678:MET:HE1	1:B:722:LEU:HD22	2.02	0.42
1:B:1016:VAL:HB	1:B:1038:VAL:HG23	2.01	0.42
1:A:989:ASN:HD22	1:A:989:ASN:N	2.18	0.42
1:A:945:MET:HE2	1:A:945:MET:HA	2.02	0.42
1:A:1359:LEU:HB2	1:A:1370:ILE:HB	2.01	0.42
1:B:1305:ALA:O	1:B:1331:THR:HA	2.20	0.42
1:A:1298:VAL:HG11	1:A:1394:MET:HB2	2.01	0.41
1:B:728:THR:HG22	1:B:728:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:PHE:O	1:B:673:SER:OG	2.36	0.41
1:A:1115:ASN:O	1:A:1119:LEU:HG	2.20	0.41
1:B:691:GLU:HA	1:B:692:TYR:CG	2.55	0.41
1:B:1318:LEU:HD22	1:B:1319:PHE:CD2	2.55	0.41
1:A:662:LEU:HA	1:A:710:ASN:ND2	2.36	0.41
1:A:661:ALA:O	1:A:710:ASN:HB3	2.21	0.41
1:A:870:PRO:HD2	1:A:881:TYR:O	2.21	0.41
1:A:731:LYS:NZ	1:B:1325:GLN:O	2.53	0.41
1:A:1190:ARG:O	1:A:1191:PRO:C	2.61	0.41
1:B:1065:VAL:HB	1:B:1122:LEU:HD11	2.02	0.41
1:A:1147:ALA:HB1	1:A:1196:ASN:HB3	2.02	0.41
1:B:652:TRP:O	1:B:653:GLU:HG2	2.21	0.41
1:A:691:GLU:HA	1:A:692:TYR:CD1	2.56	0.40
1:A:738:ALA:HA	1:A:762:ASN:HB2	2.03	0.40
1:A:1341:TYR:O	1:A:1342:PHE:C	2.63	0.40
1:B:766:TYR:OH	1:B:903[A]:MET:HE1	2.22	0.40
1:B:1268:VAL:HG13	1:B:1355:LYS:HB2	2.04	0.40
1:A:645:VAL:C	1:A:646:LEU:HD23	2.47	0.40
1:A:945:MET:HE1	1:A:1040:ILE:CG2	2.52	0.40
1:A:1309:VAL:HG12	1:A:1368:THR:HG22	2.03	0.40
1:B:1063:TYR:CD2	1:B:1402:ILE:HG22	2.56	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	861/885 (97%)	805 (94%)	53 (6%)	3 (0%)	36	56
1	B	858/885 (97%)	763 (89%)	83 (10%)	12 (1%)	9	17
All	All	1719/1770 (97%)	1568 (91%)	136 (8%)	15 (1%)	14	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	VAL
1	B	595	ASN
1	B	614	THR
1	B	694	VAL
1	B	1023	SER
1	B	1148	LEU
1	B	1258	TRP
1	B	724	ALA
1	B	801	ASN
1	B	945	MET
1	B	806	ALA
1	A	1342	PHE
1	B	576	ARG
1	A	613	ILE
1	B	1312	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	A	710/730 (97%)	662 (93%)	48 (7%)	14	30
1	B	707/730 (97%)	647 (92%)	60 (8%)	10	21
All	All	1417/1460 (97%)	1309 (92%)	108 (8%)	12	26

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	ILE
1	A	573	LYS
1	A	574	ASP
1	A	575	GLU
1	A	576	ARG
1	A	599	VAL
1	A	606	LYS
1	A	613	ILE

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Mol	Chain	Res	Type
1	A	646	LEU
1	A	662	LEU
1	A	703	SER
1	A	704	ARG
1	A	706	GLU
1	A	708	LYS
1	A	717	LEU
1	A	743	LYS
1	A	752	THR
1	A	754	ILE
1	A	777	SER
1	A	833	LYS
1	A	922	SER
1	A	927	LYS
1	A	930	THR
1	A	945	MET
1	A	960	LEU
1	A	972	SER
1	A	977	SER
1	A	989	ASN
1	A	1025	VAL
1	A	1031	THR
1	A	1083	ASN
1	A	1104	ARG
1	A	1145	ASP
1	A	1172	ILE
1	A	1180	VAL
1	A	1192	GLU
1	A	1195	GLN
1	A	1217	LYS
1	A	1265	GLN
1	A	1289	LYS
1	A	1318	LEU
1	A	1344	LYS
1	A	1347	THR
1	A	1365	ASN
1	A	1371	THR
1	A	1379	LYS
1	A	1397	ASP
1	A	1402	ILE
1	B	593	ILE
1	B	600	THR

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Mol	Chain	Res	Type
1	B	608	THR
1	B	612	THR
1	B	614	THR
1	B	615	GLU
1	B	619	ILE
1	B	620	LYS
1	B	644	LYS
1	B	646	LEU
1	B	665	GLU
1	B	678	MET
1	B	686	ILE
1	B	716	LYS
1	B	725	GLN
1	B	729	THR
1	B	779	HIS
1	B	896	GLN
1	B	903[A]	MET
1	B	903[B]	MET
1	B	913	SER
1	B	930	THR
1	B	943	VAL
1	B	949	THR
1	B	955	THR
1	B	960	LEU
1	B	962	GLN
1	B	964	THR
1	B	984	THR
1	B	986	THR
1	B	1002	ASN
1	B	1009	ASN
1	B	1010	VAL
1	B	1021	LYS
1	B	1023	SER
1	B	1025	VAL
1	B	1031	THR
1	B	1038	VAL
1	B	1048	LEU
1	B	1083	ASN
1	B	1120	LYS
1	B	1125	GLN
1	B	1143	PHE
1	B	1151	GLU

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Mol	Chain	Res	Type
1	B	1175	ASP
1	B	1186	VAL
1	B	1187	ILE
1	B	1192	GLU
1	B	1195	GLN
1	B	1217	LYS
1	B	1261	LYS
1	B	1265	GLN
1	B	1268	VAL
1	B	1289	LYS
1	B	1318	LEU
1	B	1339	LYS
1	B	1347	THR
1	B	1352	ASN
1	B	1365	ASN
1	B	1371	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	ASN
1	A	679	ASN
1	A	725	GLN
1	A	857	ASN
1	A	914	HIS
1	A	989	ASN
1	A	1074	ASN
1	A	1124	GLN
1	A	1166	GLN
1	A	1215	HIS
1	A	1265	GLN
1	A	1320	GLN
1	A	1325	GLN
1	A	1335	ASN
1	A	1361	ASN
1	A	1365	ASN
1	B	640	ASN
1	B	682	ASN
1	B	725	GLN
1	B	730	ASN
1	B	787	ASN
1	B	802	ASN

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Mol	Chain	Res	Type
1	B	896	GLN
1	B	962	GLN
1	B	989	ASN
1	B	993	HIS
1	B	1009	ASN
1	B	1083	ASN
1	B	1093	ASN
1	B	1124	GLN
1	B	1125	GLN
1	B	1126	ASN
1	B	1215	HIS
1	B	1242	GLN
1	B	1265	GLN
1	B	1325	GLN
1	B	1328	ASN
1	B	1335	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 ⓘ

4 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	C	1	2	15,15,15	0.75	0	21,21,21	2.74	5 (23%)
2	NAG	C	2	2	14,14,15	0.89	0	17,19,21	1.59	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	1	2	15,15,15	0.89	0	21,21,21	2.52	7 (33%)
2	NAG	D	2	2	14,14,15	0.60	0	17,19,21	2.34	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2	-	1/6/26/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2	-	6/6/26/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O5-C1-C2	10.42	119.98	109.52
2	D	2	NAG	C1-O5-C5	7.41	122.11	112.19
2	D	1	NAG	O5-C1-C2	5.84	115.38	109.52
2	D	1	NAG	C1-O5-C5	5.32	123.94	113.65
2	D	1	NAG	C1-C2-C3	4.19	116.26	110.54
2	C	1	NAG	C1-C2-C3	4.12	116.16	110.54
2	C	2	NAG	O4-C4-C3	-3.92	101.14	110.38
2	D	2	NAG	C8-C7-N2	3.35	121.67	116.12
2	D	1	NAG	O7-C7-C8	-3.23	116.31	122.05
2	D	1	NAG	O3-C3-C4	-3.14	102.98	110.38
2	D	1	NAG	C8-C7-N2	3.10	121.26	116.12
2	D	2	NAG	C2-N2-C7	3.03	126.95	122.90
2	C	2	NAG	O3-C3-C2	2.81	115.24	109.40
2	C	1	NAG	O7-C7-C8	-2.70	117.24	122.05
2	C	1	NAG	O1-C1-O5	-2.50	102.99	110.41
2	C	1	NAG	O7-C7-N2	2.26	125.97	121.98
2	D	1	NAG	C2-N2-C7	2.23	128.32	123.11
2	C	2	NAG	O7-C7-N2	2.17	125.81	121.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

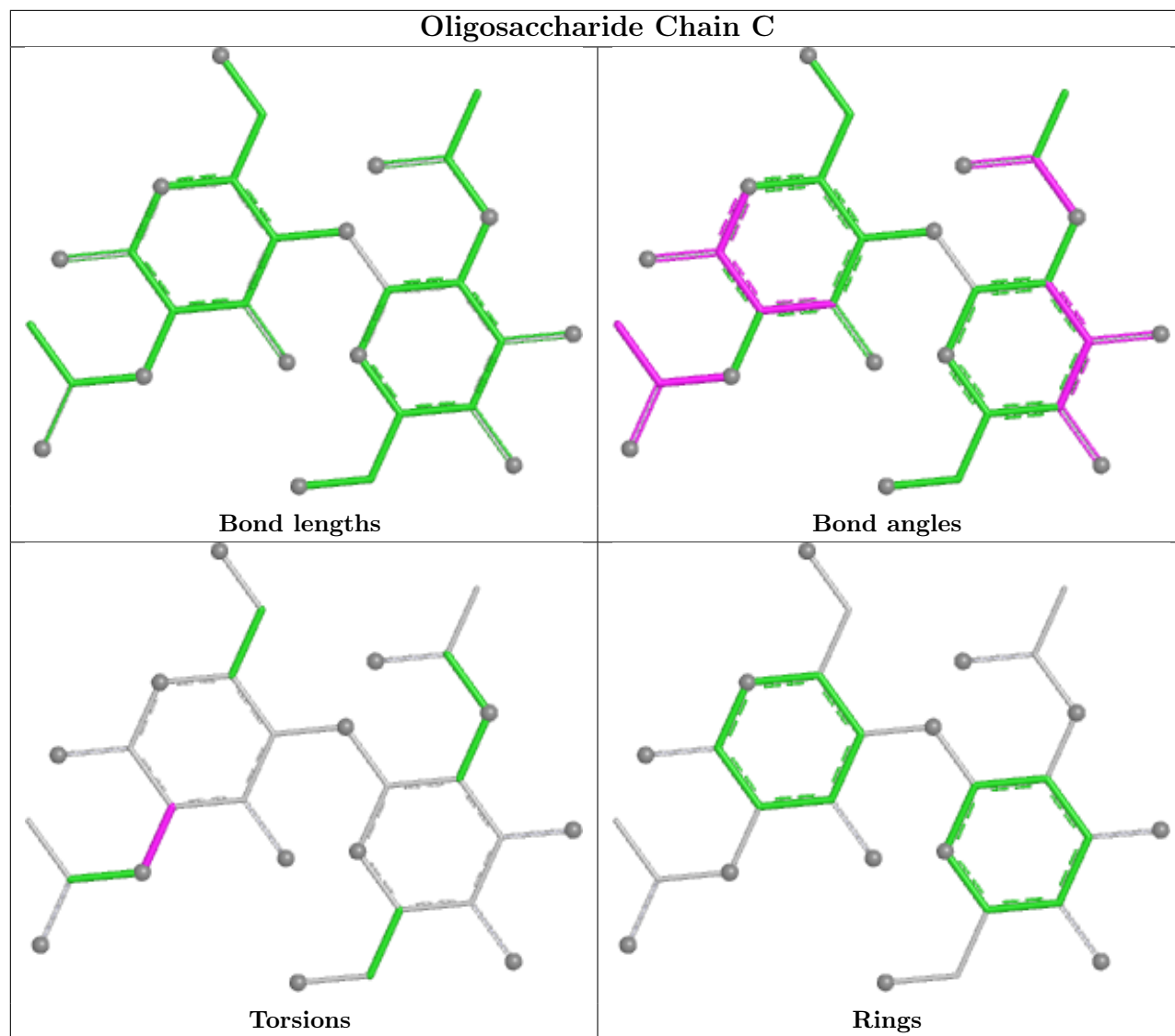
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C1-C2-N2-C7
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C1-C2-N2-C7
2	D	1	NAG	C3-C2-N2-C7

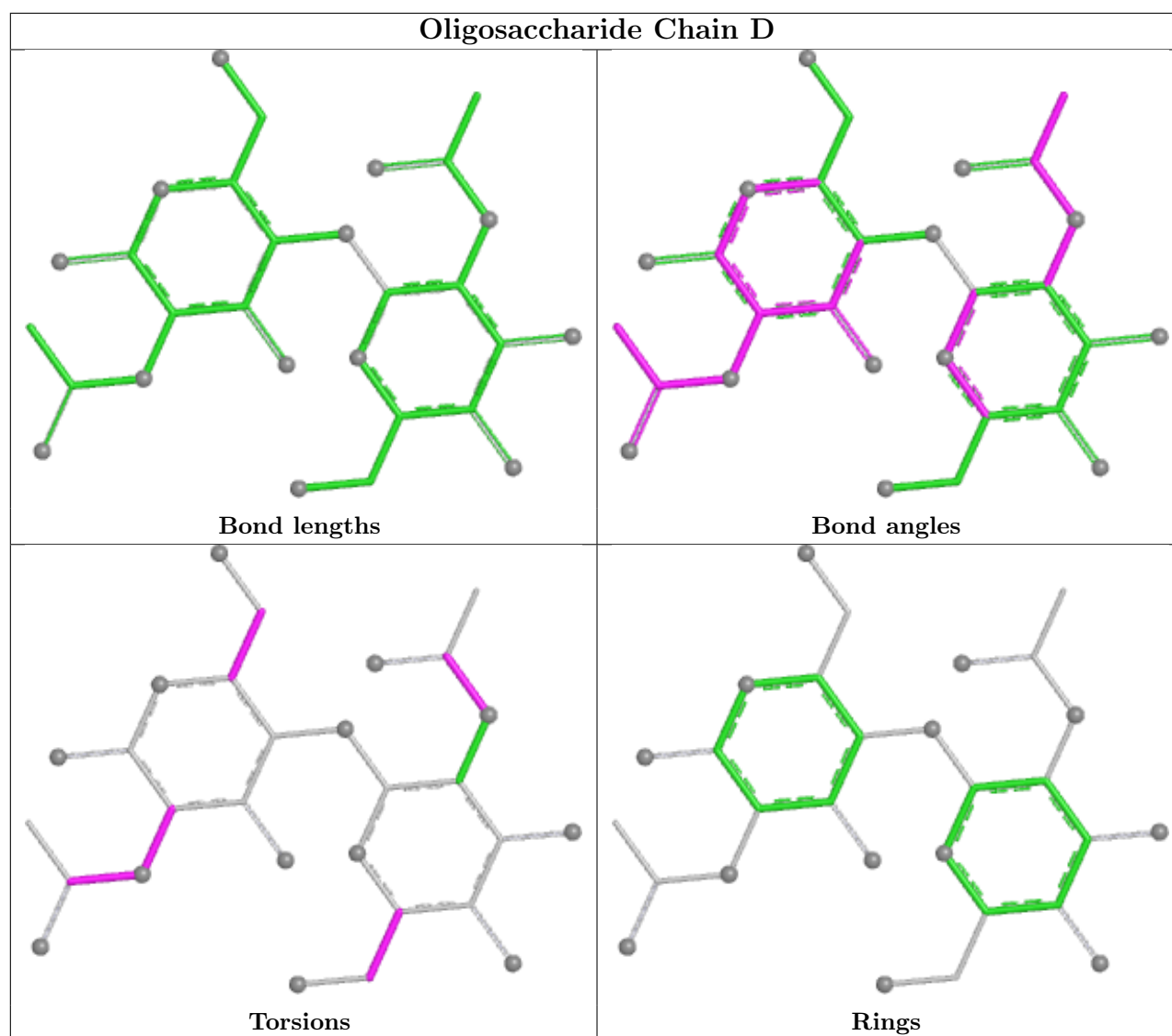
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	0
2	D	2	NAG	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 oligosaccharide.





5.6 Ligand geometry [i](#)

2 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
3	PO4	A	3003	-	4,4,4	1.71	1 (25%)	6,6,6	1.31	1 (16%)
3	PO4	B	1503	-	4,4,4	0.89	0	6,6,6	1.61	1 (16%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3003	PO4	P-O2	-2.09	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1503	PO4	O4-P-O3	-2.64	99.71	107.91
3	A	3003	PO4	O4-P-O1	-2.34	102.69	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	860/885 (97%)	-0.11	12 (1%) 73 70	17, 40, 76, 104	3 (0%)
1	B	859/885 (97%)	0.09	26 (3%) 52 47	16, 41, 81, 109	1 (0%)
All	All	1719/1770 (97%)	-0.01	38 (2%) 62 57	16, 41, 79, 109	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	613	ILE	5.6
1	A	557	VAL	5.1
1	A	613	ILE	3.9
1	B	1003	GLY	3.2
1	B	983	ILE	3.0
1	B	724	ALA	3.0
1	B	726	SER	2.9
1	B	1002	ASN	2.8
1	B	669	VAL	2.8
1	B	619	ILE	2.8
1	A	559	GLY	2.7
1	A	611	PRO	2.5
1	B	725	GLN	2.5
1	A	612	THR	2.5
1	B	925	TYR	2.5
1	A	616	ALA	2.4
1	B	722	LEU	2.4
1	B	559	GLY	2.4
1	B	929	GLY	2.4
1	B	949	THR	2.3
1	B	927	LYS	2.3
1	B	596	GLY	2.3
1	B	616	ALA	2.3
1	B	663	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	664	PRO	2.3
1	B	1007	ALA	2.2
1	A	1102	GLU	2.2
1	B	1124	GLN	2.2
1	B	982	GLY	2.2
1	A	1327	LYS	2.2
1	B	662	LEU	2.2
1	B	723	ASP	2.2
1	A	1342	PHE	2.2
1	B	627	GLU	2.1
1	B	1006	VAL	2.1
1	A	1416	ALA	2.1
1	A	660	ALA	2.0
1	A	608	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](#)

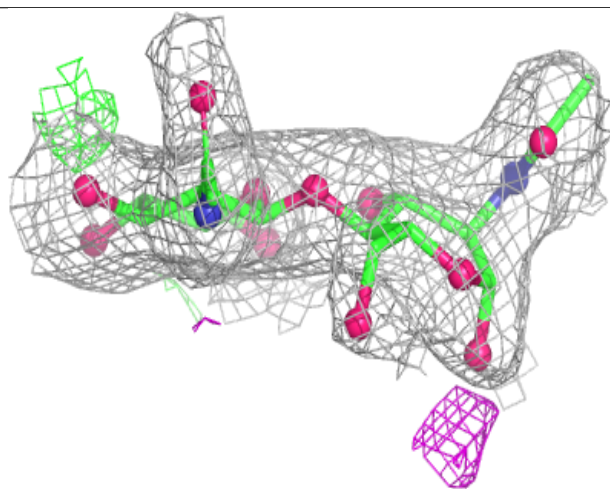
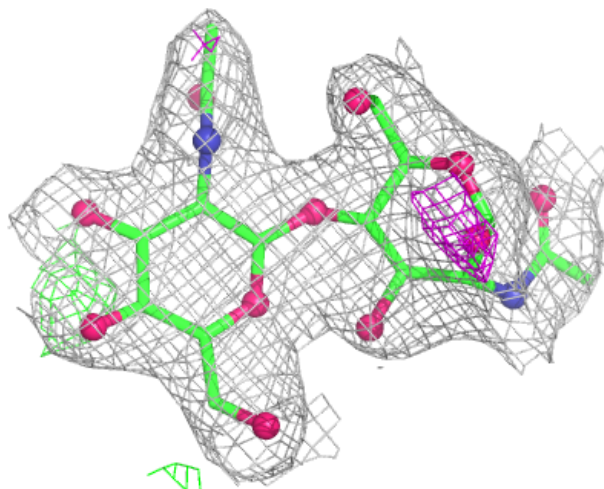
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

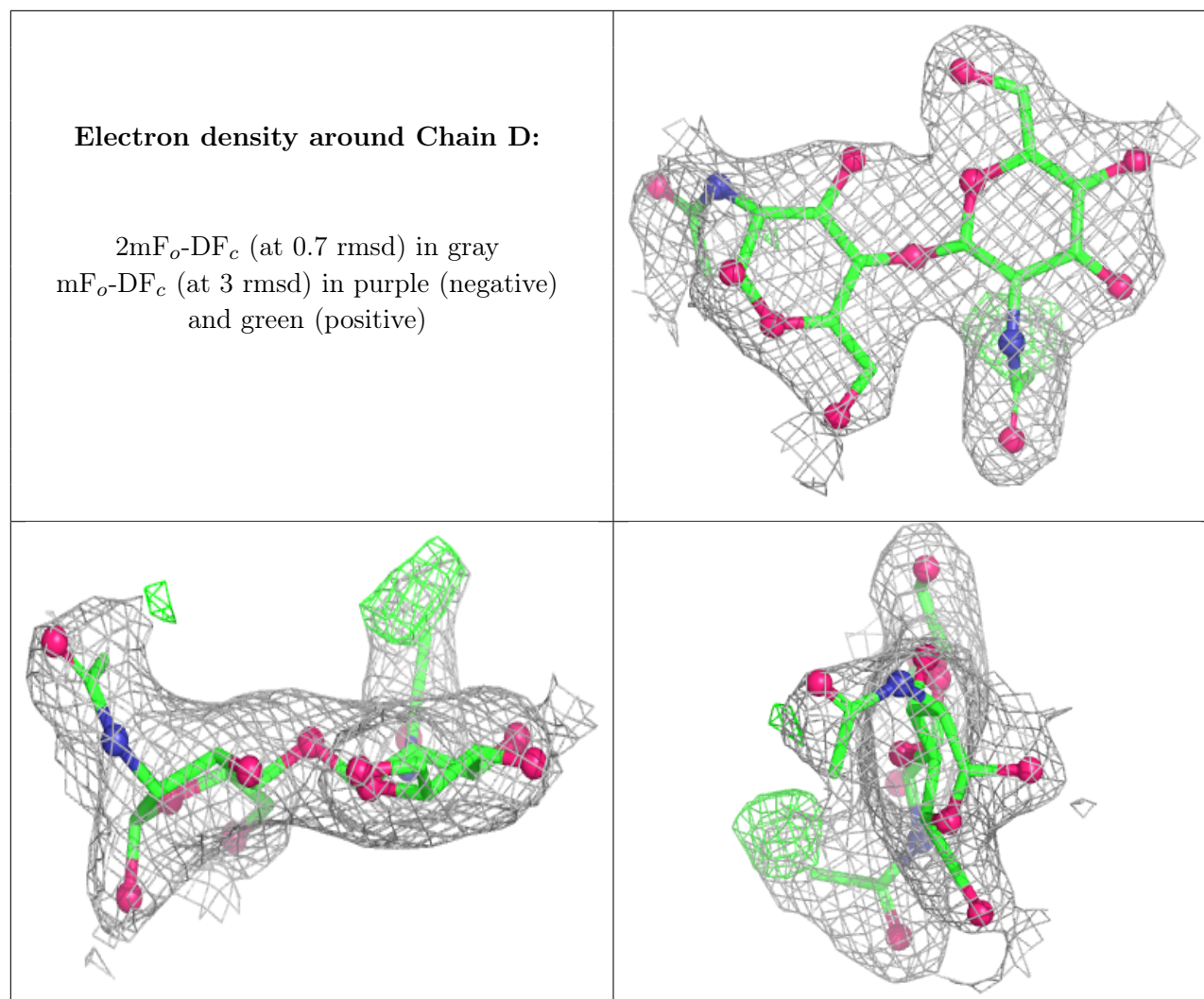
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	1	15/15	0.93	0.10	33,37,52,62	0
2	NAG	D	2	14/15	0.93	0.07	28,36,38,41	0
2	NAG	C	2	14/15	0.94	0.08	26,31,35,38	0
2	NAG	C	1	15/15	0.95	0.08	33,35,39,40	0

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 C:

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





6.4 Ligands [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
3	PO4	B	1503	5/5	0.95	0.09	41,43,48,54	0
3	PO4	A	3003	5/5	0.99	0.05	30,31,40,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.