



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:58 PM UTC

PDB ID : 4MYW / pdb_00004myw
Title : Structure of HSV-2 gD bound to nectin-1
Authors : Lu, G.; Zhang, N.; Qi, J.; Li, Y.; Chen, Z.; Zheng, C.; Yan, J.; Gao, G.F.
Deposited on : 2013-09-28
Resolution : 3.19 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

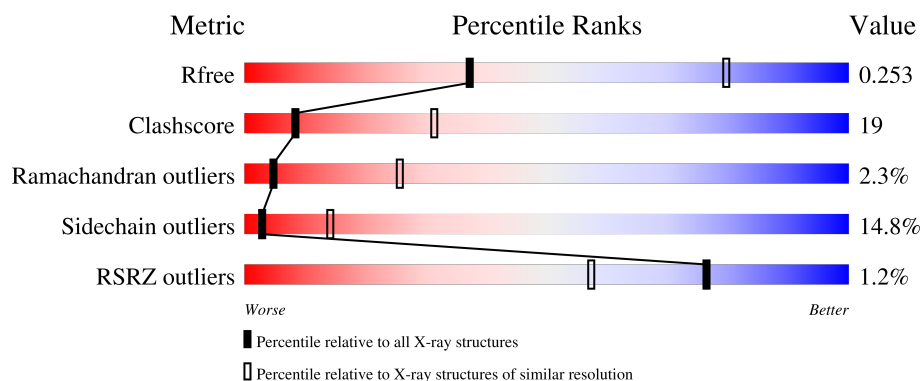
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	294	2% 44% 29% 6% 21%
1	C	294	2% 46% 27% 5% 21%
2	B	331	51% 31% 9% 8%
2	D	331	2% 53% 31% 7% 8%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8573 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 Envelope glycoprotein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1839	1184	313	332	10			
1	C	232	Total	C	N	O	S	0	0	0
			1839	1184	313	332	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P03172
A	-1	ASP	-	expression tag	UNP P03172
A	0	LEU	-	expression tag	UNP P03172
A	27	GLN	ARG	SEE REMARK 999	UNP P03172
A	286	HIS	-	expression tag	UNP P03172
A	287	HIS	-	expression tag	UNP P03172
A	288	HIS	-	expression tag	UNP P03172
A	289	HIS	-	expression tag	UNP P03172
A	290	HIS	-	expression tag	UNP P03172
A	291	HIS	-	expression tag	UNP P03172
C	-2	ALA	-	expression tag	UNP P03172
C	-1	ASP	-	expression tag	UNP P03172
C	0	LEU	-	expression tag	UNP P03172
C	27	GLN	ARG	SEE REMARK 999	UNP P03172
C	286	HIS	-	expression tag	UNP P03172
C	287	HIS	-	expression tag	UNP P03172
C	288	HIS	-	expression tag	UNP P03172
C	289	HIS	-	expression tag	UNP P03172
C	290	HIS	-	expression tag	UNP P03172
C	291	HIS	-	expression tag	UNP P03172

- Molecule 2 is a protein called Poliovirus receptor-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	303	Total 2377	C 1495	N 411	O 460	S 11	0	0	0
2	D	303	Total 2377	C 1495	N 411	O 460	S 11	0	0	0

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	MET	-	expression tag	UNP Q15223
B	17	ALA	-	expression tag	UNP Q15223
B	18	SER	-	expression tag	UNP Q15223
B	19	MET	-	expression tag	UNP Q15223
B	20	THR	-	expression tag	UNP Q15223
B	21	GLY	-	expression tag	UNP Q15223
B	22	GLY	-	expression tag	UNP Q15223
B	23	GLN	-	expression tag	UNP Q15223
B	24	GLN	-	expression tag	UNP Q15223
B	25	MET	-	expression tag	UNP Q15223
B	26	GLY	-	expression tag	UNP Q15223
B	27	ARG	-	expression tag	UNP Q15223
B	28	ASP	-	expression tag	UNP Q15223
B	29	PRO	-	expression tag	UNP Q15223
B	336	ALA	-	expression tag	UNP Q15223
B	337	ALA	-	expression tag	UNP Q15223
B	338	ALA	-	expression tag	UNP Q15223
B	339	LEU	-	expression tag	UNP Q15223
B	340	GLU	-	expression tag	UNP Q15223
B	341	HIS	-	expression tag	UNP Q15223
B	342	HIS	-	expression tag	UNP Q15223
B	343	HIS	-	expression tag	UNP Q15223
B	344	HIS	-	expression tag	UNP Q15223
B	345	HIS	-	expression tag	UNP Q15223
B	346	HIS	-	expression tag	UNP Q15223
D	16	MET	-	expression tag	UNP Q15223
D	17	ALA	-	expression tag	UNP Q15223
D	18	SER	-	expression tag	UNP Q15223
D	19	MET	-	expression tag	UNP Q15223
D	20	THR	-	expression tag	UNP Q15223
D	21	GLY	-	expression tag	UNP Q15223
D	22	GLY	-	expression tag	UNP Q15223
D	23	GLN	-	expression tag	UNP Q15223
D	24	GLN	-	expression tag	UNP Q15223
D	25	MET	-	expression tag	UNP Q15223

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Chain	Residue	Modelled	Actual	Comment	Reference
D	26	GLY	-	expression tag	UNP Q15223
D	27	ARG	-	expression tag	UNP Q15223
D	28	ASP	-	expression tag	UNP Q15223
D	29	PRO	-	expression tag	UNP Q15223
D	336	ALA	-	expression tag	UNP Q15223
D	337	ALA	-	expression tag	UNP Q15223
D	338	ALA	-	expression tag	UNP Q15223
D	339	LEU	-	expression tag	UNP Q15223
D	340	GLU	-	expression tag	UNP Q15223
D	341	HIS	-	expression tag	UNP Q15223
D	342	HIS	-	expression tag	UNP Q15223
D	343	HIS	-	expression tag	UNP Q15223
D	344	HIS	-	expression tag	UNP Q15223
D	345	HIS	-	expression tag	UNP Q15223
D	346	HIS	-	expression tag	UNP Q15223

- Molecule 3 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
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

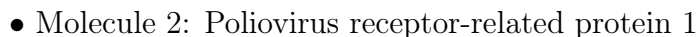


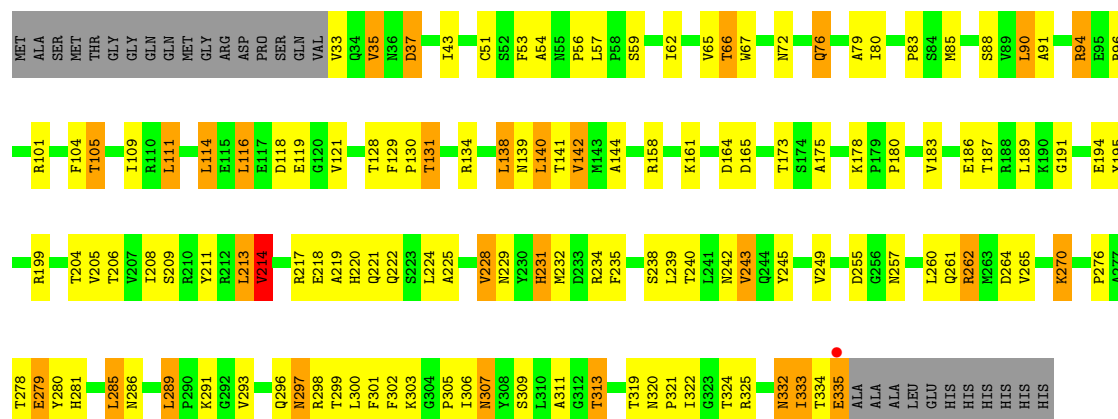
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

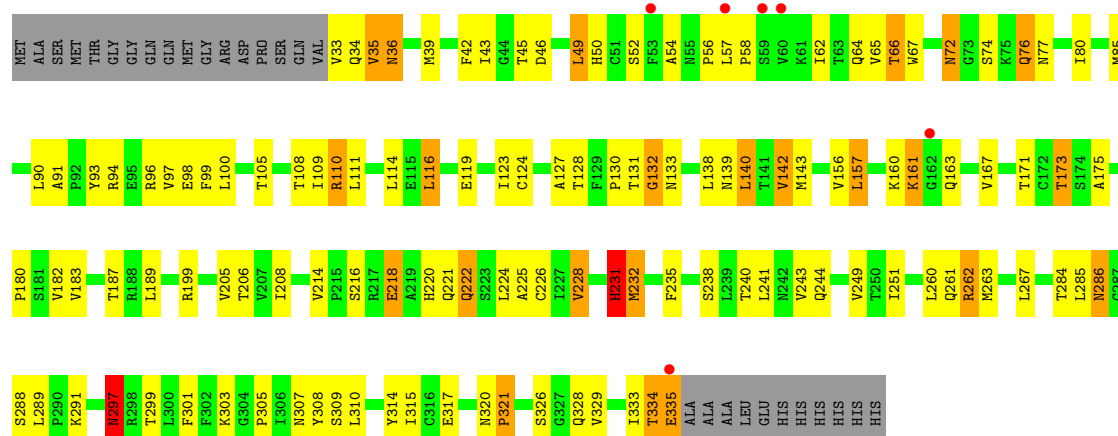
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total	O	0	0
			20	20		
5	B	13	Total	O	0	0
			13	13		
5	C	10	Total	O	0	0
			10	10		
5	D	14	Total	O	0	0
			14	14		

- Molecule 1: Envelope glycoprotein D





• Molecule 2: Poliovirus receptor-related protein 1



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 3: 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 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	53.34Å 170.86Å 192.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.93 – 3.19 38.93 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.2 (38.93-3.19) 99.3 (38.93-3.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.196 , 0.247 0.197 , 0.253	Depositor DCC
R_{free} test set	1525 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8573	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% 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: 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	0.44	0/1896	0.89	9/2595 (0.3%)
1	C	0.44	0/1896	0.90	8/2595 (0.3%)
2	B	0.37	0/2429	0.80	2/3308 (0.1%)
2	D	0.36	0/2429	0.80	2/3308 (0.1%)
All	All	0.40	0/8650	0.84	21/11806 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ILE	N-CA-C	10.11	122.25	106.88
2	B	214	VAL	CA-C-N	8.52	128.59	119.90
2	B	214	VAL	C-N-CA	8.52	128.59	119.90
1	C	170	ILE	CB-CA-C	-8.50	100.17	111.81
1	A	30	ASP	CA-C-N	6.07	126.63	120.38
1	A	30	ASP	C-N-CA	6.07	126.63	120.38
1	A	171	ASN	CB-CA-C	-6.03	109.61	116.54
1	C	197	ILE	N-CA-C	5.94	114.03	108.15
1	C	245	LYS	CA-C-N	5.58	126.12	120.38
1	C	245	LYS	C-N-CA	5.58	126.12	120.38
2	D	288	SER	N-CA-C	5.34	115.33	108.34
1	A	41	GLN	CA-C-N	5.29	124.80	119.19
1	A	41	GLN	C-N-CA	5.29	124.80	119.19
2	D	231	HIS	CB-CA-C	-5.26	110.53	116.63
1	C	41	GLN	CA-C-N	5.24	124.75	119.19
1	C	41	GLN	C-N-CA	5.24	124.75	119.19
1	C	171	ASN	N-CA-C	-5.22	99.26	108.08
1	A	193	LEU	CA-C-N	5.21	125.19	120.03
1	A	193	LEU	C-N-CA	5.21	125.19	120.03
1	A	224	ILE	CA-C-N	5.09	126.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ILE	C-N-CA	5.09	126.20	119.84

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	1839	0	1819	77	0
1	C	1839	0	1819	75	0
2	B	2377	0	2324	95	0
2	D	2377	0	2324	85	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
5	A	20	0	0	0	0
5	B	13	0	0	0	0
5	C	10	0	0	0	0
5	D	14	0	0	1	0
All	All	8573	0	8362	323	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 (323) 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)
2:D:228:VAL:HG22	2:D:235:PHE:HB3	1.51	0.93
1:A:63:GLU:HG2	1:A:184:ARG:HE	1.36	0.91
2:B:43:ILE:HD12	2:B:144:ALA:HB2	1.54	0.89
1:C:186:ARG:HG3	1:C:186:ARG:HH11	1.39	0.87
2:B:43:ILE:HD11	2:B:116:LEU:HD13	1.57	0.84
1:A:186:ARG:HH11	1:A:186:ARG:CG	1.91	0.83
1:A:85:SER:O	1:A:89:ARG:HG3	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:THR:HG23	2:B:208:ILE:HG12	1.61	0.81
1:C:253:LEU:H	1:C:254:PRO:CD	1.96	0.79
2:B:164:ASP:HA	2:B:214:VAL:HG21	1.63	0.78
2:B:297:ASN:HD22	2:B:298:ARG:H	1.33	0.76
2:D:225:ALA:HB2	2:D:238:SER:HB3	1.67	0.76
1:C:46:ASP:OD1	1:C:46:ASP:C	2.30	0.74
2:D:183:VAL:HG22	2:D:228:VAL:HG12	1.70	0.74
2:B:129:PHE:CD1	2:B:130:PRO:HA	2.24	0.73
2:B:228:VAL:HG13	2:B:235:PHE:HD1	1.54	0.73
1:C:253:LEU:H	1:C:254:PRO:HD2	1.52	0.72
1:C:170:ILE:HG22	1:C:170:ILE:O	1.87	0.72
2:D:66:THR:HG22	2:D:80:ILE:HG12	1.72	0.72
1:A:59:TYR:CD1	1:A:253:LEU:HD21	2.25	0.71
2:D:62:ILE:HA	2:D:128:THR:HG22	1.71	0.71
1:A:77:ALA:HB3	1:A:78:PRO:HD3	1.72	0.70
2:B:297:ASN:ND2	2:B:298:ARG:H	1.89	0.69
2:B:66:THR:HG23	2:B:80:ILE:HG23	1.75	0.69
2:D:100:LEU:HD21	2:D:110:ARG:HB3	1.74	0.68
2:B:91:ALA:HA	2:B:94:ARG:HG3	1.75	0.68
2:D:260:LEU:HD11	2:D:308:TYR:CE1	2.29	0.68
1:C:53:ILE:HG23	1:C:54:PRO:HD2	1.74	0.68
2:B:217:ARG:HG3	2:B:245:TYR:CD1	2.30	0.68
1:A:89:ARG:HA	1:A:120:TYR:CD1	2.30	0.67
1:C:53:ILE:HD12	1:C:173:TRP:HZ2	1.59	0.67
2:D:67:TRP:CZ3	2:D:124:CYS:HB2	2.29	0.67
1:A:53:ILE:HD12	1:A:173:TRP:HZ2	1.58	0.67
2:B:285:LEU:HD22	2:B:313:THR:HG21	1.77	0.67
2:D:43:ILE:HD11	2:D:116:LEU:HD13	1.77	0.67
1:A:186:ARG:HH11	1:A:186:ARG:HG2	1.59	0.67
2:B:119:GLU:OE2	2:B:178:LYS:HE3	1.95	0.66
1:A:215:ASP:CG	2:B:90:LEU:HD22	2.20	0.66
2:D:232:MET:HE3	2:D:232:MET:HA	1.77	0.66
2:B:54:ALA:O	2:B:56:PRO:HD3	1.95	0.66
1:A:161:ALA:HB2	1:A:183:HIS:HD2	1.61	0.66
2:D:173:THR:HG23	2:D:208:ILE:HG12	1.77	0.65
1:A:132:GLN:HG3	2:B:85:MET:SD	2.39	0.63
2:D:45:THR:HG22	2:D:46:ASP:N	2.13	0.63
1:A:63:GLU:HA	1:A:184:ARG:HB2	1.81	0.62
1:C:132:GLN:HG3	2:D:85:MET:CE	2.28	0.62
1:A:139:ASP:OD1	1:A:139:ASP:N	2.32	0.62
1:A:72:HIS:HD2	1:A:73:ALA:N	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:HH11	1:A:186:ARG:HG3	1.66	0.61
2:D:54:ALA:O	2:D:56:PRO:HD3	2.01	0.61
2:B:220:HIS:HA	2:B:243:VAL:HG23	1.83	0.61
2:D:286:ASN:H	2:D:286:ASN:HD22	1.49	0.61
2:B:83:PRO:HG2	2:B:104:PHE:CZ	2.36	0.61
2:B:262:ARG:HB3	2:B:306:ILE:HD12	1.83	0.60
2:B:175:ALA:HA	2:B:206:THR:HG23	1.84	0.60
2:D:119:GLU:HG2	2:D:142:VAL:HG23	1.84	0.60
1:A:51:PRO:HA	1:A:174:THR:HG23	1.83	0.60
1:A:186:ARG:HD3	1:A:186:ARG:N	2.17	0.60
1:C:126:VAL:HG22	1:C:126:VAL:O	2.02	0.60
1:C:220:LEU:HD22	2:D:66:THR:HG21	1.84	0.60
2:B:119:GLU:HG2	2:B:142:VAL:H	1.67	0.60
2:B:183:VAL:O	2:B:195:TYR:HE1	1.85	0.60
1:A:56:THR:HB	1:A:58:TYR:HE1	1.66	0.59
1:A:186:ARG:HD3	1:A:186:ARG:H	1.65	0.59
2:B:35:VAL:CG1	2:B:138:LEU:HB3	2.33	0.59
1:C:215:ASP:HB3	2:D:77:ASN:HB2	1.83	0.59
2:D:36:ASN:OD1	2:D:50:HIS:HB2	2.03	0.59
1:C:60:ALA:HB2	1:C:250:SER:HB3	1.85	0.59
1:C:253:LEU:O	1:C:254:PRO:C	2.46	0.58
2:D:138:LEU:C	2:D:138:LEU:HD12	2.28	0.58
1:A:101:ARG:HB2	1:A:110:ILE:HD11	1.84	0.58
2:B:270:LYS:HE2	2:B:298:ARG:HH12	1.69	0.58
1:A:127:CYS:HB3	1:A:128:PRO:HD2	1.86	0.58
1:C:241:TRP:CH2	1:C:244:PRO:HA	2.38	0.58
2:B:119:GLU:HG2	2:B:142:VAL:HG23	1.84	0.58
2:B:138:LEU:C	2:B:138:LEU:HD12	2.29	0.58
1:C:252:LEU:HD13	1:C:254:PRO:HD3	1.86	0.58
1:A:72:HIS:CD2	1:A:73:ALA:N	2.71	0.58
2:D:42:PHE:CE1	2:D:143:MET:HE3	2.39	0.58
2:D:49:LEU:HD13	2:D:138:LEU:HD21	1.85	0.58
2:B:279:GLU:CB	2:B:319:THR:HB	2.34	0.57
1:A:59:TYR:HD1	1:A:253:LEU:HD21	1.69	0.57
2:B:289:LEU:HD22	2:B:289:LEU:H	1.70	0.57
1:A:161:ALA:HB2	1:A:183:HIS:CD2	2.39	0.56
2:D:160:LYS:HB2	2:D:163:GLN:HE21	1.70	0.56
1:C:137:TYR:CD1	1:C:197:ILE:HG12	2.40	0.56
2:B:66:THR:HG22	2:B:80:ILE:HG12	1.88	0.56
1:C:46:ASP:HB2	1:C:208:TYR:HB3	1.87	0.56
1:C:186:ARG:HH11	1:C:186:ARG:CG	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ASN:HD22	2:B:309:SER:H	1.52	0.56
2:B:189:LEU:HG	2:B:222:GLN:HG2	1.86	0.56
2:B:325:ARG:HG3	2:B:325:ARG:HH11	1.71	0.56
1:C:132:GLN:HG3	2:D:85:MET:SD	2.46	0.56
2:D:317:GLU:HG2	2:D:326:SER:OG	2.05	0.56
2:D:220:HIS:CD2	2:D:221:GLN:HG3	2.41	0.56
2:D:334:THR:HG23	2:D:335:GLU:HB2	1.88	0.55
2:B:293:VAL:HG12	2:B:300:LEU:HD11	1.88	0.55
1:C:226:GLU:O	1:C:229:ARG:HB2	2.06	0.55
2:D:161:LYS:CD	2:D:161:LYS:H	2.19	0.55
2:D:161:LYS:H	2:D:161:LYS:HD2	1.70	0.55
1:C:186:ARG:HG3	1:C:186:ARG:NH1	2.16	0.55
2:D:315:ILE:HG12	2:D:328:GLN:HG2	1.89	0.55
1:C:53:ILE:HD12	1:C:173:TRP:CZ2	2.40	0.54
2:B:228:VAL:HG13	2:B:235:PHE:CD1	2.39	0.54
1:C:44:LEU:HB2	1:C:212:VAL:O	2.07	0.54
1:C:85:SER:O	1:C:89:ARG:HG3	2.08	0.54
2:D:36:ASN:OD1	2:D:36:ASN:N	2.39	0.54
1:C:47:PRO:HG3	1:C:100:TYR:CZ	2.42	0.54
1:C:108:ILE:HD13	1:C:197:ILE:HG21	1.90	0.54
1:C:139:ASP:OD1	1:C:139:ASP:N	2.38	0.54
1:C:144:VAL:O	1:C:229:ARG:NH1	2.41	0.54
1:A:75:SER:HB3	1:A:149:LEU:HD21	1.90	0.53
1:A:65:ALA:HB2	1:A:185:ALA:HB3	1.89	0.53
1:A:225:PRO:O	1:A:229:ARG:HG3	2.09	0.53
2:D:260:LEU:O	2:D:261:GLN:HB2	2.07	0.53
1:A:99:TRP:CZ3	1:A:166:ARG:HB2	2.44	0.53
1:C:147:ASP:O	1:C:148:ASN:HB2	2.08	0.53
1:A:108:ILE:HD13	1:A:197:ILE:HG21	1.89	0.53
2:B:33:VAL:CG1	2:B:134:ARG:HB3	2.39	0.53
2:B:54:ALA:C	2:B:56:PRO:HD3	2.33	0.53
2:B:307:ASN:ND2	2:B:309:SER:OG	2.42	0.53
2:D:66:THR:HG23	2:D:80:ILE:HG23	1.91	0.53
1:C:47:PRO:HG3	1:C:100:TYR:CE1	2.43	0.52
1:A:61:VAL:HG12	1:A:63:GLU:HG3	1.91	0.52
1:A:72:HIS:HD2	1:A:73:ALA:H	1.55	0.52
2:B:35:VAL:HG11	2:B:138:LEU:HB3	1.92	0.52
1:C:75:SER:O	1:C:78:PRO:HD2	2.09	0.52
2:B:279:GLU:HB2	2:B:319:THR:HB	1.90	0.52
2:B:62:ILE:HG13	2:B:128:THR:HG22	1.90	0.52
1:C:135:TRP:HB2	1:C:222:ARG:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:TYR:N	1:C:137:TYR:CD2	2.78	0.52
2:D:180:PRO:HG3	2:D:205:VAL:HG21	1.92	0.52
1:A:53:ILE:HD13	1:A:76:GLU:HG3	1.92	0.51
2:B:180:PRO:HG3	2:B:205:VAL:HG21	1.92	0.51
1:C:213:THR:O	1:C:216:SER:HB3	2.11	0.51
1:C:218:GLY:HA2	2:D:77:ASN:OD1	2.10	0.51
1:A:53:ILE:HD12	1:A:173:TRP:CZ2	2.43	0.51
2:D:72:ASN:N	2:D:72:ASN:HD22	2.07	0.51
2:B:320:ASN:HB2	2:B:321:PRO:CD	2.41	0.51
1:C:99:TRP:HB2	1:C:111:THR:HG22	1.93	0.51
1:C:253:LEU:N	1:C:254:PRO:HD2	2.23	0.51
2:D:261:GLN:HA	2:D:305:PRO:HB2	1.92	0.51
1:C:30:ASP:O	1:C:31:PRO:C	2.54	0.50
2:D:286:ASN:H	2:D:286:ASN:ND2	2.08	0.50
1:A:103:GLY:O	1:A:104:ASP:C	2.54	0.50
2:D:45:THR:CG2	2:D:46:ASP:N	2.74	0.50
2:D:54:ALA:C	2:D:56:PRO:HD3	2.37	0.50
2:D:67:TRP:CD1	2:D:109:ILE:HD13	2.47	0.50
1:A:30:ASP:HB3	1:A:34:VAL:HB	1.94	0.49
1:C:139:ASP:OD2	1:C:222:ARG:NE	2.45	0.49
1:A:47:PRO:HG3	1:A:100:TYR:CE1	2.46	0.49
1:A:108:ILE:HG12	1:A:202:CYS:HA	1.95	0.49
2:B:220:HIS:O	2:B:221:GLN:HB2	2.12	0.49
2:D:97:VAL:HG12	2:D:98:GLU:N	2.27	0.49
1:C:63:GLU:HG2	1:C:184:ARG:HE	1.78	0.49
2:B:178:LYS:HB2	2:B:204:THR:HG22	1.95	0.49
1:A:47:PRO:HG3	1:A:100:TYR:CZ	2.48	0.48
2:B:299:THR:HG21	2:B:301:PHE:CZ	2.49	0.48
1:C:37:VAL:O	1:C:131:THR:HA	2.12	0.48
2:B:57:LEU:C	2:B:59:SER:H	2.21	0.48
2:D:286:ASN:HD22	2:D:286:ASN:N	2.09	0.48
1:A:126:VAL:HG22	1:A:126:VAL:O	2.13	0.48
2:B:191:GLY:HA3	2:B:211:TYR:CE1	2.48	0.48
2:B:224:LEU:HD12	2:B:225:ALA:N	2.29	0.48
2:B:164:ASP:HA	2:B:214:VAL:CG2	2.38	0.48
1:C:231:VAL:HG12	2:D:130:PRO:HB3	1.96	0.48
2:D:138:LEU:HD12	2:D:138:LEU:O	2.14	0.48
1:C:46:ASP:OD1	1:C:47:PRO:N	2.47	0.47
1:C:253:LEU:N	1:C:254:PRO:CD	2.69	0.47
2:D:34:GLN:HG3	2:D:35:VAL:N	2.29	0.47
1:A:233:LEU:HB3	1:A:237:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TYR:C	1:A:140:SER:H	2.23	0.47
2:D:160:LYS:CB	2:D:163:GLN:HE21	2.26	0.47
1:C:46:ASP:HA	1:C:47:PRO:HD3	1.62	0.47
2:D:267:LEU:HD13	2:D:329:VAL:HG11	1.97	0.47
1:A:53:ILE:CD1	1:A:173:TRP:HZ2	2.28	0.47
1:A:87:GLU:O	1:A:90:LYS:CG	2.63	0.47
1:C:101:ARG:HB2	1:C:110:ILE:HD11	1.95	0.47
2:D:173:THR:CG2	2:D:208:ILE:HG12	2.43	0.47
1:A:65:ALA:HB2	1:A:185:ALA:CB	2.45	0.47
2:D:310:LEU:HB2	2:D:333:ILE:HD11	1.96	0.47
2:B:265:VAL:O	2:B:302:PHE:HB2	2.15	0.47
1:C:186:ARG:CG	1:C:186:ARG:NH1	2.76	0.47
1:A:87:GLU:O	1:A:90:LYS:HG3	2.14	0.46
2:D:33:VAL:HA	5:D:401:HOH:O	2.15	0.46
2:D:43:ILE:HD11	2:D:116:LEU:CD1	2.44	0.46
2:D:260:LEU:HD11	2:D:308:TYR:CZ	2.50	0.46
1:A:158:PHE:CE1	1:A:186:ARG:HA	2.51	0.46
2:D:62:ILE:HD12	2:D:62:ILE:N	2.29	0.46
2:B:94:ARG:HG3	2:B:94:ARG:H	1.48	0.46
2:B:279:GLU:HB3	2:B:319:THR:HB	1.96	0.46
1:C:169:LYS:HG3	1:C:174:THR:OG1	2.16	0.46
2:D:157:LEU:HB2	2:D:243:VAL:HG12	1.98	0.46
1:C:69:VAL:O	1:C:152:LEU:HD12	2.16	0.46
2:D:93:TYR:HB3	2:D:97:VAL:CG2	2.46	0.46
2:D:93:TYR:HB3	2:D:97:VAL:HG23	1.98	0.46
2:D:225:ALA:CB	2:D:238:SER:HB3	2.43	0.46
1:A:106:CYS:HB2	1:A:203:LEU:O	2.16	0.46
1:A:186:ARG:HG3	1:A:186:ARG:NH1	2.29	0.46
1:C:39:HIS:HE1	1:C:215:ASP:OD2	1.99	0.46
2:D:91:ALA:HA	2:D:94:ARG:HG3	1.98	0.46
2:D:127:ALA:HA	2:D:133:ASN:OD1	2.16	0.46
2:D:76:GLN:HE21	2:D:76:GLN:HB3	1.56	0.46
1:C:59:TYR:HD1	1:C:60:ALA:N	2.14	0.45
2:D:220:HIS:HB2	2:D:243:VAL:HG23	1.97	0.45
1:C:71:LEU:HD22	1:C:179:PHE:HB3	1.98	0.45
2:B:194:GLU:O	2:B:209:SER:HA	2.17	0.45
2:B:130:PRO:O	2:B:131:THR:O	2.34	0.45
1:C:127:CYS:HB3	1:C:128:PRO:HD2	1.99	0.45
1:C:195:LEU:HD23	1:C:195:LEU:HA	1.79	0.45
1:C:139:ASP:HB2	1:C:222:ARG:HD2	1.99	0.45
2:B:67:TRP:CD1	2:B:109:ILE:HD13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:LEU:CD1	2:D:138:LEU:HD11	2.47	0.44
2:D:175:ALA:HA	2:D:206:THR:HG23	1.98	0.44
1:C:240:GLY:O	1:C:241:TRP:C	2.59	0.44
2:D:189:LEU:HG	2:D:222:GLN:HG2	1.98	0.44
1:A:147:ASP:O	1:A:148:ASN:HB2	2.17	0.44
2:B:255:ASP:C	2:B:257:ASN:H	2.25	0.44
1:A:31:PRO:O	1:A:32:PRO:C	2.61	0.44
1:A:118:CYS:HA	1:A:119:PRO:HD3	1.73	0.44
2:D:187:THR:HB	2:D:224:LEU:HD12	1.99	0.44
2:B:262:ARG:O	2:B:306:ILE:HG13	2.18	0.44
1:A:186:ARG:N	1:A:186:ARG:CD	2.80	0.44
1:A:219:MET:HE2	1:A:219:MET:HB3	1.90	0.44
2:B:111:LEU:HD13	2:B:114:LEU:HD11	1.99	0.44
2:D:57:LEU:HG	2:D:58:PRO:HD2	2.00	0.44
2:D:314:TYR:O	2:D:328:GLN:HA	2.17	0.44
1:A:30:ASP:HA	1:A:31:PRO:HD2	1.66	0.44
2:B:296:GLN:HB3	2:B:297:ASN:H	1.59	0.44
1:C:77:ALA:N	1:C:78:PRO:CD	2.81	0.44
2:D:43:ILE:CD1	2:D:116:LEU:HD13	2.46	0.43
1:A:116:THR:HG22	1:A:129:ILE:HB	2.00	0.43
2:B:279:GLU:HG3	2:B:281:HIS:CE1	2.53	0.43
2:B:79:ALA:HA	2:B:88:SER:O	2.18	0.43
2:B:96:ARG:NH2	2:B:118:ASP:OD2	2.52	0.43
2:D:297:ASN:ND2	2:D:297:ASN:H	2.16	0.43
1:A:158:PHE:HE1	1:A:186:ARG:HA	1.83	0.43
1:C:62:LEU:HD13	1:C:69:VAL:HB	2.00	0.43
1:C:252:LEU:HA	1:C:252:LEU:HD23	1.78	0.43
1:A:46:ASP:HA	1:A:47:PRO:HD3	1.82	0.43
1:C:104:ASP:O	1:C:105:ASN:HB2	2.18	0.43
2:B:228:VAL:CG1	2:B:235:PHE:HD1	2.27	0.43
2:B:324:THR:O	2:B:325:ARG:HD2	2.19	0.43
1:A:99:TRP:CH2	1:A:166:ARG:HB2	2.54	0.43
2:B:119:GLU:OE2	2:B:141:THR:HG23	2.18	0.43
1:C:161:ALA:HB2	1:C:183:HIS:CD2	2.54	0.43
2:D:160:LYS:HD3	2:D:160:LYS:HA	1.89	0.43
2:B:320:ASN:C	2:B:322:ILE:H	2.27	0.43
1:C:50:PRO:HA	1:C:51:PRO:HD3	1.74	0.43
2:B:180:PRO:HG3	2:B:205:VAL:CG2	2.49	0.43
2:B:187:THR:HB	2:B:224:LEU:HD13	2.00	0.43
1:A:100:TYR:HB3	1:A:107:ALA:HB1	2.01	0.43
2:D:42:PHE:CD1	2:D:143:MET:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HE1	1:A:181:LEU:HD22	2.00	0.42
1:A:173:TRP:CH2	1:A:175:GLU:HB2	2.54	0.42
2:B:229:ASN:HD21	2:B:234:ARG:HG3	1.83	0.42
2:B:43:ILE:HD11	2:B:116:LEU:CD1	2.40	0.42
2:B:62:ILE:N	2:B:62:ILE:HD12	2.34	0.42
2:B:219:ALA:HB3	2:B:243:VAL:HG21	2.02	0.42
2:D:116:LEU:HD12	2:D:116:LEU:HA	1.78	0.42
2:D:231:HIS:HB3	2:D:232:MET:H	1.55	0.42
2:D:262:ARG:HG3	2:D:263:MET:N	2.32	0.42
2:B:116:LEU:HD21	2:B:204:THR:HG23	2.02	0.42
1:C:137:TYR:N	1:C:137:TYR:HD2	2.18	0.42
1:A:44:LEU:HD21	1:A:112:VAL:HG21	2.01	0.42
1:A:206:LYS:O	1:A:210:GLN:HG2	2.19	0.42
1:A:253:LEU:HD13	1:A:253:LEU:HA	1.88	0.42
1:C:115:TYR:N	1:C:115:TYR:CD1	2.87	0.42
1:C:252:LEU:HB3	1:C:253:LEU:H	1.66	0.42
2:D:39:MET:HB2	2:D:140:LEU:HD23	2.02	0.42
2:D:99:PHE:HA	2:D:108:THR:O	2.20	0.42
1:A:51:PRO:HB2	1:A:53:ILE:O	2.20	0.42
1:C:153:MET:HE1	1:C:181:LEU:CD2	2.49	0.42
2:B:280:TYR:HB3	2:B:297:ASN:O	2.20	0.42
2:D:307:ASN:ND2	2:D:309:SER:OG	2.53	0.42
2:B:255:ASP:C	2:B:257:ASN:N	2.77	0.42
1:C:204:THR:O	1:C:207:ALA:HB3	2.20	0.42
1:A:217:ILE:HG13	1:A:219:MET:HG3	2.02	0.42
2:D:299:THR:HG21	2:D:301:PHE:CZ	2.55	0.42
1:A:37:VAL:O	1:A:131:THR:HA	2.20	0.41
2:D:320:ASN:HB2	2:D:321:PRO:HD2	2.02	0.41
2:B:76:GLN:HE21	2:B:76:GLN:HB3	1.64	0.41
1:A:37:VAL:HG12	1:A:131:THR:HG22	2.03	0.41
1:A:246:PRO:HA	1:A:247:PRO:HD2	1.84	0.41
1:C:157:ALA:HB1	1:C:159:GLU:OE1	2.21	0.41
2:B:53:PHE:HB3	2:B:105:THR:HG22	2.01	0.41
2:B:260:LEU:HD12	2:B:335:GLU:O	2.20	0.41
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.74	0.41
2:B:319:THR:HG23	2:B:324:THR:OG1	2.20	0.41
1:C:40:ILE:HG13	1:C:131:THR:CG2	2.51	0.41
2:B:57:LEU:C	2:B:59:SER:N	2.78	0.41
2:B:261:GLN:HA	2:B:305:PRO:HB2	2.02	0.41
2:D:67:TRP:CH2	2:D:124:CYS:HB2	2.55	0.41
1:A:142:SER:HA	1:A:152:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:LEU:HD22	2:B:141:THR:N	2.35	0.41
2:B:257:ASN:O	2:B:257:ASN:CG	2.64	0.41
2:B:320:ASN:CB	2:B:321:PRO:CD	2.98	0.41
1:C:56:THR:OG1	1:C:177:THR:HG23	2.20	0.41
1:A:93:TYR:CE2	1:A:118:CYS:HB2	2.55	0.41
1:A:134:ARG:HB3	1:A:219:MET:HB3	2.02	0.41
1:A:189:CYS:SG	1:A:190:LYS:N	2.93	0.41
2:B:116:LEU:HD12	2:B:116:LEU:HA	1.88	0.41
2:B:213:LEU:C	2:B:213:LEU:CD1	2.94	0.41
2:B:262:ARG:HB3	2:B:306:ILE:CD1	2.50	0.41
2:D:52:SER:HA	2:D:105:THR:O	2.21	0.41
2:D:132:GLY:O	2:D:133:ASN:OD1	2.39	0.41
1:A:197:ILE:HA	1:A:198:PRO:HD2	1.84	0.41
1:C:141:PHE:CD2	1:C:141:PHE:N	2.89	0.41
1:C:77:ALA:HB1	1:C:170:ILE:HD11	2.03	0.40
1:C:126:VAL:O	1:C:126:VAL:CG2	2.69	0.40
2:B:33:VAL:HG11	2:B:134:ARG:HB3	2.03	0.40
2:B:231:HIS:HB3	2:B:232:MET:H	1.58	0.40
1:A:53:ILE:HG22	1:A:54:PRO:O	2.22	0.40
2:B:114:LEU:HD12	2:B:114:LEU:HA	1.83	0.40
2:B:225:ALA:HB2	2:B:238:SER:HB3	2.02	0.40
1:C:156:PRO:HB2	1:C:160:THR:OG1	2.21	0.40
1:A:36:ARG:HA	1:A:36:ARG:HD3	1.92	0.40
2:B:311:ALA:HB2	2:B:333:ILE:HD12	2.03	0.40
1:A:68:SER:O	1:A:247:PRO:HA	2.22	0.40
2:B:240:THR:HG23	1:C:86:ASP:OD2	2.22	0.40
2:B:332:ASN:O	2:B:332:ASN:ND2	2.54	0.40
2:D:216:SER:OG	2:D:218:GLU:HG2	2.21	0.40
2:D:220:HIS:HB2	2:D:243:VAL:CG2	2.51	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	230/294 (78%)	205 (89%)	20 (9%)	5 (2%)	5	26
1	C	230/294 (78%)	202 (88%)	19 (8%)	9 (4%)	2	15
2	B	301/331 (91%)	268 (89%)	28 (9%)	5 (2%)	7	32
2	D	301/331 (91%)	273 (91%)	23 (8%)	5 (2%)	7	32
All	All	1062/1250 (85%)	948 (89%)	90 (8%)	24 (2%)	5	26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	72	ASN
2	B	131	THR
1	C	252	LEU
1	C	253	LEU
1	C	65	ALA
1	C	185	ALA
2	D	132	GLY
2	D	297	ASN
1	A	104	ASP
1	C	157	ALA
1	C	246	PRO
2	D	72	ASN
1	A	139	ASP
2	B	37	ASP
1	A	31	PRO
2	B	264	ASP
1	C	31	PRO
1	C	139	ASP
2	B	276	PRO
1	C	241	TRP
2	D	96	ARG
2	D	321	PRO
1	A	32	PRO
1	A	54	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	202/255 (79%)	179 (89%)	23 (11%)	5	22
1	C	202/255 (79%)	183 (91%)	19 (9%)	8	30
2	B	264/286 (92%)	216 (82%)	48 (18%)	2	8
2	D	264/286 (92%)	216 (82%)	48 (18%)	2	8
All	All	932/1082 (86%)	794 (85%)	138 (15%)	3	14

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	25	LEU
1	A	26	ASP
1	A	37	VAL
1	A	56	THR
1	A	59	TYR
1	A	67	ARG
1	A	89	ARG
1	A	90	LYS
1	A	105	ASN
1	A	126	VAL
1	A	139	ASP
1	A	144	VAL
1	A	149	LEU
1	A	165	LEU
1	A	175	GLU
1	A	184	ARG
1	A	186	ARG
1	A	195	LEU
1	A	206	LYS
1	A	213	THR
1	A	250	SER
1	A	253	LEU
2	B	35	VAL
2	B	37	ASP
2	B	51	CYS
2	B	65	VAL
2	B	66	THR
2	B	76	GLN
2	B	90	LEU
2	B	94	ARG
2	B	101	ARG
2	B	105	THR

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Mol	Chain	Res	Type
2	B	111	LEU
2	B	114	LEU
2	B	116	LEU
2	B	121	VAL
2	B	138	LEU
2	B	139	ASN
2	B	140	LEU
2	B	142	VAL
2	B	158	ARG
2	B	161	LYS
2	B	165	ASP
2	B	186	GLU
2	B	199	ARG
2	B	213	LEU
2	B	214	VAL
2	B	218	GLU
2	B	228	VAL
2	B	231	HIS
2	B	239	LEU
2	B	242	ASN
2	B	243	VAL
2	B	249	VAL
2	B	262	ARG
2	B	270	LYS
2	B	278	THR
2	B	279	GLU
2	B	285	LEU
2	B	286	ASN
2	B	289	LEU
2	B	291	LYS
2	B	297	ASN
2	B	303	LYS
2	B	307	ASN
2	B	313	THR
2	B	332	ASN
2	B	333	ILE
2	B	334	THR
2	B	335	GLU
1	C	29	THR
1	C	37	VAL
1	C	44	LEU
1	C	57	VAL

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Mol	Chain	Res	Type
1	C	76	GLU
1	C	115	TYR
1	C	123	SER
1	C	126	VAL
1	C	139	ASP
1	C	144	VAL
1	C	165	LEU
1	C	174	THR
1	C	184	ARG
1	C	186	ARG
1	C	188	SER
1	C	195	LEU
1	C	222	ARG
1	C	252	LEU
1	C	253	LEU
2	D	35	VAL
2	D	36	ASN
2	D	49	LEU
2	D	64	GLN
2	D	65	VAL
2	D	66	THR
2	D	74	SER
2	D	76	GLN
2	D	90	LEU
2	D	110	ARG
2	D	111	LEU
2	D	114	LEU
2	D	116	LEU
2	D	123	ILE
2	D	131	THR
2	D	139	ASN
2	D	140	LEU
2	D	142	VAL
2	D	156	VAL
2	D	157	LEU
2	D	161	LYS
2	D	167	VAL
2	D	171	THR
2	D	173	THR
2	D	182	VAL
2	D	199	ARG
2	D	214	VAL

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Mol	Chain	Res	Type
2	D	218	GLU
2	D	222	GLN
2	D	226	CYS
2	D	228	VAL
2	D	231	HIS
2	D	232	MET
2	D	240	THR
2	D	241	LEU
2	D	244	GLN
2	D	249	VAL
2	D	251	ILE
2	D	262	ARG
2	D	284	THR
2	D	285	LEU
2	D	286	ASN
2	D	289	LEU
2	D	291	LYS
2	D	297	ASN
2	D	303	LYS
2	D	334	THR
2	D	335	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
1	A	210	GLN
2	B	36	ASN
2	B	64	GLN
2	B	76	GLN
2	B	221	GLN
2	B	222	GLN
2	B	229	ASN
2	B	242	ASN
2	B	274	ASN
2	B	281	HIS
2	B	286	ASN
2	B	297	ASN
2	B	307	ASN
2	B	332	ASN
1	C	39	HIS
1	C	183	HIS

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Mol	Chain	Res	Type
1	C	228	GLN
2	D	34	GLN
2	D	72	ASN
2	D	76	GLN
2	D	163	GLN
2	D	202	ASN
2	D	242	ASN
2	D	274	ASN
2	D	281	HIS
2	D	286	ASN
2	D	297	ASN
2	D	307	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	$\# Z > 2$
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	1.40	3 (17%)
3	NAG	E	2	3	14,14,15	0.39	0	17,19,21	1.20	2 (11%)
3	NAG	F	1	1,3	14,14,15	0.54	0	17,19,21	1.32	1 (5%)
3	NAG	F	2	3	14,14,15	0.43	0	17,19,21	1.08	2 (11%)

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
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	C1-O5-C5	3.58	116.99	112.19
3	E	2	NAG	C1-O5-C5	3.36	116.69	112.19
3	E	1	NAG	C4-C3-C2	3.12	115.59	111.02
3	F	2	NAG	C1-O5-C5	2.75	115.87	112.19
3	F	2	NAG	C2-N2-C7	-2.67	119.32	122.90
3	E	1	NAG	O4-C4-C3	-2.47	104.56	110.38
3	E	1	NAG	O5-C1-C2	-2.11	108.02	111.29
3	E	2	NAG	C2-N2-C7	-2.06	120.14	122.90

There are no chirality outliers.

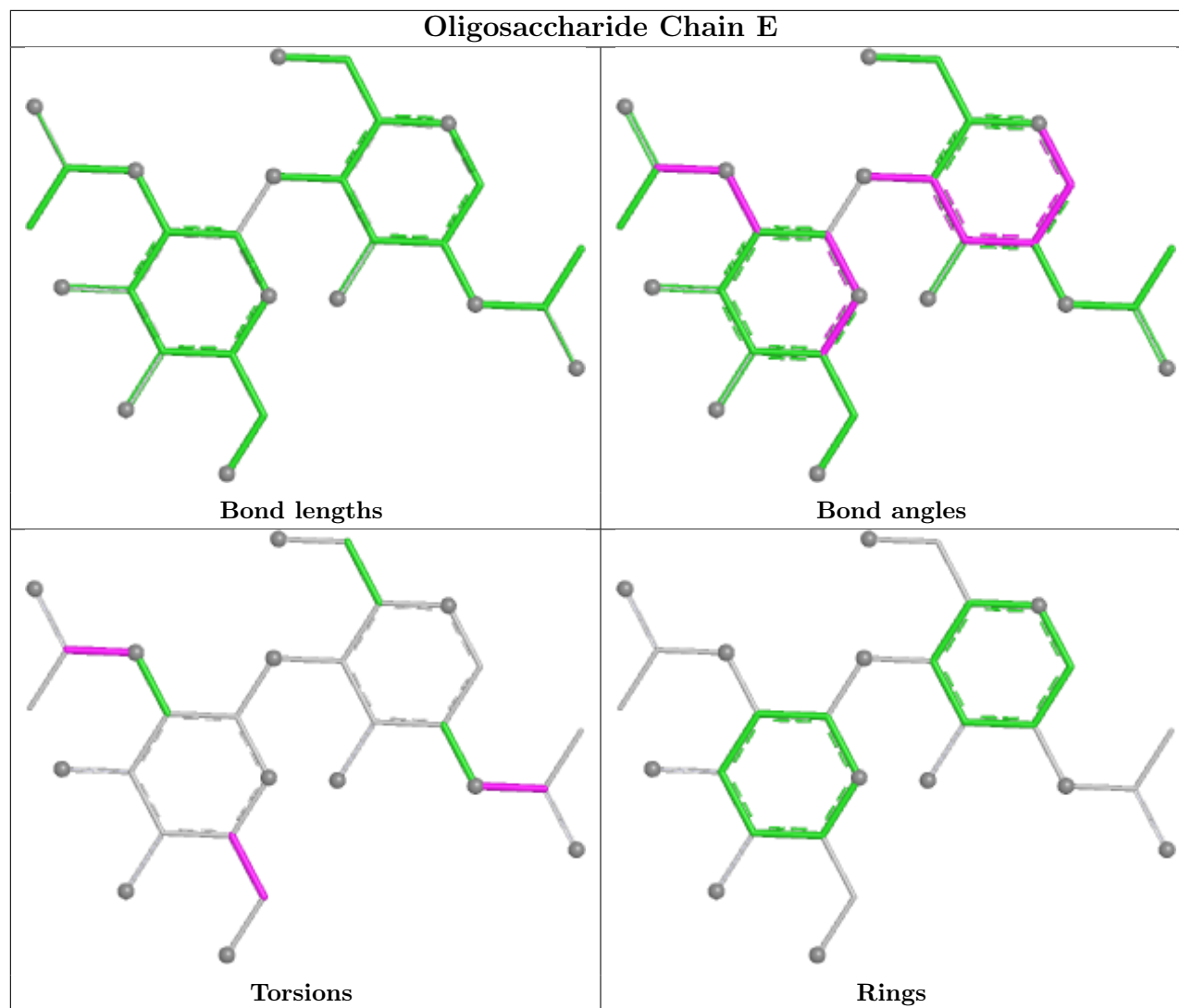
All (7) torsion outliers are listed below:

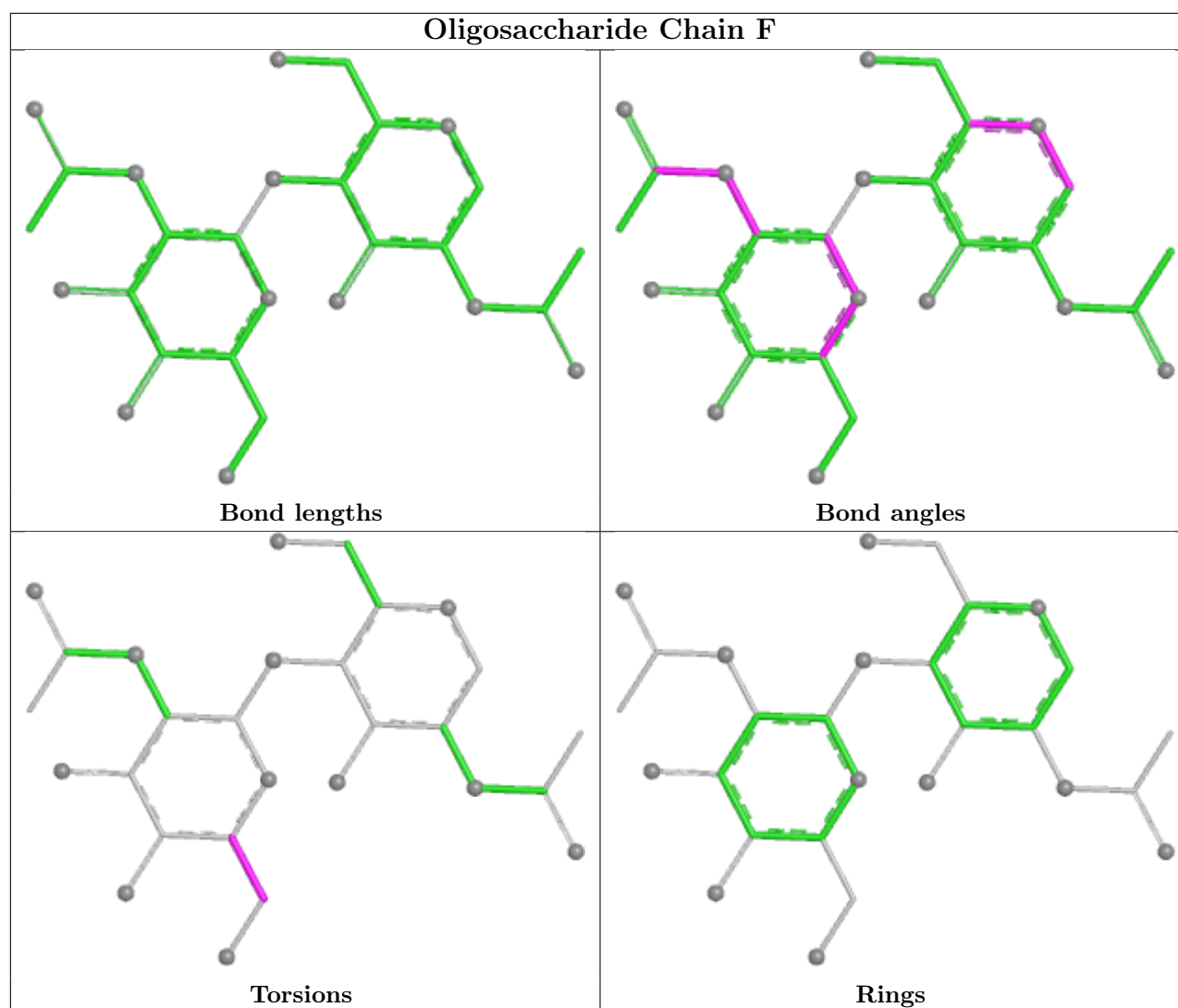
Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
3	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	NAG	C	503	1	14,14,15	0.55	0	17,19,21	0.95	0
4	NAG	A	503	1	14,14,15	0.58	0	17,19,21	0.90	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	C	503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	503	1	-	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.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503	NAG	C8-C7-N2-C2
4	C	503	NAG	O7-C7-N2-C2

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	232/294 (78%)	-0.27	2 (0%) 81 64	24, 70, 113, 178	0
1	C	232/294 (78%)	-0.08	4 (1%) 69 49	24, 78, 139, 175	0
2	B	303/331 (91%)	-0.25	1 (0%) 90 81	41, 70, 124, 182	0
2	D	303/331 (91%)	-0.18	6 (1%) 65 44	45, 78, 152, 238	0
All	All	1070/1250 (85%)	-0.20	13 (1%) 76 57	24, 75, 135, 238	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	335	GLU	3.5
2	D	162	GLY	3.4
1	A	193	LEU	2.9
1	C	23	PRO	2.8
2	B	335	GLU	2.7
2	D	57	LEU	2.6
2	D	53	PHE	2.5
1	C	187	ALA	2.4
1	C	242	HIS	2.3
1	C	24	VAL	2.3
2	D	59	SER	2.2
2	D	60	VAL	2.1
1	A	185	ALA	2.1

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

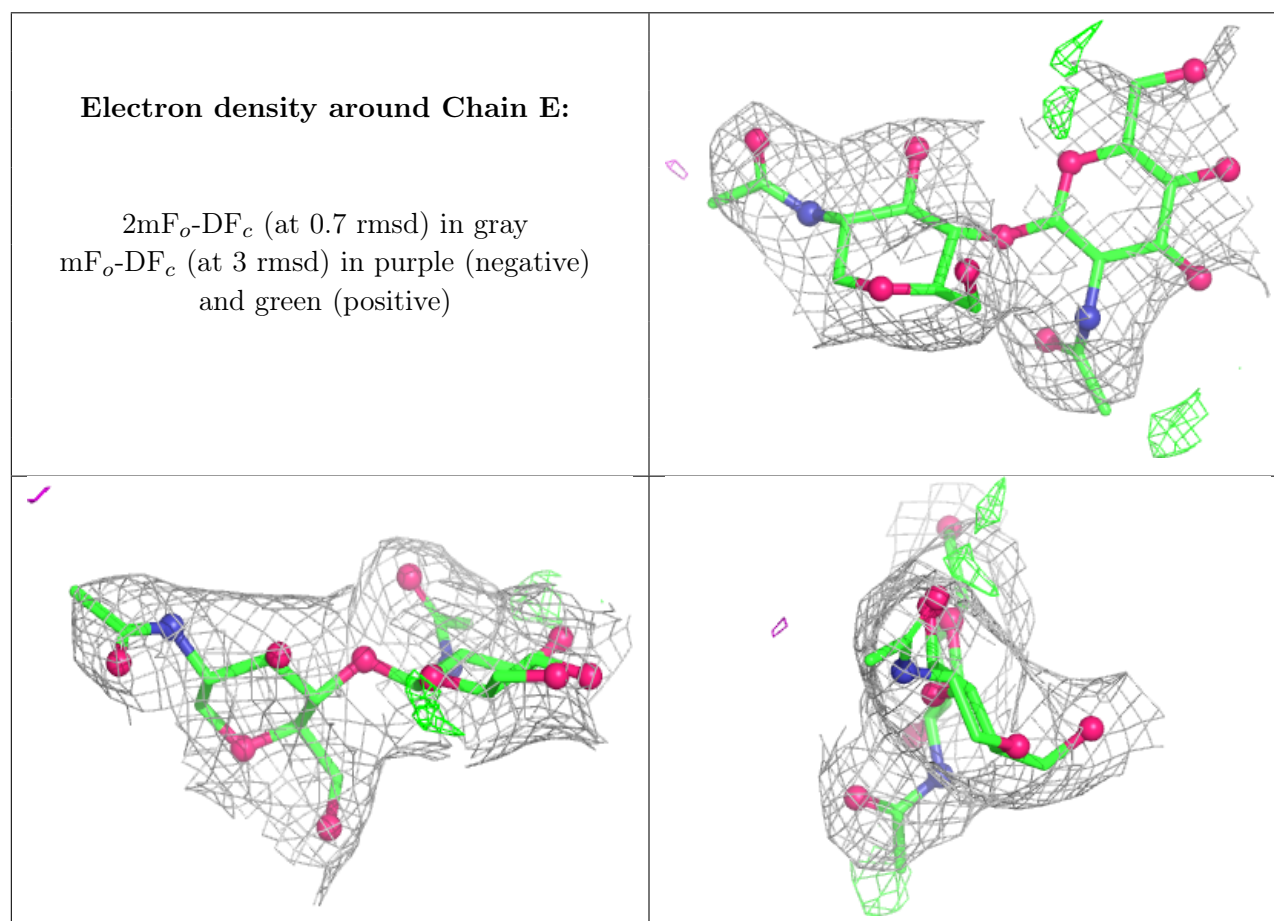
There are no non-standard protein/DNA/RNA residues in this entry.

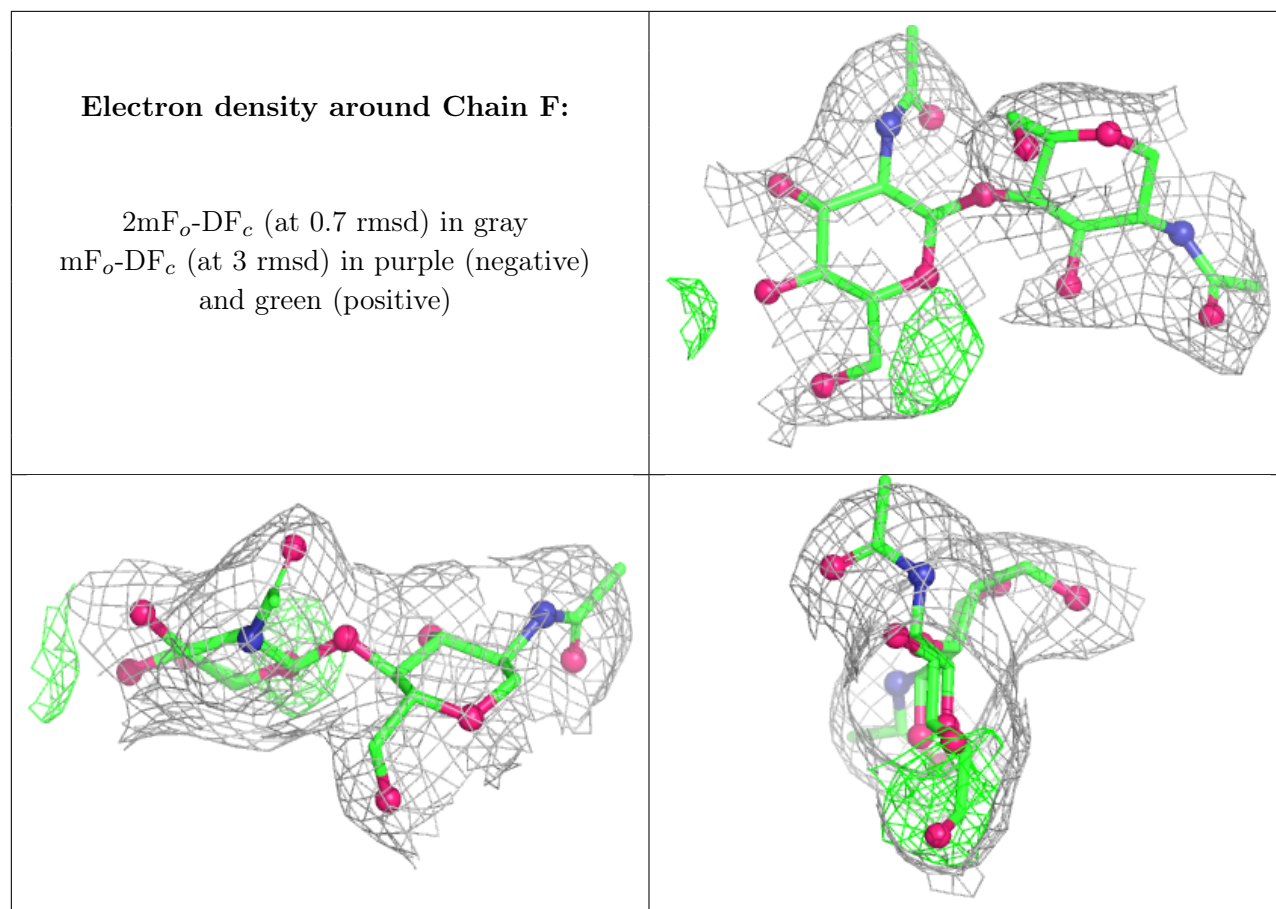
6.3 Carbohydrates [i](#)

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	NAG	E	2	14/15	0.77	0.12	86,99,109,109	0
3	NAG	F	2	14/15	0.83	0.10	73,80,90,91	0
3	NAG	E	1	14/15	0.95	0.08	59,65,75,77	0
3	NAG	F	1	14/15	0.96	0.06	62,67,71,71	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(Å ²)	Q<0.9
4	NAG	C	503	14/15	0.16	0.18	115,138,145,146	0
4	NAG	A	503	14/15	0.52	0.15	85,106,112,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.