



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:33 PM UTC

PDB ID : 8UDZ / pdb_00008udz
Title : The Structure of LTBP-49247 Fab Bound to TGFbeta1 Small Latent Complex
Authors : Streich Jr., F.C.; Nicholls, S.B.; Boston, C.J.; Ramachandran, S.
Deposited on : 2023-09-29
Resolution : 2.21 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

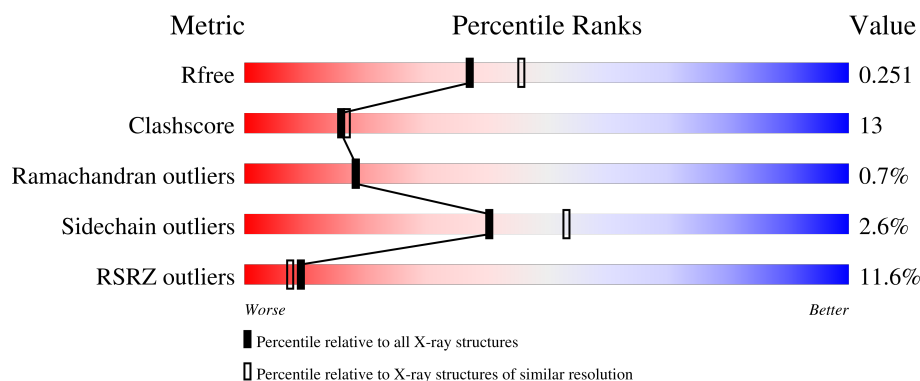
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	361	14% 46% 24% • 29%
1	B	361	11% 58% 23% • 19%
2	C	233	21% 69% 24% • 6%
2	E	233	5% 74% 22% •
3	D	218	5% 77% 21% •

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Mol	Chain	Length	Quality of chain
3	F	218	2% 88% 9% ..
4	G	5	20% 80%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11329 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 Transforming growth factor beta-1 proprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2062	1315	360	371	16			
1	B	294	Total	C	N	O	S	0	1	0
			2374	1520	413	424	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	SER	CYS	engineered mutation	UNP P01137
A	278	ALA	ARG	engineered mutation	UNP P01137
B	33	SER	CYS	engineered mutation	UNP P01137
B	278	ALA	ARG	engineered mutation	UNP P01137

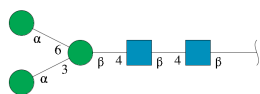
- Molecule 2 is a protein called LTBP-49247 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	220	Total	C	N	O	S	0	0	0
			1654	1044	291	313	6			
2	E	223	Total	C	N	O	S	0	0	0
			1676	1057	295	318	6			

- Molecule 3 is a protein called LTBP-49247 Fab Light Chain.

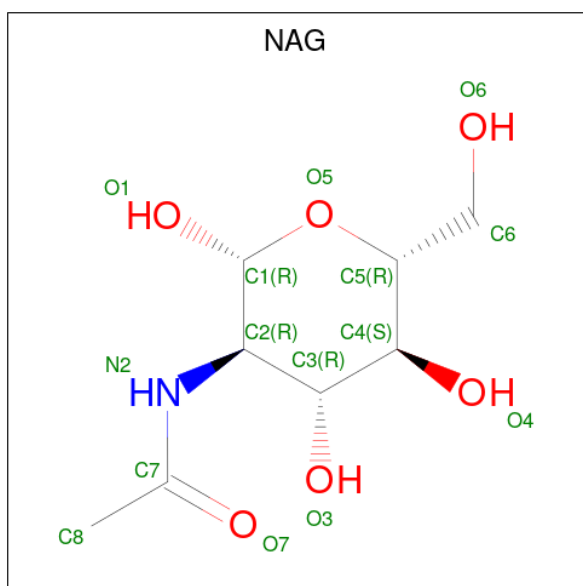
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1621	1006	270	340	5			
3	F	214	Total	C	N	O	S	0	0	0
			1621	1006	270	340	5			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

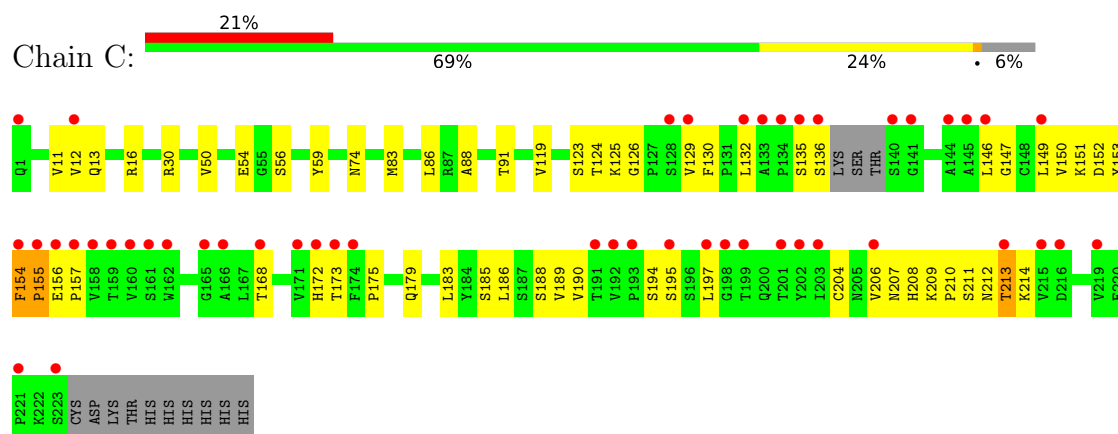
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	26	Total	O	0	0
			26	26		
6	B	30	Total	O	0	0
			30	30		
6	C	21	Total	O	0	0
			21	21		
6	D	30	Total	O	0	0
			30	30		

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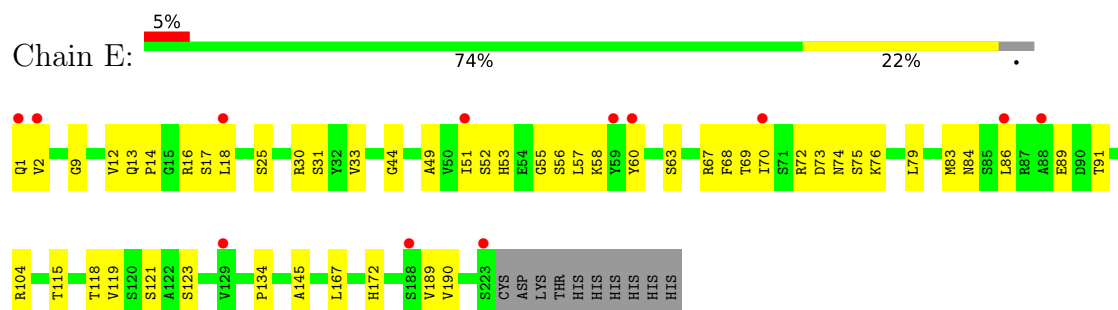
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	28	Total	O	0	0
			28	28		
6	F	97	Total	O	0	0
			97	97		

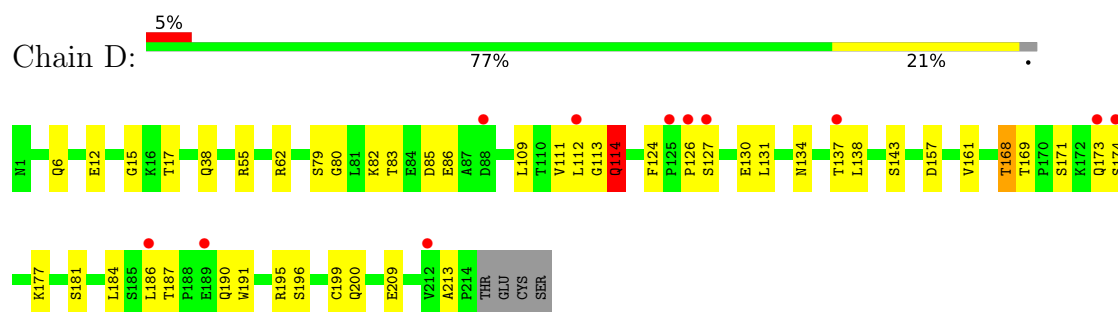
- Molecule 2: LTBP-49247 Fab Heavy Chain



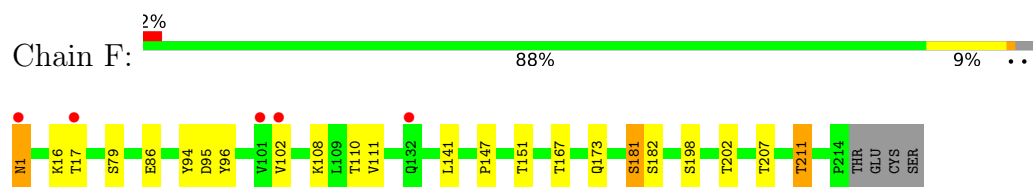
- Molecule 2: LTBP-49247 Fab Heavy Chain



- Molecule 3: LTBP-49247 Fab Light Chain



- Molecule 3: LTBP-49247 Fab Light Chain



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	73.50Å 141.91Å 186.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.50 – 2.21 73.50 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (73.50-2.21) 99.5 (73.50-2.21)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.264 (Not available) , 0.251	Depositor DCC
R_{free} test set	4924 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11329	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: BMA, NAG, MAN

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	0/2102	0.71	2/2838 (0.1%)
1	B	0.40	0/2432	0.61	0/3292
2	C	0.43	0/1693	0.63	1/2300 (0.0%)
2	E	0.35	0/1716	0.57	0/2332
3	D	0.40	0/1660	0.64	0/2267
3	F	0.47	0/1660	0.71	0/2267
All	All	0.41	0/11263	0.65	3/15296 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ASN	N-CA-C	-9.88	100.54	112.59
2	C	155	PRO	N-CA-C	-5.96	101.73	111.15
1	A	229	ASP	O-C-N	5.47	124.88	120.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	ARG	Sidechain

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	2062	0	2067	88	0
1	B	2374	0	2373	72	0
2	C	1654	0	1641	49	0
2	E	1676	0	1667	42	0
3	D	1621	0	1544	37	0
3	F	1621	0	1544	23	0
4	G	61	0	52	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
6	A	26	0	0	1	0
6	B	30	0	0	1	0
6	C	21	0	0	0	0
6	D	30	0	0	1	0
6	E	28	0	0	0	0
6	F	97	0	0	2	0
All	All	11329	0	10914	291	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 13.

All (291) 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)
3:F:17:THR:HG22	3:F:79:SER:CA	1.75	1.16
3:F:17:THR:CG2	3:F:79:SER:HA	1.88	1.03
3:F:17:THR:HG22	3:F:79:SER:HA	0.97	0.97
2:C:30:ARG:HG3	2:C:74:ASN:ND2	1.83	0.94
2:E:49:ALA:HB1	2:E:70:ILE:HD11	1.55	0.88
1:A:113:MET:SD	1:A:133:MET:HG2	2.17	0.84
1:A:80:LEU:HD12	1:A:110:ARG:HB3	1.61	0.81
1:A:228:ARG:NH1	1:B:124:PHE:CD1	2.49	0.81
1:A:113:MET:CE	1:A:256:PRO:HG2	2.13	0.79
2:E:51:ILE:HG22	2:E:58:LYS:HG2	1.64	0.79
1:B:303:ARG:HD2	1:B:315:LYS:HE2	1.65	0.79
1:A:88:VAL:HG21	1:A:195:TRP:HB2	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HD13	1:B:110:ARG:HB2	1.66	0.77
3:D:187:THR:HG1	3:D:190:GLN:H	1.33	0.76
1:A:113:MET:HE1	1:A:256:PRO:HG2	1.68	0.76
2:E:33:VAL:HG22	2:E:52:SER:HA	1.69	0.74
3:D:173:GLN:HG2	3:D:174:SER:N	2.04	0.72
2:C:155:PRO:HB2	2:C:210:PRO:HG2	1.72	0.70
2:E:83:MET:HB3	2:E:86:LEU:HD21	1.72	0.70
2:C:11:VAL:HG21	2:C:154:PHE:HZ	1.57	0.70
2:C:173:THR:HG23	2:C:188:SER:HB2	1.74	0.70
2:C:207:ASN:HA	2:C:214:LYS:HD2	1.74	0.70
1:A:289:THR:HG22	1:A:291:LYS:HG2	1.74	0.70
2:C:11:VAL:HG21	2:C:154:PHE:CZ	2.27	0.69
3:F:110:THR:HG21	3:F:147:PRO:HB3	1.74	0.69
2:C:151:LYS:NZ	2:C:152:ASP:OD2	2.23	0.69
3:D:168:THR:HG22	3:D:181:SER:H	1.55	0.69
1:A:67:GLU:OE1	1:A:67:GLU:N	2.20	0.69
3:D:86:GLU:HB2	3:D:111:VAL:HG12	1.74	0.69
1:A:88:VAL:HG21	1:A:195:TRP:CB	2.23	0.68
1:A:113:MET:SD	1:A:133:MET:HA	2.34	0.68
1:A:88:VAL:HG12	1:A:89:ALA:H	1.59	0.67
3:F:17:THR:HG22	3:F:79:SER:CB	2.25	0.66
3:D:200:GLN:HB3	3:D:209:GLU:HG3	1.79	0.65
1:A:42:LYS:O	1:A:46:ILE:HG13	1.96	0.65
3:F:167:THR:HG23	3:F:182:SER:HB3	1.78	0.65
3:D:173:GLN:HG2	3:D:174:SER:H	1.62	0.65
2:E:12:VAL:HG21	2:E:18:LEU:HG	1.79	0.64
3:D:173:GLN:OE1	3:D:177:LYS:HB2	1.98	0.64
3:F:141:LEU:HD23	3:F:181:SER:HB3	1.79	0.64
1:B:170:LEU:HD12	1:B:182:LEU:HD12	1.79	0.64
1:B:303:ARG:H	1:B:315:LYS:NZ	1.95	0.64
2:C:154:PHE:HB3	2:C:155:PRO:HD3	1.79	0.64
1:A:257:PHE:CZ	1:A:259:LEU:HB2	2.33	0.63
1:A:313:GLU:HG3	1:B:81:TYR:CE2	2.34	0.63
1:A:80:LEU:O	1:A:84:THR:HG23	1.99	0.63
1:B:66:GLY:H	1:B:68:VAL:HG22	1.64	0.63
3:F:17:THR:CG2	3:F:79:SER:CB	2.77	0.63
3:F:17:THR:CG2	3:F:79:SER:HB2	2.28	0.63
2:E:189:VAL:HG21	3:F:141:LEU:HD13	1.82	0.61
1:A:113:MET:SD	1:A:133:MET:CG	2.87	0.61
2:C:88:ALA:O	2:C:91:THR:HG22	2.01	0.60
1:A:113:MET:SD	1:A:133:MET:CB	2.89	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:186:LEU:HD22	3:D:190:GLN:NE2	2.17	0.60
2:C:194:SER:HA	2:C:197:LEU:HG	1.82	0.60
1:B:159:ARG:NH2	1:B:194:GLU:OE1	2.34	0.59
1:B:359:GLN:HB3	1:B:386:SER:OG	2.03	0.59
1:A:45:ARG:O	1:A:49:ILE:HG12	2.02	0.59
2:C:146:LEU:HB2	2:C:190:VAL:HG23	1.84	0.59
1:B:312:HIS:O	1:B:313:GLU:HG2	2.01	0.59
1:B:301:ASP:HB3	1:B:304:LYS:HB2	1.86	0.58
3:D:173:GLN:CG	3:D:174:SER:H	2.15	0.58
3:F:17:THR:HG21	3:F:79:SER:HB2	1.83	0.58
2:E:17:SER:OG	2:E:84:ASN:HA	2.04	0.58
3:D:186:LEU:HB3	3:D:190:GLN:HE21	1.69	0.57
2:E:67:ARG:O	2:E:84:ASN:HB2	2.03	0.57
1:A:88:VAL:HG11	1:A:195:TRP:C	2.29	0.57
1:A:185:ARG:NH2	1:A:198:PHE:HA	2.19	0.57
2:E:49:ALA:CB	2:E:70:ILE:HD11	2.31	0.57
3:D:113:GLY:O	3:D:114:GLN:HB3	2.04	0.57
2:C:172:HIS:HB3	2:C:189:VAL:HG12	1.85	0.57
2:E:12:VAL:HG12	2:E:13:GLN:O	2.05	0.57
1:A:168:VAL:O	1:A:184:ASN:HB2	2.04	0.57
2:E:86:LEU:HB3	2:E:119:VAL:HG21	1.87	0.56
1:A:170:LEU:HA	1:A:218:ARG:O	2.06	0.56
1:A:131:ILE:HD12	1:A:219:LEU:HD12	1.87	0.56
3:D:126:PRO:HD3	3:D:138:LEU:HD23	1.87	0.56
1:A:257:PHE:CE1	1:A:259:LEU:HB2	2.41	0.56
2:E:68:PHE:CZ	2:E:83:MET:HG2	2.40	0.56
1:A:170:LEU:HD12	1:A:218:ARG:O	2.06	0.56
1:A:162:LEU:HD12	1:A:189:PRO:HA	1.87	0.55
1:A:62:PRO:HB3	1:B:310:TRP:NE1	2.22	0.55
1:B:342:LEU:C	1:B:344:ASN:H	2.13	0.55
2:C:132:LEU:HD12	2:C:147:GLY:HA3	1.88	0.55
1:B:375:LYS:HD3	1:B:377:GLU:OE2	2.06	0.55
1:A:113:MET:HE2	1:A:256:PRO:HG2	1.89	0.55
1:B:175:SER:HB2	1:B:177:ASN:OD1	2.07	0.55
1:B:218:ARG:HE	1:B:220:SER:HG	1.53	0.55
1:A:196:LEU:HD23	1:A:197:SER:N	2.22	0.55
1:B:45:ARG:O	1:B:49:ILE:HG12	2.07	0.55
1:A:375:LYS:HE2	1:A:377:GLU:OE2	2.07	0.54
1:B:303:ARG:H	1:B:315:LYS:HZ3	1.53	0.54
1:B:342:LEU:O	1:B:344:ASN:N	2.39	0.54
2:E:17:SER:HG	2:E:84:ASN:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:THR:HG23	2:E:118:THR:HA	1.88	0.54
1:B:312:HIS:O	1:B:313:GLU:CG	2.56	0.54
1:A:223:CYS:HB3	1:A:236:ILE:HG13	1.89	0.53
2:C:208:HIS:CD2	2:C:210:PRO:HD2	2.42	0.53
1:B:174:TYR:O	1:B:175:SER:C	2.51	0.53
1:B:127:SER:OG	1:B:128:THR:N	2.42	0.53
3:D:62:ARG:HH21	3:D:85:ASP:CG	2.17	0.53
1:A:257:PHE:CD1	1:A:257:PHE:C	2.87	0.53
2:C:129:VAL:HG22	2:C:150:VAL:HG12	1.91	0.53
1:A:147:PRO:HG3	1:A:208:LEU:O	2.10	0.52
1:B:170:LEU:CD1	1:B:182:LEU:HD12	2.39	0.52
3:D:17:THR:HB	3:D:79:SER:HA	1.91	0.52
3:D:138:LEU:HD12	3:D:184:LEU:HD23	1.91	0.52
1:A:185:ARG:HH21	1:A:198:PHE:HA	1.75	0.52
3:D:62:ARG:NH2	3:D:85:ASP:OD1	2.42	0.52
1:B:113:MET:HB2	1:B:135:PHE:CZ	2.45	0.52
1:B:362:GLU:HB2	1:B:363:PRO:HD2	1.92	0.52
2:C:132:LEU:HD13	3:D:124:PHE:CE2	2.45	0.52
2:C:154:PHE:CB	2:C:155:PRO:HD3	2.40	0.52
2:E:12:VAL:HG11	2:E:86:LEU:HD12	1.92	0.52
3:F:95:ASP:O	3:F:96:TYR:HB2	2.10	0.51
1:A:84:THR:HG21	1:A:108:VAL:HG11	1.92	0.51
1:B:131:ILE:CG2	1:B:219:LEU:HB3	2.39	0.51
1:B:326:CYS:HB3	1:B:354:PRO:HB2	1.92	0.51
1:A:257:PHE:CD1	1:A:258:LEU:N	2.79	0.51
2:C:130:PHE:HD2	2:C:149:LEU:HD22	1.75	0.51
2:E:12:VAL:HG13	2:E:16:ARG:HB2	1.93	0.51
1:A:313:GLU:HB3	1:A:314:PRO:HD3	1.92	0.51
2:C:153:TYR:C	2:C:183:LEU:HD22	2.34	0.51
1:A:313:GLU:HB2	1:A:367:VAL:HB	1.93	0.51
1:A:41:VAL:HG21	1:B:323:LEU:HD22	1.93	0.50
1:A:171:TYR:HB2	1:A:218:ARG:HB2	1.93	0.50
1:A:225:CYS:HA	1:A:233:GLN:O	2.12	0.50
1:A:303:ARG:NH1	6:A:501:HOH:O	2.45	0.50
2:C:151:LYS:HG2	2:C:152:ASP:OD2	2.12	0.50
1:A:38:MET:HG2	1:A:42:LYS:HE2	1.93	0.50
1:A:111:VAL:HG21	1:A:140:LEU:HD23	1.93	0.50
1:A:141:ARG:HH21	1:A:209:SER:C	2.19	0.50
1:B:312:HIS:O	1:B:313:GLU:CD	2.55	0.50
1:A:113:MET:SD	1:A:133:MET:CA	3.00	0.49
1:B:249:THR:O	1:B:256:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLU:HB3	1:A:314:PRO:CD	2.41	0.49
1:A:204:VAL:HG11	1:A:260:LEU:HD21	1.94	0.49
1:B:347:ASN:CG	1:B:354:PRO:HG3	2.37	0.49
1:A:127:SER:OG	1:A:130:SER:N	2.38	0.49
1:A:292:ASN:O	1:A:324:GLY:HA3	2.12	0.49
1:A:45:ARG:HG2	1:B:298:LEU:HD23	1.95	0.49
1:A:145:PRO:HB2	1:A:146:GLU:OE1	2.12	0.49
2:E:104:ARG:HB3	3:F:94:TYR:CG	2.48	0.49
1:B:113:MET:HG2	1:B:114:VAL:N	2.27	0.48
2:C:129:VAL:HG21	2:C:206:VAL:HG11	1.95	0.48
1:B:177:ASN:OD1	1:B:177:ASN:N	2.46	0.48
1:B:312:HIS:O	1:B:313:GLU:OE2	2.30	0.48
3:F:17:THR:CG2	3:F:79:SER:CA	2.64	0.48
1:A:224:SER:O	1:A:234:VAL:HA	2.14	0.48
1:A:228:ARG:HA	1:A:228:ARG:NE	2.28	0.48
1:A:287:SER:O	1:A:288:SER:HB3	2.13	0.48
1:A:38:MET:HE3	1:A:42:LYS:NZ	2.29	0.48
2:C:83:MET:HE2	2:C:86:LEU:HD21	1.95	0.48
2:C:208:HIS:O	2:C:214:LYS:HE2	2.14	0.48
3:D:86:GLU:HG3	3:D:109:LEU:O	2.14	0.48
2:E:9:GLY:HA3	2:E:115:THR:HB	1.96	0.48
2:E:189:VAL:CG2	3:F:141:LEU:HD13	2.44	0.48
1:A:362:GLU:OE2	1:A:385:ARG:HD3	2.14	0.48
2:C:179:GLN:OE1	2:C:185:SER:OG	2.32	0.47
3:D:83:THR:HA	3:D:111:VAL:HG11	1.96	0.47
3:D:173:GLN:CG	3:D:174:SER:N	2.65	0.47
1:A:169:GLU:OE2	1:A:222:HIS:HD2	1.97	0.47
1:A:156:ARG:HB2	1:A:257:PHE:CD2	2.50	0.47
2:C:12:VAL:O	2:C:119:VAL:HA	2.15	0.47
2:C:30:ARG:O	2:C:30:ARG:HG2	2.14	0.47
3:D:82:LYS:O	3:D:111:VAL:HG21	2.15	0.47
3:D:168:THR:HG23	3:D:169:THR:O	2.15	0.47
2:E:172:HIS:NE2	3:F:173:GLN:OE1	2.43	0.47
1:B:113:MET:HE3	1:B:256:PRO:HB2	1.96	0.47
1:B:232:LEU:HD21	1:B:234:VAL:HG23	1.97	0.47
3:D:86:GLU:HB2	3:D:111:VAL:CG1	2.44	0.47
1:B:118:ASN:OD1	1:B:119:GLU:HG3	2.15	0.47
2:C:149:LEU:HD21	2:C:151:LYS:HB2	1.97	0.47
2:E:73:ASP:OD1	2:E:76:LYS:NZ	2.47	0.47
1:A:62:PRO:HB3	1:B:310:TRP:CD1	2.50	0.46
2:C:208:HIS:CE1	2:C:211:SER:HG	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:H	1:A:67:GLU:CD	2.19	0.46
1:B:181:TYR:OH	1:B:184:ASN:ND2	2.43	0.46
1:B:312:HIS:C	1:B:313:GLU:HG2	2.41	0.46
2:C:154:PHE:O	2:C:155:PRO:C	2.59	0.46
2:E:17:SER:OG	2:E:83:MET:O	2.25	0.46
1:A:222:HIS:HE2	1:B:169:GLU:CD	2.23	0.46
2:E:134:PRO:HA	2:E:145:ALA:O	2.15	0.46
1:B:113:MET:HE2	1:B:133:MET:HG2	1.98	0.46
2:C:150:VAL:CG2	2:C:186:LEU:HG	2.45	0.46
3:D:168:THR:CG2	3:D:181:SER:H	2.26	0.45
1:B:315:LYS:HA	1:B:315:LYS:HD2	1.69	0.45
1:B:359:GLN:HA	1:B:388:LYS:HE2	1.98	0.45
3:F:202:THR:OG1	3:F:207:THR:HG22	2.17	0.45
3:D:196:SER:HB2	3:D:213:ALA:HB2	1.97	0.45
1:B:80:LEU:HD11	1:B:108:VAL:HG12	1.98	0.45
2:C:156:GLU:O	2:C:157:PRO:C	2.60	0.45
2:C:175:PRO:HG2	3:D:171:SER:OG	2.16	0.45
1:A:141:ARG:O	1:A:145:PRO:HA	2.17	0.45
1:B:36:ILE:HD12	1:B:36:ILE:N	2.32	0.45
3:D:187:THR:OG1	3:D:190:GLN:HG3	2.17	0.45
2:E:83:MET:HB3	2:E:86:LEU:CD2	2.44	0.45
2:C:50:VAL:HG12	2:C:59:TYR:HB2	1.98	0.44
1:A:222:HIS:NE2	1:B:169:GLU:OE2	2.42	0.44
1:A:289:THR:CG2	1:A:291:LYS:HG2	2.45	0.44
2:C:124:THR:HA	2:C:154:PHE:HB3	1.98	0.44
3:D:112:LEU:HA	3:D:112:LEU:HD23	1.60	0.44
2:E:51:ILE:HD11	2:E:79:LEU:CD1	2.47	0.44
1:B:340:LEU:HG	1:B:341:ALA:H	1.81	0.44
2:E:30:ARG:HG2	2:E:74:ASN:HB3	1.99	0.44
2:E:55:GLY:O	2:E:57:LEU:N	2.51	0.44
1:A:40:LEU:HD11	2:E:31:SER:HB2	1.99	0.44
1:B:65:GLN:OE1	1:B:68:VAL:HG11	2.18	0.44
3:F:108:LYS:NZ	6:F:308:HOH:O	2.50	0.44
1:A:195:TRP:HB3	1:A:196:LEU:H	1.59	0.44
2:E:63:SER:O	2:E:67:ARG:NH2	2.45	0.44
1:A:368:TYR:HE1	1:A:377:GLU:HG3	1.82	0.44
1:A:156:ARG:HG3	1:A:257:PHE:CE2	2.53	0.43
2:C:208:HIS:HD2	2:C:210:PRO:HD2	1.82	0.43
1:A:152:ARG:HB3	1:A:261:MET:HE3	1.99	0.43
1:A:185:ARG:HG3	1:A:198:PHE:CE1	2.53	0.43
1:B:367:VAL:HG22	1:B:376:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:198:SER:OG	3:F:211:THR:HB	2.18	0.43
1:A:113:MET:SD	1:A:133:MET:HB3	2.59	0.43
2:E:14:PRO:HA	2:E:119:VAL:CG1	2.48	0.43
2:E:30:ARG:O	2:E:53:HIS:HB2	2.17	0.43
1:A:57:LEU:O	1:A:59:LEU:HD13	2.19	0.43
1:B:218:ARG:NE	1:B:220:SER:OG	2.37	0.43
2:E:83:MET:HB2	2:E:83:MET:HE3	1.75	0.43
1:B:162:LEU:HD12	1:B:163:LYS:H	1.82	0.43
2:E:44:GLY:HA3	6:F:336:HOH:O	2.19	0.43
3:D:131:LEU:HD11	3:D:191:TRP:HD1	1.83	0.43
3:D:134:ASN:O	3:D:134:ASN:ND2	2.51	0.43
1:A:136:ASN:OD1	1:A:139:GLU:HB2	2.18	0.43
2:C:13:GLN:H	2:C:13:GLN:HG2	1.70	0.43
2:E:12:VAL:CG1	2:E:16:ARG:HB2	2.49	0.43
3:D:12:GLU:O	3:D:112:LEU:HB2	2.19	0.42
1:A:67:GLU:OE2	1:B:371:GLY:O	2.37	0.42
1:B:133:MET:C	1:B:134:PHE:HD1	2.27	0.42
1:B:370:VAL:HG11	1:B:375:LYS:HE2	2.01	0.42
2:C:12:VAL:HG11	2:C:86:LEU:HD13	2.01	0.42
2:C:125:LYS:NZ	2:C:126:GLY:O	2.43	0.42
3:D:83:THR:O	3:D:111:VAL:HG11	2.20	0.42
3:D:130:GLU:OE2	3:D:137:THR:HG23	2.19	0.42
3:F:1:ASN:HB2	3:F:102:VAL:HG21	2.01	0.42
1:A:127:SER:HG	1:A:130:SER:H	1.61	0.42
2:C:130:PHE:CE2	3:D:130:GLU:HG3	2.54	0.42
1:A:380:SER:O	1:B:56:LYS:HE2	2.20	0.42
3:D:157:ASP:OD1	3:D:195:ARG:HB2	2.19	0.42
1:A:127:SER:OG	1:A:129:HIS:N	2.50	0.42
1:B:341:ALA:HB1	1:B:343:TYR:HD2	1.83	0.42
2:C:155:PRO:HG2	2:C:210:PRO:HB3	2.01	0.42
1:A:67:GLU:HG2	1:B:372:ARG:HB3	2.02	0.42
1:A:127:SER:HG	1:A:130:SER:N	2.16	0.42
1:A:323:LEU:HD22	1:B:38[B]:MET:HG2	2.02	0.42
1:B:296:ARG:HB2	1:B:321:PHE:CE1	2.54	0.42
2:C:30:ARG:HD2	2:C:74:ASN:HB3	2.01	0.42
2:C:54:GLU:OE1	2:C:56:SER:N	2.53	0.42
2:E:51:ILE:HD11	2:E:79:LEU:HD12	2.02	0.42
1:B:213:GLU:O	1:B:214:ILE:HD13	2.19	0.42
2:E:14:PRO:HD3	2:E:121:SER:OG	2.20	0.42
2:E:51:ILE:HD12	2:E:72:ARG:HD2	2.02	0.42
1:A:162:LEU:HD13	1:A:164:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASP:C	1:A:236:ILE:HD12	2.45	0.42
2:E:89:GLU:OE1	2:E:89:GLU:N	2.52	0.42
1:B:113:MET:CE	1:B:256:PRO:HD2	2.50	0.41
2:E:1:GLN:HB3	2:E:2:VAL:H	1.59	0.41
3:F:17:THR:HG21	3:F:79:SER:CB	2.45	0.41
1:A:169:GLU:O	1:A:219:LEU:HA	2.20	0.41
3:D:15:GLY:O	3:D:80:GLY:HA2	2.20	0.41
2:E:60:TYR:OH	2:E:69:THR:HA	2.20	0.41
2:C:154:PHE:CD2	2:C:155:PRO:HD3	2.55	0.41
1:B:145:PRO:HG2	1:B:149:LEU:HD12	2.02	0.41
1:A:63:PRO:O	1:A:65:GLN:HG2	2.20	0.41
2:E:68:PHE:N	2:E:68:PHE:CD1	2.89	0.41
1:A:88:VAL:HG12	1:A:89:ALA:N	2.31	0.41
1:B:340:LEU:CG	1:B:341:ALA:H	2.33	0.41
1:B:131:ILE:HD11	1:B:250:ILE:HG23	2.02	0.41
2:C:135:SER:OG	2:C:136:SER:N	2.53	0.41
3:F:16:LYS:HA	3:F:16:LYS:HD3	1.90	0.41
3:F:86:GLU:CG	3:F:111:VAL:H	2.34	0.41
1:B:56:LYS:HE3	1:B:103:TYR:O	2.21	0.40
1:B:75:GLU:HG3	6:B:503:HOH:O	2.21	0.40
2:C:12:VAL:HG22	2:C:16:ARG:HB2	2.03	0.40
2:C:209:LYS:HB2	2:C:210:PRO:HD3	2.02	0.40
2:E:167:LEU:HD21	2:E:190:VAL:HG11	2.03	0.40
2:C:83:MET:HB3	2:C:86:LEU:HD21	2.02	0.40
2:C:212:ASN:HA	2:C:214:LYS:HE3	2.03	0.40
1:A:44:LYS:N	1:A:44:LYS:HD3	2.34	0.40
1:B:359:GLN:HG3	1:B:388:LYS:HD3	2.02	0.40
1:A:84:THR:CG2	1:A:108:VAL:HG11	2.52	0.40
1:B:370:VAL:HG11	1:B:375:LYS:CE	2.51	0.40
1:B:114:VAL:HG22	1:B:134:PHE:O	2.22	0.40
1:B:185:ARG:HG3	1:B:198:PHE:CE2	2.56	0.40
2:C:213:THR:C	2:C:214:LYS:HD3	2.46	0.40
3:D:55:ARG:HD2	6:D:304:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/361 (66%)	223 (94%)	11 (5%)	3 (1%)	9	7
1	B	281/361 (78%)	258 (92%)	20 (7%)	3 (1%)	11	9
2	C	216/233 (93%)	204 (94%)	11 (5%)	1 (0%)	24	26
2	E	221/233 (95%)	211 (96%)	9 (4%)	1 (0%)	24	26
3	D	212/218 (97%)	201 (95%)	10 (5%)	1 (0%)	24	26
3	F	212/218 (97%)	205 (97%)	7 (3%)	0	100	100
All	All	1379/1624 (85%)	1302 (94%)	68 (5%)	9 (1%)	18	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	SER
2	C	154	PHE
1	A	313	GLU
2	E	56	SER
1	B	251	HIS
1	B	125	LYS
1	A	256	PRO
1	A	320	ASN
3	D	114	GLN

5.3.2 Protein sidechains [i](#)

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	143/321 (44%)	137 (96%)	6 (4%)	26	34
1	B	260/321 (81%)	257 (99%)	3 (1%)	63	76
2	C	170/195 (87%)	165 (97%)	5 (3%)	37	49
2	E	185/195 (95%)	182 (98%)	3 (2%)	55	70
3	D	187/191 (98%)	179 (96%)	8 (4%)	26	33
3	F	187/191 (98%)	183 (98%)	4 (2%)	47	61
All	All	1132/1414 (80%)	1103 (97%)	29 (3%)	40	53

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	LEU
1	A	257	PHE
1	A	313	GLU
1	A	323	LEU
1	A	388	LYS
1	A	389	CYS
1	B	174	TYR
1	B	225	CYS
1	B	296	ARG
2	C	123	SER
2	C	168	THR
2	C	195	SER
2	C	204	CYS
2	C	213	THR
3	D	6	GLN
3	D	38	GLN
3	D	114	GLN
3	D	127	SER
3	D	143	SER
3	D	161	VAL
3	D	168	THR
3	D	199	CYS
2	E	25	SER
2	E	75	SER
2	E	123	SER
3	F	1	ASN
3	F	151	THR
3	F	181	SER
3	F	211	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	GLN
1	A	381	ASN
1	B	206	GLN
2	C	53	HIS
3	D	54	GLN
3	D	134	ASN
3	D	190	GLN
3	D	200	GLN
2	E	13	GLN
2	E	82	GLN
2	E	212	ASN
3	F	203	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

5 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	G	1	1,4	14,14,15	0.37	0	17,19,21	0.67	0
4	NAG	G	2	4	14,14,15	0.36	0	17,19,21	0.77	1 (5%)
4	BMA	G	3	4	11,11,12	1.01	0	15,15,17	1.29	2 (13%)
4	MAN	G	4	4	11,11,12	1.57	3 (27%)	15,15,17	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	G	5	4	11,11,12	1.54	3 (27%)	15,15,17	1.43	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	MAN	G	5	4	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	MAN	C2-C3	3.39	1.57	1.52
4	G	4	MAN	C1-C2	3.09	1.59	1.52
4	G	4	MAN	O5-C5	2.56	1.48	1.43
4	G	5	MAN	C1-C2	2.47	1.58	1.52
4	G	5	MAN	O5-C5	2.25	1.47	1.43
4	G	4	MAN	C2-C3	2.06	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	MAN	C1-O5-C5	3.64	117.07	112.19
4	G	4	MAN	C1-O5-C5	3.17	116.43	112.19
4	G	2	NAG	C1-O5-C5	2.62	115.69	112.19
4	G	3	BMA	C1-O5-C5	2.60	115.67	112.19
4	G	5	MAN	C1-C2-C3	2.29	112.98	109.64
4	G	3	BMA	O2-C2-C3	-2.19	105.62	110.15
4	G	4	MAN	O2-C2-C3	-2.08	105.84	110.15
4	G	5	MAN	O2-C2-C3	-2.06	105.89	110.15

There are no chirality outliers.

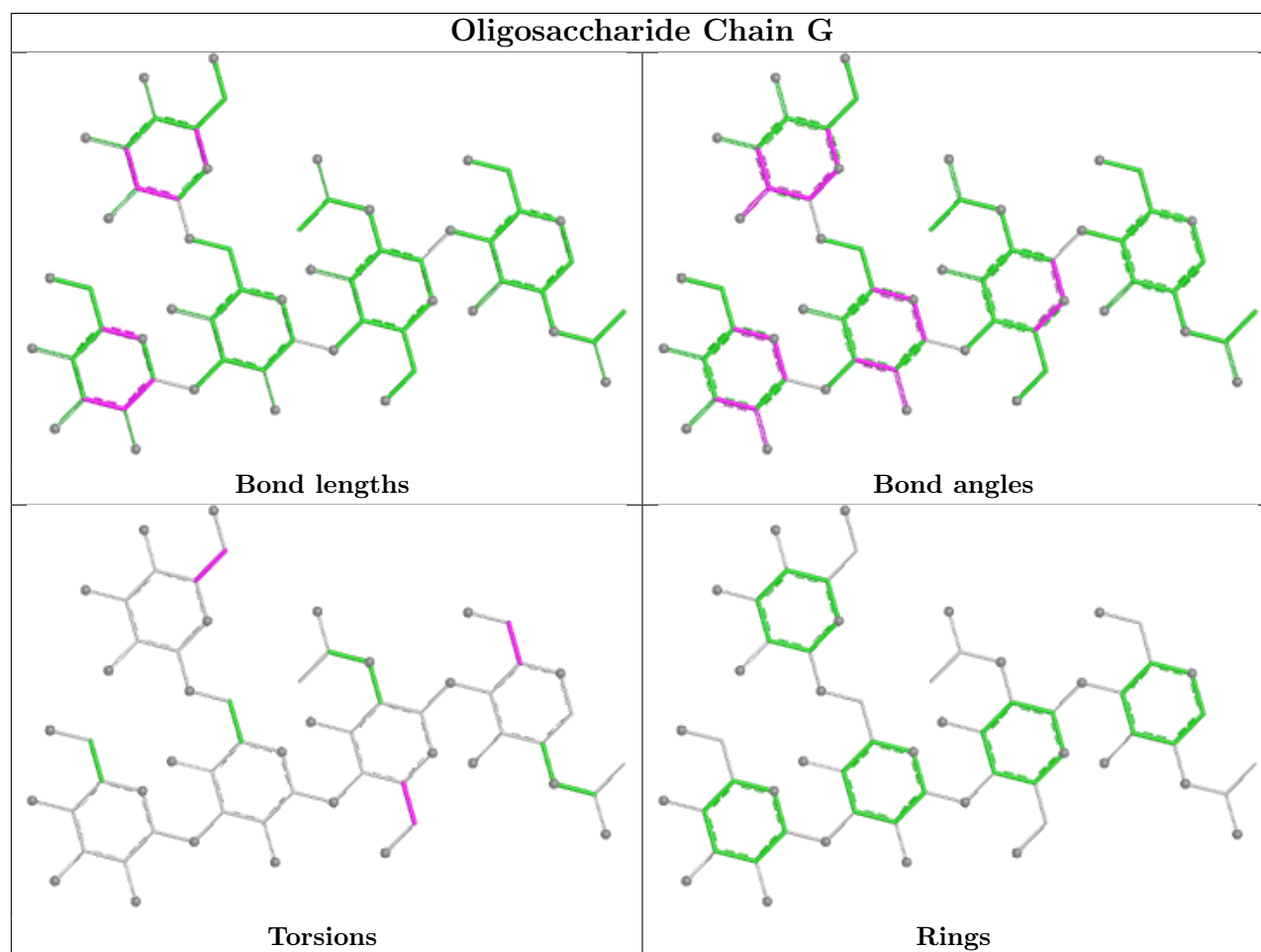
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	NAG	O5-C5-C6-O6
4	G	5	MAN	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	G	5	MAN	C4-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
5	NAG	B	401	1	14,14,15	0.75	1 (7%)	17,19,21	0.69	1 (5%)
5	NAG	A	401	1	14,14,15	0.38	0	17,19,21	0.51	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	B	401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	401	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	NAG	C1-C2	2.07	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	NAG	C1-O5-C5	2.35	115.33	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C4-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
5	B	401	NAG	O5-C5-C6-O6
5	B	401	NAG	C4-C5-C6-O6

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	257/361 (71%)	1.11	49 (19%)	3 2	30, 95, 128, 136	0
1	B	294/361 (81%)	0.92	40 (13%)	7 5	39, 76, 119, 140	1 (0%)
2	C	220/233 (94%)	1.05	48 (21%)	2 1	44, 88, 159, 186	0
2	E	223/233 (95%)	0.59	12 (5%)	31 28	54, 79, 114, 132	0
3	D	214/218 (98%)	0.56	11 (5%)	33 30	45, 78, 131, 158	0
3	F	214/218 (98%)	-0.01	5 (2%)	61 59	43, 55, 81, 112	0
All	All	1422/1624 (87%)	0.73	165 (11%)	9 7	30, 76, 132, 186	1 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	PHE	7.4
1	A	327	PRO	5.7
2	C	215	VAL	5.5
1	B	121	TYR	5.4
1	B	120	ILE	5.3
1	B	340	LEU	5.2
2	C	191	THR	5.1
1	B	342	LEU	4.8
1	A	313	GLU	4.6
2	C	154	PHE	4.6
2	E	70	ILE	4.4
2	C	213	THR	4.4
2	C	166	ALA	4.3
1	A	114	VAL	4.3
1	A	265	LEU	4.3
2	C	159	THR	4.2
1	B	174	TYR	4.2
1	B	66	GLY	4.0
1	B	241	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	131	ILE	3.9
1	A	158	LEU	3.9
2	C	160	VAL	3.9
1	B	265	LEU	3.8
2	C	162	TRP	3.8
1	B	328	TYR	3.8
1	A	89	ALA	3.8
2	C	135	SER	3.8
2	C	219	VAL	3.8
1	A	73	LEU	3.7
1	A	115	GLU	3.6
1	B	68	VAL	3.6
1	B	192	SER	3.5
2	E	223	SER	3.4
2	C	136	SER	3.4
2	C	133	ALA	3.4
1	A	70	PRO	3.3
1	A	112	LEU	3.3
1	B	250	ILE	3.3
2	C	203	ILE	3.3
1	B	70	PRO	3.3
1	A	140	LEU	3.3
1	A	314	PRO	3.2
1	B	69	PRO	3.2
1	A	195	TRP	3.2
2	C	221	PRO	3.2
3	D	186	LEU	3.1
2	C	202	TYR	3.1
1	B	36	ILE	3.1
1	B	186	LEU	3.1
1	B	231	THR	3.0
2	C	201	THR	3.0
1	B	341	ALA	3.0
1	A	90	GLY	3.0
2	C	141	GLY	3.0
1	B	187	LEU	2.9
1	B	71	GLY	2.9
1	B	238	GLY	2.9
3	D	88	ASP	2.9
1	A	226	ASP	2.9
1	A	182	LEU	2.9
1	B	161	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	69	PRO	2.8
3	D	126	PRO	2.8
1	A	218	ARG	2.8
1	A	354	PRO	2.7
2	C	197	LEU	2.7
1	A	88	VAL	2.7
1	A	128	THR	2.7
1	B	246	ASP	2.7
2	C	144	ALA	2.7
1	A	257	PHE	2.7
1	A	234	VAL	2.7
3	F	101	VAL	2.7
3	D	137	THR	2.7
2	C	161	SER	2.7
3	D	174	SER	2.7
1	A	162	LEU	2.7
2	E	59	TYR	2.7
2	C	216	ASP	2.7
2	C	158	VAL	2.6
1	A	186	LEU	2.6
3	F	1	ASN	2.6
2	C	223	SER	2.6
2	E	88	ALA	2.6
1	A	190	SER	2.6
2	C	128	SER	2.6
1	A	134	PHE	2.6
3	F	17	THR	2.5
1	A	287	SER	2.5
1	B	160	LEU	2.5
2	C	157	PRO	2.5
1	A	36	ILE	2.5
2	C	172	HIS	2.5
2	C	165	GLY	2.5
2	C	198	GLY	2.5
1	A	255	ARG	2.4
1	A	326	CYS	2.4
2	C	168	THR	2.4
1	B	343	TYR	2.4
2	C	174	PHE	2.4
3	D	173	GLN	2.4
1	A	144	VAL	2.4
1	B	239	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	51	ILE	2.4
2	C	132	LEU	2.4
3	D	112	LEU	2.4
1	A	254	ASN	2.4
3	D	189	GLU	2.4
2	C	145	ALA	2.4
1	A	46	ILE	2.4
1	B	234	VAL	2.4
2	C	206	VAL	2.4
1	A	87	ARG	2.3
2	C	146	LEU	2.3
3	F	132	GLN	2.3
2	C	155	PRO	2.3
1	B	233	GLN	2.3
1	B	87	ARG	2.3
1	A	206	GLN	2.3
2	C	171	VAL	2.3
1	A	66	GLY	2.3
2	C	199	THR	2.3
1	B	65	GLN	2.3
1	A	232	LEU	2.2
1	B	88	VAL	2.3
2	E	18	LEU	2.2
2	C	134	PRO	2.2
1	B	117	HIS	2.2
1	A	214	ILE	2.2
2	C	129	VAL	2.2
2	C	149	LEU	2.2
2	C	192	VAL	2.2
2	E	2	VAL	2.2
1	B	191	ASP	2.2
1	A	132	TYR	2.2
2	C	195	SER	2.2
1	A	157	LEU	2.2
1	B	232	LEU	2.2
1	B	226	ASP	2.2
1	A	256	PRO	2.2
1	A	207	TRP	2.2
2	E	86	LEU	2.2
1	A	127	SER	2.2
2	E	60	TYR	2.1
1	A	196	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	212	VAL	2.1
1	B	264	PRO	2.1
3	D	125	PRO	2.1
2	C	1	GLN	2.1
2	E	1	GLN	2.1
1	B	293	CYS	2.1
1	A	236	ILE	2.1
1	B	67	GLU	2.1
2	C	173	THR	2.1
3	D	127	SER	2.1
1	A	230	ASN	2.1
2	E	129	VAL	2.1
3	F	102	VAL	2.1
2	E	188	SER	2.0
1	B	165	GLU	2.0
1	A	155	LEU	2.0
2	C	12	VAL	2.0
2	C	140	SER	2.0
2	C	156	GLU	2.0
2	C	193	PRO	2.0

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

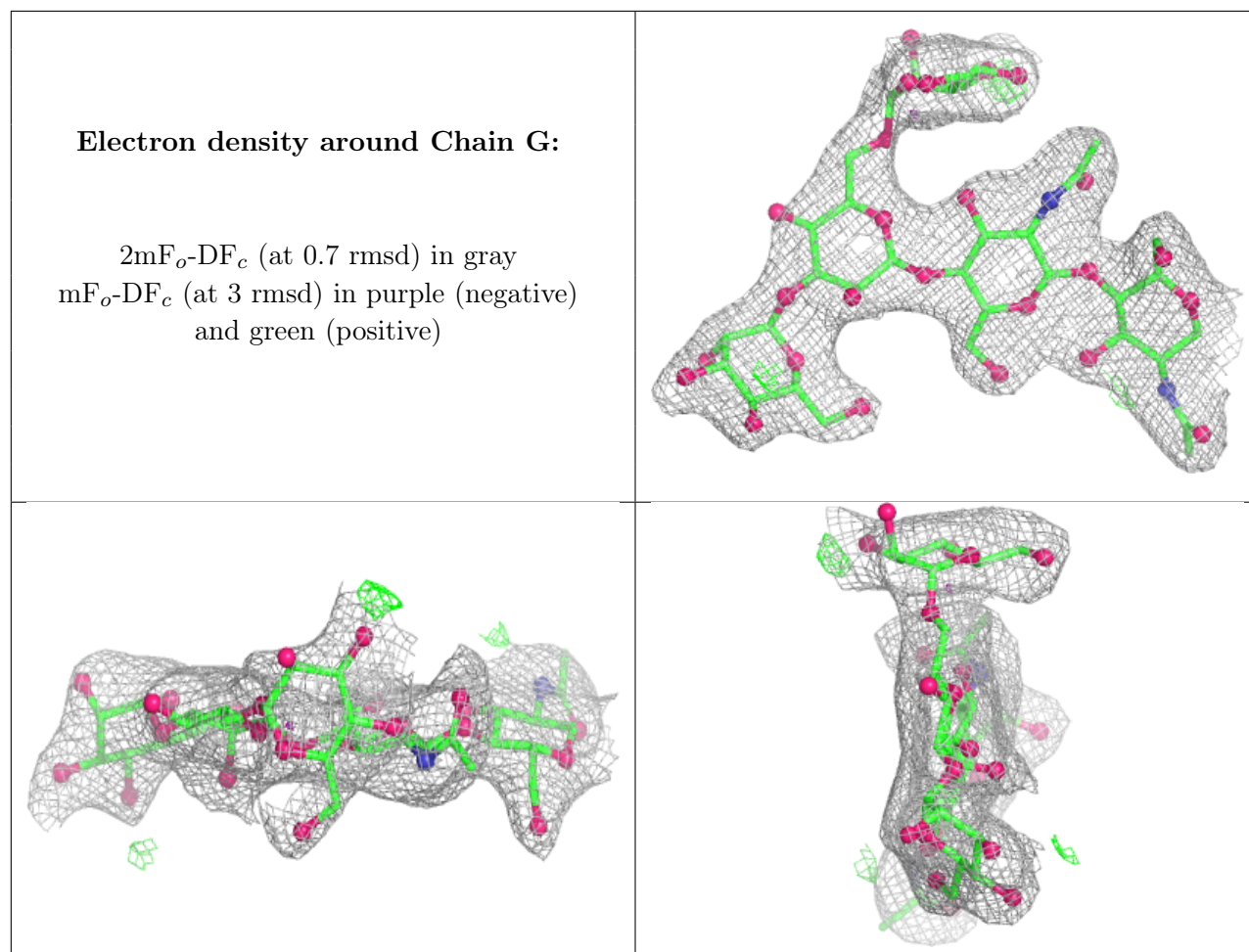
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	G	5	11/12	0.56	0.17	107,113,115,120	0
4	BMA	G	3	11/12	0.84	0.11	86,91,100,110	0
4	NAG	G	2	14/15	0.89	0.10	78,85,93,95	0
4	MAN	G	4	11/12	0.91	0.09	79,81,86,86	0
4	NAG	G	1	14/15	0.93	0.09	66,72,79,84	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
5	NAG	A	401	14/15	0.62	0.15	110,120,125,125	0
5	NAG	B	401	14/15	0.71	0.16	104,111,120,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.