Full wwPDB X-ray Structure Validation Report

Aug 7, 2023 – 05:18 AM EDT

PDB ID	:	1NAM
Title	:	MURINE ALLOREACTIVE SCFV TCR-PEPTIDE-MHC CLASS I MOLECULE COMPLEX
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Deposited on	:	2002-11-28
Resolution	:	2.70 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:

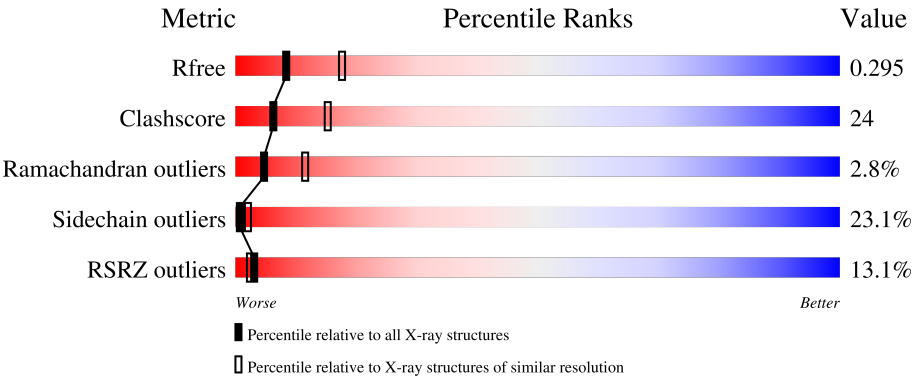
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	116	59% 25% 15%
2	B	113	% 58% 34% 7%
3	H	275	11% 56% 34% 10%
4	P	8	62% 38%
5	L	100	49% 30% 46% 23%

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Mol	Chain	Length	Quality of chain
6	C	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	C	1	X	-	-	-
6	NAG	C	2	X	-	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5091 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 BM3.3 T Cell Receptor alpha-Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			908	579	145	179	5			

- Molecule 2 is a protein called BM3.3 T Cell Receptor beta-Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			917	580	166	166	5			

- Molecule 3 is a protein called H-2 class I histocompatibility antigen, K-B alpha chain precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	275	Total	C	N	O	S	0	0	0
			2240	1413	394	424	9			

- Molecule 4 is a protein called Nucleocapsid.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	8	Total	C	N	O	0	0	0
			68	44	12	12			

- Molecule 5 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	100	Total	C	N	O	S	0	0	0
			829	529	139	153	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	cloning artifact	UNP P01887

- Molecule 6 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
6	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is water.

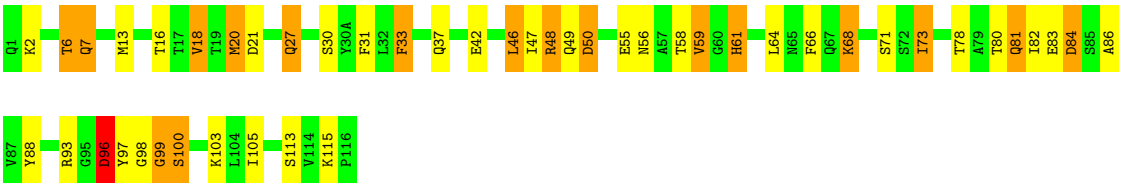
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	25	Total	O	0	0
			25	25		
7	B	32	Total	O	0	0
			32	32		
7	H	35	Total	O	0	0
			35	35		
7	P	2	Total	O	0	0
			2	2		
7	L	7	Total	O	0	0
			7	7		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

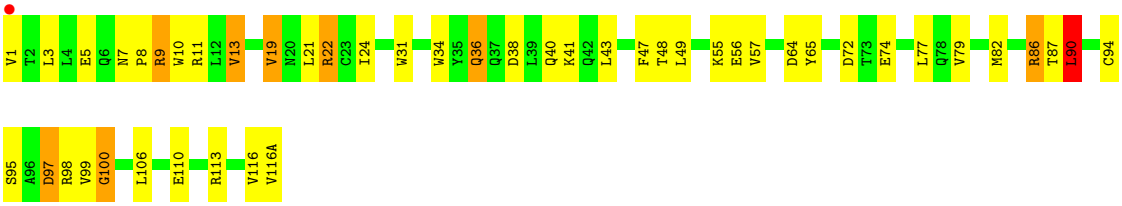
• Molecule 1: BM3.3 T Cell Receptor alpha-Chain

Chain A:



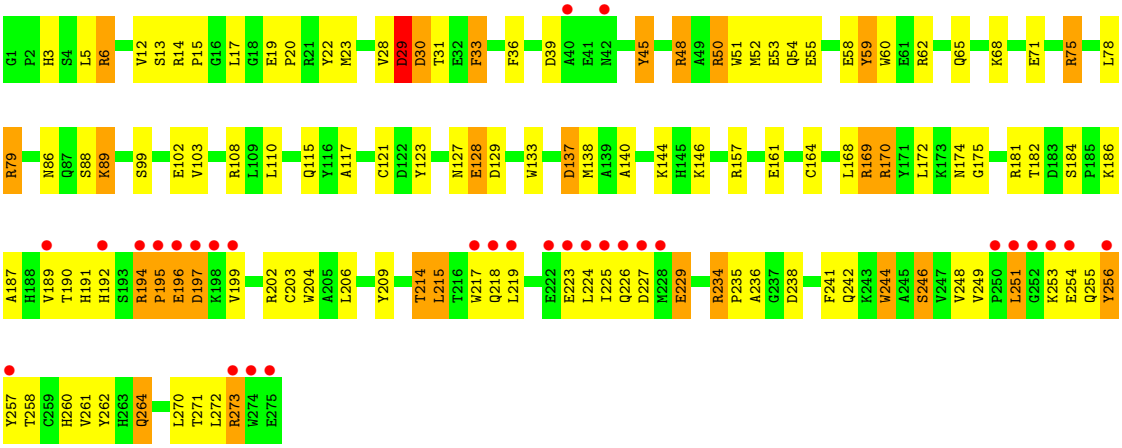
• Molecule 2: BM3.3 T Cell Receptor beta-Chain

Chain B:



• Molecule 3: H-2 class I histocompatibility antigen, K-B alpha chain precursor

Chain H:

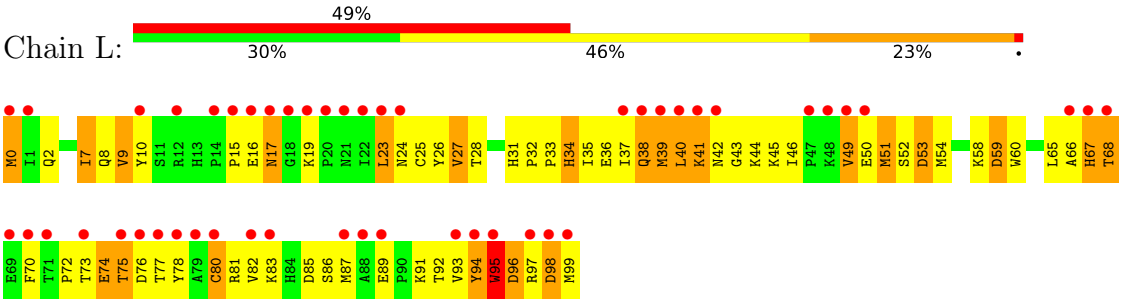


• Molecule 4: Nucleocapsid

Chain P:

• Molecule 5: Beta-2-microglobulin

Chain L:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	101.86Å 101.86Å 201.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.70 33.78 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (12.00-2.70) 96.7 (33.78-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 2.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.230 , 0.298 0.233 , 0.295	Depositor DCC
R_{free} test set	2998 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5091	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.54	0/925	0.81	3/1249 (0.2%)
2	B	0.60	0/936	0.88	4/1271 (0.3%)
3	H	0.43	0/2301	0.71	7/3125 (0.2%)
4	P	0.56	0/69	0.67	0/90
5	L	0.39	0/855	0.72	6/1158 (0.5%)
All	All	0.48	0/5086	0.77	20/6893 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	50	ASP	CB-CG-OD2	6.64	124.28	118.30
2	B	64	ASP	CB-CG-OD2	6.36	124.02	118.30
2	B	72	ASP	CB-CG-OD2	6.09	123.78	118.30
3	H	238	ASP	CB-CG-OD2	5.77	123.49	118.30
3	H	197	ASP	CB-CG-OD2	5.60	123.34	118.30
2	B	38	ASP	CB-CG-OD2	5.56	123.30	118.30
3	H	137	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	84	ASP	CB-CG-OD2	5.40	123.16	118.30
5	L	53	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	96	ASP	CB-CG-OD2	5.30	123.07	118.30
2	B	90	LEU	CA-CB-CG	-5.20	103.35	115.30
5	L	76	ASP	CB-CG-OD2	5.18	122.96	118.30
5	L	98	ASP	CB-CG-OD2	5.18	122.96	118.30
5	L	85	ASP	CB-CG-OD2	5.14	122.92	118.30
3	H	227	ASP	CB-CG-OD2	5.13	122.92	118.30
5	L	96	ASP	CB-CG-OD2	5.09	122.89	118.30
3	H	39	ASP	CB-CG-OD2	5.08	122.88	118.30
3	H	29	ASP	CB-CG-OD2	5.08	122.87	118.30
3	H	30	ASP	CB-CG-OD2	5.03	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	59	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	908	0	899	44	0
2	B	917	0	923	40	0
3	H	2240	0	2131	105	0
4	P	68	0	67	3	0
5	L	829	0	805	59	0
6	C	28	0	25	2	0
7	A	25	0	0	10	0
7	B	32	0	0	5	0
7	H	35	0	0	3	0
7	L	7	0	0	0	0
7	P	2	0	0	1	0
All	All	5091	0	4850	239	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 24.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HG3	1:A:48:ARG:HH11	1.09	1.10
3:H:128:GLU:CD	3:H:128:GLU:H	1.50	1.03
5:L:17:ASN:H	5:L:17:ASN:ND2	1.54	0.96
1:A:100:SER:HB2	1:A:103:LYS:HE3	1.46	0.95
3:H:235:PRO:O	5:L:10:TYR:OH	1.84	0.95
5:L:7:ILE:HD12	5:L:7:ILE:H	1.32	0.94
2:B:7:ASN:HD21	2:B:22:ARG:HH11	1.16	0.91
2:B:77:LEU:CD2	2:B:90:LEU:HD22	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HG3	1:A:48:ARG:NH1	1.77	0.89
3:H:204:TRP:CH2	5:L:99:MET:HA	2.07	0.88
5:L:17:ASN:H	5:L:17:ASN:HD22	1.16	0.88
5:L:27:VAL:HG21	5:L:37:ILE:HD13	1.56	0.87
3:H:157:ARG:HD2	7:H:304:HOH:O	1.74	0.87
3:H:128:GLU:CD	3:H:128:GLU:N	2.29	0.85
5:L:25:CYS:HB3	5:L:66:ALA:HB3	1.58	0.85
5:L:23:LEU:HD23	5:L:68:THR:CG2	2.07	0.84
3:H:6:ARG:NH2	3:H:102:GLU:OE2	2.12	0.83
1:A:7:GLN:HE22	1:A:21:ASP:H	1.25	0.82
5:L:15:PRO:HB3	5:L:97:ARG:HB3	1.63	0.81
3:H:17:LEU:O	3:H:17:LEU:HG	1.81	0.81
3:H:255:GLN:O	3:H:273:ARG:NH1	2.16	0.78
3:H:204:TRP:HH2	5:L:99:MET:HA	1.46	0.78
1:A:93:ARG:HB2	7:A:204:HOH:O	1.83	0.78
1:A:100:SER:HB2	1:A:103:LYS:CE	2.13	0.78
3:H:121:CYS:SG	5:L:0:MET:N	2.58	0.76
5:L:37:ILE:HG12	5:L:82:VAL:HG22	1.69	0.75
2:B:7:ASN:ND2	2:B:22:ARG:HH11	1.84	0.75
3:H:236:ALA:O	5:L:24:ASN:ND2	2.21	0.73
5:L:24:ASN:OD1	5:L:67:HIS:HB2	1.88	0.73
5:L:19:LYS:O	5:L:72:PRO:HD2	1.89	0.72
3:H:234:ARG:HG3	3:H:234:ARG:HH11	1.55	0.72
5:L:17:ASN:HD22	5:L:17:ASN:N	1.85	0.72
5:L:37:ILE:HA	5:L:81:ARG:O	1.89	0.72
3:H:51:TRP:HB2	3:H:174:ASN:O	1.89	0.72
5:L:40:LEU:O	5:L:41:LYS:HB2	1.89	0.72
1:A:98:GLY:N	7:A:212:HOH:O	2.24	0.70
1:A:99:GLY:N	7:A:212:HOH:O	2.23	0.70
1:A:100:SER:CB	1:A:103:LYS:HE3	2.21	0.70
2:B:77:LEU:HD21	2:B:90:LEU:HD22	1.72	0.70
3:H:3:HIS:CG	3:H:172:LEU:HD11	2.27	0.70
5:L:23:LEU:HD23	5:L:68:THR:HG22	1.73	0.70
3:H:256:TYR:CD1	3:H:256:TYR:N	2.60	0.69
3:H:234:ARG:HG3	3:H:234:ARG:NH1	2.07	0.69
3:H:181:ARG:HG3	3:H:182:THR:N	2.07	0.68
2:B:56:GLU:HG3	2:B:57:VAL:N	2.09	0.68
1:A:97:TYR:CE2	4:P:4:VAL:HG13	2.31	0.66
2:B:47:PHE:CE2	2:B:56:GLU:HG2	2.30	0.66
2:B:57:VAL:HG22	7:B:121:HOH:O	1.96	0.66
1:A:98:GLY:C	7:A:212:HOH:O	2.33	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:256:TYR:HD1	3:H:256:TYR:H	1.42	0.65
1:A:7:GLN:NE2	1:A:21:ASP:H	1.96	0.64
1:A:97:TYR:O	3:H:65:GLN:NE2	2.29	0.64
2:B:19:VAL:HG13	2:B:79:VAL:CG1	2.27	0.64
5:L:27:VAL:HG21	5:L:37:ILE:CD1	2.26	0.64
1:A:6:THR:HG22	1:A:7:GLN:HG3	1.79	0.64
3:H:256:TYR:N	3:H:256:TYR:HD1	1.97	0.63
1:A:98:GLY:CA	7:A:212:HOH:O	2.46	0.63
5:L:38:GLN:HA	5:L:49:VAL:HG11	1.80	0.63
5:L:41:LYS:O	5:L:42:ASN:HB2	1.98	0.62
2:B:10:TRP:O	2:B:11:ARG:HG2	1.98	0.62
2:B:113:ARG:HD3	7:B:142:HOH:O	2.00	0.62
5:L:78:TYR:O	5:L:94:TYR:CD1	2.51	0.62
2:B:47:PHE:HE2	2:B:56:GLU:HG2	1.65	0.61
5:L:17:ASN:ND2	5:L:17:ASN:N	2.32	0.61
5:L:17:ASN:HA	5:L:72:PRO:HB2	1.82	0.61
2:B:11:ARG:NH2	7:B:120:HOH:O	2.33	0.61
2:B:36:GLN:HE22	2:B:86:ARG:HH21	1.49	0.61
5:L:2:GLN:HE21	5:L:86:SER:HA	1.65	0.61
2:B:19:VAL:HG13	2:B:79:VAL:HG13	1.83	0.61
5:L:7:ILE:H	5:L:7:ILE:CD1	2.02	0.61
1:A:47:ILE:HD12	1:A:59:VAL:HG23	1.82	0.61
1:A:27:GLN:OE1	3:H:62:ARG:NH2	2.35	0.60
1:A:64:LEU:HD13	1:A:73:ILE:HD11	1.84	0.60
3:H:181:ARG:O	3:H:182:THR:HB	2.01	0.60
3:H:204:TRP:CH2	3:H:244:TRP:CD1	2.90	0.60
3:H:89:LYS:HB2	3:H:89:LYS:NZ	2.17	0.60
1:A:48:ARG:NH2	2:B:100:GLY:O	2.35	0.59
1:A:93:ARG:CB	7:A:204:HOH:O	2.47	0.59
3:H:89:LYS:NZ	3:H:89:LYS:CB	2.65	0.59
3:H:225:ILE:O	3:H:225:ILE:HG23	2.02	0.59
3:H:19:GLU:HG3	3:H:20:PRO:HD2	1.85	0.59
3:H:192:HIS:CE1	3:H:202:ARG:HB2	2.37	0.59
5:L:36:GLU:HB2	5:L:83:LYS:HB3	1.83	0.59
3:H:204:TRP:CZ3	3:H:244:TRP:HD1	2.21	0.59
1:A:7:GLN:HE22	1:A:21:ASP:N	1.98	0.59
3:H:48:ARG:NH2	5:L:53:ASP:OD1	2.35	0.59
3:H:36:PHE:HB2	3:H:45:TYR:CD2	2.36	0.58
1:A:18:VAL:CG2	1:A:80:THR:HG21	2.32	0.58
3:H:234:ARG:HH11	3:H:234:ARG:CG	2.15	0.58
1:A:66:PHE:CZ	1:A:68:LYS:HD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:GLU:HG3	2:B:57:VAL:H	1.69	0.57
3:H:55:GLU:OE2	3:H:170:ARG:NH2	2.38	0.57
3:H:229:GLU:O	3:H:246:SER:N	2.35	0.57
1:A:61:HIS:CD2	1:A:61:HIS:H	2.23	0.56
1:A:81:GLN:O	1:A:84:ASP:HB2	2.04	0.56
2:B:31:TRP:CH2	2:B:98:ARG:HD2	2.40	0.56
3:H:157:ARG:NH2	3:H:161:GLU:OE2	2.38	0.56
1:A:49:GLN:HB2	1:A:64:LEU:HD12	1.86	0.56
3:H:45:TYR:O	3:H:60:TRP:CE3	2.59	0.55
5:L:25:CYS:O	5:L:65:LEU:HD12	2.06	0.55
5:L:15:PRO:HD3	5:L:97:ARG:O	2.06	0.55
3:H:3:HIS:CD2	3:H:172:LEU:HD11	2.40	0.55
2:B:8:PRO:HD2	2:B:21:LEU:HD22	1.89	0.55
5:L:50:GLU:O	5:L:51:MET:C	2.44	0.55
5:L:38:GLN:O	5:L:81:ARG:HB3	2.06	0.55
3:H:203:CYS:HB2	3:H:217:TRP:CZ2	2.42	0.54
3:H:133:TRP:O	3:H:144:LYS:HE3	2.08	0.54
3:H:214:THR:HG23	3:H:262:TYR:HB2	1.89	0.54
3:H:215:LEU:HA	3:H:260:HIS:O	2.07	0.54
5:L:80:CYS:O	5:L:92:THR:OG1	2.14	0.54
2:B:77:LEU:HD21	2:B:90:LEU:CD2	2.37	0.53
1:A:13:MET:HE3	1:A:13:MET:HA	1.90	0.53
5:L:37:ILE:O	5:L:51:MET:SD	2.67	0.53
3:H:51:TRP:CD2	3:H:175:GLY:HA2	2.45	0.52
3:H:5:LEU:HB2	3:H:168:LEU:HD13	1.92	0.52
5:L:8:GLN:HB2	5:L:26:TYR:HB3	1.89	0.52
5:L:9:VAL:O	5:L:10:TYR:HB3	2.09	0.52
3:H:187:ALA:HA	3:H:204:TRP:O	2.09	0.52
1:A:97:TYR:CD2	4:P:4:VAL:HG13	2.45	0.51
2:B:36:GLN:NE2	2:B:65:TYR:OH	2.43	0.51
3:H:53:GLU:C	3:H:55:GLU:H	2.13	0.51
3:H:189:VAL:HG12	3:H:190:THR:N	2.25	0.51
5:L:7:ILE:HD12	5:L:7:ILE:N	2.13	0.51
1:A:56:ASN:OD1	6:C:1:NAG:N2	2.43	0.51
3:H:17:LEU:O	3:H:17:LEU:CG	2.52	0.51
1:A:48:ARG:NH1	1:A:48:ARG:CG	2.57	0.51
2:B:13:VAL:O	2:B:116:VAL:HA	2.09	0.51
2:B:9:ARG:CD	7:B:138:HOH:O	2.58	0.51
1:A:31:PHE:HD2	1:A:50:ASP:OD1	1.93	0.51
1:A:47:ILE:CD1	1:A:59:VAL:HG23	2.40	0.50
3:H:89:LYS:HB2	3:H:89:LYS:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:17:ASN:CG	5:L:97:ARG:HH22	2.15	0.50
5:L:39:MET:HG3	5:L:49:VAL:HG13	1.93	0.50
3:H:261:VAL:HB	3:H:270:LEU:HB2	1.93	0.50
1:A:61:HIS:H	1:A:61:HIS:HD2	1.58	0.50
3:H:20:PRO:HG2	3:H:75:ARG:HD2	1.93	0.49
7:A:227:HOH:O	6:C:1:NAG:H82	2.12	0.49
2:B:1:VAL:HG22	2:B:1:VAL:O	2.11	0.49
1:A:49:GLN:HB2	1:A:64:LEU:CD1	2.42	0.49
2:B:48:THR:O	2:B:49:LEU:HD23	2.12	0.49
1:A:33:PHE:CD1	1:A:33:PHE:N	2.80	0.49
5:L:32:PRO:HB2	5:L:34:HIS:CE1	2.48	0.49
3:H:128:GLU:N	3:H:128:GLU:OE2	2.45	0.48
3:H:249:VAL:HB	3:H:257:TYR:CE1	2.48	0.48
3:H:197:ASP:O	3:H:251:LEU:HB2	2.12	0.48
2:B:24:ILE:HD11	2:B:74:GLU:HG3	1.96	0.48
5:L:8:GLN:O	5:L:10:TYR:HD2	1.97	0.48
2:B:77:LEU:HD23	2:B:90:LEU:HD22	1.88	0.48
3:H:89:LYS:CB	3:H:89:LYS:HZ3	2.27	0.48
1:A:93:ARG:CA	7:A:204:HOH:O	2.62	0.48
2:B:31:TRP:O	2:B:94:CYS:HA	2.14	0.48
3:H:204:TRP:CZ3	3:H:244:TRP:CD1	3.01	0.48
1:A:18:VAL:HG22	1:A:80:THR:HG21	1.95	0.48
2:B:34:TRP:CE2	2:B:77:LEU:HB2	2.49	0.48
5:L:19:LYS:O	5:L:72:PRO:CD	2.61	0.48
1:A:37:GLN:O	1:A:86:ALA:HB1	2.14	0.47
2:B:19:VAL:O	2:B:79:VAL:HG12	2.14	0.47
2:B:99:VAL:HA	7:B:147:HOH:O	2.13	0.47
3:H:209:TYR:HD1	3:H:241:PHE:HE1	1.62	0.47
5:L:23:LEU:HD23	5:L:68:THR:HG21	1.95	0.47
3:H:192:HIS:HE1	3:H:202:ARG:HB2	1.80	0.47
2:B:24:ILE:CD1	2:B:74:GLU:HG3	2.45	0.47
2:B:56:GLU:CG	2:B:57:VAL:N	2.77	0.46
3:H:59:TYR:C	3:H:59:TYR:CD2	2.88	0.46
3:H:234:ARG:NH1	3:H:242:GLN:OE1	2.47	0.46
3:H:197:ASP:O	3:H:251:LEU:CB	2.64	0.46
5:L:25:CYS:N	5:L:66:ALA:O	2.49	0.46
1:A:71:SER:N	7:A:223:HOH:O	2.49	0.46
5:L:59:ASP:O	5:L:60:TRP:HB2	2.16	0.46
5:L:94:TYR:O	5:L:95:TRP:O	2.34	0.45
1:A:48:ARG:HH11	1:A:48:ARG:CG	1.95	0.45
3:H:36:PHE:HB2	3:H:45:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:189:VAL:CG1	3:H:190:THR:N	2.80	0.45
3:H:199:VAL:HG23	3:H:249:VAL:CG2	2.46	0.45
3:H:3:HIS:HB3	3:H:29:ASP:OD1	2.16	0.45
3:H:51:TRP:CD2	3:H:175:GLY:CA	3.00	0.45
3:H:172:LEU:HD23	3:H:172:LEU:HA	1.73	0.45
3:H:264:GLN:H	3:H:264:GLN:HG3	1.35	0.45
2:B:8:PRO:HD2	2:B:21:LEU:CD2	2.46	0.45
3:H:28:VAL:HG23	3:H:33:PHE:CD1	2.52	0.45
5:L:39:MET:CG	5:L:49:VAL:HG13	2.46	0.45
5:L:74:GLU:HB3	5:L:75:THR:H	1.49	0.45
3:H:194:ARG:O	3:H:196:GLU:N	2.49	0.45
5:L:35:ILE:HG12	5:L:37:ILE:HG13	1.99	0.45
3:H:199:VAL:HG23	3:H:199:VAL:O	2.17	0.44
5:L:7:ILE:HG21	5:L:82:VAL:HG21	1.99	0.44
3:H:123:TYR:CZ	3:H:140:ALA:HA	2.53	0.44
5:L:39:MET:H	5:L:49:VAL:CG2	2.31	0.44
2:B:79:VAL:HG13	2:B:79:VAL:O	2.18	0.43
3:H:50:ARG:HE	3:H:50:ARG:HB2	1.65	0.43
3:H:202:ARG:HG3	3:H:246:SER:CB	2.48	0.43
2:B:7:ASN:ND2	2:B:22:ARG:NH1	2.61	0.43
3:H:129:ASP:OD2	3:H:129:ASP:C	2.57	0.43
3:H:19:GLU:HG2	3:H:75:ARG:CZ	2.48	0.43
3:H:168:LEU:O	3:H:170:ARG:N	2.44	0.43
3:H:264:GLN:HE21	3:H:264:GLN:HB2	1.59	0.43
1:A:20:MET:HE1	1:A:88:TYR:CD2	2.54	0.43
1:A:18:VAL:CG2	1:A:80:THR:CG2	2.97	0.43
3:H:103:VAL:CG2	3:H:168:LEU:HD23	2.48	0.43
2:B:98:ARG:HG2	7:P:98:HOH:O	2.19	0.42
3:H:28:VAL:C	3:H:30:ASP:N	2.71	0.42
3:H:168:LEU:C	3:H:170:ARG:H	2.22	0.42
3:H:214:THR:HA	7:H:305:HOH:O	2.19	0.42
3:H:194:ARG:O	3:H:196:GLU:HB2	2.19	0.42
2:B:31:TRP:CD1	2:B:97:ASP:HA	2.54	0.42
3:H:51:TRP:CG	3:H:175:GLY:HA2	2.55	0.42
5:L:17:ASN:OD1	5:L:97:ARG:NH2	2.51	0.42
3:H:13:SER:HB3	3:H:78:LEU:HD13	2.01	0.42
3:H:103:VAL:HG21	3:H:168:LEU:HD23	2.02	0.42
3:H:137:ASP:OD2	3:H:137:ASP:C	2.58	0.42
5:L:33:PRO:O	5:L:54:MET:CE	2.68	0.42
3:H:194:ARG:O	3:H:195:PRO:C	2.58	0.41
3:H:169:ARG:HH11	3:H:169:ARG:HB3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:3:HIS:CD2	3:H:172:LEU:CD1	3.04	0.41
5:L:15:PRO:HB3	5:L:97:ARG:CB	2.44	0.41
2:B:77:LEU:CD2	2:B:90:LEU:CD2	2.85	0.41
3:H:15:PRO:C	3:H:17:LEU:H	2.23	0.41
3:H:20:PRO:HG2	3:H:75:ARG:CD	2.50	0.41
3:H:48:ARG:NH1	3:H:48:ARG:HG3	2.35	0.41
3:H:127:ASN:HB3	3:H:128:GLU:OE2	2.20	0.41
3:H:244:TRP:CE3	3:H:244:TRP:C	2.93	0.41
5:L:51:MET:HA	5:L:66:ALA:HA	2.01	0.41
3:H:22:TYR:CD2	3:H:71:GLU:HB2	2.56	0.41
3:H:110:LEU:HD23	3:H:110:LEU:HA	1.78	0.41
2:B:34:TRP:CZ2	2:B:77:LEU:HB2	2.56	0.41
3:H:146:LYS:NZ	4:P:8:LEU:OXT	2.53	0.41
5:L:31:HIS:HD2	5:L:60:TRP:O	2.04	0.41
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.86	0.41
1:A:96:ASP:HB3	7:A:217:HOH:O	2.21	0.41
3:H:79:ARG:HE	3:H:79:ARG:HB3	1.56	0.41
5:L:52:SER:OG	5:L:65:LEU:HB3	2.21	0.41
3:H:65:GLN:OE1	7:H:310:HOH:O	2.22	0.40
3:H:202:ARG:HG3	3:H:246:SER:HB3	2.03	0.40
3:H:52:MET:O	3:H:55:GLU:HB2	2.21	0.40
2:B:21:LEU:HB2	2:B:77:LEU:HB3	2.02	0.40
3:H:191:HIS:CE1	3:H:199:VAL:HG12	2.57	0.40
3:H:115:GLN:HE21	3:H:115:GLN:HB3	1.51	0.40
3:H:117:ALA:HB2	5:L:60:TRP:CE2	2.56	0.40
3:H:199:VAL:HG23	3:H:249:VAL:HG22	2.03	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	114/116 (98%)	98 (86%)	12 (10%)	4 (4%)	3 8
2	B	111/113 (98%)	108 (97%)	2 (2%)	1 (1%)	17 40
3	H	273/275 (99%)	241 (88%)	29 (11%)	3 (1%)	14 34
4	P	6/8 (75%)	5 (83%)	1 (17%)	0	100 100
5	L	98/100 (98%)	73 (74%)	16 (16%)	9 (9%)	1 0
All	All	602/612 (98%)	525 (87%)	60 (10%)	17 (3%)	5 11

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ASP
1	A	100	SER
3	H	195	PRO
5	L	41	LYS
5	L	95	TRP
1	A	99	GLY
5	L	16	GLU
5	L	58	LYS
2	B	100	GLY
3	H	54	GLN
5	L	43	GLY
5	L	51	MET
3	H	29	ASP
5	L	49	VAL
5	L	68	THR
5	L	40	LEU
1	A	73	ILE

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	102/102 (100%)	77 (76%)	25 (24%)	0 2
2	B	101/101 (100%)	81 (80%)	20 (20%)	1 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	H	233/233 (100%)	183 (78%)	50 (22%)	1 3
4	P	6/6 (100%)	5 (83%)	1 (17%)	2 5
5	L	95/95 (100%)	67 (70%)	28 (30%)	0 1
All	All	537/537 (100%)	413 (77%)	124 (23%)	1 2

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	6	THR
1	A	7	GLN
1	A	16	THR
1	A	18	VAL
1	A	20	MET
1	A	27	GLN
1	A	30	SER
1	A	33	PHE
1	A	42	GLU
1	A	46	LEU
1	A	48	ARG
1	A	55	GLU
1	A	58	THR
1	A	59	VAL
1	A	61	HIS
1	A	68	LYS
1	A	78	THR
1	A	81	GLN
1	A	82	ILE
1	A	83	GLU
1	A	96	ASP
1	A	105	ILE
1	A	113	SER
1	A	115	LYS
2	B	3	LEU
2	B	5	GLU
2	B	9	ARG
2	B	13	VAL
2	B	19	VAL
2	B	22	ARG
2	B	36	GLN
2	B	40	GLN

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Mol	Chain	Res	Type
2	B	41	LYS
2	B	43	LEU
2	B	55	LYS
2	B	82	MET
2	B	86	ARG
2	B	87	THR
2	B	90	LEU
2	B	95	SER
2	B	97	ASP
2	B	106	LEU
2	B	110	GLU
2	B	116(A)	VAL
3	H	6	ARG
3	H	12	VAL
3	H	14	ARG
3	H	23	MET
3	H	31	THR
3	H	33	PHE
3	H	45	TYR
3	H	48	ARG
3	H	50	ARG
3	H	58	GLU
3	H	59	TYR
3	H	68	LYS
3	H	75	ARG
3	H	79	ARG
3	H	86	ASN
3	H	88	SER
3	H	89	LYS
3	H	99	SER
3	H	108	ARG
3	H	128	GLU
3	H	138	MET
3	H	164	CYS
3	H	169	ARG
3	H	170	ARG
3	H	184	SER
3	H	186	LYS
3	H	194	ARG
3	H	196	GLU
3	H	206	LEU
3	H	214	THR

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Mol	Chain	Res	Type
3	H	215	LEU
3	H	218	GLN
3	H	219	LEU
3	H	223	GLU
3	H	224	LEU
3	H	226	GLN
3	H	229	GLU
3	H	234	ARG
3	H	244	TRP
3	H	246	SER
3	H	248	VAL
3	H	251	LEU
3	H	253	LYS
3	H	254	GLU
3	H	256	TYR
3	H	258	THR
3	H	264	GLN
3	H	271	THR
3	H	272	LEU
3	H	273	ARG
4	P	1	ARG
5	L	0	MET
5	L	7	ILE
5	L	9	VAL
5	L	17	ASN
5	L	23	LEU
5	L	27	VAL
5	L	28	THR
5	L	34	HIS
5	L	38	GLN
5	L	39	MET
5	L	44	LYS
5	L	45	LYS
5	L	46	ILE
5	L	67	HIS
5	L	70	PHE
5	L	73	THR
5	L	74	GLU
5	L	75	THR
5	L	77	THR
5	L	80	CYS
5	L	87	MET

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Mol	Chain	Res	Type
5	L	89	GLU
5	L	91	LYS
5	L	93	VAL
5	L	94	TYR
5	L	95	TRP
5	L	96	ASP
5	L	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	GLN
1	A	61	HIS
1	A	81	GLN
2	B	7	ASN
2	B	36	GLN
2	B	44	GLN
3	H	72	GLN
3	H	115	GLN
3	H	127	ASN
3	H	174	ASN
3	H	191	HIS
3	H	264	GLN
5	L	2	GLN
5	L	17	ASN
5	L	38	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	C	1	6,1	14,14,15	0.52	0	17,19,21	1.25	2 (11%)
6	NAG	C	2	6	14,14,15	0.45	0	17,19,21	0.89	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
6	NAG	C	1	6,1	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	C	2	6	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1	NAG	C1-O5-C5	2.47	115.54	112.19
6	C	1	NAG	O5-C1-C2	-2.24	107.76	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	1	NAG	C1
6	C	2	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1	NAG	C8-C7-N2-C2
6	C	1	NAG	O7-C7-N2-C2
6	C	2	NAG	C8-C7-N2-C2
6	C	2	NAG	O7-C7-N2-C2
6	C	2	NAG	O5-C5-C6-O6

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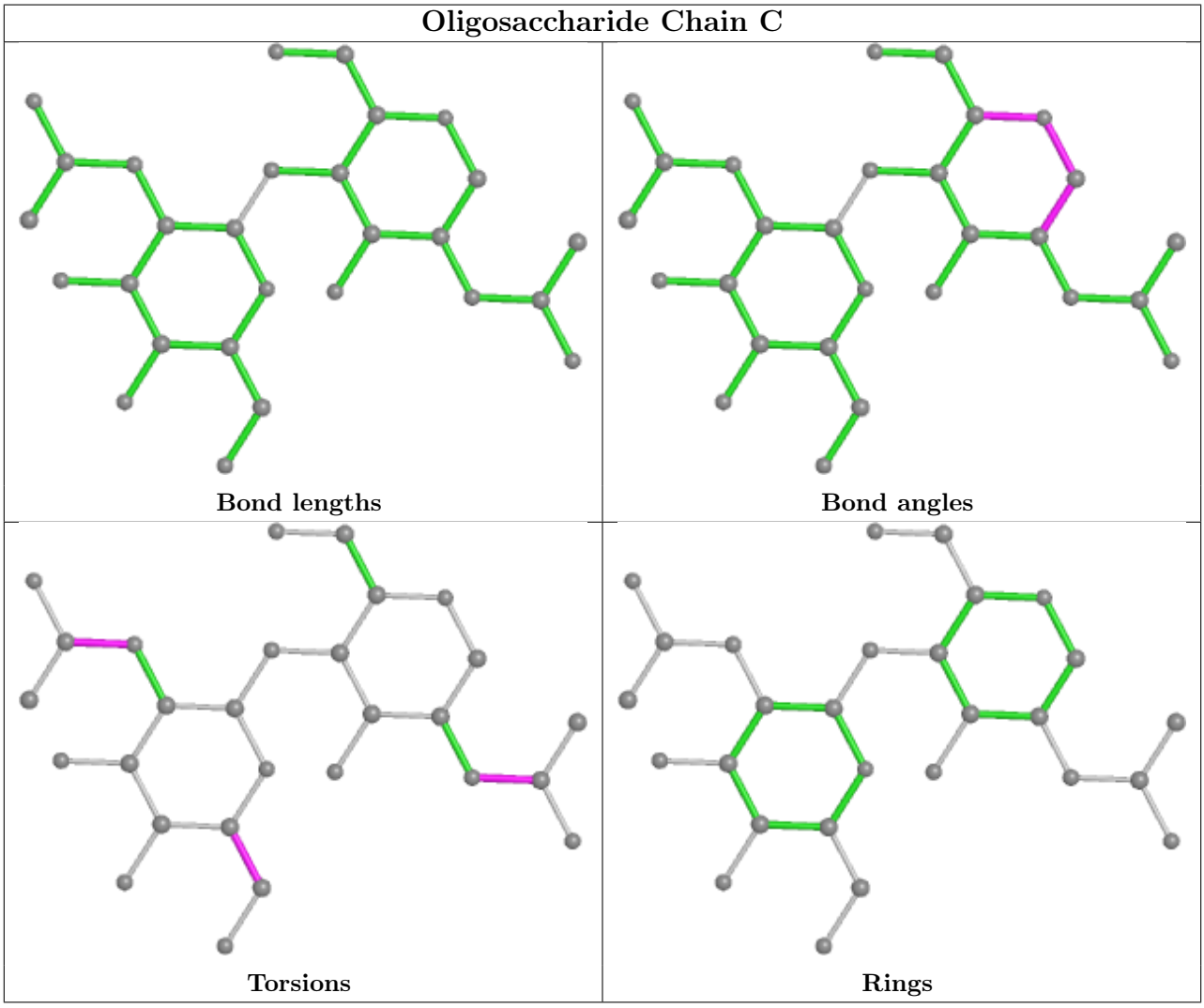
Mol	Chain	Res	Type	Atoms
6	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1	NAG	2	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

There are no ligands in this entry.

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, 95^{th} 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	116/116 (100%)	-0.02	0 100 100	18, 39, 59, 61	0
2	B	113/113 (100%)	-0.12	1 (0%) 84 85	16, 28, 44, 62	0
3	H	275/275 (100%)	0.69	30 (10%) 5 4	16, 55, 122, 135	1 (0%)
4	P	8/8 (100%)	0.57	0 100 100	28, 32, 40, 54	0
5	L	100/100 (100%)	2.34	49 (49%) 0 0	29, 98, 125, 129	0
All	All	612/612 (100%)	0.68	80 (13%) 3 2	16, 45, 121, 135	1 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	77	THR	10.9
5	L	79	ALA	10.0
3	H	195	PRO	9.2
5	L	97	ARG	8.3
5	L	68	THR	8.3
5	L	15	PRO	7.7
5	L	39	MET	7.5
3	H	250	PRO	6.4
3	H	194	ARG	6.2
5	L	94	TYR	5.6
5	L	16	GLU	5.4
5	L	22	ILE	5.3
5	L	18	GLY	5.2
3	H	224	LEU	5.2
5	L	21	ASN	5.2
5	L	48	LYS	5.1
3	H	225	ILE	4.9
5	L	38	GLN	4.9
5	L	20	PRO	4.7
5	L	88	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
3	H	251	LEU	4.5
3	H	273	ARG	4.4
5	L	76	ASP	4.4
5	L	69	GLU	4.3
3	H	252	GLY	4.3
3	H	253	LYS	4.2
5	L	47	PRO	4.1
5	L	23	LEU	4.0
5	L	95	TRP	4.0
3	H	196	GLU	4.0
5	L	78	TYR	3.9
5	L	71	THR	3.9
5	L	19	LYS	3.9
5	L	89	GLU	3.8
5	L	98	ASP	3.7
3	H	199	VAL	3.7
2	B	1	VAL	3.6
5	L	49	VAL	3.6
5	L	0	MET	3.6
5	L	37	ILE	3.5
3	H	274	TRP	3.4
3	H	228	MET	3.4
3	H	257	TYR	3.3
3	H	222	GLU	3.3
5	L	40	LEU	3.3
3	H	256	TYR	3.3
3	H	218	GLN	3.2
5	L	80	CYS	3.1
3	H	226	GLN	3.1
3	H	197	ASP	3.0
5	L	82	VAL	3.0
5	L	99	MET	3.0
3	H	192	HIS	2.8
5	L	50	GLU	2.8
3	H	227	ASP	2.8
5	L	1	ILE	2.7
3	H	223	GLU	2.7
5	L	41	LYS	2.7
3	H	275	GLU	2.6
5	L	42	ASN	2.5
5	L	87	MET	2.5
5	L	12	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
3	H	217	TRP	2.4
5	L	70	PHE	2.4
5	L	83	LYS	2.3
5	L	67	HIS	2.3
5	L	10	TYR	2.3
3	H	42	ASN	2.3
3	H	219	LEU	2.3
5	L	75	THR	2.3
3	H	198	LYS	2.3
5	L	66	ALA	2.3
5	L	14	PRO	2.2
5	L	73	THR	2.2
5	L	93	VAL	2.2
5	L	17	ASN	2.1
5	L	24	ASN	2.1
3	H	254	GLU	2.1
3	H	189	VAL	2.1
3	H	40	ALA	2.1

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)

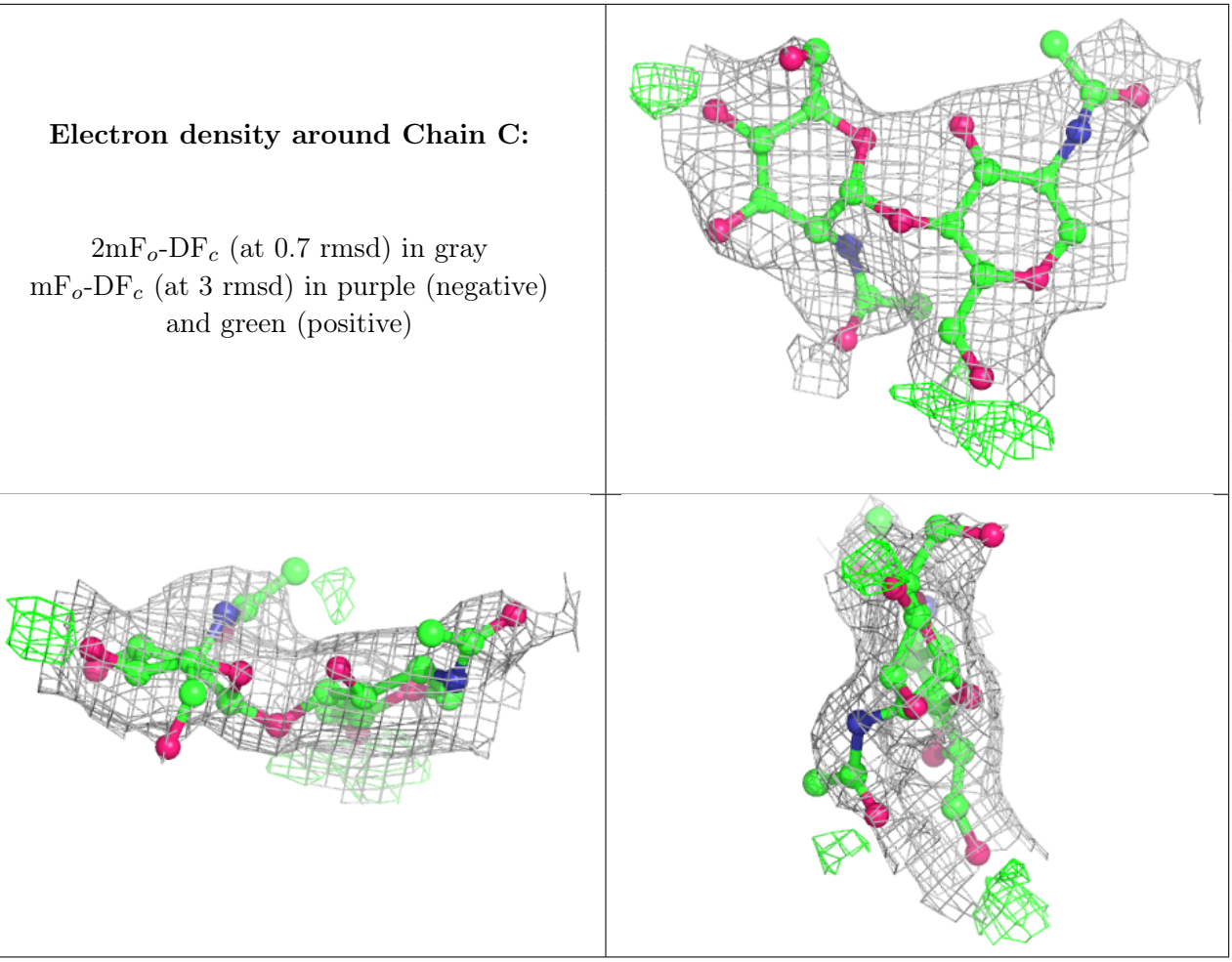
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	NAG	C	2	14/15	0.85	0.31	74,77,79,81	0
6	NAG	C	1	14/15	0.86	0.20	58,63,68,70	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.