



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:51 AM UTC

PDB ID : 5KSB / pdb_00005ksb
Title : T15-DQ8.5-glia-gamma1 complex
Authors : Petersen, J.; Rossjohn, J.; Reid, H.H.
Deposited on : 2016-07-08
Resolution : 2.90 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

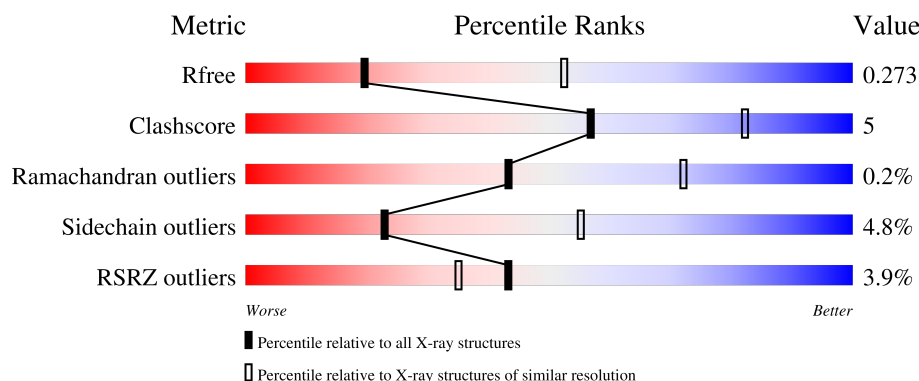
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



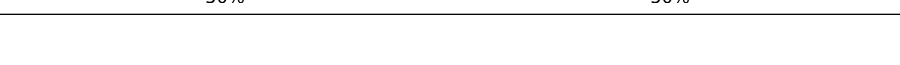
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	191	
1	C	191	
2	B	225	
2	D	225	
3	E	206	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	206	
4	F	243	
4	H	243	
5	I	11	
5	J	11	
6	K	2	
6	L	2	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13106 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 HLA class II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1432	922	234	274	2			
1	C	181	Total	C	N	O	S	0	0	0
			1432	922	234	274	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	SER	CYS	conflict	UNP P01909
A	182	THR	-	expression tag	UNP P01909
A	183	SER	-	expression tag	UNP P01909
A	184	GLY	-	expression tag	UNP P01909
A	185	ASP	-	expression tag	UNP P01909
A	186	ASP	-	expression tag	UNP P01909
A	187	ASP	-	expression tag	UNP P01909
A	188	ASP	-	expression tag	UNP P01909
A	189	LYS	-	expression tag	UNP P01909
C	44	SER	CYS	conflict	UNP P01909
C	182	THR	-	expression tag	UNP P01909
C	183	SER	-	expression tag	UNP P01909
C	184	GLY	-	expression tag	UNP P01909
C	185	ASP	-	expression tag	UNP P01909
C	186	ASP	-	expression tag	UNP P01909
C	187	ASP	-	expression tag	UNP P01909
C	188	ASP	-	expression tag	UNP P01909
C	189	LYS	-	expression tag	UNP P01909

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DQ beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	179	Total	C	N	O	S	0	0	0
			1454	923	254	270	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	178	Total	C	N	O	S	0	0	0
			1453	922	255	269	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	SER	-	linker	PDB ?
B	-12	GLY	-	linker	PDB ?
B	-11	GLY	-	linker	PDB ?
B	-10	SER	-	linker	PDB ?
B	-9	ILE	-	linker	PDB ?
B	-8	GLU	-	linker	PDB ?
B	-7	GLY	-	linker	PDB ?
B	-6	ARG	-	linker	PDB ?
B	-5	GLY	-	linker	PDB ?
B	-4	GLY	-	linker	PDB ?
B	-3	SER	-	linker	PDB ?
B	-2	GLY	-	linker	PDB ?
B	-1	ALA	-	linker	PDB ?
B	0	SER	-	linker	PDB ?
B	193	THR	-	expression tag	UNP O19707
B	194	GLY	-	expression tag	UNP O19707
B	195	GLY	-	expression tag	UNP O19707
B	196	ASP	-	expression tag	UNP O19707
B	197	ASP	-	expression tag	UNP O19707
B	198	ASP	-	expression tag	UNP O19707
B	199	ASP	-	expression tag	UNP O19707
B	200	LYS	-	expression tag	UNP O19707
D	-13	SER	-	linker	PDB ?
D	-12	GLY	-	linker	PDB ?
D	-11	GLY	-	linker	PDB ?
D	-10	SER	-	linker	PDB ?
D	-9	ILE	-	linker	PDB ?
D	-8	GLU	-	linker	PDB ?
D	-7	GLY	-	linker	PDB ?
D	-6	ARG	-	linker	PDB ?
D	-5	GLY	-	linker	PDB ?
D	-4	GLY	-	linker	PDB ?
D	-3	SER	-	linker	PDB ?
D	-2	GLY	-	linker	PDB ?
D	-1	ALA	-	linker	PDB ?
D	0	SER	-	linker	PDB ?

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	193	THR	-	expression tag	UNP O19707
D	194	GLY	-	expression tag	UNP O19707
D	195	GLY	-	expression tag	UNP O19707
D	196	ASP	-	expression tag	UNP O19707
D	197	ASP	-	expression tag	UNP O19707
D	198	ASP	-	expression tag	UNP O19707
D	199	ASP	-	expression tag	UNP O19707
D	200	LYS	-	expression tag	UNP O19707

- Molecule 3 is a protein called T15 TCR alpha TRAV20*02.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	200	Total	C	N	O	S	0	0	0
			1540	969	251	313	7			
3	G	200	Total	C	N	O	S	0	0	0
			1533	966	251	309	7			

- Molecule 4 is a protein called T15 TCR beta TRBV9*01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	241	Total	C	N	O	S	0	0	0
			1910	1205	336	364	5			
4	H	241	Total	C	N	O	S	0	0	0
			1907	1204	336	362	5			

- Molecule 5 is a protein called DQ8.5-glia-gamma1 peptide.

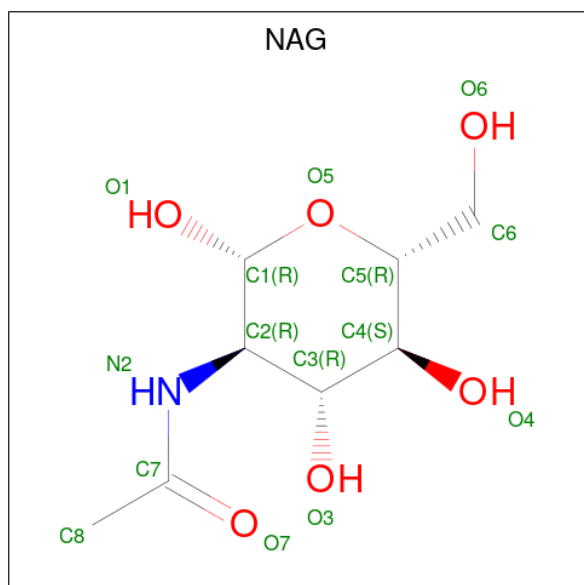
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	11	Total	C	N	O	0	0	0
			85	52	14	19			
5	J	11	Total	C	N	O	0	0	0
			85	52	14	19			

- 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	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O	0	0
			8	8		
8	B	14	Total	O	0	0
			14	14		
8	C	9	Total	O	0	0
			9	9		

Continued on next page...

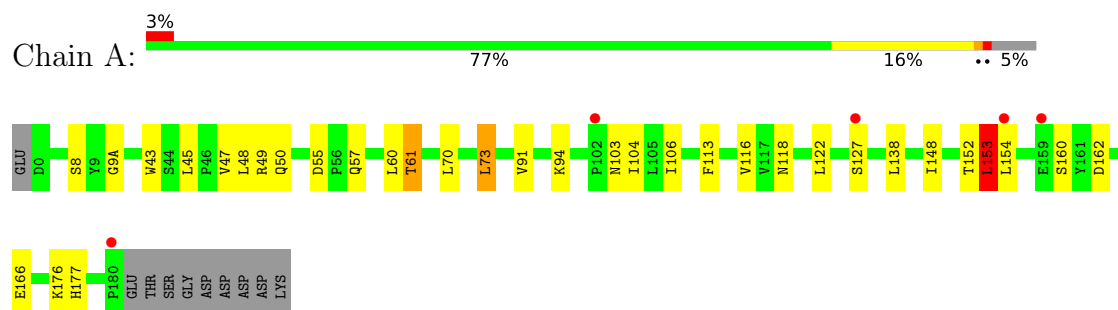
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	16	Total 16	O 16	0	0
8	E	25	Total 25	O 25	0	0
8	F	24	Total 24	O 24	0	0
8	G	30	Total 30	O 30	0	0
8	H	33	Total 33	O 33	0	0
8	I	3	Total 3	O 3	0	0
8	J	1	Total 1	O 1	0	0

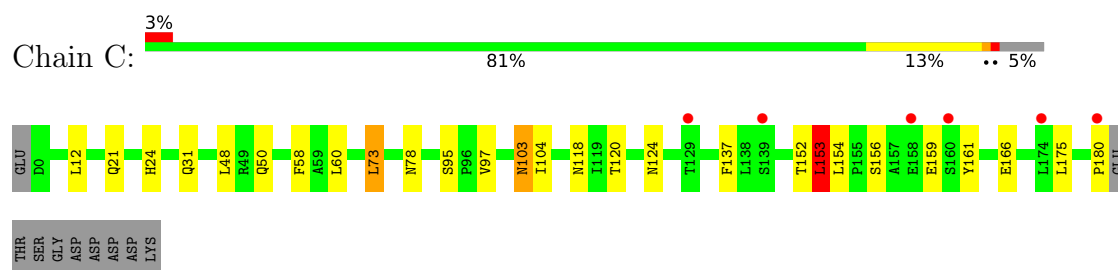
3 Residue-property plots [i](#)

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.

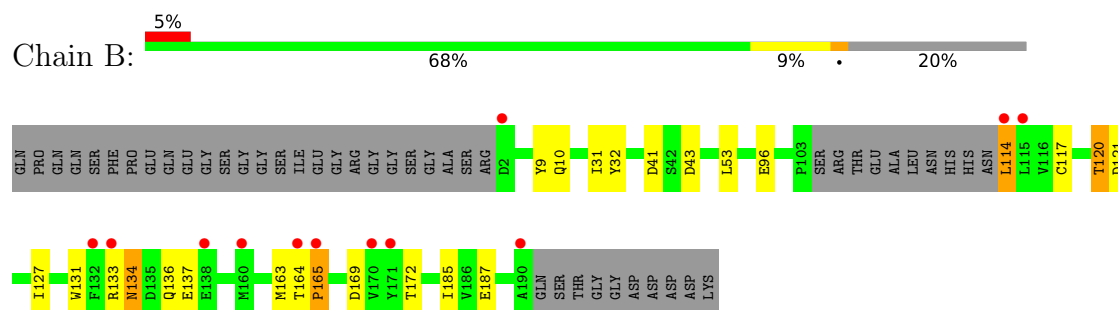
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



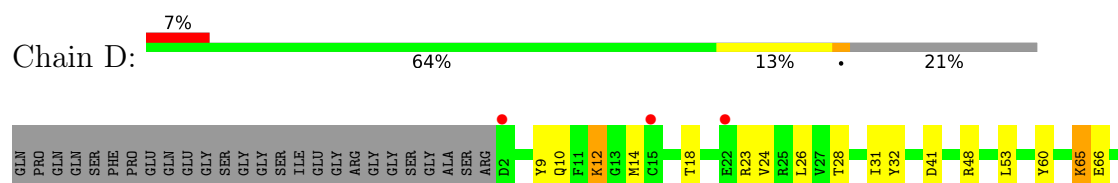
- Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain



- Molecule 2: HLA class II histocompatibility antigen, DQ beta 1 chain

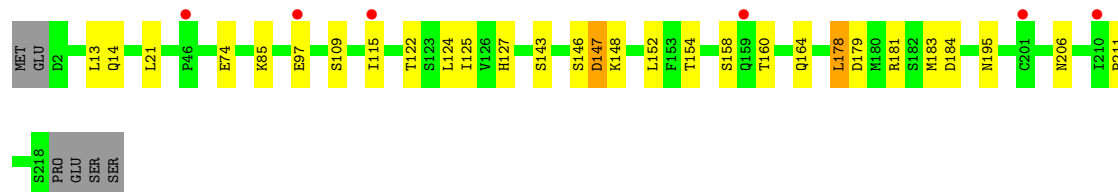
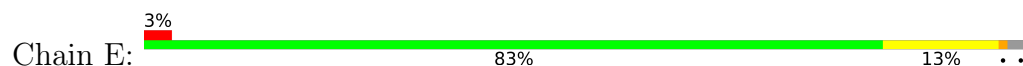


- Molecule 2: HLA class II histocompatibility antigen, DQ beta 1 chain

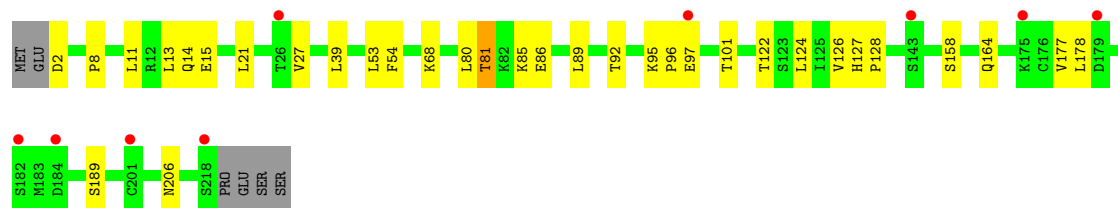
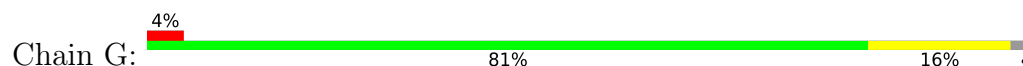




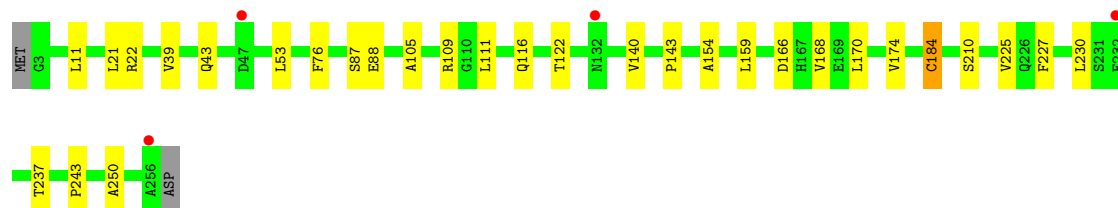
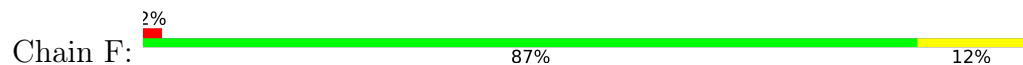
- Molecule 3: T15 TCR alpha TRAV20*02



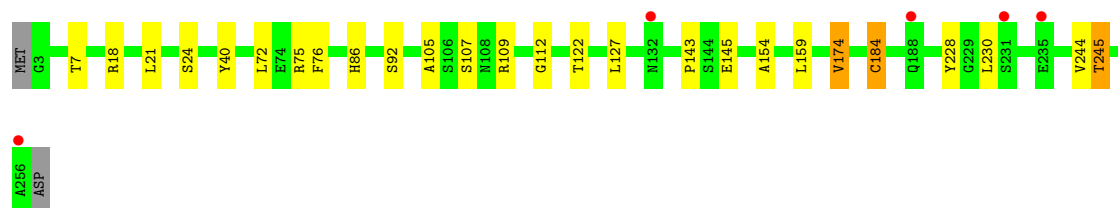
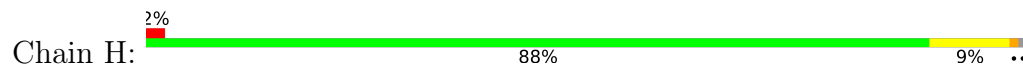
- Molecule 3: T15 TCR alpha TRAV20*02



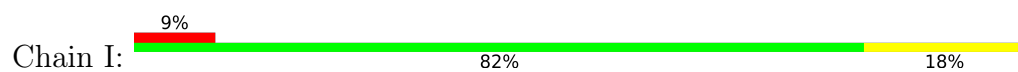
- Molecule 4: T15 TCR beta TRBV9*01



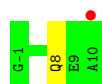
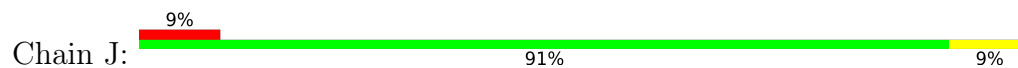
- Molecule 4: T15 TCR beta TRBV9*01



- Molecule 5: DQ8.5-glia-gamma1 peptide



- Molecule 5: DQ8.5-glia-gamma1 peptide



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.89Å 125.05Å 165.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.00 – 2.90 85.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (85.00-2.90) 99.4 (85.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.91Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.219 , 0.254 0.233 , 0.273	Depositor DCC
R_{free} test set	2710 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtrriage
Anisotropy	0.841	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13106	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5763e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.71	0/1474	1.14	5/2017 (0.2%)
1	C	0.72	0/1474	1.18	4/2017 (0.2%)
2	B	0.82	2/1491 (0.1%)	1.09	5/2035 (0.2%)
2	D	0.76	0/1490	1.13	7/2033 (0.3%)
3	E	0.70	0/1576	1.13	7/2141 (0.3%)
3	G	0.74	0/1569	1.08	1/2132 (0.0%)
4	F	0.67	0/1960	1.06	1/2669 (0.0%)
4	H	0.69	0/1957	1.07	3/2665 (0.1%)
5	I	0.60	0/87	1.02	0/117
5	J	0.71	0/87	1.07	0/117
All	All	0.72	2/13165 (0.0%)	1.11	33/17943 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	164	THR	C-N	8.05	1.41	1.33
2	B	165	PRO	N-CD	5.06	1.54	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	78	ASN	CA-CB-CG	6.78	119.38	112.60
4	F	76	PHE	CA-CB-CG	6.33	120.13	113.80
1	C	60	LEU	CA-C-N	6.29	128.71	120.28
1	C	60	LEU	C-N-CA	6.29	128.71	120.28
3	E	147	ASP	CA-CB-CG	6.04	118.64	112.60
4	H	76	PHE	CA-CB-CG	6.01	119.81	113.80
2	D	41	ASP	CA-CB-CG	5.85	118.45	112.60
3	E	115	ILE	N-CA-CB	5.68	115.36	110.08
1	A	55	ASP	CA-CB-CG	5.65	118.25	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PHE	CA-CB-CG	-5.58	108.22	113.80
3	E	195	ASN	CA-CB-CG	5.52	118.12	112.60
2	B	164	THR	CA-C-N	-5.42	112.49	120.46
2	B	164	THR	C-N-CA	-5.42	112.49	120.46
2	D	65	LYS	CA-C-N	5.39	127.45	120.44
2	D	65	LYS	C-N-CA	5.39	127.45	120.44
1	A	60	LEU	CA-C-N	5.36	127.91	120.29
1	A	60	LEU	C-N-CA	5.36	127.91	120.29
1	C	153	LEU	N-CA-C	5.36	116.95	108.96
1	A	153	LEU	N-CA-C	5.33	117.17	109.07
4	H	112	GLY	N-CA-C	5.29	119.29	112.83
2	B	41	ASP	CA-CB-CG	5.26	117.86	112.60
3	G	54	PHE	CA-CB-CG	5.13	118.93	113.80
2	B	120	THR	CA-C-N	5.08	131.25	121.54
2	B	120	THR	C-N-CA	5.08	131.25	121.54
4	H	174	VAL	N-CA-CB	5.07	117.85	111.46
2	D	28	THR	CA-C-N	5.06	128.74	121.50
2	D	28	THR	C-N-CA	5.06	128.74	121.50
3	E	154	THR	CA-C-N	5.06	129.32	122.19
3	E	154	THR	C-N-CA	5.06	129.32	122.19
2	D	12	LYS	CA-C-N	5.04	130.77	121.70
2	D	12	LYS	C-N-CA	5.04	130.77	121.70
3	E	109	SER	CA-C-N	5.01	125.55	119.98
3	E	109	SER	C-N-CA	5.01	125.55	119.98

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	1432	0	1368	22	0
1	C	1432	0	1368	16	0
2	B	1454	0	1377	14	0
2	D	1453	0	1380	27	0
3	E	1540	0	1439	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1533	0	1433	14	0
4	F	1910	0	1820	13	0
4	H	1907	0	1818	11	0
5	I	85	0	74	2	0
5	J	85	0	74	1	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
7	A	14	0	13	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
7	D	14	0	13	0	0
8	A	8	0	0	0	0
8	B	14	0	0	0	0
8	C	9	0	0	0	0
8	D	16	0	0	0	0
8	E	25	0	0	0	0
8	F	24	0	0	0	0
8	G	30	0	0	0	0
8	H	33	0	0	0	0
8	I	3	0	0	0	0
8	J	1	0	0	0	0
All	All	13106	0	12253	116	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (116) 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:166:GLN:NE2	2:D:167:ARG:O	1.88	1.05
1:A:103:ASN:O	1:A:153:LEU:HD12	1.62	1.00
2:D:172:THR:OG1	2:D:174:HIS:CD2	2.19	0.94
2:D:169:ASP:O	2:D:189:ARG:HD2	1.77	0.82
2:D:172:THR:HG1	2:D:174:HIS:CD2	1.97	0.79
1:A:160:SER:OG	1:A:177:HIS:CE1	2.42	0.72
2:D:89:THR:HG23	2:D:90:THR:H	1.56	0.69
4:H:72:LEU:HD22	4:H:75:ARG:HH11	1.59	0.66
2:B:133:ARG:O	2:B:136:GLN:CB	2.44	0.66
1:C:156:SER:HB3	1:C:159:GLU:HG3	1.78	0.66
4:F:111:LEU:HD23	5:I:5:PHE:HB3	1.79	0.65
2:B:133:ARG:O	2:B:136:GLN:N	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:THR:OG1	2:D:174:HIS:HD2	1.82	0.63
2:D:134:ASN:ND2	2:D:169:ASP:OD1	2.33	0.62
3:E:181:ARG:HG2	3:G:92:THR:HG21	1.80	0.62
4:H:109:ARG:HG2	5:J:8:GLN:HB2	1.82	0.61
2:B:133:ARG:N	2:B:136:GLN:O	2.33	0.61
3:G:13:LEU:HD12	3:G:124:LEU:HD11	1.82	0.60
4:F:21:LEU:HD22	4:F:122:THR:HG21	1.85	0.59
4:F:39:VAL:HG21	4:F:87:SER:HB2	1.86	0.58
2:B:114:LEU:HD22	2:B:163:MET:HG3	1.85	0.58
2:D:131:TRP:CE3	2:D:172:THR:O	2.57	0.58
2:D:18:THR:HB	2:D:23:ARG:HB3	1.87	0.57
4:H:21:LEU:HD22	4:H:122:THR:HG21	1.86	0.57
1:A:104:ILE:HG12	1:A:152:THR:HG22	1.86	0.56
3:E:14:GLN:HE22	3:E:158:SER:HB2	1.70	0.56
2:B:134:ASN:OD1	2:B:169:ASP:HA	2.06	0.56
1:C:95:SER:H	1:C:103:ASN:HD21	1.53	0.56
1:C:21:GLN:HE22	1:C:137:PHE:H	1.55	0.55
1:C:118:ASN:HB2	1:C:166:GLU:HB2	1.88	0.54
2:B:114:LEU:HD23	2:B:163:MET:HE3	1.90	0.54
2:D:166:GLN:HE22	2:D:167:ARG:HG2	1.72	0.54
3:E:21:LEU:HD22	3:E:122:THR:HG21	1.91	0.52
4:F:22:ARG:HG2	4:F:88:GLU:HG2	1.91	0.52
4:H:228:TYR:HA	4:H:245:THR:HB	1.91	0.52
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.92	0.52
1:A:103:ASN:O	1:A:153:LEU:CD1	2.46	0.52
4:H:40:TYR:HB2	4:H:105:ALA:HB3	1.91	0.51
4:F:105:ALA:HB1	4:F:116:GLN:HG2	1.93	0.51
2:D:48:ARG:HH22	4:H:244:VAL:HB	1.74	0.51
4:F:170:LEU:HG	4:F:225:VAL:HG22	1.93	0.51
3:E:183:MET:HE1	4:F:210:SER:HB3	1.93	0.50
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.94	0.50
4:F:140:VAL:HG23	4:F:250:ALA:HB3	1.94	0.50
1:C:73:LEU:HD22	2:D:32:TYR:HB2	1.94	0.50
1:A:45:LEU:HB2	1:A:48:LEU:HD22	1.94	0.49
2:D:166:GLN:NE2	2:D:167:ARG:N	2.60	0.49
1:C:153:LEU:C	1:C:153:LEU:CD1	2.86	0.49
1:C:153:LEU:HD23	1:C:161:TYR:CE2	2.48	0.49
2:D:176:GLU:HG3	2:D:183:PRO:HB3	1.95	0.49
2:B:172:THR:HG22	2:B:187:GLU:HB3	1.93	0.49
1:A:153:LEU:CD1	1:A:153:LEU:C	2.86	0.49
2:D:10:GLN:HB2	2:D:31:ILE:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD22	2:B:32:TYR:HB2	1.94	0.49
2:D:166:GLN:O	2:D:169:ASP:HB2	2.13	0.49
3:E:13:LEU:HD12	3:E:124:LEU:HD11	1.95	0.49
3:E:127:HIS:HB3	3:E:158:SER:HB3	1.95	0.48
3:G:21:LEU:HD22	3:G:122:THR:HG21	1.95	0.48
3:G:127:HIS:HB3	3:G:158:SER:HB3	1.95	0.48
1:A:153:LEU:C	1:A:153:LEU:HD13	2.39	0.48
1:C:24:HIS:HB3	1:C:31:GLN:HE21	1.79	0.48
3:E:160:THR:HG21	3:E:211:PRO:HD3	1.94	0.48
1:A:94:LYS:HD2	1:A:104:ILE:HD12	1.95	0.47
2:D:166:GLN:HE22	2:D:167:ARG:CG	2.26	0.47
1:A:160:SER:OG	1:A:177:HIS:NE2	2.47	0.47
4:F:143:PRO:HG2	4:F:154:ALA:HB1	1.96	0.47
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.97	0.47
1:C:124:ASN:HD21	1:C:159:GLU:HA	1.80	0.47
2:D:66:GLU:O	2:D:70:ARG:HG2	2.15	0.47
1:C:104:ILE:HG12	1:C:152:THR:HG22	1.97	0.47
4:H:40:TYR:HE1	4:H:107:SER:HB3	1.78	0.46
3:G:15:GLU:HG3	3:G:96:PRO:HD3	1.97	0.46
4:F:43:GLN:HB2	4:F:53:LEU:HD11	1.97	0.46
3:E:74:GLU:HG2	3:G:97:GLU:HG2	1.98	0.46
1:C:153:LEU:C	1:C:153:LEU:HD13	2.41	0.46
3:E:178:LEU:HB3	4:F:184:CYS:HB3	1.98	0.45
3:G:178:LEU:HB3	4:H:184:CYS:HB3	1.99	0.45
1:C:73:LEU:HD13	2:D:9:TYR:HE1	1.82	0.45
2:D:166:GLN:CD	2:D:166:GLN:C	2.85	0.45
2:D:167:ARG:O	2:D:167:ARG:HG3	2.17	0.44
2:D:12:LYS:HD3	2:D:14:MET:HE3	1.98	0.44
4:F:230:LEU:HD12	4:F:243:PRO:HD2	2.00	0.44
1:C:97:VAL:HG11	1:C:180:PRO:HB3	2.00	0.43
1:A:153:LEU:HD13	1:A:153:LEU:O	2.18	0.43
1:C:58:PHE:HB3	5:I:3:GLN:HE22	1.83	0.43
2:D:170:VAL:HA	2:D:189:ARG:HD2	2.00	0.43
2:D:85:LEU:O	2:D:89:THR:HG22	2.18	0.43
2:D:60:TYR:HA	4:H:7:THR:HG21	2.00	0.43
3:E:179:ASP:HB3	3:E:181:ARG:HD2	2.00	0.43
2:B:165:PRO:O	2:B:165:PRO:HG2	2.19	0.42
1:C:103:ASN:O	1:C:153:LEU:HD12	2.19	0.42
1:A:57:GLN:O	1:A:61:THR:HB	2.19	0.42
2:B:133:ARG:O	2:B:136:GLN:CA	2.67	0.42
3:G:39:LEU:HD13	3:G:80:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:143:SER:HB3	3:E:146:SER:HB3	2.01	0.42
3:G:21:LEU:HD12	3:G:89:LEU:HD23	2.02	0.42
1:C:156:SER:HB3	1:C:159:GLU:CG	2.49	0.41
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.55	0.41
4:H:18:ARG:HH11	4:H:92:SER:HB3	1.86	0.41
3:G:2:ASP:HA	3:G:27:VAL:HG23	2.03	0.41
1:A:43:TRP:CD1	1:A:49:ARG:HA	2.56	0.41
1:A:73:LEU:HD23	2:B:53:LEU:HD23	2.03	0.41
3:G:128:PRO:HG3	3:G:177:VAL:HG21	2.02	0.41
1:A:8:SER:C	1:A:9(A):GLY:HA2	2.46	0.41
1:A:122:LEU:HD23	1:A:127:SER:HA	2.02	0.41
1:A:91:VAL:HG23	1:A:176:LYS:HB3	2.02	0.41
1:A:43:TRP:CG	1:A:49:ARG:HA	2.56	0.41
2:D:131:TRP:HE3	2:D:172:THR:O	2.02	0.40
2:D:148:ILE:HB	2:D:156:GLN:HB3	2.02	0.40
4:F:168:VAL:HG12	4:F:227:PHE:HA	2.02	0.40
3:G:96:PRO:HA	3:G:126:VAL:HB	2.02	0.40
3:G:81:THR:HG23	3:G:85:LYS:H	1.86	0.40
4:H:143:PRO:HG2	4:H:154:ALA:HB1	2.02	0.40
1:A:70:LEU:HD13	2:B:9:TYR:HB2	2.02	0.40
1:A:106:ILE:HG23	1:A:148:ILE:HG23	2.04	0.40
3:G:8:PRO:HG3	3:G:11:LEU:HD13	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	179/191 (94%)	172 (96%)	7 (4%)	0	100	100
1	C	179/191 (94%)	174 (97%)	5 (3%)	0	100	100
2	B	175/225 (78%)	165 (94%)	9 (5%)	1 (1%)	21	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	174/225 (77%)	170 (98%)	3 (2%)	1 (1%)	21	51
3	E	198/206 (96%)	188 (95%)	10 (5%)	0	100	100
3	G	198/206 (96%)	188 (95%)	10 (5%)	0	100	100
4	F	239/243 (98%)	233 (98%)	5 (2%)	1 (0%)	30	59
4	H	239/243 (98%)	234 (98%)	5 (2%)	0	100	100
5	I	9/11 (82%)	9 (100%)	0	0	100	100
5	J	9/11 (82%)	9 (100%)	0	0	100	100
All	All	1599/1752 (91%)	1542 (96%)	54 (3%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	ASP
2	D	121	ASP
4	F	166	ASP

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	162/174 (93%)	154 (95%)	8 (5%)	22	54
1	C	162/174 (93%)	153 (94%)	9 (6%)	19	50
2	B	156/200 (78%)	148 (95%)	8 (5%)	21	53
2	D	157/200 (78%)	150 (96%)	7 (4%)	24	58
3	E	170/183 (93%)	160 (94%)	10 (6%)	18	48
3	G	168/183 (92%)	158 (94%)	10 (6%)	17	47
4	F	207/211 (98%)	201 (97%)	6 (3%)	37	71
4	H	206/211 (98%)	197 (96%)	9 (4%)	25	59
5	I	9/9 (100%)	9 (100%)	0	100	100
5	J	9/9 (100%)	9 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1406/1554 (90%)	1339 (95%)	67 (5%)	23 55

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	50	GLN
1	A	61	THR
1	A	73	LEU
1	A	116	VAL
1	A	138	LEU
1	A	153	LEU
1	A	154	LEU
2	B	43	ASP
2	B	96	GLU
2	B	114	LEU
2	B	120	THR
2	B	127	ILE
2	B	134	ASN
2	B	137	GLU
2	B	185	ILE
1	C	12	LEU
1	C	48	LEU
1	C	50	GLN
1	C	73	LEU
1	C	103	ASN
1	C	120	THR
1	C	153	LEU
1	C	154	LEU
1	C	175	LEU
2	D	24	VAL
2	D	26	LEU
2	D	53	LEU
2	D	65	LYS
2	D	166	GLN
2	D	172	THR
2	D	189	ARG
3	E	85	LYS
3	E	97	GLU
3	E	125	ILE
3	E	147	ASP
3	E	148	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	E	152	LEU
3	E	164	GLN
3	E	178	LEU
3	E	184	ASP
3	E	206	ASN
4	F	11	LEU
4	F	109	ARG
4	F	159	LEU
4	F	174	VAL
4	F	184	CYS
4	F	237	THR
3	G	14	GLN
3	G	53	LEU
3	G	68	LYS
3	G	81	THR
3	G	86	GLU
3	G	95	LYS
3	G	101	THR
3	G	164	GLN
3	G	189	SER
3	G	206	ASN
4	H	24	SER
4	H	86	HIS
4	H	127	LEU
4	H	145	GLU
4	H	159	LEU
4	H	174	VAL
4	H	184	CYS
4	H	230	LEU
4	H	245	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	111	ASN
2	B	126	GLN
1	C	21	GLN
1	C	31	GLN
1	C	50	GLN
1	C	71	ASN
1	C	101	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	103	ASN
2	D	64	GLN
2	D	84	GLN
2	D	126	GLN
2	D	150	ASN
2	D	156	GLN
2	D	166	GLN
3	E	14	GLN
3	E	131	GLN
4	F	79	GLN
4	F	90	ASN
4	F	132	ASN
4	F	180	HIS
4	F	193	GLN
4	F	219	ASN
4	F	246	GLN
4	H	132	ASN
5	J	8	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 ⓘ

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	$\# Z > 2$
6	NAG	K	1	6,1	14,14,15	0.27	0	17,19,21	0.76	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	K	2	6	14,14,15	0.30	0	17,19,21	0.43	0
6	NAG	L	1	6,1	14,14,15	0.30	0	17,19,21	0.65	1 (5%)
6	NAG	L	2	6	14,14,15	0.32	0	17,19,21	0.85	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	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	1/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	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(°)	Ideal(°)
6	K	1	NAG	C1-O5-C5	2.31	115.28	112.19
6	L	1	NAG	C1-O5-C5	2.22	115.16	112.19

There are no chirality outliers.

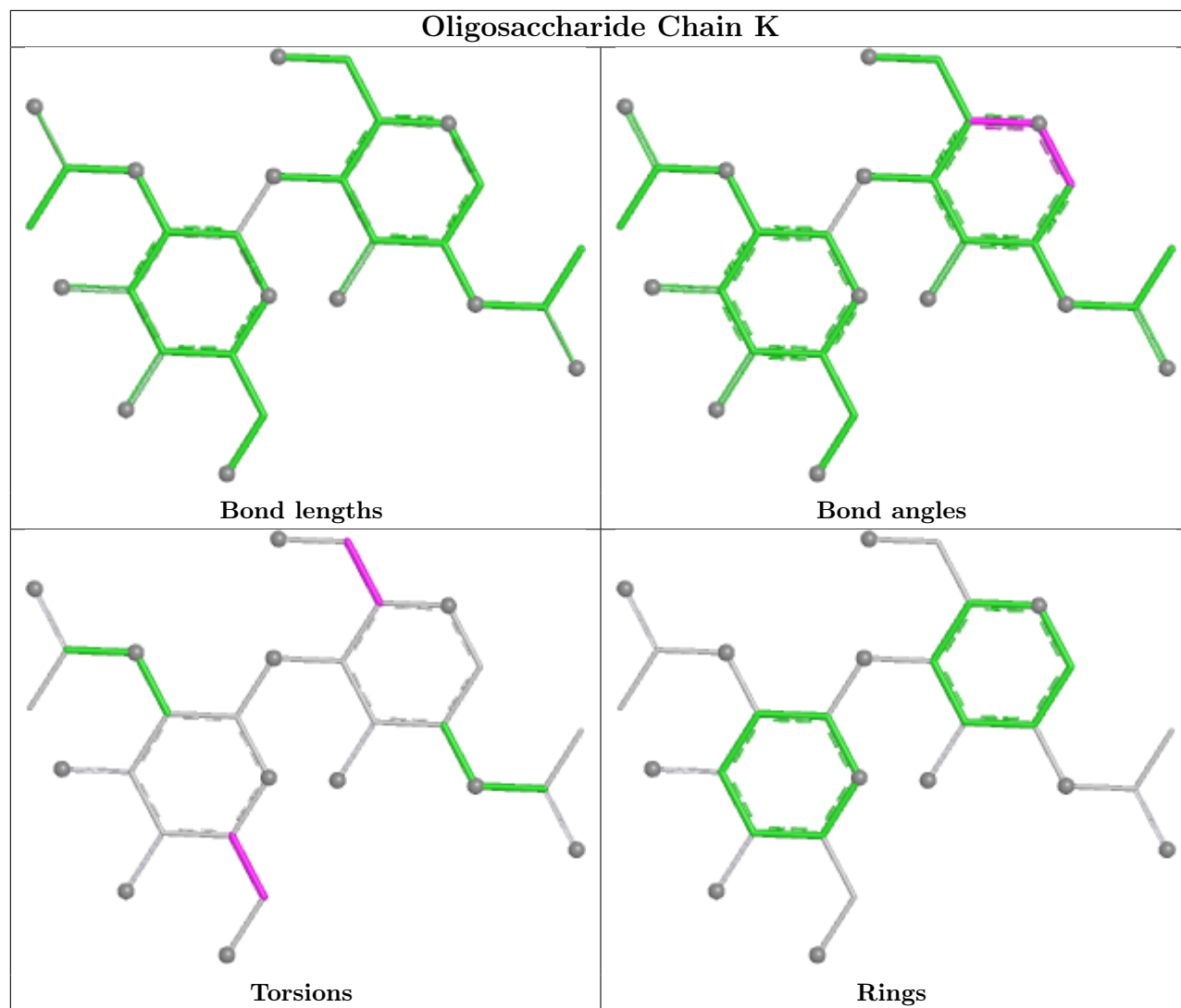
All (3) torsion outliers are listed below:

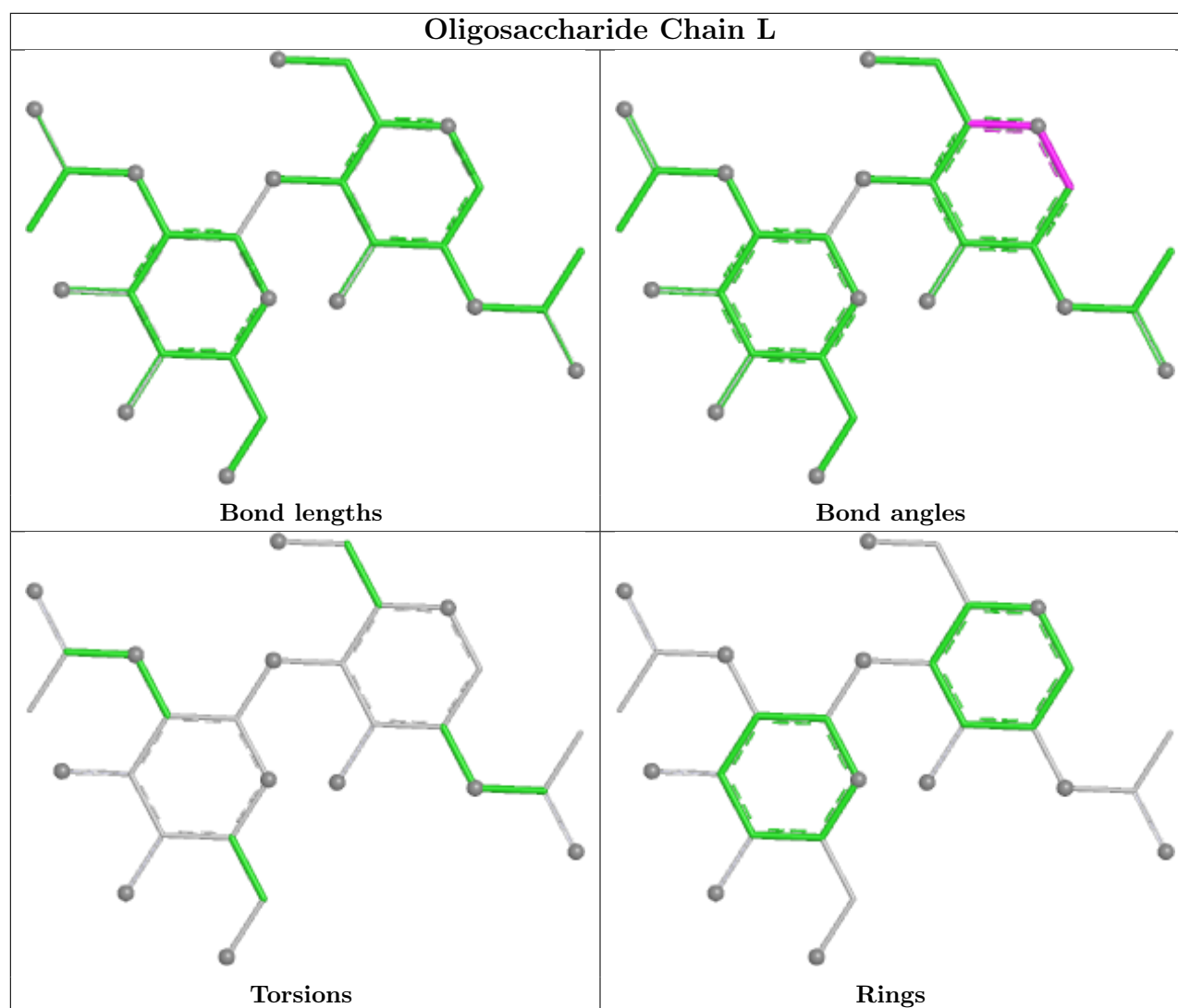
Mol	Chain	Res	Type	Atoms
6	K	1	NAG	O5-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6

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](#)

4 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	$\# Z > 2$
7	NAG	C	1000	1	14,14,15	0.40	0	17,19,21	0.88	1 (5%)
7	NAG	A	1003	1	14,14,15	0.31	0	17,19,21	1.08	3 (17%)
7	NAG	D	1000	2	14,14,15	0.40	0	17,19,21	1.80	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	B	1000	2	14,14,15	0.42	0	17,19,21	2.09	4 (23%)

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
7	NAG	C	1000	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
7	NAG	D	1000	2	-	0/6/23/26	0/1/1/1
7	NAG	B	1000	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1000	NAG	C1-O5-C5	6.82	121.32	112.19
7	D	1000	NAG	C1-O5-C5	6.62	121.06	112.19
7	C	1000	NAG	C1-O5-C5	3.18	116.45	112.19
7	B	1000	NAG	C1-C2-N2	3.16	115.41	110.43
7	D	1000	NAG	O5-C1-C2	2.90	115.77	111.29
7	B	1000	NAG	O5-C1-C2	2.73	115.52	111.29
7	A	1003	NAG	C1-O5-C5	2.61	115.69	112.19
7	A	1003	NAG	C1-C2-N2	2.51	114.39	110.43
7	B	1000	NAG	C2-N2-C7	2.43	126.16	122.90
7	A	1003	NAG	O5-C1-C2	-2.28	107.77	111.29

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1000	NAG	C1-C2-N2-C7
7	B	1000	NAG	C4-C5-C6-O6
7	B	1000	NAG	C3-C2-N2-C7

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	181/191 (94%)	0.39	5 (2%) 55 46	28, 58, 97, 108	0
1	C	181/191 (94%)	0.46	6 (3%) 49 40	32, 61, 98, 114	0
2	B	179/225 (79%)	0.53	12 (6%) 24 19	30, 55, 121, 152	0
2	D	178/225 (79%)	0.62	15 (8%) 17 14	26, 54, 121, 155	0
3	E	200/206 (97%)	0.46	6 (3%) 52 43	31, 51, 75, 105	0
3	G	200/206 (97%)	0.36	9 (4%) 38 30	22, 47, 73, 95	0
4	F	241/243 (99%)	0.13	4 (1%) 69 61	29, 45, 75, 100	0
4	H	241/243 (99%)	0.25	5 (2%) 63 54	29, 45, 73, 94	0
5	I	11/11 (100%)	0.23	1 (9%) 15 12	27, 34, 48, 60	0
5	J	11/11 (100%)	0.37	1 (9%) 15 12	31, 35, 48, 59	0
All	All	1623/1752 (92%)	0.38	64 (3%) 43 35	22, 50, 95, 155	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	256	ALA	4.2
2	B	2	ASP	4.1
5	J	10	ALA	4.1
2	D	138	GLU	3.8
5	I	10	ALA	3.7
2	B	114	LEU	3.6
2	B	190	ALA	3.5
2	D	114	LEU	3.5
2	B	165	PRO	3.5
2	D	2	ASP	3.4
2	B	138	GLU	3.3
2	B	133	ARG	3.3
1	C	180	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	182	SER	3.1
4	F	232	GLU	2.8
1	A	154	LEU	2.8
3	G	26	THR	2.7
4	F	47	ASP	2.7
3	G	201	CYS	2.7
1	A	180	PRO	2.6
3	G	218	SER	2.6
2	D	115	LEU	2.5
1	A	127	SER	2.5
2	B	164	THR	2.5
2	D	164	THR	2.5
1	C	129	THR	2.5
2	B	170	VAL	2.5
3	E	201	CYS	2.5
3	E	115	ILE	2.4
2	D	188	TRP	2.4
3	E	97	GLU	2.4
2	B	115	LEU	2.4
2	D	166	GLN	2.4
4	F	256	ALA	2.3
2	D	152	ASP	2.3
3	G	179	ASP	2.3
2	B	171	TYR	2.3
4	H	188	GLN	2.3
1	C	174	LEU	2.3
2	D	163	MET	2.2
3	G	97	GLU	2.2
4	F	132	ASN	2.2
3	E	159	GLN	2.2
1	C	139	SER	2.2
2	D	22	GLU	2.2
2	D	165	PRO	2.2
3	E	46	PRO	2.2
3	G	143	SER	2.2
4	H	231	SER	2.2
4	H	235	GLU	2.2
4	H	132	ASN	2.2
1	A	102	PRO	2.2
3	G	184	ASP	2.2
2	D	168	GLY	2.2
3	E	210	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	132	PHE	2.1
1	A	159	GLU	2.1
1	C	160	SER	2.0
2	B	160	MET	2.0
2	D	15	CYS	2.0
2	D	96	GLU	2.0
2	D	143	VAL	2.0
1	C	158	GLU	2.0
3	G	175	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

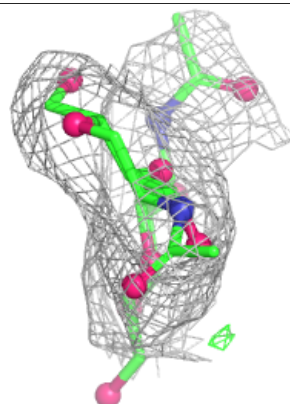
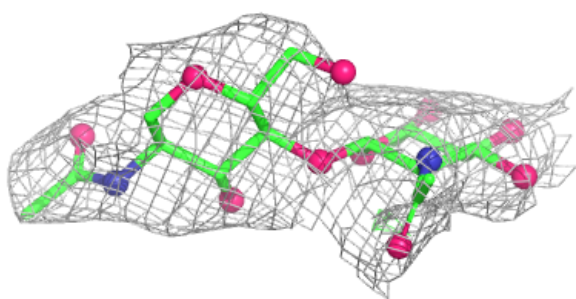
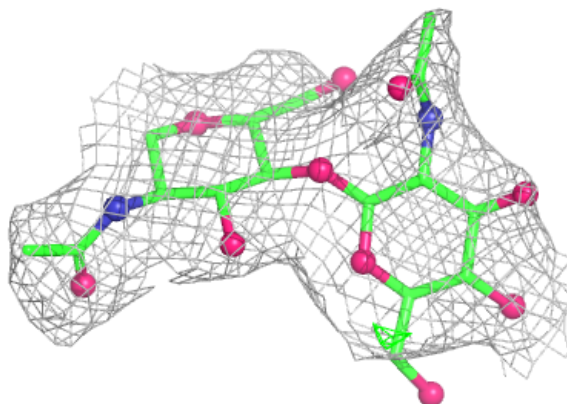
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	NAG	K	2	14/15	0.59	0.13	98,102,108,108	0
6	NAG	L	2	14/15	0.63	0.15	99,102,105,106	0
6	NAG	L	1	14/15	0.80	0.11	84,90,94,95	0
6	NAG	K	1	14/15	0.87	0.10	83,89,94,96	0

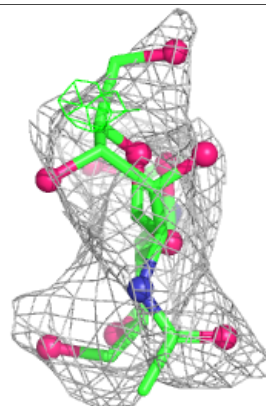
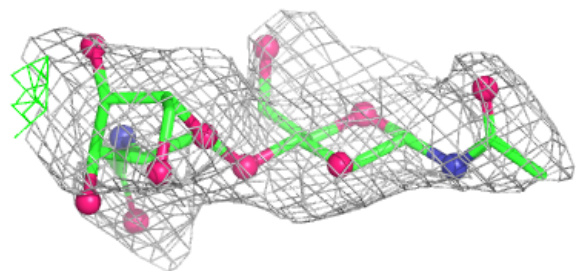
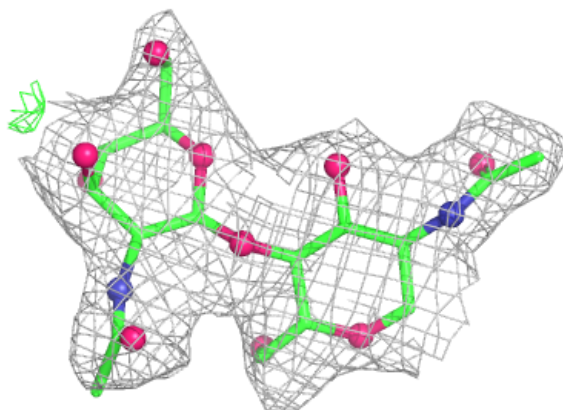
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

**Electron density around Chain L:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	NAG	D	1000	14/15	0.14	0.19	117,121,124,125	0
7	NAG	B	1000	14/15	0.26	0.19	111,113,119,119	0
7	NAG	C	1000	14/15	0.28	0.23	116,121,123,123	0
7	NAG	A	1003	14/15	0.48	0.19	94,101,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.