



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:28 PM UTC

PDB ID : 5VOC / pdb_00005voc
Title : Crystal structure of HCMV Pentamer in complex with neutralizing antibody
8I21 - Low resolution dataset for initial phasing by SAD
Authors : Malito, E.; Chandramouli, S.
Deposited on : 2017-05-02
Resolution : 3.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

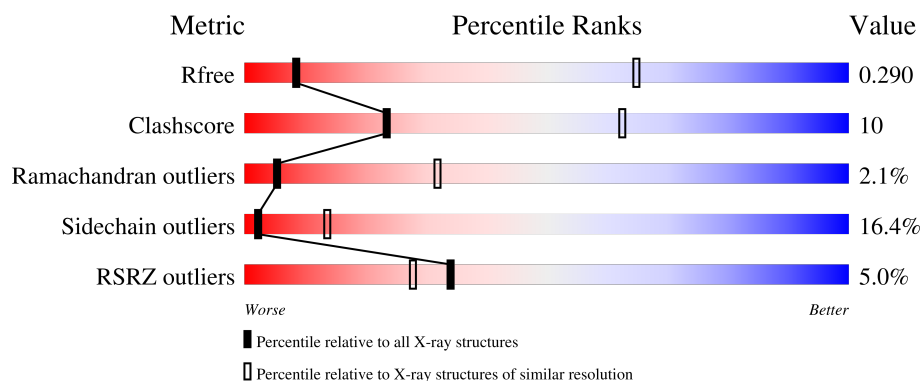
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	725	5% 58% 26% 6% 9%
2	B	278	% 55% 26% 5% 15%
3	C	171	% 42% 30% 6% 21%
4	D	252	2% 43% 20% 33%
5	E	129	2% 63% 19% 16%

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Mol	Chain	Length	Quality of chain
6	H	289	 8% 48% 16% . . 31%
7	L	235	 7% 54% 23% . . 17%
8	F	3	 33% 67%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13701 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	0	0
			5321	3402	904	990	25			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	716	GLY	-	expression tag	UNP Q6SW67
A	717	SER	-	expression tag	UNP Q6SW67
A	718	GLY	-	expression tag	UNP Q6SW67
A	719	SER	-	expression tag	UNP Q6SW67
A	720	HIS	-	expression tag	UNP Q6SW67
A	721	HIS	-	expression tag	UNP Q6SW67
A	722	HIS	-	expression tag	UNP Q6SW67
A	723	HIS	-	expression tag	UNP Q6SW67
A	724	HIS	-	expression tag	UNP Q6SW67
A	725	HIS	-	expression tag	UNP Q6SW67

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1867	1188	326	345	8			

- Molecule 3 is a protein called Envelope glycoprotein UL128.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	135	Total	C	N	O	S	0	0	0
			1090	683	197	199	11			

- Molecule 4 is a protein called Envelope glycoprotein UL130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	170	Total	C	N	O	S	0	0	0
			1388	887	243	250	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	215	GLY	-	expression tag	UNP F5HCP3
D	216	SER	-	expression tag	UNP F5HCP3
D	217	GLU	-	expression tag	UNP F5HCP3
D	218	ASN	-	expression tag	UNP F5HCP3
D	219	LEU	-	expression tag	UNP F5HCP3
D	220	TYR	-	expression tag	UNP F5HCP3
D	221	PHE	-	expression tag	UNP F5HCP3
D	222	GLN	-	expression tag	UNP F5HCP3
D	223	ALA	-	expression tag	UNP F5HCP3
D	224	GLY	-	expression tag	UNP F5HCP3
D	225	TRP	-	expression tag	UNP F5HCP3
D	226	SER	-	expression tag	UNP F5HCP3
D	227	HIS	-	expression tag	UNP F5HCP3
D	228	PRO	-	expression tag	UNP F5HCP3
D	229	GLN	-	expression tag	UNP F5HCP3
D	230	PHE	-	expression tag	UNP F5HCP3
D	231	GLU	-	expression tag	UNP F5HCP3
D	232	LYS	-	expression tag	UNP F5HCP3
D	233	GLY	-	expression tag	UNP F5HCP3
D	234	GLY	-	expression tag	UNP F5HCP3
D	235	GLY	-	expression tag	UNP F5HCP3
D	236	SER	-	expression tag	UNP F5HCP3
D	237	GLY	-	expression tag	UNP F5HCP3
D	238	GLY	-	expression tag	UNP F5HCP3
D	239	GLY	-	expression tag	UNP F5HCP3
D	240	SER	-	expression tag	UNP F5HCP3
D	241	GLY	-	expression tag	UNP F5HCP3
D	242	GLY	-	expression tag	UNP F5HCP3
D	243	GLY	-	expression tag	UNP F5HCP3
D	244	SER	-	expression tag	UNP F5HCP3
D	245	TRP	-	expression tag	UNP F5HCP3
D	246	SER	-	expression tag	UNP F5HCP3
D	247	HIS	-	expression tag	UNP F5HCP3
D	248	PRO	-	expression tag	UNP F5HCP3
D	249	GLN	-	expression tag	UNP F5HCP3
D	250	PHE	-	expression tag	UNP F5HCP3
D	251	GLU	-	expression tag	UNP F5HCP3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	252	LYS	-	expression tag	UNP F5HCP3

- Molecule 5 is a protein called Envelope glycoprotein UL131A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	108	Total	C	N	O	S	0	0	0
			893	557	168	166	2			

- Molecule 6 is a protein called Fab 8I21 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	200	Total	C	N	O	S	0	0	0
			1540	978	265	290	7			

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	228	SER	-	expression tag	UNP S6B291
H	229	SER	-	expression tag	UNP S6B291
H	230	GLY	-	expression tag	UNP S6B291
H	231	LEU	-	expression tag	UNP S6B291
H	232	GLU	-	expression tag	UNP S6B291
H	233	VAL	-	expression tag	UNP S6B291
H	234	LEU	-	expression tag	UNP S6B291
H	235	PHE	-	expression tag	UNP S6B291
H	236	GLN	-	expression tag	UNP S6B291
H	237	GLY	-	expression tag	UNP S6B291
H	238	PRO	-	expression tag	UNP S6B291
H	239	LEU	-	expression tag	UNP S6B291
H	240	GLY	-	expression tag	UNP S6B291
H	241	SER	-	expression tag	UNP S6B291
H	242	ALA	-	expression tag	UNP S6B291
H	243	TRP	-	expression tag	UNP S6B291
H	244	SER	-	expression tag	UNP S6B291
H	245	HIS	-	expression tag	UNP S6B291
H	246	PRO	-	expression tag	UNP S6B291
H	247	GLN	-	expression tag	UNP S6B291
H	248	PHE	-	expression tag	UNP S6B291
H	249	GLU	-	expression tag	UNP S6B291
H	250	LYS	-	expression tag	UNP S6B291
H	251	GLY	-	expression tag	UNP S6B291
H	252	GLY	-	expression tag	UNP S6B291

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Chain	Residue	Modelled	Actual	Comment	Reference
H	253	GLY	-	expression tag	UNP S6B291
H	254	SER	-	expression tag	UNP S6B291
H	255	GLY	-	expression tag	UNP S6B291
H	256	GLY	-	expression tag	UNP S6B291
H	257	GLY	-	expression tag	UNP S6B291
H	258	SER	-	expression tag	UNP S6B291
H	259	GLY	-	expression tag	UNP S6B291
H	260	GLY	-	expression tag	UNP S6B291
H	261	GLY	-	expression tag	UNP S6B291
H	262	SER	-	expression tag	UNP S6B291
H	263	TRP	-	expression tag	UNP S6B291
H	264	SER	-	expression tag	UNP S6B291
H	265	HIS	-	expression tag	UNP S6B291
H	266	PRO	-	expression tag	UNP S6B291
H	267	GLN	-	expression tag	UNP S6B291
H	268	PHE	-	expression tag	UNP S6B291
H	269	GLU	-	expression tag	UNP S6B291
H	270	LYS	-	expression tag	UNP S6B291

- Molecule 7 is a protein called Fab 8I21 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	194	Total	C	N	O	S	0	0	0
			1493	939	254	295	5			

There are 19 discrepancies between the modelled and reference sequences:

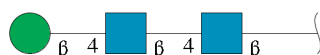
Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	THR	-	conflict	PDB ?
L	-14	GLU	-	conflict	PDB ?
L	2	THR	-	conflict	PDB ?
L	17	GLY	-	conflict	PDB ?
L	30	GLY	-	conflict	PDB ?
L	31	ILE	-	conflict	PDB ?
L	56	SER	-	conflict	PDB ?
L	58	PHE	-	conflict	PDB ?
L	76	THR	-	conflict	PDB ?
L	93	ASP	-	conflict	PDB ?
L	96	PRO	-	linker	PDB ?
L	97	TRP	-	linker	PDB ?
L	98	THR	-	linker	PDB ?
L	99	PHE	-	linker	PDB ?

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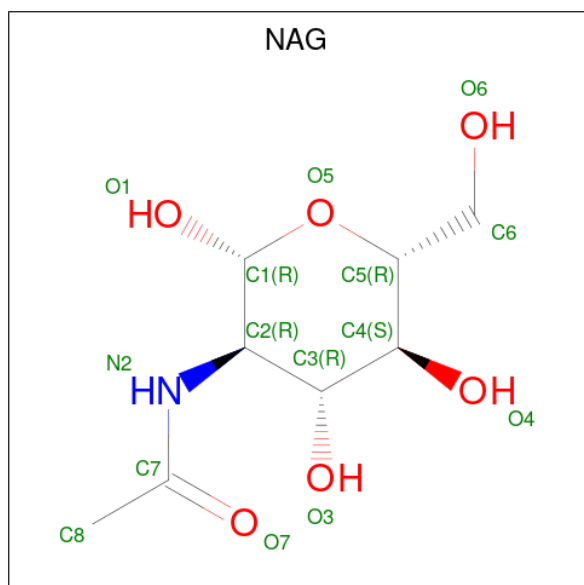
Chain	Residue	Modelled	Actual	Comment	Reference
L	100	GLY	-	linker	PDB ?
L	101	GLN	-	linker	PDB ?
L	102	GLY	-	linker	PDB ?
L	103	THR	-	linker	PDB ?
L	104	LYS	-	linker	PDB ?

- Molecule 8 is an oligosaccharide called 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
8	F	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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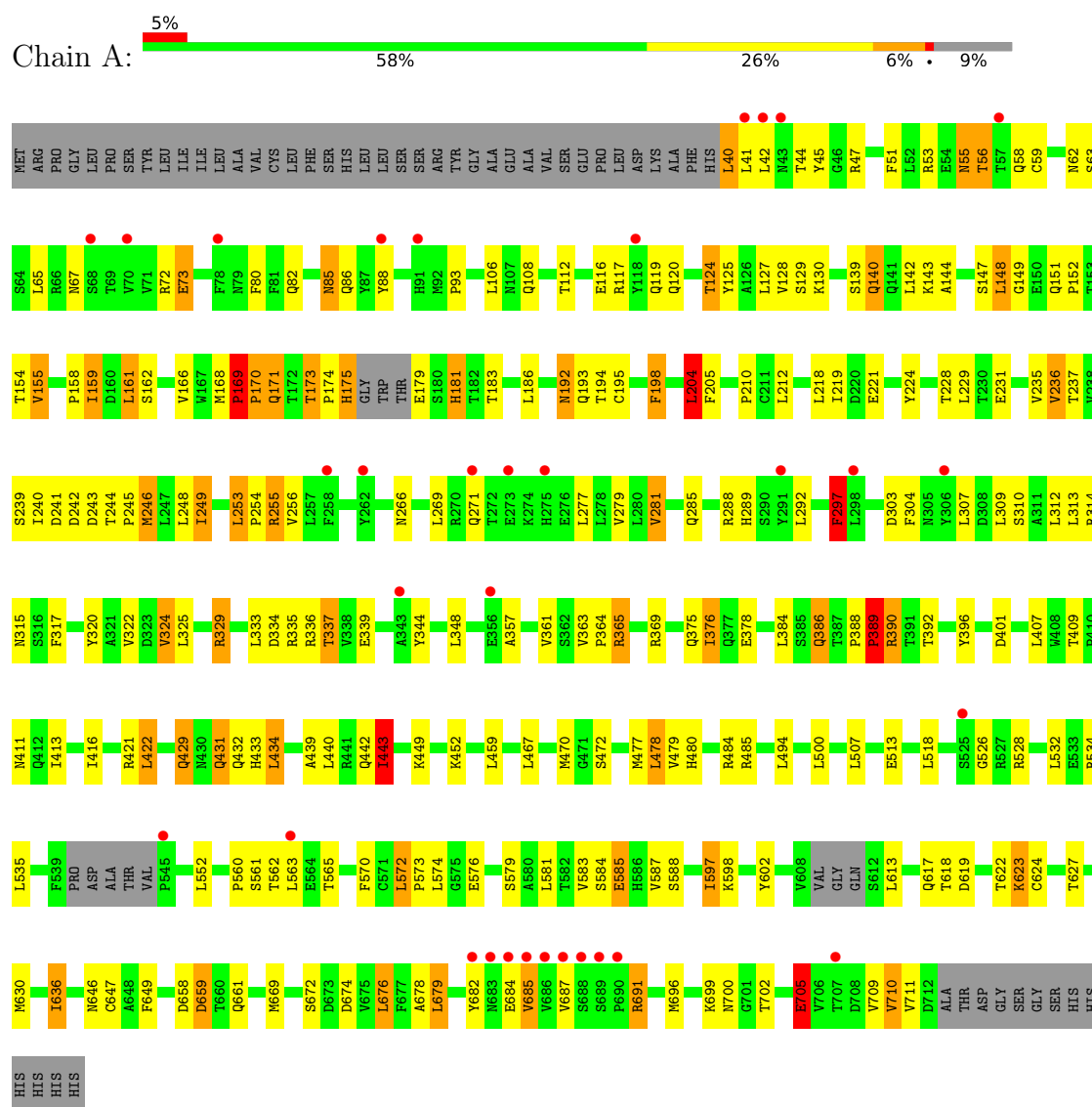
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

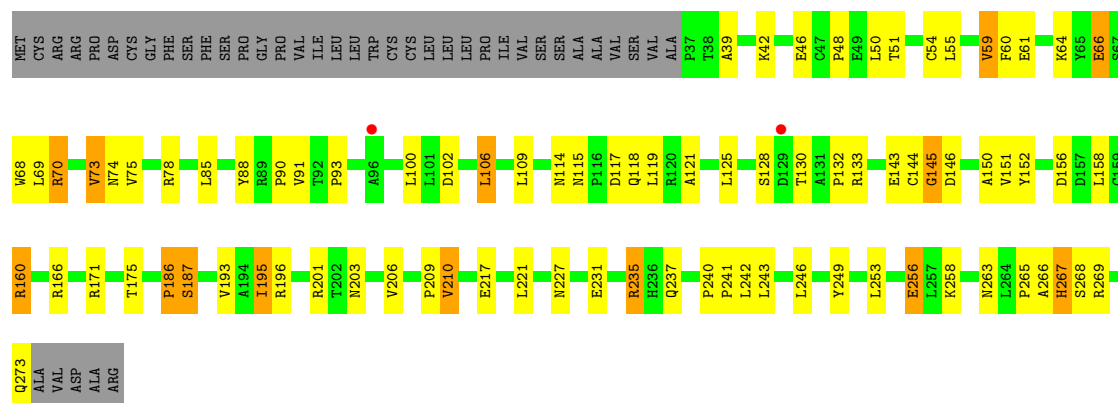
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Envelope glycoprotein H

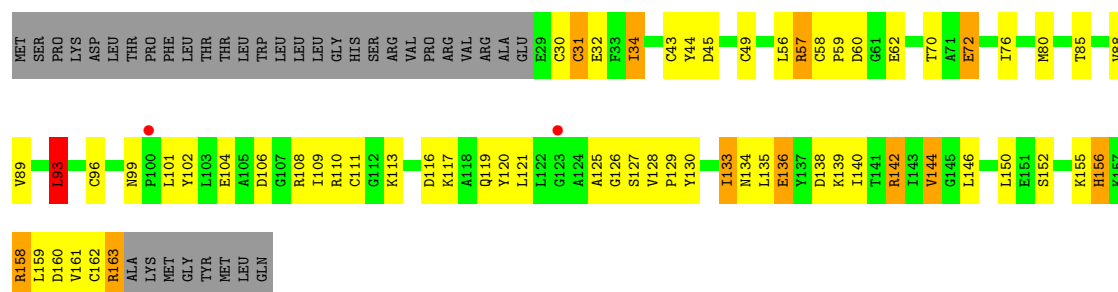


• Molecule 2: Envelope glycoprotein L

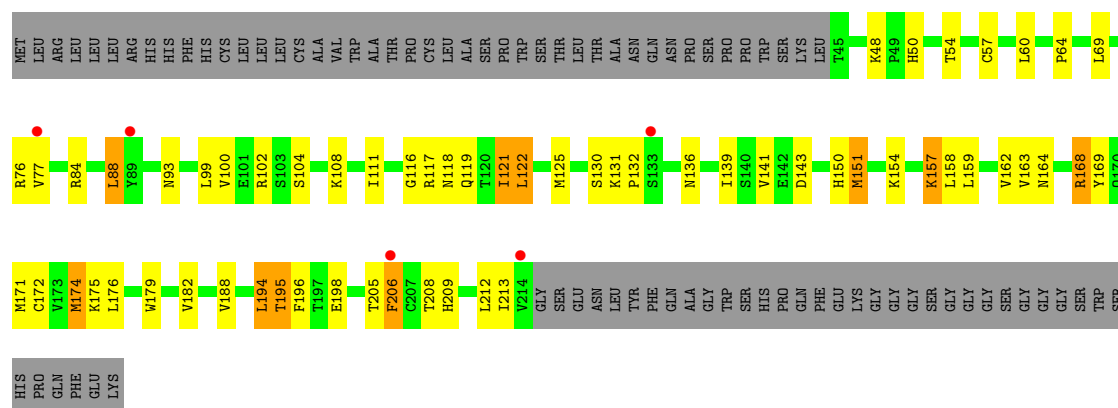




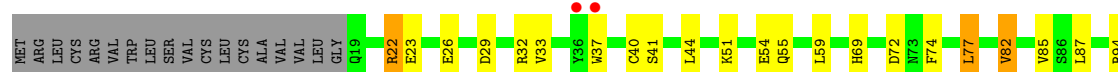
• Molecule 3: Envelope glycoprotein UL128

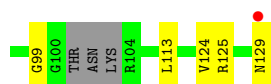


• Molecule 4: Envelope glycoprotein UL130

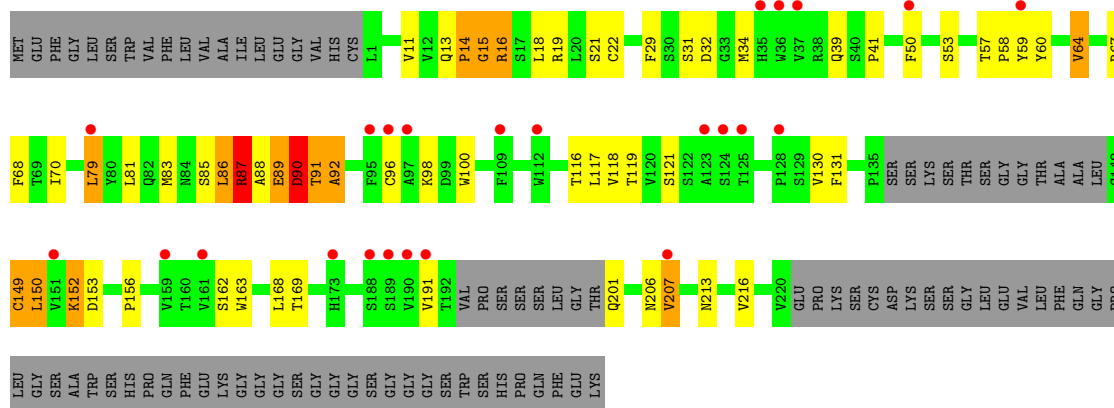


• Molecule 5: Envelope glycoprotein UL131A

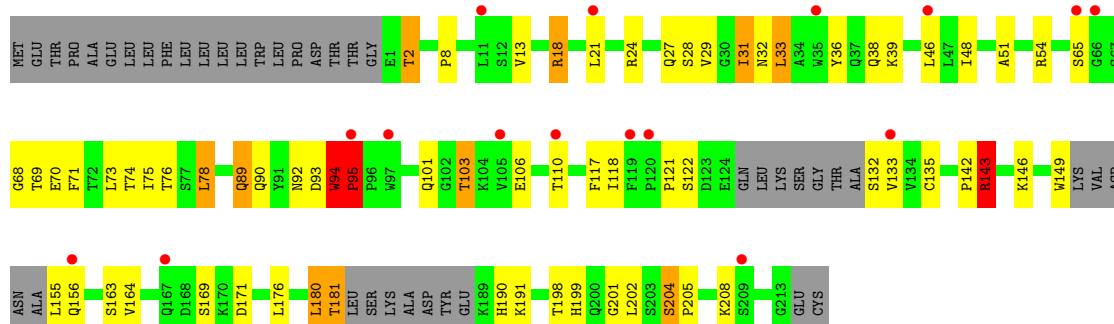




• Molecule 6: Fab 8I21 heavy chain



• Molecule 7: Fab 8I21 light chain



• Molecule 8: 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 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.42Å 146.53Å 190.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.06 – 3.99 35.06 – 3.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.06-3.99) 99.8 (35.06-3.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 4.01Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.259 , 0.276 0.270 , 0.290	Depositor DCC
R_{free} test set	1525 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	153.8	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 125.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13701	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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

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	0.91	5/5444 (0.1%)	1.41	44/7415 (0.6%)
2	B	0.93	0/1913	1.45	15/2612 (0.6%)
3	C	0.84	1/1112 (0.1%)	1.40	12/1503 (0.8%)
4	D	0.84	2/1427 (0.1%)	1.38	8/1939 (0.4%)
5	E	0.77	0/912	1.31	3/1233 (0.2%)
6	H	0.70	0/1580	1.26	11/2148 (0.5%)
7	L	0.77	2/1528 (0.1%)	1.21	7/2076 (0.3%)
All	All	0.86	10/13916 (0.1%)	1.37	100/18926 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	151	MET	SD-CE	-8.87	1.57	1.79
1	A	169	PRO	CA-C	6.22	1.57	1.52
7	L	191	LYS	CA-C	5.88	1.57	1.52
7	L	94	TRP	C-N	5.73	1.40	1.33
3	C	133	ILE	CG1-CD1	-5.61	1.29	1.51
1	A	246	MET	SD-CE	-5.39	1.66	1.79
1	A	171	GLN	CA-C	5.32	1.59	1.52
4	D	174	MET	SD-CE	-5.25	1.66	1.79
1	A	363	VAL	CA-C	5.11	1.57	1.52
1	A	173	THR	CA-C	5.07	1.59	1.52

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	136	ASN	CA-C-N	10.26	137.26	123.11
4	D	136	ASN	C-N-CA	10.26	137.26	123.11
4	D	118	ASN	CA-CB-CG	9.37	121.97	112.60
6	H	15	GLY	CA-C-N	8.66	134.68	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	15	GLY	C-N-CA	8.66	134.68	122.46
2	B	145	GLY	CA-C-N	8.64	132.22	120.38
2	B	145	GLY	C-N-CA	8.64	132.22	120.38
2	B	146	ASP	CA-CB-CG	8.54	121.14	112.60
1	A	174	PRO	CA-C-N	7.75	135.65	121.70
1	A	174	PRO	C-N-CA	7.75	135.65	121.70
1	A	472	SER	CA-C-N	7.47	130.29	120.28
1	A	472	SER	C-N-CA	7.47	130.29	120.28
3	C	116	ASP	CA-CB-CG	7.47	120.07	112.60
2	B	256	GLU	CB-CG-CD	7.39	125.16	112.60
6	H	87	ARG	CA-C-N	7.33	131.07	120.38
6	H	87	ARG	C-N-CA	7.33	131.07	120.38
1	A	409	THR	CB-CA-C	7.25	118.11	109.85
7	L	95	PRO	CA-C-O	-7.21	110.11	120.56
4	D	206	PHE	CA-CB-CG	7.10	120.90	113.80
4	D	208	THR	N-CA-C	-6.97	98.94	110.17
5	E	129	ASN	CA-CB-CG	6.92	119.52	112.60
3	C	34	ILE	N-CA-CB	6.72	118.58	110.31
1	A	192	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	390	ARG	CA-C-N	6.61	130.81	121.02
1	A	390	ARG	C-N-CA	6.61	130.81	121.02
2	B	128	SER	CA-C-N	6.60	129.79	120.28
2	B	128	SER	C-N-CA	6.60	129.79	120.28
1	A	85	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	659	ASP	CA-CB-CG	6.31	118.91	112.60
2	B	66	GLU	CB-CG-CD	6.24	123.21	112.60
7	L	171	ASP	CA-CB-CG	6.16	118.76	112.60
7	L	29	VAL	N-CA-CB	-6.06	105.11	112.33
1	A	297	PHE	CA-C-N	-6.03	112.94	122.95
1	A	297	PHE	C-N-CA	-6.03	112.94	122.95
1	A	289	HIS	CA-C-N	6.02	129.17	120.38
1	A	289	HIS	C-N-CA	6.02	129.17	120.38
6	H	16	ARG	N-CA-C	5.96	119.41	111.30
3	C	135	LEU	CA-C-N	5.93	132.87	121.54
3	C	135	LEU	C-N-CA	5.93	132.87	121.54
1	A	192	ASN	OD1-CG-ND2	5.90	128.50	122.60
1	A	375	GLN	CA-C-N	5.88	128.08	120.56
1	A	375	GLN	C-N-CA	5.88	128.08	120.56
3	C	126	GLY	CA-C-N	5.87	132.76	121.54
3	C	126	GLY	C-N-CA	5.87	132.76	121.54
1	A	443	ILE	N-CA-CB	5.87	118.52	110.54
1	A	401	ASP	CA-CB-CG	5.84	118.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	90	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	619	ASP	CA-C-N	5.67	128.15	120.38
1	A	619	ASP	C-N-CA	5.67	128.15	120.38
1	A	192	ASN	CB-CG-ND2	-5.60	108.00	116.40
4	D	111	ILE	CA-C-N	5.59	127.78	120.28
4	D	111	ILE	C-N-CA	5.59	127.78	120.28
7	L	29	VAL	N-CA-C	-5.59	107.83	113.47
5	E	51	LYS	CA-C-N	5.54	127.65	120.44
5	E	51	LYS	C-N-CA	5.54	127.65	120.44
1	A	416	ILE	CA-C-N	5.54	127.64	120.44
1	A	416	ILE	C-N-CA	5.54	127.64	120.44
1	A	171	GLN	CA-C-N	5.51	132.07	121.54
1	A	171	GLN	C-N-CA	5.51	132.07	121.54
6	H	90	ASP	CA-C-N	5.51	132.06	121.54
6	H	90	ASP	C-N-CA	5.51	132.06	121.54
1	A	237	THR	CA-C-N	-5.43	116.45	123.19
1	A	237	THR	C-N-CA	-5.43	116.45	123.19
1	A	429	GLN	N-CA-C	-5.43	101.41	109.94
2	B	195	ILE	N-CA-CB	5.42	117.49	110.99
7	L	94	TRP	CA-C-O	-5.40	112.76	120.16
1	A	204	LEU	N-CA-C	5.39	118.27	109.59
2	B	156	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	266	ALA	N-CA-C	-5.35	107.30	112.97
1	A	700	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	583	VAL	N-CA-C	5.33	116.10	110.72
1	A	429	GLN	CA-C-N	-5.32	111.38	121.54
1	A	429	GLN	C-N-CA	-5.32	111.38	121.54
1	A	563	LEU	N-CA-C	-5.30	104.81	113.19
1	A	563	LEU	CA-C-N	5.29	127.64	120.38
1	A	563	LEU	C-N-CA	5.29	127.64	120.38
4	D	93	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	623	LYS	CA-C-N	5.29	128.21	120.71
1	A	623	LYS	C-N-CA	5.29	128.21	120.71
2	B	102	ASP	CA-C-N	5.24	127.61	120.54
2	B	102	ASP	C-N-CA	5.24	127.61	120.54
3	C	162	CYS	CA-C-N	5.20	131.06	121.70
3	C	162	CYS	C-N-CA	5.20	131.06	121.70
2	B	133	ARG	N-CA-C	-5.19	105.69	112.23
2	B	242	LEU	CA-C-N	5.18	127.47	120.38
2	B	242	LEU	C-N-CA	5.18	127.47	120.38
3	C	93	LEU	CA-C-N	5.16	127.20	120.28
3	C	93	LEU	C-N-CA	5.16	127.20	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	29	PHE	CA-C-N	5.16	127.91	120.38
6	H	29	PHE	C-N-CA	5.16	127.91	120.38
7	L	95	PRO	CB-CA-C	5.16	117.21	110.92
1	A	155	VAL	N-CA-CB	5.15	117.56	111.08
3	C	72	GLU	CA-C-N	5.11	127.00	120.56
3	C	72	GLU	C-N-CA	5.11	127.00	120.56
1	A	335	ARG	CA-C-N	5.10	127.36	120.38
1	A	335	ARG	C-N-CA	5.10	127.36	120.38
1	A	51	PHE	CA-CB-CG	5.09	118.89	113.80
6	H	16	ARG	CA-C-O	-5.09	116.08	122.03
1	A	705	GLU	CB-CG-CD	5.06	121.21	112.60
7	L	143	ARG	CB-CG-CD	5.06	122.94	111.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5321	0	5274	120	0
2	B	1867	0	1859	47	0
3	C	1090	0	1075	29	0
4	D	1388	0	1360	33	0
5	E	893	0	851	14	0
6	H	1540	0	1495	38	0
7	L	1493	0	1437	31	0
8	F	39	0	34	1	0
9	A	42	0	39	2	0
9	D	28	0	26	2	0
All	All	13701	0	13450	278	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 10.

All (278) 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:169:PRO:HB2	1:A:170:PRO:HD3	1.39	1.03
7:L:13:VAL:HG11	7:L:78:LEU:HD13	1.38	1.02
2:B:121:ALA:O	2:B:125:LEU:HD13	1.64	0.97
7:L:94:TRP:HB3	7:L:95:PRO:CD	1.96	0.94
4:D:117:ARG:HG2	9:D:301:NAG:H83	1.52	0.92
6:H:41:PRO:HD3	6:H:92:ALA:HB2	1.54	0.88
2:B:125:LEU:HD11	2:B:195:ILE:HD13	1.55	0.86
7:L:21:LEU:HD13	7:L:73:LEU:HD23	1.63	0.80
1:A:159:ILE:HD12	1:A:159:ILE:H	1.44	0.80
1:A:56:THR:HG23	1:A:72:ARG:HH21	1.49	0.76
1:A:528:ARG:HH12	1:A:561:SER:HA	1.48	0.76
1:A:62:ASN:H	2:B:241:PRO:HG3	1.48	0.76
2:B:118:GLN:HE21	3:C:146:LEU:HD23	1.52	0.75
1:A:304:PHE:HZ	1:A:312:LEU:HA	1.52	0.74
7:L:94:TRP:HB3	7:L:95:PRO:HD2	1.70	0.74
1:A:56:THR:HG23	1:A:72:ARG:NH2	2.02	0.74
1:A:169:PRO:HB2	1:A:170:PRO:CD	2.16	0.73
6:H:130:VAL:HG12	6:H:216:VAL:HG11	1.72	0.72
2:B:118:GLN:HE22	3:C:146:LEU:HB3	1.55	0.72
1:A:598:LYS:HG2	1:A:627:THR:HG23	1.72	0.71
2:B:144:CYS:HB3	3:C:144:VAL:HG11	1.72	0.70
1:A:159:ILE:H	1:A:159:ILE:CD1	2.04	0.70
4:D:198:GLU:HG3	4:D:205:THR:HG21	1.74	0.69
6:H:34:MET:HE1	6:H:98:LYS:HG3	1.75	0.68
6:H:13:GLN:C	6:H:15:GLY:H	2.01	0.68
1:A:194:THR:HA	1:A:210:PRO:HA	1.75	0.68
1:A:678:ALA:HA	1:A:685:VAL:HG21	1.76	0.68
1:A:484:ARG:NH2	1:A:565:THR:HB	2.08	0.68
1:A:407:LEU:HG	1:A:422:LEU:HD11	1.77	0.66
7:L:94:TRP:CB	7:L:95:PRO:HD2	2.25	0.66
6:H:67:ARG:HH12	6:H:87:ARG:HH11	1.42	0.65
1:A:317:PHE:CE2	1:A:376:ILE:HG13	2.30	0.65
1:A:205:PHE:HD1	2:B:231:GLU:HG2	1.61	0.65
1:A:602:TYR:HB3	1:A:636:ILE:HG22	1.77	0.65
4:D:76:ARG:HH12	7:L:27:GLN:HE21	1.45	0.65
6:H:39:GLN:HE22	7:L:38:GLN:HE22	1.44	0.65
6:H:89:GLU:C	6:H:91:THR:H	2.06	0.64
7:L:94:TRP:CB	7:L:95:PRO:CD	2.74	0.64
7:L:143:ARG:HD3	7:L:164:VAL:HG21	1.79	0.63
7:L:36:TYR:HE1	7:L:89:GLN:HG2	1.64	0.63
3:C:58:CYS:HB3	3:C:59:PRO:HD2	1.81	0.63
2:B:70:ARG:HH22	2:B:74:ASN:HA	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:LEU:HD11	2:B:195:ILE:CD1	2.29	0.62
6:H:130:VAL:CG1	6:H:216:VAL:HG11	2.29	0.62
1:A:584:SER:O	1:A:585:GLU:HG3	1.99	0.62
4:D:194:LEU:HD12	5:E:85:VAL:HG11	1.81	0.61
6:H:41:PRO:HD3	6:H:92:ALA:CB	2.26	0.61
3:C:129:PRO:HB2	4:D:164:ASN:HD22	1.66	0.61
7:L:142:PRO:O	7:L:199:HIS:HE1	1.84	0.61
1:A:128:VAL:HG23	2:B:263:ASN:CG	2.25	0.61
3:C:44:TYR:CE2	3:C:57:ARG:HB3	2.36	0.61
1:A:304:PHE:CZ	1:A:312:LEU:HA	2.36	0.61
1:A:254:PRO:HG2	1:A:255:ARG:HH11	1.66	0.60
4:D:154:LYS:HD3	4:D:179:TRP:NE1	2.16	0.60
6:H:168:LEU:HD21	6:H:191:VAL:HG21	1.83	0.60
1:A:459:LEU:HD21	1:A:467:LEU:HD12	1.84	0.60
1:A:396:TYR:H	1:A:429:GLN:HE22	1.48	0.60
2:B:51:THR:HA	2:B:54:CYS:SG	2.42	0.60
7:L:8:PRO:O	7:L:103:THR:HB	2.01	0.59
7:L:31:ILE:H	7:L:31:ILE:HD12	1.67	0.59
1:A:679:LEU:HD13	1:A:710:VAL:HG23	1.85	0.58
1:A:317:PHE:CD2	1:A:376:ILE:HG13	2.39	0.58
1:A:431:GLN:CG	1:A:434:LEU:HD22	2.33	0.58
1:A:344:TYR:HD1	1:A:376:ILE:HG23	1.68	0.58
1:A:598:LYS:HG2	1:A:627:THR:CG2	2.34	0.58
1:A:246:MET:HE2	1:A:292:LEU:HD11	1.85	0.58
1:A:572:LEU:HD13	1:A:597:ILE:HD13	1.86	0.58
6:H:60:TYR:HE1	6:H:70:ILE:HG22	1.67	0.58
1:A:73:GLU:HG2	2:B:68:TRP:CD1	2.40	0.57
1:A:67:ASN:HA	1:A:85:ASN:O	2.04	0.57
1:A:142:LEU:HD23	1:A:307:LEU:HD13	1.85	0.57
1:A:239:SER:HB2	1:A:245:PRO:HB3	1.87	0.57
1:A:73:GLU:HG2	2:B:68:TRP:HD1	1.69	0.56
1:A:431:GLN:HG2	1:A:434:LEU:HD22	1.86	0.56
1:A:337:THR:HG23	1:A:384:LEU:HD21	1.87	0.56
3:C:85:THR:HG23	3:C:88:VAL:H	1.70	0.56
2:B:125:LEU:CD1	2:B:195:ILE:HD13	2.34	0.56
1:A:117:ARG:HE	1:A:120:GLN:HG3	1.70	0.56
1:A:396:TYR:H	1:A:429:GLN:NE2	2.04	0.55
4:D:119:GLN:HG3	4:D:122:LEU:HB2	1.87	0.55
7:L:94:TRP:O	7:L:95:PRO:C	2.49	0.55
2:B:118:GLN:NE2	3:C:146:LEU:HB3	2.20	0.55
2:B:66:GLU:HA	2:B:68:TRP:CZ3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ARG:HD3	1:A:585:GLU:HA	1.89	0.54
6:H:11:VAL:HG12	6:H:119:THR:HB	1.89	0.54
7:L:36:TYR:CD2	7:L:46:LEU:HA	2.43	0.54
4:D:88:LEU:HD12	4:D:102:ARG:HA	1.90	0.54
6:H:68:PHE:CE1	6:H:83:MET:HG2	2.43	0.54
4:D:122:LEU:HD11	4:D:151:MET:HE3	1.90	0.54
1:A:279:VAL:HG12	1:A:281:VAL:HG22	1.90	0.53
2:B:55:LEU:HD21	2:B:240:PRO:HB3	1.90	0.53
4:D:176:LEU:HD13	4:D:194:LEU:HD23	1.90	0.53
3:C:72:GLU:O	3:C:76:ILE:HG13	2.09	0.53
1:A:246:MET:CG	1:A:281:VAL:HG13	2.39	0.53
1:A:485:ARG:HH22	1:A:588:SER:HB3	1.74	0.53
1:A:297:PHE:O	1:A:339:GLU:OE2	2.25	0.53
1:A:166:VAL:HG11	1:A:168:MET:HE3	1.91	0.53
1:A:186:LEU:HD13	1:A:357:ALA:HB2	1.91	0.53
1:A:246:MET:HG3	1:A:281:VAL:HG13	1.91	0.52
6:H:150:LEU:HD21	6:H:152:LYS:HG3	1.91	0.52
1:A:45:TYR:HE2	2:B:209:PRO:HB3	1.74	0.52
1:A:148:LEU:HD22	1:A:310:SER:HB3	1.91	0.52
1:A:218:LEU:HA	1:A:386:GLN:HB2	1.90	0.52
4:D:54:THR:HA	4:D:57:CYS:SG	2.49	0.52
1:A:649:PHE:HD1	1:A:696:MET:HE1	1.75	0.52
2:B:106:LEU:HA	2:B:109:LEU:HD12	1.92	0.52
1:A:80:PHE:HB2	1:A:88:TYR:HB2	1.92	0.51
2:B:150:ALA:HB1	4:D:64:PRO:HG3	1.91	0.51
3:C:31:CYS:HB2	3:C:49:CYS:SG	2.51	0.51
7:L:132:SER:HB3	7:L:181:THR:HG23	1.93	0.51
1:A:80:PHE:HZ	2:B:246:LEU:HD12	1.76	0.51
1:A:166:VAL:HG12	1:A:168:MET:HG3	1.92	0.51
7:L:156:GLN:HE21	7:L:180:LEU:HD11	1.75	0.51
7:L:36:TYR:CE1	7:L:89:GLN:HG2	2.44	0.51
7:L:204:SER:HB3	7:L:205:PRO:HD2	1.92	0.50
1:A:433:HIS:CE1	1:A:434:LEU:HD13	2.47	0.50
1:A:439:ALA:O	1:A:443:ILE:HG23	2.10	0.50
4:D:76:ARG:HD3	7:L:28:SER:HB3	1.94	0.50
2:B:121:ALA:O	2:B:125:LEU:CD1	2.48	0.50
1:A:477:MET:CE	1:A:479:VAL:HG23	2.42	0.50
2:B:231:GLU:O	2:B:235:ARG:HB2	2.11	0.50
6:H:87:ARG:HH21	6:H:88:ALA:HB3	1.76	0.49
2:B:160:ARG:HG3	2:B:160:ARG:HH11	1.77	0.49
3:C:89:VAL:HG22	3:C:101:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:HB3	1:A:364:PRO:HB3	1.95	0.49
1:A:127:LEU:HD12	1:A:266:ASN:HB3	1.94	0.49
1:A:181:HIS:CE1	1:A:411:ASN:HB3	2.48	0.49
1:A:573:PRO:HG2	1:A:576:GLU:HG3	1.95	0.49
6:H:22:CYS:HB3	6:H:79:LEU:HB3	1.94	0.49
6:H:207:VAL:HG13	6:H:216:VAL:O	2.12	0.49
2:B:253:LEU:HB2	2:B:258:LYS:HE2	1.93	0.49
4:D:117:ARG:HG2	9:D:301:NAG:C8	2.36	0.48
1:A:636:ILE:HD11	1:A:705:GLU:HG2	1.95	0.48
1:A:140:GLN:HG3	1:A:303:ASP:O	2.13	0.48
1:A:320:TYR:O	1:A:324:VAL:HG13	2.13	0.48
6:H:68:PHE:HD1	6:H:81:LEU:HD11	1.79	0.48
1:A:285:GLN:HB2	1:A:288:ARG:HH12	1.79	0.48
6:H:13:GLN:HA	6:H:121:SER:O	2.14	0.48
1:A:281:VAL:HG12	1:A:285:GLN:HG3	1.95	0.47
4:D:122:LEU:HD11	4:D:151:MET:CE	2.44	0.47
6:H:16:ARG:HB2	6:H:85:SER:HA	1.95	0.47
1:A:106:LEU:C	1:A:108:GLN:H	2.21	0.47
6:H:163:TRP:HB3	6:H:168:LEU:HD23	1.96	0.47
1:A:58:GLN:HB3	2:B:59:VAL:HG13	1.95	0.47
1:A:192:ASN:OD1	9:A:801:NAG:H2	2.15	0.47
3:C:134:ASN:HB2	5:E:74:PHE:CE1	2.50	0.47
2:B:240:PRO:HD2	2:B:243:LEU:HD22	1.95	0.47
1:A:82:GLN:HE21	1:A:86:GLN:HB3	1.80	0.47
1:A:124:THR:HG23	1:A:125:TYR:HD1	1.80	0.47
3:C:99:ASN:ND2	5:E:37:TRP:H	2.13	0.47
6:H:89:GLU:C	6:H:91:THR:N	2.72	0.47
1:A:144:ALA:HB2	1:A:307:LEU:HD23	1.97	0.47
1:A:236:VAL:HG22	1:A:248:LEU:HB2	1.96	0.47
6:H:149:CYS:SG	6:H:163:TRP:CH2	3.08	0.47
1:A:56:THR:CG2	1:A:72:ARG:HH21	2.25	0.47
1:A:526:GLY:O	1:A:579:SER:HA	2.15	0.47
2:B:145:GLY:O	3:C:139:LYS:HE2	2.15	0.47
3:C:155:LYS:HE2	3:C:156:HIS:HE1	1.80	0.47
7:L:33:LEU:HD13	7:L:71:PHE:CD2	2.49	0.47
1:A:198:PHE:CD2	1:A:204:LEU:HD23	2.51	0.46
1:A:241:ASP:HB2	1:A:288:ARG:HD3	1.96	0.46
2:B:73:VAL:HG11	2:B:175:THR:HG22	1.96	0.46
6:H:13:GLN:C	6:H:15:GLY:N	2.71	0.46
1:A:452:LYS:HE3	1:A:674:ASP:OD2	2.16	0.46
6:H:16:ARG:HA	6:H:86:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:59:TYR:O	6:H:60:TYR:CD1	2.68	0.46
6:H:162:SER:HB3	6:H:206:ASN:HB2	1.97	0.46
3:C:119:GLN:C	3:C:121:LEU:H	2.24	0.46
7:L:36:TYR:HD2	7:L:46:LEU:HA	1.80	0.46
1:A:477:MET:HG3	1:A:484:ARG:HD2	1.97	0.46
1:A:253:LEU:HB3	1:A:256:VAL:HB	1.97	0.46
7:L:32:ASN:HB2	7:L:92:ASN:HB2	1.98	0.46
6:H:13:GLN:O	6:H:15:GLY:N	2.49	0.45
1:A:309:LEU:O	1:A:313:LEU:HD12	2.17	0.45
2:B:249:TYR:CE2	2:B:253:LEU:HD21	2.52	0.45
4:D:121:ILE:HG22	4:D:143:ASP:HB3	1.98	0.45
4:D:157:LYS:HE3	5:E:72:ASP:OD1	2.17	0.45
7:L:135:CYS:HB2	7:L:149:TRP:CZ2	2.51	0.45
7:L:18:ARG:HG3	7:L:76:THR:HG22	1.97	0.45
1:A:228:THR:HB	1:A:235:VAL:HB	1.98	0.45
7:L:121:PRO:HD3	7:L:133:VAL:HG22	1.99	0.45
2:B:265:PRO:C	2:B:267:HIS:H	2.24	0.45
3:C:130:TYR:CD1	5:E:82:VAL:HG13	2.51	0.45
6:H:131:PHE:HB3	7:L:122:SER:OG	2.17	0.45
4:D:130:SER:HB2	5:E:54:GLU:HB2	1.99	0.45
4:D:168:ARG:HH12	4:D:171:MET:HE2	1.80	0.45
1:A:162:SER:O	1:A:449:LYS:HE2	2.17	0.44
1:A:235:VAL:HG22	1:A:249:ILE:HG23	2.00	0.44
3:C:158:ARG:HH11	3:C:160:ASP:HB3	1.81	0.44
1:A:478:LEU:HG	1:A:565:THR:HG22	1.99	0.44
3:C:125:ALA:O	4:D:212:LEU:HA	2.17	0.44
1:A:148:LEU:O	1:A:151:GLN:HG2	2.18	0.44
1:A:467:LEU:HD11	1:A:494:LEU:HD13	1.99	0.44
1:A:485:ARG:HH11	1:A:585:GLU:H	1.65	0.44
1:A:365:ARG:O	1:A:369:ARG:HG2	2.17	0.44
7:L:149:TRP:CE2	7:L:180:LEU:HB2	2.53	0.44
1:A:329:ARG:HG2	1:A:336:ARG:HE	1.82	0.44
2:B:70:ARG:NH2	2:B:74:ASN:HA	2.31	0.44
1:A:158:PRO:HD2	1:A:161:LEU:HB2	1.98	0.44
1:A:467:LEU:HD23	1:A:470:MET:HE3	1.98	0.44
1:A:570:PHE:CE2	1:A:624:CYS:HB3	2.53	0.44
3:C:163:ARG:HD2	3:C:163:ARG:HA	1.56	0.44
4:D:121:ILE:HD13	4:D:188:VAL:HG21	2.00	0.44
4:D:104:SER:O	4:D:108:LYS:HG3	2.18	0.44
4:D:174:MET:HG3	4:D:196:PHE:CE1	2.53	0.44
6:H:130:VAL:CG1	6:H:216:VAL:CG1	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:133:ILE:HD11	4:D:162:VAL:HG13	2.00	0.43
4:D:50:HIS:HA	4:D:77:VAL:HG11	2.00	0.43
6:H:14:PRO:C	6:H:16:ARG:H	2.26	0.43
1:A:271:GLN:HE22	2:B:268:SER:HA	1.82	0.43
3:C:93:LEU:HB3	3:C:101:LEU:HD21	2.00	0.43
1:A:269:LEU:HB2	1:A:279:VAL:HG23	2.00	0.43
1:A:682:TYR:C	1:A:684:GLU:H	2.26	0.43
2:B:91:VAL:HG13	2:B:132:PRO:HB3	1.99	0.43
2:B:186:PRO:O	2:B:187:SER:CB	2.67	0.43
5:E:44:LEU:HD11	5:E:87:LEU:HB3	1.99	0.43
4:D:116:GLY:HA3	4:D:150:HIS:CE1	2.54	0.43
6:H:57:THR:HA	6:H:58:PRO:HD3	1.91	0.43
6:H:130:VAL:HG11	6:H:216:VAL:CG1	2.48	0.43
1:A:59:CYS:SG	1:A:93:PRO:HD3	2.58	0.43
3:C:102:TYR:CZ	3:C:120:TYR:HB2	2.53	0.43
6:H:31:SER:C	6:H:53:SER:OG	2.61	0.43
6:H:16:ARG:CB	6:H:85:SER:HA	2.48	0.43
1:A:702:THR:HG21	9:A:803:NAG:HN2	1.84	0.43
5:E:22:ARG:HG2	5:E:26:GLU:OE1	2.19	0.43
1:A:40:LEU:HB3	1:A:41:LEU:H	1.65	0.43
1:A:224:TYR:CD2	1:A:224:TYR:C	2.97	0.43
1:A:672:SER:O	1:A:676:LEU:HD12	2.19	0.43
2:B:46:GLU:HB3	2:B:48:PRO:HD2	2.00	0.43
2:B:115:ASN:O	2:B:118:GLN:HB2	2.19	0.43
7:L:146:LYS:HB3	7:L:198:THR:HB	2.01	0.42
1:A:322:VAL:HG22	1:A:518:LEU:HD23	2.02	0.42
4:D:175:LYS:HB3	4:D:195:THR:HG23	2.01	0.42
1:A:219:ILE:HG23	1:A:386:GLN:HG2	2.01	0.42
6:H:64:VAL:HG13	6:H:68:PHE:HB2	2.00	0.42
6:H:50:PHE:HD1	6:H:59:TYR:HD2	1.66	0.42
3:C:45:ASP:HB3	3:C:57:ARG:HB2	2.01	0.42
3:C:111:CYS:HB3	5:E:32:ARG:HD2	2.02	0.42
5:E:22:ARG:O	5:E:23:GLU:HB2	2.19	0.42
6:H:83:MET:HE2	6:H:86:LEU:HD11	2.01	0.42
1:A:344:TYR:CD1	1:A:376:ILE:HG23	2.53	0.42
1:A:477:MET:HE3	1:A:479:VAL:HG23	2.00	0.42
1:A:560:PRO:HB2	1:A:562:THR:HG22	2.02	0.42
2:B:70:ARG:H	2:B:70:ARG:HG3	1.63	0.42
1:A:388:PRO:HA	1:A:389:PRO:HD2	1.60	0.42
3:C:152:SER:O	3:C:161:VAL:HG11	2.19	0.42
1:A:587:VAL:HG23	1:A:617:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:1:NAG:H4	8:F:2:NAG:H2	1.41	0.42
7:L:143:ARG:HD2	7:L:143:ARG:O	2.20	0.42
1:A:337:THR:CG2	1:A:384:LEU:HD21	2.49	0.41
1:A:344:TYR:CZ	1:A:348:LEU:HD11	2.55	0.41
2:B:88:TYR:CE2	2:B:90:PRO:HG3	2.55	0.41
3:C:113:LYS:HE3	5:E:26:GLU:HB3	2.02	0.41
3:C:113:LYS:HG2	5:E:26:GLU:HG2	2.02	0.41
7:L:2:THR:HG23	7:L:93:ASP:HB3	2.02	0.41
2:B:93:PRO:HA	2:B:132:PRO:HB2	2.02	0.41
1:A:128:VAL:HG22	1:A:266:ASN:C	2.44	0.41
1:A:485:ARG:HH22	1:A:588:SER:CB	2.32	0.41
1:A:658:ASP:HA	1:A:691:ARG:O	2.20	0.41
4:D:159:LEU:HD22	5:E:77:LEU:HG	2.03	0.41
1:A:44:THR:HA	1:A:47:ARG:HG3	2.02	0.41
1:A:309:LEU:HD23	1:A:369:ARG:HB2	2.01	0.41
2:B:227:ASN:O	2:B:231:GLU:HB2	2.20	0.41
1:A:159:ILE:HD12	1:A:159:ILE:N	2.24	0.41
4:D:174:MET:HE3	4:D:176:LEU:HB2	2.02	0.41
2:B:152:TYR:OH	4:D:64:PRO:HG2	2.20	0.41
3:C:43:CYS:HB2	3:C:80:MET:HE1	2.03	0.41
4:D:206:PHE:O	4:D:206:PHE:HD2	2.04	0.41
2:B:39:ALA:HB3	2:B:60:PHE:HA	2.03	0.40
2:B:50:LEU:O	2:B:54:CYS:HB3	2.21	0.40
2:B:210:VAL:HG21	2:B:221:LEU:HD23	2.02	0.40
1:A:128:VAL:HG23	2:B:263:ASN:OD1	2.20	0.40
1:A:173:THR:OG1	1:A:175:HIS:ND1	2.54	0.40
1:A:333:LEU:HA	1:A:337:THR:HG21	2.04	0.40
1:A:334:ASP:H	1:A:337:THR:HB	1.87	0.40
2:B:73:VAL:HG12	2:B:75:VAL:HG22	2.04	0.40
4:D:150:HIS:ND1	5:E:69:HIS:HE1	2.19	0.40
4:D:168:ARG:NH1	4:D:171:MET:HE2	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	654/725 (90%)	599 (92%)	43 (7%)	12 (2%)	6	34
2	B	235/278 (84%)	215 (92%)	17 (7%)	3 (1%)	9	41
3	C	133/171 (78%)	108 (81%)	20 (15%)	5 (4%)	2	22
4	D	168/252 (67%)	161 (96%)	6 (4%)	1 (1%)	21	57
5	E	104/129 (81%)	98 (94%)	5 (5%)	1 (1%)	12	45
6	H	194/289 (67%)	170 (88%)	17 (9%)	7 (4%)	2	23
7	L	186/235 (79%)	169 (91%)	11 (6%)	6 (3%)	3	25
All	All	1674/2079 (80%)	1520 (91%)	119 (7%)	35 (2%)	5	32

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	169	PRO
1	A	170	PRO
1	A	297	PHE
1	A	389	PRO
3	C	30	CYS
3	C	127	SER
3	C	136	GLU
4	D	132	PRO
6	H	92	ALA
6	H	153	ASP
7	L	94	TRP
7	L	95	PRO
2	B	187	SER
3	C	117	LYS
7	L	201	GLY
1	A	55	ASN
1	A	413	ILE
1	A	661	GLN
6	H	91	THR
7	L	51	ALA
1	A	574	LEU
2	B	186	PRO
2	B	267	HIS
3	C	142	ARG
6	H	87	ARG

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Mol	Chain	Res	Type
6	H	90	ASP
1	A	140	GLN
1	A	149	GLY
6	H	14	PRO
1	A	253	LEU
7	L	68	GLY
7	L	204	SER
5	E	99	GLY
6	H	156	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/655 (92%)	506 (84%)	98 (16%)	2	14
2	B	204/238 (86%)	171 (84%)	33 (16%)	2	14
3	C	122/154 (79%)	96 (79%)	26 (21%)	1	7
4	D	156/222 (70%)	132 (85%)	24 (15%)	2	15
5	E	95/114 (83%)	82 (86%)	13 (14%)	3	17
6	H	171/239 (72%)	149 (87%)	22 (13%)	4	19
7	L	167/202 (83%)	134 (80%)	33 (20%)	1	9
All	All	1519/1824 (83%)	1270 (84%)	249 (16%)	2	14

All (249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	42	LEU
1	A	53	ARG
1	A	55	ASN
1	A	63	SER
1	A	65	LEU
1	A	73	GLU
1	A	112	THR

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Mol	Chain	Res	Type
1	A	116	GLU
1	A	119	GLN
1	A	124	THR
1	A	129	SER
1	A	130	LYS
1	A	139	SER
1	A	143	LYS
1	A	147	SER
1	A	148	LEU
1	A	154	THR
1	A	155	VAL
1	A	159	ILE
1	A	161	LEU
1	A	171	GLN
1	A	175	HIS
1	A	179	GLU
1	A	181	HIS
1	A	183	THR
1	A	193	GLN
1	A	195	CYS
1	A	198	PHE
1	A	204	LEU
1	A	212	LEU
1	A	221	GLU
1	A	229	LEU
1	A	231	GLU
1	A	236	VAL
1	A	240	ILE
1	A	242	ASP
1	A	243	ASP
1	A	244	THR
1	A	249	ILE
1	A	255	ARG
1	A	277	LEU
1	A	281	VAL
1	A	314	ARG
1	A	315	ASN
1	A	324	VAL
1	A	325	LEU
1	A	329	ARG
1	A	337	THR
1	A	361	VAL

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Mol	Chain	Res	Type
1	A	365	ARG
1	A	376	ILE
1	A	378	GLU
1	A	386	GLN
1	A	389	PRO
1	A	390	ARG
1	A	392	THR
1	A	421	ARG
1	A	422	LEU
1	A	431	GLN
1	A	432	GLN
1	A	434	LEU
1	A	440	LEU
1	A	442	GLN
1	A	443	ILE
1	A	478	LEU
1	A	480	HIS
1	A	500	LEU
1	A	507	LEU
1	A	513	GLU
1	A	532	LEU
1	A	534	ARG
1	A	535	LEU
1	A	552	LEU
1	A	572	LEU
1	A	581	LEU
1	A	585	GLU
1	A	597	ILE
1	A	613	LEU
1	A	618	THR
1	A	622	THR
1	A	623	LYS
1	A	630	MET
1	A	636	ILE
1	A	646	ASN
1	A	647	CYS
1	A	659	ASP
1	A	669	MET
1	A	676	LEU
1	A	679	LEU
1	A	685	VAL
1	A	687	VAL

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Mol	Chain	Res	Type
1	A	691	ARG
1	A	699	LYS
1	A	705	GLU
1	A	709	VAL
1	A	710	VAL
1	A	711	VAL
2	B	42	LYS
2	B	59	VAL
2	B	61	GLU
2	B	64	LYS
2	B	69	LEU
2	B	70	ARG
2	B	73	VAL
2	B	78	ARG
2	B	85	LEU
2	B	100	LEU
2	B	106	LEU
2	B	114	ASN
2	B	117	ASP
2	B	119	LEU
2	B	130	THR
2	B	143	GLU
2	B	151	VAL
2	B	158	LEU
2	B	160	ARG
2	B	166	ARG
2	B	171	ARG
2	B	193	VAL
2	B	196	ARG
2	B	201	ARG
2	B	203	ASN
2	B	206	VAL
2	B	210	VAL
2	B	217	GLU
2	B	235	ARG
2	B	237	GLN
2	B	256	GLU
2	B	269	ARG
2	B	273	GLN
3	C	31	CYS
3	C	32	GLU
3	C	34	ILE

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Mol	Chain	Res	Type
3	C	56	LEU
3	C	57	ARG
3	C	60	ASP
3	C	62	GLU
3	C	70	THR
3	C	93	LEU
3	C	96	CYS
3	C	104	GLU
3	C	106	ASP
3	C	108	ARG
3	C	109	ILE
3	C	110	ARG
3	C	128	VAL
3	C	136	GLU
3	C	138	ASP
3	C	140	ILE
3	C	142	ARG
3	C	144	VAL
3	C	150	LEU
3	C	156	HIS
3	C	158	ARG
3	C	159	LEU
3	C	163	ARG
4	D	48	LYS
4	D	60	LEU
4	D	69	LEU
4	D	84	ARG
4	D	88	LEU
4	D	99	LEU
4	D	100	VAL
4	D	121	ILE
4	D	122	LEU
4	D	125	MET
4	D	131	LYS
4	D	139	ILE
4	D	141	VAL
4	D	157	LYS
4	D	158	LEU
4	D	163	VAL
4	D	168	ARG
4	D	169	TYR
4	D	172	CYS

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Mol	Chain	Res	Type
4	D	182	VAL
4	D	194	LEU
4	D	195	THR
4	D	209	HIS
4	D	213	ILE
5	E	22	ARG
5	E	29	ASP
5	E	33	VAL
5	E	40	CYS
5	E	41	SER
5	E	55	GLN
5	E	59	LEU
5	E	77	LEU
5	E	82	VAL
5	E	94	ARG
5	E	113	LEU
5	E	124	VAL
5	E	125	ARG
6	H	18	LEU
6	H	19	ARG
6	H	21	SER
6	H	32	ASP
6	H	64	VAL
6	H	79	LEU
6	H	86	LEU
6	H	87	ARG
6	H	89	GLU
6	H	90	ASP
6	H	96	CYS
6	H	100	TRP
6	H	116	THR
6	H	117	LEU
6	H	118	VAL
6	H	149	CYS
6	H	150	LEU
6	H	152	LYS
6	H	169	THR
6	H	201	GLN
6	H	207	VAL
6	H	213	ASN
7	L	2	THR
7	L	18	ARG

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Mol	Chain	Res	Type
7	L	24	ARG
7	L	31	ILE
7	L	33	LEU
7	L	39	LYS
7	L	48	ILE
7	L	54	ARG
7	L	65	SER
7	L	69	THR
7	L	70	GLU
7	L	74	THR
7	L	75	ILE
7	L	78	LEU
7	L	89	GLN
7	L	90	GLN
7	L	94	TRP
7	L	101	GLN
7	L	103	THR
7	L	106	GLU
7	L	110	THR
7	L	117	PHE
7	L	118	ILE
7	L	143	ARG
7	L	155	LEU
7	L	163	SER
7	L	169	SER
7	L	176	LEU
7	L	180	LEU
7	L	181	THR
7	L	190	HIS
7	L	202	LEU
7	L	208	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	82	GLN
1	A	104	GLN
1	A	140	GLN
1	A	145	GLN
1	A	181	HIS
1	A	252	HIS

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Mol	Chain	Res	Type
1	A	271	GLN
1	A	289	HIS
1	A	305	ASN
1	A	429	GLN
1	A	431	GLN
1	A	433	HIS
1	A	437	GLN
1	A	480	HIS
1	A	512	HIS
1	A	559	GLN
1	A	617	GLN
1	A	621	GLN
2	B	74	ASN
2	B	118	GLN
2	B	197	ASN
2	B	203	ASN
3	C	37	ASN
3	C	90	HIS
3	C	97	ASN
3	C	99	ASN
3	C	115	ASN
3	C	119	GLN
4	D	123	GLN
4	D	136	ASN
4	D	138	GLN
4	D	164	ASN
4	D	170	GLN
4	D	211	ASN
5	E	55	GLN
5	E	69	HIS
6	H	13	GLN
6	H	39	GLN
6	H	82	GLN
6	H	208	ASN
7	L	27	GLN
7	L	37	GLN
7	L	89	GLN
7	L	156	GLN
7	L	199	HIS

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 ⓘ

3 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$
8	NAG	F	1	5,8	14,14,15	0.56	0	17,19,21	2.32	5 (29%)
8	NAG	F	2	8	14,14,15	0.75	0	17,19,21	1.95	3 (17%)
8	BMA	F	3	8	11,11,12	1.04	0	15,15,17	1.18	2 (13%)

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
8	NAG	F	1	5,8	-	4/6/23/26	0/1/1/1
8	NAG	F	2	8	-	1/6/23/26	0/1/1/1
8	BMA	F	3	8	-	0/2/19/22	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(°)
8	F	1	NAG	C1-O5-C5	5.60	119.69	112.19
8	F	2	NAG	C2-N2-C7	4.81	129.34	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	1	NAG	C3-C4-C5	4.54	118.46	110.23
8	F	1	NAG	C1-C2-N2	4.44	117.44	110.43
8	F	2	NAG	C1-C2-N2	4.06	116.83	110.43
8	F	2	NAG	C1-O5-C5	3.81	117.29	112.19
8	F	1	NAG	C2-N2-C7	2.91	126.80	122.90
8	F	3	BMA	C1-O5-C5	2.47	115.50	112.19
8	F	1	NAG	O5-C1-C2	-2.47	107.47	111.29
8	F	3	BMA	C3-C4-C5	2.28	114.36	110.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

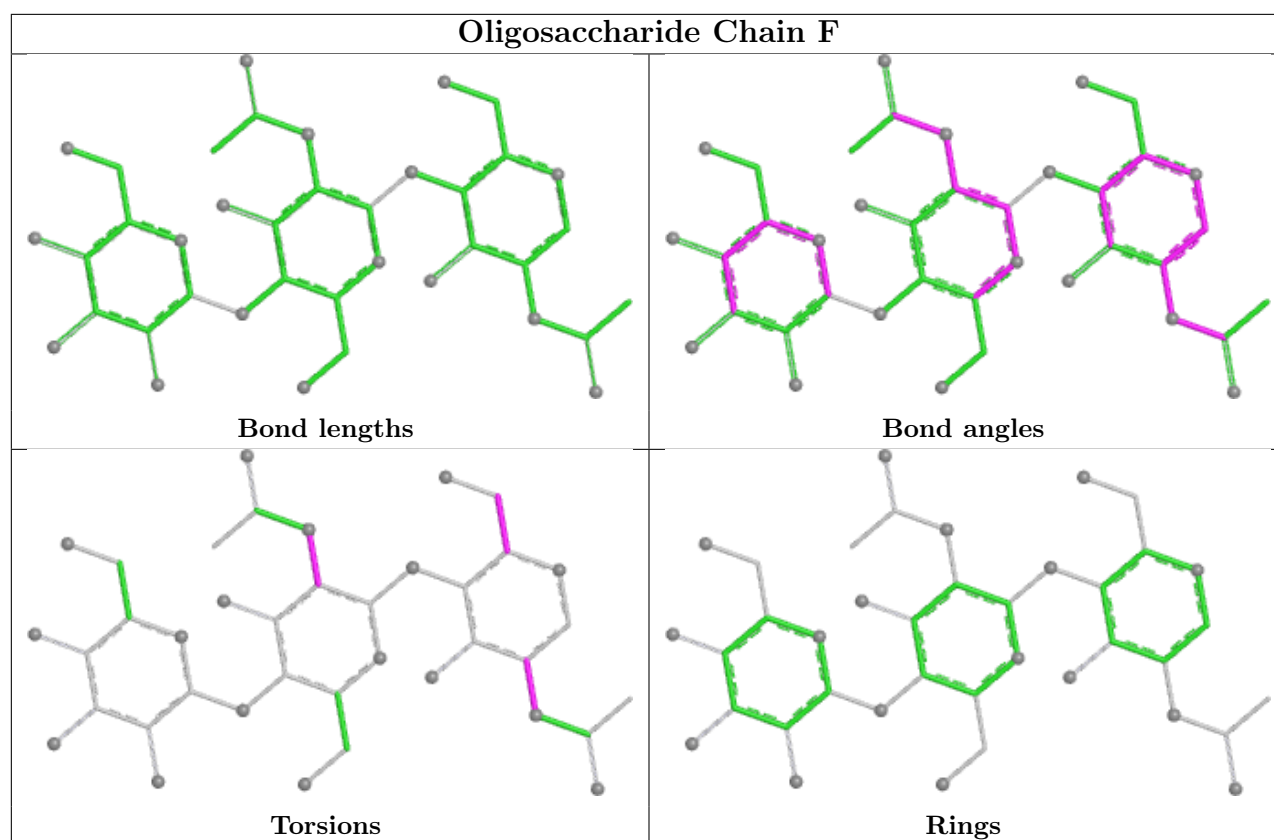
Mol	Chain	Res	Type	Atoms
8	F	1	NAG	C1-C2-N2-C7
8	F	2	NAG	C1-C2-N2-C7
8	F	1	NAG	O5-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6
8	F	1	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	1	NAG	1	0
8	F	2	NAG	1	0

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



5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
9	NAG	D	301	4	14,14,15	0.64	0	17,19,21	1.38	3 (17%)
9	NAG	D	302	4	14,14,15	0.46	0	17,19,21	0.77	1 (5%)
9	NAG	A	801	1	14,14,15	0.99	0	17,19,21	2.07	5 (29%)
9	NAG	A	802	1	14,14,15	0.72	0	17,19,21	1.75	4 (23%)
9	NAG	A	803	1	14,14,15	0.50	0	17,19,21	1.05	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	D	301	4	-	3/6/23/26	0/1/1/1
9	NAG	D	302	4	-	0/6/23/26	0/1/1/1
9	NAG	A	801	1	-	5/6/23/26	0/1/1/1
9	NAG	A	802	1	-	4/6/23/26	0/1/1/1
9	NAG	A	803	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	801	NAG	C1-C2-N2	5.15	118.55	110.43
9	A	802	NAG	C3-C4-C5	4.65	118.67	110.23
9	D	301	NAG	O5-C1-C2	3.79	117.15	111.29
9	A	801	NAG	C2-N2-C7	3.73	127.90	122.90
9	A	801	NAG	C1-O5-C5	3.54	116.92	112.19
9	A	802	NAG	C1-C2-N2	2.92	115.03	110.43
9	A	802	NAG	O3-C3-C4	2.88	117.17	110.38
9	A	803	NAG	O5-C1-C2	-2.61	107.25	111.29
9	A	801	NAG	O5-C1-C2	2.52	115.19	111.29
9	D	301	NAG	C1-O5-C5	2.45	115.47	112.19
9	D	302	NAG	O5-C1-C2	-2.36	107.64	111.29
9	D	301	NAG	C2-N2-C7	2.35	126.05	122.90
9	A	802	NAG	C2-N2-C7	2.24	125.91	122.90
9	A	803	NAG	O3-C3-C2	2.06	113.69	109.40
9	A	801	NAG	C3-C4-C5	2.03	113.92	110.23

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	801	NAG	C1-C2-N2-C7
9	A	801	NAG	O7-C7-N2-C2
9	D	301	NAG	C1-C2-N2-C7
9	A	801	NAG	C8-C7-N2-C2
9	A	801	NAG	O5-C5-C6-O6
9	A	802	NAG	C8-C7-N2-C2
9	A	802	NAG	O7-C7-N2-C2
9	D	301	NAG	C8-C7-N2-C2
9	A	801	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	D	301	NAG	O7-C7-N2-C2
9	A	803	NAG	C4-C5-C6-O6
9	A	803	NAG	O5-C5-C6-O6
9	A	802	NAG	C1-C2-N2-C7
9	A	802	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	301	NAG	2	0
9	A	801	NAG	1	0
9	A	803	NAG	1	0

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	662/725 (91%)	0.20	33 (4%) 34 28	50, 93, 133, 300	0
2	B	237/278 (85%)	0.11	2 (0%) 82 65	63, 97, 148, 166	0
3	C	135/171 (78%)	-0.02	2 (1%) 72 54	64, 101, 153, 192	2 (1%)
4	D	170/252 (67%)	0.05	5 (2%) 53 39	55, 76, 119, 182	0
5	E	108/129 (83%)	0.03	3 (2%) 55 40	55, 89, 141, 155	0
6	H	200/289 (69%)	0.78	24 (12%) 9 12	143, 203, 258, 285	0
7	L	194/235 (82%)	0.66	16 (8%) 17 19	131, 172, 278, 300	0
All	All	1706/2079 (82%)	0.26	85 (4%) 34 28	50, 101, 248, 300	2 (0%)

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	96	ALA	6.0
6	H	125	THR	5.8
1	A	685	VAL	5.4
6	H	124	SER	5.3
1	A	686	VAL	5.1
1	A	688	SER	5.1
6	H	190	VAL	4.9
6	H	188	SER	4.7
6	H	189	SER	4.6
6	H	97	ALA	4.5
1	A	683	ASN	3.9
1	A	707	THR	3.8
6	H	35	HIS	3.8
1	A	78	PHE	3.7
6	H	109	PHE	3.7
6	H	191	VAL	3.6
6	H	79	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
6	H	37	VAL	3.6
7	L	133	VAL	3.5
1	A	689	SER	3.5
1	A	275	HIS	3.5
7	L	46	LEU	3.5
6	H	151	VAL	3.4
7	L	156	GLN	3.4
1	A	298	LEU	3.4
1	A	687	VAL	3.2
7	L	209	SER	3.1
1	A	684	GLU	3.0
1	A	57	THR	2.9
1	A	42	LEU	2.9
1	A	291	TYR	2.9
1	A	545	PRO	2.8
6	H	50	PHE	2.8
7	L	65	SER	2.8
7	L	95	PRO	2.8
1	A	68	SER	2.8
6	H	123	ALA	2.8
7	L	97	TRP	2.7
1	A	690	PRO	2.7
3	C	100	PRO	2.7
6	H	112	TRP	2.6
4	D	133	SER	2.6
6	H	96	CYS	2.6
1	A	258	PHE	2.6
1	A	343	ALA	2.6
6	H	173	HIS	2.6
1	A	43	ASN	2.6
7	L	105	VAL	2.5
3	C	123	GLY	2.5
6	H	207	VAL	2.5
1	A	91	HIS	2.5
1	A	682	TYR	2.5
7	L	21	LEU	2.5
5	E	37	TRP	2.4
7	L	120	PRO	2.4
4	D	206	PHE	2.4
6	H	128	PRO	2.4
5	E	36	TYR	2.4
6	H	95	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
7	L	66	GLY	2.4
7	L	11	LEU	2.4
5	E	129	ASN	2.3
7	L	119	PHE	2.3
1	A	118	TYR	2.3
1	A	306	TYR	2.3
4	D	89	TYR	2.3
6	H	36	TRP	2.3
1	A	563	LEU	2.3
7	L	35	TRP	2.2
7	L	110	THR	2.2
6	H	161	VAL	2.2
1	A	41	LEU	2.2
1	A	356	GLU	2.2
1	A	271	GLN	2.2
1	A	262	TYR	2.1
7	L	167	GLN	2.1
1	A	273	GLU	2.1
6	H	59	TYR	2.0
1	A	70	VAL	2.0
1	A	88	TYR	2.0
2	B	129	ASP	2.0
1	A	525	SER	2.0
4	D	77	VAL	2.0
4	D	214	VAL	2.0
6	H	159	VAL	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.

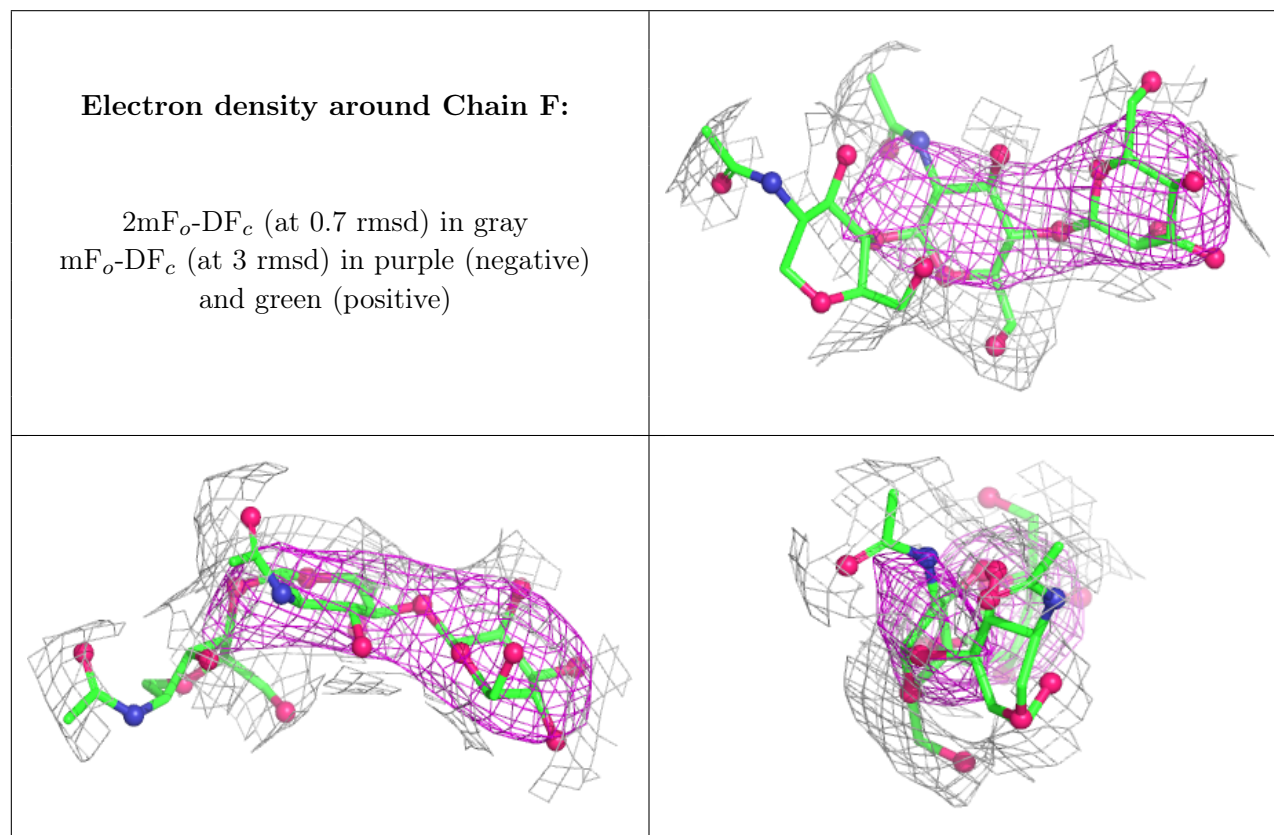
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	F	1	14/15	-	-	50,50,50,50	0
8	NAG	F	2	14/15	-	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	BMA	F	3	11/12	-	-	50,50,50,50	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 ⓘ

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
9	NAG	A	803	14/15	0.81	0.17	50,50,50,50	0
9	NAG	A	801	14/15	0.83	0.17	50,50,50,50	0
9	NAG	D	302	14/15	0.89	0.08	50,50,50,50	0
9	NAG	A	802	14/15	0.91	0.12	50,50,50,50	0
9	NAG	D	301	14/15	0.93	0.07	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.