



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:45 PM UTC

PDB ID : 9CFA / pdb_00009cfa
Title : Germline-targeting HIV-1 gp120 engineered outer domain eODgt8 in complex with Fab eOD-CL04.1
Authors : Sarkar, A.; Stanfield, R.L.; Wilson, I.A.
Deposited on : 2024-06-27
Resolution : 3.06 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

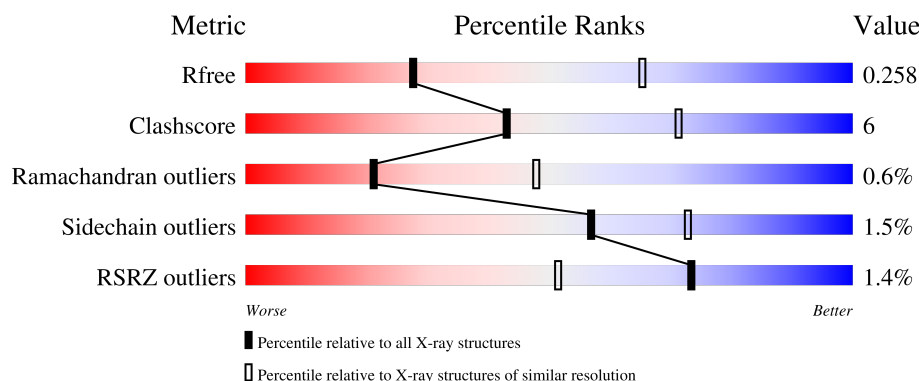
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	215	 84% 14% .
1	E	215	 84% 15%
1	L	215	 82% 18% 5%
2	B	219	 80% 18% ..
2	F	219	 83% 13% .

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Mol	Chain	Length	Quality of chain
2	H	219	% 82% 17%
3	C	183	% 74% 18% 7%
3	D	183	% 75% 14% 9%
3	G	183	81% 9% 9%
4	I	2	100%
4	J	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13622 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 Fab eOD-CL04.1 lambda light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	214	Total	C	N	O	S	0	0	0
			1602	1014	263	320	5			
1	A	214	Total	C	N	O	S	0	0	0
			1602	1014	263	320	5			
1	E	214	Total	C	N	O	S	0	0	0
			1602	1014	263	320	5			

- Molecule 2 is a protein called Fab eOD-CL04.1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1620	1017	273	323	7			
2	B	217	Total	C	N	O	S	0	0	0
			1620	1017	273	323	7			
2	F	211	Total	C	N	O	S	0	0	0
			1584	997	266	314	7			

- Molecule 3 is a protein called germline-targeting HIV-1 gp120 engineered outer domain eODgt8.

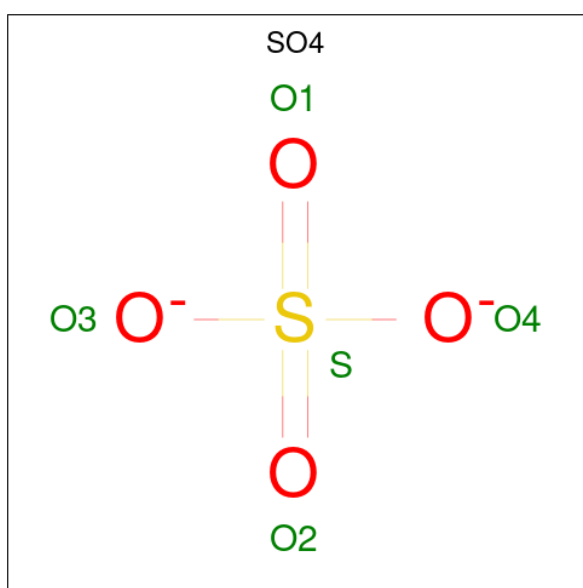
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	170	Total	C	N	O	S	0	0	0
			1293	812	228	245	8			
3	D	166	Total	C	N	O	S	0	0	0
			1265	795	223	239	8			
3	G	166	Total	C	N	O	S	0	0	0
			1265	795	223	239	8			

- Molecule 4 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
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	O	S	0	0
			5	4	1		
5	L	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

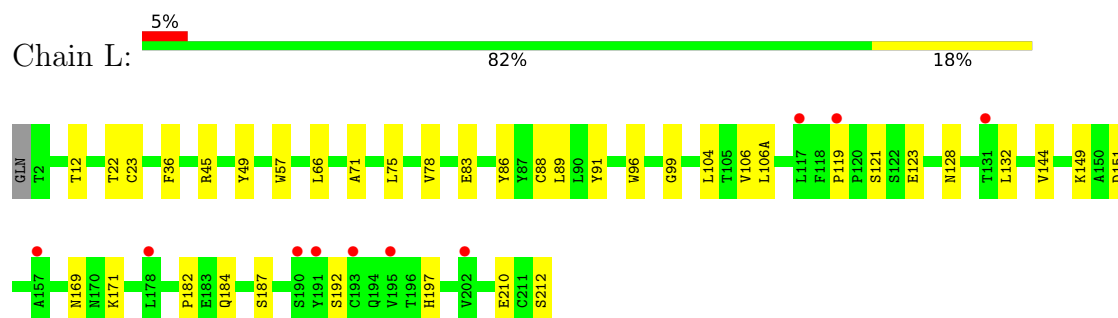


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		

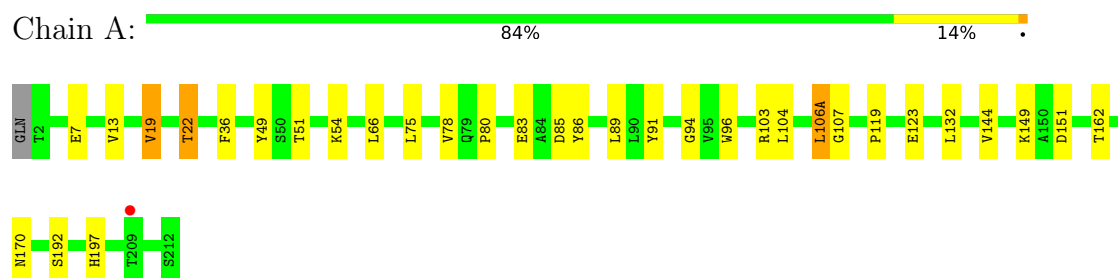
3 Residue-property plots [i](#)

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.

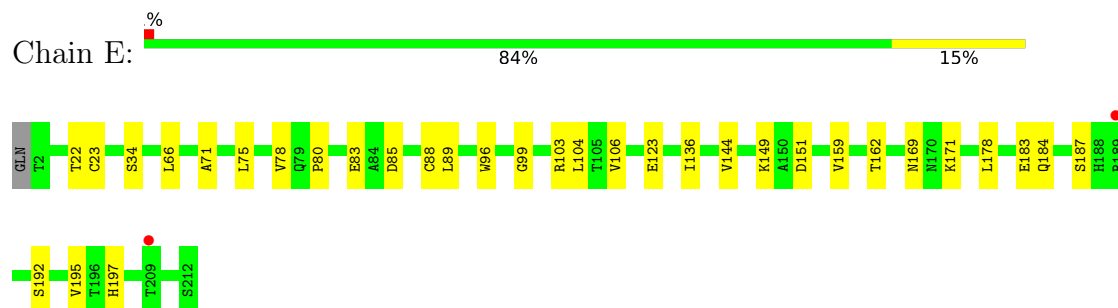
- Molecule 1: Fab eOD-CL04.1 lambda light chain



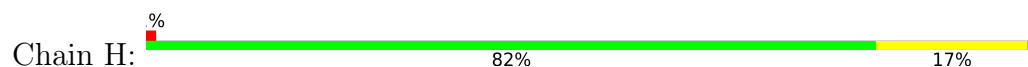
- Molecule 1: Fab eOD-CL04.1 lambda light chain

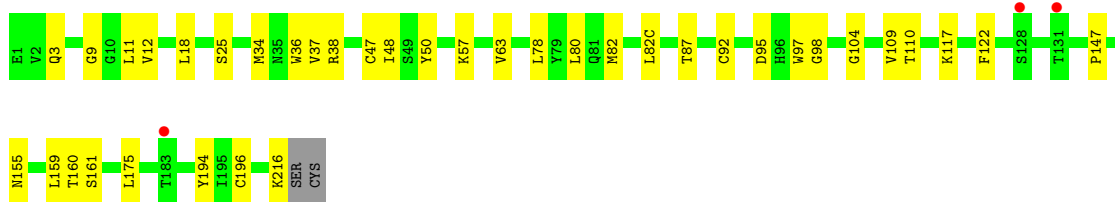


- Molecule 1: Fab eOD-CL04.1 lambda light chain

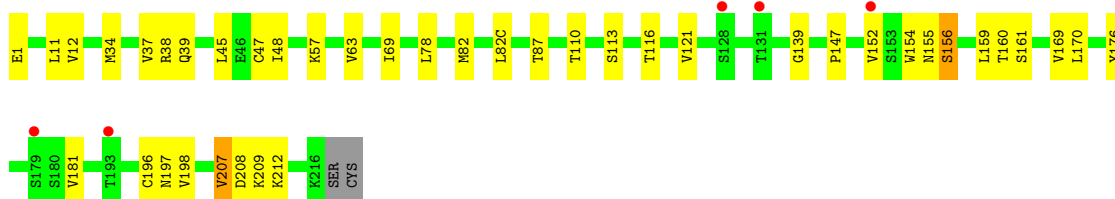
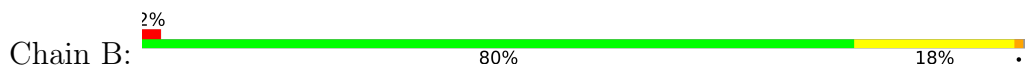


- Molecule 2: Fab eOD-CL04.1 heavy chain

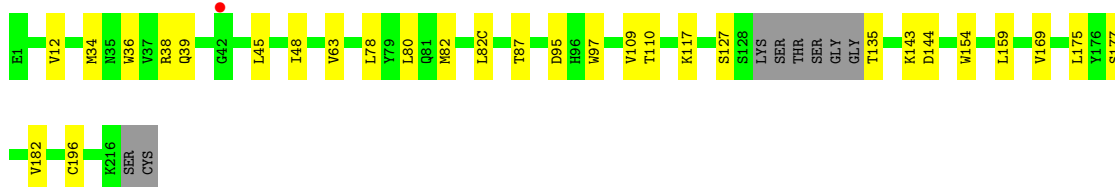
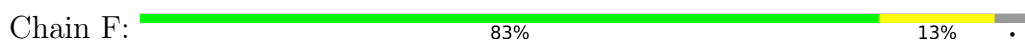




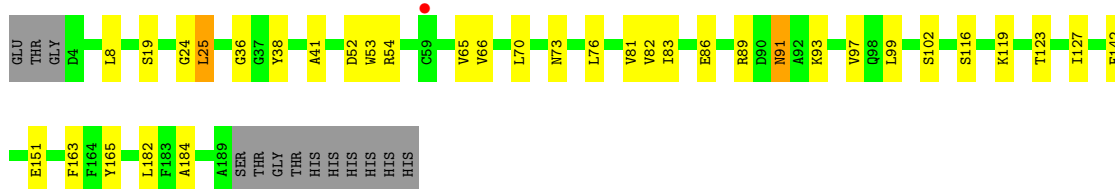
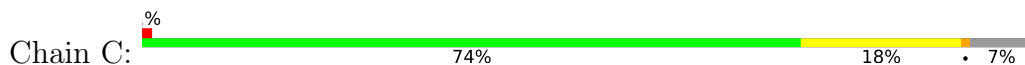
- Molecule 2: Fab eOD-CL04.1 heavy chain



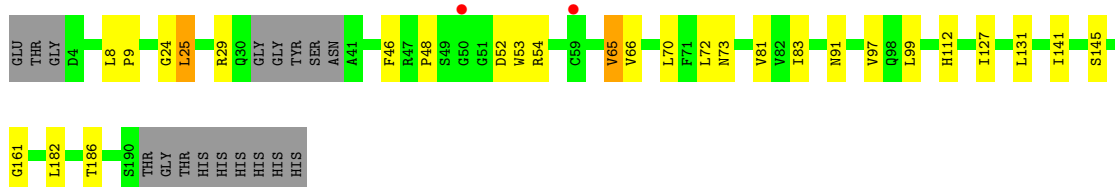
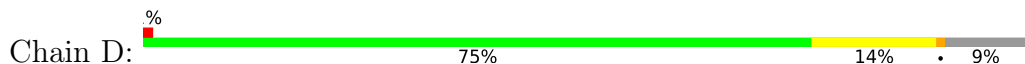
- Molecule 2: Fab eOD-CL04.1 heavy chain



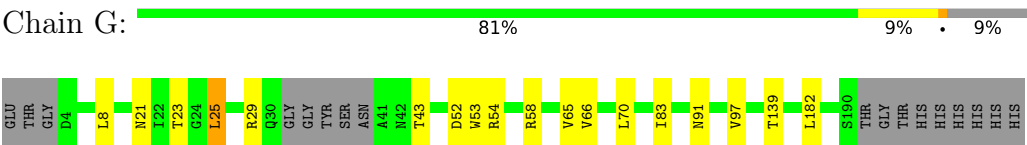
- Molecule 3: germline-targeting HIV-1 gp120 engineered outer domain eODgt8



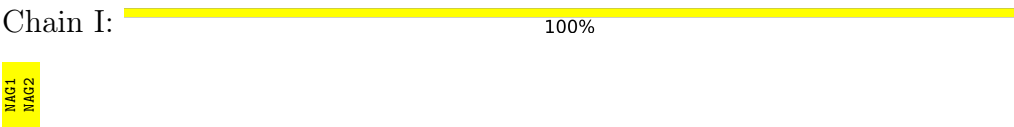
- Molecule 3: germline-targeting HIV-1 gp120 engineered outer domain eODgt8



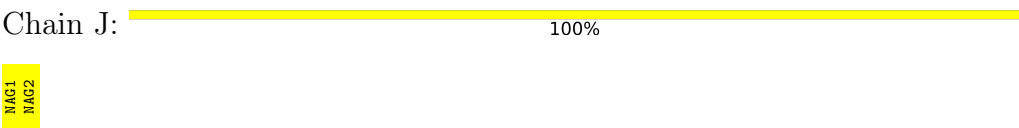
- Molecule 3: germline-targeting HIV-1 gp120 engineered outer domain eODgt8



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



- Molecule 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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.82Å 159.33Å 101.06Å 90.00° 108.23° 90.00°	Depositor
Resolution (Å)	48.22 – 3.06 48.22 – 3.06	Depositor EDS
% Data completeness (in resolution range)	93.1 (48.22-3.06) 93.4 (48.22-3.06)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, R_{free}	0.224 , 0.259 0.223 , 0.258	Depositor DCC
R_{free} test set	2118 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13622	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: SO4, 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	0.12	0/1646	0.33	0/2255
1	E	0.12	0/1646	0.31	0/2255
1	L	0.12	0/1646	0.31	0/2255
2	B	0.12	0/1658	0.35	0/2255
2	F	0.12	0/1621	0.34	0/2205
2	H	0.12	0/1658	0.33	0/2255
3	C	0.12	0/1323	0.29	0/1798
3	D	0.12	0/1293	0.32	0/1756
3	G	0.12	0/1293	0.30	0/1756
All	All	0.12	0/13784	0.32	0/18790

There are no bond length outliers.

There are no bond angle outliers.

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	1602	0	1555	21	0
1	E	1602	0	1555	19	0
1	L	1602	0	1555	23	0
2	B	1620	0	1575	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1584	0	1538	21	0
2	H	1620	0	1575	24	0
3	C	1293	0	1248	19	0
3	D	1265	0	1226	17	0
3	G	1265	0	1226	10	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
5	C	5	0	0	0	0
5	L	10	0	0	0	0
6	C	28	0	26	2	0
6	D	28	0	26	0	0
6	F	14	0	13	0	0
6	G	28	0	26	0	0
All	All	13622	0	13194	165	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 6.

All (165) 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:H:38:ARG:HD3	2:H:48:ILE:HD11	1.67	0.77
2:F:48:ILE:HG23	2:F:63:VAL:HG21	1.66	0.76
2:B:48:ILE:HG23	2:B:63:VAL:HG21	1.71	0.72
2:F:38:ARG:HD3	2:F:48:ILE:HD11	1.71	0.72
2:B:38:ARG:HD3	2:B:48:ILE:HD11	1.72	0.70
2:B:11:LEU:HB2	2:B:147:PRO:HG3	1.72	0.70
2:F:82:MET:HB3	2:F:82(C):LEU:HD21	1.74	0.68
2:H:159:LEU:O	2:H:161:SER:N	2.29	0.66
2:F:12:VAL:HG11	2:F:82(C):LEU:HD12	1.78	0.64
2:H:48:ILE:HG23	2:H:63:VAL:HG21	1.78	0.64
1:L:144:VAL:HG12	1:L:197:HIS:HB2	1.79	0.62
2:B:39:GLN:HB2	2:B:45:LEU:HD23	1.82	0.62
2:B:37:VAL:HG22	2:B:47:CYS:HA	1.81	0.62
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.81	0.61
1:E:162:THR:HG23	2:F:169:VAL:HG12	1.82	0.61
3:D:83:ILE:HG22	3:D:97:VAL:HG22	1.83	0.61
1:L:119:PRO:HA	1:L:132:LEU:HD23	1.83	0.60
3:C:83:ILE:HG22	3:C:97:VAL:HG22	1.83	0.60
2:F:87:THR:HG23	2:F:110:THR:HA	1.85	0.58
2:B:159:LEU:O	2:B:161:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:GLU:OE1	1:E:123:GLU:N	2.34	0.57
1:L:75:LEU:HG	1:L:78:VAL:HG22	1.85	0.57
3:C:91:ASN:OD1	3:C:91:ASN:N	2.38	0.56
3:C:76:LEU:HD11	3:C:102:SER:HB3	1.88	0.56
1:L:149:LYS:HB2	1:L:192:SER:HB2	1.86	0.56
2:H:37:VAL:HG22	2:H:47:CYS:HA	1.88	0.56
2:B:154:TRP:O	2:B:156:SER:N	2.37	0.56
1:E:144:VAL:HG12	1:E:197:HIS:HB2	1.88	0.55
1:A:80:PRO:O	1:A:170:ASN:ND2	2.36	0.55
1:E:80:PRO:HA	1:E:106:VAL:HG11	1.88	0.55
6:C:201:NAG:H5	6:C:202:NAG:H83	1.88	0.55
1:E:23:CYS:HB3	1:E:71:ALA:HB3	1.89	0.55
1:E:149:LYS:HB2	1:E:192:SER:HB2	1.87	0.55
1:A:149:LYS:HB2	1:A:192:SER:HB2	1.90	0.54
3:D:81:VAL:HG22	3:D:99:LEU:HA	1.89	0.54
1:E:75:LEU:HG	1:E:78:VAL:HG22	1.90	0.53
1:L:123:GLU:OE1	1:L:123:GLU:N	2.41	0.53
1:A:75:LEU:HG	1:A:78:VAL:HG22	1.90	0.53
2:B:198:VAL:HB	2:B:207:VAL:HG23	1.91	0.53
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.91	0.53
2:F:82:MET:HE1	2:F:109:VAL:HG21	1.91	0.52
2:F:97:TRP:CE2	3:G:66:VAL:HG13	2.45	0.52
3:C:19:SER:O	6:C:202:NAG:H81	2.10	0.51
3:G:83:ILE:HG22	3:G:97:VAL:HG22	1.92	0.51
3:G:8:LEU:HD11	3:G:182:LEU:HD11	1.92	0.51
3:C:142:PHE:O	3:C:184:ALA:HA	2.11	0.51
1:E:66:LEU:HD23	1:E:71:ALA:HA	1.93	0.51
3:C:116:SER:HB3	3:C:119:LYS:HE2	1.93	0.51
2:B:87:THR:HG23	2:B:110:THR:HA	1.93	0.51
1:A:144:VAL:HG12	1:A:197:HIS:HB2	1.92	0.50
1:A:89:LEU:HD11	1:A:96:TRP:HB3	1.94	0.50
2:F:39:GLN:HB2	2:F:45:LEU:HD23	1.92	0.50
3:C:25:LEU:HB3	3:C:70:LEU:HD23	1.92	0.49
2:B:121:VAL:HG11	2:B:207:VAL:HB	1.94	0.49
1:L:45:ARG:NH2	1:L:57:TRP:O	2.45	0.49
2:H:87:THR:HG23	2:H:110:THR:HA	1.94	0.49
2:H:9:GLY:HA2	2:H:109:VAL:HG22	1.94	0.49
2:H:97:TRP:CE2	3:C:66:VAL:HG13	2.48	0.49
2:H:95:ASP:OD2	3:C:54:ARG:NH2	2.44	0.49
2:B:139:GLY:HA3	2:B:181:VAL:HG12	1.95	0.49
1:L:88:CYS:O	1:L:99:GLY:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:GLY:HA2	3:C:99:LEU:HG	1.95	0.48
1:L:212:SER:HB2	2:H:216:LYS:HB3	1.95	0.48
1:A:123:GLU:OE1	1:A:123:GLU:N	2.38	0.48
3:C:151:GLU:HG3	3:C:165:TYR:HE2	1.78	0.48
2:H:117:LYS:HD2	2:H:175:LEU:HD13	1.96	0.47
2:F:117:LYS:HD2	2:F:175:LEU:HD13	1.96	0.47
3:G:54:ARG:O	3:G:58:ARG:HG3	2.14	0.47
1:L:89:LEU:HD11	1:L:96:TRP:HB3	1.96	0.47
3:C:81:VAL:HG22	3:C:99:LEU:HA	1.96	0.47
3:D:65:VAL:HG11	3:D:73:ASN:HB2	1.95	0.47
3:G:43:THR:HG22	3:G:139:THR:HB	1.96	0.47
3:G:52:ASP:OD1	3:G:53:TRP:N	2.47	0.47
1:E:89:LEU:HD11	1:E:96:TRP:HB3	1.96	0.47
2:F:34:MET:HB3	2:F:78:LEU:HD22	1.95	0.47
2:H:11:LEU:HB2	2:H:147:PRO:HG3	1.97	0.46
3:C:52:ASP:OD1	3:C:53:TRP:N	2.48	0.46
1:A:7:GLU:OE2	1:A:22:THR:HB	2.16	0.46
1:A:13:VAL:HB	1:A:19:VAL:HG13	1.96	0.46
2:B:82:MET:HB3	2:B:82(C):LEU:HD21	1.97	0.46
2:B:57:LYS:NZ	2:B:69:ILE:O	2.46	0.46
3:D:52:ASP:OD1	3:D:53:TRP:N	2.48	0.46
2:F:95:ASP:OD2	3:G:54:ARG:NH2	2.35	0.46
2:F:36:TRP:NE1	2:F:80:LEU:HB2	2.29	0.46
3:G:25:LEU:HB3	3:G:70:LEU:HD23	1.96	0.46
1:A:89:LEU:HG	1:A:96:TRP:CE3	2.51	0.46
1:A:91:TYR:HB2	1:A:96:TRP:CZ3	2.51	0.46
1:L:12:THR:HG23	1:L:106(A):LEU:HB2	1.97	0.46
1:A:94:GLY:HA2	3:D:54:ARG:NH1	2.31	0.46
3:C:36:GLY:HA2	3:C:91:ASN:ND2	2.31	0.45
1:A:51:THR:HG23	1:A:66:LEU:HG	1.98	0.45
2:B:38:ARG:CD	2:B:48:ILE:HD11	2.45	0.45
1:L:91:TYR:HB2	1:L:96:TRP:CZ3	2.51	0.45
1:E:184:GLN:HA	1:E:187:SER:HB2	1.98	0.45
1:L:45:ARG:HE	1:L:57:TRP:CD1	2.34	0.45
1:L:83:GLU:HB2	1:L:106:VAL:HG23	1.99	0.45
1:L:83:GLU:HG3	1:L:104:LEU:O	2.17	0.45
1:A:162:THR:HG23	2:B:169:VAL:HG12	1.99	0.45
2:H:155:ASN:OD1	2:H:194:TYR:HA	2.17	0.45
3:C:97:VAL:HG11	3:C:127:ILE:HG12	1.98	0.45
1:A:49:TYR:HE2	3:D:66:VAL:HG21	1.82	0.45
3:D:24:GLY:HA2	3:D:99:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:GLU:HB2	3:C:93:LYS:HD2	1.99	0.44
2:H:82:MET:HE1	2:H:109:VAL:HG21	1.99	0.44
1:A:19:VAL:HG23	1:A:75:LEU:HB3	1.98	0.44
2:B:197:ASN:HD22	2:B:208:ASP:HB3	1.82	0.44
2:B:11:LEU:HD12	2:B:110:THR:O	2.17	0.44
3:D:25:LEU:HB3	3:D:70:LEU:HD23	1.99	0.44
3:D:97:VAL:HG11	3:D:127:ILE:HG12	2.00	0.44
2:F:36:TRP:CG	2:F:80:LEU:HD22	2.53	0.44
2:F:38:ARG:CD	2:F:48:ILE:HD11	2.46	0.44
1:L:96:TRP:CZ2	2:H:98:GLY:HA2	2.52	0.44
1:A:106(A):LEU:HB3	1:A:107:GLY:H	1.66	0.44
2:B:12:VAL:HG11	2:B:82(C):LEU:HD12	2.00	0.44
2:F:154:TRP:HB2	2:F:159:LEU:HB3	1.99	0.44
1:L:66:LEU:HD23	1:L:71:ALA:HA	2.00	0.43
2:H:50:TYR:O	2:H:57:LYS:HA	2.19	0.43
2:H:92:CYS:O	2:H:104:GLY:N	2.51	0.43
3:D:46:PHE:CE1	3:D:131:LEU:HD13	2.53	0.43
2:H:3:GLN:HB2	2:H:25:SER:OG	2.19	0.43
2:H:12:VAL:HG21	2:H:18:LEU:HB2	2.01	0.43
1:E:85:ASP:OD1	1:E:103:ARG:HG2	2.18	0.43
3:D:141:ILE:HG12	3:D:186:THR:HG23	2.01	0.43
1:A:85:ASP:OD1	1:A:103:ARG:HG2	2.18	0.42
2:B:209:LYS:HE3	2:B:209:LYS:HB2	1.72	0.42
1:E:169:ASN:C	1:E:171:LYS:H	2.27	0.42
2:F:143:LYS:NZ	2:F:144:ASP:OD2	2.47	0.42
1:E:89:LEU:HG	1:E:96:TRP:CE3	2.55	0.42
3:C:65:VAL:HG21	3:C:73:ASN:HB2	2.01	0.42
1:E:136:ILE:HG21	1:E:195:VAL:HG11	2.01	0.42
2:H:34:MET:HB3	2:H:78:LEU:HD22	2.01	0.42
2:F:87:THR:HA	2:F:109:VAL:O	2.19	0.42
1:A:83:GLU:HG3	1:A:104:LEU:O	2.20	0.42
1:E:183:GLU:O	1:E:187:SER:OG	2.33	0.42
2:F:143:LYS:HA	2:F:177:SER:HB3	2.02	0.42
1:E:88:CYS:O	1:E:99:GLY:N	2.51	0.42
3:G:29:ARG:O	3:G:91:ASN:HB2	2.19	0.42
1:L:121:SER:OG	2:H:122:PHE:HB3	2.20	0.41
1:L:169:ASN:C	1:L:171:LYS:H	2.26	0.41
1:A:119:PRO:HA	1:A:132:LEU:HD23	2.02	0.41
2:B:11:LEU:HD23	2:B:116:THR:HG23	2.01	0.41
1:A:36:PHE:O	1:A:86:TYR:HA	2.20	0.41
2:B:152:VAL:HA	2:B:197:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:9:PRO:HA	3:D:112:HIS:HB3	2.01	0.41
1:L:23:CYS:HB3	1:L:71:ALA:HB3	2.02	0.41
3:G:21:ASN:O	3:G:23:THR:HG23	2.20	0.41
2:B:170:LEU:HD13	2:B:176:TYR:CZ	2.56	0.41
1:L:184:GLN:HA	1:L:187:SER:HB2	2.01	0.41
1:L:128:ASN:HA	1:L:182:PRO:HG2	2.02	0.41
3:C:8:LEU:HD11	3:C:182:LEU:HD11	2.02	0.41
1:E:34:SER:HB2	1:E:89:LEU:HB3	2.03	0.41
1:E:83:GLU:HG3	1:E:104:LEU:O	2.21	0.41
2:H:9:GLY:HA2	2:H:18:LEU:HD21	2.03	0.41
2:H:38:ARG:CD	2:H:48:ILE:HD11	2.44	0.41
1:A:54:LYS:O	3:D:161:GLY:HA2	2.21	0.41
1:E:159:VAL:HG22	1:E:178:LEU:HD13	2.03	0.41
3:D:8:LEU:HD11	3:D:182:LEU:HD11	2.03	0.40
1:L:36:PHE:O	1:L:86:TYR:HA	2.20	0.40
3:D:48:PRO:HG2	3:D:145:SER:HB2	2.02	0.40
2:F:159:LEU:HD21	2:F:182:VAL:HG21	2.03	0.40
1:L:49:TYR:HE2	3:C:66:VAL:HG21	1.86	0.40
2:H:36:TRP:NE1	2:H:80:LEU:HB2	2.36	0.40
3:D:29:ARG:O	3:D:91:ASN:HB2	2.21	0.40
3:D:65:VAL:HG21	3:D:72:LEU:HB2	2.03	0.40
2:F:143:LYS:HA	2:F:177:SER:CB	2.51	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	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	14	39
1	E	212/215 (99%)	202 (95%)	9 (4%)	1 (0%)	24	52
1	L	212/215 (99%)	202 (95%)	9 (4%)	1 (0%)	24	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	215/219 (98%)	204 (95%)	8 (4%)	3 (1%)	9	29
2	F	207/219 (94%)	201 (97%)	5 (2%)	1 (0%)	24	52
2	H	215/219 (98%)	207 (96%)	7 (3%)	1 (0%)	24	52
3	C	168/183 (92%)	153 (91%)	13 (8%)	2 (1%)	10	32
3	D	162/183 (88%)	150 (93%)	12 (7%)	0	100	100
3	G	162/183 (88%)	149 (92%)	13 (8%)	0	100	100
All	All	1765/1851 (95%)	1670 (95%)	84 (5%)	11 (1%)	21	48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	160	THR
2	B	156	SER
2	B	155	ASN
2	B	160	THR
3	C	38	TYR
2	F	127	SER
1	L	151	ASP
3	C	41	ALA
1	E	151	ASP
1	A	106(A)	LEU
1	A	151	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	179/180 (99%)	177 (99%)	2 (1%)	65	76
1	E	179/180 (99%)	178 (99%)	1 (1%)	78	81
1	L	179/180 (99%)	177 (99%)	2 (1%)	65	76
2	B	182/184 (99%)	177 (97%)	5 (3%)	39	64
2	F	178/184 (97%)	176 (99%)	2 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	182/184 (99%)	181 (100%)	1 (0%)	81	82
3	C	139/150 (93%)	133 (96%)	6 (4%)	26	53
3	D	137/150 (91%)	135 (98%)	2 (2%)	57	73
3	G	137/150 (91%)	135 (98%)	2 (2%)	57	73
All	All	1492/1542 (97%)	1469 (98%)	23 (2%)	57	73

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	22	THR
1	L	210	GLU
2	H	196	CYS
3	C	25	LEU
3	C	82	VAL
3	C	89	ARG
3	C	91	ASN
3	C	123	THR
3	C	163	PHE
1	A	19	VAL
1	A	22	THR
2	B	1	GLU
2	B	113	SER
2	B	196	CYS
2	B	207	VAL
2	B	212	LYS
3	D	25	LEU
3	D	65	VAL
1	E	22	THR
2	F	135	THR
2	F	196	CYS
3	G	25	LEU
3	G	65	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	31	ASN
2	H	81	GLN
2	H	82(A)	ASN
2	H	171	GLN

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Mol	Chain	Res	Type
3	C	98	GLN
1	A	37	GLN
2	B	76	ASN
2	B	82(A)	ASN
2	B	197	ASN
3	D	17	HIS
1	E	128	ASN
2	F	31	ASN
3	G	30	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	$\# Z > 2$
4	NAG	I	1	4,2	14,14,15	0.74	0	17,19,21	1.32	3 (17%)
4	NAG	I	2	4	14,14,15	0.83	1 (7%)	17,19,21	2.47	4 (23%)
4	NAG	J	1	4,2	14,14,15	0.71	0	17,19,21	1.00	1 (5%)
4	NAG	J	2	4	14,14,15	0.76	0	17,19,21	1.00	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	I	1	4,2	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	5/6/23/26	0/1/1/1
4	NAG	J	1	4,2	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2	NAG	C1-C2	2.17	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	2	NAG	C2-N2-C7	8.36	134.10	122.90
4	I	2	NAG	C1-C2-N2	3.00	115.17	110.43
4	I	2	NAG	C1-O5-C5	2.77	115.91	112.19
4	I	2	NAG	C8-C7-N2	2.73	120.64	116.12
4	I	1	NAG	C1-C2-N2	2.69	114.67	110.43
4	I	1	NAG	O5-C1-C2	-2.66	107.18	111.29
4	I	1	NAG	C2-N2-C7	2.64	126.43	122.90
4	J	2	NAG	C2-N2-C7	2.45	126.18	122.90
4	J	1	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

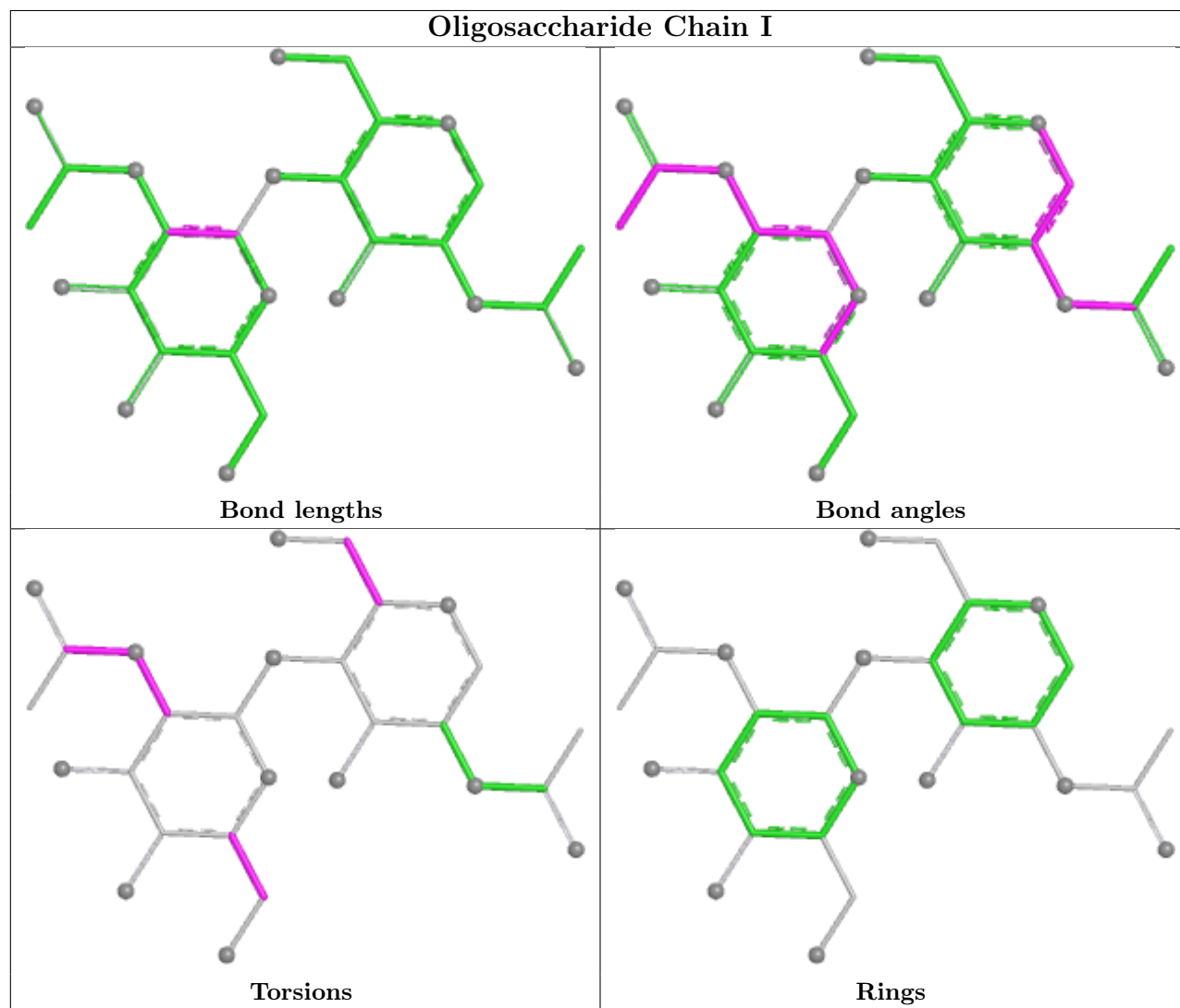
All (13) torsion outliers are listed below:

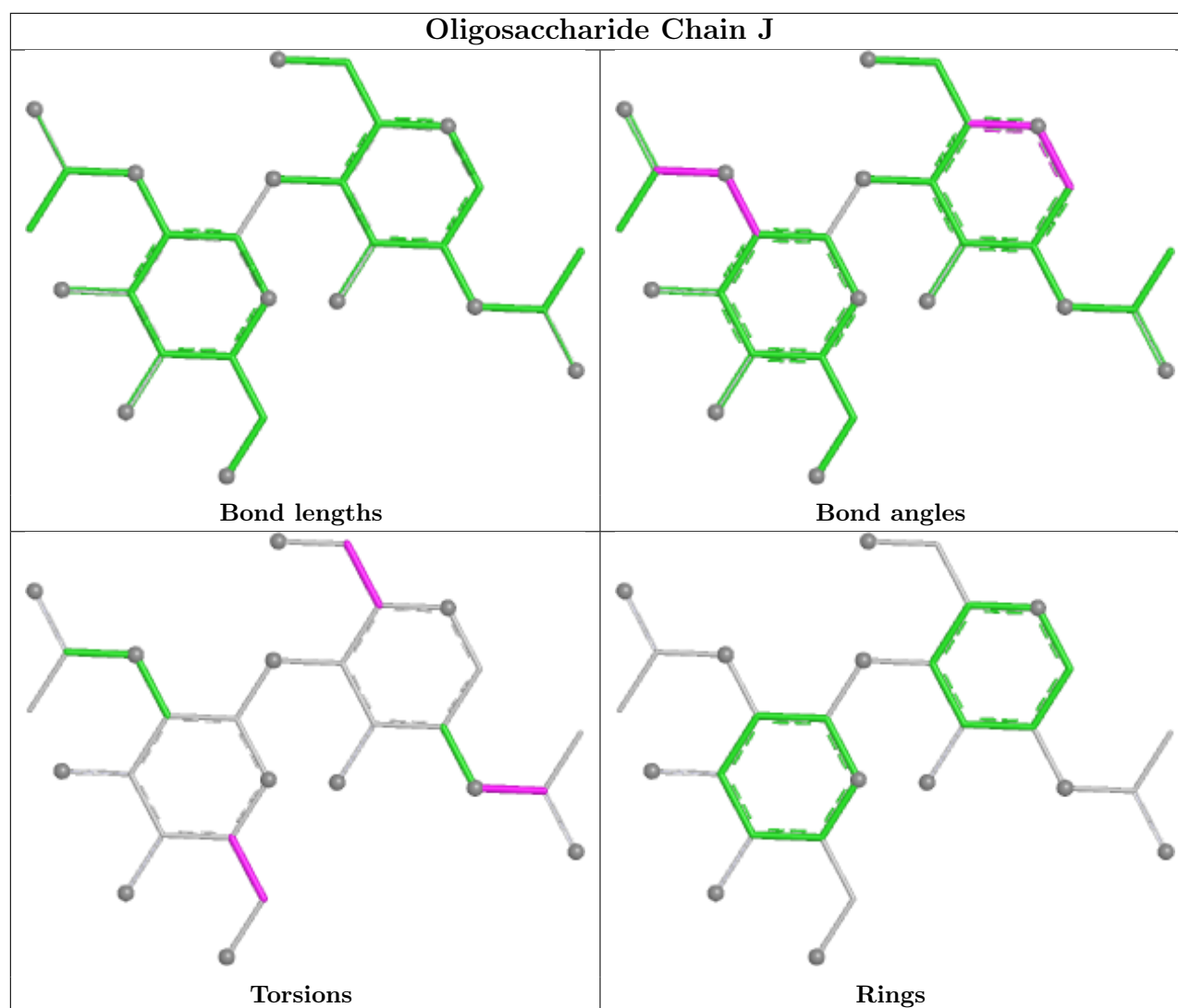
Mol	Chain	Res	Type	Atoms
4	J	1	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	I	2	NAG	C8-C7-N2-C2
4	I	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	I	2	NAG	C3-C2-N2-C7
4	I	2	NAG	C1-C2-N2-C7

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](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	C	203	-	4,4,4	0.70	0	6,6,6	0.07	0
6	NAG	G	201	3	14,14,15	0.69	0	17,19,21	0.88	0
5	SO4	L	302	-	4,4,4	0.68	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	201	3	14,14,15	0.68	0	17,19,21	1.14	1 (5%)
6	NAG	D	202	3	14,14,15	0.76	0	17,19,21	0.90	1 (5%)
5	SO4	L	301	-	4,4,4	0.70	0	6,6,6	0.07	0
6	NAG	G	202	3	14,14,15	0.77	0	17,19,21	0.89	0
6	NAG	D	201	3	14,14,15	0.73	0	17,19,21	1.03	2 (11%)
6	NAG	F	301	2	14,14,15	0.65	0	17,19,21	1.10	2 (11%)
6	NAG	C	202	3	14,14,15	0.80	0	17,19,21	2.59	6 (35%)

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	G	201	3	-	4/6/23/26	0/1/1/1
6	NAG	D	202	3	-	4/6/23/26	0/1/1/1
6	NAG	C	201	3	-	2/6/23/26	0/1/1/1
6	NAG	G	202	3	-	2/6/23/26	0/1/1/1
6	NAG	D	201	3	-	2/6/23/26	0/1/1/1
6	NAG	F	301	2	-	1/6/23/26	0/1/1/1
6	NAG	C	202	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	202	NAG	C2-N2-C7	8.02	133.65	122.90
6	C	202	NAG	C1-C2-N2	3.74	116.32	110.43
6	C	202	NAG	C4-C3-C2	2.96	115.36	111.02
6	C	201	NAG	C1-O5-C5	2.93	116.12	112.19
6	C	202	NAG	O7-C7-N2	2.67	126.70	121.98
6	C	202	NAG	C8-C7-N2	-2.62	111.77	116.12
6	C	202	NAG	O4-C4-C3	-2.49	104.50	110.38
6	F	301	NAG	C1-O5-C5	2.34	115.33	112.19
6	D	201	NAG	C1-O5-C5	2.30	115.27	112.19
6	D	202	NAG	C2-N2-C7	2.20	125.84	122.90
6	D	201	NAG	C2-N2-C7	2.16	125.80	122.90
6	F	301	NAG	O5-C1-C2	-2.11	108.02	111.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	202	NAG	C1-C2-N2-C7
6	D	201	NAG	O5-C5-C6-O6
6	G	201	NAG	O5-C5-C6-O6
6	G	201	NAG	C4-C5-C6-O6
6	D	201	NAG	C4-C5-C6-O6
6	D	202	NAG	O5-C5-C6-O6
6	C	201	NAG	C8-C7-N2-C2
6	C	201	NAG	O7-C7-N2-C2
6	D	202	NAG	C8-C7-N2-C2
6	D	202	NAG	O7-C7-N2-C2
6	G	201	NAG	C8-C7-N2-C2
6	G	201	NAG	O7-C7-N2-C2
6	G	202	NAG	C4-C5-C6-O6
6	D	202	NAG	C4-C5-C6-O6
6	G	202	NAG	O5-C5-C6-O6
6	F	301	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	201	NAG	1	0
6	C	202	NAG	2	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	214/215 (99%)	0.25	1 (0%) 87 72	48, 83, 126, 173	0
1	E	214/215 (99%)	0.16	2 (0%) 81 61	48, 70, 116, 172	0
1	L	214/215 (99%)	0.35	10 (4%) 36 19	45, 73, 150, 170	0
2	B	217/219 (99%)	0.48	5 (2%) 61 38	58, 90, 164, 190	0
2	F	211/219 (96%)	0.13	1 (0%) 87 72	51, 71, 129, 140	0
2	H	217/219 (99%)	0.28	3 (1%) 73 51	47, 76, 164, 176	0
3	C	170/183 (92%)	0.11	1 (0%) 85 69	48, 64, 96, 131	0
3	D	166/183 (90%)	0.26	2 (1%) 76 55	59, 76, 104, 123	0
3	G	166/183 (90%)	0.13	0 100 100	52, 75, 100, 120	0
All	All	1789/1851 (96%)	0.24	25 (1%) 73 51	45, 75, 142, 190	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	131	THR	3.3
1	A	209	THR	2.6
1	L	119	PRO	2.6
1	L	178	LEU	2.5
1	L	193	CYS	2.4
3	D	50	GLY	2.4
1	L	157	ALA	2.4
2	H	131	THR	2.4
1	L	195	VAL	2.3
1	E	209	THR	2.3
2	H	183	THR	2.3
2	B	193	THR	2.3
3	D	59	CYS	2.3
1	L	191	TYR	2.3
3	C	59	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	152	VAL	2.1
1	L	131	THR	2.1
2	B	179	SER	2.1
2	B	128	SER	2.1
1	L	202	VAL	2.0
1	L	190	SER	2.0
1	L	117	LEU	2.0
1	E	189	ARG	2.0
2	H	128	SER	2.0
2	F	42	GLY	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](#)

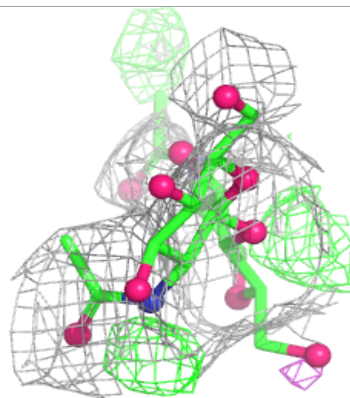
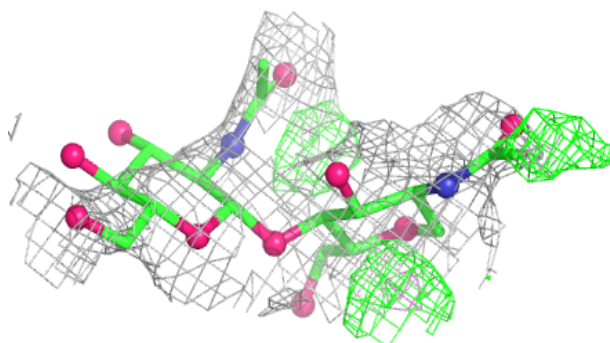
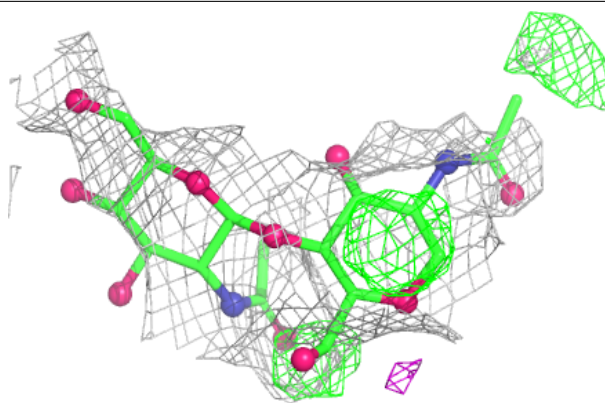
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	I	1	14/15	-	-	93,106,120,123	0
4	NAG	I	2	14/15	-	-	112,129,134,137	0
4	NAG	J	1	14/15	0.47	0.19	109,112,116,116	0
4	NAG	J	2	14/15	0.51	0.17	106,114,118,119	0

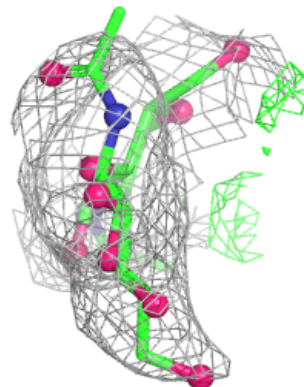
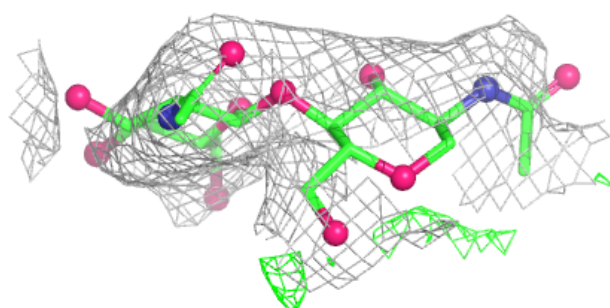
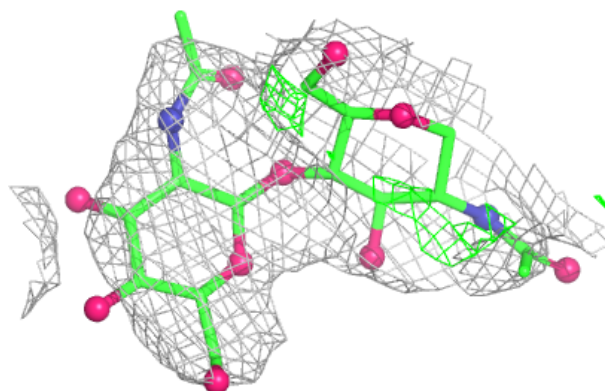
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

**Electron density around Chain J:**

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
6	NAG	F	301	14/15	0.66	0.13	95,102,107,109	0
6	NAG	D	202	14/15	0.69	0.15	82,106,119,132	0
6	NAG	C	202	14/15	0.72	0.17	86,102,112,119	0
6	NAG	G	202	14/15	0.84	0.11	79,89,95,99	0
5	SO4	L	301	5/5	0.85	0.08	75,84,95,113	0
5	SO4	L	302	5/5	0.86	0.12	71,87,98,108	0
5	SO4	C	203	5/5	0.86	0.12	80,83,100,118	0
6	NAG	D	201	14/15	0.87	0.11	63,68,72,73	0
6	NAG	G	201	14/15	0.90	0.10	62,68,75,82	0
6	NAG	C	201	14/15	0.92	0.09	57,61,73,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.