



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:04 AM UTC

PDB ID : 8TNT / pdb_00008tnt
Title : Crystal structure of Epstein-Barr virus gH/gL/gp42 in complex with antibodies F-2-1 and 769C2
Authors : Bu, W.; Kumar, A.; Board, N.; Kim, J.; Dowdell, K.; Zhang, S.; Lei, Y.; Hostal, A.; Krogmann, T.; Wang, Y.; Pittaluga, S.; Marcotrigiano, J.; Cohen, J.I.
Deposited on : 2023-08-02
Resolution : 3.15 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](#) ①) 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

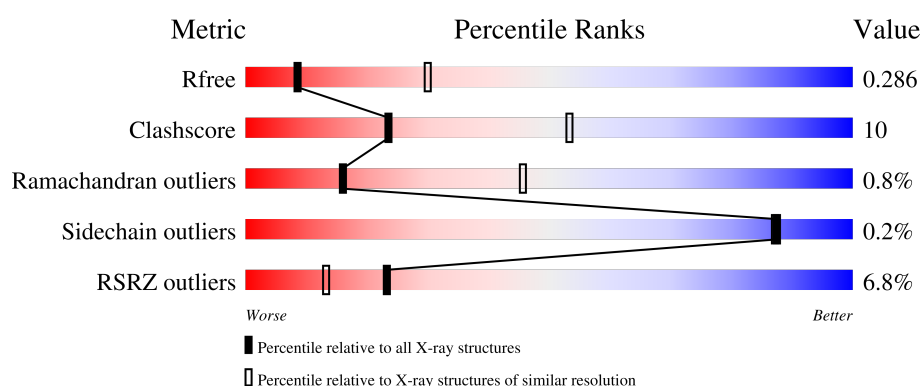
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	656	4% 81% 19%
2	B	112	74% 19% 7%
3	C	191	3% 68% 25% 7%
4	D	216	12% 75% 25%
5	E	232	7% 71% 24% 5%

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Mol	Chain	Length	Quality of chain
6	F	218	9% 74% 25%
7	G	230	11% 58% 37%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13731 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	656	Total	C	N	O	S	0	0	0
			5016	3217	819	949	31			

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			802	506	139	153	4			

- Molecule 3 is a protein called Glycoprotein 42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	178	Total	C	N	O	S	0	0	0
			1436	931	235	259	11			

- Molecule 4 is a protein called 769C2 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	214	Total	C	N	O	S	0	0	0
			1543	962	255	321	5			

- Molecule 5 is a protein called 769C2 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	220	Total	C	N	O	S	0	0	0
			1615	1016	276	316	7			

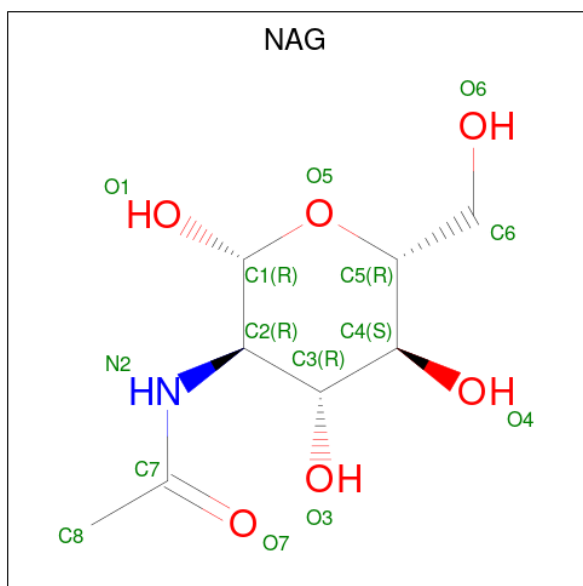
- Molecule 6 is a protein called F-2-1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	218	Total	C	N	O	S	0	0	0
			1667	1044	282	336	5			

- Molecule 7 is a protein called F-2-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	220	Total	C	N	O	S	0	0	0
			1624	1030	267	321	6			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).

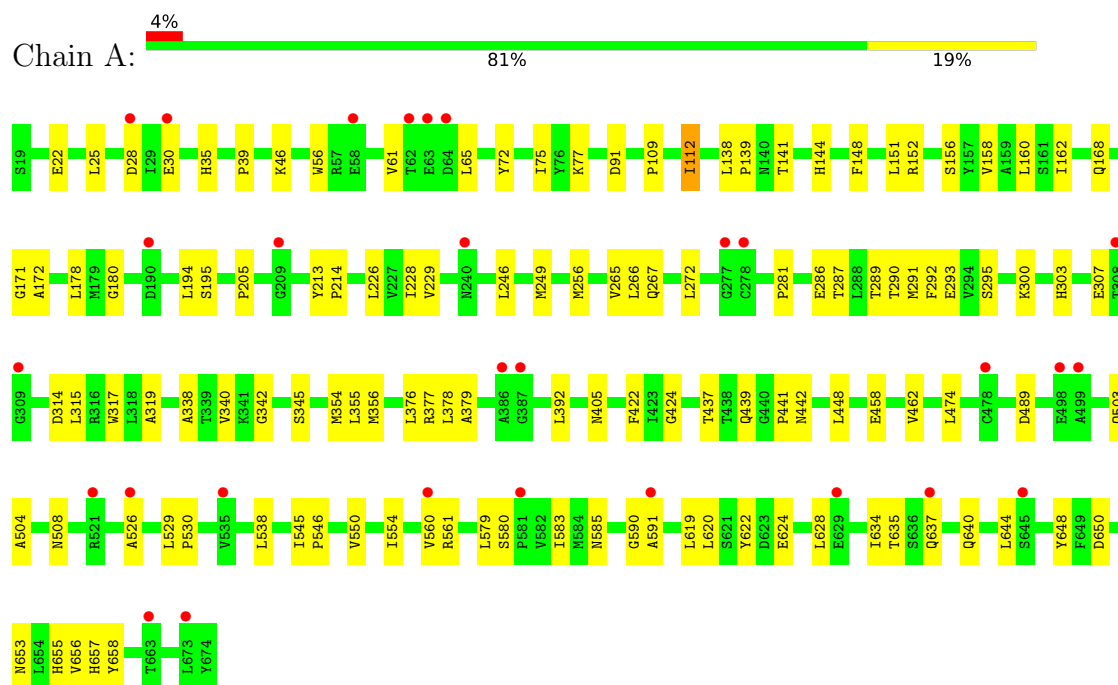


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

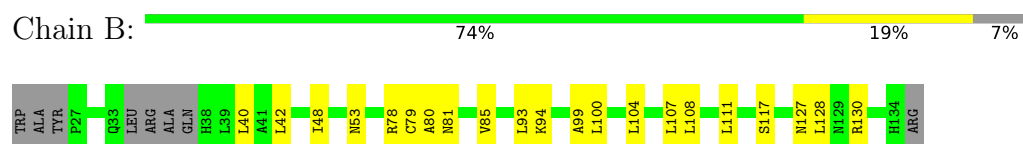
3 Residue-property plots [i](#)

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.

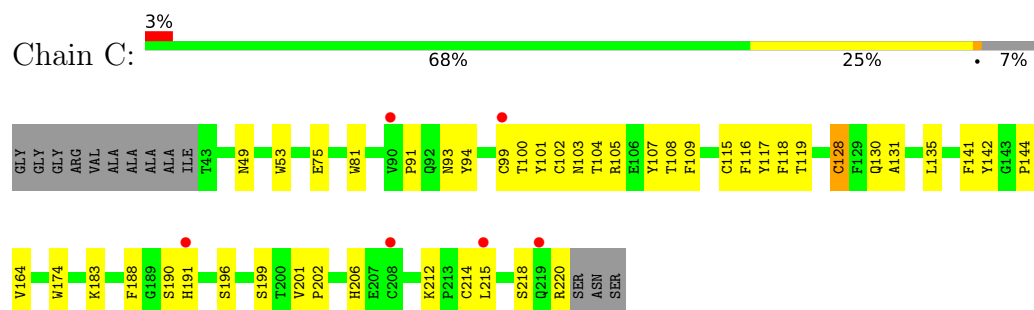
• Molecule 1: Envelope glycoprotein H



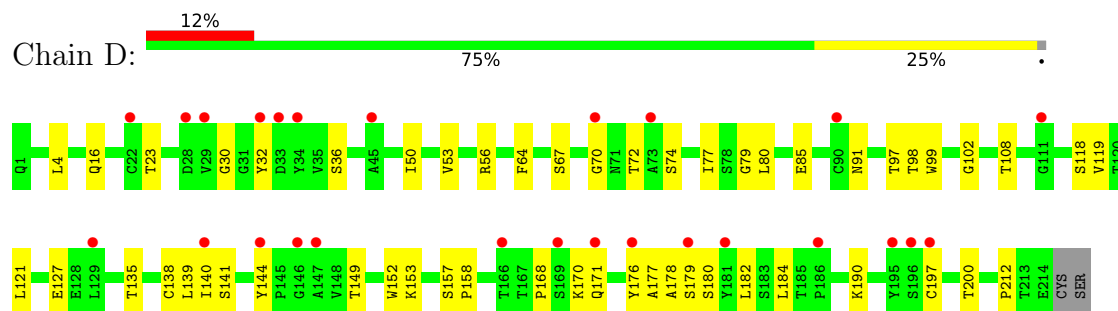
• Molecule 2: Envelope glycoprotein L



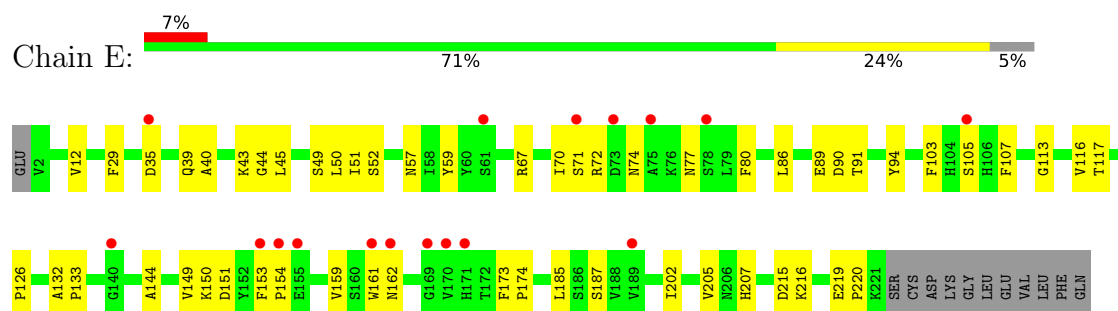
• Molecule 3: Glycoprotein 42



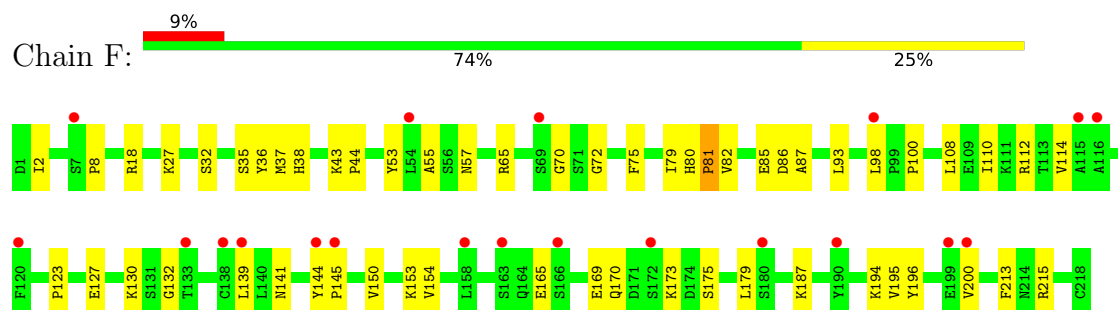
- Molecule 4: 769C2 light chain



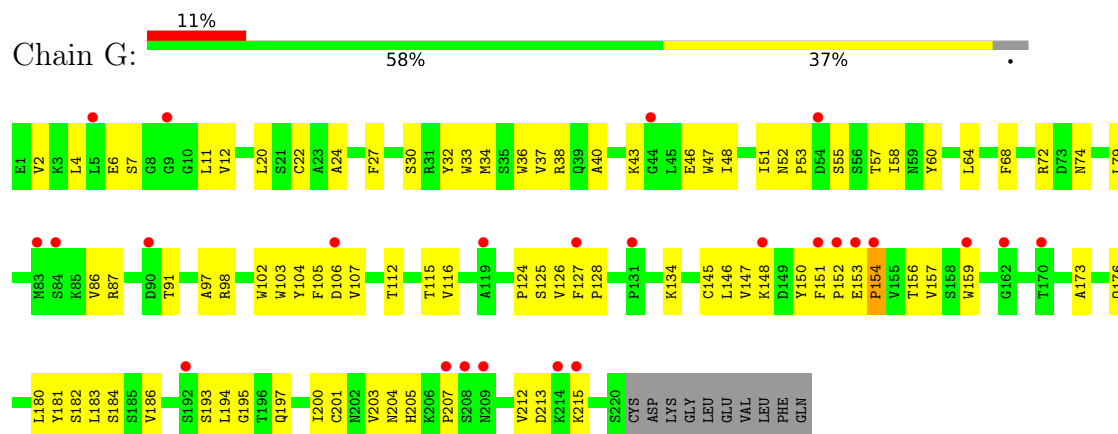
- Molecule 5: 769C2 heavy chain



- Molecule 6: F-2-1 light chain



- Molecule 7: F-2-1 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.32Å 85.17Å 119.71Å 90.00° 105.09° 90.00°	Depositor
Resolution (Å)	46.32 – 3.15 46.32 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.32-3.15) 98.5 (46.32-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.287 0.253 , 0.286	Depositor DCC
R_{free} test set	1988 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.672	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13731	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/5125	0.27	0/6975
2	B	0.09	0/816	0.30	0/1106
3	C	0.11	0/1491	0.32	0/2045
4	D	0.11	0/1579	0.36	0/2165
5	E	0.11	0/1653	0.36	0/2250
6	F	0.10	0/1705	0.30	0/2316
7	G	0.13	0/1665	0.39	0/2274
All	All	0.10	0/14034	0.32	0/19131

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 [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	5016	0	4940	82	0
2	B	802	0	786	15	0
3	C	1436	0	1344	36	0
4	D	1543	0	1447	31	0
5	E	1615	0	1561	39	0
6	F	1667	0	1622	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1624	0	1550	63	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
All	All	13731	0	13276	274	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 (274) 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)
7:G:153:GLU:HG2	7:G:154:PRO:HD3	1.48	0.94
6:F:139:LEU:HD22	7:G:186:VAL:HG21	1.58	0.86
6:F:139:LEU:HD11	6:F:141:ASN:HB3	1.56	0.86
7:G:52:ASN:HD21	7:G:57:THR:HB	1.41	0.85
1:A:650:ASP:OD2	1:A:658:TYR:OH	2.00	0.79
1:A:35:HIS:HE2	5:E:105:SER:HG	1.32	0.76
4:D:32:TYR:HB2	4:D:53:VAL:HG21	1.67	0.76
5:E:91:THR:HG23	5:E:117:THR:HA	1.69	0.74
1:A:256:MET:O	1:A:300:LYS:NZ	2.21	0.73
7:G:127:PHE:HE1	7:G:146:LEU:HD23	1.52	0.73
7:G:153:GLU:HG3	7:G:207:PRO:HG2	1.71	0.73
4:D:118:SER:H	4:D:141:SER:HB3	1.52	0.73
7:G:173:ALA:HB1	7:G:181:TYR:HB3	1.71	0.71
4:D:168:PRO:HB3	5:E:174:PRO:HG2	1.73	0.69
7:G:147:VAL:HG11	7:G:203:VAL:HG11	1.76	0.68
4:D:170:LYS:HD3	4:D:176:TYR:HA	1.76	0.68
3:C:105:ARG:NH1	7:G:32:TYR:OH	2.25	0.68
7:G:200:ILE:HG12	7:G:215:LYS:HA	1.74	0.67
4:D:153:LYS:HA	4:D:158:PRO:HD2	1.77	0.67
4:D:153:LYS:HG2	4:D:157:SER:H	1.60	0.66
1:A:138:LEU:HD13	1:A:148:PHE:HB3	1.76	0.66
6:F:194:LYS:HA	6:F:215:ARG:HG2	1.77	0.66
4:D:119:VAL:HG22	4:D:140:ILE:HG23	1.77	0.66
4:D:121:LEU:HD13	4:D:138:CYS:HB2	1.78	0.66
1:A:75:ILE:O	1:A:77:LYS:NZ	2.29	0.65
2:B:127:ASN:HB3	2:B:130:ARG:HG2	1.79	0.65
5:E:29:PHE:O	5:E:72:ARG:NH2	2.30	0.65
1:A:25:LEU:HD22	2:B:107:LEU:HD21	1.78	0.64
1:A:653:ASN:HB3	1:A:656:VAL:HG22	1.79	0.64
1:A:194:LEU:HD11	1:A:228:ILE:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLN:OE1	1:A:442:ASN:ND2	2.30	0.63
1:A:152:ARG:NH2	3:C:75:GLU:OE1	2.31	0.63
6:F:44:PRO:HG2	6:F:169:GLU:HG3	1.79	0.63
1:A:35:HIS:NE2	5:E:105:SER:OG	2.27	0.62
1:A:561:ARG:HA	1:A:591:ALA:H	1.64	0.62
6:F:35:SER:HB2	6:F:55:ALA:HB2	1.82	0.62
1:A:168:GLN:HE21	3:C:81:TRP:HB2	1.64	0.62
4:D:85:GLU:HB2	4:D:108:THR:HA	1.80	0.61
7:G:154:PRO:HG3	7:G:205:HIS:CD2	2.35	0.61
7:G:205:HIS:HD2	7:G:207:PRO:HD2	1.64	0.61
1:A:504:ALA:O	1:A:508:ASN:ND2	2.32	0.61
1:A:25:LEU:HG	2:B:48:ILE:HD11	1.82	0.61
7:G:205:HIS:CD2	7:G:207:PRO:HD2	2.35	0.61
7:G:4:LEU:HD12	7:G:107:VAL:HG12	1.83	0.60
3:C:149:LEU:HD11	3:C:202:PRO:HD3	1.83	0.60
5:E:161:TRP:NE1	5:E:187:SER:OG	2.33	0.60
5:E:67:ARG:NH2	5:E:90:ASP:OD2	2.34	0.60
1:A:138:LEU:HB2	1:A:151:LEU:H	1.67	0.60
1:A:624:GLU:OE2	1:A:657:HIS:NE2	2.35	0.60
1:A:637:GLN:OE1	3:C:49:ASN:ND2	2.33	0.60
3:C:100:THR:HG1	7:G:103:TRP:HZ3	1.49	0.59
1:A:287:THR:HG22	1:A:291:MET:HE3	1.85	0.59
1:A:554:ILE:HG21	1:A:628:LEU:HD21	1.85	0.58
5:E:40:ALA:HB3	5:E:43:LYS:HB3	1.85	0.57
6:F:170:GLN:HE21	6:F:175:SER:HB3	1.69	0.57
7:G:91:THR:HG23	7:G:115:THR:HA	1.85	0.57
1:A:61:VAL:HG23	2:B:85:VAL:HG22	1.87	0.57
7:G:34:MET:HB3	7:G:79:LEU:HD22	1.86	0.57
5:E:133:PRO:HD2	5:E:220:PRO:HB3	1.86	0.57
3:C:118:PHE:HE1	3:C:215:LEU:HD12	1.70	0.56
7:G:157:VAL:HG22	7:G:203:VAL:HG22	1.88	0.56
1:A:267:GLN:HG2	1:A:474:LEU:HD13	1.88	0.56
4:D:152:TRP:CE2	4:D:197:CYS:HB3	2.40	0.56
7:G:151:PHE:CD2	7:G:152:PRO:HD2	2.41	0.55
4:D:140:ILE:HG22	4:D:141:SER:H	1.71	0.55
7:G:2:VAL:HB	7:G:107:VAL:HG21	1.88	0.55
4:D:67:SER:HB3	4:D:74:SER:HB3	1.89	0.54
6:F:165:GLU:HB2	6:F:179:LEU:HD21	1.89	0.54
7:G:98:ARG:NH1	7:G:106:ASP:OD2	2.40	0.54
1:A:249:MET:HE3	1:A:289:THR:HG23	1.89	0.54
5:E:202:ILE:HD11	5:E:215:ASP:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:93:LEU:HD11	6:F:100:PRO:HB2	1.90	0.53
1:A:72:TYR:O	1:A:77:LYS:NZ	2.34	0.53
1:A:405:ASN:OD1	1:A:635:THR:OG1	2.26	0.53
7:G:126:VAL:HG11	7:G:212:VAL:HG11	1.90	0.53
1:A:550:VAL:HG12	1:A:583:ILE:HA	1.91	0.53
6:F:38:HIS:CE1	7:G:104:TYR:HB3	2.44	0.53
5:E:215:ASP:OD1	5:E:215:ASP:N	2.42	0.53
7:G:36:TRP:O	7:G:48:ILE:HG12	2.09	0.52
3:C:144:PRO:HD2	3:C:164:VAL:HB	1.91	0.52
6:F:127:GLU:HA	6:F:130:LYS:HE2	1.91	0.52
1:A:158:VAL:HG22	1:A:340:VAL:HG22	1.92	0.52
6:F:87:ALA:HA	6:F:108:LEU:HD23	1.91	0.52
5:E:51:ILE:HB	5:E:70:ILE:HG21	1.92	0.52
5:E:149:VAL:HG11	5:E:205:VAL:HG21	1.92	0.52
5:E:35:ASP:HB2	5:E:107:PHE:HE2	1.76	0.51
1:A:622:TYR:CE1	1:A:657:HIS:HB2	2.46	0.51
3:C:100:THR:HB	3:C:220:ARG:HA	1.91	0.51
6:F:100:PRO:HD2	7:G:47:TRP:CD2	2.45	0.51
1:A:22:GLU:HG2	1:A:39:PRO:HA	1.92	0.51
3:C:107:TYR:HA	3:C:117:TYR:HD1	1.76	0.51
5:E:71:SER:HB2	5:E:80:PHE:HB2	1.92	0.51
7:G:24:ALA:HB1	7:G:27:PHE:HE1	1.75	0.51
1:A:554:ILE:HG13	1:A:579:LEU:HG	1.93	0.51
5:E:161:TRP:O	5:E:162:ASN:ND2	2.44	0.51
6:F:110:ILE:H	6:F:170:GLN:HE22	1.58	0.51
1:A:441:PRO:HB2	3:C:53:TRP:CD1	2.45	0.51
3:C:190:SER:OG	3:C:191:HIS:N	2.42	0.50
4:D:80:LEU:H	4:D:80:LEU:HD12	1.76	0.50
5:E:89:GLU:N	5:E:89:GLU:OE1	2.44	0.50
3:C:100:THR:O	6:F:36:TYR:OH	2.18	0.50
2:B:53:ASN:HB3	2:B:117:SER:HB3	1.94	0.50
7:G:153:GLU:HG2	7:G:154:PRO:CD	2.33	0.50
3:C:108:THR:HG22	3:C:109:PHE:HD1	1.76	0.50
3:C:119:THR:HG22	3:C:135:LEU:HD22	1.93	0.50
5:E:49:SER:HB2	5:E:70:ILE:HD11	1.94	0.50
6:F:80:HIS:HB3	6:F:81:PRO:HD3	1.93	0.50
1:A:178:LEU:HD11	1:A:295:SER:HB3	1.94	0.50
4:D:23:THR:HA	4:D:72:THR:HA	1.94	0.49
1:A:148:PHE:HE2	1:A:205:PRO:HG2	1.77	0.49
3:C:183:LYS:O	3:C:201:VAL:HG11	2.12	0.49
4:D:64:PHE:HD1	4:D:77:ILE:HG12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:146:LEU:HD12	7:G:183:LEU:O	2.13	0.49
1:A:376:LEU:HD22	1:A:424:GLY:HA2	1.94	0.49
4:D:168:PRO:HD2	4:D:179:SER:HA	1.93	0.49
4:D:171:GLN:H	4:D:177:ALA:HB2	1.76	0.49
2:B:40:LEU:HD22	2:B:78:ARG:HH11	1.76	0.49
5:E:159:VAL:HG21	5:E:187:SER:HB2	1.95	0.49
7:G:38:ARG:NE	7:G:46:GLU:OE1	2.45	0.49
7:G:11:LEU:HD12	7:G:115:THR:HB	1.95	0.48
7:G:148:LYS:HA	7:G:182:SER:HA	1.95	0.48
1:A:30:GLU:HB3	5:E:52:SER:HB2	1.95	0.48
2:B:81:ASN:O	2:B:85:VAL:HG23	2.12	0.48
7:G:195:GLY:O	7:G:197:GLN:N	2.44	0.48
3:C:99:CYS:SG	3:C:100:THR:N	2.85	0.48
1:A:65:LEU:HB3	2:B:128:LEU:HD22	1.95	0.48
1:A:139:PRO:HB2	1:A:141:THR:HG23	1.95	0.48
4:D:99:TRP:HE1	5:E:50:LEU:HD12	1.78	0.48
1:A:634:ILE:HD11	1:A:640:GLN:HG3	1.96	0.48
4:D:4:LEU:HD11	4:D:102:GLY:HA2	1.96	0.48
7:G:20:LEU:HD21	7:G:112:THR:HG21	1.95	0.48
7:G:6:GLU:OE1	7:G:6:GLU:N	2.47	0.47
1:A:91:ASP:HB2	1:A:317:TRP:HE1	1.79	0.47
1:A:319:ALA:HB1	1:A:377:ARG:HB3	1.95	0.47
1:A:356:MET:HA	1:A:356:MET:HE2	1.96	0.47
1:A:437:THR:HG22	1:A:439:GLN:H	1.79	0.47
7:G:97:ALA:HB1	7:G:105:PHE:HB3	1.95	0.47
4:D:190:LYS:HA	4:D:212:PRO:HG2	1.97	0.47
6:F:2:ILE:HD11	6:F:27:LYS:HB2	1.97	0.47
7:G:53:PRO:O	7:G:55:SER:N	2.41	0.47
1:A:249:MET:HE2	1:A:292:PHE:HD2	1.80	0.47
1:A:356:MET:HE3	1:A:378:LEU:HB2	1.96	0.47
1:A:458:GLU:O	1:A:462:VAL:HG23	2.15	0.47
1:A:526:ALA:HB1	1:A:529:LEU:HB2	1.96	0.47
7:G:33:TRP:CH2	7:G:52:ASN:HB3	2.50	0.47
1:A:112:ILE:HG22	1:A:355:LEU:HD12	1.97	0.47
3:C:220:ARG:HG2	7:G:103:TRP:CZ2	2.50	0.46
6:F:70:GLY:HA3	6:F:75:PHE:HA	1.96	0.46
7:G:32:TYR:O	7:G:72:ARG:NH2	2.43	0.46
5:E:126:PRO:HD3	5:E:207:HIS:HD1	1.80	0.46
5:E:43:LYS:HG2	5:E:44:GLY:H	1.81	0.46
1:A:226:LEU:HD21	1:A:246:LEU:HD22	1.97	0.46
5:E:132:ALA:HB1	5:E:220:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:128:PRO:HA	7:G:145:CYS:HA	1.98	0.46
3:C:104:THR:HG21	7:G:32:TYR:CD2	2.50	0.46
3:C:163:TRP:CZ2	3:C:212:LYS:HD2	2.51	0.46
3:C:174:TRP:CZ2	3:C:190:SER:HB2	2.50	0.46
4:D:97:THR:O	4:D:99:TRP:N	2.49	0.46
6:F:123:PRO:HB3	6:F:213:PHE:CZ	2.51	0.46
4:D:85:GLU:O	4:D:85:GLU:HG2	2.16	0.46
6:F:36:TYR:CE2	7:G:102:TRP:HD1	2.34	0.46
7:G:193:SER:O	7:G:195:GLY:N	2.49	0.46
6:F:114:VAL:HG13	6:F:145:PRO:HG2	1.98	0.46
2:B:94:LYS:HD2	2:B:108:LEU:HD21	1.97	0.45
1:A:286:GLU:O	1:A:290:THR:OG1	2.33	0.45
7:G:91:THR:OG1	7:G:116:VAL:HG22	2.15	0.45
1:A:265:VAL:HG22	1:A:293:GLU:HB3	1.99	0.45
7:G:7:SER:O	7:G:112:THR:OG1	2.24	0.45
7:G:125:SER:OG	7:G:148:LYS:O	2.27	0.45
6:F:65:ARG:HB2	6:F:81:PRO:HD2	1.98	0.45
6:F:65:ARG:NE	6:F:86:ASP:OD2	2.45	0.45
7:G:146:LEU:HD13	7:G:184:SER:HB3	1.99	0.45
1:A:213:TYR:N	1:A:214:PRO:HD2	2.30	0.45
4:D:56:ARG:NH2	4:D:64:PHE:O	2.44	0.45
5:E:133:PRO:HA	5:E:144:ALA:HB3	1.98	0.45
6:F:154:VAL:HG13	6:F:196:TYR:CE2	2.52	0.45
6:F:196:TYR:HB2	6:F:213:PHE:CE1	2.52	0.45
7:G:86:VAL:HB	7:G:116:VAL:HG11	1.99	0.45
1:A:619:LEU:HD21	1:A:648:TYR:HE2	1.81	0.45
3:C:99:CYS:HB2	6:F:32:SER:HB3	1.99	0.45
3:C:149:LEU:CD1	3:C:202:PRO:HD3	2.45	0.45
5:E:133:PRO:HB3	5:E:144:ALA:N	2.32	0.45
6:F:132:GLY:HA2	6:F:187:LYS:HD3	1.98	0.45
6:F:43:LYS:NZ	6:F:85:GLU:O	2.34	0.45
1:A:46:LYS:HE2	2:B:99:ALA:HB1	1.99	0.44
1:A:61:VAL:HG22	2:B:80:ALA:HB1	1.98	0.44
1:A:448:LEU:HB2	1:A:546:PRO:HD2	1.98	0.44
1:A:489:ASP:OD1	1:A:489:ASP:N	2.50	0.44
4:D:127:GLU:HG3	5:E:216:LYS:HE2	1.99	0.44
5:E:150:LYS:HZ2	5:E:151:ASP:CG	2.26	0.44
7:G:37:VAL:HG12	7:G:38:ARG:N	2.32	0.44
7:G:87:ARG:O	7:G:116:VAL:HG21	2.16	0.44
7:G:200:ILE:HG21	7:G:213:ASP:C	2.42	0.44
1:A:144:HIS:NE2	1:A:195:SER:OG	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD21	1:A:422:PHE:HZ	1.83	0.44
5:E:94:TYR:O	5:E:113:GLY:HA2	2.17	0.44
7:G:12:VAL:O	7:G:116:VAL:HA	2.17	0.44
1:A:171:GLY:HA2	1:A:180:GLY:HA2	2.00	0.43
5:E:57:ASN:OD1	5:E:57:ASN:N	2.47	0.43
5:E:91:THR:HA	5:E:116:VAL:O	2.17	0.43
3:C:128:CYS:HA	3:C:131:ALA:HB3	2.01	0.43
5:E:219:GLU:HG3	5:E:220:PRO:HD2	2.00	0.43
7:G:40:ALA:HB3	7:G:43:LYS:HB3	2.00	0.43
4:D:16:GLN:O	4:D:79:GLY:N	2.40	0.43
1:A:56:TRP:CD2	2:B:42:LEU:HD13	2.54	0.43
6:F:153:LYS:HA	6:F:153:LYS:HD3	1.82	0.43
1:A:172:ALA:O	1:A:178:LEU:HD12	2.19	0.43
1:A:148:PHE:HE1	1:A:229:VAL:HG21	1.83	0.43
1:A:272:LEU:HD21	1:A:287:THR:HA	2.01	0.43
6:F:173:LYS:C	6:F:175:SER:H	2.26	0.43
1:A:28:ASP:OD2	5:E:103:PHE:N	2.47	0.43
1:A:538:LEU:HD23	1:A:538:LEU:H	1.84	0.43
7:G:33:TRP:CZ3	7:G:52:ASN:HB3	2.54	0.43
7:G:134:LYS:HD3	7:G:134:LYS:H	1.84	0.43
7:G:156:THR:HB	7:G:204:ASN:O	2.18	0.43
1:A:213:TYR:H	1:A:214:PRO:HD2	1.84	0.42
5:E:39:GLN:HB2	5:E:45:LEU:HD23	2.01	0.42
3:C:94:TYR:CZ	3:C:130:GLN:HB2	2.54	0.42
3:C:188:PHE:CD1	3:C:206:HIS:HB3	2.54	0.42
6:F:150:VAL:HG23	6:F:200:VAL:HG12	2.01	0.42
1:A:249:MET:HE2	1:A:292:PHE:CD2	2.54	0.42
1:A:624:GLU:HG3	1:A:655:HIS:O	2.19	0.42
5:E:12:VAL:HG11	5:E:86:LEU:HD13	2.01	0.42
7:G:30:SER:HB3	7:G:74:ASN:HB3	2.02	0.42
3:C:116:PHE:CZ	3:C:148:ILE:HG21	2.54	0.42
3:C:115:CYS:HB2	3:C:218:SER:OG	2.19	0.42
5:E:173:PHE:O	5:E:185:LEU:HB2	2.19	0.42
7:G:58:ILE:HD12	7:G:60:TYR:OH	2.20	0.42
1:A:156:SER:HB3	1:A:342:GLY:HA3	2.02	0.42
1:A:314:ASP:OD1	1:A:315:LEU:N	2.52	0.42
1:A:503:GLN:H	1:A:503:GLN:CD	2.26	0.42
1:A:545:ILE:HD11	1:A:620:LEU:HD11	2.00	0.42
3:C:103:ASN:O	3:C:107:TYR:HB3	2.20	0.42
3:C:142:TYR:HD2	3:C:215:LEU:HD21	1.84	0.42
6:F:37:MET:HG2	6:F:75:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:79:ILE:HB	6:F:82:VAL:HG12	2.00	0.42
1:A:530:PRO:HB2	1:A:585:ASN:HB3	2.01	0.42
2:B:93:LEU:HB3	2:B:108:LEU:HD22	2.01	0.42
3:C:196:SER:H	3:C:199:SER:HG	1.64	0.42
4:D:36:SER:OG	4:D:91:ASN:HB3	2.20	0.42
4:D:139:LEU:HA	4:D:180:SER:HA	2.01	0.42
6:F:112:ARG:HD3	6:F:144:TYR:HB2	2.02	0.42
7:G:64:LEU:HG	7:G:68:PHE:CE2	2.55	0.42
1:A:303:HIS:CD2	1:A:307:GLU:HG3	2.55	0.41
1:A:561:ARG:HG3	1:A:590:GLY:HA2	2.03	0.41
3:C:101:TYR:O	3:C:218:SER:HB2	2.19	0.41
4:D:141:SER:HA	4:D:178:ALA:HB2	2.02	0.41
6:F:195:VAL:HA	6:F:213:PHE:O	2.20	0.41
1:A:303:HIS:NE2	1:A:307:GLU:HG3	2.35	0.41
3:C:141:PHE:CE1	3:C:214:CYS:HB3	2.55	0.41
5:E:153:PHE:HB3	5:E:154:PRO:HD3	2.03	0.41
7:G:150:TYR:HE2	7:G:154:PRO:HD2	1.84	0.41
6:F:53:TYR:O	6:F:57:ASN:HB2	2.21	0.41
7:G:176:GLN:N	7:G:180:LEU:O	2.48	0.41
7:G:51:ILE:HB	7:G:58:ILE:HG22	2.02	0.41
6:F:18:ARG:HA	6:F:79:ILE:O	2.20	0.41
2:B:100:LEU:HG	2:B:104:LEU:HB2	2.02	0.41
3:C:91:PRO:O	3:C:93:ASN:N	2.49	0.41
3:C:101:TYR:CG	3:C:102:CYS:N	2.88	0.41
4:D:149:THR:HG23	4:D:200:THR:HB	2.02	0.41
6:F:98:LEU:O	6:F:100:PRO:HD3	2.20	0.41
1:A:109:PRO:HA	1:A:354:MET:HE3	2.03	0.41
1:A:162:ILE:HD12	1:A:281:PRO:HB2	2.03	0.41
5:E:50:LEU:HD22	5:E:59:TYR:CD1	2.55	0.41
1:A:168:GLN:HG2	3:C:81:TRP:CE3	2.57	0.40
5:E:74:ASN:O	5:E:77:ASN:HB2	2.22	0.40
7:G:51:ILE:HD13	7:G:72:ARG:HB2	2.02	0.40
1:A:560:VAL:HG11	1:A:580:SER:HB3	2.03	0.40
1:A:160:LEU:HB3	1:A:338:ALA:HB2	2.04	0.40
1:A:379:ALA:HB1	1:A:392:LEU:HD13	2.03	0.40
2:B:111:LEU:HD23	2:B:111:LEU:HA	1.88	0.40
4:D:50:ILE:HD13	4:D:50:ILE:HA	1.92	0.40
7:G:159:TRP:HA	7:G:201:CYS:HA	2.03	0.40
4:D:135:THR:HG22	4:D:184:LEU:HD12	2.03	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	654/656 (100%)	595 (91%)	56 (9%)	3 (0%)	24	55
2	B	100/112 (89%)	94 (94%)	6 (6%)	0	100	100
3	C	176/191 (92%)	161 (92%)	15 (8%)	0	100	100
4	D	212/216 (98%)	177 (84%)	30 (14%)	5 (2%)	4	23
5	E	218/232 (94%)	197 (90%)	21 (10%)	0	100	100
6	F	216/218 (99%)	198 (92%)	15 (7%)	3 (1%)	9	34
7	G	218/230 (95%)	190 (87%)	25 (12%)	3 (1%)	9	34
All	All	1794/1855 (97%)	1612 (90%)	168 (9%)	14 (1%)	16	46

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	644	LEU
4	D	182	LEU
7	G	194	LEU
4	D	70	GLY
4	D	98	THR
6	F	81	PRO
7	G	154	PRO
1	A	345	SER
6	F	72	GLY
4	D	30	GLY
1	A	112	ILE
6	F	8	PRO
4	D	144	TYR
7	G	124	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	542/562 (96%)	542 (100%)	0	100	100
2	B	92/98 (94%)	91 (99%)	1 (1%)	65	75
3	C	161/169 (95%)	160 (99%)	1 (1%)	78	81
4	D	169/183 (92%)	169 (100%)	0	100	100
5	E	178/195 (91%)	178 (100%)	0	100	100
6	F	188/189 (100%)	188 (100%)	0	100	100
7	G	176/196 (90%)	175 (99%)	1 (1%)	78	81
All	All	1506/1592 (95%)	1503 (100%)	3 (0%)	87	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	79	CYS
3	C	128	CYS
7	G	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	168	GLN
1	A	426	HIS
3	C	186	GLN
3	C	206	HIS
4	D	71	ASN
5	E	171	HIS
6	F	170	GLN
7	G	197	GLN
7	G	202	ASN
7	G	205	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	NAG	B	201	2	14,14,15	0.26	0	17,19,21	0.51	0
8	NAG	A	701	1	14,14,15	0.25	0	17,19,21	0.40	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
8	NAG	B	201	2	-	4/6/23/26	0/1/1/1
8	NAG	A	701	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

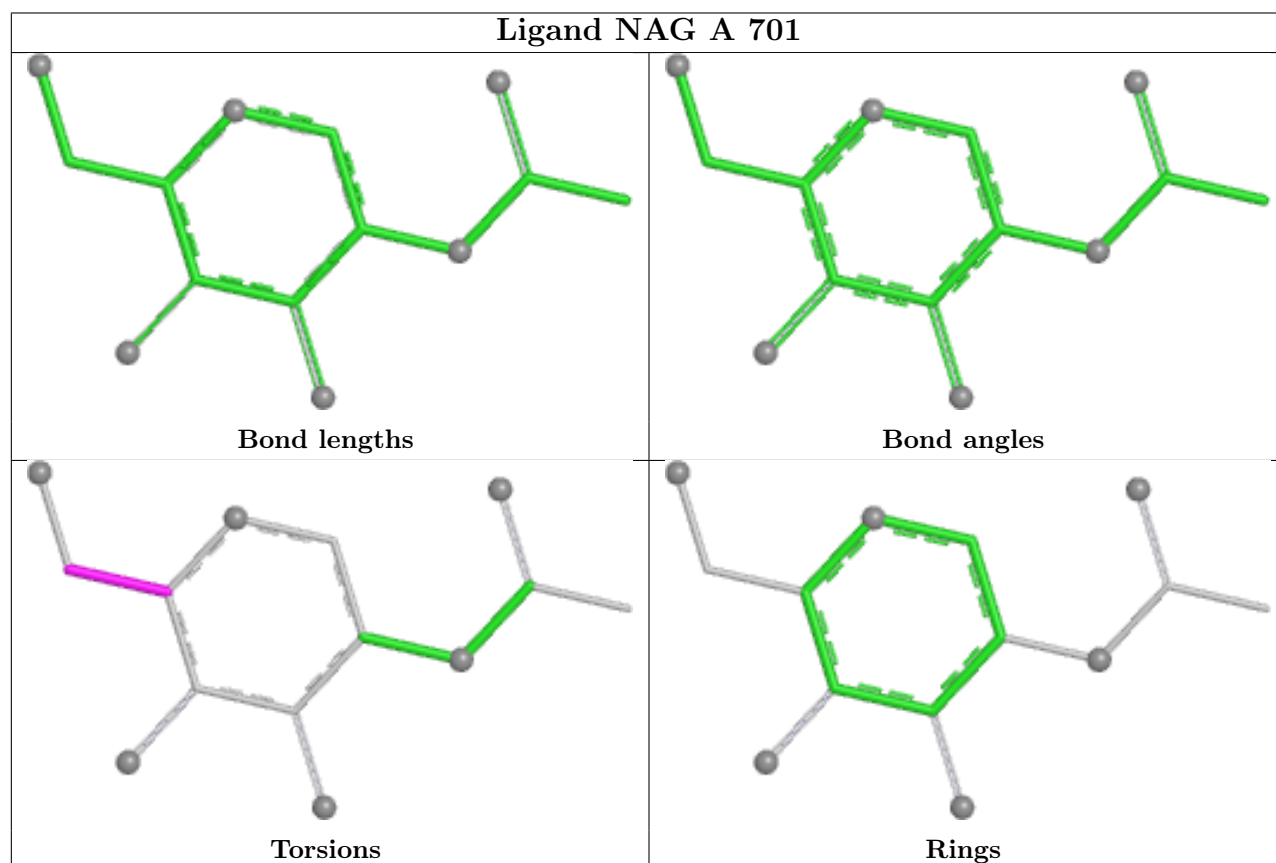
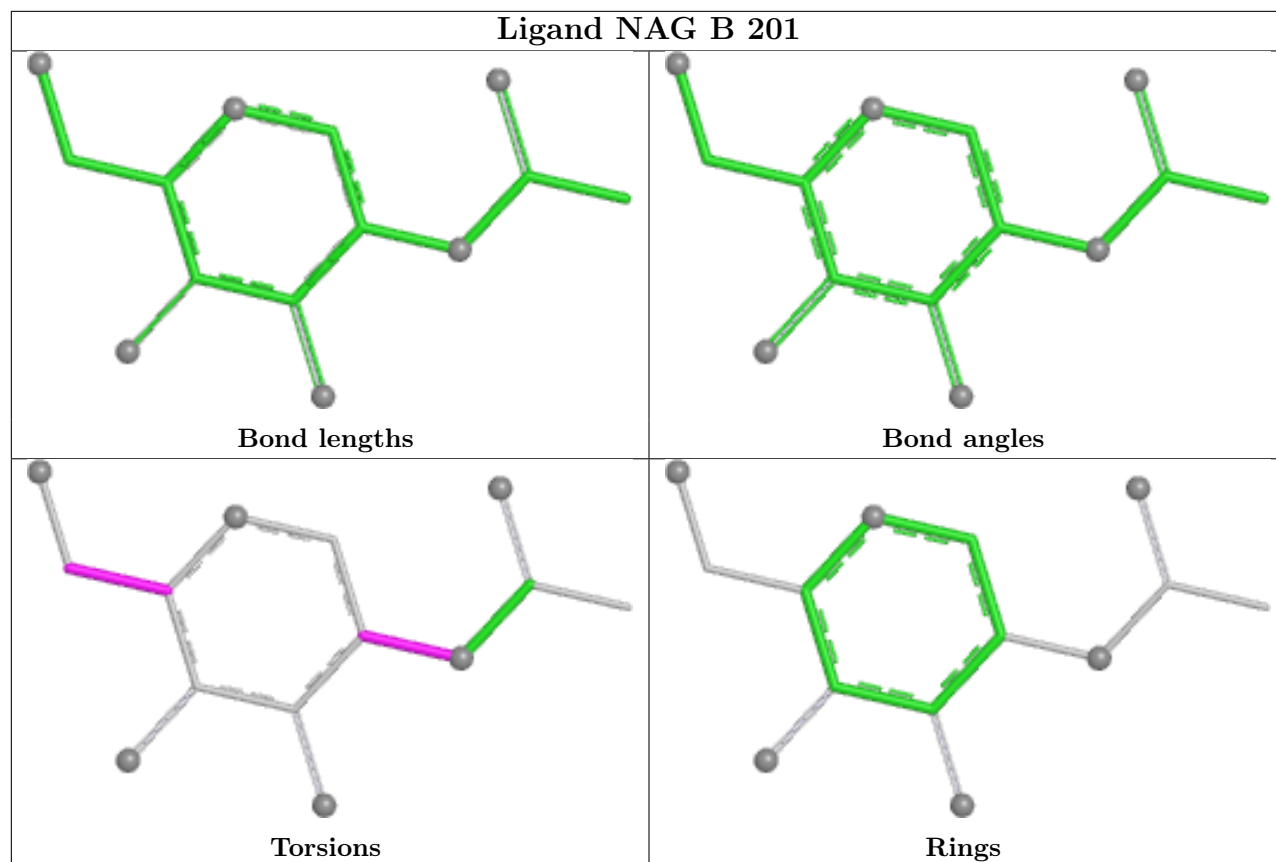
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	701	NAG	C4-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	B	201	NAG	O5-C5-C6-O6
8	B	201	NAG	C4-C5-C6-O6
8	B	201	NAG	C1-C2-N2-C7
8	B	201	NAG	C3-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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	656/656 (100%)	0.49	29 (4%) 39 22	31, 67, 129, 178	0
2	B	104/112 (92%)	0.43	0 100 100	40, 70, 110, 149	0
3	C	178/191 (93%)	0.44	6 (3%) 48 28	39, 65, 115, 156	0
4	D	214/216 (99%)	0.91	26 (12%) 8 5	41, 93, 138, 200	0
5	E	220/232 (94%)	0.73	17 (7%) 19 11	43, 75, 153, 215	0
6	F	218/218 (100%)	0.83	20 (9%) 14 8	59, 103, 169, 217	0
7	G	220/230 (95%)	0.90	25 (11%) 10 6	58, 110, 201, 266	0
All	All	1810/1855 (97%)	0.65	123 (6%) 23 13	31, 79, 154, 266	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	151	PHE	4.6
7	G	131	PRO	4.5
5	E	153	PHE	4.3
5	E	171	HIS	4.1
4	D	181	TYR	4.0
6	F	138	CYS	3.9
1	A	308	THR	3.9
1	A	581	PRO	3.8
6	F	98	LEU	3.7
4	D	45	ALA	3.7
6	F	69	SER	3.7
1	A	560	VAL	3.6
6	F	190	TYR	3.6
4	D	179	SER	3.6
1	A	30	GLU	3.5
1	A	63	GLU	3.4
7	G	192	SER	3.4

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Mol	Chain	Res	Type	RSRZ
7	G	54	ASP	3.3
4	D	144	TYR	3.2
1	A	209	GLY	3.2
1	A	498	GLU	3.2
4	D	33	ASP	3.2
5	E	155	GLU	3.2
1	A	478	CYS	3.2
5	E	154	PRO	3.2
7	G	159	TRP	3.1
3	C	99	CYS	3.1
5	E	189	VAL	3.1
4	D	22	CYS	3.1
7	G	162	GLY	3.0
5	E	170	VAL	3.0
6	F	115	ALA	3.0
5	E	162	ASN	3.0
1	A	591	ALA	3.0
3	C	208	CYS	3.0
6	F	116	ALA	2.9
7	G	208	SER	2.9
6	F	7	SER	2.9
1	A	309	GLY	2.9
6	F	163	SER	2.8
7	G	90	ASP	2.8
5	E	140	GLY	2.8
7	G	83	MET	2.8
4	D	176	TYR	2.8
5	E	161	TRP	2.8
4	D	195	TYR	2.8
7	G	170	THR	2.7
6	F	200	VAL	2.7
4	D	146	GLY	2.7
1	A	386	ALA	2.7
1	A	526	ALA	2.7
7	G	153	GLU	2.6
4	D	196	SER	2.6
1	A	637	GLN	2.6
6	F	199	GLU	2.6
7	G	214	LYS	2.6
1	A	28	ASP	2.6
1	A	521	ARG	2.6
7	G	215	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	D	73	ALA	2.5
6	F	120	PHE	2.5
1	A	645	SER	2.5
3	C	215	LEU	2.5
4	D	28	ASP	2.5
5	E	73	ASP	2.5
4	D	166	THR	2.5
5	E	105	SER	2.5
6	F	54	LEU	2.5
4	D	29	VAL	2.5
1	A	278	CYS	2.4
1	A	64	ASP	2.4
1	A	277	GLY	2.4
4	D	169	SER	2.4
6	F	166	SER	2.4
5	E	169	GLY	2.4
5	E	61	SER	2.4
1	A	629	GLU	2.4
1	A	190	ASP	2.4
7	G	152	PRO	2.4
3	C	191	HIS	2.3
4	D	129	LEU	2.3
7	G	127	PHE	2.3
1	A	58	GLU	2.3
6	F	144	TYR	2.3
7	G	209	ASN	2.3
4	D	171	GLN	2.3
4	D	197	CYS	2.3
7	G	207	PRO	2.3
7	G	44	GLY	2.3
6	F	139	LEU	2.3
4	D	90	CYS	2.3
3	C	90	VAL	2.3
4	D	32	TYR	2.2
1	A	535	VAL	2.2
5	E	78	SER	2.2
4	D	70	GLY	2.2
4	D	147	ALA	2.2
6	F	133	THR	2.2
4	D	186	PRO	2.2
7	G	106	ASP	2.2
1	A	673	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	75	ALA	2.1
4	D	34	TYR	2.1
4	D	140	ILE	2.1
3	C	219	GLN	2.1
1	A	499	ALA	2.1
1	A	387	GLY	2.1
1	A	62	THR	2.1
7	G	5	LEU	2.1
7	G	119	ALA	2.1
6	F	180	SER	2.1
1	A	240	ASN	2.1
6	F	158	LEU	2.1
4	D	111	GLY	2.1
7	G	148	LYS	2.0
5	E	71	SER	2.0
7	G	84	SER	2.0
5	E	35	ASP	2.0
6	F	145	PRO	2.0
7	G	154	PRO	2.0
6	F	172	SER	2.0
1	A	663	THR	2.0
7	G	9	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](#)

There are no oligosaccharides in this entry.

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
8	NAG	B	201	14/15	0.57	0.12	88,115,134,136	0

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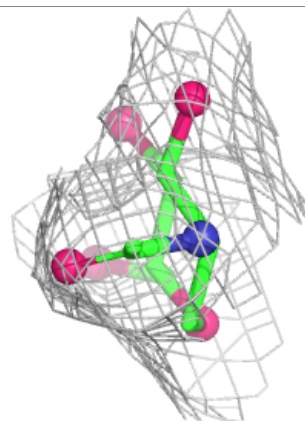
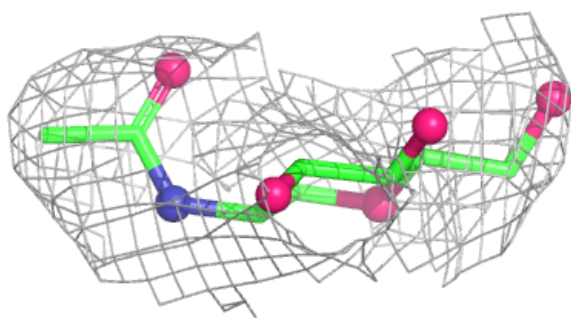
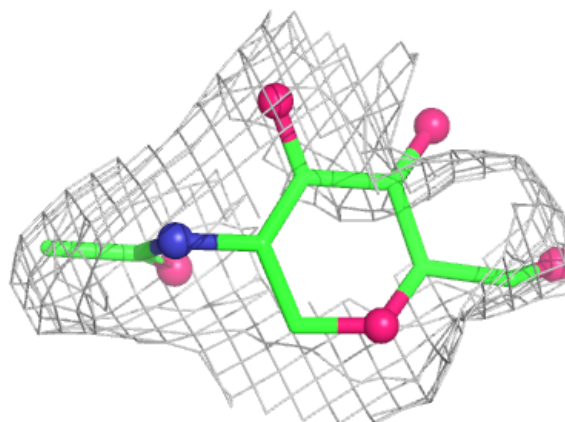
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	NAG	A	701	14/15	0.86	0.13	83,88,99,106	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

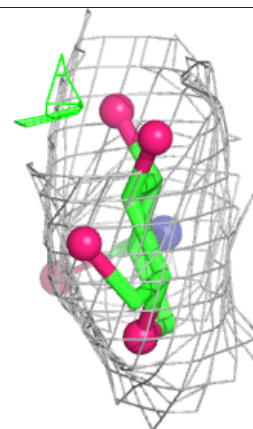
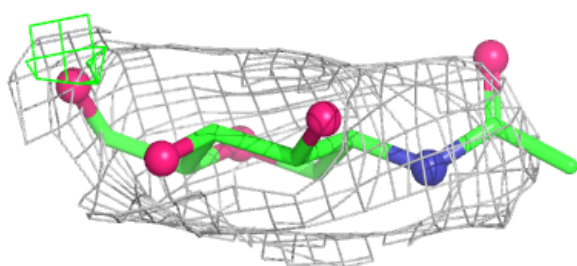
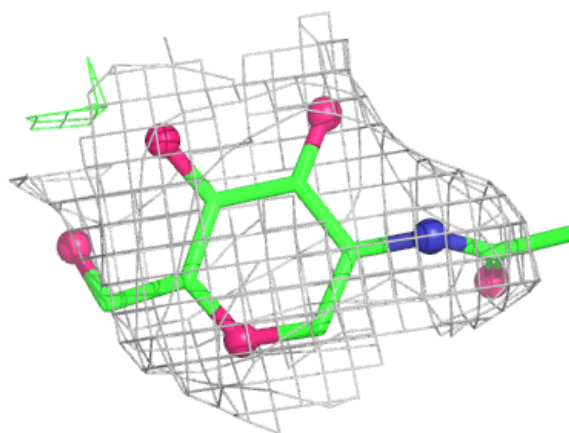
Electron density around NAG B 201:

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 NAG A 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.