



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2024 – 06:05 PM EDT

PDB ID : 8TNT
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

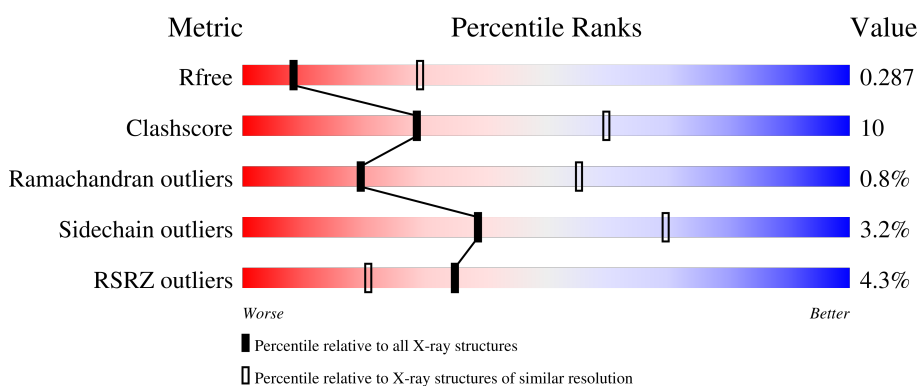
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



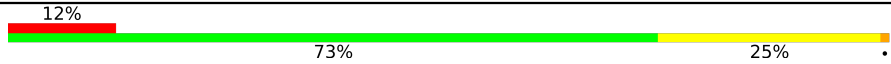

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div>
2	B	112	<div style="display: flex; align-items: center;"> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
3	C	191	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 68%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
4	D	216	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 0%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>
5	E	232	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 71%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 24%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	F	218	
7	G	230	

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	656	5016	3217	819	949	31	0	0	0

- Molecule 2 is a protein called Envelope glycoprotein L.

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

- Molecule 3 is a protein called Glycoprotein 42.

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

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

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

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

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

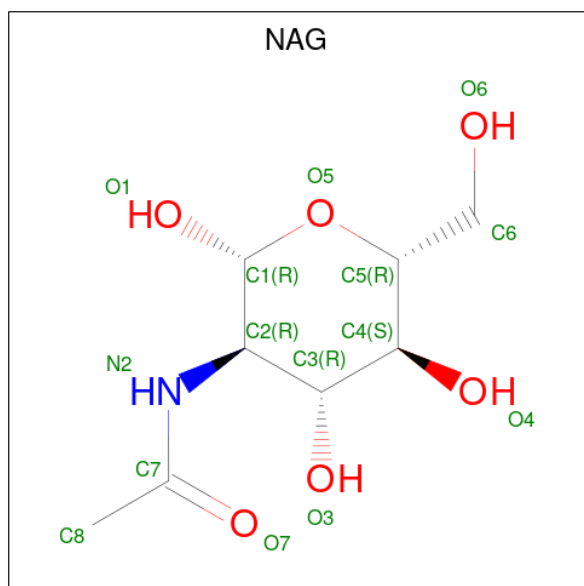
- Molecule 6 is a protein called F-2-1 light chain.

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

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

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

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

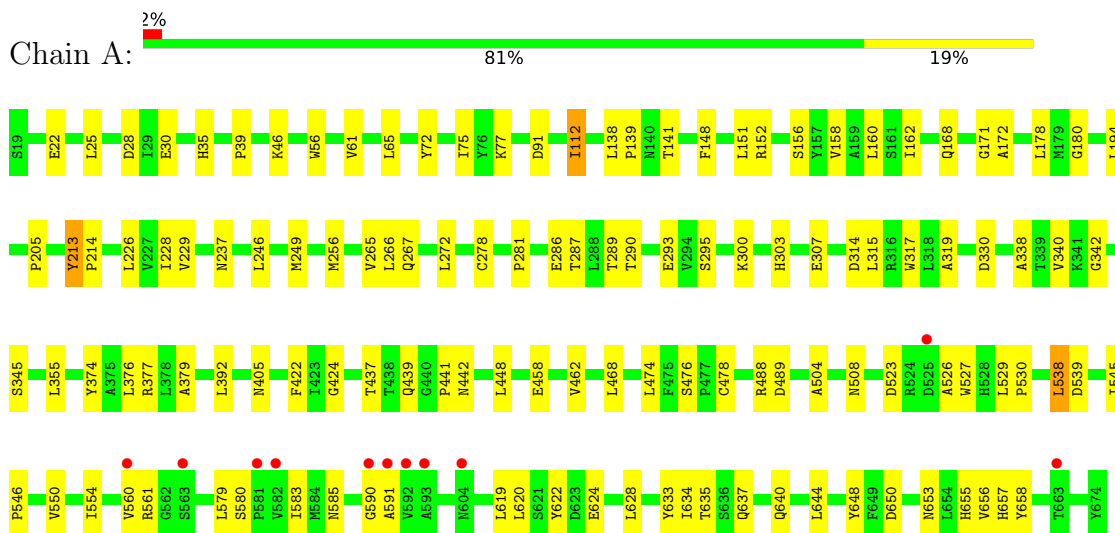


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	14	8	1	5	0	0
8	B	1	14	8	1	5	0	0

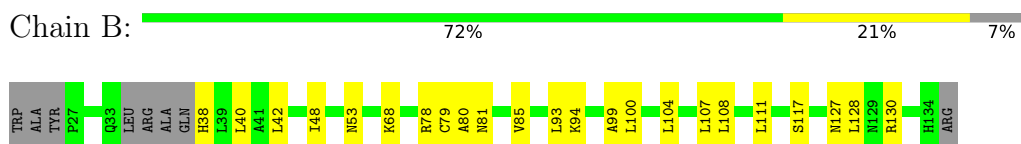
3 Residue-property plots [i](#)

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

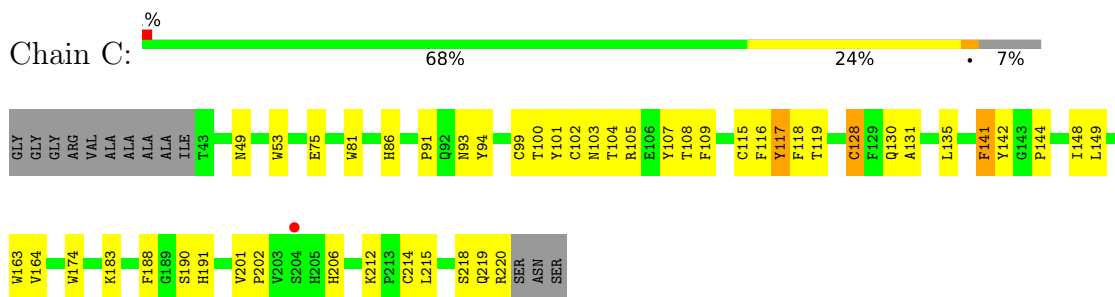
- Molecule 1: Envelope glycoprotein H



- Molecule 2: Envelope glycoprotein L

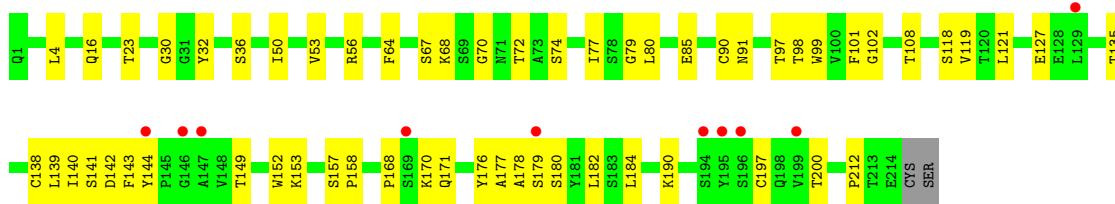


- Molecule 3: Glycoprotein 42

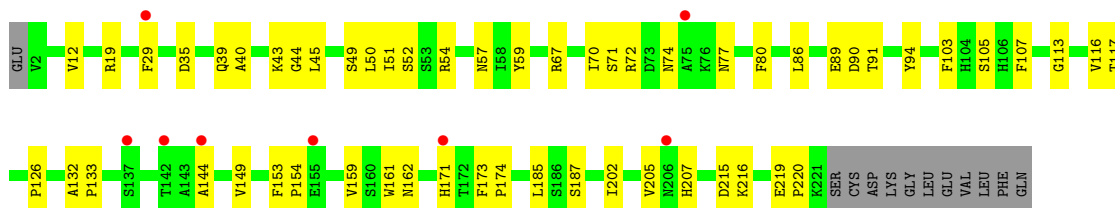


- Molecule 4: 769C2 light chain

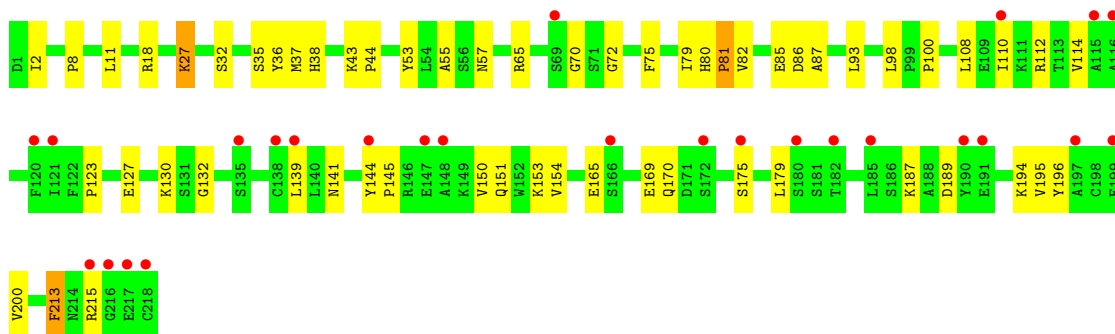




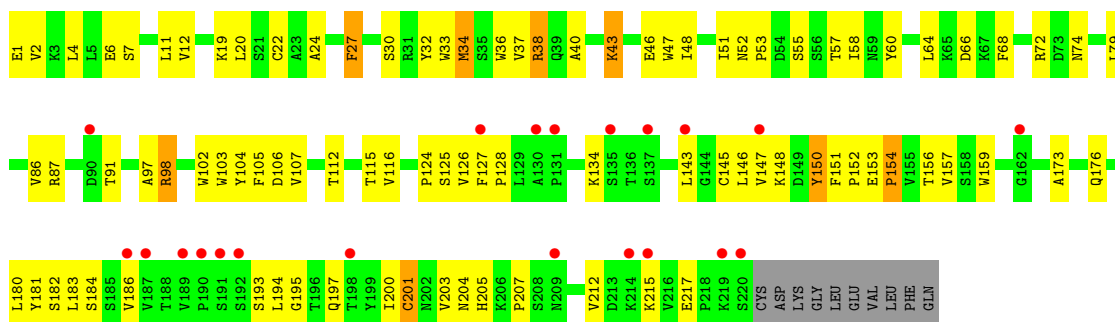
- Molecule 5: 769C2 heavy chain



- Molecule 6: F-2-1 light chain



- Molecule 7: F-2-1 heavy chain



4 Data and refinement statistics i

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 47.82 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.32-3.15) 98.5 (47.82-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.255 , 0.287 0.254 , 0.287	Depositor DCC
R_{free} test set	1987 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtrriage
Anisotropy	0.672	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.014 for l,-k,h	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	13731	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage'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	0.24	0/5125	0.47	0/6975
2	B	0.24	0/816	0.46	0/1106
3	C	0.25	0/1491	0.46	0/2045
4	D	0.25	0/1579	0.49	0/2165
5	E	0.25	0/1653	0.52	0/2250
6	F	0.25	0/1705	0.49	0/2316
7	G	0.25	0/1665	0.50	0/2274
All	All	0.25	0/14034	0.48	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	74	0
2	B	802	0	786	15	0
3	C	1436	0	1344	35	0
4	D	1543	0	1447	31	0
5	E	1615	0	1561	38	0
6	F	1667	0	1622	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1624	0	1550	62	0
8	A	14	0	13	0	0
8	B	14	0	13	0	0
All	All	13731	0	13276	262	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 (262) 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
4:D:32:TYR:HB2	4:D:53:VAL:HG21	1.67	0.76
1:A:35:HIS:HE2	5:E:105:SER:HG	1.32	0.75
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

Continued on next page...

Continued from previous page...

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: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
5:E:202:ILE:HD11	5:E:215:ASP:HB2	1.89	0.53
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:190:SER:OG	3:C:191:HIS:N	2.42	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:249:MET:HE3	1:A:289:THR:HA	1.94	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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:489:ASP:OD1	1:A:489:ASP:N	2.50	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
4:D:127:GLU:HG3	5:E:216:LYS:HE2	1.99	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
6:F:79:ILE:HB	6:F:82:VAL:HG12	2.00	0.42
3:C:101:TYR:CG	3:C:102:CYS:N	2.88	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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 [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	654/656 (100%)	595 (91%)	56 (9%)	3 (0%)	29	65
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%)	6	30
5	E	218/232 (94%)	197 (90%)	21 (10%)	0	100	100
6	F	216/218 (99%)	198 (92%)	15 (7%)	3 (1%)	11	43
7	G	218/230 (95%)	190 (87%)	25 (12%)	3 (1%)	11	43
All	All	1794/1855 (97%)	1612 (90%)	168 (9%)	14 (1%)	19	55

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	542/562 (96%)	528 (97%)	14 (3%)	46	74
2	B	92/98 (94%)	89 (97%)	3 (3%)	38	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	161/169 (95%)	156 (97%)	5 (3%)	40	70
4	D	169/183 (92%)	164 (97%)	5 (3%)	41	71
5	E	178/195 (91%)	175 (98%)	3 (2%)	60	82
6	F	188/189 (100%)	183 (97%)	5 (3%)	44	73
7	G	176/196 (90%)	163 (93%)	13 (7%)	13	43
All	All	1506/1592 (95%)	1458 (97%)	48 (3%)	39	70

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	TYR
1	A	237	ASN
1	A	278	CYS
1	A	330	ASP
1	A	374	TYR
1	A	468	LEU
1	A	476	SER
1	A	478	CYS
1	A	488	ARG
1	A	523	ASP
1	A	527	TRP
1	A	538	LEU
1	A	539	ASP
1	A	633	TYR
2	B	38	HIS
2	B	68	LYS
2	B	79	CYS
3	C	86	HIS
3	C	117	TYR
3	C	128	CYS
3	C	141	PHE
3	C	219	GLN
4	D	68	LYS
4	D	90	CYS
4	D	101	PHE
4	D	142	ASP
4	D	143	PHE
5	E	19	ARG
5	E	54	ARG
5	E	171	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	11	LEU
6	F	27	LYS
6	F	151	GLN
6	F	189	ASP
6	F	213	PHE
7	G	1	GLU
7	G	19	LYS
7	G	22	CYS
7	G	27	PHE
7	G	34	MET
7	G	38	ARG
7	G	43	LYS
7	G	66	ASP
7	G	98	ARG
7	G	143	LEU
7	G	150	TYR
7	G	201	CYS
7	G	217	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
7	G	205	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	A	701	1	14,14,15	0.24	0	17,19,21	0.38	0
8	NAG	B	201	2	14,14,15	0.24	0	17,19,21	0.48	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	A	701	1	-	2/6/23/26	0/1/1/1
8	NAG	B	201	2	-	4/6/23/26	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:

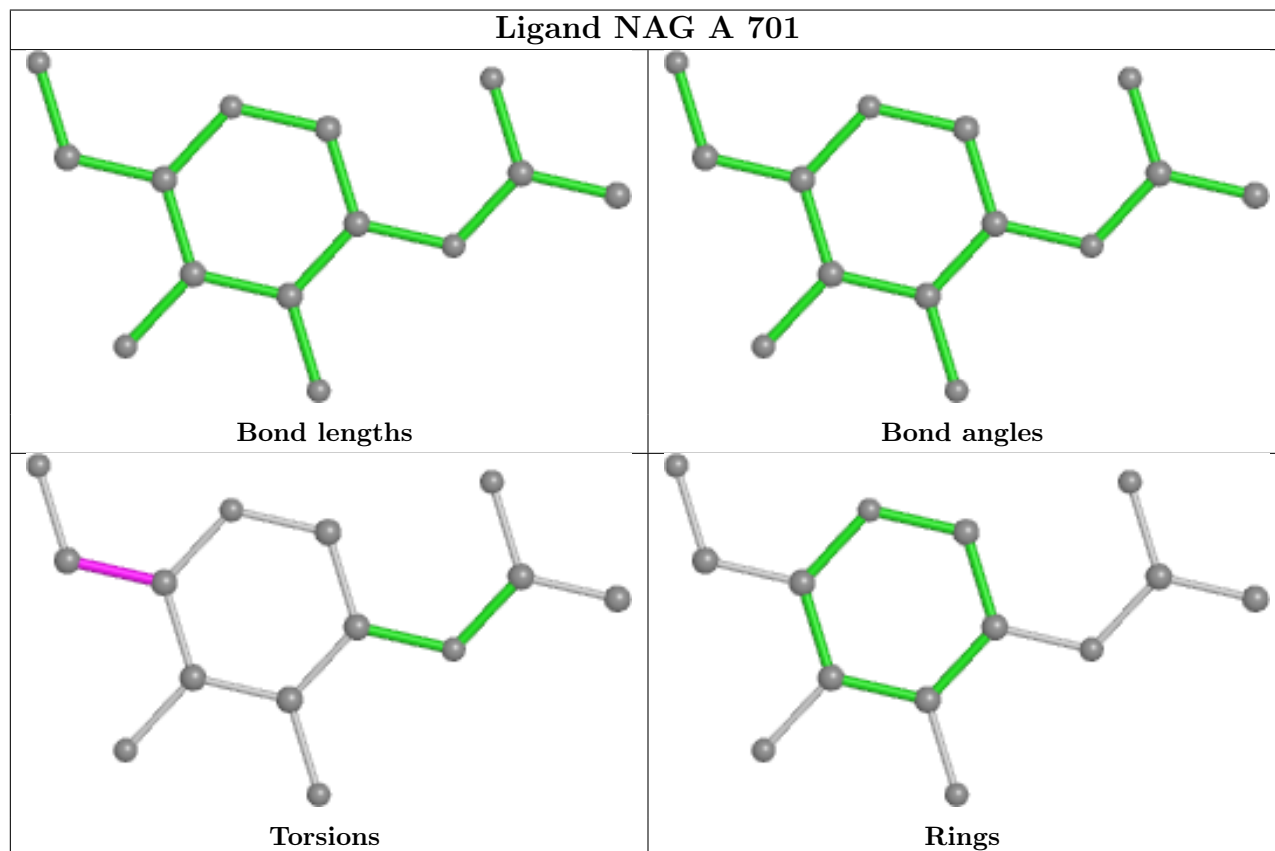
Mol	Chain	Res	Type	Atoms
8	A	701	NAG	C4-C5-C6-O6
8	A	701	NAG	O5-C5-C6-O6
8	B	201	NAG	O5-C5-C6-O6
8	B	201	NAG	C4-C5-C6-O6
8	B	201	NAG	C3-C2-N2-C7
8	B	201	NAG	C1-C2-N2-C7

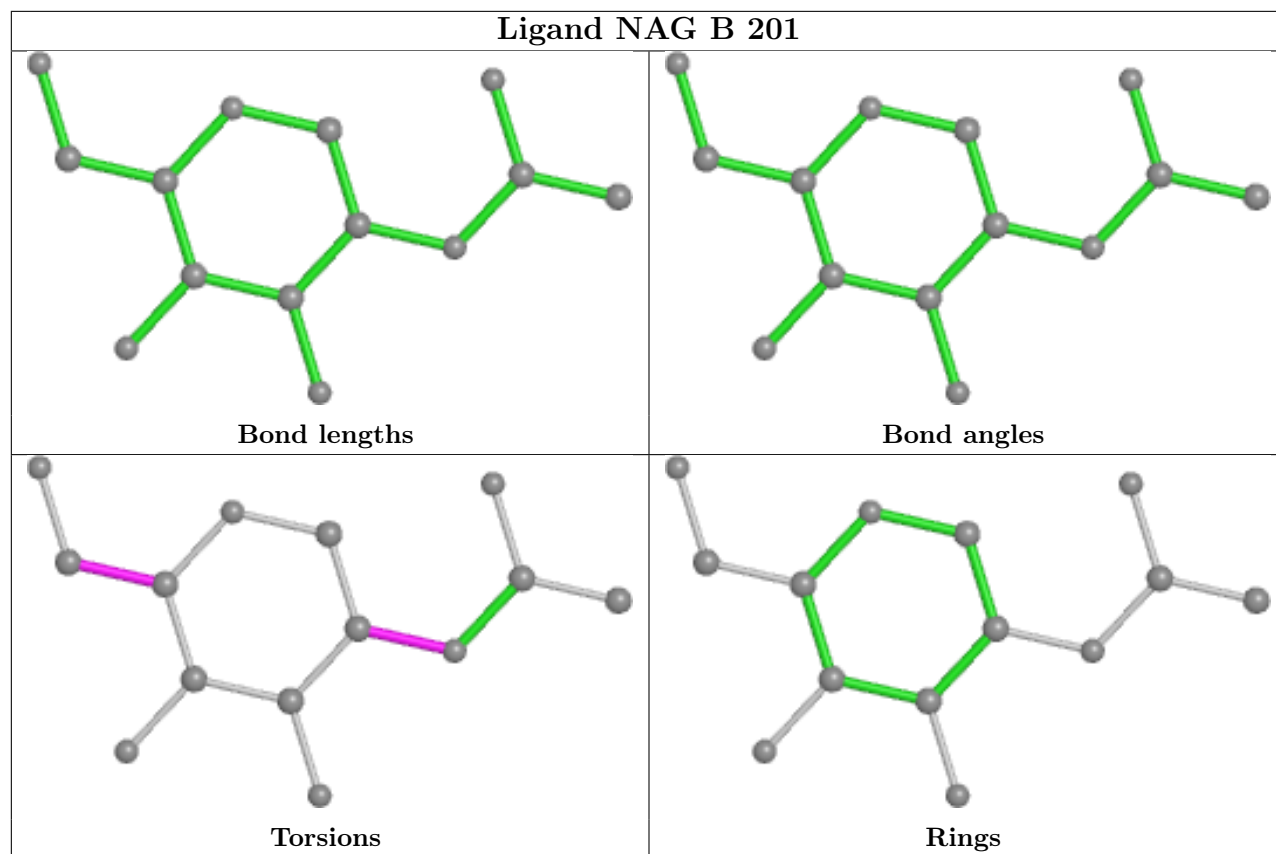
There are no ring outliers.

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 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 [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 i

6.1 Protein, DNA and RNA chains i

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%)	0.06	11 (1%) 70 57	31, 67, 129, 178	0
2	B	104/112 (92%)	-0.07	0 100 100	40, 70, 110, 149	0
3	C	178/191 (93%)	0.08	1 (0%) 89 84	39, 65, 115, 156	0
4	D	214/216 (99%)	0.37	10 (4%) 31 17	41, 93, 138, 200	0
5	E	220/232 (94%)	0.23	8 (3%) 42 26	43, 75, 153, 215	0
6	F	218/218 (100%)	0.61	26 (11%) 4 2	59, 103, 169, 217	0
7	G	220/230 (95%)	0.61	21 (9%) 8 4	58, 110, 201, 266	0
All	All	1810/1855 (97%)	0.25	77 (4%) 35 21	31, 79, 154, 266	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	131	PRO	8.1
1	A	592	VAL	7.0
7	G	215	LYS	5.6
6	F	138	CYS	5.5
1	A	591	ALA	5.3
1	A	593	ALA	5.2
7	G	192	SER	5.1
1	A	581	PRO	4.9
6	F	190	TYR	4.5
5	E	75	ALA	4.5
6	F	218	CYS	4.4
7	G	186	VAL	4.3
7	G	220	SER	4.1
5	E	142	THR	4.1
6	F	116	ALA	4.0
6	F	191	GLU	3.9
6	F	115	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	190	PRO	3.9
6	F	121	ILE	3.8
6	F	147	GLU	3.7
7	G	127	PHE	3.7
7	G	130	ALA	3.7
4	D	196	SER	3.7
7	G	214	LYS	3.7
4	D	146	GLY	3.6
6	F	180	SER	3.6
4	D	147	ALA	3.5
6	F	139	LEU	3.5
7	G	137	SER	3.5
1	A	525	ASP	3.4
7	G	147	VAL	3.4
1	A	560	VAL	3.4
1	A	590	GLY	3.3
5	E	144	ALA	3.2
7	G	187	VAL	3.2
4	D	169	SER	3.1
7	G	135	SER	3.1
6	F	172	SER	2.9
6	F	197	ALA	2.9
1	A	582	VAL	2.9
7	G	198	THR	2.8
6	F	217	GLU	2.8
6	F	110	ILE	2.8
6	F	120	PHE	2.8
1	A	563	SER	2.8
1	A	663	THR	2.8
6	F	144	TYR	2.8
7	G	90	ASP	2.8
6	F	166	SER	2.8
6	F	135	SER	2.7
4	D	144	TYR	2.7
7	G	143	LEU	2.7
5	E	171	HIS	2.6
6	F	182	THR	2.6
3	C	204	SER	2.6
4	D	195	TYR	2.6
6	F	216	GLY	2.5
5	E	155	GLU	2.5
4	D	199	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	209	ASN	2.5
1	A	604	ASN	2.4
5	E	29	PHE	2.4
6	F	69	SER	2.4
6	F	148	ALA	2.4
7	G	162	GLY	2.3
6	F	199	GLU	2.3
5	E	206	ASN	2.2
6	F	185	LEU	2.2
6	F	215	ARG	2.2
7	G	219	LYS	2.2
5	E	137	SER	2.2
6	F	175	SER	2.2
4	D	194	SER	2.1
7	G	189	VAL	2.1
7	G	191	SER	2.1
4	D	179	SER	2.1
4	D	129	LEU	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 monosaccharides in this entry.

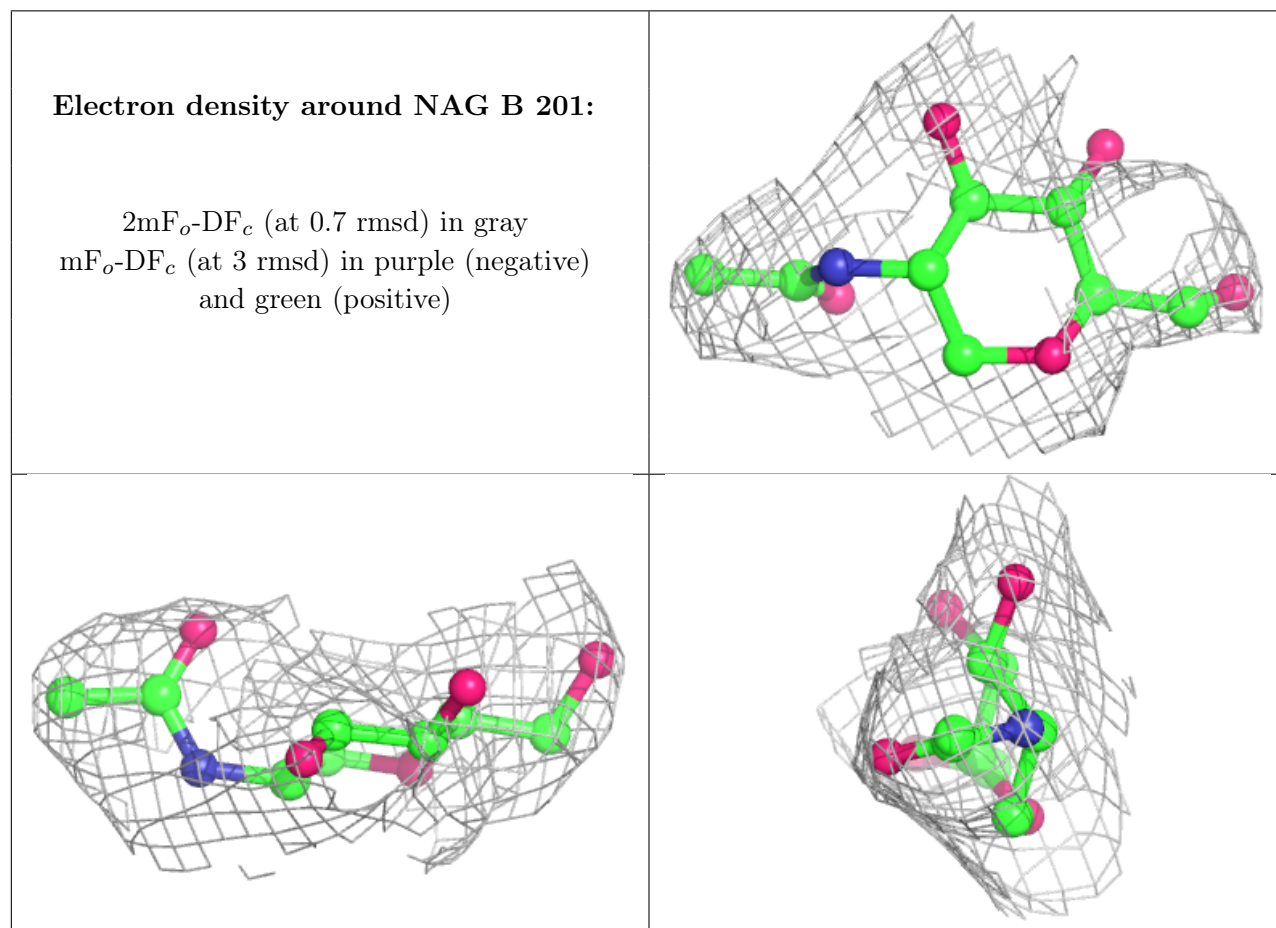
6.4 Ligands [i](#)

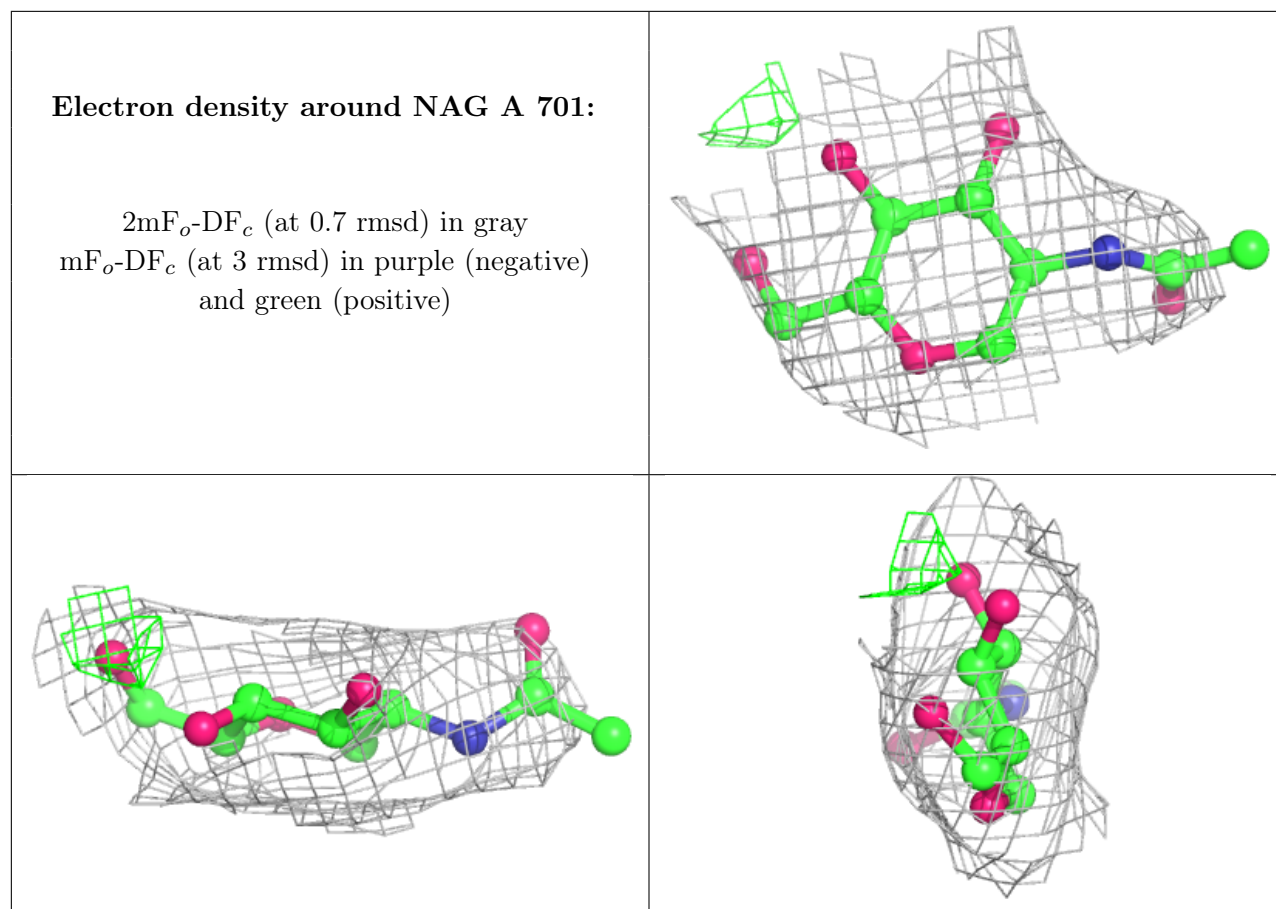
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NAG	B	201	14/15	0.83	0.19	88,115,134,136	0
8	NAG	A	701	14/15	0.88	0.22	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.