



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 07:41 PM JST

PDB ID : 7YCN
Title : Crystal structure of SARS-CoV-2 Spike RBD in complex with IY-2A Fab
Authors : Mohapatra, A.; Chen, X.
Deposited on : 2022-07-01
Resolution : 2.85 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (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

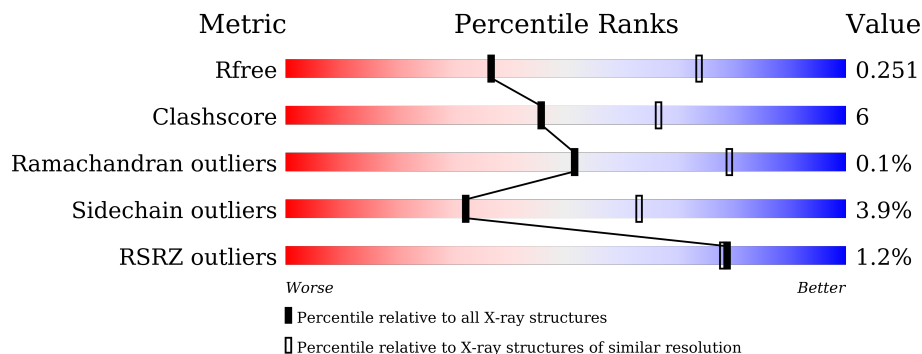
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	195	 % 90% 9% .
1	B	195	 4% 88% 11% ..
1	G	195	 87% 13% .
1	J	195	 % 85% 14% ..
2	C	228	 75% 22% ..
2	E	228	 5% 74% 21% ..

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Mol	Chain	Length	Quality of chain
2	H	228	 <p>77% 18% . .</p>
2	K	228	 <p>77% 16% . .</p>
3	D	216	 <p>77% 20% .</p>
3	F	216	 <p>84% 16%</p>
3	I	216	 <p>80% 18% ..</p>
3	L	216	 <p>85% 12% ..</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19094 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	J	194	1536	985	256	287	8	0	0	0
1	A	194	1536	985	256	287	8	0	0	0
1	B	194	1530	982	253	287	8	0	0	0
1	G	194	1530	982	253	287	8	0	0	0

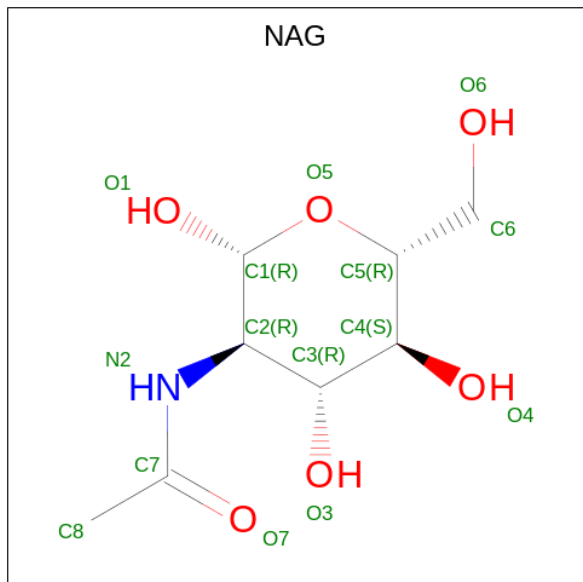
- Molecule 2 is a protein called IY-2A Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	K	219	1625	1039	267	315	4	0	0	0
2	E	220	1625	1037	266	318	4	0	0	0
2	C	223	1650	1052	271	323	4	0	0	0
2	H	221	1633	1042	268	319	4	0	0	0

- Molecule 3 is a protein called IY-2A Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	212	1593	992	265	331	5	0	0	0
3	F	215	1615	1004	268	337	6	0	0	0
3	D	212	1593	992	265	331	5	0	0	0
3	I	213	1600	996	266	333	5	0	0	0

- Molecule 4 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).

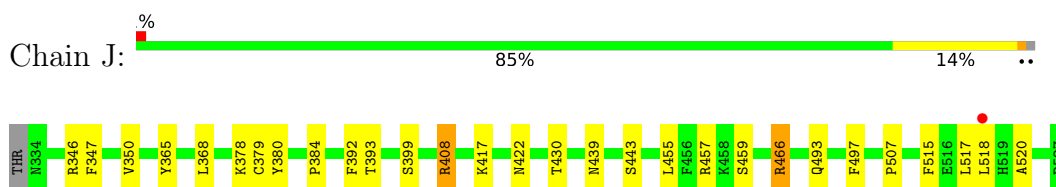


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	J	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

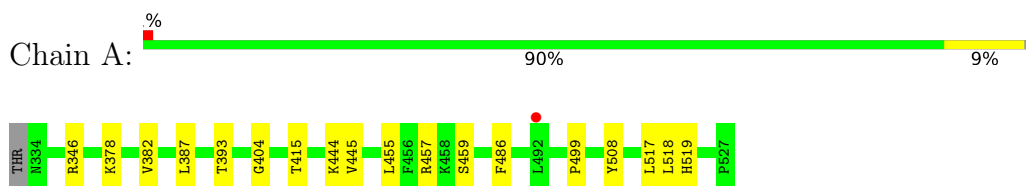
3 Residue-property plots [i](#)

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.

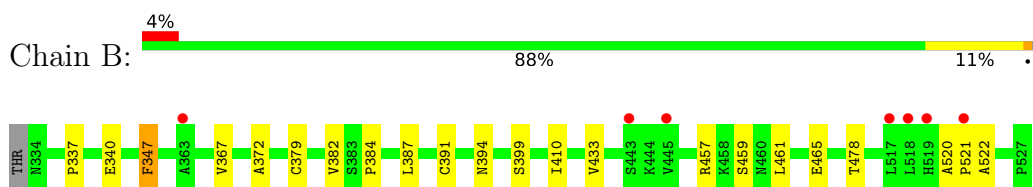
- Molecule 1: Spike protein S1



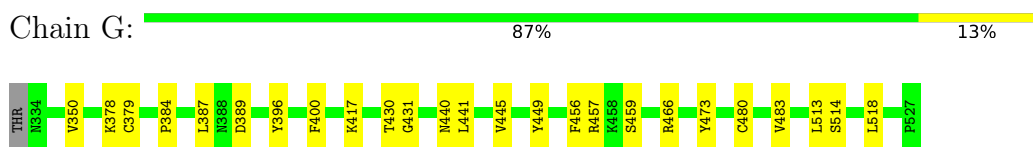
- Molecule 1: Spike protein S1



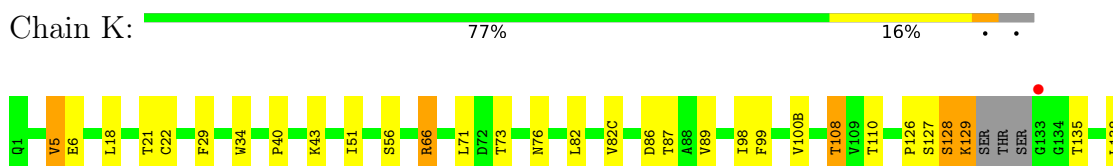
- Molecule 1: Spike protein S1



- Molecule 1: Spike protein S1

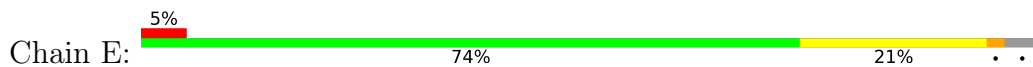


- Molecule 2: IY-2A Fab heavy chain

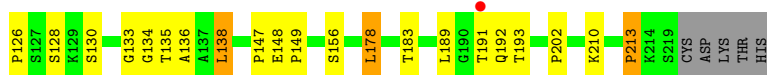
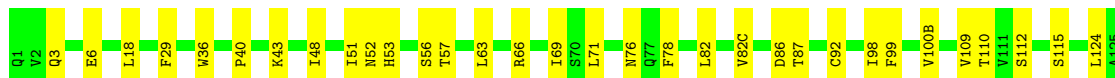




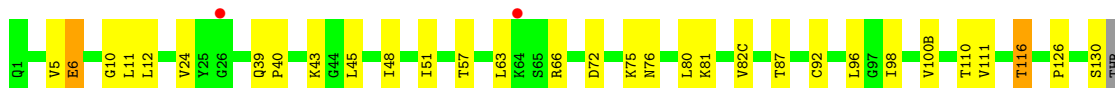
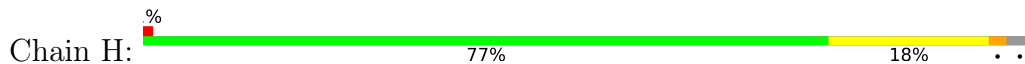
• Molecule 2: IY-2A Fab heavy chain



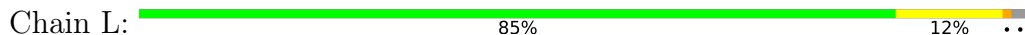
• Molecule 2: IY-2A Fab heavy chain



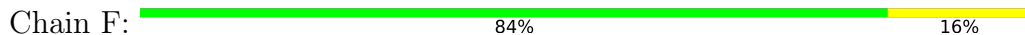
• Molecule 2: IY-2A Fab heavy chain



• Molecule 3: IY-2A Fab light chain

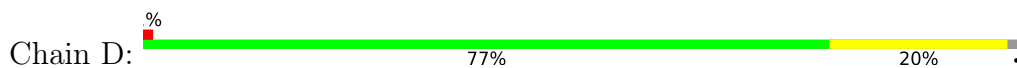


• Molecule 3: IY-2A Fab light chain

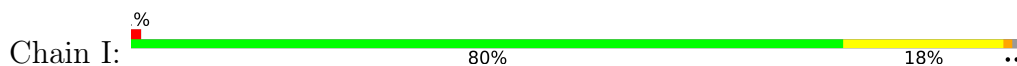




• Molecule 3: IY-2A Fab light chain



• Molecule 3: IY-2A Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	193.02Å 225.15Å 95.52Å 90.00° 96.16° 90.00°	Depositor
Resolution (Å)	33.64 – 2.85 33.64 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.64-2.85) 99.9 (33.64-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.85Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.211 , 0.250 0.213 , 0.251	Depositor DCC
R_{free} test set	4687 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19094	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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	0.46	0/1580	0.65	0/2151
1	B	0.44	0/1574	0.66	0/2144
1	G	0.49	0/1574	0.66	0/2144
1	J	0.53	0/1580	0.72	0/2151
2	C	0.49	1/1692 (0.1%)	0.69	1/2314 (0.0%)
2	E	0.47	0/1666	0.69	0/2280
2	H	0.45	0/1674	0.68	0/2289
2	K	0.57	0/1666	0.73	1/2277 (0.0%)
3	D	0.51	0/1633	0.73	0/2231
3	F	0.55	0/1655	0.70	0/2261
3	I	0.47	0/1640	0.68	0/2241
3	L	0.59	0/1633	0.74	0/2231
All	All	0.50	1/19567 (0.0%)	0.69	2/26714 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	124	LEU	C-N	5.42	1.46	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	178	LEU	CB-CG-CD1	-5.89	100.98	111.00
2	K	178	LEU	CB-CG-CD1	-5.45	101.74	111.00

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	1536	0	1452	15	0
1	B	1530	0	1441	15	0
1	G	1530	0	1442	12	1
1	J	1536	0	1452	18	0
2	C	1650	0	1640	33	1
2	E	1625	0	1607	27	0
2	H	1633	0	1618	31	0
2	K	1625	0	1619	29	0
3	D	1593	0	1519	24	0
3	F	1615	0	1537	18	0
3	I	1600	0	1526	22	0
3	L	1593	0	1519	13	0
4	B	14	0	13	0	0
4	J	14	0	13	1	0
All	All	19094	0	18398	237	1

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 (237) 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:C:128:SER:HB2	2:C:213:PRO:HB3	1.52	0.92
2:H:130:SER:O	2:H:133:GLY:N	2.08	0.86
2:K:100(B):VAL:O	3:L:91:TYR:OH	1.96	0.83
2:H:11:LEU:O	2:H:12:LEU:HD23	1.82	0.80
3:I:194:GLN:HG3	3:I:203:GLU:HB3	1.63	0.79
3:F:80:THR:HA	3:F:106:VAL:HG21	1.64	0.79
2:C:100(B):VAL:O	3:D:91:TYR:OH	2.01	0.76
2:C:128:SER:HB2	2:C:213:PRO:CB	2.19	0.73
2:C:148:GLU:HG2	2:C:149:PRO:HA	1.70	0.72
2:H:171:GLN:NE2	2:H:177:SER:OG	2.23	0.71
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.72	0.70
3:F:83:GLU:HG3	3:F:106:VAL:HG22	1.74	0.67
3:D:136:ILE:HG12	3:D:195:VAL:HG11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:161:THR:HG23	3:L:176:SER:HB2	1.77	0.67
2:K:40:PRO:HG2	2:K:43:LYS:HB2	1.77	0.67
2:H:100(B):VAL:O	3:I:91:TYR:OH	2.11	0.67
2:H:11:LEU:N	2:H:11:LEU:HD12	2.12	0.65
2:K:66:ARG:NH2	2:K:86:ASP:OD2	2.30	0.64
2:K:126:PRO:HD3	2:K:138:LEU:HB3	1.79	0.64
2:C:51:ILE:HG13	2:C:57:THR:HG22	1.77	0.64
1:A:457:ARG:HD3	1:A:459:SER:O	1.99	0.63
3:I:39:ARG:NH1	3:I:81:GLU:O	2.31	0.63
2:H:10:GLY:C	2:H:11:LEU:HD12	2.20	0.62
3:F:39:ARG:NH1	3:F:81:GLU:O	2.31	0.62
3:I:192:SER:OG	3:I:205:THR:HG22	2.00	0.61
2:E:40:PRO:HG2	2:E:43:LYS:HB2	1.82	0.61
2:K:159:LEU:HD21	2:K:182:VAL:HG11	1.83	0.61
3:L:192:SER:OG	3:L:205:THR:HG23	2.00	0.61
3:I:194:GLN:CG	3:I:203:GLU:HB3	2.31	0.60
1:A:393:THR:HG23	1:A:517:LEU:HA	1.83	0.60
2:C:40:PRO:HG2	2:C:43:LYS:HB2	1.82	0.60
2:C:126:PRO:HD3	2:C:138:LEU:HB3	1.83	0.60
3:F:180:LEU:HD21	3:F:191:TYR:CZ	2.37	0.59
1:J:380:TYR:O	1:J:430:THR:HA	2.02	0.59
2:E:142:VAL:HG11	2:E:150:VAL:HG11	1.85	0.59
2:E:38:ARG:NH1	2:E:86:ASP:OD1	2.35	0.58
3:D:161:THR:HG22	3:D:176:SER:OG	2.03	0.58
3:I:149:LYS:HG3	3:I:192:SER:HB2	1.84	0.58
3:I:185:TRP:HH2	3:I:206:VAL:HG12	1.67	0.58
1:J:457:ARG:HD3	1:J:459:SER:O	2.04	0.57
2:C:18:LEU:HB3	2:C:82:LEU:HB3	1.86	0.57
2:H:210:LYS:HE3	2:H:212:GLU:OE2	2.03	0.57
2:H:11:LEU:N	2:H:11:LEU:CD1	2.68	0.57
2:E:126:PRO:HD3	2:E:138:LEU:HB3	1.87	0.57
1:A:393:THR:HG23	1:A:517:LEU:HD12	1.86	0.57
2:K:6:GLU:HA	2:K:21:THR:O	2.04	0.57
2:K:51:ILE:HD13	2:K:71:LEU:HB2	1.87	0.57
3:D:180:LEU:HD21	3:D:191:TYR:CZ	2.40	0.57
2:E:33:TYR:HB3	2:E:50:LEU:HD13	1.86	0.57
1:A:518:LEU:HD22	1:A:519:HIS:CD2	2.41	0.56
1:B:337:PRO:O	1:B:340:GLU:HG2	2.06	0.56
3:D:2:ASN:O	3:D:27:SER:HB2	2.05	0.56
2:C:87:THR:HG23	2:C:110:THR:HA	1.87	0.55
1:B:387:LEU:HD12	2:C:98:ILE:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:LEU:HD12	2:C:98:ILE:CD1	2.36	0.55
3:L:68:SER:O	3:L:68:SER:OG	2.24	0.55
2:H:126:PRO:HD3	2:H:138:LEU:HB3	1.87	0.55
2:E:210:LYS:HE2	2:E:212:GLU:OE2	2.07	0.55
1:G:378:LYS:HD3	3:I:29:ALA:O	2.08	0.54
2:C:29:PHE:O	2:C:53:HIS:HB2	2.08	0.54
3:F:39:ARG:HG3	3:F:84:ALA:HB2	1.89	0.54
2:C:6:GLU:HG3	2:C:92:CYS:SG	2.47	0.54
2:K:135:THR:HG21	1:A:455:LEU:CD2	2.38	0.54
2:C:29:PHE:HE1	2:C:76:ASN:HA	1.73	0.54
1:G:379:CYS:SG	1:G:384:PRO:HG3	2.48	0.54
1:G:440:ASN:ND2	1:G:441:LEU:HG	2.23	0.53
3:L:109:PRO:HB2	1:A:415:THR:HG23	1.90	0.53
3:I:181:THR:HG23	3:I:184:GLN:H	1.73	0.53
3:D:83:GLU:HG3	3:D:106:VAL:HG23	1.90	0.53
2:E:119:PRO:HD3	2:E:200:HIS:CD2	2.44	0.53
2:C:52:ASN:HD21	2:C:56:SER:HB2	1.74	0.52
2:C:133:GLY:O	2:C:135:THR:N	2.42	0.52
3:D:18:THR:HG23	3:D:76:SER:HA	1.92	0.52
3:F:133:VAL:HG22	3:F:177:TYR:CD2	2.45	0.52
1:B:457:ARG:HD3	1:B:459:SER:O	2.10	0.52
2:K:18:LEU:HB3	2:K:82:LEU:HB3	1.91	0.51
2:C:193:THR:HG23	2:C:210:LYS:HE3	1.91	0.51
2:K:140:CYS:HG	2:K:196:CYS:CB	2.23	0.51
3:L:151:ASP:OD1	3:L:189:ARG:HG2	2.11	0.51
3:I:20:THR:HG22	3:I:74:THR:HG23	1.91	0.51
2:C:136:ALA:HB2	2:C:189:LEU:HD22	1.92	0.51
1:J:379:CYS:SG	1:J:384:PRO:HG3	2.51	0.51
2:K:66:ARG:HH22	2:K:86:ASP:CG	2.15	0.51
2:K:127:SER:O	2:K:128:SER:C	2.48	0.51
2:H:203:SER:OG	2:H:205:THR:HG23	2.10	0.51
2:E:140:CYS:HG	2:E:196:CYS:HG	1.56	0.50
2:C:136:ALA:CB	2:C:189:LEU:HD22	2.40	0.50
1:J:365:TYR:CD1	2:K:98:ILE:HD12	2.46	0.50
3:L:38:GLN:O	3:L:84:ALA:HB1	2.12	0.50
1:J:518:LEU:O	1:J:518:LEU:HG	2.12	0.50
3:D:105:THR:HG21	3:D:141:PRO:HB3	1.93	0.50
1:B:382:VAL:HG21	1:B:387:LEU:HD21	1.93	0.50
1:G:457:ARG:HD3	1:G:459:SER:O	2.12	0.50
3:F:13:GLU:HG3	3:F:17:LYS:HB2	1.93	0.49
3:F:17:LYS:O	3:F:78:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:6:GLU:N	2:K:6:GLU:OE1	2.45	0.49
1:J:497:PHE:CE2	1:J:507:PRO:HB3	2.47	0.49
3:D:61:ARG:HH21	3:D:82:ASP:CG	2.15	0.49
2:H:51:ILE:HG13	2:H:57:THR:HG22	1.94	0.49
2:K:214:LYS:C	2:K:214:LYS:HD3	2.33	0.49
2:H:24:VAL:HB	2:H:76:ASN:OD1	2.13	0.49
1:B:372:ALA:O	3:D:94:GLY:HA3	2.12	0.49
3:D:181:THR:HG23	3:D:184:GLN:H	1.78	0.49
2:K:98:ILE:HG22	2:K:99:PHE:CD2	2.49	0.48
2:H:6:GLU:HG2	2:H:92:CYS:SG	2.53	0.48
2:H:12:LEU:HB2	2:H:111:VAL:HG22	1.94	0.48
3:L:194:GLN:HG2	3:L:203:GLU:HG3	1.95	0.48
1:B:367:VAL:O	2:C:99:PHE:HA	2.13	0.48
1:G:480:CYS:O	1:G:483:VAL:HG12	2.13	0.48
2:H:130:SER:C	2:H:133:GLY:O	2.52	0.48
4:J:601:NAG:H83	4:J:601:NAG:H3	1.96	0.48
2:C:18:LEU:HD13	2:C:109:VAL:HG11	1.96	0.48
2:K:5:VAL:O	2:K:22:CYS:HA	2.13	0.48
2:H:159:LEU:HD21	2:H:182:VAL:HG11	1.96	0.47
3:I:61:ARG:HD2	3:I:77:GLY:H	1.80	0.47
2:E:140:CYS:SG	2:E:196:CYS:SG	3.08	0.47
2:H:80:LEU:HD12	2:H:81:LYS:H	1.79	0.47
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.47	0.47
3:I:146:VAL:HG22	3:I:195:VAL:HG13	1.95	0.47
1:B:410:ILE:O	1:B:433:VAL:HG21	2.15	0.47
3:I:55:PRO:HD2	3:I:58:VAL:HG21	1.96	0.47
1:A:378:LYS:HD3	3:F:29:ALA:O	2.15	0.47
3:L:167:GLN:OE1	3:L:173:ALA:HB2	2.15	0.46
1:J:347:PHE:CE2	1:J:399:SER:HB2	2.49	0.46
3:L:161:THR:HG23	3:L:176:SER:CB	2.43	0.46
3:F:79:ARG:HB3	3:F:81:GLU:OE2	2.14	0.46
2:H:87:THR:HG23	2:H:110:THR:HA	1.97	0.46
3:I:17:LYS:O	3:I:78:LEU:HB2	2.15	0.46
2:C:66:ARG:NH2	2:C:86:ASP:OD2	2.45	0.46
2:E:29:PHE:O	2:E:53:HIS:HB2	2.16	0.46
2:E:71:LEU:HD12	2:E:78:PHE:HB3	1.97	0.46
2:C:71:LEU:HD12	2:C:78:PHE:HB3	1.97	0.46
1:J:518:LEU:HD23	1:J:518:LEU:H	1.79	0.46
1:G:431:GLY:HA3	1:G:513:LEU:O	2.16	0.46
2:E:6:GLU:OE1	2:E:104:GLY:HA3	2.16	0.46
1:B:347:PHE:CE2	1:B:399:SER:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:GLU:CG	3:D:106:VAL:H	2.28	0.46
2:H:48:ILE:HG23	2:H:63:LEU:HD22	1.98	0.46
2:E:155:ASN:HA	2:E:195:ILE:HG13	1.98	0.46
2:K:29:PHE:HE2	2:K:76:ASN:HA	1.81	0.45
2:C:48:ILE:HG23	2:C:63:LEU:HD22	1.98	0.45
2:E:32:TYR:CZ	2:E:94:ARG:NH1	2.84	0.45
2:E:119:PRO:HD3	2:E:200:HIS:HD2	1.82	0.45
3:F:123:GLU:O	3:F:126:GLN:HB2	2.17	0.45
1:J:497:PHE:CD2	1:J:507:PRO:HB3	2.51	0.45
2:C:191:THR:HG23	2:C:192:GLN:N	2.31	0.45
2:E:206:LYS:HB3	2:E:206:LYS:HE3	1.79	0.45
2:E:144:ASP:HB3	2:E:175:LEU:HD13	1.99	0.45
2:E:39:GLN:HB2	2:E:45:LEU:HD23	1.98	0.44
2:C:36:TRP:HD1	2:C:69:ILE:HD11	1.82	0.44
3:D:196:THR:HG22	3:D:201:THR:OG1	2.17	0.44
3:I:38:GLN:O	3:I:84:ALA:HB1	2.17	0.44
1:J:393:THR:HG21	1:J:520:ALA:HB3	2.00	0.44
2:E:131:THR:HB	2:E:132:SER:H	1.60	0.44
3:F:81:GLU:CD	3:F:81:GLU:H	2.19	0.44
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.48	0.44
2:E:13:LYS:HG3	2:E:14:PRO:HD2	2.00	0.44
3:F:148:TRP:CD1	3:F:159:VAL:HG22	2.53	0.44
3:I:82:ASP:O	3:I:104:LEU:HD23	2.18	0.44
1:J:350:VAL:HG22	1:J:422:ASN:HB3	1.98	0.43
2:K:192:GLN:HE22	1:A:486:PHE:HA	1.83	0.43
1:J:392:PHE:CE1	1:J:515:PHE:HB3	2.53	0.43
1:B:391:CYS:HB3	1:B:522:ALA:HB1	1.99	0.43
2:H:169:VAL:O	2:H:176:TYR:HA	2.19	0.43
3:I:159:VAL:HG22	3:I:178:LEU:HD13	2.00	0.43
1:J:466:ARG:HE	1:J:466:ARG:HB2	1.49	0.43
1:G:350:VAL:HG23	1:G:400:PHE:CD1	2.54	0.43
3:F:144:VAL:HG12	3:F:197:HIS:HB2	2.00	0.43
2:C:178:LEU:HD12	2:C:178:LEU:HA	1.82	0.43
3:D:117:LEU:HD12	3:D:133:VAL:O	2.19	0.43
2:H:43:LYS:HA	2:H:43:LYS:HE2	2.01	0.43
1:B:387:LEU:HA	1:B:387:LEU:HD23	1.80	0.43
3:D:51:ASP:OD1	3:D:66:ILE:HD11	2.19	0.43
3:I:181:THR:CG2	3:I:184:GLN:H	2.32	0.43
1:B:379:CYS:SG	1:B:384:PRO:HG3	2.59	0.43
1:J:455:LEU:HD22	1:J:493:GLN:HG3	2.01	0.42
3:L:61:ARG:HD2	3:L:76:SER:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:189:LEU:HD23	2:E:189:LEU:HA	1.77	0.42
3:D:78:LEU:HA	3:D:78:LEU:HD12	1.69	0.42
2:K:135:THR:HG21	1:A:455:LEU:HD22	2.01	0.42
2:K:148:GLU:HG2	2:K:149:PRO:HA	2.01	0.42
1:J:517:LEU:HD12	1:J:517:LEU:HA	1.85	0.42
2:K:192:GLN:OE1	1:A:486:PHE:N	2.52	0.42
3:D:181:THR:CG2	3:D:184:GLN:H	2.32	0.42
2:K:29:PHE:HD1	2:K:34:TRP:CE2	2.37	0.42
1:B:384:PRO:HG2	3:D:32:TYR:CE2	2.55	0.42
2:C:29:PHE:CD2	2:C:71:LEU:HD11	2.55	0.42
1:G:417:LYS:HA	1:G:417:LYS:HD3	1.74	0.42
2:K:129:LYS:HB2	2:K:129:LYS:HE2	1.29	0.42
3:F:35:TRP:CD2	3:F:73:LEU:HB2	2.55	0.42
2:H:75:LYS:HE2	2:H:75:LYS:HB3	1.93	0.42
3:I:180:LEU:HD11	3:I:191:TYR:CE2	2.54	0.42
1:J:408:ARG:HD3	3:F:112:ALA:HB2	2.01	0.42
3:I:197:HIS:CE1	3:I:198:GLU:HG2	2.55	0.42
2:E:36:TRP:CG	2:E:80:LEU:HD22	2.55	0.42
3:F:150:ALA:HB2	3:F:191:TYR:CE2	2.54	0.42
1:G:518:LEU:HD12	1:G:518:LEU:HA	1.77	0.42
2:H:72:ASP:OD2	2:H:75:LYS:HB2	2.20	0.42
1:A:393:THR:CG2	1:A:517:LEU:HD12	2.50	0.42
1:A:387:LEU:HB2	2:E:98:ILE:HD11	2.01	0.41
1:A:404:GLY:HA2	1:A:508:TYR:CD1	2.55	0.41
1:A:444:LYS:O	1:A:499:PRO:HD3	2.19	0.41
2:H:80:LEU:HD12	2:H:81:LYS:N	2.34	0.41
2:E:47:TRP:CB	3:F:96:TRP:HB2	2.51	0.41
3:D:146:VAL:HA	3:D:194:GLN:O	2.21	0.41
2:K:178:LEU:HA	2:K:178:LEU:HD12	1.88	0.41
1:B:461:LEU:HD22	1:B:465:GLU:HB3	2.02	0.41
2:C:147:PRO:HD2	2:C:202:PRO:HB3	2.02	0.41
2:E:165:THR:HA	2:E:180:SER:HA	2.02	0.41
1:G:387:LEU:HB2	2:H:98:ILE:HD11	2.03	0.41
1:G:456:PHE:HB3	1:G:473:TYR:CD2	2.55	0.41
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.01	0.41
2:C:69:ILE:HG21	2:C:69:ILE:HD13	1.77	0.41
2:C:98:ILE:HG21	2:C:98:ILE:HD13	1.86	0.41
1:J:368:LEU:HD13	2:K:56:SER:HB2	2.03	0.41
2:K:87:THR:HG23	2:K:110:THR:HA	2.02	0.41
2:E:6:GLU:HA	2:E:21:THR:O	2.20	0.41
2:C:193:THR:HG23	2:C:210:LYS:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:37:GLN:HB2	3:D:86:TYR:CE1	2.56	0.41
3:I:150:ALA:O	3:I:151:ASP:HB2	2.19	0.41
2:K:89:VAL:HG22	2:K:108:THR:HG22	2.03	0.41
3:D:165:SER:O	3:D:172:TYR:HA	2.20	0.41
1:G:396:TYR:HB2	1:G:514:SER:HB2	2.01	0.41
2:H:82(C):VAL:HG13	2:H:111:VAL:HG11	2.03	0.41
2:H:96:LEU:HD23	2:H:96:LEU:HA	1.90	0.41
2:H:210:LYS:HE3	2:H:212:GLU:CD	2.41	0.41
3:I:83:GLU:CG	3:I:106:VAL:H	2.34	0.41
1:J:439:ASN:O	1:J:443:SER:HB2	2.21	0.41
3:D:5:LEU:HD22	3:D:23:CYS:SG	2.61	0.41
3:D:133:VAL:HG22	3:D:177:TYR:CD2	2.56	0.40
2:K:181:VAL:HG22	2:K:182:VAL:N	2.37	0.40
3:L:133:VAL:HG22	3:L:177:TYR:CD2	2.56	0.40
1:A:518:LEU:HD22	1:A:519:HIS:NE2	2.36	0.40
3:D:167:GLN:OE1	3:D:173:ALA:HB2	2.21	0.40
2:C:52:ASN:ND2	2:C:56:SER:HB2	2.37	0.40
2:H:116:THR:HA	2:H:146:PHE:O	2.22	0.40
2:E:119:PRO:HB2	2:E:142:VAL:HG13	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:SER:OG	1:G:449:TYR:OH[1_556]	1.94	0.26

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	192/195 (98%)	180 (94%)	12 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	192/195 (98%)	179 (93%)	13 (7%)	0	100	100
1	G	192/195 (98%)	180 (94%)	12 (6%)	0	100	100
1	J	192/195 (98%)	181 (94%)	11 (6%)	0	100	100
2	C	221/228 (97%)	207 (94%)	12 (5%)	2 (1%)	17	43
2	E	216/228 (95%)	200 (93%)	16 (7%)	0	100	100
2	H	217/228 (95%)	205 (94%)	12 (6%)	0	100	100
2	K	215/228 (94%)	200 (93%)	14 (6%)	1 (0%)	29	57
3	D	210/216 (97%)	199 (95%)	11 (5%)	0	100	100
3	F	213/216 (99%)	203 (95%)	10 (5%)	0	100	100
3	I	211/216 (98%)	200 (95%)	11 (5%)	0	100	100
3	L	210/216 (97%)	202 (96%)	8 (4%)	0	100	100
All	All	2481/2556 (97%)	2336 (94%)	142 (6%)	3 (0%)	51	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	134	GLY
2	K	128	SER
2	C	213	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	167/168 (99%)	164 (98%)	3 (2%)	59	82
1	B	166/168 (99%)	163 (98%)	3 (2%)	59	82
1	G	166/168 (99%)	162 (98%)	4 (2%)	49	77
1	J	167/168 (99%)	162 (97%)	5 (3%)	41	72
2	C	188/194 (97%)	181 (96%)	7 (4%)	34	65
2	E	184/194 (95%)	172 (94%)	12 (6%)	17	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	185/194 (95%)	178 (96%)	7 (4%)	33	64
2	K	184/194 (95%)	175 (95%)	9 (5%)	25	54
3	D	182/185 (98%)	175 (96%)	7 (4%)	33	64
3	F	185/185 (100%)	177 (96%)	8 (4%)	29	59
3	I	183/185 (99%)	177 (97%)	6 (3%)	38	68
3	L	182/185 (98%)	170 (93%)	12 (7%)	16	40
All	All	2139/2188 (98%)	2056 (96%)	83 (4%)	32	63

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	346	ARG
1	J	378	LYS
1	J	408	ARG
1	J	417	LYS
1	J	466	ARG
2	K	5	VAL
2	K	66	ARG
2	K	73	THR
2	K	82(C)	VAL
2	K	108	THR
2	K	129	LYS
2	K	153	SER
2	K	201	LYS
2	K	214	LYS
3	L	2	ASN
3	L	4	MET
3	L	23	CYS
3	L	26	SER
3	L	68	SER
3	L	105	THR
3	L	110	LYS
3	L	115	VAL
3	L	121	SER
3	L	136	ILE
3	L	161	THR
3	L	205	THR
1	A	346	ARG
1	A	382	VAL
1	A	445	VAL

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Mol	Chain	Res	Type
2	E	66	ARG
2	E	105	GLN
2	E	135	THR
2	E	138	LEU
2	E	169	VAL
2	E	183	THR
2	E	188	SER
2	E	193	THR
2	E	200	HIS
2	E	201	LYS
2	E	206	LYS
2	E	212	GLU
3	F	105	THR
3	F	110	LYS
3	F	115	VAL
3	F	136	ILE
3	F	175	SER
3	F	181	THR
3	F	186	LYS
3	F	189	ARG
1	B	347	PHE
1	B	394	ASN
1	B	478	THR
2	C	3	GLN
2	C	82(C)	VAL
2	C	112	SER
2	C	115	SER
2	C	138	LEU
2	C	156	SER
2	C	183	THR
3	D	23	CYS
3	D	63	SER
3	D	65	SER
3	D	149	LYS
3	D	155	VAL
3	D	171	LYS
3	D	200	SER
1	G	389	ASP
1	G	430	THR
1	G	445	VAL
1	G	466	ARG
2	H	5	VAL

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Mol	Chain	Res	Type
2	H	6	GLU
2	H	66	ARG
2	H	116	THR
2	H	138	LEU
2	H	191	THR
2	H	205	THR
3	I	6	THR
3	I	105	THR
3	I	116	THR
3	I	149	LYS
3	I	187	SER
3	I	203	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	G	440	ASN
2	H	171	GLN

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 [i](#)

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
4	NAG	B	601	1	14,14,15	0.30	0	17,19,21	0.76	0
4	NAG	J	601	1	14,14,15	0.95	1 (7%)	17,19,21	1.55	3 (17%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	J	601	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	601	NAG	C1-C2	2.76	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	601	NAG	C2-N2-C7	4.29	129.01	122.90
4	J	601	NAG	C1-O5-C5	3.54	116.99	112.19
4	J	601	NAG	C1-C2-N2	2.24	114.31	110.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

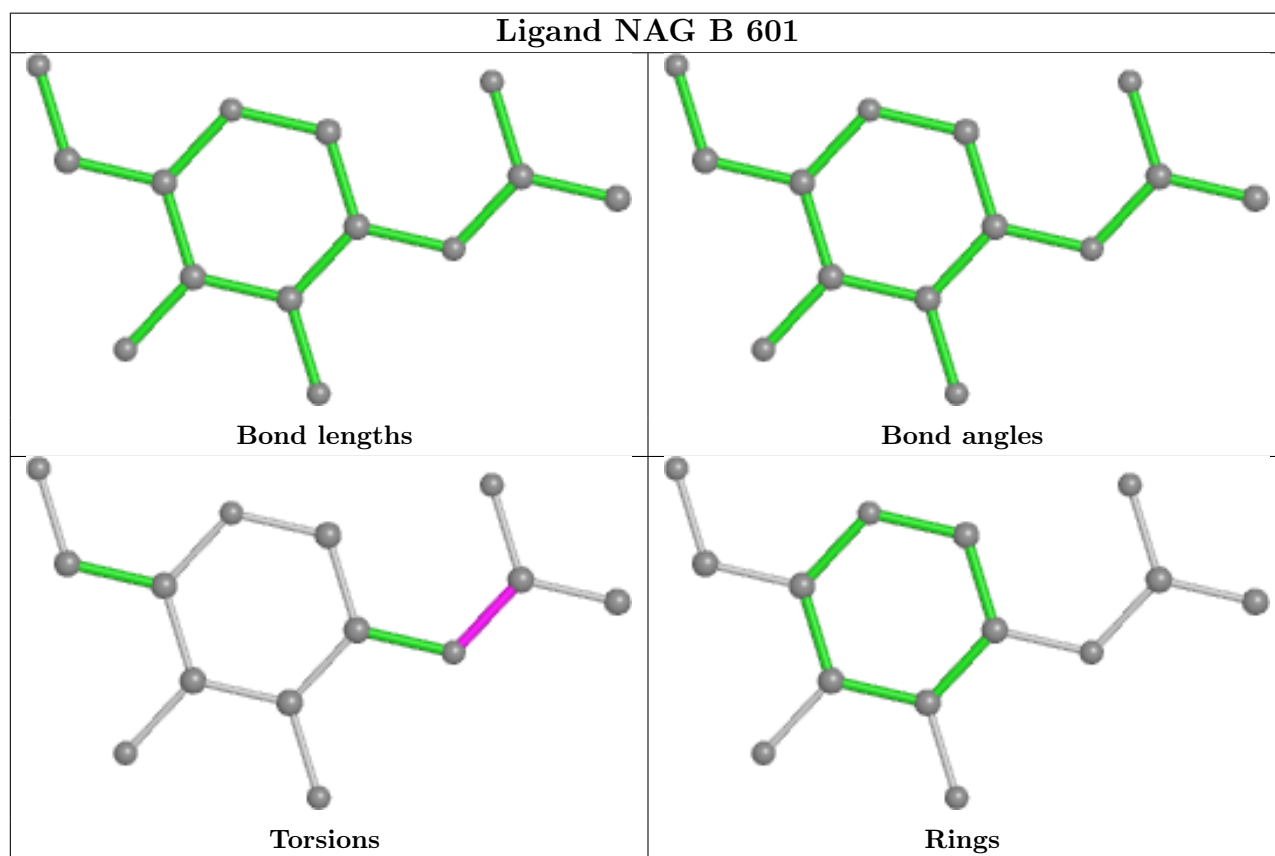
Mol	Chain	Res	Type	Atoms
4	J	601	NAG	C8-C7-N2-C2
4	J	601	NAG	O7-C7-N2-C2
4	B	601	NAG	C8-C7-N2-C2
4	B	601	NAG	O7-C7-N2-C2
4	J	601	NAG	C3-C2-N2-C7

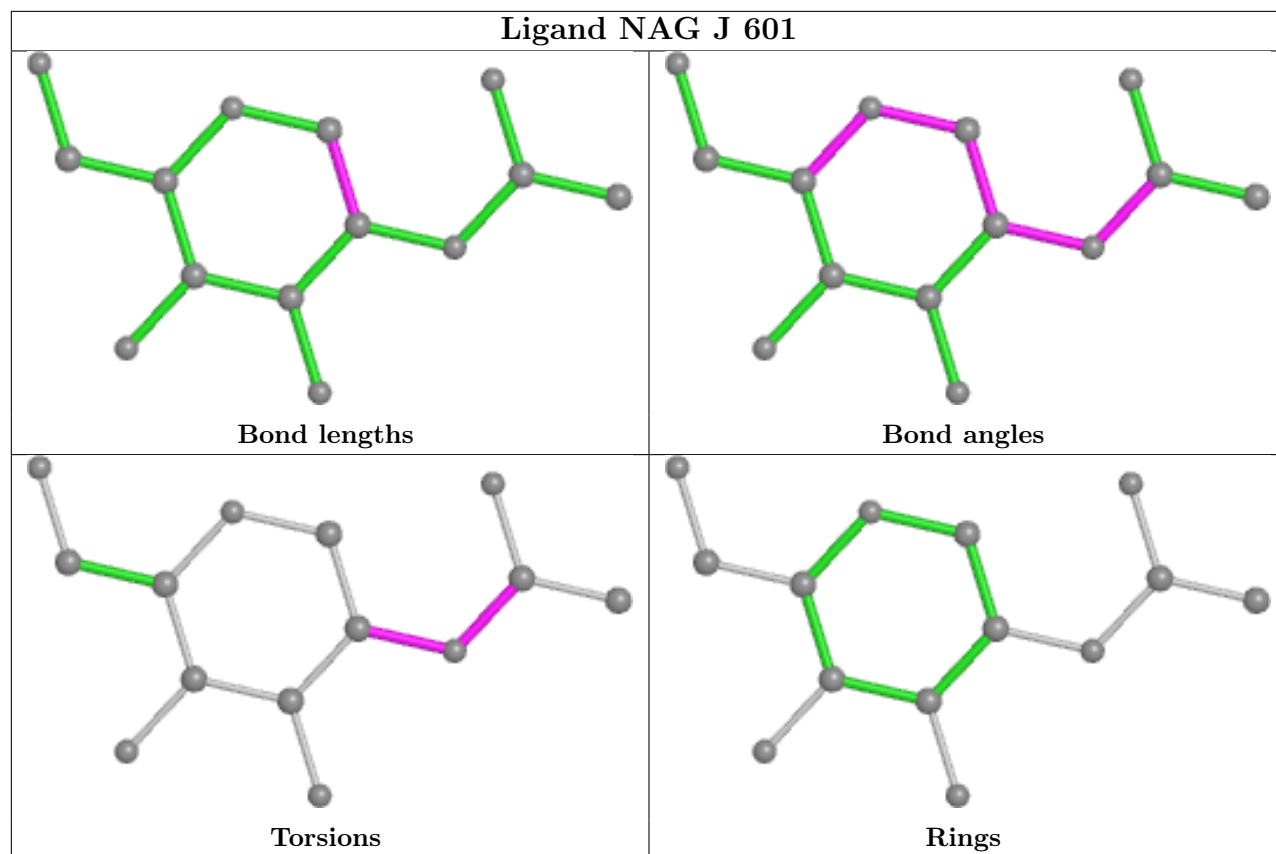
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	601	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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	194/195 (99%)	-0.21	1 (0%) 91 90	42, 65, 95, 148	0
1	B	194/195 (99%)	0.03	7 (3%) 42 37	53, 83, 118, 145	0
1	G	194/195 (99%)	-0.36	0 100 100	43, 59, 90, 125	0
1	J	194/195 (99%)	-0.46	1 (0%) 91 90	30, 44, 80, 112	0
2	C	223/228 (97%)	-0.21	1 (0%) 92 92	45, 66, 108, 153	0
2	E	220/228 (96%)	0.15	11 (5%) 28 24	51, 78, 117, 160	0
2	H	221/228 (96%)	-0.02	2 (0%) 84 84	47, 73, 117, 144	0
2	K	219/228 (96%)	-0.38	1 (0%) 91 90	28, 49, 88, 132	0
3	D	212/216 (98%)	-0.39	2 (0%) 84 84	35, 54, 94, 126	0
3	F	215/216 (99%)	-0.44	0 100 100	32, 51, 94, 151	0
3	I	213/216 (98%)	-0.22	3 (1%) 75 74	39, 63, 103, 129	0
3	L	212/216 (98%)	-0.51	0 100 100	27, 43, 75, 98	0
All	All	2511/2556 (98%)	-0.25	29 (1%) 79 78	27, 62, 106, 160	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	132	SER	7.0
1	B	363	ALA	4.7
1	B	518	LEU	4.6
2	E	191	THR	3.6
2	E	204	ASN	3.3
2	K	133	GLY	3.3
2	E	28	SER	3.2
1	B	521	PRO	3.1
2	E	131	THR	2.9
2	C	191	THR	2.9
3	D	149	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	219	SER	2.8
3	I	147	ALA	2.7
2	E	73	THR	2.6
2	E	64	LYS	2.6
1	B	519	HIS	2.5
1	B	443	SER	2.5
2	H	26	GLY	2.5
1	J	518	LEU	2.5
3	D	150	ALA	2.5
2	E	30	SER	2.5
2	E	29	PHE	2.4
3	I	189	ARG	2.2
2	E	116	THR	2.2
2	H	64	LYS	2.2
1	B	517	LEU	2.1
3	I	151	ASP	2.1
1	A	492	LEU	2.1
1	B	445	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

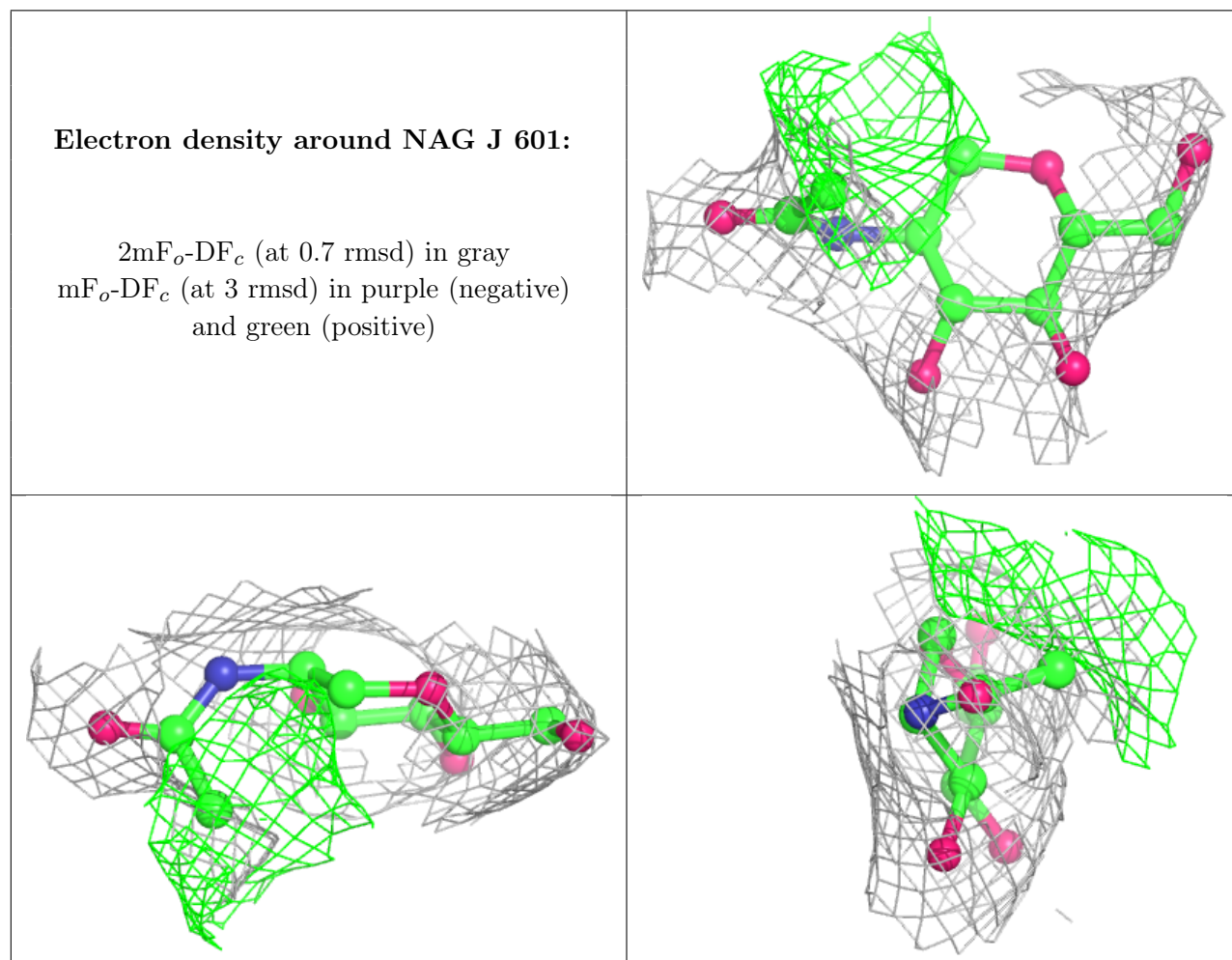
6.4 Ligands [i](#)

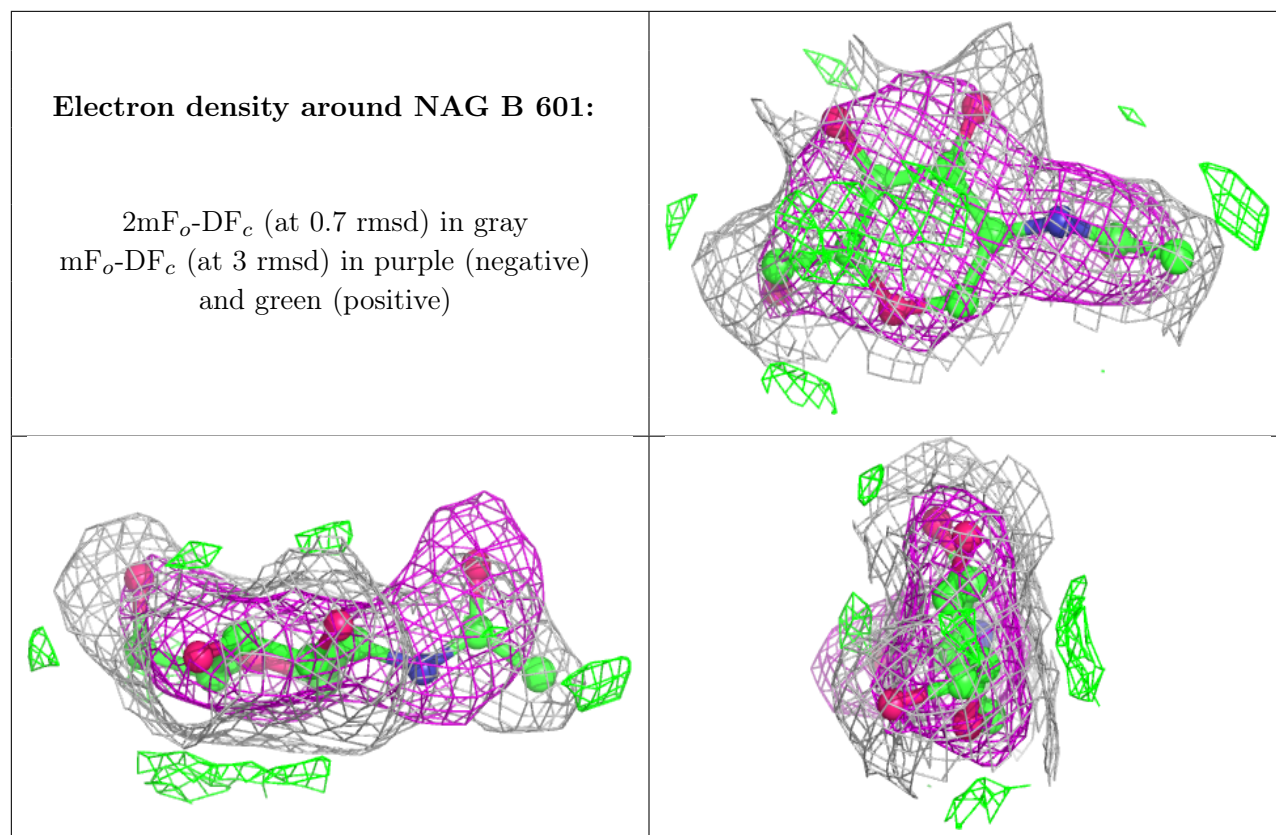
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	J	601	14/15	0.78	0.18	116,130,135,138	0
4	NAG	B	601	14/15	0.82	0.40	30,30,30,30	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.