



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2020 – 11:33 PM EST

PDB ID : 6VVU
Title : Anti-Tryptase fab E104.v1 bound to tryptase
Authors : Ultsch, M.; Koerber, J.T.
Deposited on : 2020-02-18
Resolution : 3.00 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 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 : 2.16
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) : 2.16

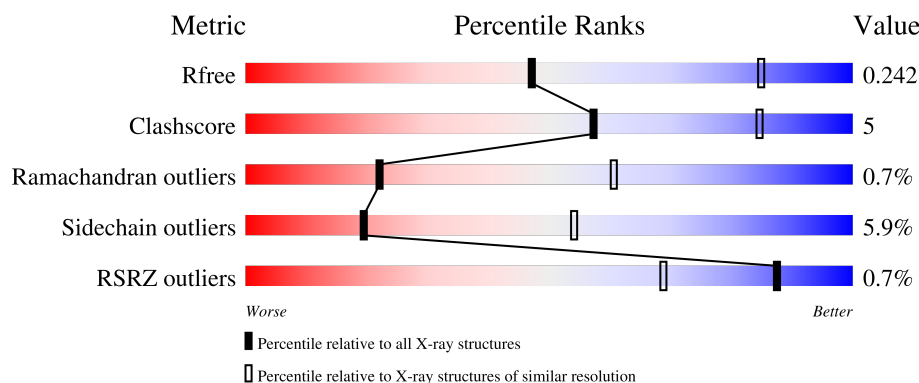
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	275	 75% 13% 12%
1	B	275	 77% 11% 11%
1	C	275	 76% 12% 12%
1	D	275	 77% 10% 12%
2	E	230	 76% 16% • 6%

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Mol	Chain	Length	Quality of chain
2	G	230	<div><div></div><div>79%14%6%</div></div>
2	H	230	<div><div>%</div><div></div><div>80%13%6%</div></div>
2	J	230	<div><div>3%</div><div></div><div>80%13%5%</div></div>
3	F	217	<div><div></div><div>79%21%</div></div>
3	I	217	<div><div></div><div>85%14%</div></div>
3	K	217	<div><div>%</div><div></div><div>73%23%</div></div>
3	L	217	<div><div></div><div>84%14%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20793 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 Tryptase alpha/beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1919	1228	338	341	12			
1	B	244	Total	C	N	O	S	0	0	0
			1928	1234	340	342	12			
1	D	242	Total	C	N	O	S	0	0	0
			1910	1222	336	340	12			
1	C	242	Total	C	N	O	S	0	0	0
			1910	1222	336	340	12			

- Molecule 2 is a protein called Fab E104.v1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	216	Total	C	N	O	S	0	0	0
			1599	1018	265	312	4			
2	G	217	Total	C	N	O	S	0	0	0
			1608	1023	266	315	4			
2	H	216	Total	C	N	O	S	0	0	0
			1599	1018	265	312	4			
2	J	219	Total	C	N	O	S	0	0	0
			1620	1030	269	316	5			

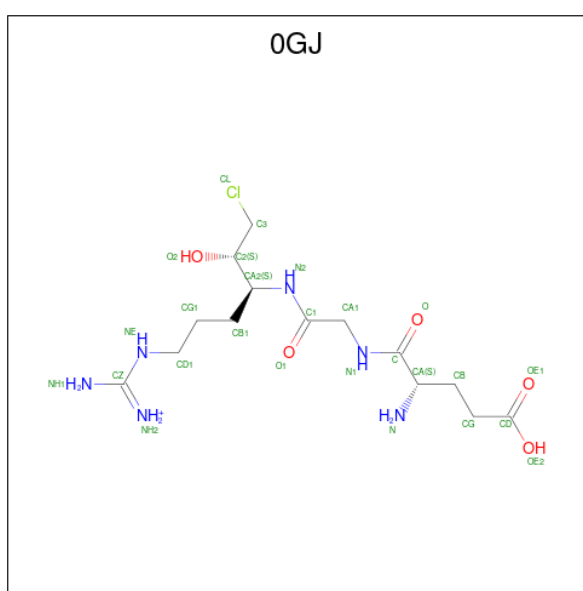
- Molecule 3 is a protein called Fab E104.v1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	216	Total	C	N	O	S	0	0	0
			1651	1030	277	339	5			
3	I	216	Total	C	N	O	S	0	0	0
			1651	1030	277	339	5			
3	K	216	Total	C	N	O	S	0	0	0
			1650	1029	277	338	6			
3	L	215	Total	C	N	O	S	0	0	0
			1643	1026	276	336	5			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		

- Molecule 5 is L-alpha-glutamyl-N-{(1S)-4-[[amino(iminio)methyl]amino]-1-[(1S)-2-chloro-1-hydroxyethyl]butyl}glycinamide (three-letter code: 0GJ) (formula: C₁₄H₂₈ClN₆O₅).



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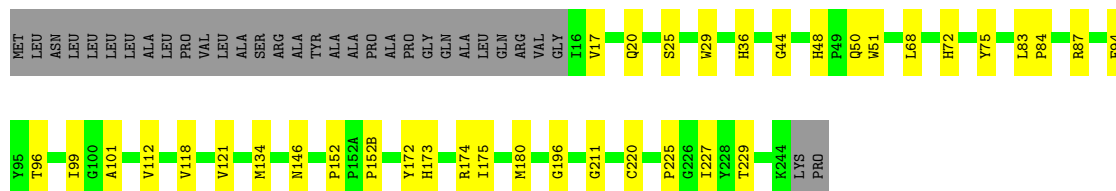
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	K	1	Total	O	0	0
			1	1		

3 Residue-property plots


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

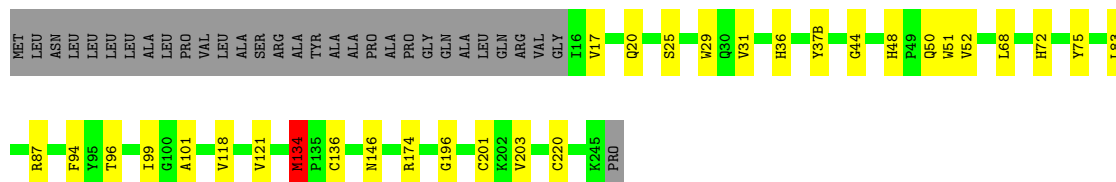
• Molecule 1: Tryptase alpha/beta-1

Chain A: 




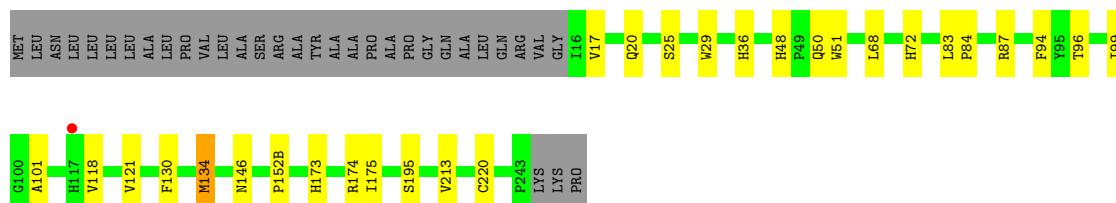
• Molecule 1: Tryptase alpha/beta-1

Chain B: 




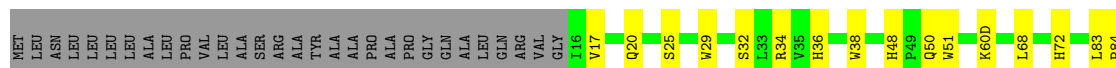
• Molecule 1: Tryptase alpha/beta-1

Chain D: 



• Molecule 1: Tryptase alpha/beta-1

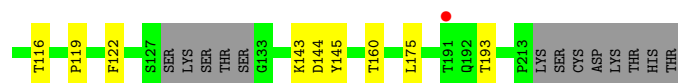
Chain C: 





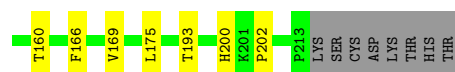
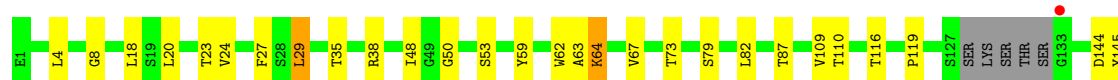
- Molecule 2: Fab E104.v1 heavy chain

Chain E: 76% 16% 6%



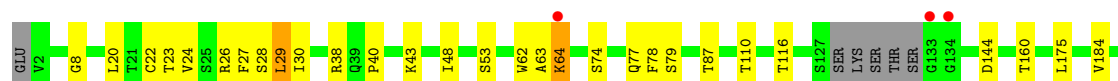
- Molecule 2: Fab E104.v1 heavy chain

Chain G: 79% 14% 6%



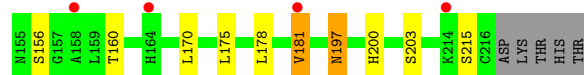
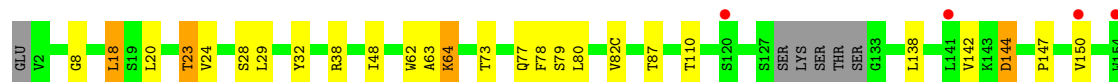
- Molecule 2: Fab E104.v1 heavy chain

Chain H: 80% 13% 6%



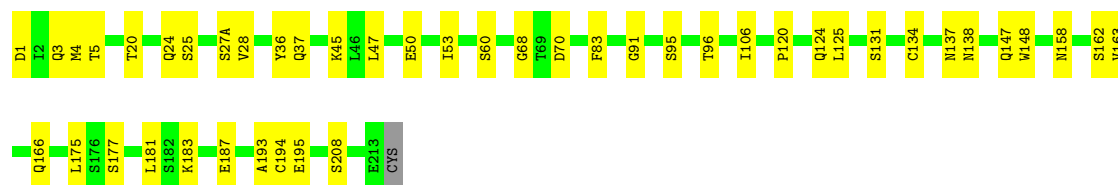
- Molecule 2: Fab E104.v1 heavy chain

Chain I: 80% 13% 5%

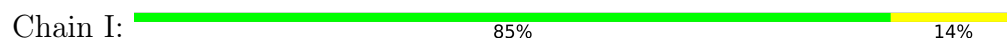


- Molecule 3: Fab E104.v1 light chain

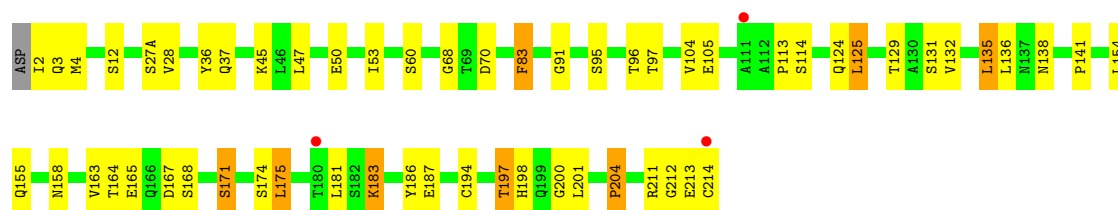
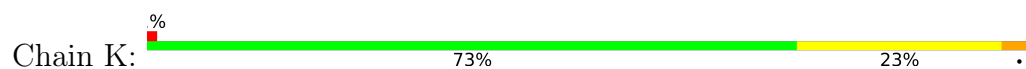
Chain F: 79% 21%



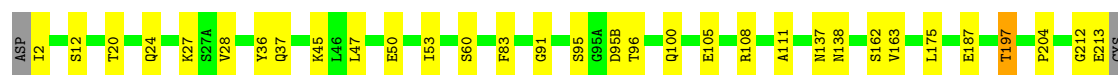
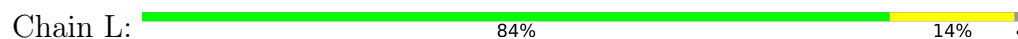
- Molecule 3: Fab E104.v1 light chain



- Molecule 3: Fab E104.v1 light chain



- Molecule 3: Fab E104.v1 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.57Å 168.81Å 114.65Å 90.00° 109.97° 90.00°	Depositor
Resolution (Å)	90.83 – 3.00 84.41 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (90.83-3.00) 97.8 (84.41-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.187 , 0.232 0.200 , 0.242	Depositor DCC
R_{free} test set	1266 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20793	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.50	0/1984	0.70	0/2720
1	B	0.53	0/1993	0.72	1/2731 (0.0%)
1	C	0.49	0/1975	0.69	0/2709
1	D	0.46	0/1975	0.68	0/2709
2	E	0.49	0/1637	0.76	0/2238
2	G	0.47	0/1646	0.72	0/2250
2	H	0.51	0/1637	0.74	0/2238
2	J	0.55	0/1658	0.79	0/2265
3	F	0.45	0/1684	0.71	0/2283
3	I	0.42	0/1684	0.68	0/2283
3	K	0.56	0/1683	0.78	0/2280
3	L	0.51	0/1676	0.74	0/2272
All	All	0.50	0/21232	0.72	1/28978 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	MET	C-N-CD	5.23	139.39	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1919	0	1847	19	0
1	B	1928	0	1862	22	0
1	C	1910	0	1834	15	0
1	D	1910	0	1834	14	0
2	E	1599	0	1600	24	0
2	G	1608	0	1607	21	0
2	H	1599	0	1598	16	0
2	J	1620	0	1620	21	0
3	F	1651	0	1607	17	0
3	I	1651	0	1607	8	0
3	K	1650	0	1604	24	0
3	L	1643	0	1600	11	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	25	0	24	0	0
5	B	25	0	24	0	0
5	C	25	0	24	0	0
5	D	25	0	24	0	0
6	D	1	0	0	0	0
6	K	1	0	0	0	0
All	All	20793	0	20316	201	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 5.

All (201) 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:E:22:CYS:SG	2:E:92:CYS:SG	1.30	1.28
1:B:136:CYS:SG	1:B:201:CYS:CB	2.35	1.14
1:B:136:CYS:SG	1:B:201:CYS:SG	1.13	1.13
2:G:24:VAL:HG21	2:G:29:LEU:HD13	1.33	1.09
2:J:24:VAL:HG21	2:J:29:LEU:HD22	1.34	1.09
1:B:134:MET:CE	1:B:203:VAL:HG22	1.88	1.04
2:E:22:CYS:SG	2:E:92:CYS:CB	2.49	0.99
2:G:24:VAL:HG21	2:G:29:LEU:CD1	1.96	0.95
2:E:24:VAL:HG21	2:E:29:LEU:HD11	1.55	0.87
3:L:2:ILE:HD13	3:L:27:LYS:HG3	1.59	0.83
1:B:134:MET:HE2	1:B:203:VAL:HG22	1.61	0.80
2:J:29:LEU:HD21	2:J:78:PHE:HE2	1.53	0.73
3:K:211:ARG:HG2	3:K:212:GLY:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:LEU:CD2	2:J:78:PHE:HE2	2.03	0.71
3:K:2:ILE:HA	3:K:97:THR:HG21	1.71	0.71
3:K:211:ARG:HG2	3:K:212:GLY:H	1.56	0.70
3:K:91:GLY:HA2	3:K:96:THR:HG22	1.72	0.70
2:G:4:LEU:HD23	2:G:24:VAL:HG22	1.72	0.69
2:H:24:VAL:HG11	2:H:29:LEU:HD13	1.74	0.69
3:L:91:GLY:HA2	3:L:96:THR:HG22	1.74	0.69
1:B:134:MET:HE3	1:B:203:VAL:HG22	1.74	0.69
3:F:91:GLY:HA2	3:F:96:THR:HG22	1.74	0.69
3:I:91:GLY:HA2	3:I:96:THR:HG22	1.75	0.67
2:E:144:ASP:HB3	2:E:175:LEU:HD13	1.77	0.67
1:A:75:TYR:HE1	1:B:72:HIS:CD2	2.13	0.65
2:H:24:VAL:HG21	2:H:29:LEU:HD11	1.78	0.65
3:L:2:ILE:HD12	3:L:95(B):ASP:OD2	1.95	0.65
2:J:24:VAL:HG21	2:J:29:LEU:CD2	2.21	0.64
3:I:50:GLU:HB2	3:I:53:ILE:HD12	1.82	0.62
2:H:24:VAL:HG21	2:H:29:LEU:CD1	2.30	0.62
3:K:163:VAL:HG22	3:K:175:LEU:HB2	1.80	0.62
3:F:50:GLU:HB2	3:F:53:ILE:HD12	1.83	0.60
3:F:134:CYS:HB2	3:F:148:TRP:CZ2	2.36	0.60
1:C:68:LEU:HD13	1:C:118:VAL:HG11	1.84	0.59
3:L:50:GLU:HB2	3:L:53:ILE:HD12	1.83	0.59
3:I:163:VAL:HG22	3:I:175:LEU:HD12	1.84	0.59
2:J:181:VAL:HG21	3:K:135:LEU:HG	1.84	0.59
2:J:29:LEU:HD21	2:J:78:PHE:CE2	2.37	0.59
2:J:156:SER:H	2:J:197:ASN:HD21	1.51	0.58
2:J:18:LEU:HD23	2:J:82(C):VAL:HG11	1.85	0.58
2:E:18:LEU:HD22	2:E:109:VAL:HG11	1.84	0.58
3:K:50:GLU:HB2	3:K:53:ILE:HD12	1.86	0.57
1:D:130:PHE:HA	1:D:134:MET:HE2	1.86	0.57
2:E:8:GLY:HA3	2:E:20:LEU:HD23	1.87	0.57
2:H:62:TRP:O	2:H:63:ALA:HB3	2.05	0.57
2:J:144:ASP:HB3	2:J:175:LEU:HD23	1.87	0.57
1:C:68:LEU:HG	1:C:83:LEU:HD11	1.87	0.56
2:E:62:TRP:O	2:E:63:ALA:HB3	2.06	0.56
3:K:83:PHE:HD1	3:K:104:VAL:O	1.89	0.56
3:K:125:LEU:HD21	3:K:186:TYR:CD2	2.41	0.56
2:H:28:SER:OG	2:H:30:ILE:HG12	2.07	0.55
3:F:163:VAL:HG22	3:F:175:LEU:HD12	1.88	0.55
2:H:62:TRP:CE3	2:H:63:ALA:HB2	2.41	0.55
3:K:197:THR:HG23	3:K:204:PRO:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:62:TRP:CE3	2:J:63:ALA:HB2	2.41	0.55
1:B:68:LEU:HD13	1:B:118:VAL:HG11	1.88	0.55
3:L:197:THR:HG23	3:L:204:PRO:HG3	1.88	0.55
1:D:68:LEU:HG	1:D:83:LEU:HD11	1.89	0.54
3:F:147:GLN:HB3	3:F:195:GLU:HB3	1.90	0.54
2:G:24:VAL:HG11	2:G:27:PHE:HD2	1.72	0.53
2:H:8:GLY:HA3	2:H:20:LEU:HD23	1.91	0.53
3:L:163:VAL:HG22	3:L:175:LEU:HD12	1.90	0.53
3:K:198:HIS:CD2	3:K:200:GLY:H	2.27	0.52
3:K:167:ASP:O	3:K:171:SER:HA	2.10	0.52
1:D:96:THR:OG1	1:D:99:ILE:HD12	2.09	0.52
3:K:164:THR:HG22	3:K:174:SER:H	1.74	0.52
2:E:29:LEU:HD22	2:E:94:ARG:HD3	1.92	0.52
2:E:24:VAL:HG11	2:E:29:LEU:HD21	1.91	0.52
1:A:68:LEU:HD13	1:A:118:VAL:HG11	1.92	0.51
2:E:38:ARG:HB3	2:E:48:ILE:HD11	1.93	0.51
1:D:68:LEU:HD13	1:D:118:VAL:HG11	1.92	0.51
2:J:8:GLY:HA3	2:J:20:LEU:HD23	1.90	0.51
2:G:8:GLY:HA3	2:G:20:LEU:HD23	1.92	0.51
1:B:68:LEU:HG	1:B:83:LEU:HD11	1.93	0.51
3:F:147:GLN:O	3:F:194:CYS:HA	2.11	0.50
2:J:62:TRP:CZ3	2:J:63:ALA:HB2	2.47	0.50
3:K:125:LEU:HD23	3:K:183:LYS:HB2	1.93	0.50
1:D:195:SER:HA	1:D:213:VAL:HB	1.93	0.50
2:H:62:TRP:CZ3	2:H:63:ALA:HB2	2.47	0.50
1:A:75:TYR:CE1	1:B:72:HIS:CD2	2.98	0.50
2:J:23:THR:HG23	2:J:77:GLN:HG2	1.94	0.50
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.93	0.49
2:J:62:TRP:O	2:J:63:ALA:HB3	2.12	0.49
2:G:18:LEU:HG	2:G:82:LEU:HB3	1.92	0.49
2:E:119:PRO:HB3	2:E:145:TYR:HB3	1.95	0.49
1:A:146:ASN:HD21	1:A:220:CYS:H	1.59	0.48
2:G:24:VAL:HG21	2:G:29:LEU:HD11	1.90	0.48
1:A:68:LEU:HG	1:A:83:LEU:HD11	1.93	0.48
1:B:146:ASN:HD21	1:B:220:CYS:H	1.60	0.48
2:G:62:TRP:CE3	2:G:63:ALA:HB2	2.49	0.48
1:C:146:ASN:HD21	1:C:220:CYS:H	1.61	0.48
1:D:146:ASN:HD21	1:D:220:CYS:H	1.61	0.48
3:K:155:GLN:HB3	3:K:158:ASN:HD21	1.79	0.48
1:C:51:TRP:HH2	1:C:87:ARG:HH21	1.62	0.47
2:G:38:ARG:HB3	2:G:48:ILE:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:141:PRO:HG2	3:I:143:GLU:HG3	1.96	0.47
1:A:75:TYR:HB2	1:B:75:TYR:CE1	2.49	0.47
2:E:87:THR:HG23	2:E:110:THR:HA	1.96	0.47
2:G:144:ASP:HB3	2:G:175:LEU:HD13	1.97	0.47
1:B:31:VAL:HG21	1:B:52:VAL:HG11	1.97	0.47
3:K:124:GLN:HE22	3:K:131:SER:HB2	1.80	0.47
2:G:62:TRP:O	2:G:63:ALA:HB3	2.15	0.47
3:K:91:GLY:CA	3:K:96:THR:HG22	2.41	0.47
1:D:51:TRP:HH2	1:D:87:ARG:HH21	1.61	0.46
2:H:144:ASP:HB3	2:H:175:LEU:HD13	1.97	0.46
2:H:87:THR:HG23	2:H:110:THR:HA	1.98	0.46
2:H:23:THR:HG23	2:H:77:GLN:HG2	1.98	0.46
2:J:38:ARG:HB3	2:J:48:ILE:HD11	1.97	0.46
1:A:96:THR:OG1	1:A:99:ILE:HD12	2.15	0.46
3:F:134:CYS:HB2	3:F:148:TRP:CH2	2.51	0.46
1:C:48:HIS:HB3	1:C:51:TRP:HB2	1.98	0.46
3:F:4:MET:HE3	3:F:4:MET:HB2	1.86	0.46
1:B:48:HIS:HB3	1:B:51:TRP:HB2	1.98	0.45
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.52	0.45
3:L:12:SER:HA	3:L:105:GLU:O	2.16	0.45
1:D:29:TRP:CG	1:D:121:VAL:HB	2.51	0.45
2:E:40:PRO:HB2	2:E:43:LYS:HB2	1.99	0.45
3:L:108:ARG:HH21	3:L:111:ALA:HB2	1.82	0.45
1:C:29:TRP:CG	1:C:121:VAL:HB	2.52	0.45
2:G:87:THR:HG23	2:G:110:THR:HA	1.99	0.45
3:K:124:GLN:HE22	3:K:131:SER:CB	2.30	0.45
1:A:29:TRP:CG	1:A:121:VAL:HB	2.52	0.45
1:C:96:THR:OG1	1:C:99:ILE:HD12	2.17	0.44
3:F:125:LEU:O	3:F:183:LYS:HD2	2.17	0.44
1:C:94:PHE:HB2	1:C:101:ALA:O	2.18	0.44
1:A:94:PHE:HB2	1:A:101:ALA:O	2.18	0.44
1:C:34:ARG:HD2	1:C:38:TRP:O	2.18	0.44
1:D:17:VAL:HG21	1:D:220:CYS:HB3	1.99	0.44
2:J:142:VAL:HG11	2:J:150:VAL:HG11	1.99	0.44
1:D:48:HIS:HB3	1:D:51:TRP:HB2	2.00	0.44
2:E:59:TYR:HD2	2:E:64:LYS:HE3	1.81	0.44
3:K:113:PRO:HD3	3:K:198:HIS:CD2	2.52	0.44
3:F:4:MET:HG2	3:F:25:SER:HB3	2.00	0.44
2:J:150:VAL:HG12	2:J:178:LEU:HD21	2.00	0.44
3:K:135:LEU:HD22	3:K:136:LEU:H	1.83	0.44
3:L:36:TYR:HA	3:L:45:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:200:HIS:HD2	2:J:203:SER:H	1.64	0.44
3:K:37:GLN:HB2	3:K:47:LEU:HD11	2.00	0.44
1:A:17:VAL:HG21	1:A:220:CYS:HB3	2.00	0.44
1:B:29:TRP:CG	1:B:121:VAL:HB	2.53	0.44
1:C:17:VAL:HG21	1:C:220:CYS:HB3	2.00	0.44
2:E:23:THR:HG23	2:E:77:GLN:HG2	1.99	0.44
2:E:96:PRO:HD2	2:E:100(E):ARG:O	2.18	0.43
3:F:193:ALA:HB2	3:F:208:SER:HB3	2.00	0.43
3:K:12:SER:HA	3:K:105:GLU:O	2.17	0.43
2:J:87:THR:HG23	2:J:110:THR:HA	2.00	0.43
1:B:94:PHE:HB2	1:B:101:ALA:O	2.18	0.43
1:C:72:HIS:HB3	1:C:152(B):PRO:O	2.19	0.43
2:G:18:LEU:HD22	2:G:109:VAL:HG11	2.00	0.43
3:L:91:GLY:CA	3:L:96:THR:HG22	2.45	0.43
1:A:48:HIS:HB3	1:A:51:TRP:HB2	2.00	0.43
1:C:200:VAL:HG12	1:C:209:GLN:HA	2.00	0.43
1:A:173:HIS:CE1	1:A:175:ILE:HD12	2.53	0.43
1:B:44:GLY:HA2	1:B:196:GLY:O	2.19	0.43
2:E:59:TYR:HB2	2:E:64:LYS:HG2	2.01	0.43
2:G:35:THR:HG22	2:G:50:GLY:HA3	2.01	0.43
3:I:36:TYR:HA	3:I:45:LYS:O	2.19	0.43
1:B:136:CYS:SG	1:B:201:CYS:HB3	2.50	0.43
1:B:17:VAL:HG21	1:B:220:CYS:HB3	2.01	0.43
2:G:63:ALA:O	2:G:67:VAL:HG12	2.18	0.43
1:A:180:MET:HB3	1:A:227:ILE:HG23	2.02	0.42
1:C:84:PRO:HD3	2:E:53:SER:HB3	2.01	0.42
3:F:36:TYR:HA	3:F:45:LYS:O	2.19	0.42
2:H:40:PRO:HB2	2:H:43:LYS:HB2	2.00	0.42
1:A:72:HIS:HB3	1:A:152(B):PRO:O	2.20	0.42
2:J:29:LEU:HA	2:J:32:TYR:HD2	1.85	0.42
3:K:36:TYR:HA	3:K:45:LYS:O	2.20	0.42
1:B:134:MET:HE2	1:B:203:VAL:CG2	2.42	0.42
1:D:84:PRO:HD3	2:G:53:SER:HB3	2.01	0.42
3:F:106:ILE:H	3:F:166:GLN:HE22	1.67	0.42
1:D:173:HIS:CE1	1:D:175:ILE:HD12	2.55	0.42
3:F:120:PRO:HB3	3:F:131:SER:H	1.85	0.42
2:G:59:TYR:HB2	2:G:64:LYS:HG2	2.01	0.42
1:D:94:PHE:HB2	1:D:101:ALA:O	2.19	0.42
2:E:18:LEU:HG	2:E:82:LEU:HB3	2.02	0.42
3:I:12:SER:HA	3:I:105:GLU:O	2.19	0.42
2:G:200:HIS:CD2	2:G:202:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:35:THR:HG22	2:E:50:GLY:HA3	2.02	0.41
1:B:96:THR:OG1	1:B:99:ILE:HD12	2.21	0.41
1:A:152:PRO:HB3	1:B:37(B):TYR:CD1	2.56	0.41
2:E:20:LEU:HD12	2:E:80:LEU:HD23	2.02	0.41
3:F:91:GLY:CA	3:F:96:THR:HG22	2.46	0.41
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.03	0.41
1:B:99:ILE:HG13	1:C:99:ILE:HG13	2.01	0.41
3:I:37:GLN:HB2	3:I:47:LEU:HD11	2.02	0.41
2:E:122:PHE:CE2	3:F:124:GLN:HG3	2.56	0.41
2:E:29:LEU:HB3	2:E:32:TYR:CD2	2.55	0.41
2:E:62:TRP:O	2:E:63:ALA:CB	2.69	0.41
1:A:44:GLY:HA2	1:A:196:GLY:O	2.20	0.41
3:F:37:GLN:HB2	3:F:47:LEU:HD11	2.03	0.41
3:K:141:PRO:O	3:K:198:HIS:HE1	2.04	0.41
1:A:172:TYR:CE1	1:A:225:PRO:HD2	2.56	0.40
1:C:173:HIS:CE1	1:C:175:ILE:HD12	2.56	0.40
1:D:72:HIS:HB3	1:D:152(B):PRO:O	2.20	0.40
2:G:119:PRO:HB3	2:G:145:TYR:HB3	2.03	0.40
1:A:211:GLY:HA2	1:A:229:THR:O	2.22	0.40
1:A:84:PRO:HD3	2:H:53:SER:HB3	2.03	0.40
2:J:20:LEU:HD12	2:J:80:LEU:HD23	2.03	0.40
2:G:62:TRP:CZ3	2:G:63:ALA:HB2	2.56	0.40
2:H:22:CYS:HB3	2:H:78:PHE:HB2	2.04	0.40
2:G:166:PHE:CE2	3:I:176:SER:HB3	2.56	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	241/275 (88%)	232 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	242/275 (88%)	232 (96%)	10 (4%)	0	100	100
1	C	240/275 (87%)	231 (96%)	9 (4%)	0	100	100
1	D	240/275 (87%)	232 (97%)	8 (3%)	0	100	100
2	E	212/230 (92%)	197 (93%)	13 (6%)	2 (1%)	17	55
2	G	213/230 (93%)	197 (92%)	15 (7%)	1 (0%)	29	68
2	H	212/230 (92%)	196 (92%)	14 (7%)	2 (1%)	17	55
2	J	215/230 (94%)	198 (92%)	13 (6%)	4 (2%)	8	36
3	F	214/217 (99%)	197 (92%)	14 (6%)	3 (1%)	11	43
3	I	214/217 (99%)	203 (95%)	9 (4%)	2 (1%)	17	55
3	K	214/217 (99%)	198 (92%)	13 (6%)	3 (1%)	11	43
3	L	213/217 (98%)	200 (94%)	11 (5%)	2 (1%)	17	55
All	All	2670/2888 (92%)	2513 (94%)	138 (5%)	19 (1%)	22	60

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	64	LYS
2	J	144	ASP
3	F	138	ASN
3	F	158	ASN
2	H	64	LYS
2	J	64	LYS
3	K	138	ASN
2	E	63	ALA
3	I	138	ASN
2	J	28	SER
2	G	64	LYS
2	H	26	ARG
3	L	138	ASN
3	K	204	PRO
3	L	212	GLY
3	I	68	GLY
3	K	68	GLY
3	F	68	GLY
2	J	147	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	208/231 (90%)	200 (96%)	8 (4%)	33	69
1	B	209/231 (90%)	202 (97%)	7 (3%)	38	73
1	C	207/231 (90%)	199 (96%)	8 (4%)	32	69
1	D	207/231 (90%)	201 (97%)	6 (3%)	42	76
2	E	181/195 (93%)	170 (94%)	11 (6%)	18	53
2	G	182/195 (93%)	174 (96%)	8 (4%)	28	65
2	H	181/195 (93%)	172 (95%)	9 (5%)	24	60
2	J	184/195 (94%)	173 (94%)	11 (6%)	19	53
3	F	189/190 (100%)	173 (92%)	16 (8%)	10	38
3	I	189/190 (100%)	175 (93%)	14 (7%)	13	44
3	K	189/190 (100%)	163 (86%)	26 (14%)	3	17
3	L	188/190 (99%)	176 (94%)	12 (6%)	17	51
All	All	2314/2464 (94%)	2178 (94%)	136 (6%)	19	54

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	25	SER
1	A	36	HIS
1	A	50	GLN
1	A	87	ARG
1	A	112	VAL
1	A	134	MET
1	A	174	ARG
1	B	20	GLN
1	B	25	SER
1	B	36	HIS
1	B	50	GLN
1	B	87	ARG
1	B	134	MET

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Mol	Chain	Res	Type
1	B	174	ARG
1	D	20	GLN
1	D	25	SER
1	D	36	HIS
1	D	50	GLN
1	D	134	MET
1	D	174	ARG
1	C	20	GLN
1	C	25	SER
1	C	32	SER
1	C	36	HIS
1	C	50	GLN
1	C	60(D)	LYS
1	C	134	MET
1	C	174	ARG
2	E	23	THR
2	E	24	VAL
2	E	26	ARG
2	E	29	LEU
2	E	64	LYS
2	E	73	THR
2	E	79	SER
2	E	116	THR
2	E	143	LYS
2	E	160	THR
2	E	193	THR
3	F	1	ASP
3	F	3	GLN
3	F	5	THR
3	F	20	THR
3	F	24	GLN
3	F	27(A)	SER
3	F	28	VAL
3	F	60	SER
3	F	70	ASP
3	F	83	PHE
3	F	95	SER
3	F	137	ASN
3	F	162	SER
3	F	177	SER
3	F	181	LEU
3	F	187	GLU

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Mol	Chain	Res	Type
2	G	23	THR
2	G	29	LEU
2	G	73	THR
2	G	79	SER
2	G	116	THR
2	G	160	THR
2	G	169	VAL
2	G	193	THR
2	H	27	PHE
2	H	29	LEU
2	H	64	LYS
2	H	74	SER
2	H	79	SER
2	H	116	THR
2	H	160	THR
2	H	193	THR
2	H	197	ASN
3	I	1	ASP
3	I	5	THR
3	I	20	THR
3	I	27(A)	SER
3	I	28	VAL
3	I	60	SER
3	I	83	PHE
3	I	95	SER
3	I	137	ASN
3	I	158	ASN
3	I	162	SER
3	I	187	GLU
3	I	197	THR
3	I	213	GLU
2	J	18	LEU
2	J	23	THR
2	J	64	LYS
2	J	73	THR
2	J	79	SER
2	J	138	LEU
2	J	160	THR
2	J	170	LEU
2	J	181	VAL
2	J	197	ASN
2	J	215	SER

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Mol	Chain	Res	Type
3	K	3	GLN
3	K	4	MET
3	K	27(A)	SER
3	K	28	VAL
3	K	60	SER
3	K	70	ASP
3	K	83	PHE
3	K	95	SER
3	K	114	SER
3	K	125	LEU
3	K	129	THR
3	K	132	VAL
3	K	135	LEU
3	K	154	LEU
3	K	165	GLU
3	K	168	SER
3	K	171	SER
3	K	175	LEU
3	K	181	LEU
3	K	183	LYS
3	K	187	GLU
3	K	194	CYS
3	K	197	THR
3	K	201	LEU
3	K	213	GLU
3	K	214	CYS
3	L	20	THR
3	L	24	GLN
3	L	28	VAL
3	L	60	SER
3	L	83	PHE
3	L	95	SER
3	L	100	GLN
3	L	137	ASN
3	L	162	SER
3	L	187	GLU
3	L	197	THR
3	L	213	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	192	GLN
1	B	36	HIS
1	B	72	HIS
1	B	146	ASN
1	D	146	ASN
1	C	36	HIS
1	C	146	ASN
2	E	164	HIS
2	E	199	ASN
3	F	24	GLN
3	F	37	GLN
3	F	137	ASN
3	F	166	GLN
2	G	164	HIS
2	G	199	ASN
2	H	164	HIS
2	H	199	ASN
3	I	37	GLN
3	I	124	GLN
3	I	137	ASN
3	I	138	ASN
3	I	166	GLN
2	J	77	GLN
2	J	197	ASN
2	J	199	ASN
2	J	200	HIS
3	K	124	GLN
3	K	198	HIS
3	L	24	GLN
3	L	37	GLN
3	L	137	ASN
3	L	138	ASN
3	L	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	0GJ	D	302	1,4	20,24,25	2.41	5 (25%)	23,30,31	1.09	2 (8%)
5	0GJ	A	302	1,4	20,24,25	2.14	5 (25%)	23,30,31	1.35	2 (8%)
5	0GJ	C	301	1	20,24,25	2.23	4 (20%)	23,30,31	1.22	3 (13%)
5	0GJ	B	302	1,4	20,24,25	2.31	4 (20%)	23,30,31	1.37	3 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	0GJ	D	302	1,4	-	4/27/29/31	-
5	0GJ	A	302	1,4	-	10/27/29/31	-
5	0GJ	C	301	1	-	8/27/29/31	-
5	0GJ	B	302	1,4	-	5/27/29/31	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	302	0GJ	C-N1	6.08	1.46	1.33
5	B	302	0GJ	C-N1	5.85	1.46	1.33
5	D	302	0GJ	CZ-NE	5.81	1.44	1.33
5	C	301	0GJ	CZ-NE	5.74	1.44	1.33
5	B	302	0GJ	CZ-NE	5.73	1.44	1.33
5	C	301	0GJ	C-N1	5.48	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	302	0GJ	C-N1	5.40	1.45	1.33
5	A	302	0GJ	CZ-NE	5.10	1.43	1.33
5	D	302	0GJ	C1-N2	4.48	1.43	1.34
5	C	301	0GJ	C1-N2	4.07	1.42	1.34
5	B	302	0GJ	C1-N2	4.05	1.42	1.34
5	A	302	0GJ	C1-N2	4.01	1.42	1.34
5	B	302	0GJ	O2-C2	3.36	1.52	1.43
5	D	302	0GJ	O2-C2	3.19	1.51	1.43
5	C	301	0GJ	O2-C2	3.08	1.51	1.43
5	A	302	0GJ	O2-C2	2.54	1.50	1.43
5	A	302	0GJ	C3-C2	2.17	1.58	1.51
5	D	302	0GJ	C3-C2	2.08	1.58	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	302	0GJ	CG-CB-CA	3.39	121.74	113.84
5	B	302	0GJ	CB1-CA2-N2	3.32	114.70	110.33
5	C	301	0GJ	CA2-N2-C1	-3.31	117.89	123.48
5	A	302	0GJ	O1-C1-N2	-2.98	117.92	122.95
5	C	301	0GJ	CG1-CB1-CA2	2.79	119.63	113.93
5	A	302	0GJ	CG-CB-CA	2.79	120.34	113.84
5	B	302	0GJ	CG1-CB1-CA2	2.69	119.43	113.93
5	D	302	0GJ	NH1-CZ-NE	2.37	124.66	119.19
5	D	302	0GJ	CB1-CA2-C2	2.19	116.31	112.51
5	C	301	0GJ	CA1-N1-C	-2.14	116.08	121.37

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	302	0GJ	O2-C2-CA2-N2
5	A	302	0GJ	C3-C2-CA2-N2
5	A	302	0GJ	O2-C2-CA2-CB1
5	A	302	0GJ	N2-CA2-CB1-CG1
5	C	301	0GJ	O2-C2-CA2-CB1
5	C	301	0GJ	N2-CA2-CB1-CG1
5	C	301	0GJ	C2-CA2-CB1-CG1
5	B	302	0GJ	N2-CA2-CB1-CG1
5	B	302	0GJ	C2-CA2-CB1-CG1
5	D	302	0GJ	N2-CA2-CB1-CG1
5	D	302	0GJ	C2-CA2-CB1-CG1

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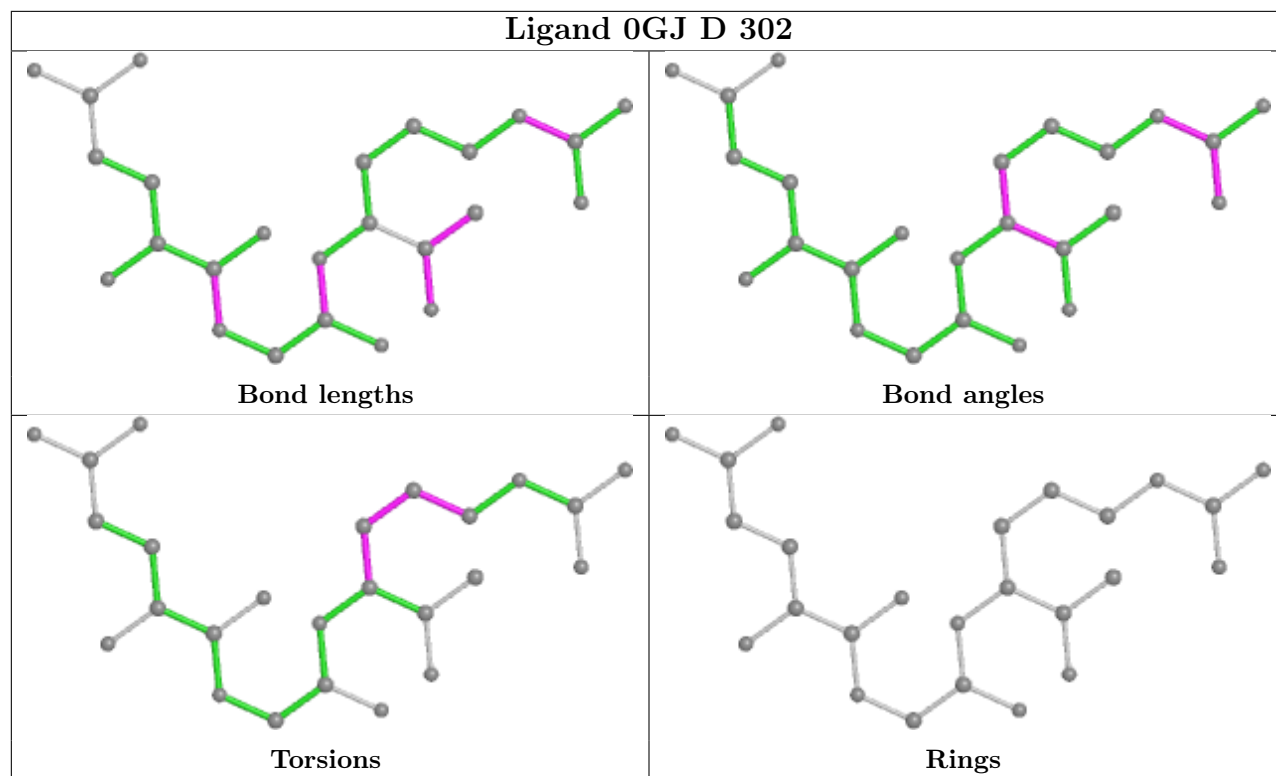
Mol	Chain	Res	Type	Atoms
5	B	302	0GJ	NE-CD1-CG1-CB1
5	C	301	0GJ	NE-CD1-CG1-CB1
5	D	302	0GJ	NE-CD1-CG1-CB1
5	A	302	0GJ	NE-CD1-CG1-CB1
5	A	302	0GJ	CA2-CB1-CG1-CD1
5	C	301	0GJ	CA2-CB1-CG1-CD1
5	D	302	0GJ	CA2-CB1-CG1-CD1
5	C	301	0GJ	C3-C2-CA2-N2
5	A	302	0GJ	C-CA-CB-CG
5	B	302	0GJ	CA2-CB1-CG1-CD1
5	A	302	0GJ	C3-C2-CA2-CB1
5	A	302	0GJ	C2-CA2-CB1-CG1
5	C	301	0GJ	O2-C2-CA2-N2
5	C	301	0GJ	C3-C2-CA2-CB1
5	A	302	0GJ	N-CA-CB-CG
5	B	302	0GJ	C3-C2-CA2-N2

There are no ring outliers.

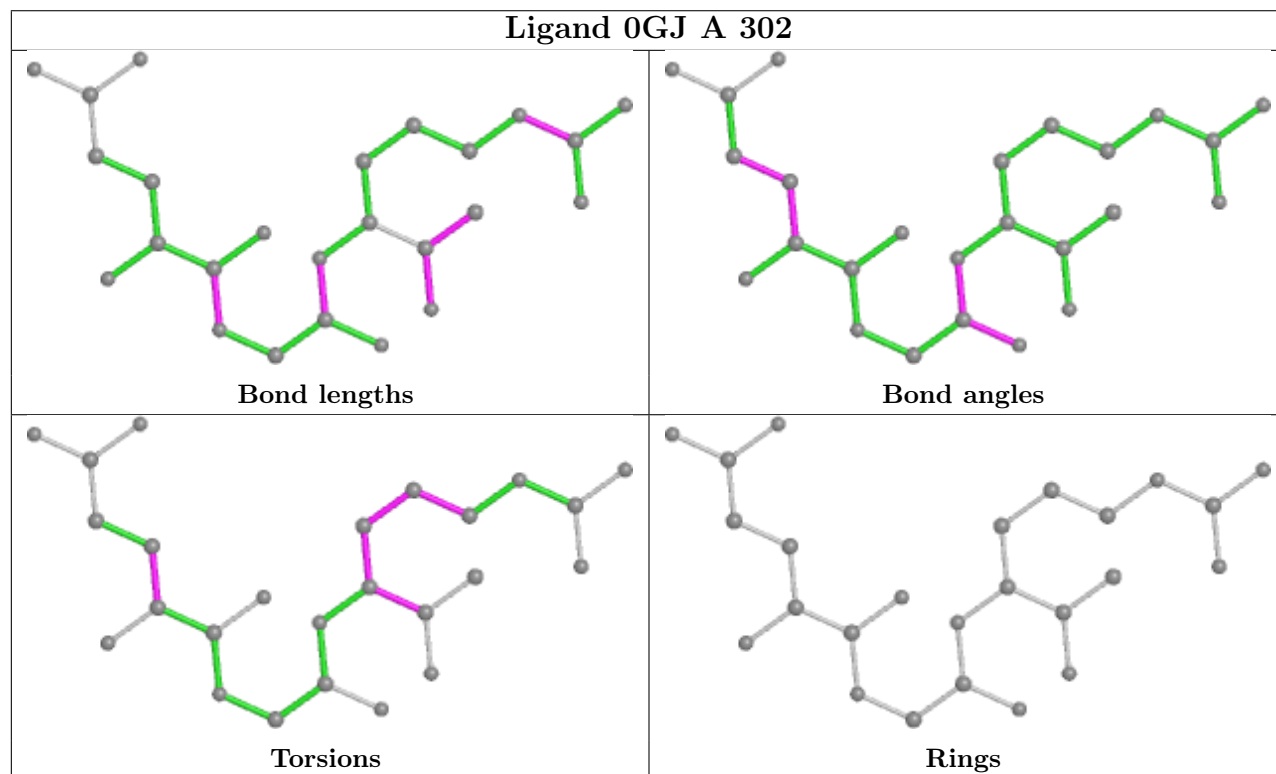
No monomer is involved in short contacts.

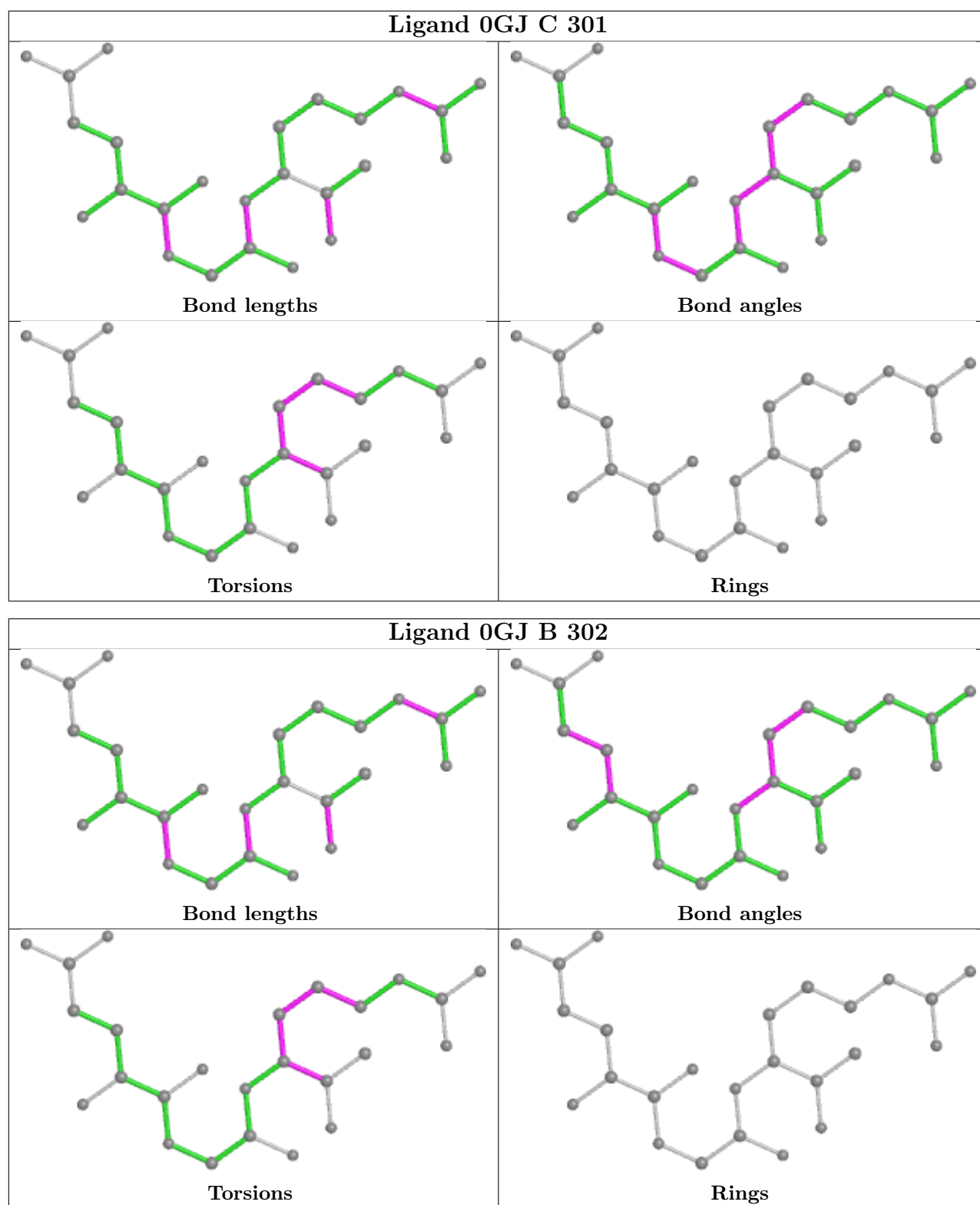
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 0GJ D 302



Ligand 0GJ A 302





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	243/275 (88%)	-0.43	0 100 100	32, 50, 76, 95	0
1	B	244/275 (88%)	-0.46	0 100 100	30, 47, 72, 95	0
1	C	242/275 (88%)	-0.33	1 (0%) 92 79	37, 59, 96, 120	0
1	D	242/275 (88%)	-0.29	1 (0%) 92 79	42, 60, 83, 106	0
2	E	216/230 (93%)	-0.25	1 (0%) 91 75	48, 78, 124, 142	0
2	G	217/230 (94%)	-0.21	1 (0%) 91 75	53, 79, 108, 128	0
2	H	216/230 (93%)	-0.38	3 (1%) 75 49	32, 68, 94, 124	0
2	J	219/230 (95%)	-0.01	8 (3%) 41 17	37, 78, 114, 134	0
3	F	216/217 (99%)	-0.35	0 100 100	52, 89, 123, 144	0
3	I	216/217 (99%)	-0.42	1 (0%) 91 75	53, 87, 132, 159	0
3	K	216/217 (99%)	-0.16	3 (1%) 75 49	30, 78, 124, 154	0
3	L	215/217 (99%)	-0.39	0 100 100	32, 67, 113, 135	0
All	All	2702/2888 (93%)	-0.31	19 (0%) 87 69	30, 69, 114, 159	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	117	HIS	4.3
2	J	214	LYS	4.3
2	J	141	LEU	3.5
2	J	158	ALA	3.2
2	J	150	VAL	3.0
2	J	120	SER	3.0
2	E	191	THR	2.9
1	C	117	HIS	2.8
3	I	154	LEU	2.7
2	G	133	GLY	2.6
2	J	154	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
3	K	180	THR	2.5
2	H	133	GLY	2.5
2	J	181	VAL	2.5
3	K	214	CYS	2.3
3	K	111	ALA	2.2
2	H	134	GLY	2.2
2	H	64	LYS	2.1
2	J	164	HIS	2.1

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](#)

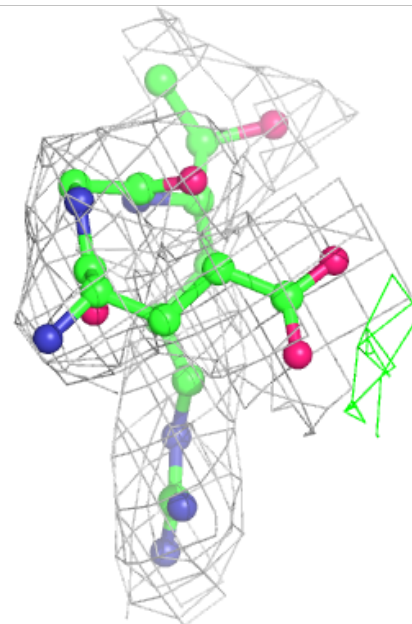
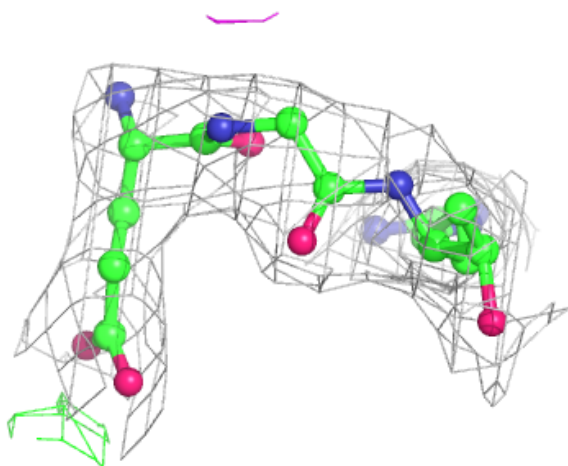
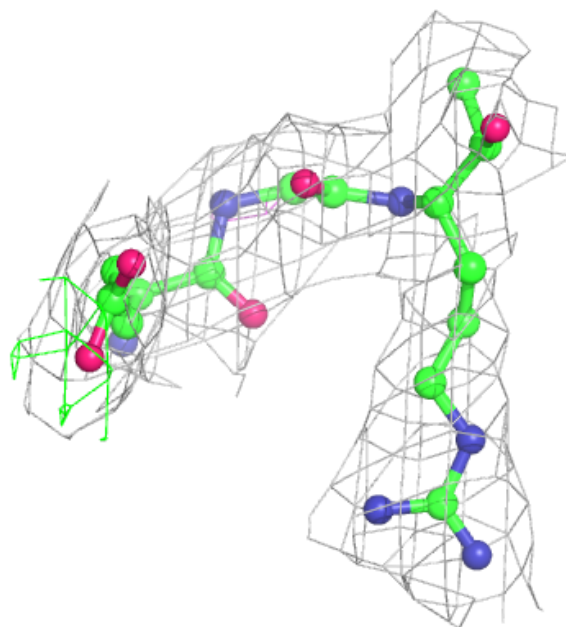
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CA	A	301	1/1	0.85	0.18	98,98,98,98	0
5	0GJ	C	301	25/26	0.94	0.18	35,45,70,72	0
4	CA	D	301	1/1	0.95	0.09	81,81,81,81	0
5	0GJ	A	302	25/26	0.95	0.17	34,46,60,64	0
5	0GJ	D	302	25/26	0.96	0.19	37,50,70,73	0
5	0GJ	B	302	25/26	0.97	0.20	34,43,68,71	0
4	CA	B	301	1/1	0.97	0.13	76,76,76,76	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.

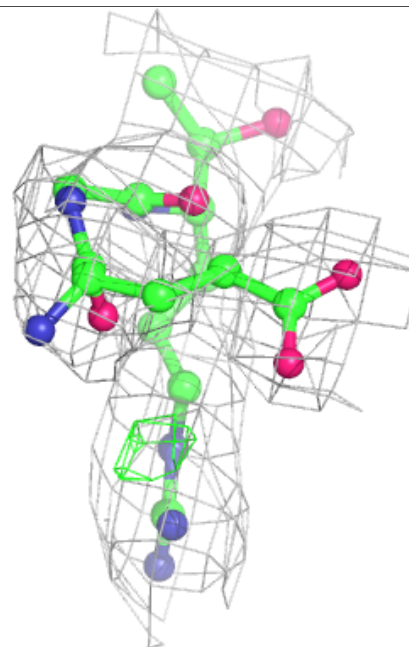
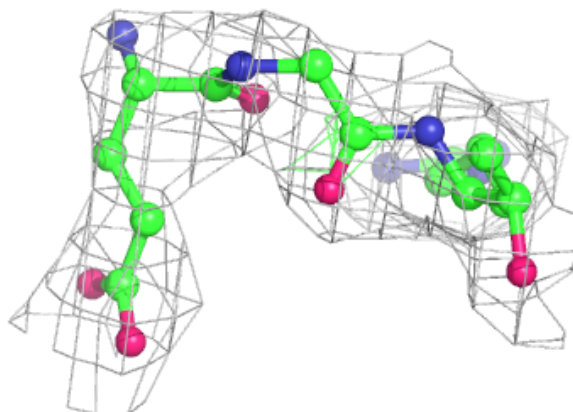
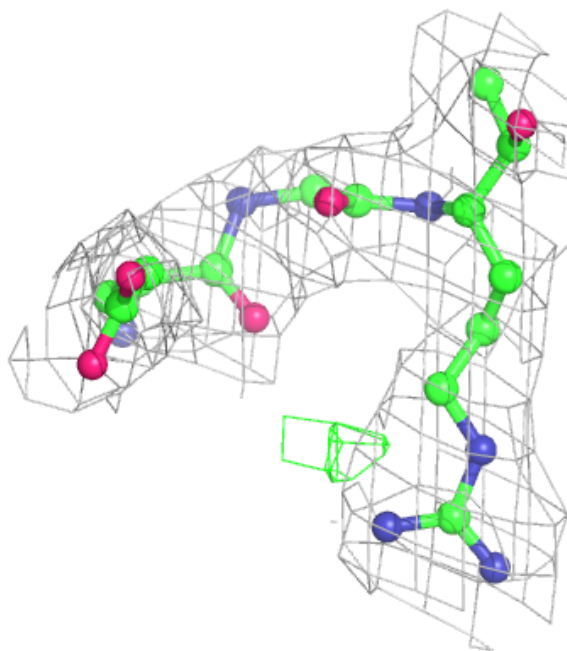
Electron density around 0GJ C 301:

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



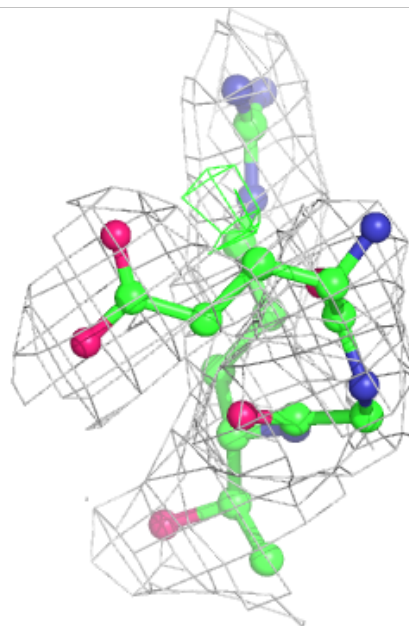
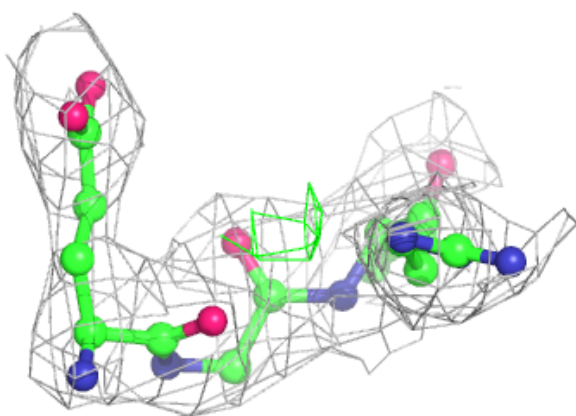
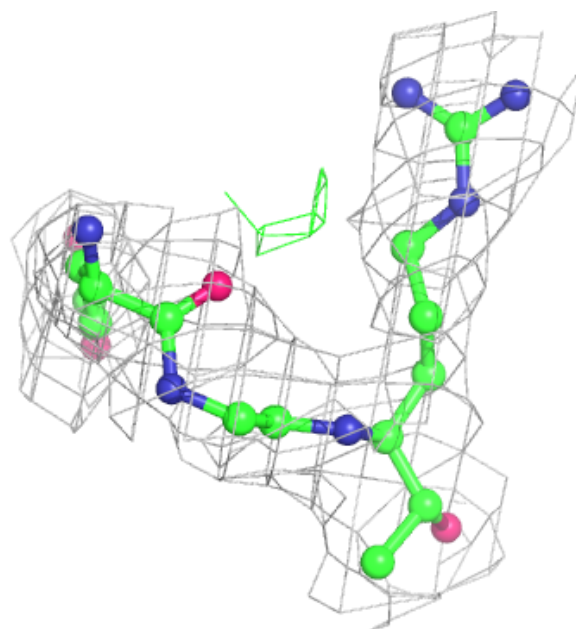
Electron density around 0GJ A 302:

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



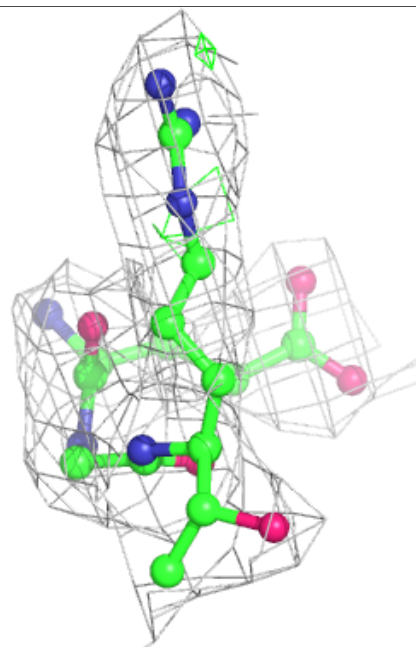
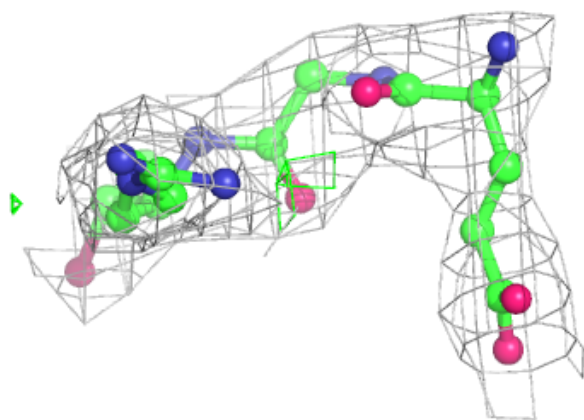
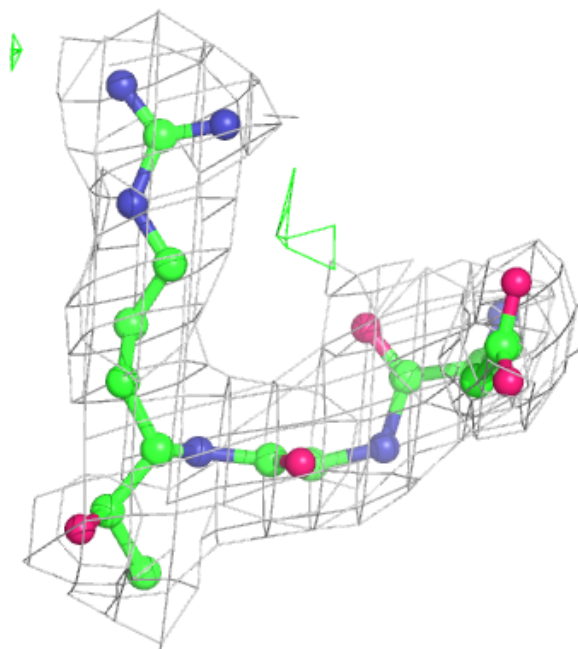
Electron density around 0GJ D 302:

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



Electron density around 0GJ B 302:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.