



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:00 PM UTC

PDB ID : 7QT0 / pdb_00007qt0
Title : Antibody FenAb136 - fentanyl complex
Authors : Zeelen, J.P.; Straaten van, M.; Stebbins, C.E.
Deposited on : 2022-01-14
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

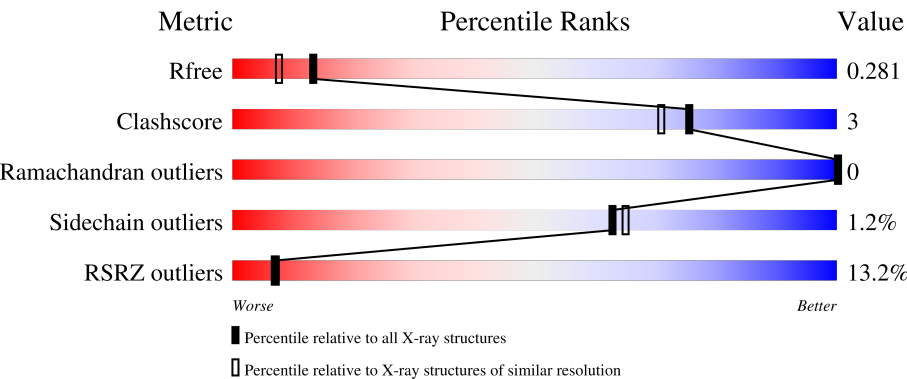
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	225	8% 89%5% . .
1	C	225	4% 88%8% .
1	E	225	8% 88%8% .
1	G	225	8% 90%5% 5%
1	I	225	7% 88%7% 5%

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Mol	Chain	Length	Quality of chain
1	K	225	15% 84% 10% 5%
2	B	214	15% 90% 7%
2	D	214	14% 93% 5%
2	F	214	14% 91% 7%
2	H	214	14% 89% 10%
2	J	214	30% 87% 12%
2	L	214	17% 86% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21106 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.

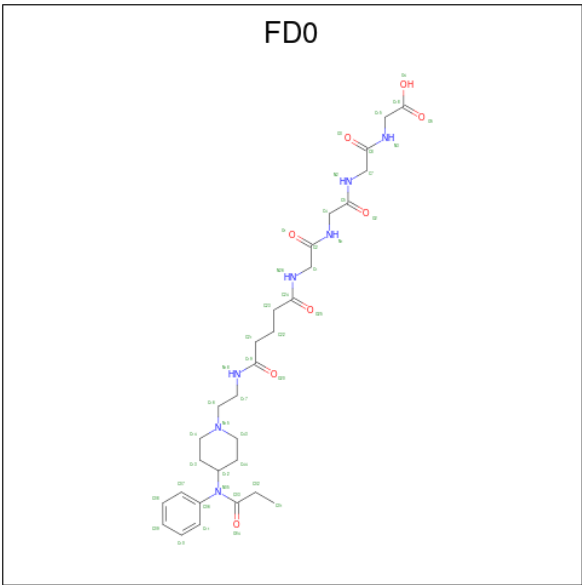
- Molecule 1 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1625	1032	264	321	8			
1	C	216	Total	C	N	O	S	0	1	0
			1645	1044	268	325	8			
1	E	217	Total	C	N	O	S	0	1	0
			1646	1043	265	330	8			
1	G	214	Total	C	N	O	S	0	0	0
			1629	1034	264	323	8			
1	I	213	Total	C	N	O	S	0	0	0
			1618	1029	261	320	8			
1	K	214	Total	C	N	O	S	0	0	0
			1618	1028	260	322	8			

- Molecule 2 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	1	0
			1630	1014	272	337	7			
2	D	212	Total	C	N	O	S	0	2	0
			1643	1021	278	338	6			
2	F	211	Total	C	N	O	S	0	3	0
			1643	1021	276	339	7			
2	H	212	Total	C	N	O	S	0	2	0
			1649	1024	278	340	7			
2	J	212	Total	C	N	O	S	0	0	0
			1629	1010	274	338	7			
2	L	211	Total	C	N	O	S	0	1	0
			1631	1014	275	336	6			

- Molecule 3 is 2-[2-[2-[2-[[5-oxidanylidene-5-[2-[4-[phenyl(propanoyl)amino]piperidin-1-yl]ethylamino]pentanoyl]amino]ethanoylamino]ethanoylamino]ethanoylamino]ethanoic acid (CCD ID: FD0) (formula: C₂₉H₄₃N₇O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	21	4	3		
3	C	1	Total	C	N	O	0	0
			28	21	4	3		
3	E	1	Total	C	N	O	0	0
			28	21	4	3		
3	G	1	Total	C	N	O	0	0
			28	21	4	3		
3	I	1	Total	C	N	O	0	0
			32	23	5	4		
3	K	1	Total	C	N	O	0	0
			28	21	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total	O	0	0
			121	121		
4	B	111	Total	O	0	0
			111	111		
4	C	136	Total	O	0	0
			136	136		
4	D	96	Total	O	0	0
			96	96		
4	E	146	Total	O	0	0
			146	146		
4	F	98	Total	O	0	0
			98	98		

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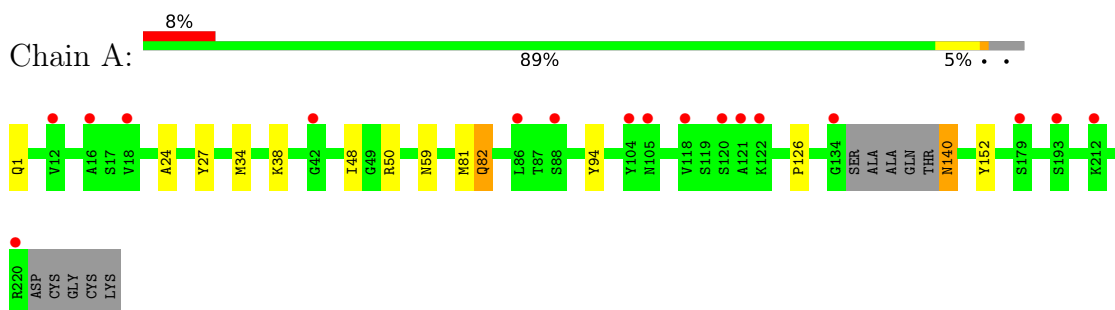
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	122	Total 122	O 122	0	0
4	H	93	Total 93	O 93	0	0
4	I	132	Total 132	O 132	0	0
4	J	71	Total 71	O 71	0	0
4	K	114	Total 114	O 114	0	0
4	L	88	Total 88	O 88	0	0

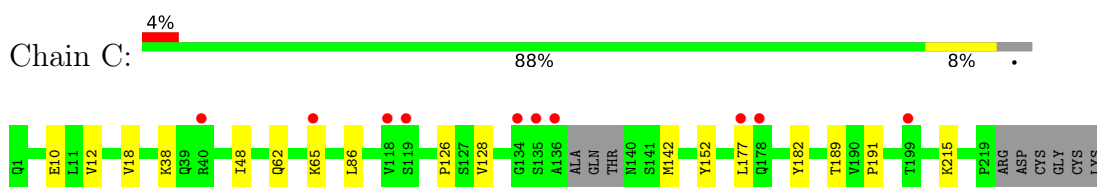
3 Residue-property plots [i](#)

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.

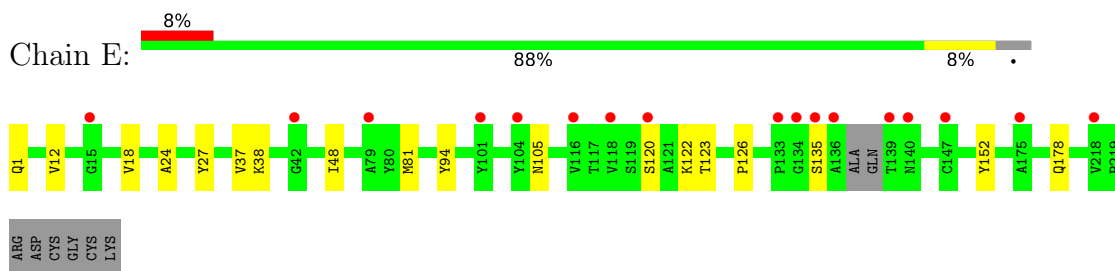
- Molecule 1: Antibody heavy chain



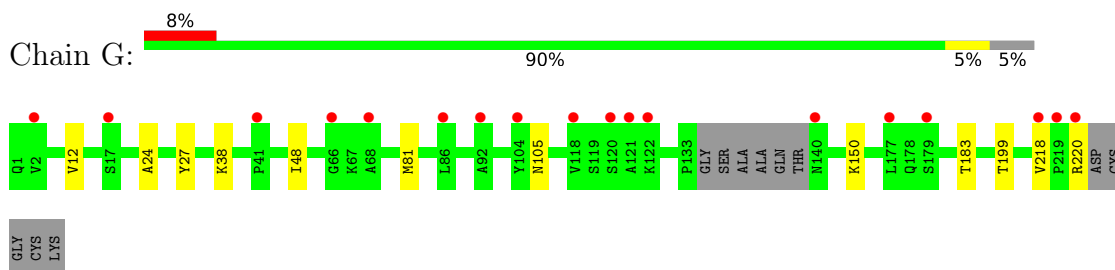
- Molecule 1: Antibody heavy chain



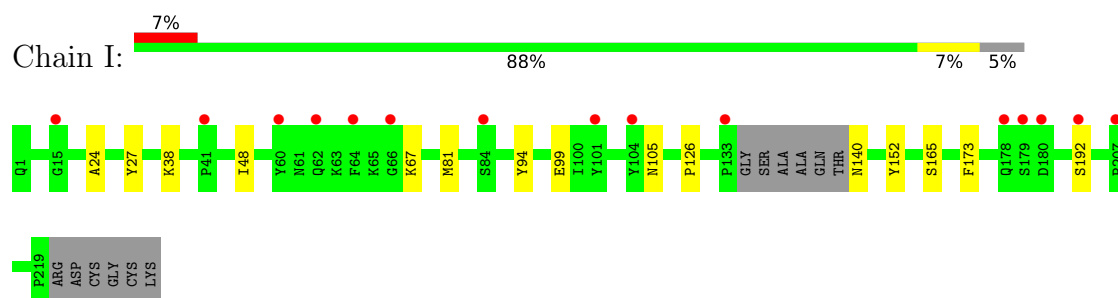
- Molecule 1: Antibody heavy chain



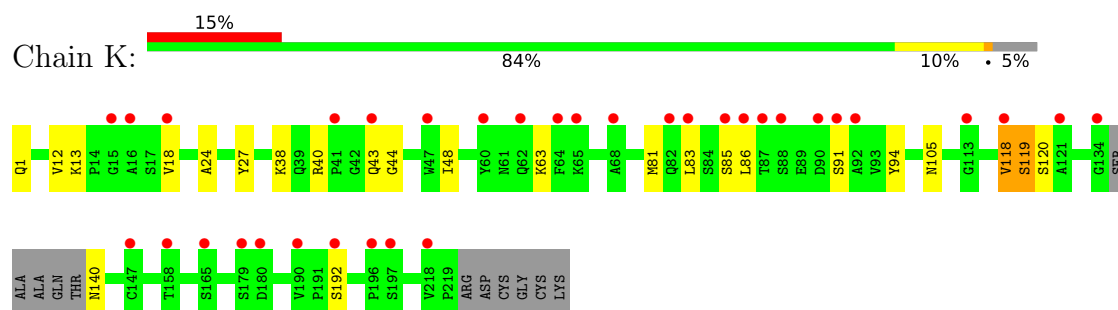
- Molecule 1: Antibody heavy chain



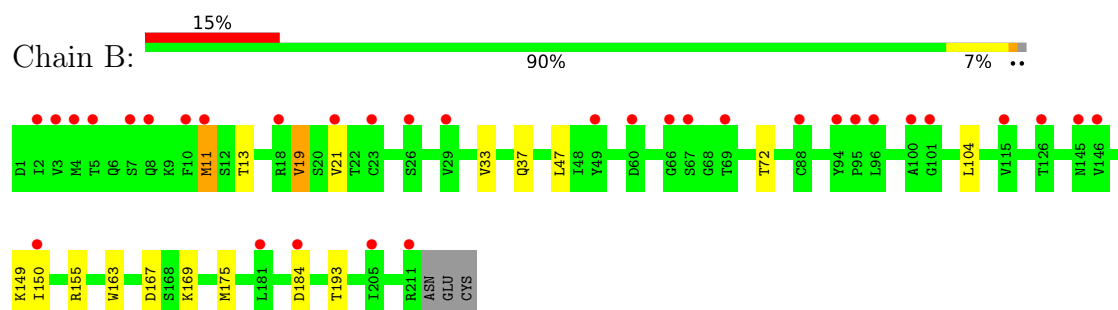
- Molecule 1: Antibody heavy chain



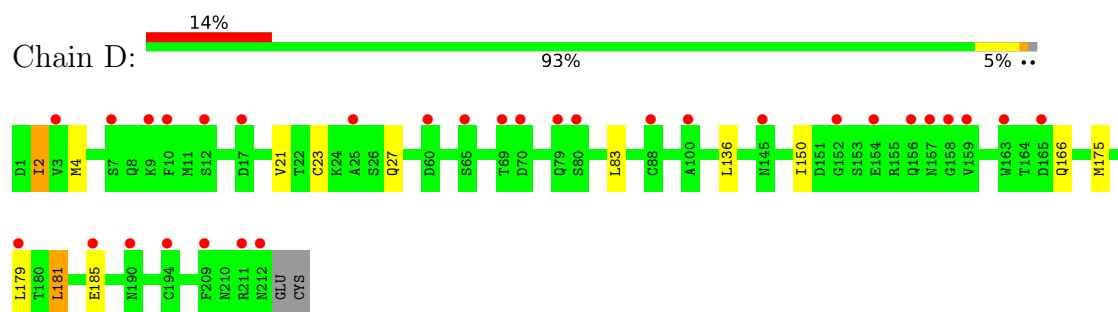
- Molecule 1: Antibody heavy chain



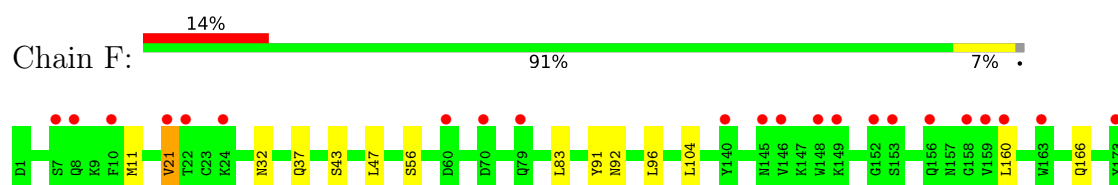
- Molecule 2: Antibody light chain

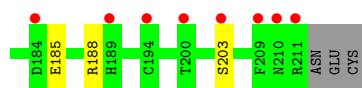


- Molecule 2: Antibody light chain

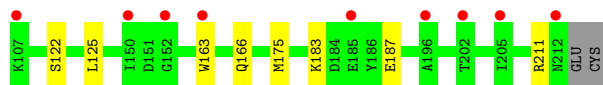
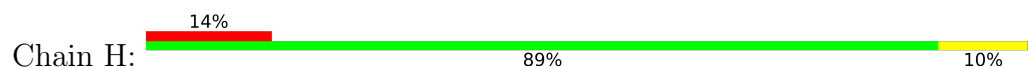


- Molecule 2: Antibody light chain

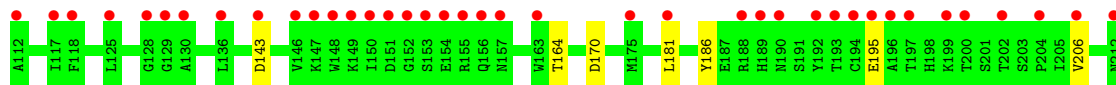
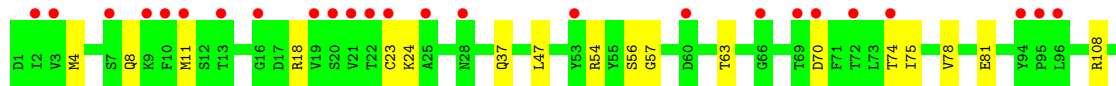
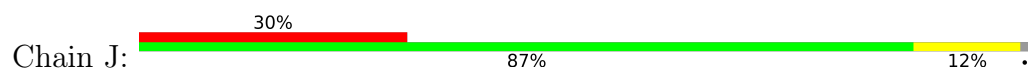




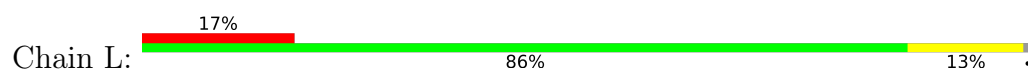
• Molecule 2: Antibody light chain



• Molecule 2: Antibody light chain



• Molecule 2: Antibody 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	182.98Å 105.84Å 172.78Å 90.00° 112.24° 90.00°	Depositor
Resolution (Å)	54.52 – 2.07 54.52 – 2.07	Depositor EDS
% Data completeness (in resolution range)	96.9 (54.52-2.07) 84.6 (54.52-2.07)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.242 , 0.282 0.243 , 0.281	Depositor DCC
R_{free} test set	1991 reflections (1.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	21106	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.98% 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: FD0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.09	0/1670	0.27	0/2288
1	C	0.09	0/1690	0.28	0/2314
1	E	0.09	0/1691	0.29	0/2317
1	G	0.09	0/1674	0.27	0/2293
1	I	0.08	0/1663	0.26	0/2278
1	K	0.15	0/1663	0.33	0/2279
2	B	0.19	1/1666 (0.1%)	0.31	0/2266
2	D	0.08	0/1679	0.26	0/2284
2	F	0.08	0/1679	0.26	0/2283
2	H	0.09	0/1685	0.28	0/2291
2	J	0.08	0/1665	0.25	0/2266
2	L	0.08	0/1667	0.25	0/2268
All	All	0.10	1/20092 (0.0%)	0.28	0/27427

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	11	MET	SD-CE	-5.68	1.65	1.79

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	1625	0	1565	10	0
1	C	1645	0	1594	12	0
1	E	1646	0	1583	9	0
1	G	1629	0	1572	6	0
1	I	1618	0	1566	9	0
1	K	1618	0	1556	16	0
2	B	1630	0	1532	8	0
2	D	1643	0	1548	6	0
2	F	1643	0	1550	9	0
2	H	1649	0	1550	11	0
2	J	1629	0	1519	14	0
2	L	1631	0	1538	14	0
3	A	28	0	0	0	0
3	C	28	0	0	0	0
3	E	28	0	0	0	0
3	G	28	0	0	0	0
3	I	32	0	0	1	0
3	K	28	0	0	0	0
4	A	121	0	0	0	0
4	B	111	0	0	0	0
4	C	136	0	0	1	0
4	D	96	0	0	0	0
4	E	146	0	0	0	0
4	F	98	0	0	0	0
4	G	122	0	0	0	0
4	H	93	0	0	0	0
4	I	132	0	0	1	0
4	J	71	0	0	0	0
4	K	114	0	0	0	0
4	L	88	0	0	0	0
All	All	21106	0	18673	117	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 3.

All (117) 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:L:195:GLU:HG2	2:L:206:VAL:HG22	1.64	0.79
1:C:62:GLN:HA	1:C:65:LYS:HG3	1.76	0.67
1:K:12:VAL:HG11	1:K:86:LEU:HD12	1.75	0.67
1:K:12:VAL:HG21	1:K:18:VAL:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASN:N	1:A:140:ASN:HD22	1.95	0.65
2:B:13:THR:HB	2:B:19:VAL:HG13	1.82	0.62
1:C:38:LYS:HB2	1:C:48:ILE:HD11	1.81	0.61
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.82	0.61
1:E:12:VAL:HG11	1:E:18:VAL:HB	1.83	0.60
1:K:83:LEU:HB3	1:K:86:LEU:HD21	1.82	0.60
2:F:185:GLU:OE1	2:F:188:ARG:NH1	2.35	0.59
2:H:37:GLN:HB2	2:H:47:LEU:HD11	1.83	0.59
2:B:150:ILE:HD12	2:B:155:ARG:HG3	1.85	0.58
1:E:178:GLN:HG3	2:F:160:LEU:HD11	1.84	0.58
1:C:62:GLN:HG2	1:C:65:LYS:HE2	1.87	0.57
1:E:38:LYS:HB2	1:E:48:ILE:HD11	1.87	0.57
1:I:67:LYS:NZ	4:I:402:HOH:O	2.38	0.57
1:K:38:LYS:HB2	1:K:48:ILE:HD11	1.87	0.56
2:J:18:ARG:HD3	2:J:74:THR:HG23	1.88	0.56
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.87	0.56
1:A:140:ASN:N	1:A:140:ASN:ND2	2.53	0.55
1:I:38:LYS:HB2	1:I:48:ILE:HD11	1.89	0.55
1:G:38:LYS:HB2	1:G:48:ILE:HD11	1.89	0.54
2:D:4:MET:HE3	2:D:23:CYS:SG	2.48	0.54
1:A:38:LYS:HB2	1:A:48:ILE:HD11	1.89	0.54
1:C:142:MET:HE3	1:C:189:THR:HG22	1.90	0.53
1:K:81:MET:HE1	1:K:94:TYR:CD1	2.44	0.53
2:H:163:TRP:NE1	2:H:175:MET:HE3	2.23	0.53
1:I:126:PRO:HB3	1:I:152:TYR:HB3	1.91	0.53
2:H:13:THR:HB	2:H:19:VAL:HG13	1.91	0.52
2:L:4:MET:HE3	2:L:23:CYS:SG	2.50	0.52
2:D:181:LEU:HB3	2:D:185:GLU:OE1	2.10	0.51
1:C:215:LYS:NZ	4:C:406:HOH:O	2.40	0.51
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.91	0.51
1:K:40:ARG:HH11	1:K:40:ARG:HG2	1.76	0.51
2:H:91:TYR:HA	2:H:96:LEU:HD22	1.91	0.51
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.92	0.51
1:C:12:VAL:HG21	1:C:18:VAL:HB	1.92	0.51
2:L:32:ASN:HB2	2:L:92:ASN:HB2	1.91	0.51
2:F:11:MET:SD	2:F:21:VAL:HG22	2.50	0.51
2:J:75:ILE:HG22	2:J:78:VAL:HG12	1.93	0.51
2:J:24:LYS:HE2	2:J:70:ASP:HA	1.93	0.51
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.93	0.51
2:F:83:LEU:HD13	2:F:166:GLN:HB3	1.92	0.50
2:F:91:TYR:HA	2:F:96:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:183:LYS:NZ	2:H:187:GLU:OE2	2.35	0.50
2:L:184:ASP:O	2:L:188:ARG:HG3	2.11	0.50
2:B:21:VAL:O	2:B:72:THR:HA	2.13	0.49
2:D:136:LEU:HD13	2:D:175:MET:HG2	1.94	0.49
2:L:161:ASN:HB3	2:L:175:MET:HE3	1.94	0.49
1:K:63:LYS:HB2	1:K:63:LYS:HE2	1.65	0.48
1:K:140:ASN:O	1:K:192:SER:OG	2.31	0.48
2:L:14:SER:HB2	2:L:17:ASP:OD1	2.13	0.48
2:J:195:GLU:HG2	2:J:206:VAL:HG22	1.94	0.48
1:G:218:VAL:HB	1:G:220:ARG:HD2	1.96	0.47
1:C:126:PRO:HB3	1:C:152:TYR:HB3	1.95	0.47
2:J:4:MET:HE3	2:J:23:CYS:SG	2.54	0.47
2:L:115:VAL:HA	2:L:135:PHE:O	2.15	0.47
2:B:167:ASP:OD2	2:B:169:LYS:HD2	2.14	0.47
1:G:105:ASN:HB3	2:H:56:SER:HB2	1.96	0.47
1:K:13:LYS:HD3	1:K:120:SER:HA	1.96	0.47
1:A:34:MET:HE2	1:A:34:MET:HB2	1.85	0.47
1:C:18:VAL:HG12	1:C:86:LEU:HD11	1.97	0.46
1:I:99:GLU:OE2	3:I:301:FD0:N18	2.47	0.46
2:D:83:LEU:HD13	2:D:166:GLN:HB3	1.97	0.46
2:J:108:ARG:NH1	2:J:170:ASP:O	2.48	0.46
2:H:19:VAL:HG22	2:H:78:VAL:HG21	1.96	0.46
1:C:10:GLU:HG2	1:C:18:VAL:HG21	1.97	0.46
2:L:166:GLN:HG3	2:L:173:TYR:CZ	2.52	0.45
2:F:11:MET:HE3	2:F:104:LEU:HB2	1.98	0.45
2:J:181:LEU:CD1	2:J:186:TYR:HB2	2.47	0.45
1:K:105:ASN:HB3	2:L:56:SER:HB2	1.99	0.45
1:I:105:ASN:HB3	2:J:56:SER:HB2	1.99	0.45
2:H:211:ARG:HG2	2:H:211:ARG:HH11	1.81	0.45
1:K:12:VAL:O	1:K:118:VAL:HA	2.17	0.45
1:K:1:GLN:OE1	1:K:1:GLN:N	2.47	0.44
1:G:24:ALA:HB1	1:G:27:TYR:CE1	2.51	0.44
2:J:81:GLU:H	2:J:81:GLU:CD	2.25	0.44
1:K:24:ALA:HB1	1:K:27:TYR:CE1	2.51	0.44
1:K:40:ARG:HG2	1:K:40:ARG:NH1	2.33	0.44
1:C:191:PRO:HB3	2:J:57:GLY:HA2	2.00	0.43
1:I:173:PHE:CD2	2:J:164:THR:HG23	2.53	0.43
1:I:24:ALA:HB1	1:I:27:TYR:CE1	2.53	0.43
1:A:50:ARG:HG2	1:A:59:ASN:HB2	1.99	0.43
1:K:13:LYS:NZ	1:K:119:SER:O	2.47	0.43
1:A:126:PRO:HB3	1:A:152:TYR:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:61:ARG:HB3	2:L:76:SER:O	2.19	0.43
2:H:83:LEU:HD13	2:H:166:GLN:HB3	2.00	0.43
1:E:1:GLN:OE1	1:E:1:GLN:N	2.36	0.43
2:F:32:ASN:HB2	2:F:92:ASN:HB2	2.01	0.42
1:G:150:LYS:HA	1:G:183:THR:HG23	2.01	0.42
1:G:81:MET:HE2	1:G:81:MET:HB3	1.90	0.42
2:J:54:ARG:HH12	2:J:63:THR:HG22	1.83	0.42
1:I:81:MET:HE1	1:I:94:TYR:CD2	2.53	0.42
1:E:126:PRO:HB3	1:E:152:TYR:HB3	2.01	0.42
1:A:81:MET:HE1	1:A:94:TYR:CD1	2.55	0.42
2:B:163:TRP:CE2	2:B:175:MET:HG3	2.54	0.42
1:A:24:ALA:HB1	1:A:27:TYR:CE1	2.55	0.42
1:A:82:GLN:HE21	1:A:82:GLN:HB3	1.52	0.42
2:D:2:ILE:HD13	2:D:27:GLN:HB2	2.00	0.42
1:E:81:MET:HE1	1:E:94:TYR:CD1	2.55	0.42
1:I:140:ASN:O	1:I:192:SER:OG	2.31	0.42
1:E:105:ASN:HB3	2:F:56:SER:HB2	2.02	0.41
1:C:128:VAL:O	1:C:215:LYS:HE3	2.20	0.41
2:B:149:LYS:HB2	2:B:193:THR:HB	2.03	0.41
2:D:150:ILE:HD11	2:D:179:LEU:HD21	2.03	0.41
1:A:1:GLN:OE1	1:A:1:GLN:N	2.48	0.41
2:B:11:MET:SD	2:B:104:LEU:HD13	2.61	0.41
1:C:177:LEU:HD13	1:C:182:TYR:CZ	2.56	0.41
1:E:24:ALA:HB1	1:E:27:TYR:CE1	2.55	0.41
2:J:8:GLN:HG3	2:J:11:MET:HE1	2.03	0.41
1:E:122:LYS:HE3	1:E:123:THR:H	1.87	0.40
2:L:169:LYS:HD3	2:L:169:LYS:HA	1.90	0.40
2:H:122:SER:HA	2:H:125:LEU:HD12	2.04	0.40
1:K:43:GLN:CD	1:K:44:GLY:H	2.29	0.40
2:H:32:ASN:HB2	2:H:92:ASN:HB2	2.04	0.40
2:L:39:LYS:HG2	2:L:84:ALA:HB2	2.02	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	211/225 (94%)	207 (98%)	4 (2%)	0	100	100
1	C	213/225 (95%)	211 (99%)	2 (1%)	0	100	100
1	E	214/225 (95%)	210 (98%)	4 (2%)	0	100	100
1	G	210/225 (93%)	205 (98%)	5 (2%)	0	100	100
1	I	209/225 (93%)	204 (98%)	5 (2%)	0	100	100
1	K	210/225 (93%)	208 (99%)	2 (1%)	0	100	100
2	B	210/214 (98%)	203 (97%)	7 (3%)	0	100	100
2	D	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
2	F	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
2	H	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
2	J	210/214 (98%)	206 (98%)	4 (2%)	0	100	100
2	L	210/214 (98%)	204 (97%)	6 (3%)	0	100	100
All	All	2532/2634 (96%)	2480 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	184/195 (94%)	182 (99%)	2 (1%)	65	68
1	C	187/195 (96%)	187 (100%)	0	100	100
1	E	188/195 (96%)	185 (98%)	3 (2%)	55	55
1	G	186/195 (95%)	184 (99%)	2 (1%)	65	68
1	I	185/195 (95%)	184 (100%)	1 (0%)	81	85
1	K	184/195 (94%)	180 (98%)	4 (2%)	45	43
2	B	184/190 (97%)	181 (98%)	3 (2%)	55	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	185/190 (97%)	182 (98%)	3 (2%)	55	55
2	F	186/190 (98%)	182 (98%)	4 (2%)	45	43
2	H	186/190 (98%)	183 (98%)	3 (2%)	55	55
2	J	183/190 (96%)	182 (100%)	1 (0%)	81	85
2	L	184/190 (97%)	182 (99%)	2 (1%)	65	68
All	All	2222/2310 (96%)	2194 (99%)	28 (1%)	63	62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	140	ASN
2	B	19	VAL
2	B	33	VAL
2	B	184	ASP
2	D	2	ILE
2	D	21	VAL
2	D	181	LEU
1	E	37	VAL
1	E	120	SER
1	E	135	SER
2	F	21	VAL
2	F	43[A]	SER
2	F	43[B]	SER
2	F	203	SER
1	G	12	VAL
1	G	199	THR
2	H	8	GLN
2	H	33	VAL
2	H	50	SER
1	I	165	SER
2	J	143	ASP
1	K	85	SER
1	K	91	SER
1	K	118	VAL
1	K	119	SER
2	L	5	THR
2	L	210	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	210	ASN
2	D	42	GLN
2	D	137	ASN
1	E	43	GLN
1	E	171	HIS
2	F	137	ASN
2	F	156	GLN
2	H	137	ASN
1	I	3	GLN
2	J	8	GLN
2	J	137	ASN
2	J	145	ASN
2	J	212	ASN
2	L	161	ASN
2	L	189	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
3	FD0	G	301	-	29,29,45	2.37	7 (24%)	36,37,57	1.05	3 (8%)
3	FD0	E	301	-	29,29,45	2.38	7 (24%)	36,37,57	1.05	4 (11%)
3	FD0	K	301	-	29,29,45	2.36	7 (24%)	36,37,57	1.11	3 (8%)
3	FD0	C	301	-	29,29,45	2.41	7 (24%)	36,37,57	1.47	5 (13%)
3	FD0	I	301	-	33,33,45	2.51	9 (27%)	41,42,57	1.05	4 (9%)
3	FD0	A	301	-	29,29,45	2.42	7 (24%)	36,37,57	1.06	3 (8%)

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
3	FD0	G	301	-	-	1/26/36/56	0/2/2/2
3	FD0	E	301	-	-	2/26/36/56	0/2/2/2
3	FD0	K	301	-	-	4/26/36/56	0/2/2/2
3	FD0	C	301	-	-	4/26/36/56	0/2/2/2
3	FD0	I	301	-	-	3/31/41/56	0/2/2/2
3	FD0	A	301	-	-	8/26/36/56	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	FD0	C03-N05	7.69	1.49	1.36
3	E	301	FD0	C03-N05	7.44	1.48	1.36
3	C	301	FD0	C03-N05	7.42	1.48	1.36
3	I	301	FD0	C03-N05	7.41	1.48	1.36
3	G	301	FD0	C03-N05	7.39	1.48	1.36
3	K	301	FD0	C03-N05	7.37	1.48	1.36
3	I	301	FD0	C24-N26	6.25	1.48	1.33
3	A	301	FD0	C19-N18	6.22	1.48	1.33
3	C	301	FD0	C19-N18	6.21	1.48	1.33
3	I	301	FD0	C19-N18	6.09	1.47	1.33
3	E	301	FD0	C19-N18	6.08	1.47	1.33
3	K	301	FD0	C19-N18	6.05	1.47	1.33
3	G	301	FD0	C19-N18	6.05	1.47	1.33
3	K	301	FD0	C24-N26	4.77	1.48	1.32
3	G	301	FD0	C24-N26	4.76	1.48	1.32
3	A	301	FD0	C24-N26	4.75	1.48	1.32
3	C	301	FD0	C24-N26	4.75	1.48	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	FD0	C24-N26	4.72	1.48	1.32
3	I	301	FD0	C2-N1	3.94	1.45	1.32
3	A	301	FD0	C02-C03	3.41	1.56	1.51
3	G	301	FD0	C02-C03	3.36	1.56	1.51
3	C	301	FD0	C02-C03	3.35	1.56	1.51
3	E	301	FD0	C02-C03	3.32	1.56	1.51
3	I	301	FD0	C02-C03	3.30	1.56	1.51
3	K	301	FD0	C02-C03	3.24	1.56	1.51
3	C	301	FD0	O20-C19	-2.71	1.17	1.23
3	K	301	FD0	O20-C19	-2.70	1.17	1.23
3	G	301	FD0	O20-C19	-2.69	1.17	1.23
3	E	301	FD0	O20-C19	-2.68	1.17	1.23
3	I	301	FD0	C23-C24	2.68	1.56	1.51
3	I	301	FD0	O20-C19	-2.67	1.18	1.23
3	A	301	FD0	O20-C19	-2.63	1.18	1.23
3	I	301	FD0	C06-N05	2.57	1.47	1.43
3	G	301	FD0	C06-N05	2.56	1.47	1.43
3	E	301	FD0	C06-N05	2.56	1.47	1.43
3	K	301	FD0	C06-N05	2.54	1.47	1.43
3	C	301	FD0	C06-N05	2.53	1.47	1.43
3	C	301	FD0	C21-C19	2.47	1.56	1.51
3	I	301	FD0	C21-C19	2.45	1.56	1.51
3	E	301	FD0	C21-C19	2.45	1.56	1.51
3	A	301	FD0	C21-C19	2.43	1.56	1.51
3	G	301	FD0	C21-C19	2.42	1.56	1.51
3	K	301	FD0	C21-C19	2.38	1.56	1.51
3	A	301	FD0	C06-N05	2.18	1.46	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	FD0	C43-N15-C14	4.57	118.69	108.84
3	C	301	FD0	C44-C43-N15	3.55	116.81	111.08
3	A	301	FD0	C43-N15-C14	3.28	115.91	108.84
3	C	301	FD0	C06-N05-C03	-3.12	119.04	121.72
3	K	301	FD0	C06-N05-C03	-3.06	119.09	121.72
3	C	301	FD0	C06-N05-C12	2.76	122.64	119.25
3	K	301	FD0	C06-N05-C12	2.59	122.43	119.25
3	C	301	FD0	C13-C14-N15	2.56	115.22	111.08
3	G	301	FD0	C06-N05-C03	-2.52	119.56	121.72
3	I	301	FD0	C06-N05-C03	-2.42	119.64	121.72
3	E	301	FD0	C43-N15-C14	2.34	113.88	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	301	FD0	C06-N05-C12	2.31	122.08	119.25
3	A	301	FD0	C06-N05-C03	-2.27	119.77	121.72
3	E	301	FD0	C06-N05-C03	-2.26	119.78	121.72
3	G	301	FD0	C43-N15-C14	2.18	113.54	108.84
3	I	301	FD0	C43-N15-C14	2.13	113.44	108.84
3	E	301	FD0	C06-N05-C12	2.10	121.83	119.25
3	I	301	FD0	C21-C19-N18	2.05	120.08	116.34
3	A	301	FD0	C06-N05-C12	-2.04	116.74	119.25
3	I	301	FD0	C06-N05-C12	2.03	121.74	119.25
3	K	301	FD0	C21-C19-N18	2.01	120.01	116.34
3	E	301	FD0	C21-C19-N18	2.00	120.00	116.34

There are no chirality outliers.

All (22) torsion outliers are listed below:

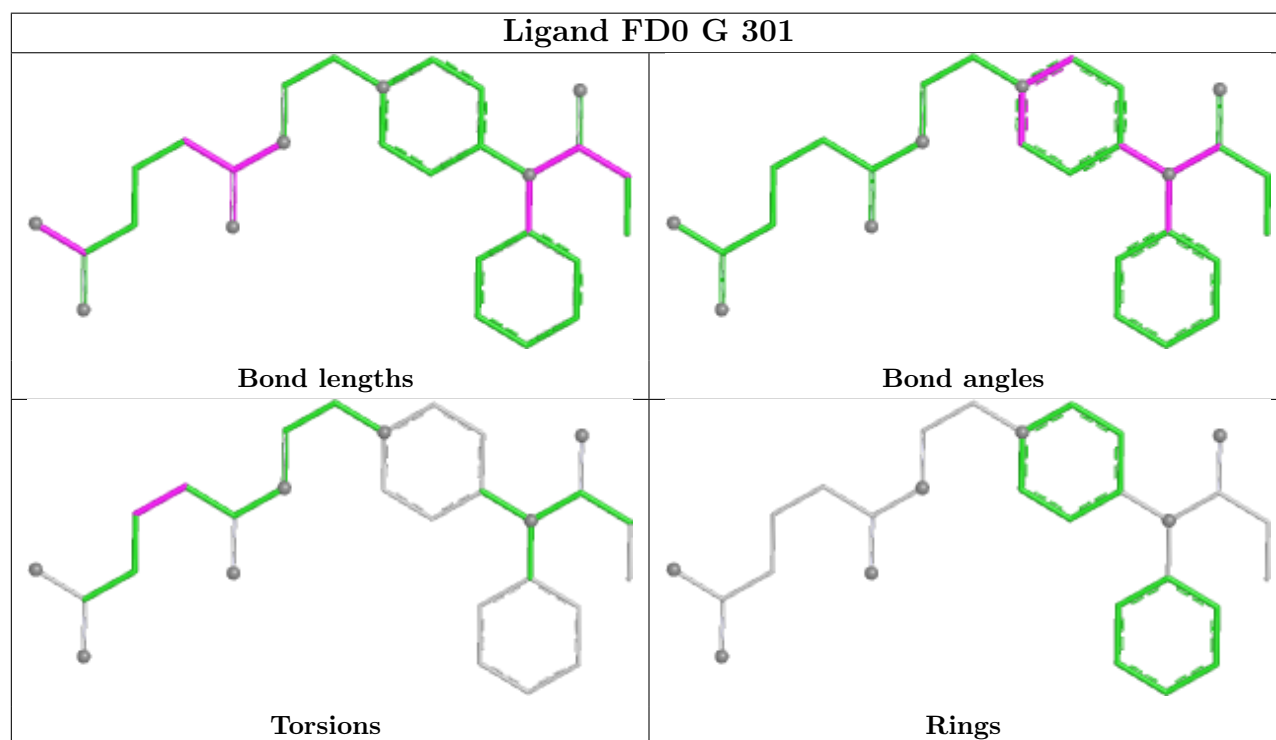
Mol	Chain	Res	Type	Atoms
3	I	301	FD0	N26-C1-C2-O1
3	K	301	FD0	C19-C21-C22-C23
3	A	301	FD0	N15-C16-C17-N18
3	C	301	FD0	C17-C16-N15-C43
3	A	301	FD0	C19-C21-C22-C23
3	K	301	FD0	N15-C16-C17-N18
3	I	301	FD0	N26-C1-C2-N1
3	I	301	FD0	C19-C21-C22-C23
3	K	301	FD0	C22-C23-C24-N26
3	K	301	FD0	C22-C23-C24-O25
3	C	301	FD0	C21-C22-C23-C24
3	A	301	FD0	C21-C22-C23-C24
3	A	301	FD0	C22-C23-C24-O25
3	G	301	FD0	C19-C21-C22-C23
3	A	301	FD0	C22-C23-C24-N26
3	C	301	FD0	N15-C16-C17-N18
3	E	301	FD0	C17-C16-N15-C14
3	A	301	FD0	C13-C12-N05-C03
3	A	301	FD0	C44-C12-N05-C03
3	A	301	FD0	C17-C16-N15-C43
3	C	301	FD0	C19-C21-C22-C23
3	E	301	FD0	C17-C16-N15-C43

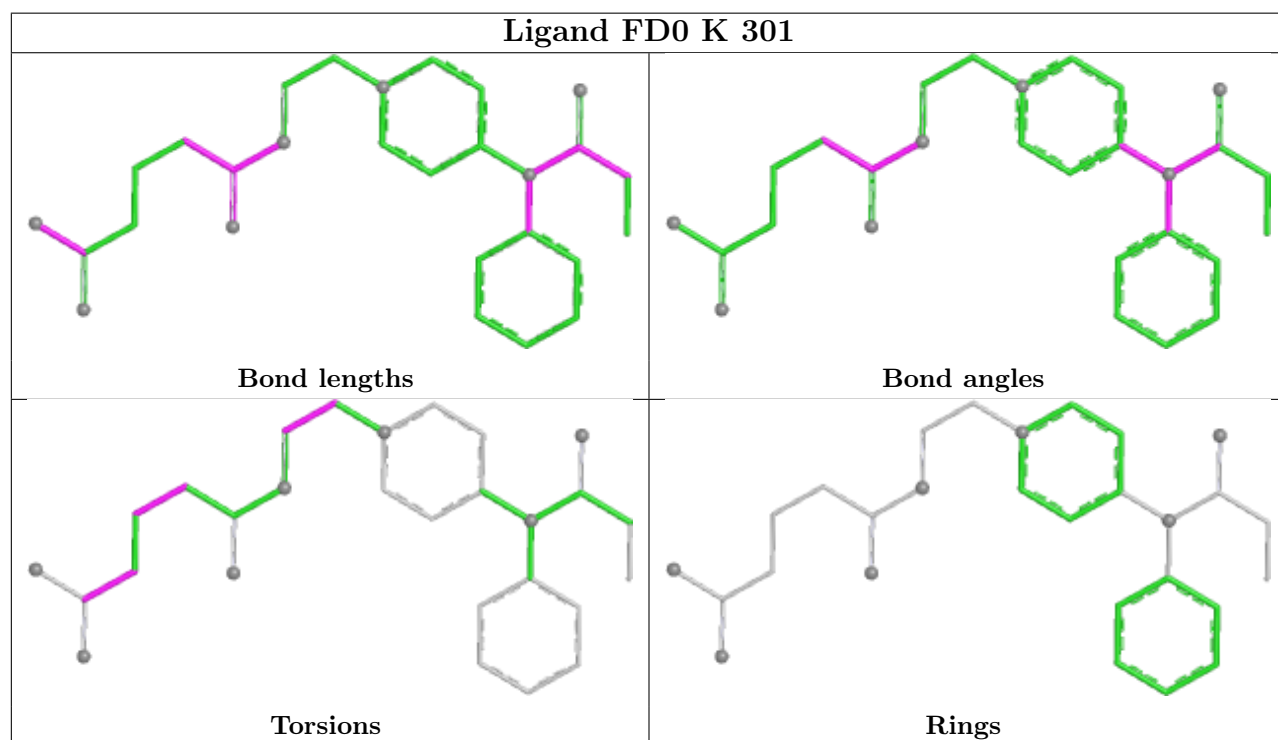
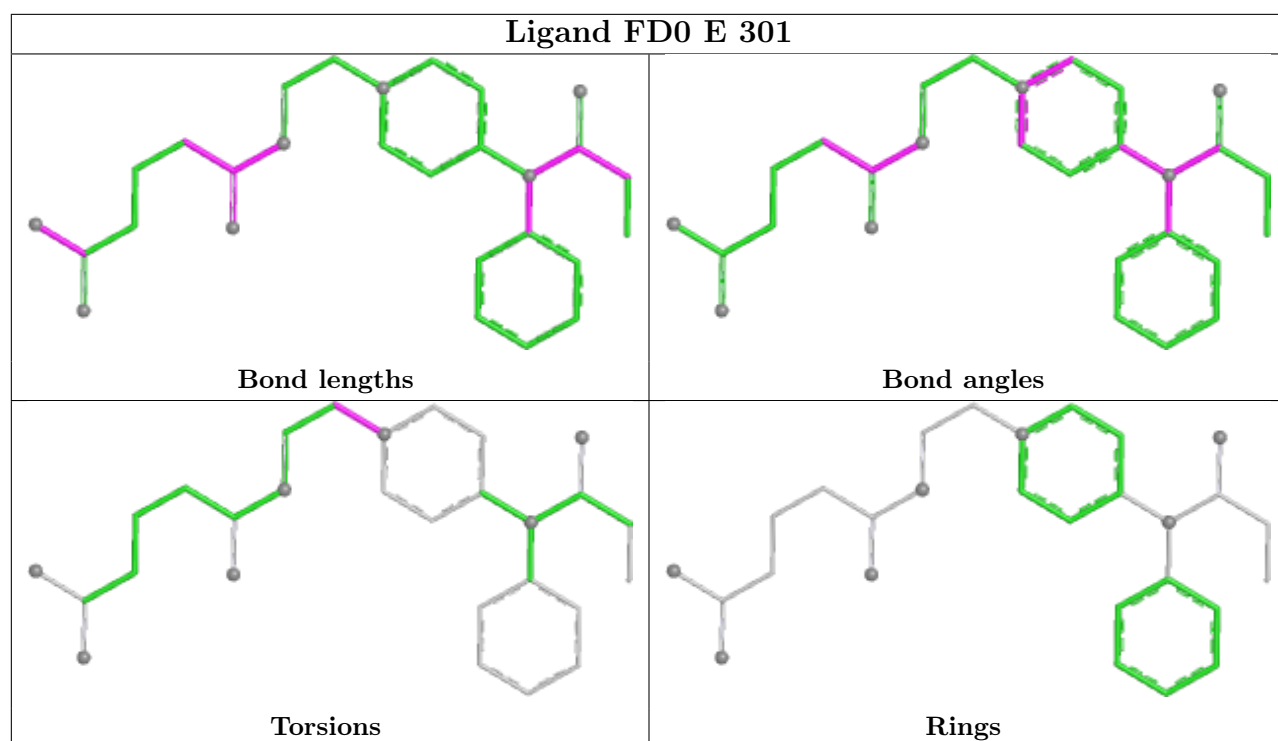
There are no ring outliers.

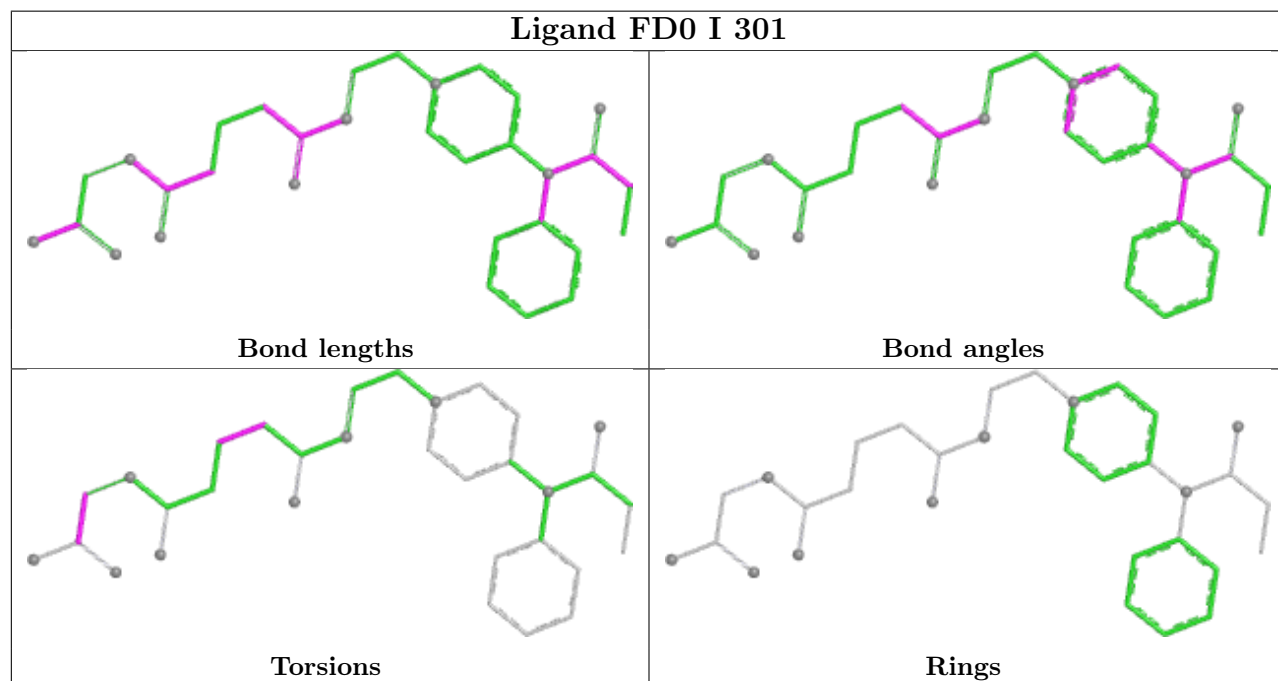
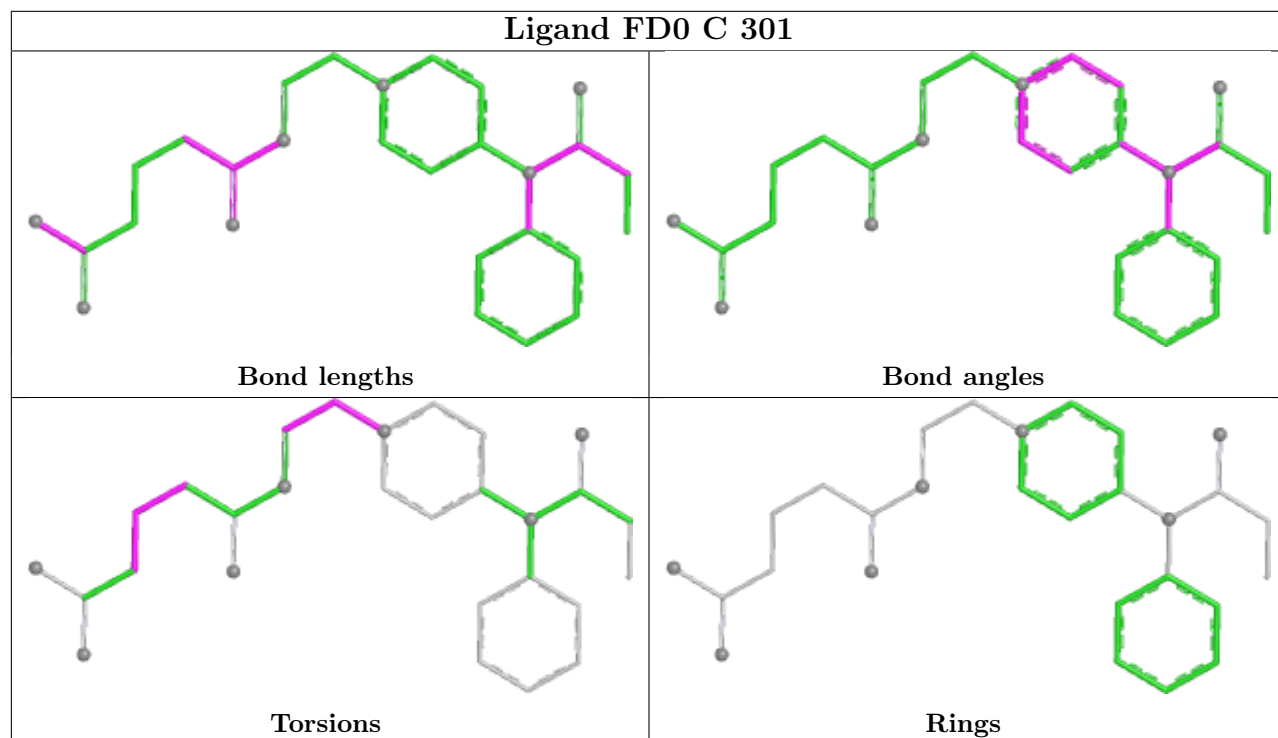
1 monomer is involved in 1 short contact:

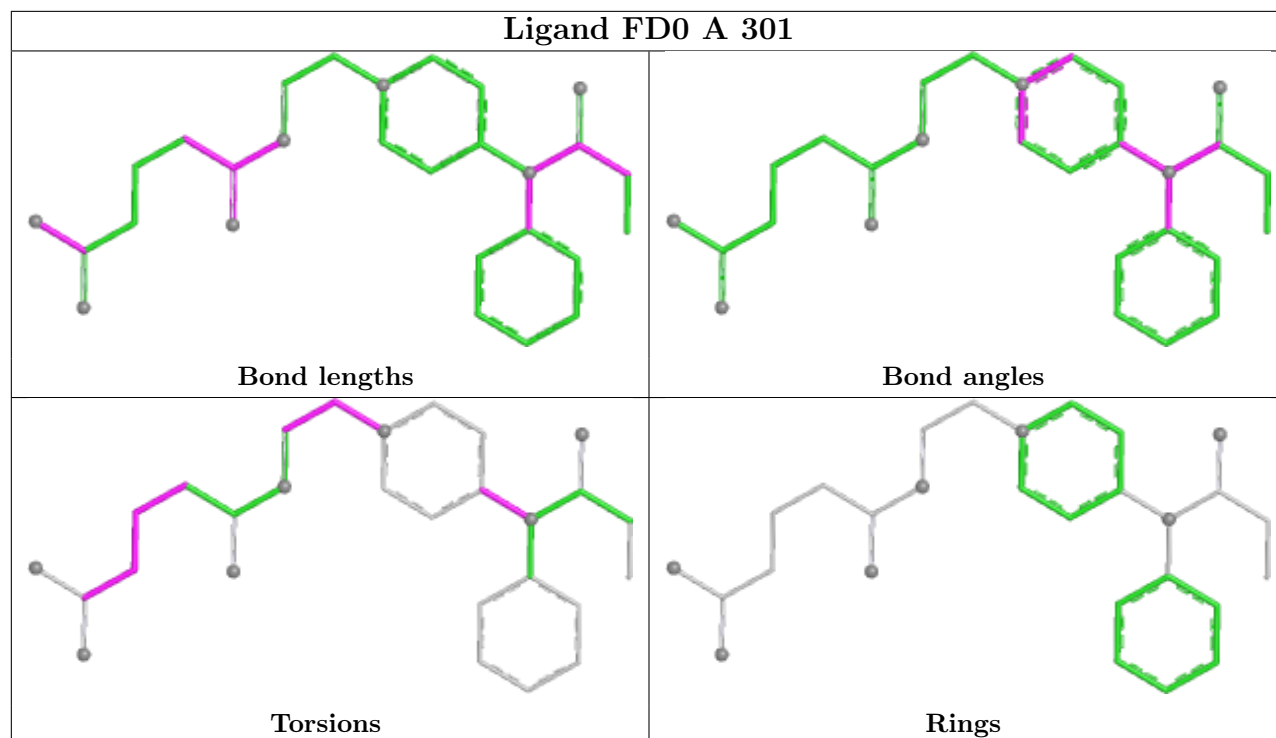
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	301	FD0	1	0

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 ⓘ

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	215/225 (95%)	1.04	17 (7%)	18 19	32, 41, 58, 75	0
1	C	216/225 (96%)	0.93	10 (4%)	37 37	23, 39, 55, 99	1 (0%)
1	E	217/225 (96%)	1.00	17 (7%)	19 19	24, 38, 55, 87	1 (0%)
1	G	214/225 (95%)	1.02	18 (8%)	17 17	32, 41, 60, 89	0
1	I	213/225 (94%)	0.97	15 (7%)	22 22	31, 40, 59, 71	0
1	K	214/225 (95%)	1.21	34 (15%)	5 5	30, 42, 68, 77	0
2	B	211/214 (98%)	1.26	33 (15%)	5 5	22, 45, 64, 74	1 (0%)
2	D	212/214 (99%)	1.13	31 (14%)	6 5	18, 44, 62, 75	2 (0%)
2	F	211/214 (98%)	1.16	30 (14%)	6 6	20, 43, 64, 82	2 (0%)
2	H	212/214 (99%)	1.29	31 (14%)	6 5	22, 48, 69, 83	2 (0%)
2	J	212/214 (99%)	1.57	64 (30%)	1 1	31, 51, 78, 97	0
2	L	211/214 (98%)	1.32	37 (17%)	4 3	19, 48, 69, 85	1 (0%)
All	All	2558/2634 (97%)	1.16	337 (13%)	7 7	18, 43, 67, 99	10 (0%)

All (337) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	ALA	5.3
2	J	150	ILE	5.0
1	E	136	ALA	4.7
2	J	146	VAL	4.7
1	E	133	PRO	4.7
1	K	118	VAL	4.6
2	F	163	TRP	4.4
2	B	7	SER	4.3
2	B	11	MET	4.3
1	A	120	SER	4.2
1	A	134	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	J	148	TRP	4.0
2	J	188	ARG	3.9
2	J	21	VAL	3.8
2	D	10	PHE	3.8
1	A	16	ALA	3.7
1	I	192	SER	3.6
2	H	70[A]	ASP	3.6
2	B	126	THR	3.6
2	J	202	THR	3.5
1	K	121	ALA	3.5
2	B	145[A]	ASN	3.5
1	C	135	SER	3.4
2	J	189	HIS	3.4
2	B	66	GLY	3.4
1	K	82	GLN	3.4
2	L	21	VAL	3.3
2	H	88	CYS	3.3
1	E	139	THR	3.3
2	L	160	LEU	3.3
1	K	134	GLY	3.3
2	B	5	THR	3.2
1	C	40[A]	ARG	3.2
2	J	206	VAL	3.2
2	H	163	TRP	3.2
2	J	96	LEU	3.2
1	A	179	SER	3.2
2	H	66	GLY	3.2
2	H	7	SER	3.2
2	J	212	ASN	3.2
1	G	86	LEU	3.1
2	B	94	TYR	3.1
2	L	94	TYR	3.1
2	L	209	PHE	3.1
2	L	1	ASP	3.1
2	F	148	TRP	3.1
2	F	7	SER	3.1
1	E	134	GLY	3.1
1	K	41	PRO	3.1
2	J	156	GLN	3.1
2	J	190	ASN	3.1
2	L	181	LEU	3.1
2	J	10	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	194	CYS	3.0
2	L	134	CYS	3.0
2	H	79[A]	GLN	3.0
1	G	140	ASN	3.0
1	I	60	TYR	3.0
2	H	53	TYR	3.0
1	K	65	LYS	3.0
1	A	121	ALA	3.0
2	F	146	VAL	3.0
2	F	160	LEU	3.0
2	L	127	SER	3.0
2	J	95	PRO	3.0
2	H	10	PHE	3.0
2	J	20	SER	3.0
2	L	196	ALA	3.0
1	A	118	VAL	3.0
1	K	165	SER	2.9
2	B	96	LEU	2.9
2	B	101	GLY	2.9
2	L	145	ASN	2.9
1	G	122	LYS	2.9
2	H	202	THR	2.9
1	K	16	ALA	2.9
1	K	113	GLY	2.9
1	G	104	TYR	2.9
2	H	94	TYR	2.9
1	I	66	GLY	2.9
2	F	194	CYS	2.8
2	J	193	THR	2.8
2	B	95	PRO	2.8
2	H	69	THR	2.8
2	D	156	GLN	2.8
2	J	154	GLU	2.8
2	H	150	ILE	2.8
2	L	205	ILE	2.8
2	B	4	MET	2.7
1	K	180	ASP	2.7
2	J	147	LYS	2.7
2	J	136	LEU	2.7
2	F	200	THR	2.7
2	H	33	VAL	2.7
2	B	26	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	47	TRP	2.7
2	F	158	GLY	2.7
2	F	10	PHE	2.7
2	J	192	TYR	2.7
2	J	157	ASN	2.7
2	B	23	CYS	2.7
2	F	184	ASP	2.7
2	F	79	GLN	2.7
2	J	200	THR	2.7
1	I	41	PRO	2.7
1	E	116	VAL	2.7
1	K	197	SER	2.7
2	D	159	VAL	2.7
2	B	60	ASP	2.7
2	D	70	ASP	2.7
2	H	185	GLU	2.6
2	H	212	ASN	2.6
1	K	179	SER	2.6
2	J	94	TYR	2.6
2	B	3	VAL	2.6
1	I	178	GLN	2.6
1	K	62	GLN	2.6
2	F	22	THR	2.6
2	J	181	LEU	2.6
2	L	106	LEU	2.6
1	E	135	SER	2.6
2	H	29	VAL	2.6
1	C	178	GLN	2.6
2	H	41	GLY	2.6
2	B	69	THR	2.6
2	D	209	PHE	2.6
1	A	220	ARG	2.6
2	D	211	ARG	2.6
1	I	104	TYR	2.6
1	G	220	ARG	2.6
2	J	13	THR	2.6
1	G	17	SER	2.6
2	L	156	GLN	2.5
1	A	18	VAL	2.5
1	C	118	VAL	2.5
2	F	152	GLY	2.5
2	L	147	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	211[A]	ARG	2.5
2	J	155	ARG	2.5
1	A	88	SER	2.5
1	K	88	SER	2.5
2	B	67	SER	2.5
2	J	129	GLY	2.5
1	E	140	ASN	2.5
2	L	210	ASN	2.5
1	I	133	PRO	2.5
1	K	43	GLN	2.5
2	J	197	THR	2.5
1	K	83	LEU	2.5
2	H	71	PHE	2.5
2	B	29	VAL	2.5
2	L	146	VAL	2.5
2	F	140	TYR	2.5
2	F	70	ASP	2.5
2	L	31	THR	2.5
1	G	41	PRO	2.5
1	G	92	ALA	2.5
2	H	95	PRO	2.5
1	C	177	LEU	2.5
2	L	104	LEU	2.5
2	F	145[A]	ASN	2.5
2	L	60	ASP	2.4
2	L	184	ASP	2.4
2	D	65	SER	2.4
2	L	153	SER	2.4
1	G	68	ALA	2.4
1	G	121	ALA	2.4
2	B	100	ALA	2.4
2	D	9	LYS	2.4
2	F	189	HIS	2.4
1	K	64	PHE	2.4
1	A	105	ASN	2.4
1	I	101	TYR	2.4
2	L	23	CYS	2.4
2	D	7	SER	2.4
2	H	26	SER	2.4
2	J	204	PRO	2.4
2	L	157	ASN	2.4
2	J	143	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	218	VAL	2.4
1	C	119	SER	2.4
2	J	175	MET	2.4
2	J	199	LYS	2.4
2	J	66	GLY	2.4
1	I	180	ASP	2.4
2	H	87	PHE	2.4
1	G	219	PRO	2.4
2	D	88	CYS	2.4
2	D	185	GLU	2.3
2	H	100	ALA	2.3
2	B	181	LEU	2.3
2	F	156	GLN	2.3
1	A	42	GLY	2.3
2	B	184	ASP	2.3
2	B	18	ARG	2.3
1	A	193	SER	2.3
2	B	21	VAL	2.3
2	B	115	VAL	2.3
2	F	203	SER	2.3
2	J	74	THR	2.3
2	D	154	GLU	2.3
2	J	194	CYS	2.3
2	D	25	ALA	2.3
2	D	100	ALA	2.3
2	J	196	ALA	2.3
1	K	15	GLY	2.3
2	J	16	GLY	2.3
2	J	128	GLY	2.3
2	J	60	ASP	2.3
2	J	9	LYS	2.3
2	J	149	LYS	2.3
1	G	179	SER	2.3
2	D	12	SER	2.3
2	J	153	SER	2.3
2	H	205	ILE	2.3
2	J	2	ILE	2.3
2	L	189	HIS	2.3
1	I	207	PRO	2.3
1	K	196	PRO	2.3
2	D	157	ASN	2.3
2	J	23	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	112	ALA	2.3
2	H	152	GLY	2.3
2	J	125	LEU	2.3
2	J	151	ASP	2.3
2	L	152	GLY	2.3
2	J	11	MET	2.3
1	I	179	SER	2.3
1	K	192	SER	2.3
2	J	7	SER	2.3
2	J	195	GLU	2.3
2	D	3	VAL	2.3
2	J	22	THR	2.3
1	A	122	LYS	2.3
2	F	149	LYS	2.3
1	K	86	LEU	2.3
2	J	53	TYR	2.3
1	G	118	VAL	2.2
2	L	53	TYR	2.2
2	L	188	ARG	2.2
1	K	87	THR	2.2
1	E	218	VAL	2.2
2	L	17	ASP	2.2
1	E	15	GLY	2.2
1	K	92	ALA	2.2
2	D	179	LEU	2.2
1	I	62	GLN	2.2
1	A	104	TYR	2.2
2	F	173	TYR	2.2
1	K	91	SER	2.2
2	J	163	TRP	2.2
2	H	22	THR	2.2
2	L	71	PHE	2.2
2	J	70	ASP	2.2
2	H	21	VAL	2.2
2	J	3	VAL	2.2
1	C	134	GLY	2.2
2	F	153	SER	2.2
1	E	101	TYR	2.2
2	B	49	TYR	2.2
2	F	24	LYS	2.2
2	D	163	TRP	2.2
1	C	199	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	2	VAL	2.1
2	D	152	GLY	2.1
2	H	27	GLN	2.1
2	J	152	GLY	2.1
1	K	68	ALA	2.1
1	I	84	SER	2.1
2	L	67	SER	2.1
2	L	201	SER	2.1
1	E	104	TYR	2.1
2	D	212	ASN	2.1
2	D	17	ASP	2.1
2	B	205	ILE	2.1
1	E	42	GLY	2.1
1	G	66	GLY	2.1
1	I	15	GLY	2.1
2	D	158	GLY	2.1
2	F	159	VAL	2.1
2	L	29	VAL	2.1
1	A	86	LEU	2.1
2	H	24	LYS	2.1
1	K	147	CYS	2.1
2	B	88	CYS	2.1
2	D	80	SER	2.1
1	K	90	ASP	2.1
2	D	165	ASP	2.1
1	K	60	TYR	2.1
2	D	69	THR	2.1
2	B	10	PHE	2.1
2	F	209	PHE	2.1
1	K	218	VAL	2.1
2	J	19	VAL	2.1
2	J	130	ALA	2.1
1	G	177	LEU	2.1
1	K	85	SER	2.1
2	L	7	SER	2.1
1	E	147	CYS	2.1
2	L	88	CYS	2.1
2	L	105	GLU	2.1
2	F	210	ASN	2.1
2	D	60	ASP	2.1
2	F	60	ASP	2.1
2	J	72	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	150	ILE	2.1
2	J	117	ILE	2.1
1	E	118	VAL	2.1
1	K	18	VAL	2.1
2	F	21	VAL	2.1
2	J	118	PHE	2.1
2	L	15	VAL	2.1
2	L	159	VAL	2.1
1	E	120	SER	2.1
1	G	120	SER	2.1
2	H	12	SER	2.1
2	D	190	ASN	2.0
2	D	79	GLN	2.0
2	B	211	ARG	2.0
1	K	158	THR	2.0
1	A	212	LYS	2.0
1	C	65	LYS	2.0
2	B	2	ILE	2.0
1	A	12	VAL	2.0
1	I	64	PHE	2.0
1	K	190	VAL	2.0
2	B	146	VAL	2.0
1	E	79	ALA	2.0
1	E	175	ALA	2.0
2	H	196	ALA	2.0
2	J	25	ALA	2.0
2	D	145	ASN	2.0
2	J	28	ASN	2.0
2	B	8	GLN	2.0
2	F	8	GLN	2.0
2	H	107	LYS	2.0
2	J	69	THR	2.0

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

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

6.3 Carbohydrates ⓘ

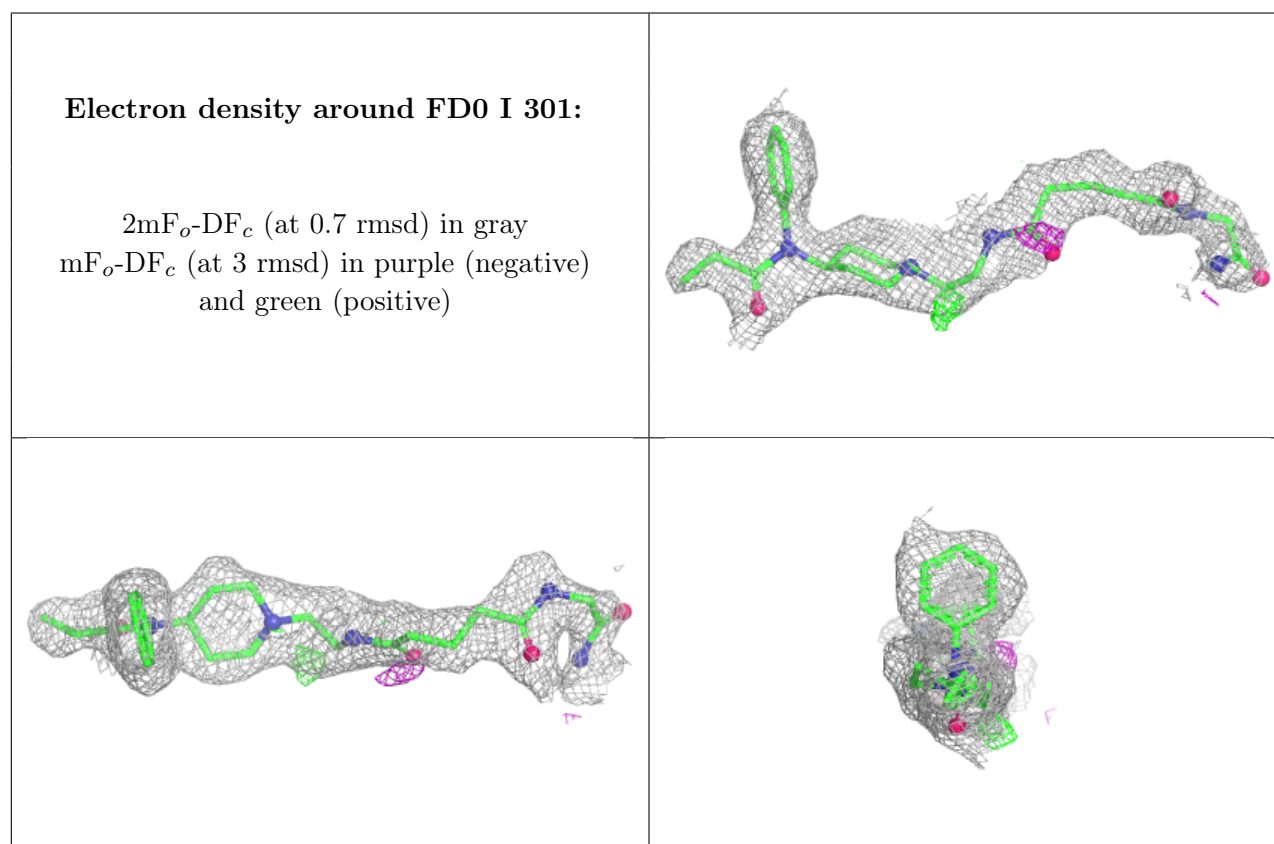
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

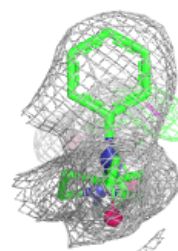
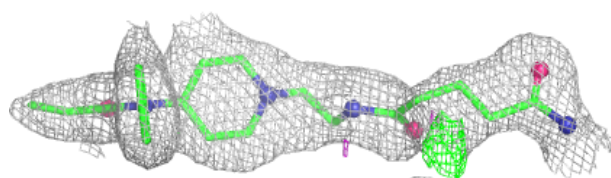
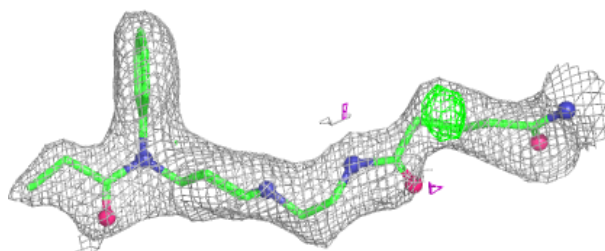
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FD0	I	301	32/44	0.83	0.16	40,49,66,78	0
3	FD0	G	301	28/44	0.85	0.15	38,45,54,57	0
3	FD0	K	301	28/44	0.85	0.15	36,43,58,66	0
3	FD0	C	301	28/44	0.87	0.14	33,42,59,61	0
3	FD0	A	301	28/44	0.87	0.15	34,43,53,63	0
3	FD0	E	301	28/44	0.88	0.13	31,37,52,60	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.

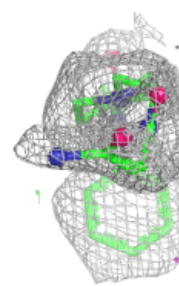
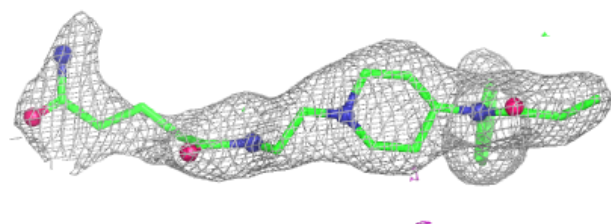
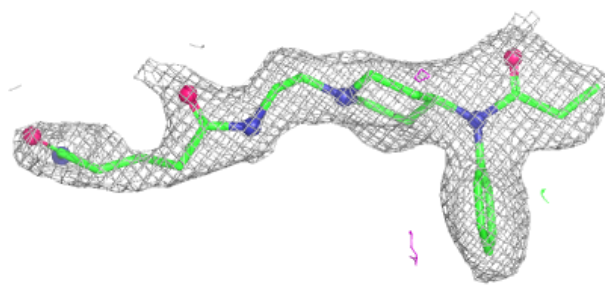


Electron density around FD0 G 301:

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

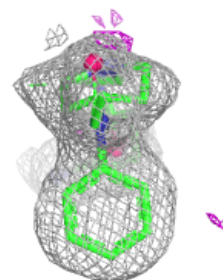
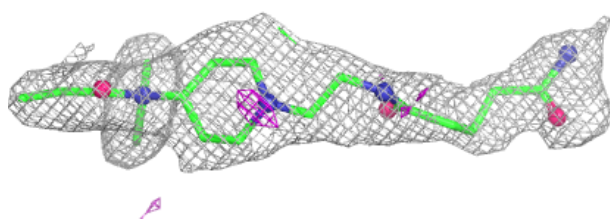
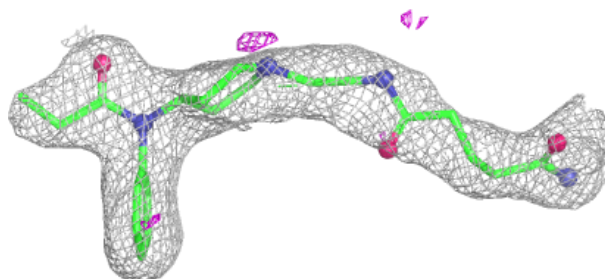
**Electron density around FD0 K 301:**

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

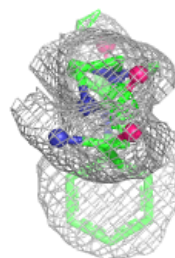
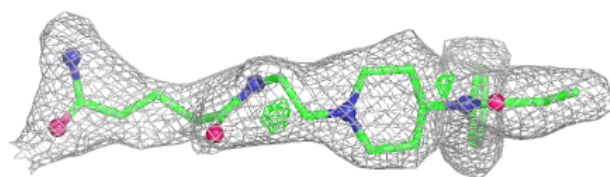
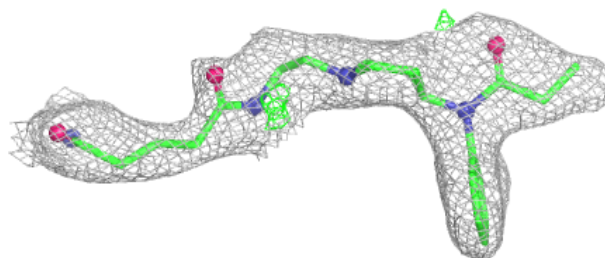


Electron density around FD0 C 301:

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

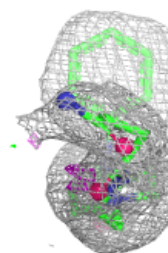
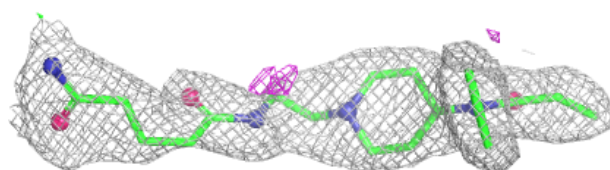
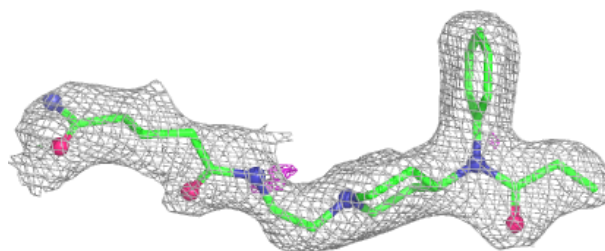
**Electron density around FD0 A 301:**

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



Electron density around FD0 E 301:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.