



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:29 am BST

PDB ID : 1FLR
Title : 4-4-20 FAB FRAGMENT
Authors : Whitlow, M.
Deposited on : 1995-01-19
Resolution : 1.85 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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

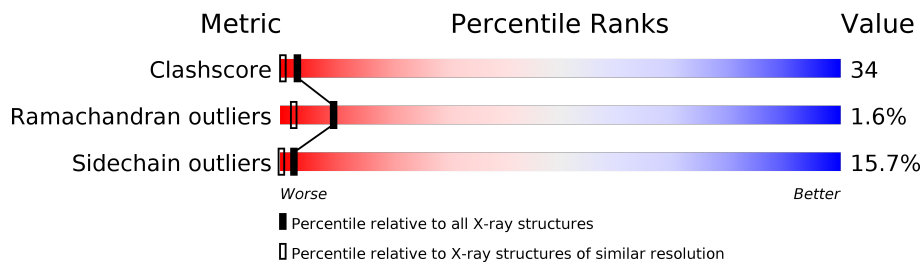
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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 on 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	219	58% 32% 9% .
2	H	219	37% 44% 14% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLU	L	600	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3700 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 4-4-20 (IG*G2A=KAPPA=) FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	1711	1068	293	343	7	0	4	0

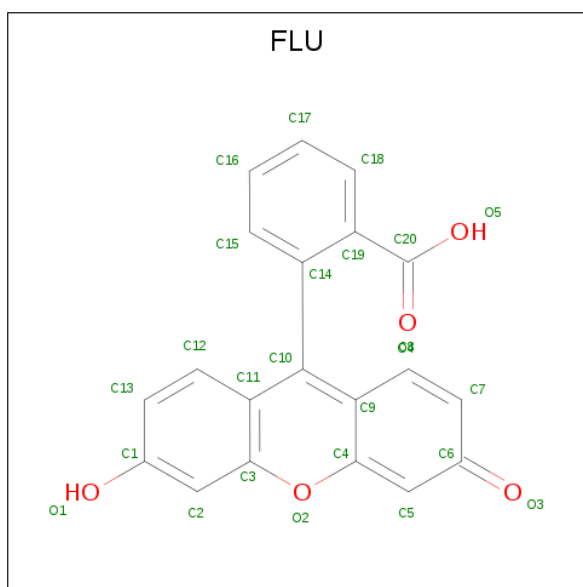
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	VAL	ILE	CONFLICT	GB 1589925
L	7	THR	SER	CONFLICT	GB 1589925
L	29	LEU	VAL	CONFLICT	GB 1589925
L	39	ARG	GLU	CONFLICT	GB 1589925
L	41	TYR	PHE	CONFLICT	GB 1589925
L	51	VAL	LEU	CONFLICT	GB 1589925
L	92	PHE	TYR	CONFLICT	GB 1589925
L	94	SER	PHE	CONFLICT	GB 1589925
L	96	SER	ALA	CONFLICT	GB 1589925
L	97	THR	SER	CONFLICT	GB 1589925
L	217	ASN	GLY	CONFLICT	GB 1589925

- Molecule 2 is a protein called 4-4-20 (IG*G2A=KAPPA=) FAB FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	216	1672	1062	274	326	10	0	6	0

- Molecule 3 is 2-(6-HYDROXY-3-OXO-3H-XANTHEN-9-YL)-BENZOIC ACID (three-letter code: FLU) (formula: C₂₀H₁₂O₅).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	C O	0	0
			25	20 5		

- Molecule 4 is water.

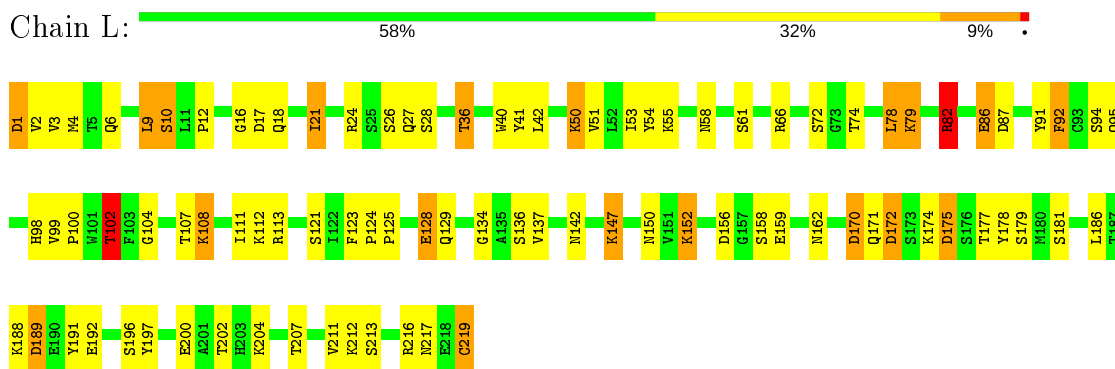
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	148	Total	O	0	1
			149	149		
4	H	142	Total	O	0	1
			143	143		

3 Residue-property plots [i](#)

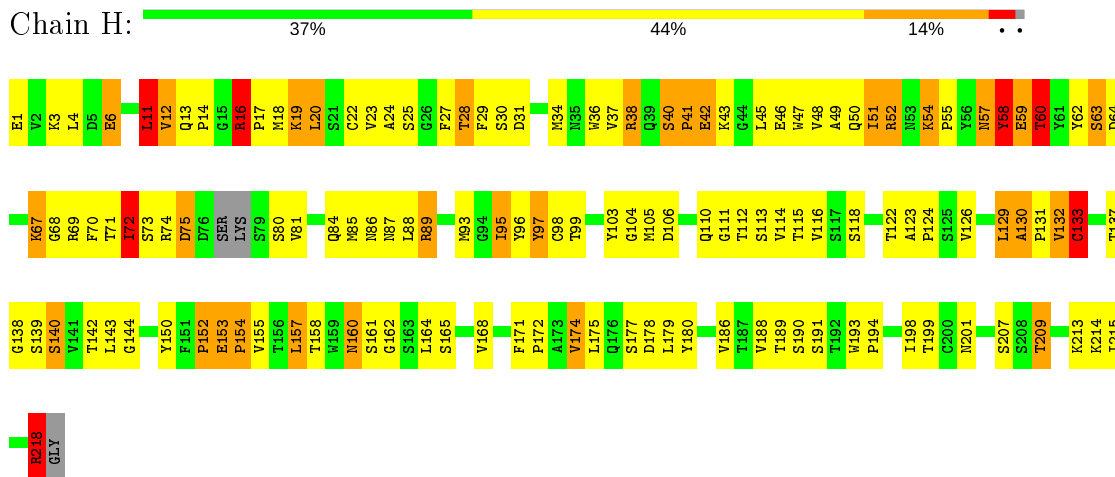
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: 4-4-20 (IG*G2A=KAPPA=) FAB FRAGMENT



- Molecule 2: 4-4-20 (IG*G2A=KAPPA=) FAB FRAGMENT



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	42.75Å 43.87Å 58.17Å 95.15° 86.85° 98.01°	Depositor
Resolution (Å)	10.00 – 1.85	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.85)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.188 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3700	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

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: FLU

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	L	1.08	2/1771 (0.1%)	1.83	37/2400 (1.5%)
2	H	7.04	2/1744 (0.1%)	2.11	40/2378 (1.7%)
All	All	5.02	4/3515 (0.1%)	1.97	77/4778 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	133[A]	CYS	N-CA	205.83	5.58	1.46
2	H	133[B]	CYS	N-CA	205.83	5.58	1.46
1	L	40	TRP	CG-CD1	6.33	1.45	1.36
1	L	134	GLY	N-CA	5.07	1.53	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	VAL	C-N-CA	-37.37	28.27	121.70
2	H	133[A]	CYS	N-CA-CB	-18.43	77.42	110.60
2	H	133[B]	CYS	N-CA-CB	-18.43	77.42	110.60
2	H	133[A]	CYS	N-CA-C	-18.37	61.39	111.00
2	H	133[B]	CYS	N-CA-C	-18.37	61.39	111.00
1	L	66	ARG	NE-CZ-NH2	11.47	126.03	120.30
2	H	52	ARG	CD-NE-CZ	10.77	138.68	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	152	PRO	C-N-CA	10.69	148.42	121.70
1	L	128	GLU	CA-CB-CG	10.52	136.55	113.40
1	L	86	GLU	CA-CB-CG	10.18	135.80	113.40
2	H	52	ARG	NE-CZ-NH1	10.03	125.31	120.30
1	L	189	ASP	CB-CG-OD1	-9.50	109.75	118.30
1	L	186	LEU	CA-CB-CG	9.43	136.99	115.30
1	L	175	ASP	CB-CG-OD1	9.39	126.75	118.30
1	L	87	ASP	CB-CG-OD2	-8.86	110.32	118.30
2	H	106	ASP	CB-CG-OD2	8.59	126.03	118.30
2	H	218	ARG	NE-CZ-NH1	8.49	124.54	120.30
2	H	154	PRO	N-CA-C	8.27	133.60	112.10
2	H	103	TYR	CB-CG-CD2	-7.97	116.22	121.00
2	H	89	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	L	170	ASP	CB-CG-OD1	7.91	125.42	118.30
1	L	40	TRP	CB-CG-CD2	7.65	136.55	126.60
2	H	38	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	L	92	PHE	CB-CG-CD1	-7.27	115.71	120.80
1	L	216	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	H	112	THR	N-CA-CB	7.03	123.66	110.30
1	L	192	GLU	OE1-CD-OE2	6.98	131.68	123.30
1	L	102	THR	N-CA-CB	-6.74	97.50	110.30
1	L	86	GLU	N-CA-CB	6.63	122.54	110.60
1	L	102	THR	CA-CB-CG2	6.62	121.67	112.40
2	H	45	LEU	CB-CA-C	6.44	122.43	110.20
2	H	103	TYR	CB-CG-CD1	6.40	124.84	121.00
1	L	170	ASP	CA-CB-CG	6.34	127.35	113.40
2	H	16	ARG	CD-NE-CZ	6.25	132.34	123.60
1	L	78	LEU	CA-CB-CG	6.24	129.66	115.30
1	L	40	TRP	CB-CG-CD1	-6.21	118.92	127.00
2	H	72[A]	ILE	N-CA-CB	6.17	124.98	110.80
2	H	72[B]	ILE	N-CA-CB	6.17	124.98	110.80
2	H	58	TYR	CB-CG-CD2	-6.11	117.34	121.00
1	L	36	THR	N-CA-CB	5.99	121.68	110.30
1	L	172	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	H	59	GLU	N-CA-CB	5.98	121.36	110.60
2	H	11[A]	LEU	CA-CB-CG	5.88	128.82	115.30
2	H	11[B]	LEU	CA-CB-CG	5.88	128.82	115.30
1	L	82	ARG	CA-CB-CG	5.80	126.16	113.40
1	L	10	SER	O-C-N	5.78	131.95	122.70
2	H	97	TYR	O-C-N	5.77	131.94	122.70
2	H	133[A]	CYS	C-N-CA	5.77	134.41	122.30
2	H	133[B]	CYS	C-N-CA	5.77	134.41	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	42	GLU	CA-CB-CG	5.76	126.07	113.40
2	H	209	THR	CA-CB-CG2	5.70	120.38	112.40
1	L	191	TYR	CD1-CE1-CZ	5.70	124.93	119.80
1	L	192	GLU	CG-CD-OE2	-5.67	106.95	118.30
2	H	130	ALA	CB-CA-C	5.64	118.56	110.10
1	L	197	TYR	CB-CG-CD2	-5.62	117.63	121.00
2	H	174	VAL	CA-CB-CG1	5.54	119.22	110.90
2	H	52	ARG	CG-CD-NE	5.53	123.41	111.80
1	L	213	SER	N-CA-CB	-5.47	102.30	110.50
1	L	158	SER	N-CA-CB	5.43	118.65	110.50
2	H	154	PRO	O-C-N	-5.41	114.04	122.70
2	H	104	GLY	CA-C-O	-5.40	110.89	120.60
2	H	6	GLU	CA-CB-CG	5.39	125.27	113.40
2	H	60	THR	N-CA-CB	-5.39	100.06	110.30
1	L	53	ILE	CA-CB-CG1	5.37	121.21	111.00
1	L	92	PHE	N-CA-CB	-5.36	100.96	110.60
1	L	54	TYR	CB-CG-CD1	-5.35	117.79	121.00
1	L	219	CYS	CA-CB-SG	5.34	123.61	114.00
1	L	41	TYR	O-C-N	5.31	131.19	122.70
1	L	10	SER	N-CA-CB	5.26	118.39	110.50
2	H	36	TRP	N-CA-CB	5.26	120.06	110.60
1	L	137	VAL	C-N-CA	5.24	134.81	121.70
2	H	104	GLY	O-C-N	5.18	131.00	122.70
1	L	178	TYR	CB-CG-CD2	5.16	124.10	121.00
2	H	28	THR	O-C-N	5.11	130.87	122.70
1	L	189	ASP	CB-CG-OD2	5.08	122.88	118.30
1	L	17	ASP	CA-CB-CG	5.01	124.43	113.40
2	H	179	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	132	VAL	Peptide

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	L	1711	0	1661	61	1
2	H	1672	0	1607	174	0
3	L	25	0	10	1	0
4	H	143	0	0	15	0
4	L	149	0	0	13	0
All	All	3700	0	3278	228	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 34.

All (228) 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:H:164:LEU:HD13	4:H:836:HOH:O	1.31	1.30
2:H:12:VAL:HG12	2:H:18:MET:CE	1.78	1.13
2:H:49:ALA:HB1	2:H:72[A]:ILE:HD11	1.32	1.09
2:H:51:ILE:HD13	2:H:74:ARG:CD	1.83	1.07
2:H:51:ILE:CD1	2:H:74:ARG:HG2	1.86	1.06
1:L:50:LYS:NZ	4:L:702:HOH:O	1.76	1.04
2:H:54:LYS:HB3	2:H:55:PRO:HD3	1.38	1.02
2:H:19:LYS:HG3	2:H:84:GLN:HG3	1.40	1.01
1:L:172:ASP:OD2	1:L:174:LYS:HG2	1.59	1.00
2:H:51:ILE:HD13	2:H:74:ARG:HD2	1.44	0.99
2:H:12:VAL:HB	2:H:16:ARG:NH2	1.78	0.99
2:H:12:VAL:HG12	2:H:18:MET:HE3	1.45	0.98
2:H:16:ARG:HH11	2:H:16:ARG:HB3	1.27	0.98
2:H:153[A]:GLU:HB2	2:H:154:PRO:HD3	1.44	0.97
2:H:161:SER:H	2:H:201:ASN:ND2	1.62	0.96
2:H:48:VAL:O	2:H:63:SER:OG	1.85	0.94
2:H:161:SER:H	2:H:201:ASN:HD21	1.03	0.94
2:H:12:VAL:HG12	2:H:18:MET:HE1	1.47	0.93
2:H:23:VAL:HG12	2:H:80:SER:OG	1.70	0.92
1:L:152:LYS:HE2	1:L:159:GLU:HG2	1.51	0.92
2:H:51:ILE:HD13	2:H:74:ARG:CG	2.01	0.89
1:L:150:ASN:ND2	4:L:742:HOH:O	2.06	0.88
2:H:12:VAL:CG1	2:H:18:MET:CE	2.51	0.88
1:L:99:VAL:HG13	1:L:100:PRO:HA	1.55	0.88
2:H:17:PRO:HB3	2:H:86:ASN:HA	1.56	0.87
2:H:12:VAL:HB	2:H:16:ARG:CZ	2.06	0.86
2:H:20:LEU:HD22	2:H:85:MET:SD	2.15	0.86
2:H:43:LYS:NZ	2:H:43:LYS:HB3	1.91	0.86
2:H:62:TYR:O	4:H:780:HOH:O	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HD13	2:H:74:ARG:HG2	1.54	0.85
2:H:16:ARG:CB	2:H:16:ARG:HH11	1.89	0.85
2:H:49:ALA:HB1	2:H:72[A]:ILE:CD1	2.07	0.85
2:H:154:PRO:HB3	4:H:822:HOH:O	1.77	0.83
2:H:70:PHE:O	4:H:704:HOH:O	1.96	0.83
2:H:48:VAL:HA	2:H:63:SER:OG	1.80	0.82
2:H:54:LYS:HB3	2:H:55:PRO:CD	2.10	0.81
2:H:55:PRO:HG3	4:H:777:HOH:O	1.79	0.81
1:L:202:THR:HG23	4:L:754:HOH:O	1.82	0.80
2:H:16:ARG:O	2:H:88:LEU:HB2	1.82	0.80
2:H:16:ARG:NH1	2:H:16:ARG:HB3	1.99	0.77
2:H:154:PRO:CB	4:H:822:HOH:O	2.32	0.77
2:H:12:VAL:CG1	2:H:18:MET:HE1	2.12	0.77
2:H:153[B]:GLU:HB2	2:H:154:PRO:HD3	1.66	0.75
2:H:54:LYS:CB	2:H:55:PRO:HD3	2.15	0.75
2:H:20:LEU:CD2	2:H:85:MET:SD	2.74	0.75
2:H:12:VAL:CG1	2:H:18:MET:HE3	2.13	0.74
2:H:89:ARG:NH2	4:H:789:HOH:O	2.16	0.73
2:H:51:ILE:HD12	2:H:74:ARG:HG2	1.71	0.72
2:H:43:LYS:HZ3	2:H:43:LYS:HB3	1.53	0.71
1:L:147:LYS:HD2	4:L:603:HOH:O	1.90	0.71
1:L:99:VAL:CG1	1:L:100:PRO:HA	2.21	0.71
2:H:157:LEU:HD12	2:H:158:THR:N	2.06	0.70
2:H:207:SER:OG	2:H:209:THR:HG23	1.91	0.70
2:H:12:VAL:CB	2:H:16:ARG:NH2	2.55	0.68
2:H:51:ILE:HB	2:H:72[B]:ILE:HG12	1.73	0.68
2:H:70:PHE:CD1	2:H:85:MET:HA	2.28	0.68
1:L:147:LYS:CD	4:L:603:HOH:O	2.42	0.68
1:L:156:ASP:HA	1:L:196:SER:OG	1.94	0.67
2:H:168:VAL:HG12	2:H:186:VAL:HG23	1.77	0.67
2:H:70:PHE:CZ	2:H:85:MET:HE3	2.29	0.67
2:H:38:ARG:NH1	2:H:96:TYR:OH	2.26	0.67
1:L:58:ASN:OD1	4:L:643:HOH:O	2.11	0.66
2:H:140:SER:HA	2:H:189:THR:HA	1.77	0.66
1:L:111:ILE:H	1:L:171:GLN:HE22	1.41	0.66
1:L:2:VAL:O	1:L:102:THR:HG21	1.95	0.66
2:H:13[B]:GLN:NE2	4:H:762:HOH:O	2.29	0.66
1:L:9:LEU:O	1:L:108[A]:LYS:HD2	1.96	0.65
2:H:28:THR:HG21	2:H:31:ASP:OD2	1.96	0.65
1:L:100:PRO:HB3	2:H:47:TRP:CZ3	2.32	0.65
2:H:67:LYS:HD3	2:H:68:GLY:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:SER:N	2:H:201:ASN:HD21	1.87	0.64
2:H:67:LYS:HB3	4:H:782:HOH:O	1.96	0.64
1:L:136:SER:O	4:L:602:HOH:O	2.15	0.64
2:H:70:PHE:CE2	2:H:85:MET:HE3	2.34	0.63
1:L:6[B]:GLN:NE2	1:L:91:TYR:O	2.25	0.63
2:H:12:VAL:HB	2:H:16:ARG:HH22	1.58	0.63
2:H:161:SER:N	2:H:201:ASN:ND2	2.43	0.63
2:H:24:ALA:HB3	2:H:29:PHE:CD2	2.34	0.62
2:H:6:GLU:OE2	2:H:97:TYR:HA	1.97	0.62
2:H:43:LYS:CB	2:H:43:LYS:HZ3	2.12	0.62
2:H:51:ILE:CD1	2:H:74:ARG:CG	2.63	0.62
2:H:43:LYS:CB	2:H:43:LYS:NZ	2.63	0.61
2:H:54:LYS:CB	2:H:55:PRO:CD	2.75	0.61
2:H:164:LEU:CD1	4:H:836:HOH:O	2.12	0.61
1:L:121:SER:OG	2:H:142:THR:HG21	2.02	0.60
1:L:219:CYS:HA	2:H:133[B]:CYS:HA	1.83	0.60
1:L:100:PRO:HB3	2:H:47:TRP:HZ3	1.66	0.60
2:H:193:TRP:HB2	2:H:198:ILE:HD12	1.83	0.59
1:L:21:ILE:HD13	1:L:107:THR:OG1	2.03	0.59
1:L:152:LYS:HE2	1:L:159:GLU:CG	2.28	0.59
2:H:87:ASN:HA	4:H:861:HOH:O	2.03	0.59
2:H:51:ILE:HG23	2:H:74:ARG:HD2	1.84	0.59
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.83	0.58
2:H:12:VAL:HB	2:H:16:ARG:NH1	2.18	0.58
2:H:158:THR:CG2	2:H:162:GLY:N	2.66	0.58
1:L:121:SER:OG	2:H:142:THR:CG2	2.52	0.58
2:H:158:THR:HG23	2:H:162:GLY:N	2.18	0.58
2:H:70:PHE:HA	2:H:84:GLN:O	2.04	0.57
2:H:34:MET:HB2	2:H:51:ILE:HG22	1.85	0.57
2:H:85:MET:HE2	2:H:88:LEU:HD21	1.87	0.57
2:H:126:VAL:O	2:H:213:LYS:NZ	2.37	0.57
2:H:49:ALA:HB1	2:H:72[A]:ILE:CG1	2.35	0.57
2:H:12:VAL:HG22	2:H:116:VAL:HG22	1.87	0.56
1:L:6[B]:GLN:HG3	1:L:21:ILE:HD11	1.86	0.56
2:H:43:LYS:HZ2	2:H:43:LYS:HB3	1.70	0.56
1:L:189:ASP:HB2	4:L:858:HOH:O	2.05	0.56
1:L:100:PRO:CB	2:H:47:TRP:CZ3	2.88	0.56
2:H:218:ARG:CG	2:H:218:ARG:O	2.54	0.56
1:L:6[A]:GLN:HG3	1:L:104:GLY:HA3	1.88	0.55
2:H:16:ARG:HG2	2:H:17:PRO:CD	2.36	0.55
1:L:95:GLN:HE21	1:L:102:THR:HB	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:MET:HG2	1:L:102:THR:CG2	2.37	0.55
2:H:123:ALA:HB1	2:H:209:THR:HG21	1.89	0.55
2:H:158:THR:HG22	2:H:201:ASN:HD22	1.71	0.54
1:L:6[B]:GLN:CG	1:L:21:ILE:HD11	2.38	0.54
2:H:193:TRP:CD1	2:H:198:ILE:HD12	2.43	0.54
2:H:37:VAL:HG13	2:H:46:GLU:O	2.08	0.54
2:H:110[A]:GLN:HG3	2:H:111:GLY:N	2.23	0.53
2:H:18:MET:O	2:H:85:MET:N	2.34	0.53
2:H:139:SER:O	2:H:140:SER:O	2.27	0.53
2:H:12:VAL:CG1	2:H:16:ARG:HH22	2.21	0.53
2:H:95:ILE:HD12	2:H:95:ILE:N	2.24	0.53
2:H:62:TYR:CE1	2:H:72[A]:ILE:HD12	2.43	0.53
2:H:69:ARG:HB3	2:H:86:ASN:O	2.09	0.53
1:L:172:ASP:OD2	1:L:174:LYS:CG	2.45	0.52
2:H:62:TYR:OH	2:H:71:THR:HA	2.10	0.52
2:H:164:LEU:HD21	2:H:186:VAL:HG21	1.91	0.52
2:H:16:ARG:HH22	2:H:18:MET:HE3	1.75	0.52
1:L:156:ASP:HA	1:L:196:SER:HG	1.73	0.52
2:H:31:ASP:OD1	4:H:857:HOH:O	2.19	0.51
2:H:165:SER:O	2:H:168:VAL:HG13	2.11	0.51
2:H:62:TYR:CZ	2:H:72[A]:ILE:HD12	2.45	0.51
2:H:23:VAL:HG12	2:H:80:SER:CB	2.41	0.51
1:L:12:PRO:HB2	1:L:112[A]:LYS:HB2	1.91	0.51
2:H:16:ARG:HG2	2:H:17:PRO:HD2	1.93	0.51
2:H:24:ALA:HB3	2:H:29:PHE:HD2	1.74	0.51
1:L:200:GLU:HG3	1:L:211:VAL:HG22	1.93	0.51
1:L:175:ASP:OD1	1:L:177:THR:OG1	2.22	0.50
2:H:130:ALA:HB1	2:H:131:PRO:HD2	1.93	0.50
1:L:2:VAL:HG21	1:L:98:HIS:ND1	2.26	0.50
2:H:193:TRP:HB2	2:H:198:ILE:CD1	2.42	0.50
1:L:2:VAL:HA	1:L:26:SER:OG	2.11	0.49
2:H:93:MET:HG3	2:H:114:VAL:O	2.11	0.49
2:H:73:SER:O	2:H:81:VAL:HA	2.10	0.49
2:H:153[B]:GLU:CD	4:H:795:HOH:O	2.51	0.49
2:H:67:LYS:C	2:H:67:LYS:CD	2.81	0.49
2:H:157:LEU:C	2:H:157:LEU:HD12	2.33	0.49
2:H:12:VAL:CB	2:H:16:ARG:HH22	2.23	0.49
2:H:133[B]:CYS:N	2:H:218:ARG:HD3	2.28	0.49
2:H:18:MET:N	2:H:85:MET:O	2.30	0.49
2:H:70:PHE:CZ	2:H:85:MET:CE	2.94	0.49
1:L:129:GLN:NE2	4:L:632:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:VAL:HG12	2:H:80:SER:HG	1.76	0.48
2:H:14:PRO:HA	2:H:88:LEU:O	2.13	0.48
1:L:150:ASN:HB3	1:L:202:THR:OG1	2.13	0.48
1:L:50:LYS:HE2	1:L:50:LYS:HB2	1.43	0.48
2:H:57:ASN:O	2:H:59:GLU:N	2.47	0.48
2:H:25:SER:O	4:H:679:HOH:O	2.20	0.48
1:L:28:SER:HA	1:L:74:THR:HG22	1.95	0.48
2:H:4:LEU:HD23	2:H:98:CYS:SG	2.53	0.47
2:H:133[B]:CYS:N	2:H:218:ARG:CG	2.77	0.47
2:H:38:ARG:NE	2:H:46:GLU:OE1	2.29	0.47
2:H:87:ASN:CA	4:H:861:HOH:O	2.61	0.47
1:L:61:SER:O	1:L:61:SER:OG	2.31	0.47
2:H:171:PHE:HA	2:H:172:PRO:HD3	1.73	0.47
2:H:38:ARG:HA	2:H:95:ILE:O	2.14	0.47
2:H:139:SER:HA	2:H:190:SER:HB2	1.97	0.47
2:H:17:PRO:HA	2:H:88:LEU:HD12	1.96	0.47
2:H:62:TYR:CE1	2:H:72[A]:ILE:CD1	2.98	0.47
1:L:147:LYS:HD3	4:L:603:HOH:O	2.13	0.47
3:L:600:FLU:C15	3:L:600:FLU:H8	2.43	0.47
2:H:75:ASP:OD1	2:H:75:ASP:C	2.54	0.46
2:H:140:SER:HA	2:H:188:VAL:O	2.15	0.46
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.50	0.46
2:H:70:PHE:CE1	2:H:85:MET:HB3	2.51	0.46
1:L:112[A]:LYS:HG3	1:L:113:ARG:N	2.31	0.46
2:H:3:LYS:HE2	2:H:3:LYS:HB3	1.76	0.46
2:H:75:ASP:O	2:H:75:ASP:OD1	2.33	0.46
1:L:28:SER:O	1:L:98:HIS:HE1	1.99	0.46
2:H:193:TRP:CG	2:H:194:PRO:HA	2.51	0.45
1:L:42:LEU:HD13	1:L:91:TYR:CZ	2.52	0.45
2:H:177:SER:O	2:H:178:ASP:HB2	2.16	0.45
2:H:6:GLU:OE2	2:H:98:CYS:N	2.42	0.45
1:L:125:PRO:O	2:H:218:ARG:NH2	2.41	0.45
1:L:123:PHE:HA	1:L:124:PRO:HD3	1.85	0.45
2:H:40:SER:O	2:H:42:GLU:N	2.50	0.44
1:L:2:VAL:HG22	1:L:27:GLN:HB2	1.98	0.44
2:H:51:ILE:HG23	2:H:51:ILE:O	2.17	0.44
2:H:48:VAL:C	2:H:63:SER:OG	2.55	0.44
2:H:96:TYR:O	2:H:111:GLY:HA2	2.16	0.44
2:H:193:TRP:CD1	2:H:194:PRO:HA	2.52	0.44
2:H:22:CYS:HB3	2:H:81:VAL:HG13	1.99	0.44
1:L:79:LYS:HB2	4:L:873:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:175:LEU:HG	2:H:180:TYR:CE1	2.53	0.44
2:H:85:MET:HB3	2:H:85:MET:HE2	1.69	0.44
2:H:160:ASN:ND2	2:H:199:THR:H	2.16	0.43
2:H:37:VAL:CG1	2:H:46:GLU:O	2.66	0.43
2:H:16:ARG:HH11	2:H:16:ARG:CG	2.31	0.43
2:H:42:GLU:N	2:H:42:GLU:OE1	2.50	0.43
2:H:52:ARG:O	2:H:74:ARG:NH1	2.51	0.43
1:L:100:PRO:HB2	2:H:47:TRP:CE3	2.54	0.43
1:L:4:MET:HA	1:L:24:ARG:O	2.18	0.43
1:L:6[A]:GLN:OE1	1:L:92:PHE:HA	2.19	0.43
2:H:42:GLU:HB2	2:H:43:LYS:H	1.61	0.43
2:H:62:TYR:CZ	2:H:72[B]:ILE:HG22	2.54	0.42
2:H:54:LYS:HG3	2:H:58:TYR:OH	2.19	0.42
2:H:11[A]:LEU:HD23	2:H:12:VAL:H	1.84	0.42
2:H:50:GLN:O	2:H:60:THR:HA	2.19	0.42
2:H:129:LEU:HB2	2:H:144:GLY:C	2.39	0.42
2:H:110[A]:GLN:HG3	2:H:111:GLY:H	1.85	0.42
2:H:12:VAL:O	2:H:116:VAL:HA	2.20	0.41
2:H:12:VAL:HG12	2:H:16:ARG:HH22	1.86	0.41
2:H:138:GLY:HA2	2:H:190:SER:OG	2.21	0.41
2:H:150:TYR:CE2	2:H:155:VAL:HG13	2.55	0.41
1:L:1:ASP:HA	4:L:622:HOH:O	2.21	0.41
2:H:131:PRO:O	2:H:218:ARG:HD2	2.20	0.41
2:H:16:ARG:HH11	2:H:16:ARG:C	2.25	0.41
1:L:142:ASN:HD22	1:L:179:SER:HB3	1.86	0.41
1:L:3:VAL:HB	1:L:26:SER:HB3	2.03	0.40
1:L:16:GLY:HA2	1:L:82:ARG:HD2	2.03	0.40
2:H:49:ALA:CB	2:H:72[A]:ILE:CG1	2.99	0.40
1:L:188:LYS:HE3	4:L:740:HOH:O	2.21	0.40
1:L:36:THR:O	1:L:55:LYS:HA	2.21	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)
1:L:27:GLN:OE1	1:L:82:ARG:NH2[1_655]	2.08	0.12

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	L	221/219 (101%)	216 (98%)	4 (2%)	1 (0%)	29	15
2	H	216/219 (99%)	185 (86%)	23 (11%)	8 (4%)	3	0
All	All	437/438 (100%)	401 (92%)	27 (6%)	9 (2%)	9	1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	162	ASN
2	H	58	TYR
2	H	133[A]	CYS
2	H	133[B]	CYS
2	H	140	SER
2	H	41	PRO
2	H	137	THR
2	H	153[A]	GLU
2	H	153[B]	GLU

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	L	200/197 (102%)	175 (88%)	25 (12%)	4	0
2	H	191/192 (100%)	152 (80%)	39 (20%)	1	0
All	All	391/389 (100%)	327 (84%)	64 (16%)	2	0

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	9	LEU
1	L	10	SER
1	L	18	GLN
1	L	21	ILE
1	L	50	LYS
1	L	51	VAL
1	L	72	SER
1	L	78	LEU
1	L	79	LYS
1	L	82	ARG
1	L	86	GLU
1	L	94	SER
1	L	102	THR
1	L	108[A]	LYS
1	L	108[B]	LYS
1	L	128	GLU
1	L	147	LYS
1	L	152	LYS
1	L	170	ASP
1	L	181	SER
1	L	204	LYS
1	L	207	THR
1	L	212	LYS
1	L	217	ASN
2	H	1	GLU
2	H	11[A]	LEU
2	H	11[B]	LEU
2	H	12	VAL
2	H	16	ARG
2	H	19	LYS
2	H	20	LEU
2	H	30	SER
2	H	40	SER
2	H	41	PRO
2	H	51	ILE
2	H	54	LYS
2	H	57	ASN
2	H	60	THR
2	H	63	SER
2	H	64	ASP
2	H	67	LYS

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Mol	Chain	Res	Type
2	H	72[A]	ILE
2	H	72[B]	ILE
2	H	75	ASP
2	H	95	ILE
2	H	99	THR
2	H	105	MET
2	H	113	SER
2	H	115	THR
2	H	118	SER
2	H	122	THR
2	H	129	LEU
2	H	133[A]	CYS
2	H	133[B]	CYS
2	H	143	LEU
2	H	152	PRO
2	H	157	LEU
2	H	160	ASN
2	H	174	VAL
2	H	191	SER
2	H	214	LYS
2	H	215	ILE
2	H	218	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	31	HIS
1	L	47	GLN
1	L	58	ASN
1	L	98	HIS
1	L	129	GLN
1	L	142	ASN
1	L	162	ASN
1	L	171	GLN
1	L	194	HIS
1	L	215	ASN
1	L	217	ASN
2	H	160	ASN
2	H	176	GLN
2	H	196	GLN
2	H	201	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	FLU	L	600	-	24,28,28	4.37	12 (50%)	28,41,41	6.59	22 (78%)

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	FLU	L	600	-	-	0/4/12/12	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	600	FLU	C14-C10	-14.76	1.32	1.50
3	L	600	FLU	O2-C3	7.46	1.49	1.36
3	L	600	FLU	C19-C20	-5.88	1.41	1.47
3	L	600	FLU	O1-C1	-5.71	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	600	FLU	C11-C3	-5.60	1.33	1.41
3	L	600	FLU	C10-C11	-5.25	1.33	1.43
3	L	600	FLU	C9-C10	4.44	1.46	1.39
3	L	600	FLU	C13-C1	-2.66	1.33	1.38
3	L	600	FLU	C2-C1	2.61	1.42	1.37
3	L	600	FLU	C17-C16	2.25	1.44	1.38
3	L	600	FLU	C12-C13	2.24	1.41	1.36
3	L	600	FLU	C5-C4	2.13	1.41	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	600	FLU	C9-C10-C11	-18.15	104.18	119.63
3	L	600	FLU	C8-C9-C10	-16.90	111.88	122.70
3	L	600	FLU	C10-C11-C3	10.65	129.23	119.21
3	L	600	FLU	O2-C4-C5	-9.00	105.36	116.03
3	L	600	FLU	C12-C11-C10	-8.69	109.69	122.47
3	L	600	FLU	C14-C10-C11	7.31	131.73	119.42
3	L	600	FLU	C17-C18-C19	6.17	130.75	120.33
3	L	600	FLU	C1-C2-C3	-5.58	112.58	120.42
3	L	600	FLU	C13-C12-C11	-5.48	113.51	121.13
3	L	600	FLU	C16-C17-C18	-5.01	112.56	120.19
3	L	600	FLU	C7-C6-C5	4.10	123.63	117.49
3	L	600	FLU	C12-C11-C3	3.96	121.08	116.50
3	L	600	FLU	C18-C19-C14	-3.94	114.76	118.67
3	L	600	FLU	C18-C19-C20	-3.91	114.38	120.20
3	L	600	FLU	O2-C3-C2	-3.72	111.74	116.11
3	L	600	FLU	C16-C15-C14	3.65	126.50	120.33
3	L	600	FLU	C5-C4-C9	3.48	125.03	118.69
3	L	600	FLU	C12-C13-C1	3.31	123.96	120.15
3	L	600	FLU	C7-C8-C9	-2.86	115.44	120.33
3	L	600	FLU	C15-C14-C10	2.53	124.61	119.41
3	L	600	FLU	C2-C3-C11	2.51	125.83	123.05
3	L	600	FLU	O1-C1-C2	-2.09	114.99	120.98

There are no chirality outliers.

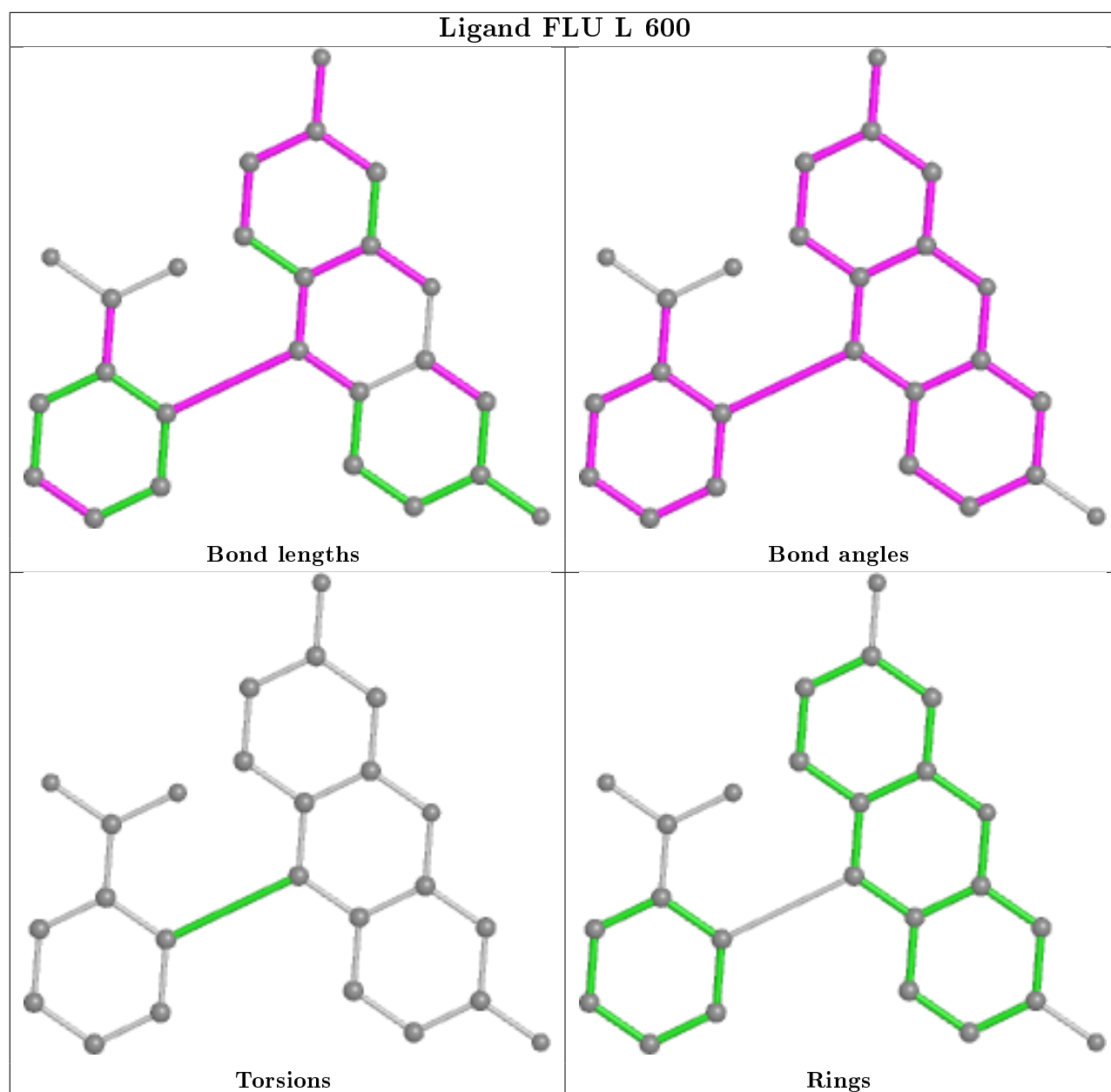
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	600	FLU	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	132:VAL	C	133[B]:CYS	N	4.51
1	H	138:GLY	C	139:SER	N	3.29

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.