



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 AM UTC

PDB ID : 1FLR / pdb_00001flr
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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

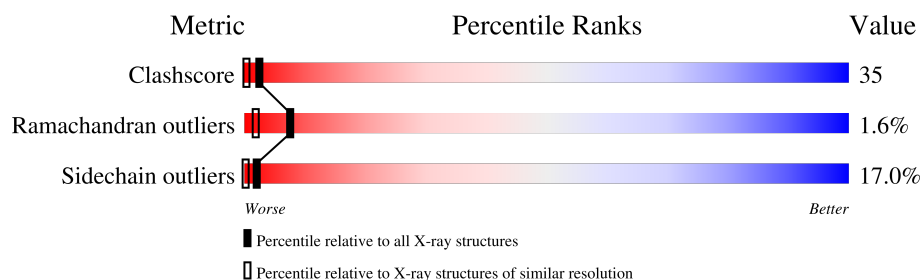
1 Overall quality at a glance

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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	219	52% 35% 12% .
2	H	219	26% 43% 24% 5% .

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

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
1	L	219	Total	C	N	O	S	0	4	0
			1711	1068	293	343	7			

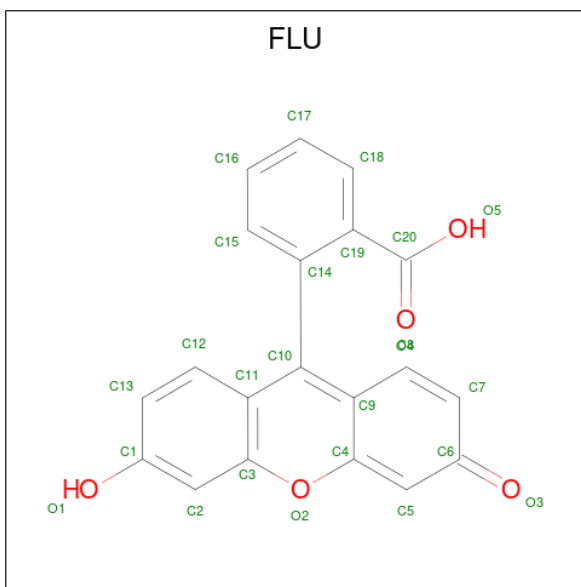
There are 11 discrepancies between the modelled and reference sequences:

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
2	H	216	Total	C	N	O	S	0	6	0
			1672	1062	274	326	10			

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



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

- Molecule 4 is water.

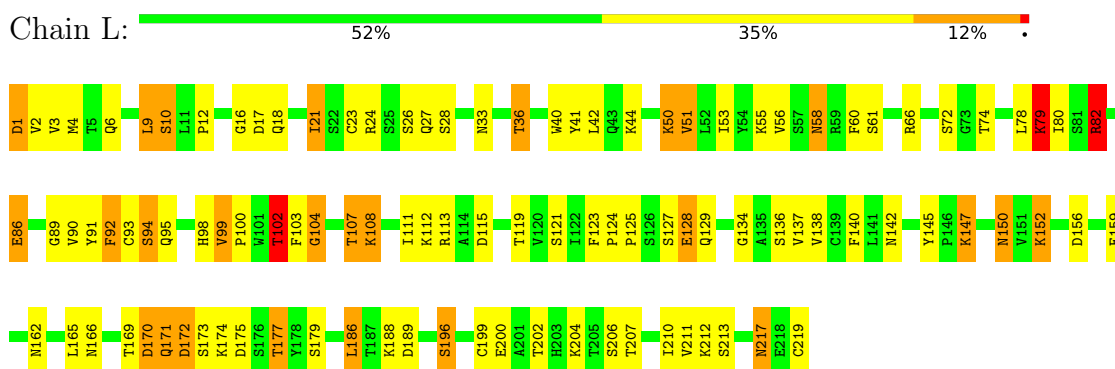
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	148	Total	O	0	1
			149	149		
4	H	142	Total	O	0	1
			143	143		

3 Residue-property plots

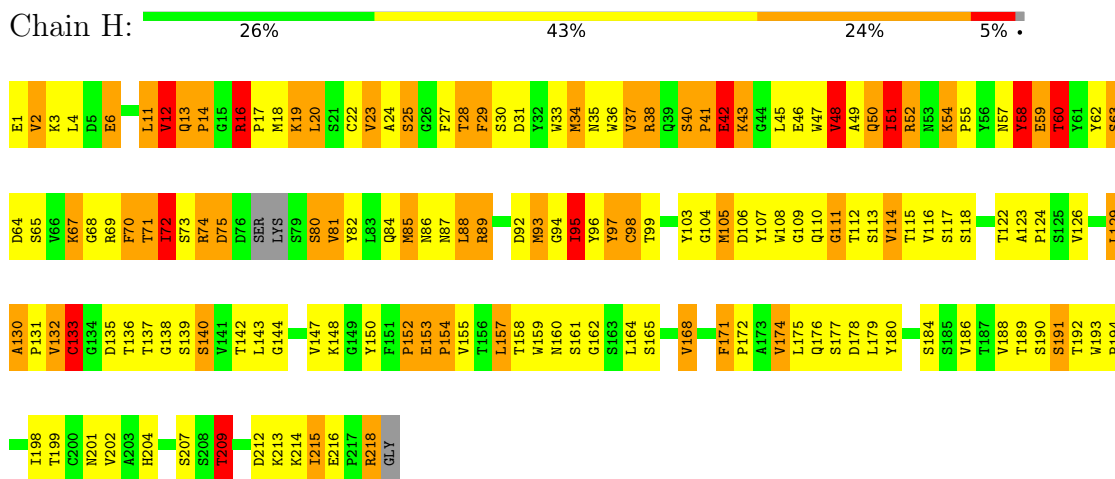
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Xtriage (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.	Xtriage
Total number of atoms	3700	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.40	5/1771 (0.3%)	2.23	63/2400 (2.6%)
2	H	1.26	5/1744 (0.3%)	2.68	111/2378 (4.7%)
All	All	1.33	10/3515 (0.3%)	2.46	174/4778 (3.6%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	134	GLY	N-CA	8.65	1.53	1.44
1	L	41	TYR	CA-C	7.17	1.61	1.52
2	H	136	THR	CA-CB	6.60	1.61	1.53
1	L	137	VAL	CA-C	5.83	1.60	1.52
1	L	93	CYS	N-CA	5.82	1.52	1.45
2	H	38	ARG	N-CA	5.61	1.53	1.45
2	H	60	THR	CA-CB	5.54	1.63	1.53
2	H	106	ASP	N-CA	5.42	1.52	1.46
1	L	177	THR	CA-CB	5.19	1.61	1.53
2	H	35	ASN	CA-C	5.06	1.58	1.52

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	VAL	CA-C-N	-48.83	28.27	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	VAL	C-N-CA	-48.83	28.27	121.54
1	L	170	ASP	CA-CB-CG	14.75	127.35	112.60
1	L	17	ASP	CA-CB-CG	11.83	124.43	112.60
1	L	128	GLU	CA-CB-CG	11.23	136.55	114.10
2	H	212	ASP	CA-CB-CG	11.08	123.68	112.60
2	H	152	PRO	CA-C-N	10.91	148.42	121.80
2	H	152	PRO	C-N-CA	10.91	148.42	121.80
1	L	86	GLU	CA-CB-CG	10.85	135.80	114.10
2	H	154	PRO	N-CA-C	10.26	133.60	112.47
2	H	52	ARG	CD-NE-CZ	10.20	138.68	124.40
1	L	115	ASP	CA-CB-CG	10.17	122.77	112.60
2	H	13[A]	GLN	N-CA-C	-9.20	98.52	109.93
2	H	13[B]	GLN	N-CA-C	-9.20	98.52	109.93
1	L	137	VAL	CA-C-N	9.07	134.81	123.10
1	L	137	VAL	C-N-CA	9.07	134.81	123.10
1	L	103	PHE	CA-CB-CG	8.95	122.75	113.80
2	H	25	SER	N-CA-C	8.50	123.86	111.87
1	L	33	ASN	OD1-CG-ND2	8.44	131.04	122.60
2	H	104	GLY	CA-C-O	-8.40	110.89	119.20
2	H	136	THR	N-CA-C	8.34	121.16	109.15
2	H	37	VAL	CA-C-N	-8.20	109.71	122.59
2	H	37	VAL	C-N-CA	-8.20	109.71	122.59
1	L	102	THR	N-CA-CB	-8.16	97.50	111.69
2	H	59	GLU	N-CA-CB	8.14	121.36	110.29
2	H	6	GLU	CB-CG-CD	7.76	125.80	112.60
2	H	70	PHE	CA-CB-CG	7.74	121.54	113.80
2	H	35	ASN	CA-CB-CG	7.70	120.30	112.60
2	H	45	LEU	CB-CA-C	7.69	122.43	109.75
1	L	166	ASN	CA-CB-CG	7.66	120.26	112.60
2	H	112	THR	N-CA-CB	7.65	123.66	110.81
1	L	66	ARG	NE-CZ-NH2	7.59	126.03	119.20
1	L	217	ASN	CA-CB-CG	7.48	120.08	112.60
1	L	92	PHE	CA-C-O	-7.43	112.68	120.70
1	L	128	GLU	CB-CG-CD	7.42	125.21	112.60
2	H	42	GLU	CB-CG-CD	7.37	125.12	112.60
2	H	111	GLY	N-CA-C	-7.24	105.07	111.95
2	H	106	ASP	CA-CB-CG	7.11	119.71	112.60
1	L	10	SER	O-C-N	7.04	131.95	123.36
2	H	104	GLY	O-C-N	7.00	131.00	122.25
1	L	36	THR	N-CA-CB	6.98	121.68	110.65
1	L	40	TRP	CB-CG-CD2	6.96	136.55	126.80
2	H	108	TRP	CA-C-N	-6.96	114.90	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	108	TRP	C-N-CA	-6.96	114.90	122.55
2	H	64	ASP	CA-C-N	6.79	133.61	120.99
2	H	64	ASP	C-N-CA	6.79	133.61	120.99
2	H	97	TYR	O-C-N	6.73	131.94	123.19
1	L	86	GLU	N-CA-CB	6.71	122.54	110.32
1	L	58	ASN	OD1-CG-ND2	6.68	129.28	122.60
2	H	133[A]	CYS	CA-C-N	6.63	134.41	121.41
2	H	133[A]	CYS	C-N-CA	6.63	134.41	121.41
2	H	133[B]	CYS	CA-C-N	6.63	134.41	121.41
2	H	133[B]	CYS	C-N-CA	6.63	134.41	121.41
2	H	204	HIS	O-C-N	6.59	126.77	121.17
1	L	102	THR	CA-CB-CG2	6.57	121.67	110.50
2	H	81	VAL	CA-C-O	-6.55	113.55	120.76
1	L	127	SER	O-C-N	6.54	129.05	122.12
2	H	130	ALA	CB-CA-C	6.50	118.56	108.61
2	H	135	ASP	CA-C-N	6.50	131.80	121.66
2	H	135	ASP	C-N-CA	6.50	131.80	121.66
1	L	41	TYR	O-C-N	6.46	131.19	123.24
1	L	89	GLY	CA-C-O	6.45	126.14	121.04
1	L	44[A]	LYS	N-CA-C	-6.42	101.42	110.29
1	L	44[B]	LYS	N-CA-C	-6.42	101.42	110.29
1	L	80	ILE	N-CA-C	-6.41	99.13	108.11
2	H	50	GLN	CA-C-N	6.41	131.81	123.10
2	H	50	GLN	C-N-CA	6.41	131.81	123.10
2	H	60	THR	N-CA-CB	-6.40	100.06	110.81
2	H	12	VAL	O-C-N	6.38	130.54	122.57
2	H	192	THR	N-CA-C	6.37	117.92	110.97
2	H	154	PRO	O-C-N	-6.37	114.04	122.64
1	L	53	ILE	CA-CB-CG1	6.36	121.21	110.40
2	H	33	TRP	CA-C-O	-6.27	113.71	120.92
1	L	138	VAL	CA-C-O	6.25	127.85	120.72
2	H	82	TYR	CA-C-O	-6.25	114.13	121.44
1	L	171	GLN	CA-C-O	6.23	127.75	120.96
1	L	199	CYS	CA-C-O	-6.23	113.80	120.46
2	H	28	THR	O-C-N	6.19	130.87	122.57
1	L	51	VAL	O-C-N	6.15	129.98	122.72
2	H	65	SER	N-CA-C	6.15	120.25	112.87
2	H	109	GLY	CA-C-N	6.12	128.98	120.29
2	H	109	GLY	C-N-CA	6.12	128.98	120.29
2	H	98	CYS	O-C-N	6.07	130.13	123.27
2	H	80	SER	N-CA-C	6.07	118.40	109.24
1	L	82	ARG	CA-CB-CG	6.03	126.16	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	107	THR	CA-C-O	-6.02	112.86	120.20
2	H	25	SER	CA-C-O	-6.02	113.25	120.65
1	L	140	PHE	CA-CB-CG	6.01	119.81	113.80
2	H	136	THR	CA-C-N	6.00	133.00	121.54
2	H	136	THR	C-N-CA	6.00	133.00	121.54
2	H	42	GLU	CA-CB-CG	5.99	126.07	114.10
2	H	117	SER	O-C-N	5.97	130.17	123.48
2	H	94	GLY	O-C-N	5.96	129.64	123.92
2	H	114	VAL	O-C-N	5.96	128.81	123.03
1	L	66	ARG	CA-C-O	5.95	126.73	119.11
2	H	36	TRP	N-CA-CB	5.92	120.06	110.77
1	L	186	LEU	CA-CB-CG	5.91	136.99	116.30
2	H	93	MET	O-C-N	5.91	129.95	123.04
1	L	145	TYR	CA-C-O	-5.84	112.16	120.16
2	H	85	MET	O-C-N	5.84	130.16	123.27
2	H	104	GLY	N-CA-C	5.82	122.81	115.42
2	H	209	THR	CA-CB-CG2	5.81	120.38	110.50
1	L	206	SER	CA-C-N	5.75	128.46	120.29
1	L	206	SER	C-N-CA	5.75	128.46	120.29
1	L	169	THR	N-CA-C	-5.73	102.28	110.59
2	H	94	GLY	CA-C-O	-5.69	115.38	121.35
2	H	103	TYR	CA-C-N	5.68	130.75	122.28
2	H	103	TYR	C-N-CA	5.68	130.75	122.28
1	L	169	THR	N-CA-CB	5.68	119.06	110.42
2	H	16	ARG	CD-NE-CZ	5.67	132.34	124.40
1	L	92	PHE	N-CA-CB	-5.67	100.96	110.83
2	H	74	ARG	CA-C-N	5.67	131.96	123.23
2	H	74	ARG	C-N-CA	5.67	131.96	123.23
1	L	79	LYS	CA-C-N	-5.64	115.75	123.14
1	L	79	LYS	C-N-CA	-5.64	115.75	123.14
2	H	48	VAL	CB-CA-C	5.63	120.52	111.29
2	H	89	ARG	NE-CZ-NH2	5.63	124.26	119.20
2	H	159	TRP	N-CA-CB	5.62	119.59	110.77
2	H	33	TRP	N-CA-C	-5.61	100.54	109.96
2	H	6	GLU	CA-CB-CG	5.58	125.27	114.10
2	H	171	PHE	CA-CB-CG	-5.58	108.22	113.80
2	H	191	SER	CA-C-N	5.55	127.98	120.65
2	H	191	SER	C-N-CA	5.55	127.98	120.65
1	L	94	SER	CA-C-O	-5.51	113.76	120.54
1	L	196	SER	O-C-N	5.51	129.50	123.22
1	L	99	VAL	N-CA-CB	5.50	118.91	111.21
1	L	90	VAL	O-C-N	5.50	129.20	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	173	SER	CA-C-N	5.50	128.10	120.63
1	L	173	SER	C-N-CA	5.50	128.10	120.63
2	H	28	THR	CA-C-O	-5.48	115.06	120.98
1	L	210	ILE	N-CA-C	-5.48	100.00	107.99
1	L	92	PHE	O-C-N	5.47	130.34	123.23
1	L	104	GLY	N-CA-C	-5.46	104.27	112.89
2	H	148	LYS	CA-C-N	5.46	132.10	121.41
2	H	148	LYS	C-N-CA	5.46	132.10	121.41
1	L	150	ASN	CB-CA-C	5.43	120.11	109.35
2	H	202	VAL	N-CA-C	5.43	115.71	108.11
1	L	172	ASP	CA-CB-CG	-5.43	107.17	112.60
1	L	56	VAL	N-CA-C	5.42	120.60	109.34
1	L	213	SER	N-CA-CB	-5.40	102.30	111.69
2	H	29	PHE	CA-C-N	5.38	128.03	120.28
2	H	29	PHE	C-N-CA	5.38	128.03	120.28
2	H	38	ARG	NE-CZ-NH2	5.34	124.01	119.20
2	H	71	THR	CA-C-O	-5.34	114.56	120.33
2	H	215	ILE	CB-CG1-CD1	5.34	125.01	113.80
2	H	176	GLN	N-CA-CB	5.32	119.37	110.53
1	L	40	TRP	CB-CG-CD1	-5.32	118.92	126.90
2	H	216	GLU	CB-CG-CD	5.32	121.64	112.60
2	H	51	ILE	N-CA-C	5.29	115.13	106.72
1	L	119	THR	O-C-N	5.28	129.34	123.05
2	H	64	ASP	CA-C-O	5.28	127.19	121.02
2	H	88	LEU	CB-CA-C	5.26	117.38	110.06
2	H	16	ARG	CA-C-N	5.26	126.41	119.84
2	H	16	ARG	C-N-CA	5.26	126.41	119.84
1	L	51	VAL	N-CA-CB	5.23	117.42	110.26
2	H	60	THR	OG1-CB-CG2	5.21	119.72	109.30
2	H	45	LEU	N-CA-C	-5.19	100.78	109.24
2	H	52	ARG	CG-CD-NE	5.19	123.41	112.00
2	H	174	VAL	CA-CB-CG1	5.19	119.22	110.40
2	H	58	TYR	O-C-N	5.16	129.45	122.59
2	H	107	TYR	CA-C-O	-5.16	115.13	120.70
2	H	23	VAL	O-C-N	5.06	128.41	122.99
2	H	95	ILE	O-C-N	5.03	128.27	122.93
2	H	59	GLU	N-CA-C	-5.03	103.84	110.33
2	H	72[A]	ILE	O-C-N	5.03	128.90	122.61
2	H	72[B]	ILE	O-C-N	5.03	128.90	122.61
2	H	147	VAL	CB-CA-C	5.03	118.07	111.53
2	H	2	VAL	O-C-N	5.03	128.66	122.83
2	H	35	ASN	O-C-N	5.03	129.25	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	53	ILE	CB-CG1-CD1	5.01	124.33	113.80
2	H	184	SER	CA-CB-OG	5.01	121.12	111.10
1	L	80	ILE	CA-C-O	-5.00	115.14	120.39
2	H	14	PRO	CB-CA-C	-5.00	104.99	111.39
2	H	174	VAL	CB-CA-C	5.00	118.20	110.50

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	63	1
2	H	1672	0	1607	181	0
3	L	25	0	10	1	0
4	H	143	0	0	14	0
4	L	149	0	0	13	0
All	All	3700	0	3278	235	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 35.

All (235) 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
1:L:50:LYS:NZ	4:L:702:HOH:O	1.76	1.19
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:12:VAL:HG12	2:H:18:MET:HE3	1.42	1.00
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: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
1:L:152:LYS:HE2	1:L:159:GLU:HG2	1.51	0.92
2:H:23:VAL:HG12	2:H:80:SER:OG	1.70	0.92
2:H:12:VAL:HG12	2:H:18:MET:HE1	1.50	0.90
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
1:L:99:VAL:HG13	1:L:100:PRO:HA	1.55	0.88
2:H:12:VAL:CG1	2:H:18:MET:CE	2.51	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:HB3	2:H:43:LYS:NZ	1.91	0.86
2:H:62:TYR:O	4:H:780:HOH:O	1.92	0.85
2:H:51:ILE:HD13	2:H:74:ARG:HG2	1.54	0.85
2:H:16:ARG:HH11	2:H:16:ARG:CB	1.89	0.85
2:H:49:ALA:HB1	2:H:72[A]:ILE:CD1	2.07	0.85
2:H:70:PHE:O	4:H:704:HOH:O	1.96	0.83
2:H:154:PRO:HB3	4:H:822:HOH:O	1.77	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:12:VAL:CG1	2:H:18:MET:HE3	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:HB3	2:H:16:ARG:NH1	1.99	0.77
2:H:154:PRO:CB	4:H:822:HOH:O	2.32	0.77
2:H:54:LYS:CB	2:H:55:PRO:HD3	2.15	0.75
2:H:153[B]:GLU:HB2	2:H:154:PRO:HD3	1.66	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:HE1	2.15	0.74
2:H:89:ARG:NH2	4:H:789:HOH:O	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HD12	2:H:74:ARG:HG2	1.71	0.72
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:43:LYS:HB3	2:H:43:LYS:HZ2	1.55	0.70
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
1:L:60:PHE:CD1	2:H:105:MET:HE2	2.27	0.69
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
2:H:70:PHE:CZ	2:H:85:MET:HE3	2.28	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: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
1:L:111:ILE:H	1:L:171:GLN:HE22	1.41	0.66
2:H:140:SER:HA	2:H:189:THR:HA	1.77	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
2:H:67:LYS:HB3	4:H:782:HOH:O	1.96	0.64
2:H:161:SER:N	2:H:201:ASN:HD21	1.87	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	2.33	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:6:GLU:OE2	2:H:97:TYR:HA	1.97	0.62
2:H:24:ALA:HB3	2:H:29:PHE:CD2	2.34	0.62
2:H:51:ILE:CD1	2:H:74:ARG:CG	2.63	0.62
2:H:43:LYS:NZ	2:H:43:LYS:CB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:29:PHE:HE2	2:H:34:MET:HE2	1.67	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:85:MET:HE2	2:H:88:LEU:HD21	1.85	0.58
2:H:158:THR:CG2	2:H:162:GLY:N	2.66	0.58
2:H:43:LYS:HB3	2:H:43:LYS:HZ3	1.67	0.58
2:H:29:PHE:CE2	2:H:34:MET:HE2	2.38	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: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
1:L:6[B]:GLN:HG3	1:L:21:ILE:HD11	1.86	0.56
2:H:12:VAL:HG22	2:H:116:VAL:HG22	1.87	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
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:67:LYS:C	2:H:67:LYS:CD	2.81	0.54
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:157:LEU:HD12	2:H:157:LEU:C	2.33	0.54
2:H:18:MET:O	2:H:85:MET:N	2.34	0.53
2:H:110[A]:GLN:HG3	2:H:111:GLY:N	2.23	0.53
2:H:12:VAL:CG1	2:H:16:ARG:HH22	2.21	0.53
2:H:95:ILE:N	2:H:95:ILE:HD12	2.24	0.53
2:H:139:SER:O	2:H:140:SER:O	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.74	0.51
2:H:31:ASP:OD1	4:H:857:HOH:O	2.19	0.51
2:H:62:TYR:CZ	2:H:72[A]:ILE:HD12	2.45	0.51
2:H:165:SER:O	2:H:168:VAL:HG13	2.11	0.51
1:L:12:PRO:HB2	1:L:112[A]:LYS:HB2	1.91	0.51
2:H:23:VAL:HG12	2:H:80:SER:CB	2.41	0.51
1:L:200:GLU:HG3	1:L:211:VAL:HG22	1.93	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
2:H:75:ASP:OD1	2:H:75:ASP:C	2.54	0.50
1:L:2:VAL:HG21	1:L:98:HIS:ND1	2.26	0.50
2:H:130:ALA:HB1	2:H:131:PRO:HD2	1.93	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:12:VAL:CB	2:H:16:ARG:HH22	2.23	0.49
2:H:18:MET:N	2:H:85:MET:O	2.30	0.49
2:H:133[B]:CYS:N	2:H:218:ARG:HD3	2.28	0.49
2:H:48:VAL:C	2:H:63:SER:OG	2.55	0.49
2:H:70:PHE:CZ	2:H:85:MET:CE	2.94	0.49
1:L:61:SER:O	1:L:61:SER:OG	2.31	0.49
1:L:129:GLN:NE2	4:L:632:HOH:O	2.46	0.49
1:L:60:PHE:CE1	2:H:105:MET:HE2	2.47	0.48
1:L:150:ASN:HB3	1:L:202:THR:OG1	2.13	0.48
2:H:14:PRO:HA	2:H:88:LEU:O	2.13	0.48
2:H:43:LYS:CB	2:H:43:LYS:HZ3	2.26	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
1:L:28:SER:HA	1:L:74:THR:HG22	1.95	0.48
2:H:25:SER:O	4:H:679:HOH:O	2.20	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
2:H:38:ARG:HA	2:H:95:ILE:O	2.14	0.47
2:H:171:PHE:HA	2:H:172:PRO:HD3	1.73	0.47
2:H:17:PRO:HA	2:H:88:LEU:HD12	1.96	0.47
2:H:139:SER:HA	2:H:190:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:147:LYS:HD3	4:L:603:HOH:O	2.13	0.47
2:H:62:TYR:CE1	2:H:72[A]:ILE:CD1	2.98	0.47
2:H:129:LEU:HB2	2:H:144:GLY:C	2.39	0.47
3:L:600:FLU:C15	3:L:600:FLU:H8	2.43	0.47
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.50	0.46
2:H:140:SER:HA	2:H:188:VAL:O	2.15	0.46
1:L:4:MET:HE3	1:L:23:CYS:SG	2.56	0.46
1:L:112[A]:LYS:HG3	1:L:113:ARG:N	2.31	0.46
2:H:70:PHE:CE1	2:H:85:MET:HB3	2.51	0.46
2:H:3:LYS:HB3	2:H:3:LYS:HE2	1.76	0.46
2:H:75:ASP:OD1	2:H:75:ASP:O	2.33	0.46
1:L:28:SER:O	1:L:98:HIS:HE1	1.99	0.46
2:H:16:ARG:HH11	2:H:16:ARG:C	2.25	0.45
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
1:L:125:PRO:O	2:H:218:ARG:NH2	2.41	0.45
2:H:6:GLU:OE2	2:H:98:CYS:N	2.42	0.45
2:H:177:SER:O	2:H:178:ASP:HB2	2.16	0.45
1:L:175:ASP:OD1	1:L:177:THR:OG1	2.22	0.45
1:L:123:PHE:HA	1:L:124:PRO:HD3	1.85	0.45
1:L:2:VAL:HG22	1:L:27:GLN:HB2	1.98	0.44
2:H:40:SER:O	2:H:42:GLU:N	2.50	0.44
2:H:51:ILE:HG23	2:H:51:ILE:O	2.17	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
1:L:79:LYS:HB2	4:L:873:HOH:O	2.18	0.44
2:H:22:CYS:HB3	2:H:81:VAL:HG13	1.99	0.44
2:H:69:ARG:HH22	2:H:92:ASP:CG	2.25	0.44
2:H:175:LEU:HG	2:H:180:TYR:CE1	2.53	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:67:LYS:HD3	2:H:67:LYS:C	2.42	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
2:H:85:MET:HE2	2:H:85:MET:HB3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:57:ASN:O	2:H:58:TYR:C	2.63	0.41
2:H:48:VAL:C	2:H:63:SER:HG	2.26	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
1:L:1:ASP:HA	4:L:622:HOH:O	2.21	0.41
2:H:150:TYR:CE2	2:H:155:VAL:HG13	2.55	0.41
2:H:178:ASP:C	2:H:179:LEU:HD22	2.45	0.41
1:L:142:ASN:HD22	1:L:179:SER:HB3	1.86	0.41
2:H:131:PRO:O	2:H:218:ARG:HD2	2.20	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:36:THR:O	1:L:55:LYS:HA	2.21	0.40
1:L:188:LYS:HE3	4:L:740:HOH:O	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%)	24 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	216/219 (99%)	185 (86%)	23 (11%)	8 (4%)	2	0
All	All	437/438 (100%)	401 (92%)	27 (6%)	9 (2%)	7	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 ⓘ

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%)	174 (87%)	26 (13%)	4	0
2	H	191/192 (100%)	148 (78%)	43 (22%)	1	0
All	All	391/389 (100%)	322 (82%)	69 (18%)	2	0

All (69) 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

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Mol	Chain	Res	Type
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	165	LEU
1	L	170	ASP
1	L	186	LEU
1	L	204	LYS
1	L	207	THR
1	L	212	LYS
1	L	217	ASN
2	H	1	GLU
2	H	2	VAL
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	34	MET
2	H	40	SER
2	H	41	PRO
2	H	42	GLU
2	H	43	LYS
2	H	48	VAL
2	H	51	ILE
2	H	54	LYS
2	H	60	THR
2	H	63	SER
2	H	67	LYS
2	H	72[A]	ILE
2	H	72[B]	ILE
2	H	75	ASP

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Mol	Chain	Res	Type
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	168	VAL
2	H	174	VAL
2	H	191	SER
2	H	209	THR
2	H	214	LYS
2	H	215	ILE
2	H	218	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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	95	GLN
1	L	98	HIS
1	L	129	GLN
1	L	143	ASN
1	L	162	ASN
1	L	171	GLN
1	L	194	HIS
1	L	215	ASN
1	L	217	ASN
2	H	57	ASN
2	H	84	GLN
2	H	160	ASN
2	H	176	GLN
2	H	196	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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	-	28,28,28	4.20	16 (57%)	41,41,41	4.70	30 (73%)

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	-	-	2/6/12/12	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	600	FLU	C14-C10	-12.64	1.32	1.49
3	L	600	FLU	O2-C4	-8.04	1.22	1.37
3	L	600	FLU	O2-C3	7.53	1.49	1.38
3	L	600	FLU	O1-C1	-5.92	1.23	1.37
3	L	600	FLU	O4-C20	5.63	1.38	1.22
3	L	600	FLU	C11-C10	-5.07	1.33	1.47
3	L	600	FLU	C9-C4	-4.93	1.33	1.43
3	L	600	FLU	C11-C3	-3.77	1.33	1.40
3	L	600	FLU	C19-C20	-3.67	1.41	1.49
3	L	600	FLU	C7-C6	-3.56	1.37	1.46
3	L	600	FLU	C8-C7	2.87	1.42	1.35
3	L	600	FLU	C13-C1	-2.74	1.33	1.39
3	L	600	FLU	C17-C16	2.60	1.44	1.38
3	L	600	FLU	C5-C6	-2.47	1.39	1.45
3	L	600	FLU	C9-C10	2.36	1.46	1.40
3	L	600	FLU	C12-C11	2.21	1.43	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	600	FLU	C14-C10-C11	9.15	131.73	119.91
3	L	600	FLU	C3-C11-C10	7.97	129.23	118.65
3	L	600	FLU	O2-C4-C9	7.74	129.61	120.36
3	L	600	FLU	O2-C4-C5	-7.63	105.36	116.73
3	L	600	FLU	C4-C5-C6	-7.40	113.02	120.66
3	L	600	FLU	C11-C10-C9	-7.38	104.18	120.00
3	L	600	FLU	C12-C11-C10	-6.88	109.69	123.22
3	L	600	FLU	C3-O2-C4	-6.52	108.14	119.73
3	L	600	FLU	C7-C6-C5	6.41	123.63	117.12
3	L	600	FLU	C16-C17-C18	-6.23	112.56	120.24
3	L	600	FLU	C17-C18-C19	6.06	130.75	119.80
3	L	600	FLU	O5-C20-C19	5.85	131.90	115.28
3	L	600	FLU	C8-C9-C10	-5.81	111.88	123.90
3	L	600	FLU	C10-C9-C4	5.68	126.38	119.37
3	L	600	FLU	O4-C20-C19	-5.54	108.75	121.97
3	L	600	FLU	C13-C12-C11	-4.46	113.51	120.86
3	L	600	FLU	C3-C2-C1	-4.07	112.58	118.98
3	L	600	FLU	C18-C19-C14	-4.01	114.76	119.26
3	L	600	FLU	C12-C13-C1	3.86	123.96	119.88
3	L	600	FLU	C19-C14-C10	-3.76	118.16	123.42
3	L	600	FLU	C16-C15-C14	3.71	126.50	119.80
3	L	600	FLU	C15-C14-C10	3.26	124.61	118.36
3	L	600	FLU	C14-C10-C9	3.06	124.07	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	600	FLU	C8-C9-C4	3.05	121.73	115.59
3	L	600	FLU	C7-C8-C9	-3.04	115.44	121.16
3	L	600	FLU	O3-C6-C5	-2.91	117.29	121.43
3	L	600	FLU	O2-C3-C2	-2.89	111.74	115.83
3	L	600	FLU	C13-C1-C2	2.46	122.88	120.19
3	L	600	FLU	C2-C3-C11	2.36	125.83	121.39
3	L	600	FLU	C12-C11-C3	2.18	121.08	118.21

There are no chirality outliers.

All (2) torsion outliers are listed below:

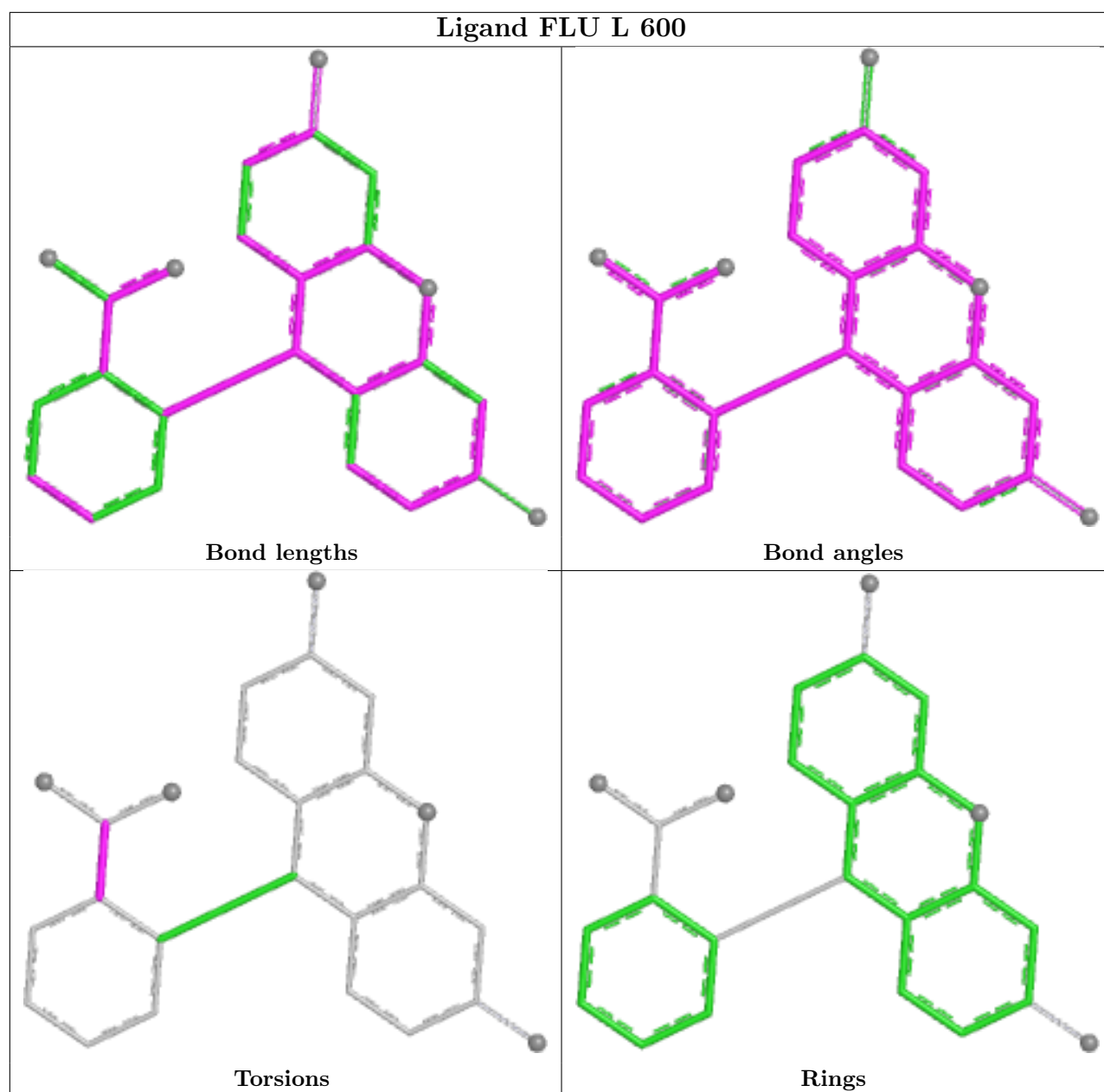
Mol	Chain	Res	Type	Atoms
3	L	600	FLU	C18-C19-C20-O5
3	L	600	FLU	C14-C19-C20-O5

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.