



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:59 PM UTC

PDB ID : 7GCH / pdb_00007gch
Title : STRUCTURE OF CHYMOTRYPSIN-*TRIFLUOROMETHYL KETONE
INHIBITOR COMPLEXES. COMPARISON OF SLOWLY AND RAPIDLY
EQUILIBRATING INHIBITORS
Authors : Brady, K.; Ringe, D.; Abeles, R.H.
Deposited on : 1990-04-06
Resolution : 1.80 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

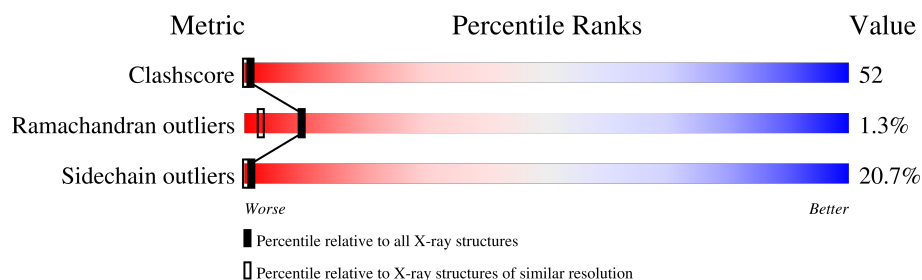
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	E	13	
2	F	131	
3	G	97	

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
4	LPF	G	246	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1863 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 GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	11	Total	C	N	O	S	0	0	1
			69	45	12	11	1			

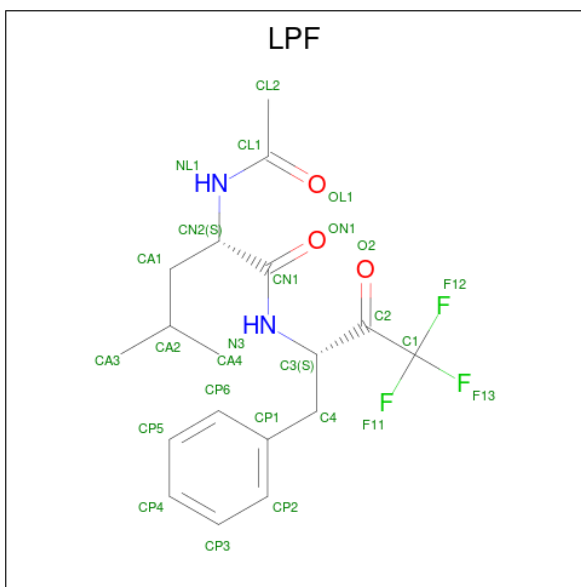
- Molecule 2 is a protein called GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	131	Total	C	N	O	S	0	0	0
			980	618	162	196	4			

- Molecule 3 is a protein called GAMMA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	95	Total	C	N	O	S	0	0	0
			689	429	120	133	7			

- Molecule 4 is 1,1,1-TRIFLUORO-3-((N-ACETYL)-L-LEUCYLAMIDO)-4-PHENYL-BUTAN-2-ONE(N-ACETYL-L-LEUCYL-L-PHENYLALANYL TRIFLUOROMETHYL KETONE) (CCD ID: LPF) (formula: C₁₈H₂₃F₃N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	G	1	Total	C	F	N	O	0	0
			26	18	3	2	3		

- Molecule 5 is water.

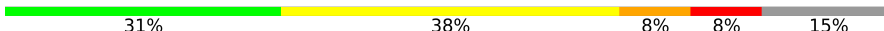
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total	O	0	0
			2	2		
5	F	49	Total	O	0	0
			49	49		
5	G	48	Total	O	0	0
			48	48		

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.

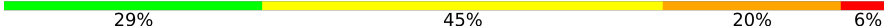
Note EDS was not executed.

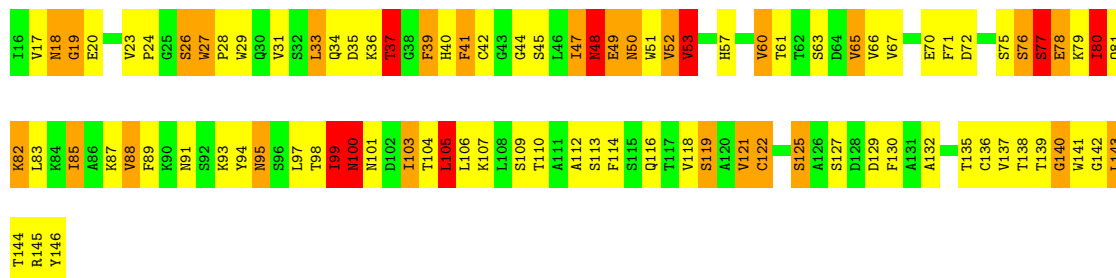
• Molecule 1: GAMMA-CHYMOTRYPSIN A

Chain E: 



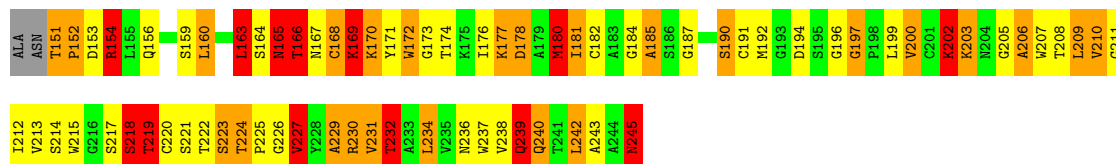
• Molecule 2: GAMMA-CHYMOTRYPSIN A

Chain F: 



• Molecule 3: GAMMA-CHYMOTRYPSIN A

Chain G: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.30 Å 69.30 Å 97.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1863	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: LPF

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	E	1.27	0/70	2.31	4/97 (4.1%)
2	F	1.54	5/1000 (0.5%)	2.74	88/1361 (6.5%)
3	G	1.49	4/702 (0.6%)	2.70	75/955 (7.9%)
All	All	1.51	9/1772 (0.5%)	2.71	167/2413 (6.9%)

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
1	E	0	1
2	F	0	1
3	G	0	2
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	245	ASN	C-OXT	7.38	1.38	1.23
2	F	121	VAL	N-CA	6.35	1.54	1.46
2	F	125	SER	N-CA	6.17	1.53	1.45
2	F	50	ASN	CA-CB	5.93	1.63	1.53
2	F	85	ILE	N-CA	5.92	1.53	1.46
3	G	156	GLN	N-CA	5.83	1.52	1.45
3	G	160	LEU	N-CA	5.28	1.53	1.46
3	G	165	ASN	N-CA	5.28	1.52	1.46
2	F	105	LEU	C-O	5.01	1.30	1.23

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	50	ASN	CA-CB-CG	-15.52	97.08	112.60
2	F	50	ASN	OD1-CG-ND2	12.10	134.70	122.60
2	F	72	ASP	CA-CB-CG	11.12	123.72	112.60
3	G	240	GLN	CB-CG-CD	10.87	131.09	112.60
2	F	78	GLU	CB-CG-CD	10.37	130.23	112.60
3	G	202	LYS	CA-C-N	9.77	136.61	122.44
3	G	202	LYS	C-N-CA	9.77	136.61	122.44
2	F	113	SER	CA-C-O	-9.55	110.14	120.36
2	F	26	SER	CA-C-N	9.52	133.33	122.85
2	F	26	SER	C-N-CA	9.52	133.33	122.85
2	F	118	VAL	CB-CA-C	9.34	121.84	110.73
3	G	232	THR	OG1-CB-CG2	8.80	126.90	109.30
3	G	153	ASP	CA-C-N	8.70	133.86	121.42
3	G	153	ASP	C-N-CA	8.70	133.86	121.42
2	F	70	GLU	CA-C-O	8.51	130.25	120.80
2	F	49	GLU	CB-CG-CD	8.33	126.76	112.60
3	G	163	LEU	CA-CB-CG	8.18	144.93	116.30
3	G	219	THR	CA-CB-OG1	-8.07	97.49	109.60
2	F	125	SER	CA-C-O	-8.07	111.67	121.36
2	F	143	LEU	CB-CA-C	8.05	122.67	109.70
2	F	76	SER	N-CA-C	-8.05	103.67	113.97
2	F	39	PHE	CA-CB-CG	8.03	121.83	113.80
3	G	232	THR	N-CA-CB	-7.99	98.38	110.12
3	G	165	ASN	CB-CA-C	7.97	123.50	110.90
2	F	26	SER	N-CA-C	7.95	122.97	113.28
3	G	172	TRP	CA-C-N	7.78	132.68	120.00
3	G	172	TRP	C-N-CA	7.78	132.68	120.00
2	F	20	GLU	O-C-N	7.67	132.17	123.27
2	F	141	TRP	CA-C-N	7.61	128.73	120.44
2	F	141	TRP	C-N-CA	7.61	128.73	120.44
3	G	168	CYS	CA-C-O	-7.55	112.41	120.42
3	G	165	ASN	CA-CB-CG	-7.52	105.08	112.60
2	F	122	CYS	N-CA-CB	7.52	121.72	110.29
2	F	72	ASP	N-CA-CB	-7.51	99.43	110.84
2	F	100	ASN	N-CA-CB	7.41	121.71	110.45
3	G	200	VAL	CA-C-N	7.38	133.40	122.99
3	G	200	VAL	C-N-CA	7.38	133.40	122.99
3	G	240	GLN	CA-CB-CG	7.35	128.79	114.10
3	G	165	ASN	N-CA-CB	-7.34	99.43	110.07
3	G	181	ILE	CB-CG1-CD1	7.31	129.16	113.80
2	F	18	ASN	CA-CB-CG	7.31	119.91	112.60
2	F	99	ILE	N-CA-CB	7.24	123.18	111.23
2	F	50	ASN	O-C-N	7.23	130.99	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	140	GLY	CA-C-N	7.15	134.03	122.67
2	F	140	GLY	C-N-CA	7.15	134.03	122.67
2	F	66	VAL	N-CA-C	-7.07	99.55	108.89
2	F	77	SER	N-CA-C	7.07	120.78	112.72
2	F	125	SER	N-CA-C	-6.93	99.30	110.32
3	G	166	THR	CA-CB-OG1	-6.89	99.26	109.60
2	F	70	GLU	CG-CD-OE1	6.87	134.21	118.40
2	F	48	ASN	CA-CB-CG	6.86	119.46	112.60
2	F	27	TRP	CA-C-N	6.84	126.54	119.56
2	F	27	TRP	C-N-CA	6.84	126.54	119.56
2	F	50	ASN	CB-CA-C	-6.75	98.76	110.17
3	G	224	THR	CA-CB-OG1	-6.67	99.59	109.60
3	G	224	THR	CA-C-N	6.66	126.42	119.76
3	G	224	THR	C-N-CA	6.66	126.42	119.76
2	F	37	THR	N-CA-CB	-6.60	100.06	110.28
3	G	234	LEU	O-C-N	6.57	129.89	122.27
1	E	8	PRO	CA-C-O	-6.56	114.21	121.23
2	F	103	ILE	CB-CG1-CD1	6.52	127.48	113.80
3	G	221	SER	CA-C-O	-6.50	114.04	121.19
3	G	219	THR	N-CA-CB	-6.50	100.80	110.61
3	G	242	LEU	O-C-N	6.48	130.25	122.27
3	G	230	ARG	CB-CA-C	6.45	121.10	110.78
2	F	72	ASP	CB-CA-C	6.42	120.31	110.62
2	F	18	ASN	CA-C-N	-6.41	115.50	122.55
2	F	18	ASN	C-N-CA	-6.41	115.50	122.55
3	G	178	ASP	CA-C-O	-6.40	113.72	120.63
2	F	80	ILE	CA-C-O	-6.39	114.25	121.98
2	F	101	ASN	CA-C-O	-6.36	114.90	122.27
2	F	81	GLN	CA-C-O	-6.34	113.51	120.36
3	G	232	THR	CA-C-N	6.33	133.93	121.58
3	G	232	THR	C-N-CA	6.33	133.93	121.58
2	F	107	LYS	O-C-N	-6.30	116.03	123.22
3	G	190	SER	N-CA-C	-6.24	102.12	110.55
2	F	20	GLU	CA-C-O	-6.24	113.83	121.06
2	F	89	PHE	O-C-N	6.23	130.32	122.84
3	G	218	SER	CA-C-O	6.19	129.36	120.51
3	G	223	SER	N-CA-C	-6.18	106.06	113.97
3	G	159	SER	CA-C-O	-6.16	113.97	121.36
3	G	224	THR	CB-CA-C	6.14	116.86	109.31
2	F	51	TRP	CA-C-O	6.11	127.80	120.28
1	E	3	VAL	CB-CA-C	6.10	122.46	111.36
2	F	118	VAL	CA-C-O	-6.08	114.35	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	24	PRO	CA-C-O	-6.08	114.69	121.32
3	G	230	ARG	CD-NE-CZ	6.07	132.90	124.40
3	G	224	THR	N-CA-CB	-6.07	100.55	109.90
2	F	138	THR	CA-CB-OG1	-6.05	100.52	109.60
3	G	200	VAL	CA-CB-CG1	6.03	120.66	110.40
3	G	206	ALA	CA-C-N	6.02	130.45	121.72
3	G	206	ALA	C-N-CA	6.02	130.45	121.72
3	G	152	PRO	CA-C-O	-6.01	114.59	121.56
2	F	88	VAL	CB-CA-C	5.98	119.26	110.77
2	F	80	ILE	CB-CA-C	-5.98	105.02	111.59
3	G	176	ILE	CB-CA-C	-5.96	104.80	111.23
3	G	172	TRP	CB-CA-C	5.96	119.02	109.02
2	F	70	GLU	CB-CG-CD	5.95	122.71	112.60
3	G	231	VAL	N-CA-C	5.95	119.38	111.17
2	F	103	ILE	CA-C-N	5.94	132.59	122.37
2	F	103	ILE	C-N-CA	5.94	132.59	122.37
2	F	95	ASN	CA-C-O	5.93	130.76	120.85
3	G	239	GLN	CA-C-N	5.90	128.77	120.28
3	G	239	GLN	C-N-CA	5.90	128.77	120.28
3	G	203	LYS	CA-CB-CG	5.86	125.82	114.10
2	F	119	SER	CA-C-O	-5.81	115.23	121.45
3	G	243	ALA	O-C-N	5.81	128.05	122.07
2	F	94	TYR	N-CA-CB	5.77	118.51	109.69
2	F	41	PHE	CB-CA-C	5.72	118.29	109.03
3	G	197	GLY	O-C-N	-5.71	116.06	121.77
3	G	232	THR	CB-CA-C	5.68	120.23	110.79
2	F	49	GLU	CA-C-N	5.68	131.29	122.49
2	F	49	GLU	C-N-CA	5.68	131.29	122.49
1	E	2	GLY	N-CA-C	5.67	122.91	115.36
2	F	19	GLY	N-CA-C	-5.67	102.58	112.55
2	F	65	VAL	CB-CA-C	5.66	119.01	110.63
3	G	170	LYS	CB-CA-C	5.66	121.54	110.67
2	F	85	ILE	CA-C-O	-5.65	114.53	120.57
2	F	121	VAL	N-CA-C	-5.65	101.60	109.45
3	G	165	ASN	N-CA-C	-5.64	105.05	111.14
3	G	229	ALA	CA-C-O	-5.62	114.86	121.16
2	F	95	ASN	CA-C-N	5.60	128.55	120.38
2	F	95	ASN	C-N-CA	5.60	128.55	120.38
1	E	8	PRO	N-CA-C	-5.55	102.49	111.03
3	G	226	GLY	CA-C-N	-5.55	115.94	122.93
3	G	226	GLY	C-N-CA	-5.55	115.94	122.93
3	G	154	ARG	NE-CZ-NH1	5.54	127.04	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	154	ARG	CA-CB-CG	-5.53	103.05	114.10
2	F	78	GLU	N-CA-CB	5.51	119.61	110.63
3	G	172	TRP	N-CA-CB	-5.47	103.62	110.90
3	G	205	GLY	N-CA-C	5.46	122.30	115.21
2	F	27	TRP	CA-C-O	5.44	127.27	121.28
2	F	89	PHE	CA-C-O	-5.43	114.43	121.11
2	F	66	VAL	CA-CB-CG2	5.42	119.62	110.40
3	G	164	SER	O-C-N	5.41	129.00	122.94
2	F	61	THR	N-CA-CB	5.41	120.03	111.43
2	F	135	THR	CA-CB-OG1	-5.41	101.49	109.60
2	F	47	ILE	O-C-N	5.39	127.70	122.25
3	G	196	GLY	CA-C-O	5.38	124.87	119.27
3	G	151	THR	CA-CB-OG1	-5.36	101.56	109.60
3	G	185	ALA	N-CA-C	-5.36	105.38	112.24
2	F	101	ASN	CA-C-N	5.34	130.81	122.26
2	F	101	ASN	C-N-CA	5.34	130.81	122.26
2	F	51	TRP	CA-CB-CG	5.33	123.72	113.60
3	G	184	GLY	O-C-N	5.32	130.99	123.39
3	G	229	ALA	CA-C-N	-5.30	115.95	122.84
3	G	229	ALA	C-N-CA	-5.30	115.95	122.84
2	F	60	VAL	CA-C-N	5.27	131.68	122.82
2	F	60	VAL	C-N-CA	5.27	131.68	122.82
3	G	210	VAL	CB-CA-C	5.25	119.90	111.29
2	F	97	LEU	N-CA-C	-5.25	105.23	111.69
2	F	52	VAL	CA-C-N	-5.24	116.34	123.10
2	F	52	VAL	C-N-CA	-5.24	116.34	123.10
3	G	163	LEU	N-CA-C	-5.24	102.14	109.69
3	G	219	THR	OG1-CB-CG2	5.17	119.64	109.30
3	G	154	ARG	N-CA-C	5.16	118.36	110.20
3	G	227	VAL	CB-CA-C	5.15	117.85	110.84
2	F	35	ASP	CA-CB-CG	5.13	117.73	112.60
2	F	82	LYS	CB-CG-CD	5.12	123.09	111.30
3	G	180	MET	CA-CB-CG	5.08	124.27	114.10
2	F	50	ASN	N-CA-CB	-5.08	102.94	110.61
2	F	78	GLU	CA-C-N	5.05	129.66	122.08
2	F	78	GLU	C-N-CA	5.05	129.66	122.08
3	G	154	ARG	CB-CA-C	-5.04	101.01	109.53
2	F	100	ASN	N-CA-C	-5.03	103.76	110.55
2	F	33	LEU	CA-C-O	-5.03	114.66	120.49
3	G	223	SER	CA-C-O	5.00	124.33	118.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	LEU	Mainchain
2	F	53	VAL	Mainchain
3	G	154	ARG	Sidechain
3	G	169	LYS	Mainchain

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	E	69	0	76	10	0
2	F	980	0	951	107	4
3	G	689	0	686	87	1
4	G	26	0	23	13	0
5	E	2	0	0	0	0
5	F	49	0	0	19	0
5	G	48	0	0	22	3
All	All	1863	0	1736	181	4

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 52.

All (181) 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)
4:G:246:LPG:F13	4:G:246:LPG:C1	1.59	1.39
4:G:246:LPG:C1	4:G:246:LPG:F12	1.62	1.36
3:G:167:ASN:HA	3:G:170:LYS:CD	1.60	1.31
2:F:33:LEU:HD12	2:F:42:CYS:CB	1.65	1.24
3:G:167:ASN:CA	3:G:170:LYS:HD2	1.68	1.23
3:G:199:LEU:N	5:G:425:HOH:O	1.65	1.16
3:G:211:GLY:O	5:G:425:HOH:O	1.61	1.16
2:F:40:HIS:HA	5:F:331:HOH:O	1.44	1.14
3:G:177:LYS:HG2	3:G:180:MET:HE3	1.22	1.13
3:G:172:TRP:N	5:G:372:HOH:O	1.80	1.12
3:G:168:CYS:O	5:G:372:HOH:O	1.65	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:163:LEU:HB3	5:G:367:HOH:O	1.48	1.11
2:F:18:ASN:ND2	3:G:187:GLY:O	1.92	1.03
2:F:40:HIS:CA	5:F:331:HOH:O	1.99	1.03
2:F:33:LEU:CD1	2:F:42:CYS:HB2	1.90	1.01
2:F:33:LEU:HD12	2:F:42:CYS:HB2	1.01	1.01
2:F:105:LEU:HD21	3:G:238:VAL:HG22	1.42	0.97
3:G:167:ASN:HA	3:G:170:LYS:HD2	1.00	0.97
2:F:57:HIS:CG	4:G:246:LPF:HA43	1.99	0.96
4:G:246:LPF:CP4	5:G:428:HOH:O	2.18	0.91
2:F:95:ASN:CG	2:F:98:THR:OG1	2.15	0.90
2:F:33:LEU:O	5:F:331:HOH:O	1.91	0.89
3:G:222:THR:C	5:G:409:HOH:O	2.14	0.89
2:F:41:PHE:N	5:F:331:HOH:O	2.06	0.88
2:F:143:LEU:HD12	3:G:192:MET:HB2	1.56	0.87
3:G:177:LYS:HG2	3:G:180:MET:CE	2.05	0.87
3:G:217:SER:HB2	3:G:224:THR:HG21	1.60	0.84
3:G:167:ASN:HA	3:G:170:LYS:CE	2.07	0.84
3:G:224:THR:HG22	5:G:400:HOH:O	1.77	0.84
2:F:53:VAL:CG1	2:F:105:LEU:HD11	2.10	0.82
3:G:199:LEU:HB3	5:G:425:HOH:O	1.78	0.82
3:G:238:VAL:O	3:G:242:LEU:HD13	1.78	0.81
3:G:171:TYR:HB2	5:G:372:HOH:O	1.80	0.81
3:G:190:SER:O	5:G:428:HOH:O	1.98	0.81
3:G:239:GLN:NE2	3:G:239:GLN:HA	1.94	0.80
3:G:199:LEU:CA	5:G:425:HOH:O	2.19	0.80
2:F:47:ILE:HG23	2:F:53:VAL:HG22	1.67	0.77
2:F:95:ASN:ND2	2:F:98:THR:OG1	2.17	0.77
2:F:105:LEU:HD22	3:G:237:TRP:CZ3	2.19	0.76
2:F:33:LEU:HD12	2:F:42:CYS:HB3	1.67	0.76
3:G:177:LYS:CG	3:G:180:MET:HE3	2.12	0.75
3:G:167:ASN:C	3:G:170:LYS:HD2	2.12	0.75
2:F:47:ILE:HG23	2:F:53:VAL:CG2	2.17	0.74
2:F:39:PHE:O	5:F:331:HOH:O	2.04	0.74
2:F:53:VAL:HG13	2:F:105:LEU:HD11	1.70	0.73
2:F:34:GLN:HA	5:F:331:HOH:O	1.86	0.73
2:F:53:VAL:HG13	2:F:105:LEU:CD1	2.19	0.73
3:G:239:GLN:HA	3:G:239:GLN:HE21	1.53	0.73
5:F:356:HOH:O	3:G:232:THR:CG2	2.36	0.73
2:F:53:VAL:CG1	2:F:105:LEU:CD1	2.67	0.72
3:G:222:THR:O	5:G:409:HOH:O	2.05	0.72
2:F:78:GLU:OE1	5:F:456:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:LEU:HD22	3:G:237:TRP:CH2	2.25	0.71
5:F:356:HOH:O	3:G:232:THR:HG23	1.90	0.70
4:G:246:LPF:CA3	4:G:246:LPF:HL1	2.06	0.69
2:F:19:GLY:N	5:F:394:HOH:O	2.18	0.69
2:F:83:LEU:HD23	2:F:110:THR:HG23	1.73	0.69
2:F:71:PHE:HE2	3:G:154:ARG:HH11	1.41	0.69
2:F:83:LEU:CD2	2:F:110:THR:HG23	2.23	0.68
2:F:80:ILE:CD1	2:F:82:LYS:HE3	2.24	0.68
2:F:47:ILE:CG2	2:F:53:VAL:CG2	2.73	0.67
2:F:87:LYS:HG2	2:F:88:VAL:H	1.60	0.66
3:G:217:SER:HB2	3:G:224:THR:CG2	2.26	0.66
2:F:60:VAL:HG23	5:F:301:HOH:O	1.96	0.65
3:G:209:LEU:HD13	3:G:231:VAL:HG21	1.79	0.63
2:F:45:SER:O	2:F:53:VAL:HG23	2.00	0.62
3:G:199:LEU:CB	5:G:425:HOH:O	2.35	0.62
1:E:4:PRO:HB3	2:F:28:PRO:HG3	1.82	0.61
2:F:27:TRP:CD1	2:F:139:THR:HG21	2.35	0.61
2:F:17:VAL:HG11	3:G:222:THR:CG2	2.29	0.61
3:G:213:VAL:HG13	5:G:412:HOH:O	2.01	0.61
2:F:95:ASN:O	2:F:99:ILE:N	2.29	0.60
4:G:246:LPF:NL1	4:G:246:LPF:HA33	2.16	0.60
2:F:40:HIS:CD2	2:F:40:HIS:C	2.80	0.59
3:G:169:LYS:HE3	5:G:561:HOH:O	2.03	0.59
3:G:215:TRP:CH2	3:G:227:VAL:HG21	2.36	0.59
2:F:33:LEU:CD1	2:F:42:CYS:CB	2.60	0.59
3:G:172:TRP:HB2	5:G:372:HOH:O	2.02	0.58
4:G:246:LPF:HL1	4:G:246:LPF:HA33	1.68	0.58
2:F:53:VAL:HG12	2:F:105:LEU:CD1	2.33	0.58
2:F:57:HIS:CD2	4:G:246:LPF:HA43	2.39	0.57
2:F:17:VAL:CG1	3:G:222:THR:CG2	2.82	0.57
2:F:47:ILE:CG2	2:F:53:VAL:HG21	2.33	0.57
3:G:230:ARG:NE	5:G:610:HOH:O	2.36	0.57
3:G:166:THR:C	3:G:170:LYS:HE3	2.29	0.57
1:E:9:VAL:HG22	2:F:23:VAL:CG2	2.35	0.56
2:F:57:HIS:ND1	4:G:246:LPF:HA43	2.20	0.56
2:F:144:THR:HG23	3:G:152:PRO:HD3	1.87	0.56
3:G:167:ASN:HA	3:G:170:LYS:NZ	2.20	0.56
3:G:217:SER:O	3:G:219:THR:N	2.40	0.55
2:F:142:GLY:O	2:F:143:LEU:C	2.50	0.55
2:F:83:LEU:HD22	2:F:110:THR:O	2.06	0.55
5:F:340:HOH:O	3:G:197:GLY:HA3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:PRO:HB2	2:F:119:SER:OG	2.08	0.54
3:G:219:THR:O	3:G:220:CYS:HB2	2.08	0.54
2:F:53:VAL:HG12	2:F:105:LEU:HD11	1.90	0.54
3:G:181:ILE:HG13	3:G:182:CYS:N	2.21	0.54
3:G:217:SER:C	3:G:219:THR:N	2.64	0.53
2:F:127:SER:CB	5:F:462:HOH:O	2.55	0.53
2:F:80:ILE:HG13	2:F:80:ILE:O	2.09	0.53
3:G:217:SER:C	3:G:219:THR:H	2.17	0.53
2:F:47:ILE:CG2	2:F:53:VAL:HG22	2.36	0.53
2:F:129:ASP:OD2	5:F:384:HOH:O	2.18	0.53
2:F:40:HIS:C	5:F:331:HOH:O	2.31	0.52
2:F:122:CYS:O	3:G:208:THR:HA	2.09	0.52
4:G:246:LPF:CA3	4:G:246:LPF:NL1	2.68	0.52
2:F:53:VAL:HG13	2:F:105:LEU:HD12	1.92	0.52
2:F:130:PHE:CE2	3:G:210:VAL:HG21	2.45	0.52
2:F:48:ASN:C	2:F:48:ASN:HD22	2.18	0.51
4:G:246:LPF:HP4	5:G:428:HOH:O	2.01	0.51
2:F:39:PHE:C	5:F:331:HOH:O	2.52	0.51
2:F:27:TRP:N	2:F:28:PRO:CD	2.74	0.51
2:F:34:GLN:HA	2:F:39:PHE:O	2.11	0.50
1:E:8:PRO:HG3	2:F:26:SER:O	2.12	0.49
2:F:146:TYR:CE2	3:G:219:THR:OG1	2.65	0.49
2:F:26:SER:C	2:F:28:PRO:HD3	2.38	0.49
2:F:31:VAL:HG22	2:F:44:GLY:C	2.37	0.49
2:F:19:GLY:CA	5:F:394:HOH:O	2.59	0.49
1:E:4:PRO:HB3	2:F:28:PRO:CG	2.43	0.49
3:G:200:VAL:HG23	3:G:207:TRP:CE3	2.48	0.49
1:E:9:VAL:HG22	2:F:23:VAL:HG21	1.94	0.49
2:F:17:VAL:HG12	3:G:222:THR:HG21	1.95	0.48
2:F:95:ASN:C	2:F:95:ASN:OD1	2.56	0.48
3:G:174:THR:HA	5:G:374:HOH:O	2.14	0.48
3:G:202:LYS:HA	3:G:206:ALA:O	2.12	0.48
3:G:166:THR:HG22	3:G:170:LYS:HZ2	1.78	0.48
3:G:171:TYR:CB	5:G:372:HOH:O	2.49	0.48
2:F:127:SER:HB3	5:F:462:HOH:O	2.13	0.48
2:F:87:LYS:HG2	2:F:88:VAL:N	2.27	0.48
3:G:166:THR:O	3:G:170:LYS:HE3	2.14	0.48
2:F:23:VAL:O	2:F:26:SER:OG	2.28	0.48
3:G:166:THR:HA	3:G:169:LYS:HE2	1.95	0.47
3:G:169:LYS:HD2	5:G:561:HOH:O	2.13	0.47
1:E:5:ALA:CB	2:F:116:GLN:HG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:PHE:CE1	3:G:210:VAL:HG22	2.50	0.47
2:F:17:VAL:HG11	3:G:222:THR:HG23	1.96	0.47
2:F:34:GLN:HG2	2:F:40:HIS:HA	1.97	0.47
2:F:130:PHE:CZ	3:G:210:VAL:CG2	2.99	0.46
2:F:83:LEU:HD23	2:F:110:THR:CG2	2.44	0.46
3:G:212:ILE:HB	3:G:229:ALA:HB3	1.97	0.46
3:G:214:SER:HB3	3:G:227:VAL:O	2.15	0.46
2:F:48:ASN:HD22	2:F:49:GLU:N	2.15	0.45
2:F:143:LEU:HD12	3:G:192:MET:CB	2.38	0.44
2:F:99:ILE:CD1	4:G:246:LPF:HA31	2.48	0.44
2:F:95:ASN:HD21	2:F:98:THR:HG23	1.83	0.44
2:F:100:ASN:HD22	2:F:100:ASN:HA	1.56	0.44
2:F:103:ILE:HD12	3:G:212:ILE:CD1	2.48	0.44
3:G:185:ALA:HB2	3:G:225:PRO:HG3	1.99	0.44
2:F:140:GLY:HA3	3:G:194:ASP:OD2	2.18	0.43
1:E:4:PRO:HB3	2:F:28:PRO:CD	2.47	0.43
2:F:37:THR:HG22	2:F:39:PHE:H	1.83	0.43
3:G:165:ASN:ND2	3:G:230:ARG:NH1	2.66	0.43
3:G:245:ASN:N	3:G:245:ASN:ND2	2.66	0.43
2:F:17:VAL:CG1	3:G:222:THR:HG21	2.46	0.43
2:F:83:LEU:HD22	2:F:110:THR:HG23	1.99	0.43
3:G:167:ASN:CA	3:G:170:LYS:CE	2.89	0.43
3:G:154:ARG:H	3:G:154:ARG:HG2	1.58	0.42
2:F:29:TRP:CG	2:F:121:VAL:HB	2.55	0.42
3:G:181:ILE:HG13	3:G:182:CYS:H	1.85	0.42
4:G:246:LPF:F13	4:G:246:LPF:C2	2.44	0.42
1:E:5:ALA:HB1	2:F:116:GLN:HG2	2.01	0.42
2:F:48:ASN:HD22	2:F:50:ASN:H	1.68	0.42
3:G:211:GLY:HA2	3:G:229:ALA:O	2.19	0.42
1:E:9:VAL:HG22	2:F:23:VAL:HG23	2.02	0.41
2:F:103:ILE:HD12	3:G:212:ILE:HD11	2.01	0.41
3:G:169:LYS:HB2	3:G:173:GLY:HA2	2.02	0.41
3:G:217:SER:O	3:G:218:SER:C	2.63	0.41
2:F:112:ALA:HB3	2:F:114:PHE:HE1	1.85	0.41
2:F:27:TRP:N	2:F:28:PRO:HD3	2.36	0.41
2:F:103:ILE:CG2	3:G:234:LEU:HD13	2.51	0.41
3:G:165:ASN:O	3:G:168:CYS:N	2.53	0.41
1:E:3:VAL:HA	1:E:4:PRO:HD2	1.98	0.41
2:F:99:ILE:HG22	2:F:99:ILE:O	2.20	0.41
2:F:91:ASN:ND2	3:G:237:TRP:CD2	2.89	0.41
2:F:136:CYS:C	2:F:137:VAL:HG23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:SER:HA	5:F:344:HOH:O	2.22	0.41
3:G:192:MET:HB2	3:G:192:MET:HE2	1.96	0.41
2:F:53:VAL:CG1	2:F:105:LEU:HD12	2.47	0.40
2:F:93:LYS:HE3	2:F:93:LYS:HB3	1.80	0.40
2:F:52:VAL:HB	2:F:106:LEU:HB2	2.03	0.40
3:G:167:ASN:CA	3:G:170:LYS:NZ	2.84	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:116:GLN:NE2	5:G:477:HOH:O[5_656]	1.54	0.66
2:F:76:SER:OG	3:G:236:ASN:OD1[6_476]	1.62	0.58
2:F:146:TYR:OH	5:G:589:HOH:O[2_675]	1.79	0.41
2:F:132:ALA:O	5:G:367:HOH:O[8_777]	1.99	0.21

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	E	9/13 (69%)	9 (100%)	0	0	100	100
2	F	129/131 (98%)	123 (95%)	4 (3%)	2 (2%)	7	2
3	G	93/97 (96%)	87 (94%)	5 (5%)	1 (1%)	11	3
All	All	231/241 (96%)	219 (95%)	9 (4%)	3 (1%)	9	3

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	218	SER
2	F	48	ASN
2	F	99	ILE

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	E	8/10 (80%)	7 (88%)	1 (12%)	4	1
2	F	109/109 (100%)	90 (83%)	19 (17%)	2	0
3	G	76/77 (99%)	56 (74%)	20 (26%)	0	0
All	All	193/196 (98%)	153 (79%)	40 (21%)	1	0

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	VAL
2	F	36	LYS
2	F	37	THR
2	F	48	ASN
2	F	53	VAL
2	F	63	SER
2	F	65	VAL
2	F	67	VAL
2	F	75	SER
2	F	77	SER
2	F	79	LYS
2	F	80	ILE
2	F	85	ILE
2	F	99	ILE
2	F	100	ASN
2	F	104	THR
2	F	105	LEU
2	F	109	SER
2	F	125	SER
2	F	145	ARG
3	G	151	THR
3	G	160	LEU
3	G	163	LEU
3	G	165	ASN
3	G	166	THR
3	G	169	LYS

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Mol	Chain	Res	Type
3	G	177	LYS
3	G	178	ASP
3	G	180	MET
3	G	191	CYS
3	G	202	LYS
3	G	203	LYS
3	G	209	LEU
3	G	219	THR
3	G	223	SER
3	G	227	VAL
3	G	232	THR
3	G	239	GLN
3	G	240	GLN
3	G	245	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	48	ASN
2	F	73	GLN
2	F	100	ASN
3	G	165	ASN
3	G	236	ASN
3	G	239	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
4	LPF	G	246	3	25,26,26	5.47	11 (44%)	34,36,36	3.42	13 (38%)

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
4	LPF	G	246	3	-	7/29/30/30	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	246	LPF	O2-C2	18.54	1.51	1.21
4	G	246	LPF	CL2-CL1	-10.89	1.28	1.50
4	G	246	LPF	OL1-CL1	10.35	1.46	1.23
4	G	246	LPF	F12-C1	7.29	1.62	1.32
4	G	246	LPF	F13-C1	6.47	1.59	1.32
4	G	246	LPF	F11-C1	5.56	1.55	1.32
4	G	246	LPF	CN1-N3	3.81	1.42	1.34
4	G	246	LPF	CP2-CP1	-3.11	1.32	1.38
4	G	246	LPF	CP6-CP1	-2.92	1.33	1.38
4	G	246	LPF	CP5-CP6	-2.19	1.35	1.38
4	G	246	LPF	CL1-NL1	-2.18	1.27	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	246	LPF	O2-C2-C1	-10.45	109.11	117.06
4	G	246	LPF	ON1-CN1-CN2	7.05	135.24	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	246	LPF	OL1-CL1-CL2	-6.94	109.70	122.05
4	G	246	LPF	O2-C2-C3	-6.28	105.29	119.80
4	G	246	LPF	CN2-CN1-N3	-5.16	105.62	116.63
4	G	246	LPF	CP1-C4-C3	4.87	126.31	113.36
4	G	246	LPF	CA1-CN2-CN1	4.58	121.44	110.59
4	G	246	LPF	OL1-CL1-NL1	4.26	129.52	121.98
4	G	246	LPF	F13-C1-C2	-3.54	104.26	112.14
4	G	246	LPF	CL2-CL1-NL1	2.78	120.73	116.12
4	G	246	LPF	C4-C3-C2	-2.74	106.86	110.46
4	G	246	LPF	ON1-CN1-N3	-2.20	119.02	122.96
4	G	246	LPF	CP5-CP6-CP1	2.11	123.57	120.61

There are no chirality outliers.

All (7) torsion outliers are listed below:

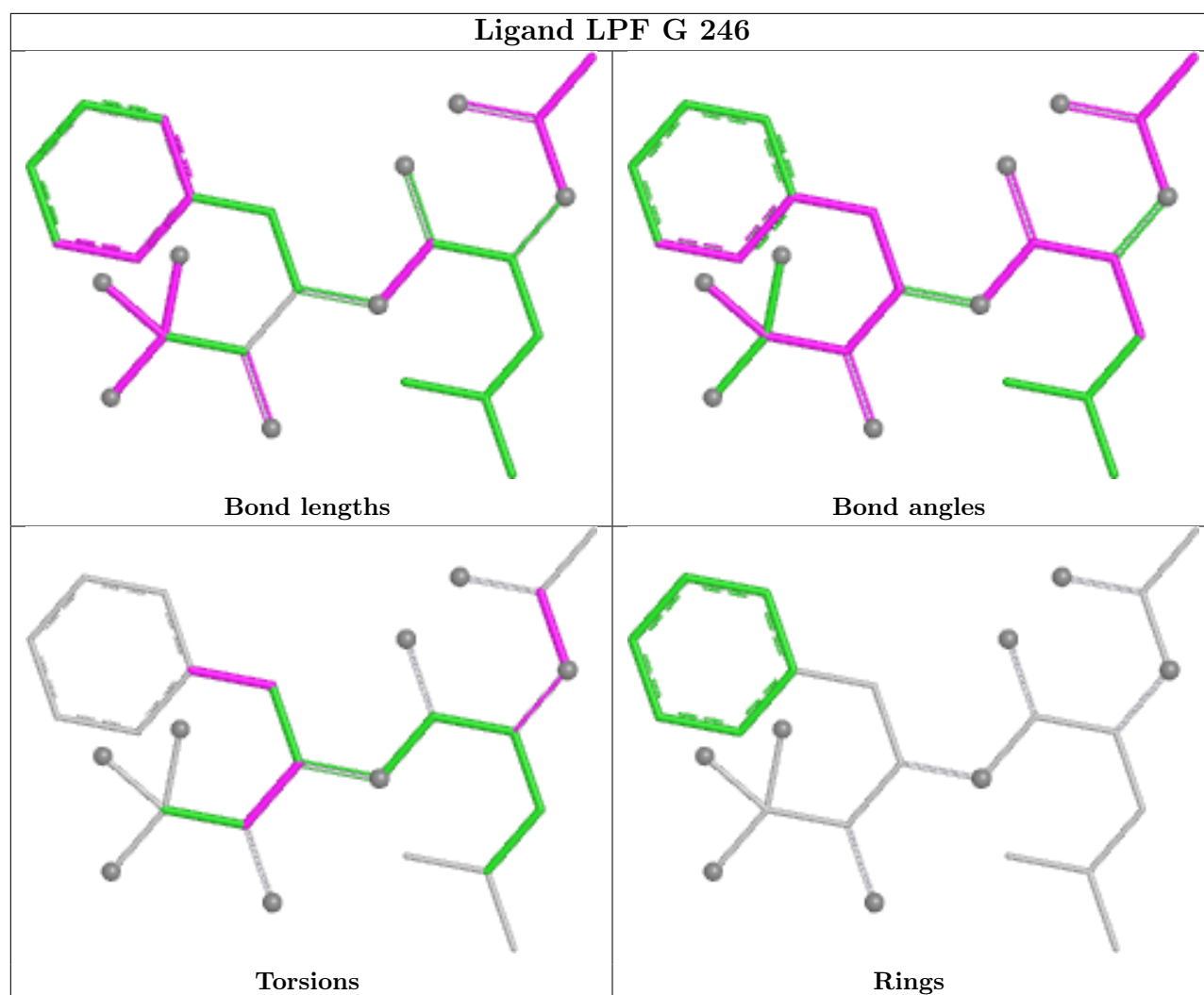
Mol	Chain	Res	Type	Atoms
4	G	246	LPF	OL1-CL1-NL1-CN2
4	G	246	LPF	CL2-CL1-NL1-CN2
4	G	246	LPF	CN1-CN2-NL1-CL1
4	G	246	LPF	C3-C4-CP1-CP6
4	G	246	LPF	C3-C4-CP1-CP2
4	G	246	LPF	O2-C2-C3-C4
4	G	246	LPF	O2-C2-C3-N3

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	246	LPF	13	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

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.