Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:15 pm BST

PDB ID	:	7GCH
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 following versions of software and data (see references ①) were used in the production of this report:

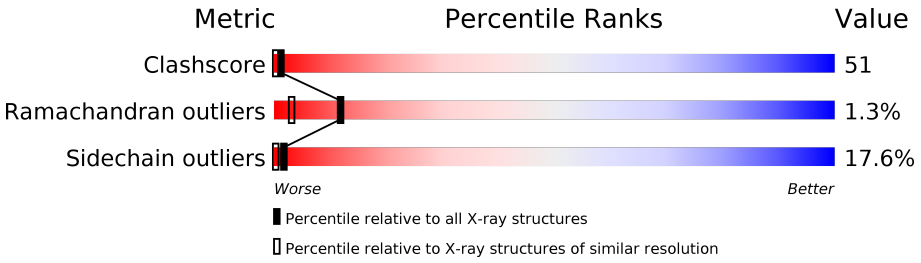
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	13	38% 38% 8% 15%
2	F	131	38% 50% 8% •
3	G	97	32% 42% 16% 7% •

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			

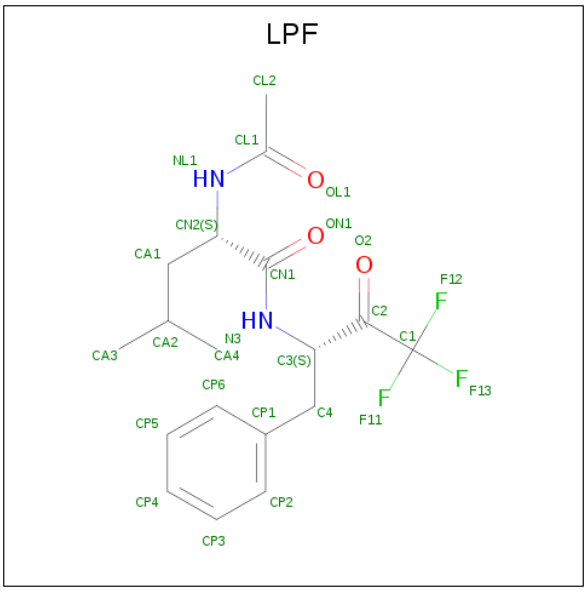
- Molecule 2 is a protein called GAMMA-CHYMOTRYPSIN A.

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) (three-letter code: LPF) (formula: $C_{18}H_{23}F_3N_2O_3$).



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		

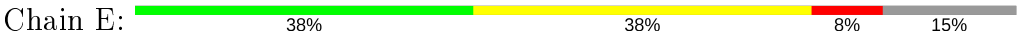
3 Residue-property plots (i)

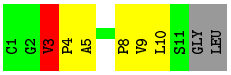
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Chain E:



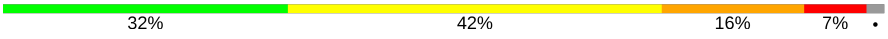


- Molecule 2: GAMMA-CHYMOTRYPSIN A

Chain F:

- Molecule 3: GAMMA-CHYMOTRYPSIN A

Chain G:



4 Data and refinement statistics (i)

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	69.30Å 69.30Å 97.60Å 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	1.02	0/70	1.62	1/97 (1.0%)
2	F	1.26	6/1000 (0.6%)	2.03	28/1361 (2.1%)
3	G	1.16	1/702 (0.1%)	2.06	26/955 (2.7%)
All	All	1.21	7/1772 (0.4%)	2.03	55/2413 (2.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	245	ASN	C-OXT	7.88	1.38	1.23
2	F	78	GLU	CD-OE2	7.12	1.33	1.25
2	F	21	GLU	CD-OE2	6.77	1.33	1.25
2	F	70	GLU	CD-OE2	6.61	1.32	1.25
2	F	49	GLU	CD-OE2	5.17	1.31	1.25
2	F	20	GLU	CD-OE2	5.09	1.31	1.25
2	F	146	TYR	C-OXT	5.06	1.32	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	154	ARG	NE-CZ-NH1	13.47	127.04	120.30
3	G	163	LEU	CA-CB-CG	12.88	144.93	115.30
2	F	114	PHE	CB-CG-CD1	-9.63	114.06	120.80
2	F	70	GLU	CG-CD-OE1	7.95	134.21	118.30
2	F	114	PHE	CB-CG-CD2	7.66	126.16	120.80
3	G	240	GLN	CB-CG-CD	7.50	131.09	111.60
2	F	50	ASN	CA-CB-CG	-7.42	97.08	113.40
3	G	232	THR	OG1-CB-CG2	7.35	126.90	110.00
2	F	72	ASP	CB-CG-OD1	-7.03	111.97	118.30
3	G	240	GLN	CA-CB-CG	7.00	128.79	113.40
2	F	89	PHE	CB-CG-CD1	-6.97	115.92	120.80
2	F	70	GLU	OE1-CD-OE2	-6.73	115.22	123.30
3	G	230	ARG	CD-NE-CZ	6.64	132.90	123.60
2	F	143	LEU	CB-CA-C	6.56	122.67	110.20
3	G	165	ASN	CB-CA-C	6.55	123.50	110.40
3	G	200	VAL	CA-CB-CG1	6.50	120.66	110.90
2	F	128	ASP	CB-CG-OD2	-6.48	112.47	118.30
3	G	180	MET	CA-CB-CG	6.45	124.27	113.30
3	G	230	ARG	NE-CZ-NH2	-6.37	117.11	120.30
3	G	232	THR	N-CA-CB	-6.27	98.38	110.30
2	F	72	ASP	N-CA-CB	-6.21	99.43	110.60
3	G	165	ASN	N-CA-CB	-6.21	99.43	110.60
2	F	58	CYS	CA-CB-SG	6.19	125.14	114.00
2	F	122	CYS	N-CA-CB	6.18	121.72	110.60
2	F	100	ASN	N-CA-CB	6.17	121.71	110.60
2	F	71	PHE	CB-CG-CD1	-6.04	116.57	120.80
3	G	202	LYS	C-N-CA	5.96	136.61	121.70
2	F	78	GLU	CB-CG-CD	5.94	130.23	114.20
3	G	245	ASN	CA-C-O	-5.93	107.64	120.10
2	F	20	GLU	O-C-N	5.92	132.17	122.70
2	F	50	ASN	CB-CA-C	-5.82	98.76	110.40
1	E	3	VAL	CB-CA-C	5.82	122.46	111.40
2	F	66	VAL	CA-CB-CG2	5.82	119.62	110.90
3	G	244	ALA	CB-CA-C	5.65	118.57	110.10
3	G	203	LYS	CA-CB-CG	5.64	125.82	113.40
3	G	170	LYS	CB-CA-C	5.57	121.54	110.40
2	F	50	ASN	OD1-CG-ND2	5.56	134.70	121.90
2	F	118	VAL	CB-CA-C	5.50	121.84	111.40
3	G	219	THR	CA-CB-OG1	-5.48	97.49	109.00
3	G	181	ILE	CB-CG1-CD1	5.45	129.16	113.90
2	F	128	ASP	CB-CG-OD1	5.42	123.18	118.30
2	F	37	THR	N-CA-CB	-5.39	100.06	110.30
2	F	99	ILE	N-CA-CB	5.38	123.18	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	230	ARG	CB-CA-C	5.35	121.10	110.40
3	G	154	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	F	51	TRP	CA-CB-CG	5.27	123.72	113.70
3	G	184	GLY	O-C-N	5.18	130.99	122.70
2	F	50	ASN	O-C-N	5.18	130.99	122.70
3	G	224	THR	N-CA-CB	-5.13	100.55	110.30
2	F	61	THR	N-CA-CB	5.12	120.03	110.30
2	F	95	ASN	CA-C-O	5.08	130.76	120.10
3	G	213	VAL	CA-CB-CG2	5.05	118.48	110.90
3	G	160	LEU	CA-CB-CG	5.01	126.83	115.30
2	F	78	GLU	N-CA-CB	5.00	119.61	110.60
3	G	219	THR	N-CA-CB	-5.00	100.80	110.30

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	105	4
3	G	689	0	686	86	1
4	G	26	0	23	13	0
5	E	2	0	0	0	0
5	F	49	0	0	18	0
5	G	48	0	0	22	3
All	All	1863	0	1736	178	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 51.

All (178) 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:LPF:F13	4:G:246:LPF:C1	1.59	1.39
4:G:246:LPF:C1	4:G:246:LPF: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: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
3:G:163:LEU:HB3	5:G:367:HOH:O	1.48	1.11
2:F:40:HIS:CA	5:F:331:HOH:O	1.99	1.03
2:F:18:ASN:ND2	3:G:187:GLY:O	1.92	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:33:LEU:O	5:F:331:HOH:O	1.91	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
2:F:95:ASN:CG	2:F:98:THR:OG1	2.15	0.85
3:G:177:LYS:HG2	3:G:180:MET:HE3	1.57	0.85
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:222:THR:C	5:G:409:HOH:O	2.14	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:HA	3:G:239:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:222:THR:O	5:G:409:HOH:O	2.05	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
2:F:78:GLU:OE1	5:F:456:HOH:O	2.07	0.71
2:F:105:LEU:HD22	3:G:237:TRP:CH2	2.25	0.71
3:G:167:ASN:C	3:G:170:LYS:HD2	2.12	0.70
5:F:356:HOH:O	3:G:232:THR:HG23	1.90	0.70
4:G:246:LPF:HL1	4:G:246:LPF:CA3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:230:ARG:NE	5:G:610:HOH:O	2.36	0.57
1:E:9:VAL:HG22	2:F:23:VAL:CG2	2.35	0.56
2:F:144:THR:HG23	3:G:152:PRO:HD3	1.87	0.56
3:G:177:LYS:HG2	3:G:180:MET:HE1	1.87	0.56
2:F:57:HIS:ND1	4:G:246:LPF:HA43	2.20	0.56
3:G:167:ASN:HA	3:G:170:LYS:NZ	2.20	0.56
3:G:181:ILE:HG13	3:G:182:CYS:N	2.21	0.55
2:F:40:HIS:CD2	2:F:40:HIS:C	2.80	0.55
3:G:217:SER:O	3:G:219:THR:N	2.40	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
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
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
2:F:129:ASP:OD2	5:F:384:HOH:O	2.18	0.53
2:F:47:ILE:CG2	2:F:53:VAL:HG22	2.36	0.53
2:F:122:CYS:O	3:G:208:THR:HA	2.09	0.52
3:G:166:THR:C	3:G:170:LYS:HE3	2.29	0.52
4:G:246:LPF:NL1	4:G:246:LPF:CA3	2.68	0.52
2:F:130:PHE:CE2	3:G:210:VAL:HG21	2.45	0.52
2:F:53:VAL:HG13	2:F:105:LEU:HD12	1.92	0.52
3:G:217:SER:C	3:G:219:THR:N	2.64	0.51
4:G:246:LPF:HP4	5:G:428:HOH:O	2.01	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
2:F:142:GLY:O	2:F:143:LEU:C	2.50	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:48:ASN:HD22	2:F:48:ASN:C	2.18	0.47
3:G:217:SER:C	3:G:219:THR:H	2.17	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:95:ASN:C	2:F:95:ASN:OD1	2.56	0.45
2:F:26:SER:C	2:F:28:PRO:HD3	2.38	0.45
2:F:31:VAL:HG22	2:F:44:GLY:C	2.37	0.45
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:HA	2:F:100:ASN:HD22	1.56	0.44
3:G:185:ALA:HB2	3:G:225:PRO:HG3	1.99	0.44
2:F:103:ILE:HD12	3:G:212:ILE:CD1	2.48	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:ND2	3:G:245:ASN:N	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
2:F:39:PHE:C	5:F:331:HOH:O	2.52	0.42
3:G:154:ARG:HG2	3:G:154:ARG:H	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
3:G:167:ASN:O	3:G:170:LYS:HD2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:169:LYS:HB2	3:G:173:GLY:HA2	2.02	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
3:G:165:ASN:O	3:G:168:CYS:N	2.53	0.41
2:F:103:ILE:CG2	3:G:234:LEU:HD13	2.51	0.41
1:E:3:VAL:HA	1:E:4:PRO:HD2	1.98	0.41
2:F:17:VAL:O	2:F:18:ASN:HB2	2.20	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
3:G:166:THR:HG22	3:G:170:LYS:HZ2	1.85	0.41
2:F:77:SER:HA	5:F:344:HOH:O	2.22	0.41
2:F:53:VAL:CG1	2:F:105:LEU:HD12	2.47	0.40
2:F:93:LYS:HB3	2:F:93:LYS:HE3	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%)	9 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	93/97 (96%)	87 (94%)	5 (5%)	1 (1%)	14 4
All	All	231/241 (96%)	219 (95%)	9 (4%)	3 (1%)	12 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 (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	E	8/10 (80%)	7 (88%)	1 (12%)	4 1
2	F	109/109 (100%)	94 (86%)	15 (14%)	3 1
3	G	76/77 (99%)	58 (76%)	18 (24%)	1 0
All	All	193/196 (98%)	159 (82%)	34 (18%)	2 0

All (34) 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	67	VAL
2	F	75	SER
2	F	77	SER
2	F	79	LYS
2	F	100	ASN
2	F	104	THR

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Mol	Chain	Res	Type
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	166	THR
3	G	169	LYS
3	G	177	LYS
3	G	178	ASP
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	48	ASN
2	F	100	ASN
3	G	165	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 (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	$\#\|Z\| > 2$
4	LPF	G	246	3	26,26,26	5.23	11 (42%)	33,36,36	3.38	11 (33%)

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	-	5/29/30/30	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	17.55	1.51	1.21
4	G	246	LPF	CL2-CL1	-10.87	1.28	1.50
4	G	246	LPF	OL1-CL1	10.24	1.46	1.23
4	G	246	LPF	F12-C1	6.99	1.62	1.32
4	G	246	LPF	F13-C1	6.21	1.59	1.32
4	G	246	LPF	F11-C1	5.34	1.55	1.32
4	G	246	LPF	C3-C2	-4.40	1.45	1.52
4	G	246	LPF	CN1-N3	3.71	1.42	1.34
4	G	246	LPF	CP2-CP1	-2.79	1.32	1.38
4	G	246	LPF	CP6-CP1	-2.62	1.33	1.38
4	G	246	LPF	CL1-NL1	-2.05	1.27	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	246	LPF	O2-C2-C1	-10.45	109.11	117.06
4	G	246	LPF	ON1-CN1-CN2	7.03	135.24	120.45
4	G	246	LPF	OL1-CL1-CL2	-6.65	109.70	122.06
4	G	246	LPF	O2-C2-C3	-6.19	105.29	119.96
4	G	246	LPF	CN2-CN1-N3	-5.05	105.62	116.70
4	G	246	LPF	CP1-C4-C3	4.69	126.31	113.39
4	G	246	LPF	CA1-CN2-CN1	4.57	121.44	110.57
4	G	246	LPF	OL1-CL1-NL1	4.11	129.52	121.95
4	G	246	LPF	F13-C1-C2	-3.54	104.26	112.14
4	G	246	LPF	CL2-CL1-NL1	2.74	120.73	116.10
4	G	246	LPF	ON1-CN1-N3	-2.11	119.02	122.93

There are no chirality outliers.

All (5) 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

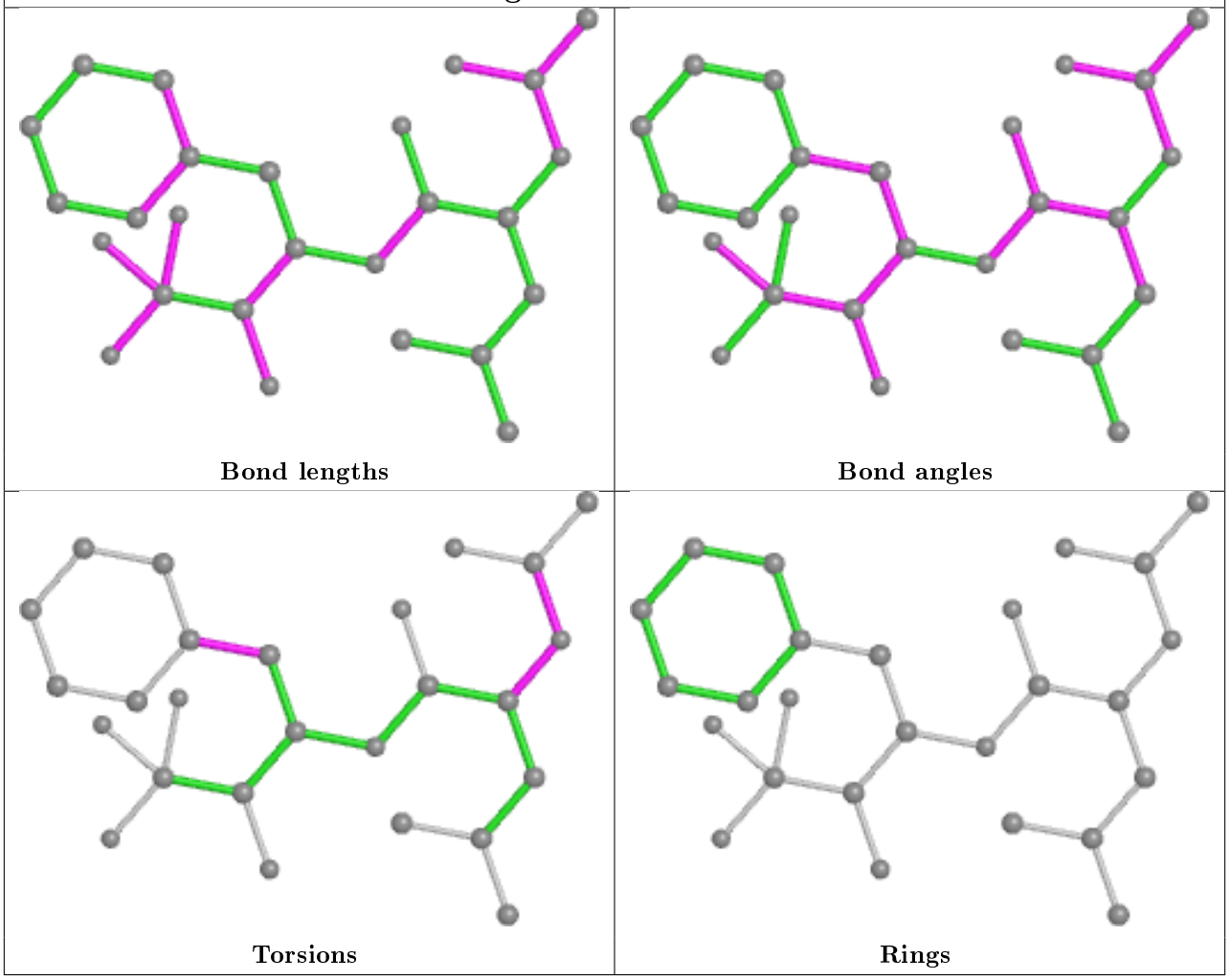
There are no ring outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LPF G 246



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.