



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 AM UTC

PDB ID : 2GCH / pdb_00002gch
Title : REFINED CRYSTAL STRUCTURE OF GAMMA-CHYMOTRYPSIN AT
1.9 ANGSTROMS RESOLUTION
Authors : Cohen, G.H.; Davies, D.R.; Silverton, E.W.
Deposited on : 1980-05-21
Resolution : 1.90 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

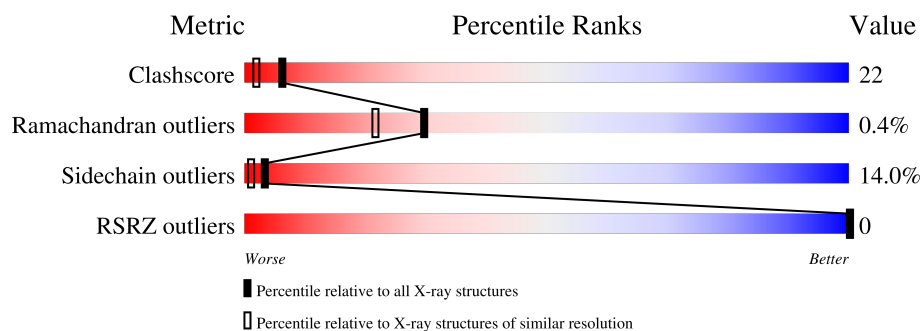
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	13	
2	F	131	
3	G	97	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1889 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 water.

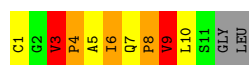
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	4	Total	O	0	0
			4	4		
4	F	83	Total	O	0	0
			83	83		
4	G	64	Total	O	0	0
			64	64		

3 Residue-property plots

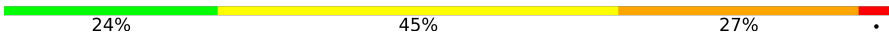
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

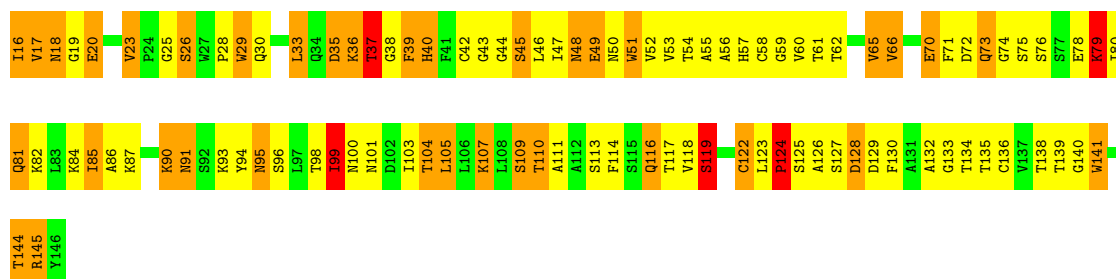
• Molecule 1: GAMMA-CHYMOTRYPSIN A

Chain E: 

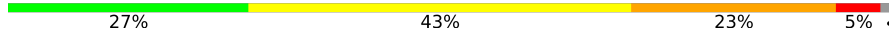


• Molecule 2: GAMMA-CHYMOTRYPSIN A

Chain F: 



• Molecule 3: GAMMA-CHYMOTRYPSIN A

Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.60Å 69.60Å 97.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 1.90 7.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-1.90) 76.5 (7.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available) 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 85.1	EDS
L-test for twinning ¹	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1889	wwPDB-VP
Average B, all atoms (Å ²)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	2.41	6/70 (8.6%)	3.41	14/97 (14.4%)
2	F	2.55	57/1000 (5.7%)	3.05	143/1361 (10.5%)
3	G	2.48	33/702 (4.7%)	3.12	97/955 (10.2%)
All	All	2.52	96/1772 (5.4%)	3.09	254/2413 (10.5%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	65	VAL	C-O	-11.43	1.12	1.24
2	F	40	HIS	CG-CD2	10.81	1.47	1.35
2	F	57	HIS	ND1-CE1	-10.18	1.22	1.32
2	F	47	ILE	C-O	9.24	1.36	1.24
2	F	30	GLN	C-O	9.17	1.34	1.23
2	F	30	GLN	C-N	-8.86	1.21	1.33
2	F	110	THR	CA-CB	8.63	1.66	1.53
3	G	202	LYS	CA-CB	-8.51	1.41	1.53
2	F	94	TYR	CA-CB	8.34	1.67	1.53
2	F	43	GLY	N-CA	7.91	1.52	1.44
2	F	103	ILE	C-O	7.90	1.31	1.24
2	F	71	PHE	CA-CB	7.85	1.66	1.53
2	F	23	VAL	CA-C	7.75	1.59	1.53
2	F	44	GLY	CA-C	7.53	1.59	1.51
2	F	55	ALA	C-N	7.38	1.44	1.34
2	F	58	CYS	C-N	-7.33	1.26	1.33
3	G	208	THR	C-O	7.25	1.32	1.23
1	E	4	PRO	C-N	-7.21	1.24	1.33
3	G	211	GLY	N-CA	7.17	1.53	1.45
3	G	225	PRO	C-O	7.06	1.31	1.23
2	F	51	TRP	C-O	-7.00	1.15	1.23
3	G	163	LEU	CB-CG	-6.99	1.39	1.53
2	F	79	LYS	N-CA	6.98	1.56	1.46
3	G	229	ALA	CA-C	6.98	1.62	1.52
3	G	232	THR	CA-CB	6.93	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	222	THR	CB-OG1	-6.81	1.32	1.43
2	F	133	GLY	C-N	-6.80	1.24	1.33
3	G	232	THR	N-CA	6.73	1.54	1.46
3	G	234	LEU	CA-CB	6.68	1.63	1.54
2	F	26	SER	CB-OG	-6.67	1.28	1.42
2	F	72	ASP	CG-OD1	-6.62	1.12	1.25
2	F	44	GLY	C-O	-6.61	1.17	1.23
2	F	103	ILE	N-CA	6.55	1.54	1.46
2	F	33	LEU	N-CA	6.51	1.54	1.46
3	G	198	PRO	C-O	-6.50	1.16	1.23
3	G	244	ALA	N-CA	6.42	1.54	1.46
2	F	82	LYS	C-O	6.40	1.31	1.24
2	F	35	ASP	CA-CB	6.38	1.62	1.53
2	F	72	ASP	C-O	6.36	1.31	1.24
3	G	183	ALA	C-O	6.34	1.31	1.23
2	F	101	ASN	C-O	-6.34	1.15	1.23
2	F	130	PHE	N-CA	6.29	1.54	1.46
2	F	66	VAL	C-N	-6.25	1.25	1.33
1	E	10	LEU	C-N	-6.21	1.24	1.33
2	F	70	GLU	C-N	-6.19	1.25	1.33
2	F	40	HIS	CA-CB	6.09	1.60	1.53
2	F	101	ASN	N-CA	6.07	1.55	1.46
2	F	65	VAL	N-CA	6.01	1.52	1.46
2	F	62	THR	CB-OG1	5.97	1.53	1.43
2	F	119	SER	N-CA	-5.97	1.37	1.46
2	F	90	LYS	N-CA	5.94	1.53	1.46
3	G	215	TRP	C-N	-5.93	1.27	1.33
2	F	116	GLN	N-CA	-5.92	1.38	1.46
1	E	9	VAL	N-CA	5.92	1.54	1.46
1	E	3	VAL	N-CA	5.91	1.53	1.46
3	G	172	TRP	C-O	-5.86	1.16	1.24
3	G	189	SER	C-O	-5.85	1.15	1.23
2	F	74	GLY	C-N	-5.81	1.25	1.33
2	F	117	THR	CA-C	-5.81	1.45	1.52
3	G	172	TRP	CA-CB	5.68	1.62	1.53
3	G	241	THR	C-O	-5.62	1.17	1.24
3	G	153	ASP	C-O	-5.60	1.16	1.24
2	F	119	SER	CB-OG	-5.60	1.30	1.42
1	E	7	GLN	CD-OE1	5.57	1.34	1.23
2	F	16	ILE	CA-C	5.57	1.64	1.52
2	F	40	HIS	CE1-NE2	5.55	1.38	1.32
3	G	231	VAL	C-N	-5.55	1.26	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	138	THR	C-O	5.54	1.30	1.23
2	F	57	HIS	CD2-NE2	-5.53	1.31	1.37
3	G	164	SER	N-CA	5.51	1.53	1.45
3	G	177	LYS	CE-NZ	5.41	1.65	1.49
3	G	198	PRO	N-CD	5.40	1.55	1.47
2	F	45	SER	C-O	-5.36	1.17	1.24
1	E	7	GLN	CD-NE2	5.35	1.44	1.33
3	G	244	ALA	C-O	5.34	1.30	1.24
2	F	117	THR	CA-CB	5.34	1.61	1.53
3	G	159	SER	C-O	-5.34	1.17	1.23
2	F	52	VAL	CA-C	5.32	1.59	1.52
2	F	51	TRP	CG-CD2	5.28	1.53	1.43
3	G	165	ASN	CB-CG	5.26	1.65	1.52
3	G	180	MET	CA-C	5.23	1.58	1.52
3	G	216	GLY	C-N	-5.22	1.26	1.33
3	G	236	ASN	N-CA	5.22	1.52	1.46
2	F	134	THR	CA-C	5.21	1.59	1.52
3	G	196	GLY	CA-C	5.19	1.58	1.51
2	F	144	THR	CB-OG1	5.17	1.52	1.43
2	F	96	SER	N-CA	5.16	1.53	1.46
2	F	56	ALA	CA-C	-5.16	1.45	1.52
2	F	141	TRP	CA-C	5.13	1.59	1.53
3	G	194	ASP	C-N	-5.10	1.26	1.33
2	F	122	CYS	N-CA	5.06	1.52	1.45
3	G	203	LYS	CA-C	5.05	1.58	1.52
2	F	82	LYS	CE-NZ	5.03	1.64	1.49
2	F	138	THR	N-CA	5.02	1.51	1.45
2	F	114	PHE	C-N	-5.02	1.26	1.33
3	G	200	VAL	C-O	5.01	1.29	1.24

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	153	ASP	CA-CB-CG	17.31	129.91	112.60
3	G	202	LYS	CA-CB-CG	15.02	144.13	114.10
2	F	73	GLN	CB-CG-CD	14.43	137.12	112.60
3	G	229	ALA	O-C-N	13.03	138.95	122.93
2	F	128	ASP	CA-CB-CG	12.70	125.30	112.60
3	G	165	ASN	CA-CB-CG	-12.36	100.24	112.60
2	F	116	GLN	OE1-CD-NE2	12.21	134.81	122.60
1	E	7	GLN	OE1-CD-NE2	-11.68	110.92	122.60
3	G	160	LEU	O-C-N	11.46	130.77	121.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	76	SER	CA-C-O	-11.30	106.62	119.05
3	G	157	GLN	OE1-CD-NE2	-11.25	111.35	122.60
3	G	224	THR	CA-CB-OG1	-11.12	92.92	109.60
3	G	236	ASN	OD1-CG-ND2	-10.85	111.75	122.60
2	F	129	ASP	CA-CB-CG	-10.81	101.78	112.60
3	G	223	SER	O-C-N	9.83	133.79	122.20
2	F	61	THR	CA-CB-CG2	9.74	127.06	110.50
3	G	244	ALA	CB-CA-C	9.63	129.58	110.42
2	F	78	GLU	CA-C-O	-9.60	109.84	121.36
2	F	116	GLN	CB-CG-CD	-9.23	96.91	112.60
3	G	178	ASP	CA-CB-CG	8.96	121.56	112.60
2	F	76	SER	O-C-N	8.94	133.34	122.35
3	G	202	LYS	N-CA-CB	8.83	124.27	109.87
2	F	46	LEU	O-C-N	8.80	133.26	123.22
2	F	116	GLN	CA-CB-CG	-8.70	96.70	114.10
2	F	39	PHE	CA-C-N	8.47	134.87	121.66
2	F	39	PHE	C-N-CA	8.47	134.87	121.66
2	F	91	ASN	O-C-N	-8.46	111.48	123.07
2	F	110	THR	CA-CB-OG1	-8.39	97.02	109.60
2	F	20	GLU	CG-CD-OE1	8.36	137.63	118.40
3	G	236	ASN	CA-CB-CG	8.26	120.86	112.60
2	F	84	LYS	CG-CD-CE	8.25	130.28	111.30
3	G	229	ALA	CA-C-O	-8.23	111.34	120.81
1	E	10	LEU	N-CA-CB	-8.10	96.73	110.50
2	F	138	THR	O-C-N	-8.04	112.33	123.11
2	F	135	THR	CA-C-O	8.02	128.94	120.36
2	F	37	THR	CA-CB-CG2	7.93	123.99	110.50
2	F	140	GLY	O-C-N	7.90	131.44	123.78
2	F	20	GLU	O-C-N	7.88	133.40	123.15
3	G	199	LEU	N-CA-CB	7.87	123.70	110.87
3	G	189	SER	O-C-N	7.84	132.14	123.52
3	G	241	THR	CA-CB-OG1	-7.83	97.85	109.60
2	F	38	GLY	CA-C-N	7.83	133.08	121.72
2	F	38	GLY	C-N-CA	7.83	133.08	121.72
3	G	189	SER	CB-CA-C	-7.82	97.13	109.72
1	E	6	ILE	CB-CG1-CD1	7.77	130.11	113.80
2	F	40	HIS	CB-CG-ND1	7.77	134.35	122.70
2	F	81	GLN	CG-CD-NE2	-7.75	104.77	116.40
2	F	40	HIS	CB-CG-CD2	-7.74	121.13	131.20
3	G	194	ASP	CA-C-O	-7.74	109.71	119.31
3	G	198	PRO	N-CA-C	7.68	124.51	111.68
2	F	91	ASN	CB-CA-C	7.67	120.72	110.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	37	THR	CA-C-O	7.62	128.95	119.05
3	G	190	SER	O-C-N	-7.59	113.91	122.86
3	G	244	ALA	O-C-N	-7.59	112.50	122.59
3	G	152	PRO	CB-CA-C	-7.58	101.53	111.23
2	F	23	VAL	N-CA-C	-7.48	102.20	108.63
2	F	37	THR	CA-CB-OG1	-7.47	98.39	109.60
3	G	151	THR	CA-CB-OG1	7.46	120.79	109.60
2	F	101	ASN	CA-C-O	-7.42	112.97	121.65
1	E	3	VAL	CA-CB-CG1	7.41	123.00	110.40
3	G	167	ASN	CA-C-O	7.36	128.44	119.97
3	G	243	ALA	CA-C-O	-7.32	112.79	120.55
2	F	51	TRP	CB-CG-CD1	7.30	137.85	126.90
2	F	145	ARG	NE-CZ-NH1	-7.30	114.20	121.50
2	F	30	GLN	CA-C-N	7.21	134.46	122.57
2	F	30	GLN	C-N-CA	7.21	134.46	122.57
3	G	174	THR	CA-CB-OG1	-7.20	98.80	109.60
1	E	10	LEU	CA-C-N	7.19	130.57	116.20
2	F	110	THR	N-CA-CB	-7.07	99.62	110.65
3	G	194	ASP	N-CA-CB	7.01	121.82	110.40
3	G	184	GLY	CA-C-O	-7.00	112.51	121.05
3	G	219	THR	O-C-N	-6.97	113.77	122.35
3	G	151	THR	CA-C-N	6.93	126.92	119.78
3	G	151	THR	C-N-CA	6.93	126.92	119.78
3	G	232	THR	CA-C-N	6.91	134.22	122.26
3	G	232	THR	C-N-CA	6.91	134.22	122.26
2	F	45	SER	CA-C-O	6.91	127.99	120.32
2	F	73	GLN	CA-CB-CG	6.88	127.86	114.10
2	F	113	SER	CA-C-O	6.88	127.69	120.54
3	G	185	ALA	N-CA-C	-6.85	104.22	112.58
2	F	71	PHE	CA-C-O	6.83	130.28	120.51
3	G	190	SER	CA-C-O	6.83	129.00	121.56
1	E	10	LEU	CA-C-O	-6.75	109.33	120.80
2	F	36	LYS	CA-CB-CG	6.70	127.50	114.10
2	F	25	GLY	CA-C-N	6.67	132.81	121.14
2	F	25	GLY	C-N-CA	6.67	132.81	121.14
2	F	66	VAL	CA-C-N	6.66	131.43	122.90
2	F	66	VAL	C-N-CA	6.66	131.43	122.90
3	G	239	GLN	CA-C-O	6.63	127.54	119.38
3	G	204	ASN	CA-CB-CG	6.61	119.21	112.60
3	G	194	ASP	CA-CB-CG	6.58	119.18	112.60
2	F	99	ILE	O-C-N	6.56	130.77	122.57
1	E	7	GLN	O-C-N	6.53	127.25	121.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	54	THR	CA-CB-CG2	6.53	121.60	110.50
3	G	198	PRO	CA-C-N	6.51	132.33	122.95
3	G	198	PRO	C-N-CA	6.51	132.33	122.95
2	F	55	ALA	CA-C-N	-6.51	110.42	120.31
2	F	55	ALA	C-N-CA	-6.51	110.42	120.31
2	F	35	ASP	CA-C-O	-6.49	113.97	121.82
2	F	129	ASP	CA-C-N	-6.47	113.36	123.13
2	F	129	ASP	C-N-CA	-6.47	113.36	123.13
2	F	51	TRP	O-C-N	6.46	131.15	123.33
2	F	19	GLY	O-C-N	6.45	129.01	122.88
3	G	203	LYS	N-CA-CB	-6.40	100.34	110.77
2	F	110	THR	CA-CB-CG2	6.39	121.36	110.50
3	G	152	PRO	N-CD-CG	-6.36	93.66	103.20
3	G	220	CYS	CA-C-O	-6.32	112.97	120.81
2	F	132	ALA	N-CA-C	-6.31	101.09	110.23
3	G	218	SER	CA-C-N	6.31	132.29	122.26
3	G	218	SER	C-N-CA	6.31	132.29	122.26
3	G	212	ILE	CA-CB-CG1	6.30	121.11	110.40
2	F	46	LEU	CA-C-N	-6.29	114.24	122.16
2	F	46	LEU	C-N-CA	-6.29	114.24	122.16
3	G	174	THR	OG1-CB-CG2	6.27	121.85	109.30
3	G	231	VAL	CA-C-N	6.26	129.30	120.28
3	G	231	VAL	C-N-CA	6.26	129.30	120.28
2	F	91	ASN	N-CA-CB	-6.26	99.02	109.28
2	F	124	PRO	CA-C-N	6.26	131.35	122.09
2	F	124	PRO	C-N-CA	6.26	131.35	122.09
1	E	10	LEU	CB-CA-C	6.25	121.98	110.10
2	F	119	SER	N-CA-C	6.24	117.65	108.86
2	F	113	SER	CB-CA-C	6.19	120.68	110.78
2	F	62	THR	CA-CB-OG1	-6.18	100.33	109.60
2	F	126	ALA	O-C-N	6.18	130.43	122.39
3	G	166	THR	CA-CB-OG1	-6.17	100.34	109.60
3	G	223	SER	CA-C-O	-6.16	111.92	119.18
2	F	105	LEU	CA-C-O	-6.16	114.02	121.28
2	F	109	SER	CB-CA-C	-6.16	97.82	110.38
2	F	70	GLU	CG-CD-OE1	6.15	132.55	118.40
2	F	72	ASP	CA-C-O	-6.13	114.16	120.54
3	G	175	LYS	CA-C-O	-6.13	113.17	120.10
3	G	244	ALA	N-CA-CB	-6.12	100.14	110.49
3	G	154	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
2	F	71	PHE	O-C-N	-6.09	114.49	122.59
2	F	79	LYS	CB-CA-C	6.06	121.80	111.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	98	THR	CA-CB-CG2	6.02	120.74	110.50
3	G	173	GLY	O-C-N	6.00	129.07	123.19
2	F	87	LYS	CA-CB-CG	-5.99	102.11	114.10
2	F	101	ASN	O-C-N	5.97	129.74	122.58
2	F	81	GLN	CG-CD-OE1	5.95	132.70	120.80
2	F	126	ALA	N-CA-C	-5.94	105.13	112.38
3	G	159	SER	N-CA-CB	5.93	120.08	110.41
1	E	4	PRO	CA-C-N	5.92	128.69	120.29
1	E	4	PRO	C-N-CA	5.92	128.69	120.29
1	E	9	VAL	CA-C-O	5.92	126.99	120.48
2	F	98	THR	O-C-N	5.89	129.59	122.35
2	F	85	ILE	CA-C-O	-5.86	114.21	120.59
3	G	160	LEU	CB-CA-C	5.84	117.86	109.92
2	F	141	TRP	CA-C-N	5.83	127.11	120.53
2	F	141	TRP	C-N-CA	5.83	127.11	120.53
3	G	223	SER	N-CA-CB	5.82	119.48	110.80
3	G	219	THR	CA-C-O	5.81	125.44	119.05
2	F	109	SER	O-C-N	5.81	130.12	122.33
3	G	154	ARG	CA-C-N	5.81	129.12	120.87
3	G	154	ARG	C-N-CA	5.81	129.12	120.87
3	G	164	SER	O-C-N	5.81	129.52	122.96
3	G	232	THR	OG1-CB-CG2	5.77	120.83	109.30
3	G	232	THR	N-CA-CB	-5.75	101.36	110.22
2	F	38	GLY	O-C-N	-5.75	115.19	122.32
2	F	93	LYS	CB-CG-CD	5.74	124.50	111.30
2	F	42	CYS	O-C-N	5.73	129.78	123.25
2	F	95	ASN	OD1-CG-ND2	5.72	128.32	122.60
3	G	222	THR	O-C-N	5.72	129.77	122.39
3	G	163	LEU	O-C-N	5.72	130.58	123.15
2	F	73	GLN	OE1-CD-NE2	-5.71	116.89	122.60
2	F	57	HIS	CE1-NE2-CD2	5.71	114.71	109.00
3	G	232	THR	O-C-N	-5.70	115.55	122.22
3	G	197	GLY	CA-C-N	5.69	126.17	120.14
3	G	197	GLY	C-N-CA	5.69	126.17	120.14
3	G	175	LYS	O-C-N	5.68	128.87	122.22
2	F	129	ASP	N-CA-C	5.66	117.74	108.52
2	F	110	THR	CA-C-N	5.65	128.87	120.90
2	F	110	THR	C-N-CA	5.65	128.87	120.90
2	F	94	TYR	CA-CB-CG	-5.64	103.75	113.90
3	G	225	PRO	O-C-N	-5.64	116.33	123.10
1	E	6	ILE	CB-CA-C	-5.60	103.40	111.19
3	G	170	LYS	CA-C-O	-5.58	113.56	119.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	109	SER	N-CA-CB	5.57	118.89	110.30
2	F	145	ARG	CA-C-O	5.56	127.01	120.89
2	F	45	SER	CA-C-N	5.56	130.03	122.19
2	F	45	SER	C-N-CA	5.56	130.03	122.19
3	G	214	SER	CA-CB-OG	5.56	122.22	111.10
2	F	114	PHE	CB-CA-C	5.55	118.77	109.89
2	F	87	LYS	N-CA-C	5.54	117.52	108.76
2	F	17	VAL	O-C-N	5.53	129.63	122.77
3	G	223	SER	CA-CB-OG	-5.53	100.05	111.10
2	F	37	THR	N-CA-CB	-5.50	100.76	110.39
2	F	104	THR	N-CA-CB	5.50	120.05	110.81
2	F	78	GLU	CA-C-N	-5.49	114.64	122.77
2	F	78	GLU	C-N-CA	-5.49	114.64	122.77
3	G	208	THR	CA-CB-CG2	5.49	119.84	110.50
2	F	59	GLY	CA-C-N	5.49	127.86	120.50
2	F	59	GLY	C-N-CA	5.49	127.86	120.50
2	F	57	HIS	ND1-CE1-NE2	-5.48	102.92	108.40
2	F	130	PHE	CB-CA-C	5.47	120.42	111.23
3	G	210	VAL	CG1-CB-CG2	5.46	122.81	110.80
1	E	7	GLN	CG-CD-OE1	5.44	131.69	120.80
2	F	84	LYS	CA-CB-CG	-5.44	103.22	114.10
2	F	144	THR	CA-CB-OG1	-5.44	101.44	109.60
3	G	229	ALA	N-CA-C	-5.43	101.82	109.96
2	F	45	SER	O-C-N	-5.42	116.97	123.31
2	F	51	TRP	CG-CD2-CE3	-5.40	128.50	133.90
3	G	163	LEU	CA-CB-CG	5.39	135.17	116.30
2	F	70	GLU	O-C-N	-5.39	116.37	123.16
2	F	61	THR	CA-CB-OG1	-5.38	101.54	109.60
3	G	193	GLY	CA-C-O	5.35	124.99	119.27
3	G	240	GLN	N-CA-C	-5.34	105.90	112.90
3	G	170	LYS	O-C-N	5.33	128.83	122.27
2	F	132	ALA	CA-C-O	-5.33	115.33	121.19
2	F	90	LYS	O-C-N	-5.33	117.00	123.13
3	G	231	VAL	N-CA-C	5.32	117.70	111.05
2	F	86	ALA	CA-C-O	5.32	126.49	120.00
2	F	105	LEU	O-C-N	5.31	129.20	123.10
3	G	152	PRO	CA-C-O	-5.30	115.41	121.56
3	G	184	GLY	O-C-N	5.28	131.00	123.56
2	F	110	THR	CB-CA-C	5.28	118.92	110.16
2	F	40	HIS	ND1-CE1-NE2	5.27	113.67	108.40
2	F	107	LYS	N-CA-CB	-5.27	101.32	110.17
2	F	26	SER	CA-CB-OG	5.25	121.61	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	194	ASP	O-C-N	5.23	129.68	122.46
1	E	8	PRO	CB-CA-C	-5.23	104.71	111.46
2	F	138	THR	CA-CB-OG1	-5.23	101.76	109.60
2	F	28	PRO	CB-CA-C	5.22	119.26	111.85
3	G	190	SER	N-CA-C	-5.22	103.14	110.50
2	F	139	THR	CA-CB-OG1	-5.22	101.78	109.60
2	F	35	ASP	CA-CB-CG	-5.19	107.41	112.60
2	F	80	ILE	CA-C-O	-5.17	115.72	121.98
2	F	29	TRP	CA-C-O	5.16	125.72	119.11
2	F	75	SER	CA-CB-OG	-5.15	100.80	111.10
3	G	210	VAL	CA-C-N	-5.15	115.10	121.38
3	G	210	VAL	C-N-CA	-5.15	115.10	121.38
2	F	33	LEU	O-C-N	5.15	129.09	123.22
2	F	20	GLU	CG-CD-OE2	-5.14	106.58	118.40
3	G	175	LYS	CG-CD-CE	5.14	123.12	111.30
3	G	175	LYS	CA-CB-CG	-5.13	103.83	114.10
3	G	182	CYS	O-C-N	5.13	129.00	123.10
3	G	199	LEU	CA-C-O	5.13	127.66	120.52
2	F	70	GLU	CB-CG-CD	5.12	121.31	112.60
2	F	104	THR	CA-C-O	-5.12	113.98	120.28
2	F	60	VAL	CA-C-N	-5.12	113.69	123.32
2	F	60	VAL	C-N-CA	-5.12	113.69	123.32
2	F	123	LEU	CD1-CG-CD2	5.11	122.04	110.80
2	F	132	ALA	O-C-N	5.11	129.16	122.87
3	G	245	ASN	CA-CB-CG	-5.10	107.50	112.60
3	G	192	MET	CG-SD-CE	5.09	112.10	100.90
2	F	140	GLY	CA-C-O	-5.09	116.64	121.83
3	G	181	ILE	CB-CG1-CD1	-5.08	103.12	113.80
2	F	145	ARG	NE-CZ-NH2	5.06	123.76	119.20
3	G	208	THR	CB-CA-C	5.06	119.37	109.35
2	F	80	ILE	CA-C-N	-5.03	115.90	123.00
2	F	80	ILE	C-N-CA	-5.03	115.90	123.00
2	F	116	GLN	O-C-N	5.03	129.40	122.46
2	F	49	GLU	CA-C-N	-5.03	114.15	121.99
2	F	49	GLU	C-N-CA	-5.03	114.15	121.99

There are no chirality outliers.

There are no planarity outliers.

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	E	69	0	76	12	0
2	F	980	0	951	54	0
3	G	689	0	687	28	0
4	E	4	0	0	0	0
4	F	83	0	0	14	0
4	G	64	0	0	6	0
All	All	1889	0	1714	77	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (77) 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:F:40:HIS:HD2	4:F:161:HOH:O	1.29	1.12
1:E:5:ALA:HB3	2:F:116:GLN:HG3	1.40	1.03
2:F:73:GLN:NE2	4:F:216:HOH:O	1.98	0.96
2:F:48:ASN:HD22	2:F:50:ASN:H	1.11	0.94
2:F:16:ILE:HD13	4:F:196:HOH:O	1.69	0.93
1:E:5:ALA:CB	2:F:116:GLN:HG3	1.99	0.93
3:G:239:GLN:HE21	3:G:239:GLN:HA	1.34	0.91
2:F:17:VAL:O	2:F:18:ASN:HB2	1.76	0.84
2:F:48:ASN:ND2	2:F:50:ASN:H	1.80	0.80
2:F:70:GLU:OE1	4:F:208:HOH:O	1.98	0.78
2:F:51:TRP:CZ2	2:F:107:LYS:HD3	2.20	0.77
2:F:53:VAL:HG12	2:F:105:LEU:HD23	1.69	0.74
2:F:40:HIS:CD2	4:F:161:HOH:O	2.15	0.73
3:G:178:ASP:OD1	4:G:284:HOH:O	2.09	0.70
2:F:35:ASP:OD2	2:F:37:THR:HB	1.92	0.70
3:G:239:GLN:HA	3:G:239:GLN:NE2	2.06	0.70
2:F:16:ILE:CD1	4:F:196:HOH:O	2.33	0.69
2:F:17:VAL:O	2:F:18:ASN:CB	2.40	0.69
2:F:125:SER:HB2	2:F:128:ASP:CG	2.19	0.68
3:G:165:ASN:ND2	4:G:294:HOH:O	2.20	0.67
1:E:9:VAL:HB	2:F:23:VAL:HG21	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:LEU:CD2	2:F:66:VAL:HG22	2.26	0.66
3:G:218:SER:OG	4:G:308:HOH:O	2.12	0.65
2:F:119:SER:HB2	4:F:185:HOH:O	1.96	0.65
2:F:16:ILE:CG2	4:F:196:HOH:O	2.46	0.64
2:F:95:ASN:O	2:F:99:ILE:N	2.31	0.64
2:F:53:VAL:HG12	2:F:105:LEU:CD2	2.28	0.63
2:F:111:ALA:HB1	4:F:199:HOH:O	2.00	0.60
1:E:6:ILE:HD11	2:F:116:GLN:HG2	1.85	0.58
1:E:6:ILE:CD1	2:F:116:GLN:HG2	2.34	0.58
2:F:16:ILE:HG21	4:F:196:HOH:O	2.02	0.57
3:G:232:THR:HB	4:G:251:HOH:O	2.05	0.57
2:F:141:TRP:O	3:G:151:THR:HB	2.05	0.56
2:F:144:THR:HG23	3:G:152:PRO:HD3	1.87	0.56
2:F:125:SER:HB2	2:F:128:ASP:OD2	2.06	0.56
2:F:124:PRO:HD3	3:G:209:LEU:O	2.06	0.55
3:G:245:ASN:ND2	3:G:245:ASN:H	2.01	0.55
2:F:18:ASN:HB3	3:G:188:VAL:HG12	1.89	0.55
3:G:220:CYS:HA	4:G:285:HOH:O	2.07	0.54
2:F:90:LYS:O	2:F:91:ASN:C	2.51	0.53
2:F:100:ASN:HD22	3:G:180:MET:HE3	1.75	0.52
2:F:100:ASN:ND2	3:G:180:MET:HE3	2.25	0.51
3:G:211:GLY:HA2	3:G:229:ALA:O	2.10	0.51
2:F:36:LYS:NZ	4:F:201:HOH:O	2.45	0.50
1:E:9:VAL:HB	2:F:23:VAL:CG2	2.41	0.50
2:F:37:THR:HG22	2:F:39:PHE:HB2	1.95	0.49
1:E:9:VAL:O	1:E:9:VAL:HG12	2.13	0.48
3:G:181:ILE:HD13	3:G:181:ILE:HG21	1.57	0.48
3:G:239:GLN:HB3	4:G:267:HOH:O	2.12	0.48
2:F:16:ILE:CG1	4:F:196:HOH:O	2.59	0.48
3:G:169:LYS:HG2	3:G:173:GLY:O	2.12	0.48
3:G:245:ASN:ND2	3:G:245:ASN:N	2.62	0.48
2:F:136:CYS:HB3	3:G:200:VAL:O	2.15	0.47
3:G:219:THR:O	3:G:220:CYS:HB2	2.16	0.46
2:F:23:VAL:O	2:F:26:SER:OG	2.25	0.45
3:G:230:ARG:HG2	3:G:232:THR:HG22	1.98	0.45
3:G:163:LEU:HD11	3:G:225:PRO:HB3	1.99	0.44
2:F:145:ARG:NH1	4:F:228:HOH:O	2.49	0.44
1:E:3:VAL:O	1:E:3:VAL:CG2	2.65	0.43
2:F:16:ILE:O	2:F:144:THR:HA	2.17	0.43
2:F:79:LYS:O	2:F:79:LYS:HG2	2.17	0.43
2:F:81:GLN:NE2	2:F:118:VAL:HG21	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100:ASN:ND2	3:G:177:LYS:HB2	2.34	0.43
2:F:116:GLN:O	2:F:116:GLN:CG	2.67	0.43
3:G:197:GLY:O	3:G:213:VAL:HG23	2.19	0.43
2:F:125:SER:C	2:F:127:SER:N	2.76	0.42
1:E:1:CYS:C	2:F:122:CYS:SG	3.02	0.42
2:F:85:ILE:HG21	2:F:85:ILE:HD13	1.77	0.42
3:G:210:VAL:O	3:G:210:VAL:HG12	2.19	0.42
2:F:29:TRP:O	2:F:45:SER:HA	2.20	0.41
1:E:5:ALA:HB1	2:F:116:GLN:HG3	1.94	0.41
3:G:165:ASN:ND2	3:G:230:ARG:HH11	2.19	0.41
2:F:16:ILE:HD13	2:F:16:ILE:HG21	1.74	0.41
3:G:169:LYS:HA	3:G:173:GLY:H	1.86	0.41
2:F:79:LYS:N	4:F:203:HOH:O	2.40	0.41
1:E:4:PRO:HG2	1:E:8:PRO:HD3	2.04	0.40
1:E:8:PRO:HA	2:F:26:SER:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	5 (4%)	1 (1%)	16	8
3	G	93/97 (96%)	90 (97%)	3 (3%)	0	100	100
All	All	231/241 (96%)	222 (96%)	8 (4%)	1 (0%)	30	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	6 (75%)	2 (25%)	0	0
2	F	109/109 (100%)	96 (88%)	13 (12%)	5	2
3	G	76/77 (99%)	64 (84%)	12 (16%)	2	1
All	All	193/196 (98%)	166 (86%)	27 (14%)	3	1

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	VAL
1	E	9	VAL
2	F	18	ASN
2	F	20	GLU
2	F	37	THR
2	F	48	ASN
2	F	49	GLU
2	F	65	VAL
2	F	79	LYS
2	F	99	ILE
2	F	104	THR
2	F	109	SER
2	F	110	THR
2	F	119	SER
2	F	124	PRO
3	G	163	LEU
3	G	166	THR
3	G	202	LYS
3	G	203	LYS
3	G	208	THR
3	G	212	ILE
3	G	219	THR
3	G	221	SER
3	G	223	SER
3	G	232	THR
3	G	239	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	245	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	48	ASN
2	F	50	ASN
2	F	73	GLN
2	F	100	ASN
3	G	165	ASN
3	G	239	GLN
3	G	245	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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	11/13 (84%)	-0.14	0 100 100	8, 10, 25, 27	0
2	F	131/131 (100%)	-0.71	0 100 100	2, 7, 16, 20	0
3	G	95/97 (97%)	-0.65	0 100 100	2, 6, 16, 21	0
All	All	237/241 (98%)	-0.66	0 100 100	2, 7, 18, 27	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.