



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:16 AM UTC

PDB ID : 4CHA / pdb_00004cha
Title : STRUCTURE OF ALPHA-*CHYMOTRYPSIN REFINED AT 1.68
ANGSTROMS RESOLUTION
Authors : Tsukada, H.; Blow, D.M.
Deposited on : 1984-11-26
Resolution : 1.68 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

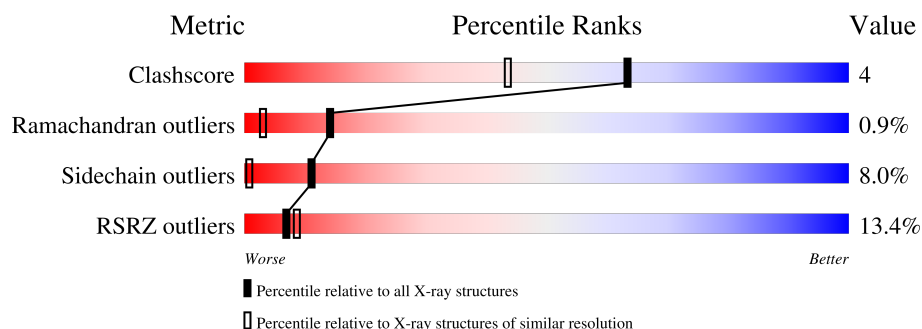
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	A	13	31% 54% 23% 8% 15%
1	E	13	15% 46% 31% 23%
2	B	131	15% 68% 27% • •
2	F	131	15% 67% 26% 5% •
3	C	97	9% 70% 24% • •
3	G	97	9% 67% 26% 5% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3591 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 ALPHA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	11	Total	C	N	O	S	0	0	0
			74	48	12	13	1			
1	E	10	Total	C	N	O	S	0	0	0
			68	45	11	11	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	97	Total	C	N	O	S	0	0	0
			702	436	123	136	7			
3	G	97	Total	C	N	O	S	0	0	0
			702	436	123	136	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	23	Total	O	0	0
			23	23		
4	C	18	Total	O	0	0
			18	18		
4	F	21	Total	O	0	0
			21	21		

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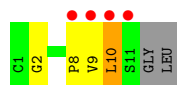
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	22	Total	O	0	0
			22	22		

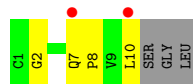
3 Residue-property plots [i](#)

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.

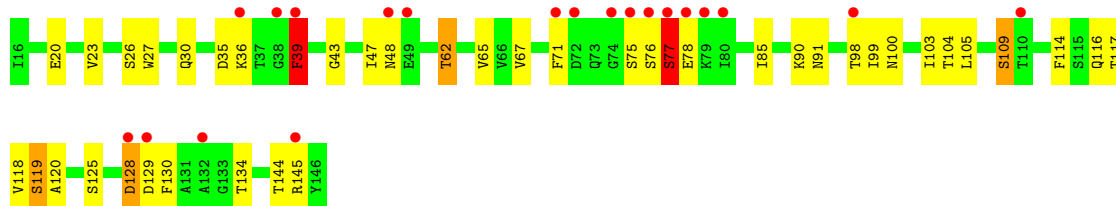
• Molecule 1: ALPHA-CHYMOTRYPSIN A



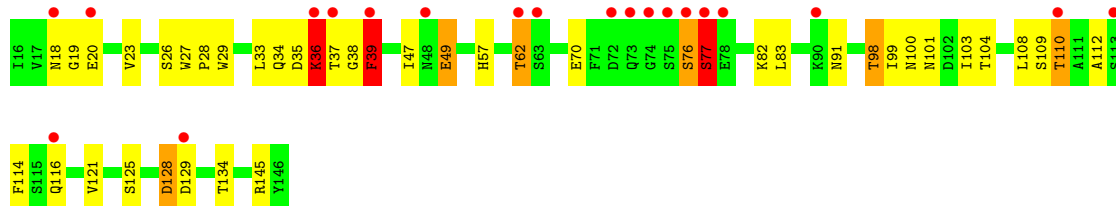
• Molecule 1: ALPHA-CHYMOTRYPSIN A



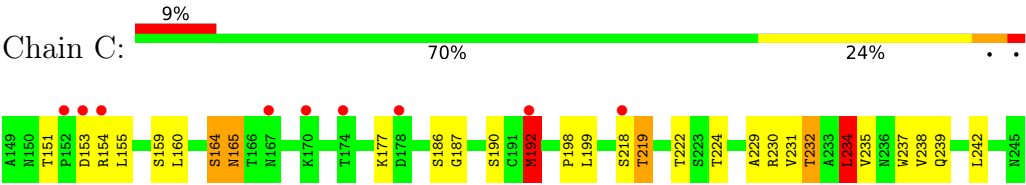
• Molecule 2: ALPHA-CHYMOTRYPSIN A



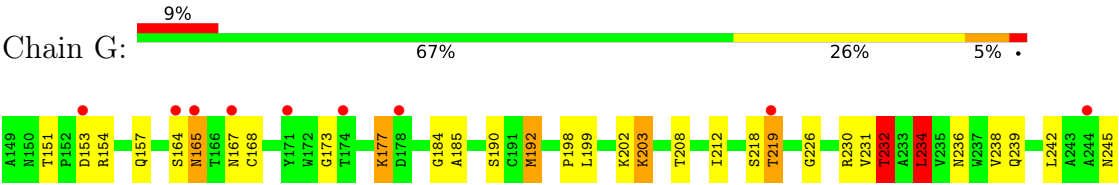
• Molecule 2: ALPHA-CHYMOTRYPSIN A



• Molecule 3: ALPHA-CHYMOTRYPSIN A



• Molecule 3: ALPHA-CHYMOTRYPSIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.23Å 67.39Å 65.99Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.68 64.59 – 1.69	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-1.68) 94.4 (64.59-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.70Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.236 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3591	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	A	0.95	0/75	2.35	5/103 (4.9%)
1	E	1.01	0/69	2.17	1/95 (1.1%)
2	B	1.17	2/1000 (0.2%)	2.25	43/1361 (3.2%)
2	F	1.20	1/1000 (0.1%)	2.30	49/1361 (3.6%)
3	C	1.23	1/715 (0.1%)	2.16	33/973 (3.4%)
3	G	1.23	0/715	2.20	34/973 (3.5%)
All	All	1.19	4/3574 (0.1%)	2.24	165/4866 (3.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	199	LEU	CA-C	6.19	1.59	1.52
2	B	43	GLY	N-CA	5.23	1.49	1.44
2	F	27	TRP	N-CA	5.15	1.52	1.46
2	B	91	ASN	N-CA	5.02	1.52	1.46

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	128	ASP	CA-CB-CG	17.82	130.42	112.60
2	B	128	ASP	CA-CB-CG	15.71	128.31	112.60
2	B	91	ASN	CA-CB-CG	13.61	126.21	112.60
2	B	47	ILE	CA-C-N	10.98	139.88	121.87
2	B	47	ILE	C-N-CA	10.98	139.88	121.87
2	F	39	PHE	CA-CB-CG	10.88	124.67	113.80
3	G	232	THR	N-CA-CB	-10.65	94.08	110.06
2	F	18	ASN	OD1-CG-ND2	10.13	132.73	122.60
3	G	232	THR	CB-CA-C	9.86	127.45	110.68
2	F	128	ASP	CB-CG-OD1	9.24	139.66	118.40
2	F	47	ILE	CA-C-N	9.20	137.53	121.80
2	F	47	ILE	C-N-CA	9.20	137.53	121.80
2	B	125	SER	N-CA-CB	8.69	124.12	110.56
3	G	153	ASP	CA-CB-CG	8.59	121.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	77	SER	CA-C-N	8.54	135.88	121.87
2	F	77	SER	C-N-CA	8.54	135.88	121.87
3	C	219	THR	N-CA-CB	-8.54	97.86	110.49
3	C	232	THR	N-CA-CB	-8.50	97.31	110.06
3	C	218	SER	CA-C-N	8.37	136.35	122.54
3	C	218	SER	C-N-CA	8.37	136.35	122.54
2	B	71	PHE	O-C-N	8.19	129.81	121.79
2	F	129	ASP	CA-CB-CG	-8.18	104.42	112.60
2	B	76	SER	CA-C-N	8.11	137.03	121.54
2	B	76	SER	C-N-CA	8.11	137.03	121.54
3	G	234	LEU	N-CA-CB	-8.08	98.77	110.80
3	C	235	VAL	CA-C-O	-7.72	112.13	120.47
2	B	23	VAL	N-CA-CB	7.60	117.15	110.08
2	F	76	SER	CA-C-N	7.54	135.94	121.54
2	F	76	SER	C-N-CA	7.54	135.94	121.54
3	G	219	THR	N-CA-CB	-7.49	99.12	110.73
2	F	125	SER	N-CA-CB	7.49	122.24	110.56
3	C	232	THR	CB-CA-C	7.47	123.37	110.68
2	F	109	SER	CA-C-N	7.45	133.48	123.05
2	F	109	SER	C-N-CA	7.45	133.48	123.05
2	B	65	VAL	CA-CB-CG1	7.34	122.88	110.40
3	G	212	ILE	CA-C-O	-7.33	112.69	120.39
2	F	114	PHE	CA-CB-CG	7.33	121.13	113.80
2	B	91	ASN	CB-CA-C	7.32	121.78	109.84
2	F	145	ARG	CA-CB-CG	7.29	128.67	114.10
2	B	23	VAL	N-CA-C	-7.27	101.83	108.95
2	F	91	ASN	CA-CB-CG	7.23	119.83	112.60
2	F	101	ASN	OD1-CG-ND2	7.22	129.82	122.60
3	C	234	LEU	N-CA-CB	-7.10	100.72	110.95
2	F	33	LEU	O-C-N	7.00	131.18	123.27
2	F	35	ASP	CA-CB-CG	6.95	119.55	112.60
2	B	114	PHE	CA-CB-CG	6.94	120.74	113.80
3	G	184	GLY	CA-C-O	6.91	126.72	120.64
3	G	198	PRO	N-CA-C	6.89	123.28	111.77
1	A	10	LEU	N-CA-CB	-6.87	101.71	112.08
3	C	199	LEU	N-CA-CB	6.86	121.27	110.84
1	A	2	GLY	N-CA-C	6.86	124.45	114.10
2	B	39	PHE	CA-CB-CG	6.85	120.65	113.80
2	F	23	VAL	N-CA-C	-6.85	102.74	108.63
2	F	145	ARG	NE-CZ-NH2	6.82	125.34	119.20
3	C	190	SER	N-CA-C	-6.79	100.92	110.50
2	F	37	THR	CA-C-N	6.57	130.87	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	37	THR	C-N-CA	6.57	130.87	122.00
3	C	186	SER	N-CA-CB	-6.55	100.57	110.73
3	G	219	THR	CA-CB-OG1	-6.51	99.84	109.60
3	C	198	PRO	N-CA-C	6.51	121.46	111.57
2	F	18	ASN	CB-CG-ND2	-6.42	106.77	116.40
3	G	177	LYS	CA-CB-CG	6.41	126.92	114.10
3	C	235	VAL	O-C-N	6.39	129.03	121.80
1	E	2	GLY	N-CA-C	6.38	124.11	114.61
3	G	190	SER	N-CA-C	-6.36	101.07	110.48
2	F	49	GLU	CB-CG-CD	6.31	123.33	112.60
3	G	245	ASN	CA-CB-CG	6.31	118.91	112.60
3	C	231	VAL	CA-C-O	-6.30	114.40	120.95
2	B	35	ASP	CA-CB-CG	6.30	118.90	112.60
2	F	110	THR	CB-CA-C	6.29	120.50	110.19
2	B	48	ASN	CA-C-O	-6.27	114.74	121.45
3	G	192	MET	CA-CB-CG	-6.27	101.55	114.10
3	C	218	SER	CA-C-O	6.25	127.17	120.55
3	G	231	VAL	CA-C-O	-6.21	113.93	120.57
3	C	164	SER	N-CA-CB	6.19	119.86	110.45
2	F	128	ASP	OD1-CG-OD2	-6.18	108.07	122.90
3	G	219	THR	CA-CB-CG2	6.14	120.94	110.50
3	C	224	THR	O-C-N	6.11	126.83	121.39
3	C	153	ASP	N-CA-C	-6.07	104.95	112.90
3	C	239	GLN	OE1-CD-NE2	-6.05	116.55	122.60
3	G	190	SER	N-CA-CB	6.03	119.46	110.29
2	B	145	ARG	CD-NE-CZ	6.03	132.84	124.40
3	C	229	ALA	N-CA-CB	5.99	118.78	109.85
3	G	199	LEU	N-CA-CB	5.97	119.92	110.84
2	B	77	SER	CA-C-N	5.93	132.79	122.82
2	B	77	SER	C-N-CA	5.93	132.79	122.82
3	C	229	ALA	CA-C-O	-5.93	113.99	120.81
2	B	48	ASN	N-CA-C	5.93	117.80	108.96
3	G	208	THR	O-C-N	5.92	130.92	123.23
2	F	104	THR	CA-CB-CG2	5.91	120.55	110.50
3	G	199	LEU	N-CA-C	-5.89	97.53	108.02
1	A	9	VAL	CA-CB-CG1	5.89	120.41	110.40
2	B	128	ASP	CB-CG-OD1	5.87	131.91	118.40
3	G	154	ARG	NE-CZ-NH2	5.87	124.48	119.20
3	C	192	MET	CA-CB-CG	-5.86	102.38	114.10
2	B	129	ASP	CA-C-O	5.85	126.68	120.36
2	F	37	THR	N-CA-C	-5.85	106.14	113.28
3	C	232	THR	CA-C-O	5.85	126.95	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	177	LYS	CA-C-N	5.83	128.09	120.28
3	C	177	LYS	C-N-CA	5.83	128.09	120.28
3	C	199	LEU	N-CA-C	-5.83	97.64	108.02
2	B	67	VAL	O-C-N	5.80	129.35	123.20
3	G	226	GLY	N-CA-C	-5.80	103.80	113.02
2	B	91	ASN	OD1-CG-ND2	-5.80	116.80	122.60
2	B	120	ALA	N-CA-C	5.79	119.50	110.17
3	G	184	GLY	N-CA-C	5.78	118.56	111.45
2	F	28	PRO	O-C-N	5.77	130.15	122.30
2	B	118	VAL	O-C-N	5.77	129.18	123.18
2	F	34	GLN	CG-CD-NE2	-5.73	107.81	116.40
3	G	185	ALA	CA-C-O	5.71	127.06	120.32
3	C	164	SER	N-CA-C	-5.69	102.86	110.55
2	B	62	THR	CA-CB-CG2	5.67	120.13	110.50
3	C	154	ARG	NE-CZ-NH2	5.64	124.28	119.20
3	G	203	LYS	CB-CG-CD	5.64	124.26	111.30
2	B	30	GLN	CB-CG-CD	5.57	122.06	112.60
2	F	36	LYS	CB-CG-CD	5.56	124.09	111.30
3	C	160	LEU	O-C-N	5.54	126.15	121.83
3	G	165	ASN	CA-CB-CG	5.53	118.12	112.60
2	B	76	SER	CA-C-O	5.51	126.37	120.20
2	F	38	GLY	CA-C-N	-5.50	114.96	122.93
2	F	38	GLY	C-N-CA	-5.50	114.96	122.93
3	C	219	THR	CA-CB-OG1	-5.47	101.39	109.60
2	F	110	THR	CA-CB-CG2	5.45	119.76	110.50
2	F	125	SER	N-CA-C	-5.42	102.03	110.42
2	B	117	THR	N-CA-C	5.36	119.97	113.38
3	G	239	GLN	OE1-CD-NE2	-5.34	117.26	122.60
3	G	218	SER	CA-C-O	5.33	126.39	120.63
2	F	98	THR	CA-CB-CG2	5.32	119.55	110.50
2	B	144	THR	CA-CB-OG1	-5.32	101.62	109.60
2	B	23	VAL	CA-C-O	-5.30	114.78	119.71
2	B	119	SER	CA-CB-OG	-5.30	100.50	111.10
2	F	19	GLY	N-CA-C	-5.27	105.06	112.60
2	F	57	HIS	CA-CB-CG	5.27	119.07	113.80
3	G	236	ASN	OD1-CG-ND2	-5.24	117.36	122.60
2	F	112	ALA	CA-C-O	-5.23	115.09	121.05
3	G	168	CYS	O-C-N	5.22	128.69	122.27
2	F	82	LYS	N-CA-C	-5.21	100.67	108.96
2	B	134	THR	CA-C-O	-5.21	115.46	121.19
2	B	130	PHE	CB-CA-C	5.20	119.97	111.23
2	F	62	THR	CA-CB-OG1	-5.20	101.80	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	VAL	CA-C-N	5.20	129.72	122.08
1	A	9	VAL	C-N-CA	5.20	129.72	122.08
2	F	70	GLU	CA-CB-CG	5.19	124.49	114.10
2	B	109	SER	N-CA-C	-5.18	105.54	111.14
2	B	30	GLN	OE1-CD-NE2	-5.17	117.43	122.60
2	B	104	THR	CA-CB-OG1	-5.17	101.85	109.60
3	G	173	GLY	CA-C-N	5.17	128.95	120.63
3	G	173	GLY	C-N-CA	5.17	128.95	120.63
2	B	39	PHE	N-CA-C	5.15	117.88	109.59
2	F	91	ASN	CB-CA-C	5.14	118.22	109.84
2	B	27	TRP	CB-CA-C	5.14	119.16	111.14
2	B	104	THR	CA-CB-CG2	5.14	119.23	110.50
2	F	27	TRP	CB-CA-C	5.14	119.15	111.14
3	C	165	ASN	CB-CG-ND2	5.13	124.10	116.40
2	F	110	THR	N-CA-CB	-5.13	102.49	110.55
3	C	155	LEU	O-C-N	5.13	129.31	122.95
2	F	134	THR	CA-C-O	-5.12	115.55	121.19
2	B	62	THR	CA-CB-OG1	-5.12	101.92	109.60
2	F	98	THR	N-CA-CB	-5.11	102.67	110.33
3	C	239	GLN	CB-CG-CD	5.08	121.24	112.60
3	G	202	LYS	CA-C-O	5.06	126.81	121.05
3	G	199	LEU	CA-C-O	-5.05	114.88	120.33
3	C	219	THR	CA-CB-CG2	5.04	119.07	110.50
3	G	219	THR	CB-CA-C	5.03	119.23	110.72
2	B	125	SER	N-CA-C	-5.00	102.67	110.42

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	A	74	0	81	1	0
1	E	68	0	76	3	0
2	B	980	0	951	7	0
2	F	980	0	951	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	702	0	698	10	0
3	G	702	0	698	11	1
4	A	1	0	0	0	0
4	B	23	0	0	0	0
4	C	18	0	0	0	0
4	F	21	0	0	0	0
4	G	22	0	0	1	0
All	All	3591	0	3455	28	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 4.

All (28) 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)
3:C:192:MET:HG2	3:G:192:MET:HG2	1.66	0.78
2:F:98:THR:HG22	2:F:100:ASN:HB2	1.73	0.70
2:B:39:PHE:HE2	3:G:151:THR:HG21	1.64	0.61
3:G:165:ASN:HD21	3:G:230:ARG:HH11	1.48	0.60
2:B:98:THR:HG22	2:B:100:ASN:HB2	1.85	0.58
2:F:103:ILE:HG21	3:G:234:LEU:HG	1.88	0.55
2:F:83:LEU:HD13	2:F:108:LEU:HD13	1.89	0.53
3:C:151:THR:HG21	2:F:39:PHE:CZ	2.44	0.52
2:F:36:LYS:HA	2:F:36:LYS:HE2	1.95	0.48
2:B:105:LEU:HD23	3:C:237:TRP:CZ3	2.49	0.47
3:C:187:GLY:C	3:C:222:THR:HB	2.40	0.47
2:B:39:PHE:CE2	3:G:151:THR:HG21	2.47	0.46
3:C:151:THR:HG21	2:F:39:PHE:HZ	1.80	0.45
2:F:29:TRP:CG	2:F:121:VAL:HB	2.52	0.45
2:F:98:THR:HG23	3:G:177:LYS:HE2	1.98	0.45
1:E:10:LEU:HD22	3:G:157:GLN:HE21	1.83	0.44
3:C:238:VAL:O	3:C:242:LEU:HG	2.18	0.44
2:B:62:THR:HG23	2:B:85:ILE:O	2.18	0.43
3:G:238:VAL:O	3:G:242:LEU:HG	2.18	0.43
1:E:7:GLN:HA	1:E:8:PRO:HD3	1.92	0.43
3:G:232:THR:HB	4:G:570:HOH:O	2.16	0.43
3:C:165:ASN:HD21	3:C:230:ARG:HH11	1.66	0.43
3:C:165:ASN:ND2	3:C:230:ARG:HH11	2.17	0.42
3:G:164:SER:HB2	3:G:167:ASN:OD1	2.20	0.42
2:B:103:ILE:HG21	3:C:234:LEU:HG	2.01	0.41
3:C:192:MET:HG2	3:G:192:MET:CG	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:PRO:HA	2:F:26:SER:HB2	2.02	0.41
1:A:8:PRO:HA	2:B:26:SER:HB2	2.03	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)
2:F:76:SER:CB	3:G:167:ASN:ND2[1_455]	2.16	0.04

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	A	9/13 (69%)	9 (100%)	0	0	100	100
1	E	8/13 (62%)	8 (100%)	0	0	100	100
2	B	129/131 (98%)	125 (97%)	2 (2%)	2 (2%)	7	0
2	F	129/131 (98%)	125 (97%)	2 (2%)	2 (2%)	7	0
3	C	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
3	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
All	All	465/482 (96%)	448 (96%)	13 (3%)	4 (1%)	14	3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	77	SER
2	B	77	SER
2	B	99	ILE
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	A	9/10 (90%)	8 (89%)	1 (11%)	6	0
1	E	8/10 (80%)	8 (100%)	0	100	100
2	B	109/109 (100%)	98 (90%)	11 (10%)	7	0
2	F	109/109 (100%)	100 (92%)	9 (8%)	10	1
3	C	77/77 (100%)	71 (92%)	6 (8%)	11	1
3	G	77/77 (100%)	73 (95%)	4 (5%)	21	3
All	All	389/392 (99%)	358 (92%)	31 (8%)	11	1

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
2	B	20	GLU
2	B	36	LYS
2	B	39	PHE
2	B	75	SER
2	B	77	SER
2	B	78	GLU
2	B	90	LYS
2	B	109	SER
2	B	116	GLN
2	B	119	SER
2	B	128	ASP
3	C	159	SER
3	C	164	SER
3	C	192	MET
3	C	219	THR
3	C	232	THR
3	C	234	LEU
2	F	20	GLU
2	F	36	LYS
2	F	39	PHE
2	F	49	GLU

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Mol	Chain	Res	Type
2	F	62	THR
2	F	77	SER
2	F	110	THR
2	F	116	GLN
2	F	128	ASP
3	G	203	LYS
3	G	219	THR
3	G	232	THR
3	G	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	18	ASN
2	B	34	GLN
2	B	48	ASN
3	C	165	ASN
2	F	34	GLN
3	G	150	ASN
3	G	157	GLN
3	G	165	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	A	11/13 (84%)	1.62	4 (36%) 1 1	10, 14, 29, 30	0
1	E	10/13 (76%)	1.28	2 (20%) 3 3	9, 12, 19, 22	0
2	B	131/131 (100%)	0.92	20 (15%) 5 6	5, 13, 27, 36	0
2	F	131/131 (100%)	0.87	20 (15%) 5 6	6, 14, 26, 35	0
3	C	97/97 (100%)	0.60	9 (9%) 14 17	5, 12, 20, 21	0
3	G	97/97 (100%)	0.65	9 (9%) 14 17	5, 12, 22, 23	0
All	All	477/482 (98%)	0.81	64 (13%) 7 9	5, 13, 23, 36	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	74	GLY	7.7
1	E	10	LEU	7.6
2	F	76	SER	5.2
3	G	244	ALA	5.0
2	F	39	PHE	4.9
1	A	10	LEU	4.8
2	F	75	SER	4.3
2	B	39	PHE	4.0
2	B	77	SER	4.0
3	G	167	ASN	3.9
2	B	79	LYS	3.9
2	B	76	SER	3.8
2	B	75	SER	3.8
2	F	74	GLY	3.7
1	A	11	SER	3.5
2	B	78	GLU	3.4
2	F	78	GLU	3.4
2	F	36	LYS	3.3
2	B	36	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	129	ASP	3.2
2	B	110	THR	3.2
3	G	164	SER	3.1
3	G	178	ASP	3.0
2	B	48	ASN	3.0
2	F	72	ASP	3.0
2	F	48	ASN	3.0
1	A	9	VAL	2.9
2	B	72	ASP	2.9
2	B	71	PHE	2.7
2	F	129	ASP	2.7
2	F	110	THR	2.7
3	C	153	ASP	2.7
3	C	178	ASP	2.7
2	F	77	SER	2.6
2	B	38	GLY	2.6
3	C	192	MET	2.6
2	B	98	THR	2.6
2	B	80	ILE	2.6
2	F	62	THR	2.5
3	C	174	THR	2.5
2	F	90	LYS	2.5
3	G	219	THR	2.4
3	G	165	ASN	2.4
2	F	73	GLN	2.4
2	F	63	SER	2.3
2	B	49	GLU	2.3
3	G	153	ASP	2.3
2	F	37	THR	2.2
3	C	167	ASN	2.2
2	F	20	GLU	2.2
3	C	170	LYS	2.2
2	B	128	ASP	2.2
3	G	171	TYR	2.2
2	F	18	ASN	2.1
2	B	145	ARG	2.1
3	C	154	ARG	2.1
1	A	8	PRO	2.1
3	C	152	PRO	2.1
3	C	218	SER	2.0
3	G	174	THR	2.0
1	E	7	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	116	GLN	2.0
2	B	132	ALA	2.0
2	F	113	SER	2.0

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.