



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 PM UTC

PDB ID : 5GCH / pdb_00005gch
Title : CHEMISTRY OF CAGED ENZYMES /II\$. PHOTOACTIVATION OF INHIBITED CHYMOTRYPSIN
Authors : Stoddard, B.L.; Ringe, D.; Petsko, G.A.
Deposited on : 1989-09-25
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
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

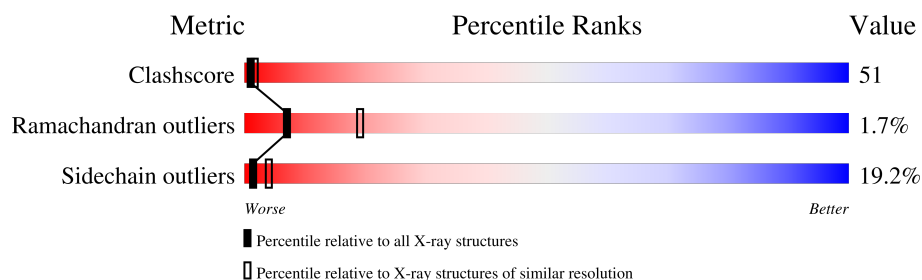
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1814 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
			979	618	162	195	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
			688	429	120	132	7			

- Molecule 4 is water.

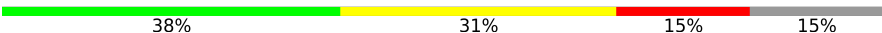
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	5	Total	O	0	0
			5	5		
4	F	50	Total	O	0	0
			50	50		
4	G	23	Total	O	0	0
			23	23		

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. 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.

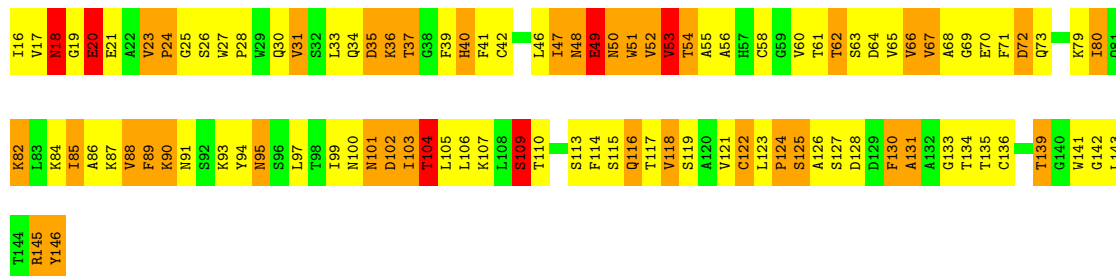
• Molecule 1: GAMMA-CHYMOTRYPSIN A

Chain E: 



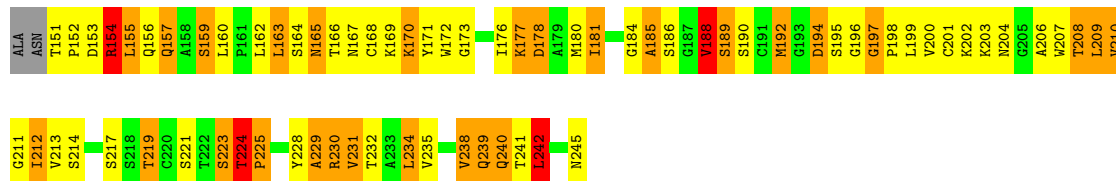
• Molecule 2: GAMMA-CHYMOTRYPSIN A

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	69.70 Å 69.70 Å 97.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1814	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

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	1.26	0/70	2.72	7/97 (7.2%)
2	F	1.38	2/999 (0.2%)	2.51	80/1361 (5.9%)
3	G	1.32	1/701 (0.1%)	2.46	43/955 (4.5%)
All	All	1.35	3/1770 (0.2%)	2.50	130/2413 (5.4%)

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
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	19	GLY	N-CA	5.53	1.48	1.44
3	G	198	PRO	N-CD	5.32	1.55	1.47
2	F	104	THR	CA-C	5.14	1.58	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	204	ASN	CA-CB-CG	13.88	126.48	112.60
2	F	64	ASP	CA-CB-CG	12.47	125.07	112.60
2	F	93	LYS	CA-CB-CG	10.22	134.55	114.10
3	G	197	GLY	CA-C-N	9.43	129.19	119.76
3	G	197	GLY	C-N-CA	9.43	129.19	119.76
3	G	204	ASN	OD1-CG-ND2	-9.37	113.23	122.60
3	G	177	LYS	CA-C-O	-9.21	110.46	121.60
2	F	101	ASN	CA-CB-CG	-8.89	103.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	GLN	OE1-CD-NE2	-8.88	113.72	122.60
2	F	95	ASN	OD1-CG-ND2	8.80	131.40	122.60
2	F	95	ASN	CA-CB-CG	-8.32	104.28	112.60
2	F	104	THR	N-CA-CB	8.32	125.30	111.08
2	F	18	ASN	CA-CB-CG	-8.25	104.35	112.60
2	F	51	TRP	CA-C-O	-8.23	111.18	120.32
3	G	155	LEU	CA-C-O	8.02	130.06	120.92
3	G	157	GLN	OE1-CD-NE2	8.01	130.61	122.60
1	E	9	VAL	O-C-N	8.00	131.68	123.20
2	F	110	THR	CA-CB-OG1	-7.96	97.67	109.60
3	G	190	SER	CA-C-O	-7.91	112.69	121.87
3	G	223	SER	CA-CB-OG	-7.89	95.31	111.10
3	G	154	ARG	CA-CB-CG	-7.84	98.42	114.10
3	G	198	PRO	N-CA-C	7.83	123.48	111.19
3	G	224	THR	O-C-N	7.80	130.16	121.43
3	G	245	ASN	CA-C-O	-7.62	107.85	120.80
2	F	125	SER	CA-C-O	-7.61	112.72	121.47
2	F	19	GLY	N-CA-C	-7.52	102.43	112.81
2	F	136	CYS	CA-C-O	-7.30	110.07	120.51
2	F	80	ILE	CA-C-O	-7.30	112.83	121.80
2	F	113	SER	CA-C-O	-7.25	112.70	120.46
3	G	224	THR	N-CA-C	-7.25	100.63	109.83
2	F	36	LYS	CA-CB-CG	7.22	128.54	114.10
2	F	31	VAL	CA-C-O	-7.18	111.81	120.78
2	F	126	ALA	N-CA-C	-7.13	102.62	111.75
2	F	130	PHE	CA-C-N	7.11	130.97	120.87
2	F	130	PHE	C-N-CA	7.11	130.97	120.87
2	F	54	THR	CA-CB-OG1	-7.10	98.95	109.60
2	F	19	GLY	O-C-N	7.07	130.67	123.11
2	F	103	ILE	CB-CA-C	7.05	119.71	110.12
3	G	157	GLN	CA-C-O	-7.02	113.75	121.33
2	F	18	ASN	OD1-CG-ND2	7.01	129.61	122.60
2	F	104	THR	CA-CB-CG2	6.95	122.32	110.50
2	F	145	ARG	O-C-N	6.92	131.30	123.27
3	G	165	ASN	CA-C-N	6.87	129.81	120.54
3	G	165	ASN	C-N-CA	6.87	129.81	120.54
2	F	21	GLU	CG-CD-OE2	-6.82	102.70	118.40
3	G	196	GLY	N-CA-C	-6.80	105.08	114.67
3	G	198	PRO	CB-CA-C	-6.54	102.51	111.21
2	F	109	SER	CA-CB-OG	6.51	124.12	111.10
2	F	145	ARG	CD-NE-CZ	-6.45	115.37	124.40
3	G	155	LEU	N-CA-C	6.43	119.68	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	35	ASP	CA-C-O	-6.34	114.65	121.94
2	F	69	GLY	N-CA-C	-6.32	106.99	115.21
2	F	36	LYS	N-CA-CB	6.29	121.13	110.49
2	F	49	GLU	CB-CG-CD	6.28	123.27	112.60
2	F	61	THR	N-CA-C	-6.24	100.96	109.95
3	G	201	CYS	N-CA-C	-6.22	99.59	109.23
2	F	146	TYR	CA-CB-CG	-6.20	102.73	113.90
3	G	224	THR	CA-CB-OG1	-6.19	100.31	109.60
2	F	49	GLU	CA-CB-CG	6.19	126.48	114.10
2	F	62	THR	CA-CB-OG1	-6.15	100.37	109.60
3	G	171	TYR	O-C-N	6.11	129.34	122.32
3	G	194	ASP	CA-CB-CG	-6.09	106.51	112.60
3	G	212	ILE	CA-C-O	6.07	126.70	120.39
3	G	186	SER	N-CA-CB	-6.05	102.23	110.95
3	G	157	GLN	CB-CG-CD	-6.04	102.33	112.60
2	F	145	ARG	CA-C-O	-6.02	114.08	121.06
2	F	143	LEU	CA-C-O	-5.99	114.97	121.44
2	F	52	VAL	CA-C-O	-5.94	114.97	121.92
3	G	178	ASP	CA-C-O	-5.82	113.28	119.97
3	G	214	SER	CA-C-O	-5.81	112.40	119.61
2	F	64	ASP	CB-CA-C	5.81	119.45	109.51
2	F	20	GLU	CG-CD-OE1	5.78	131.68	118.40
3	G	230	ARG	CA-C-O	5.78	127.86	121.39
2	F	85	ILE	N-CA-C	5.76	116.72	107.73
3	G	231	VAL	CB-CA-C	5.76	120.73	111.29
2	F	135	THR	CA-CB-OG1	-5.75	100.97	109.60
2	F	35	ASP	CA-CB-CG	5.74	118.34	112.60
1	E	3	VAL	CA-C-N	5.73	127.00	119.84
1	E	3	VAL	C-N-CA	5.73	127.00	119.84
3	G	189	SER	O-C-N	5.73	130.01	123.48
2	F	31	VAL	O-C-N	5.71	129.71	122.57
2	F	20	GLU	CG-CD-OE2	-5.68	105.34	118.40
2	F	126	ALA	CA-C-O	5.64	126.52	120.20
3	G	185	ALA	CA-C-O	5.64	127.99	121.28
2	F	89	PHE	CA-CB-CG	5.62	119.42	113.80
2	F	93	LYS	N-CA-CB	5.60	119.81	110.41
2	F	53	VAL	N-CA-CB	5.58	118.90	111.64
2	F	84	LYS	CB-CG-CD	5.57	124.11	111.30
2	F	102	ASP	CB-CA-C	5.53	120.65	112.03
2	F	145	ARG	CB-CA-C	-5.52	97.30	109.56
2	F	115	SER	CA-C-O	-5.51	112.63	120.51
2	F	25	GLY	CA-C-N	5.51	132.32	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	25	GLY	C-N-CA	5.51	132.32	121.58
2	F	64	ASP	O-C-N	-5.51	116.89	123.06
3	G	238	VAL	CA-C-N	5.48	127.89	120.38
3	G	238	VAL	C-N-CA	5.48	127.89	120.38
3	G	188	VAL	CA-C-O	-5.43	115.97	121.67
2	F	40	HIS	ND1-CE1-NE2	5.42	113.82	108.40
2	F	67	VAL	CB-CA-C	5.41	118.23	110.33
2	F	102	ASP	N-CA-CB	-5.41	103.27	110.57
2	F	50	ASN	OD1-CG-ND2	5.40	128.00	122.60
3	G	242	LEU	O-C-N	5.31	127.82	122.09
3	G	241	THR	O-C-N	5.29	128.78	122.27
2	F	47	ILE	CA-C-O	5.29	124.80	119.20
3	G	185	ALA	CB-CA-C	5.29	119.24	111.73
1	E	10	LEU	N-CA-C	5.27	125.77	111.00
2	F	35	ASP	O-C-N	5.27	129.13	122.65
2	F	85	ILE	CB-CG1-CD1	5.26	124.85	113.80
3	G	164	SER	CA-C-O	-5.26	115.89	121.94
2	F	123	LEU	N-CA-C	-5.24	103.58	110.39
2	F	104	THR	N-CA-C	-5.24	101.34	109.72
2	F	121	VAL	CA-C-O	-5.23	116.08	121.93
2	F	82	LYS	CA-C-N	5.22	129.81	122.09
2	F	82	LYS	C-N-CA	5.22	129.81	122.09
2	F	72	ASP	CA-C-O	-5.22	115.50	120.92
2	F	50	ASN	N-CA-CB	-5.21	104.11	110.98
2	F	122	CYS	CA-C-O	-5.17	114.70	120.54
2	F	103	ILE	O-C-N	-5.15	117.72	123.03
3	G	229	ALA	CB-CA-C	5.10	118.37	109.65
2	F	131	ALA	N-CA-C	5.08	117.80	110.28
2	F	110	THR	CA-CB-CG2	5.07	119.12	110.50
3	G	178	ASP	N-CA-CB	5.07	118.13	110.28
3	G	234	LEU	N-CA-CB	-5.06	103.90	110.88
1	E	7	GLN	CA-C-N	5.04	124.97	119.78
1	E	7	GLN	C-N-CA	5.04	124.97	119.78
2	F	66	VAL	CB-CA-C	-5.03	104.32	111.21
2	F	23	VAL	CB-CA-C	5.03	115.61	110.94
2	F	63	SER	N-CA-C	-5.03	106.93	113.16
2	F	118	VAL	CB-CA-C	5.03	117.20	110.42
2	F	121	VAL	O-C-N	5.01	128.37	122.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	LEU	Mainchain
2	F	145	ARG	Sidechain

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	11	0
2	F	979	0	951	112	1
3	G	688	0	687	85	4
4	E	5	0	0	1	4
4	F	50	0	0	14	4
4	G	23	0	0	7	1
All	All	1814	0	1714	177	8

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 (177) 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:G:180:MET:O	4:G:316:HOH:O	1.56	1.23
3:G:239:GLN:HE21	3:G:239:GLN:HA	1.03	1.15
3:G:230:ARG:NE	4:G:316:HOH:O	1.77	1.15
2:F:58:CYS:HB2	4:F:271:HOH:O	1.49	1.10
2:F:48:ASN:C	2:F:48:ASN:HD22	1.63	1.03
2:F:28:PRO:HA	4:F:278:HOH:O	1.58	1.03
3:G:239:GLN:HA	3:G:239:GLN:NE2	1.67	0.99
1:E:5:ALA:CB	2:F:116:GLN:HG3	1.94	0.96
3:G:180:MET:C	4:G:316:HOH:O	2.04	0.95
1:E:5:ALA:HB3	2:F:116:GLN:HG3	1.54	0.90
2:F:71:PHE:O	3:G:154:ARG:HA	1.75	0.86
2:F:28:PRO:HB2	2:F:119:SER:OG	1.75	0.86
2:F:49:GLU:C	4:F:272:HOH:O	2.19	0.85
2:F:50:ASN:N	4:F:272:HOH:O	2.09	0.84
2:F:73:GLN:N	3:G:153:ASP:O	2.10	0.84
2:F:51:TRP:HH2	2:F:89:PHE:CE1	1.99	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:PRO:O	4:F:261:HOH:O	2.00	0.79
3:G:230:ARG:CZ	4:G:316:HOH:O	2.21	0.78
2:F:48:ASN:C	2:F:48:ASN:ND2	2.42	0.77
2:F:35:ASP:OD2	2:F:37:THR:HB	1.85	0.77
2:F:48:ASN:ND2	2:F:50:ASN:H	1.84	0.76
3:G:177:LYS:HG2	3:G:180:MET:HE3	1.66	0.75
2:F:51:TRP:CH2	2:F:89:PHE:CE1	2.76	0.74
2:F:90:LYS:HA	2:F:104:THR:CG2	2.18	0.73
3:G:212:ILE:HB	3:G:229:ALA:HB3	1.71	0.73
2:F:90:LYS:O	2:F:91:ASN:C	2.32	0.72
3:G:172:TRP:CZ2	3:G:224:THR:HG21	2.24	0.72
1:E:6:ILE:HG21	4:F:261:HOH:O	1.88	0.72
2:F:95:ASN:O	2:F:99:ILE:N	2.26	0.69
1:E:5:ALA:HB1	2:F:116:GLN:HG3	1.75	0.68
2:F:33:LEU:HD13	2:F:60:VAL:CG2	2.23	0.68
2:F:88:VAL:HG13	2:F:106:LEU:CD2	2.23	0.68
2:F:23:VAL:O	2:F:26:SER:OG	2.10	0.68
2:F:90:LYS:HA	2:F:104:THR:HG22	1.74	0.68
2:F:117:THR:O	4:F:278:HOH:O	2.11	0.67
2:F:33:LEU:HD13	2:F:60:VAL:HG21	1.76	0.67
3:G:167:ASN:O	3:G:170:LYS:HB2	1.94	0.67
3:G:172:TRP:CZ2	3:G:224:THR:CG2	2.78	0.67
3:G:165:ASN:O	3:G:168:CYS:HB3	1.96	0.66
2:F:124:PRO:O	3:G:235:VAL:HG21	1.96	0.66
3:G:162:LEU:HD22	3:G:181:ILE:HD11	1.77	0.66
3:G:172:TRP:HB2	3:G:176:ILE:HD11	1.78	0.64
2:F:51:TRP:CH2	2:F:89:PHE:CD1	2.86	0.64
2:F:90:LYS:CG	2:F:104:THR:HG23	2.28	0.63
2:F:31:VAL:HG12	2:F:68:ALA:HB2	1.80	0.63
2:F:90:LYS:CA	2:F:104:THR:HG22	2.29	0.62
3:G:177:LYS:CG	3:G:180:MET:HE3	2.29	0.62
2:F:51:TRP:HH2	2:F:89:PHE:CD1	2.17	0.62
3:G:177:LYS:HB2	3:G:180:MET:HE3	1.82	0.62
1:E:6:ILE:HD11	2:F:116:GLN:HG2	1.81	0.61
3:G:209:LEU:O	3:G:231:VAL:HG11	2.01	0.61
2:F:95:ASN:C	2:F:95:ASN:OD1	2.43	0.61
3:G:177:LYS:HG2	3:G:180:MET:CE	2.31	0.61
3:G:228:TYR:OH	4:G:318:HOH:O	2.16	0.60
2:F:90:LYS:N	2:F:104:THR:HG22	2.17	0.60
2:F:17:VAL:N	3:G:189:SER:O	2.29	0.60
2:F:146:TYR:CD2	3:G:219:THR:HA	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:165:ASN:N	4:G:311:HOH:O	2.30	0.58
3:G:230:ARG:NH1	4:G:316:HOH:O	2.34	0.58
2:F:48:ASN:HD22	2:F:50:ASN:H	1.52	0.58
2:F:124:PRO:HB2	2:F:128:ASP:HB2	1.84	0.58
3:G:200:VAL:HG23	3:G:207:TRP:CE3	2.39	0.58
2:F:142:GLY:C	3:G:151:THR:HG22	2.30	0.57
2:F:53:VAL:HG13	2:F:105:LEU:HD23	1.88	0.56
3:G:177:LYS:CB	3:G:180:MET:HE3	2.35	0.56
2:F:62:THR:HG22	2:F:85:ILE:HG22	1.88	0.56
2:F:133:GLY:N	3:G:162:LEU:O	2.28	0.56
1:E:10:LEU:HD12	4:F:254:HOH:O	2.05	0.55
2:F:125:SER:C	2:F:127:SER:N	2.58	0.55
2:F:47:ILE:HG23	2:F:53:VAL:HG22	1.87	0.55
2:F:27:TRP:CD1	2:F:139:THR:HG21	2.42	0.54
3:G:167:ASN:HA	3:G:170:LYS:HD3	1.89	0.54
2:F:48:ASN:HD22	2:F:49:GLU:N	2.03	0.54
2:F:51:TRP:CE2	2:F:107:LYS:HD3	2.42	0.54
2:F:16:ILE:N	3:G:194:ASP:OD1	2.40	0.54
2:F:40:HIS:CD2	2:F:40:HIS:C	2.86	0.53
2:F:114:PHE:CD1	2:F:118:VAL:HG12	2.44	0.53
3:G:165:ASN:HD21	3:G:181:ILE:HA	1.74	0.53
2:F:134:THR:HB	3:G:162:LEU:HD12	1.92	0.52
2:F:139:THR:HG22	3:G:157:GLN:HB3	1.91	0.52
2:F:53:VAL:HG13	2:F:105:LEU:CD2	2.39	0.52
2:F:90:LYS:HG2	2:F:104:THR:HG23	1.92	0.52
2:F:146:TYR:CE1	3:G:192:MET:CE	2.93	0.51
2:F:89:PHE:C	2:F:104:THR:HG22	2.36	0.51
2:F:124:PRO:HB2	2:F:128:ASP:CB	2.41	0.51
2:F:47:ILE:O	2:F:48:ASN:HB3	2.11	0.50
3:G:160:LEU:HD12	3:G:184:GLY:CA	2.41	0.50
3:G:169:LYS:O	3:G:173:GLY:HA2	2.11	0.50
3:G:224:THR:HG22	3:G:225:PRO:HD2	1.94	0.50
2:F:141:TRP:CD2	3:G:155:LEU:HD13	2.47	0.50
2:F:18:ASN:HB3	3:G:188:VAL:HA	1.94	0.50
2:F:103:ILE:HG21	3:G:234:LEU:HD13	1.93	0.50
3:G:200:VAL:HA	3:G:208:THR:O	2.12	0.49
3:G:159:SER:O	3:G:160:LEU:HB3	2.12	0.49
3:G:217:SER:OG	3:G:219:THR:HG23	2.13	0.49
3:G:157:GLN:O	3:G:157:GLN:HG3	2.11	0.49
2:F:18:ASN:O	3:G:188:VAL:HG12	2.12	0.49
2:F:72:ASP:C	2:F:72:ASP:OD2	2.56	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ILE:CD1	2:F:116:GLN:HG2	2.43	0.48
3:G:239:GLN:NE2	3:G:239:GLN:CA	2.56	0.48
2:F:94:TYR:HA	2:F:101:ASN:HB2	1.95	0.48
2:F:104:THR:HG21	4:F:287:HOH:O	2.13	0.48
2:F:31:VAL:CG1	2:F:68:ALA:HB2	2.43	0.48
3:G:213:VAL:HG22	3:G:228:TYR:HE2	1.79	0.48
2:F:139:THR:HG22	3:G:156:GLN:O	2.14	0.48
3:G:172:TRP:CB	3:G:176:ILE:HD11	2.44	0.48
3:G:238:VAL:O	3:G:242:LEU:HD12	2.14	0.48
2:F:130:PHE:CE2	3:G:203:LYS:HD3	2.49	0.47
2:F:17:VAL:O	2:F:18:ASN:CB	2.63	0.47
2:F:49:GLU:HG3	4:F:269:HOH:O	2.14	0.47
2:F:90:LYS:HG3	2:F:104:THR:HG23	1.96	0.47
2:F:87:LYS:HE3	2:F:87:LYS:HB3	1.64	0.47
3:G:163:LEU:HD12	3:G:163:LEU:N	2.30	0.46
2:F:30:GLN:HG2	3:G:155:LEU:HD21	1.98	0.46
2:F:90:LYS:HA	2:F:104:THR:HG23	1.94	0.46
2:F:146:TYR:CE1	3:G:192:MET:HE1	2.49	0.46
3:G:160:LEU:HD12	3:G:184:GLY:HA2	1.98	0.46
2:F:66:VAL:HG23	2:F:85:ILE:HD11	1.98	0.46
3:G:200:VAL:CG2	3:G:207:TRP:CE3	2.98	0.46
3:G:235:VAL:O	3:G:239:GLN:HB2	2.16	0.46
2:F:141:TRP:CE3	3:G:155:LEU:HD13	2.51	0.46
2:F:88:VAL:HG13	2:F:106:LEU:HD21	1.95	0.46
4:F:258:HOH:O	3:G:156:GLN:HG3	2.15	0.46
3:G:194:ASP:HB3	3:G:213:VAL:HG11	1.98	0.45
3:G:203:LYS:HB2	3:G:208:THR:HG21	1.98	0.45
3:G:211:GLY:HA2	3:G:229:ALA:O	2.16	0.45
2:F:54:THR:OG1	2:F:55:ALA:N	2.48	0.45
2:F:31:VAL:HG12	2:F:68:ALA:CB	2.46	0.45
2:F:34:GLN:HA	2:F:39:PHE:O	2.17	0.45
2:F:90:LYS:HG3	4:F:287:HOH:O	2.16	0.45
3:G:172:TRP:CZ2	3:G:224:THR:HG22	2.51	0.45
1:E:5:ALA:N	4:E:296:HOH:O	2.47	0.44
2:F:31:VAL:HB	2:F:66:VAL:HG13	1.99	0.44
2:F:49:GLU:HA	4:F:272:HOH:O	2.17	0.44
2:F:86:ALA:HB2	2:F:109:SER:HA	1.99	0.44
2:F:51:TRP:HA	2:F:106:LEU:O	2.18	0.44
3:G:165:ASN:O	3:G:168:CYS:CB	2.65	0.44
1:E:10:LEU:HD23	1:E:10:LEU:HA	1.61	0.44
2:F:62:THR:HA	2:F:85:ILE:HB	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:ALA:HB2	2:F:109:SER:CA	2.47	0.44
2:F:131:ALA:O	2:F:134:THR:OG1	2.31	0.44
2:F:100:ASN:O	2:F:101:ASN:HB2	2.18	0.43
2:F:47:ILE:HD13	2:F:47:ILE:HG21	1.87	0.43
2:F:41:PHE:CD1	2:F:41:PHE:C	2.96	0.43
2:F:52:VAL:N	2:F:106:LEU:O	2.45	0.43
2:F:141:TRP:CE2	3:G:155:LEU:HD13	2.53	0.43
2:F:28:PRO:C	4:F:278:HOH:O	2.58	0.43
2:F:100:ASN:HD22	2:F:100:ASN:HA	1.39	0.43
3:G:185:ALA:CB	3:G:223:SER:O	2.66	0.43
2:F:41:PHE:CE1	2:F:42:CYS:HB2	2.54	0.43
2:F:125:SER:C	2:F:127:SER:H	2.26	0.42
3:G:221:SER:C	3:G:223:SER:H	2.27	0.42
2:F:20:GLU:O	3:G:157:GLN:HG2	2.19	0.42
2:F:90:LYS:CA	2:F:104:THR:CG2	2.90	0.42
2:F:70:GLU:CA	2:F:80:ILE:HG22	2.49	0.42
3:G:212:ILE:O	3:G:229:ALA:N	2.42	0.42
1:E:5:ALA:HB1	2:F:116:GLN:CG	2.48	0.42
1:E:3:VAL:HG12	3:G:206:ALA:HB2	2.01	0.42
3:G:197:GLY:O	3:G:213:VAL:HG23	2.19	0.42
2:F:49:GLU:HB3	2:F:114:PHE:CE1	2.55	0.42
3:G:151:THR:HB	3:G:152:PRO:HD2	2.01	0.42
3:G:234:LEU:O	3:G:238:VAL:HG23	2.20	0.42
2:F:35:ASP:C	2:F:37:THR:H	2.27	0.42
3:G:172:TRP:CH2	3:G:224:THR:HG21	2.55	0.42
2:F:67:VAL:HG22	2:F:82:LYS:HG2	2.02	0.41
2:F:103:ILE:CG2	3:G:234:LEU:HD13	2.50	0.41
3:G:154:ARG:H	3:G:154:ARG:HG2	1.14	0.41
3:G:172:TRP:HB2	3:G:176:ILE:CD1	2.47	0.41
3:G:192:MET:SD	3:G:192:MET:N	2.93	0.41
2:F:56:ALA:HB3	2:F:102:ASP:OD2	2.19	0.41
2:F:70:GLU:N	2:F:80:ILE:HG22	2.36	0.41
2:F:122:CYS:O	3:G:208:THR:HA	2.21	0.41
3:G:168:CYS:C	3:G:170:LYS:N	2.78	0.41
3:G:199:LEU:HD23	3:G:210:VAL:HG12	2.02	0.41
3:G:213:VAL:HG22	3:G:228:TYR:CE2	2.56	0.40
2:F:70:GLU:HA	2:F:80:ILE:CG2	2.51	0.40
3:G:160:LEU:N	3:G:160:LEU:HD23	2.36	0.40

All (8) 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)
3:G:240:GLN:NE2	4:E:251:HOH:O[5_646]	0.78	1.42
3:G:240:GLN:CD	4:E:251:HOH:O[5_646]	0.97	1.23
4:F:273:HOH:O	4:F:273:HOH:O[2_675]	1.10	1.10
4:F:274:HOH:O	4:F:286:HOH:O[2_675]	1.45	0.75
3:G:240:GLN:CG	4:E:251:HOH:O[5_646]	1.74	0.46
2:F:82:LYS:NZ	4:F:302:HOH:O[6_476]	1.95	0.25
4:F:291:HOH:O	4:G:312:HOH:O[3_654]	2.11	0.09
3:G:240:GLN:OE1	4:E:251:HOH:O[5_646]	2.15	0.05

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%)	7 (78%)	2 (22%)	0	100	100
2	F	129/131 (98%)	116 (90%)	10 (8%)	3 (2%)	5	13
3	G	93/97 (96%)	86 (92%)	6 (6%)	1 (1%)	11	29
All	All	231/241 (96%)	209 (90%)	18 (8%)	4 (2%)	7	19

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	195	SER
2	F	18	ASN
2	F	79	LYS
2	F	24	PRO

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	11
2	F	109/109 (100%)	93 (85%)	16 (15%)	3	8
3	G	76/77 (99%)	56 (74%)	20 (26%)	0	2
All	All	193/196 (98%)	156 (81%)	37 (19%)	1	4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	3	VAL
2	F	20	GLU
2	F	36	LYS
2	F	37	THR
2	F	46	LEU
2	F	48	ASN
2	F	49	GLU
2	F	53	VAL
2	F	65	VAL
2	F	88	VAL
2	F	90	LYS
2	F	97	LEU
2	F	104	THR
2	F	109	SER
2	F	116	GLN
2	F	124	PRO
2	F	139	THR
3	G	154	ARG
3	G	159	SER
3	G	163	LEU
3	G	166	THR
3	G	170	LYS
3	G	178	ASP
3	G	181	ILE
3	G	188	VAL
3	G	192	MET
3	G	202	LYS
3	G	208	THR
3	G	209	LEU
3	G	210	VAL
3	G	219	THR
3	G	224	THR

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Mol	Chain	Res	Type
3	G	225	PRO
3	G	232	THR
3	G	239	GLN
3	G	240	GLN
3	G	242	LEU

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

Mol	Chain	Res	Type
1	E	7	GLN
2	F	34	GLN
2	F	48	ASN
2	F	100	ASN
2	F	116	GLN
3	G	165	ASN
3	G	239	GLN

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 ⓘ

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.