



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:38 AM UTC

PDB ID : 5CHA / pdb_00005cha
Title : THE REFINEMENT AND THE STRUCTURE OF THE DIMER OF
ALPHA-*CHYMOTRYPSIN AT 1.67-*ANGSTROMS RESOLUTION
Authors : Blevins, R.A.; Tulinsky, A.
Deposited on : 1985-01-22
Resolution : 1.67 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
Xtrriage (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

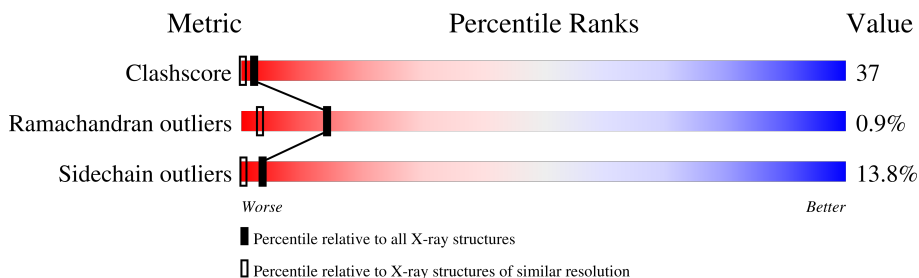
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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)

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	A	13	15% 38% 8% 8% 31%
1	E	13	31% 31% 8% 31%
2	B	131	32% 37% 23% 8%
2	F	131	31% 38% 24% 7%
3	C	97	28% 39% 29% .
3	G	97	32% 49% 15% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3719 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
			Total	C	N	O	S			
1	A	9	Total 54	C 34	N 10	O 9	S 1	0	0	1
1	E	9	Total 54	C 34	N 10	O 9	S 1	0	0	1

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

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

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total 9 O 9	0	0
4	B	75	Total 75 O 75	0	0
4	C	57	Total 57 O 57	0	0
4	E	3	Total 3 O 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	59	Total O 59 59	0	0
4	G	44	Total O 44 44	0	0

3 Residue-property plots

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

Note EDS was not executed.

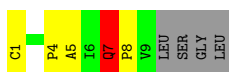
- Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain A: 

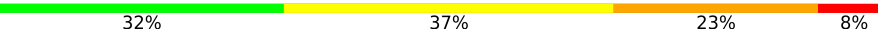


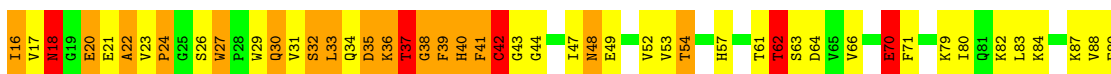
- Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain E: 

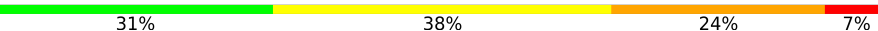


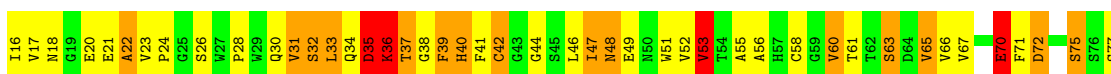
- Molecule 2: ALPHA-CHYMOTRYPSIN A

Chain B: 

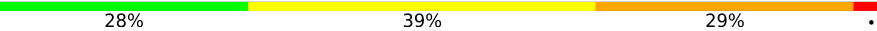


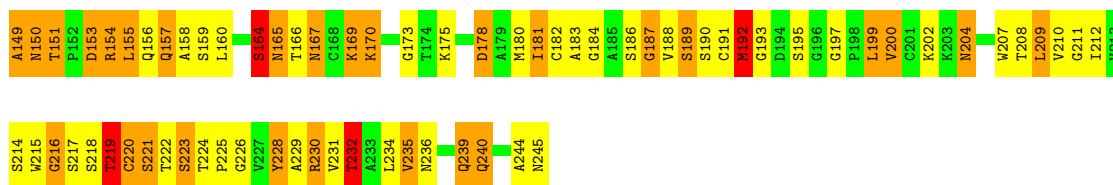
- Molecule 2: ALPHA-CHYMOTRYPSIN A

Chain F: 




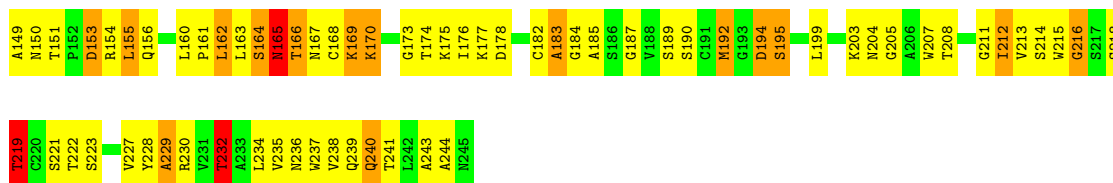
- Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain C:  28% 39% 29%



• Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain G:  32% 49% 15%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.29Å 67.48Å 65.94Å 90.00° 102.02° 90.00°	Depositor
Resolution (Å)	(Not available) – 1.67	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.67)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3719	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	1.82	0/55	4.09	10/76 (13.2%)
1	E	1.41	0/55	3.00	9/76 (11.8%)
2	B	1.53	6/1000 (0.6%)	2.89	107/1361 (7.9%)
2	F	1.44	3/1000 (0.3%)	2.88	96/1361 (7.1%)
3	C	1.78	8/715 (1.1%)	3.01	85/973 (8.7%)
3	G	1.74	12/715 (1.7%)	2.85	78/973 (8.0%)
All	All	1.61	29/3540 (0.8%)	2.93	385/4820 (8.0%)

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
2	F	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	154	ARG	NE-CZ	18.68	1.53	1.33
3	C	215	TRP	N-CA	7.58	1.55	1.46
3	G	216	GLY	CA-C	7.45	1.59	1.52
2	B	44	GLY	N-CA	7.26	1.53	1.45
3	C	199	LEU	CA-C	7.18	1.61	1.52
2	B	43	GLY	N-CA	6.95	1.50	1.44
3	G	213	VAL	N-CA	6.92	1.55	1.46
3	C	207	TRP	N-CA	6.88	1.54	1.46
3	C	193	GLY	CA-C	5.91	1.59	1.51
3	G	239	GLN	N-CA	5.81	1.53	1.46
2	B	57	HIS	C-O	5.68	1.31	1.24
3	G	241	THR	CA-CB	5.65	1.62	1.53
2	F	22	ALA	N-CA	5.60	1.53	1.45
2	F	32	SER	N-CA	5.57	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	212	ILE	CA-C	5.56	1.60	1.52
3	G	199	LEU	CA-C	5.50	1.59	1.52
3	G	215	TRP	N-CA	5.46	1.52	1.46
3	C	154	ARG	CG-CD	-5.41	1.36	1.52
3	C	235	VAL	N-CA	5.36	1.52	1.46
3	G	208	THR	CB-OG1	5.36	1.52	1.43
3	G	232	THR	N-CA	5.28	1.52	1.46
3	G	194	ASP	C-O	5.27	1.30	1.24
3	C	212	ILE	C-O	-5.26	1.18	1.24
2	F	44	GLY	N-CA	5.24	1.51	1.45
3	G	228	TYR	C-N	-5.23	1.26	1.33
2	B	112	ALA	C-N	-5.14	1.26	1.33
2	B	140	GLY	CA-C	5.10	1.57	1.51
2	B	105	LEU	N-CA	5.07	1.52	1.46
3	G	216	GLY	N-CA	5.04	1.50	1.45

All (385) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	ASP	CA-CB-CG	22.99	135.59	112.60
3	C	204	ASN	OD1-CG-ND2	-20.48	102.12	122.60
2	F	35	ASP	CA-CB-CG	-18.38	94.22	112.60
2	F	39	PHE	CA-CB-CG	18.14	131.94	113.80
2	F	128	ASP	CA-CB-CG	16.75	129.34	112.60
3	C	204	ASN	CB-CG-ND2	15.69	139.93	116.40
1	A	1	CYS	CA-C-O	-14.28	96.52	120.80
2	B	97	LEU	CA-C-O	13.95	135.17	119.41
3	C	157	GLN	OE1-CD-NE2	-13.60	109.00	122.60
3	G	239	GLN	OE1-CD-NE2	-13.38	109.22	122.60
2	B	40	HIS	CA-C-O	-13.10	106.65	120.80
1	A	1	CYS	CA-C-N	12.83	146.55	121.41
1	A	1	CYS	C-N-CA	12.83	146.55	121.41
2	F	70	GLU	CA-CB-CG	11.81	137.72	114.10
3	C	200	VAL	CA-C-O	11.37	135.84	121.40
2	B	98	THR	N-CA-CB	-11.35	93.85	110.53
3	G	205	GLY	CA-C-O	-11.20	104.92	119.25
2	B	116	GLN	CB-CG-CD	11.09	131.46	112.60
2	F	37	THR	N-CA-C	-10.70	100.22	113.28
2	F	18	ASN	CA-C-N	10.61	132.78	122.27
2	F	18	ASN	C-N-CA	10.61	132.78	122.27
2	B	48	ASN	CA-CB-CG	-10.51	102.09	112.60
2	B	63	SER	CB-CA-C	10.50	127.92	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	53	VAL	O-C-N	10.38	134.07	123.18
2	F	95	ASN	CA-C-O	-10.34	109.39	120.46
2	B	95	ASN	OD1-CG-ND2	-10.29	112.31	122.60
2	B	95	ASN	CB-CG-ND2	10.03	131.44	116.40
3	C	167	ASN	OD1-CG-ND2	9.97	132.57	122.60
2	F	115	SER	CA-C-O	-9.96	110.59	121.05
3	C	151	THR	CA-C-O	9.88	129.38	120.19
2	B	106	LEU	O-C-N	9.55	134.35	123.27
1	E	7	GLN	CG-CD-NE2	9.47	130.60	116.40
2	B	18	ASN	OD1-CG-ND2	9.43	132.03	122.60
2	B	18	ASN	CA-CB-CG	9.43	122.03	112.60
3	G	239	GLN	CG-CD-NE2	9.39	130.48	116.40
2	F	42	CYS	O-C-N	9.37	132.74	123.46
3	C	180	MET	CA-C-N	9.35	137.00	122.70
3	C	180	MET	C-N-CA	9.35	137.00	122.70
2	F	119	SER	CB-CA-C	-9.29	94.23	110.95
2	F	144	THR	CA-C-O	9.25	129.69	119.15
3	G	155	LEU	CA-C-O	9.25	131.36	121.19
3	C	232	THR	N-CA-CB	-9.20	95.60	110.14
1	A	4	PRO	CA-C-N	9.18	133.33	120.29
1	A	4	PRO	C-N-CA	9.18	133.33	120.29
3	G	219	THR	CA-CB-CG2	9.17	126.09	110.50
2	F	56	ALA	O-C-N	9.08	133.43	122.27
3	G	177	LYS	CA-C-N	9.07	135.61	121.19
3	G	177	LYS	C-N-CA	9.07	135.61	121.19
3	G	232	THR	N-CA-CB	-9.06	96.47	110.06
3	G	219	THR	N-CA-CB	-9.00	96.79	110.73
3	C	156	GLN	OE1-CD-NE2	-8.98	113.62	122.60
2	B	116	GLN	CG-CD-NE2	-8.95	102.97	116.40
2	F	95	ASN	CA-CB-CG	-8.94	103.66	112.60
1	E	7	GLN	OE1-CD-NE2	-8.89	113.71	122.60
2	B	135	THR	CA-C-O	-8.88	111.08	120.58
2	F	34	GLN	OE1-CD-NE2	8.88	131.48	122.60
3	G	227	VAL	O-C-N	8.78	132.74	123.26
3	C	224	THR	O-C-N	8.59	129.74	121.66
1	A	4	PRO	CB-CA-C	8.59	122.54	111.46
3	G	183	ALA	CA-C-O	-8.49	112.15	121.23
3	C	240	GLN	CA-C-O	8.47	129.40	120.42
2	F	128	ASP	N-CA-CB	8.40	122.27	110.17
3	C	184	GLY	N-CA-C	8.39	121.77	111.45
3	C	219	THR	N-CA-CB	-8.37	98.90	110.95
2	B	34	GLN	OE1-CD-NE2	8.27	130.87	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	140	GLY	O-C-N	8.21	131.74	123.78
2	F	134	THR	CA-C-O	-8.19	112.04	120.96
3	C	190	SER	N-CA-C	-8.15	99.77	110.53
2	F	81	GLN	OE1-CD-NE2	8.13	130.73	122.60
2	F	106	LEU	CA-C-O	-8.12	111.39	120.32
3	C	232	THR	OG1-CB-CG2	8.08	125.47	109.30
2	F	20	GLU	CA-CB-CG	8.05	130.21	114.10
3	G	237	TRP	CA-C-O	8.02	129.24	120.82
3	G	239	GLN	CB-CG-CD	7.98	126.16	112.60
2	B	115	SER	CA-C-O	-7.93	109.17	120.51
3	G	153	ASP	CA-CB-CG	-7.91	104.69	112.60
1	A	5	ALA	CB-CA-C	-7.86	97.48	110.85
3	C	223	SER	CB-CA-C	-7.84	94.66	109.72
3	G	166	THR	CB-CA-C	7.83	124.17	110.85
3	C	210	VAL	O-C-N	7.83	130.41	122.04
3	G	150	ASN	OD1-CG-ND2	7.81	130.41	122.60
2	B	54	THR	CA-CB-OG1	-7.79	97.91	109.60
2	B	24	PRO	N-CA-CB	7.79	110.24	103.31
2	B	20	GLU	CG-CD-OE2	-7.78	100.50	118.40
2	F	38	GLY	CA-C-N	-7.77	109.92	122.36
2	F	38	GLY	C-N-CA	-7.77	109.92	122.36
3	G	176	ILE	CA-C-O	7.77	130.31	120.76
3	G	234	LEU	O-C-N	7.67	131.17	122.27
2	B	39	PHE	CA-CB-CG	-7.67	106.13	113.80
2	B	98	THR	OG1-CB-CG2	7.67	124.63	109.30
3	C	158	ALA	O-C-N	7.65	131.94	123.52
2	B	116	GLN	CG-CD-OE1	7.63	136.07	120.80
3	C	167	ASN	CA-CB-CG	-7.62	104.97	112.60
2	B	97	LEU	O-C-N	-7.60	111.57	122.36
3	G	155	LEU	O-C-N	-7.59	113.54	122.87
2	F	103	ILE	CA-C-O	-7.54	112.83	120.90
2	F	115	SER	O-C-N	7.54	131.39	122.72
3	G	232	THR	CB-CA-C	7.49	123.41	110.68
2	F	38	GLY	CA-C-O	-7.45	110.91	118.96
3	C	153	ASP	N-CA-C	-7.42	103.69	112.89
2	F	92	SER	CA-C-O	-7.42	109.75	119.10
3	C	232	THR	O-C-N	-7.41	113.76	122.20
2	F	47	ILE	O-C-N	7.37	131.46	122.03
3	G	232	THR	OG1-CB-CG2	7.34	123.99	109.30
2	B	31	VAL	O-C-N	7.34	130.83	122.97
2	F	40	HIS	N-CA-C	7.30	120.84	109.96
3	G	239	GLN	O-C-N	-7.27	114.53	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	34	GLN	CG-CD-NE2	-7.24	105.54	116.40
3	C	149	ALA	N-CA-CB	7.24	121.25	110.40
2	F	145	ARG	CD-NE-CZ	-7.24	114.27	124.40
2	B	125	SER	CA-C-O	-7.22	112.85	121.66
2	F	121	VAL	CA-C-O	-7.20	112.95	121.80
2	F	75	SER	CA-C-O	-7.19	113.04	120.80
3	C	223	SER	N-CA-CB	-7.14	99.25	110.46
3	C	230	ARG	NE-CZ-NH2	-7.13	112.78	119.20
1	E	4	PRO	CA-C-N	7.13	130.42	120.29
1	E	4	PRO	C-N-CA	7.13	130.42	120.29
3	C	209	LEU	CA-C-O	-7.10	112.25	120.49
2	B	140	GLY	O-C-N	7.10	130.91	123.81
2	B	106	LEU	CA-C-O	-7.08	112.72	120.30
3	C	169	LYS	O-C-N	7.07	130.97	122.27
2	B	104	THR	CA-CB-OG1	-7.07	99.00	109.60
3	C	219	THR	OG1-CB-CG2	7.07	123.44	109.30
2	B	66	VAL	CA-C-O	-7.05	113.03	120.57
2	B	135	THR	O-C-N	7.03	131.37	122.93
2	B	97	LEU	CA-C-N	7.00	134.02	121.92
2	B	97	LEU	C-N-CA	7.00	134.02	121.92
3	C	221	SER	CA-C-O	-6.99	113.50	121.19
3	C	210	VAL	CB-CA-C	6.98	117.21	111.06
2	F	95	ASN	O-C-N	6.98	131.93	123.13
3	C	240	GLN	OE1-CD-NE2	6.97	129.57	122.60
3	G	216	GLY	N-CA-C	-6.96	101.43	110.69
3	C	239	GLN	OE1-CD-NE2	-6.95	115.66	122.60
2	B	70	GLU	N-CA-C	6.92	120.77	109.76
2	F	101	ASN	O-C-N	6.92	130.88	122.58
3	G	190	SER	N-CA-C	-6.90	100.78	110.50
2	B	123	LEU	CA-C-O	-6.89	113.54	120.63
3	G	223	SER	CB-CA-C	6.87	122.45	110.64
2	F	112	ALA	CA-C-O	-6.84	113.60	121.47
3	G	166	THR	CA-C-O	-6.84	113.17	120.42
2	F	85	ILE	O-C-N	6.84	131.10	123.10
3	G	207	TRP	CA-C-O	-6.83	112.99	120.43
1	A	1	CYS	CB-CA-C	-6.82	97.14	110.10
3	G	216	GLY	O-C-N	6.81	130.46	123.92
3	C	155	LEU	CA-C-N	6.81	134.22	122.64
3	C	155	LEU	C-N-CA	6.81	134.22	122.64
2	B	38	GLY	CA-C-N	-6.79	111.21	122.21
2	B	38	GLY	C-N-CA	-6.79	111.21	122.21
3	G	204	ASN	CB-CG-ND2	6.75	126.53	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	178	ASP	CB-CG-OD1	6.71	133.82	118.40
3	C	193	GLY	O-C-N	6.70	130.22	122.65
3	G	208	THR	O-C-N	6.69	131.93	123.23
2	F	89	PHE	CA-C-O	6.68	132.00	120.85
3	G	162	LEU	CA-C-O	-6.67	113.94	121.81
2	F	31	VAL	CA-C-N	-6.66	112.95	122.94
2	F	31	VAL	C-N-CA	-6.66	112.95	122.94
2	B	112	ALA	N-CA-C	-6.65	101.75	110.53
1	A	7	GLN	CA-C-O	6.64	126.44	119.80
3	C	204	ASN	CA-CB-CG	6.59	119.19	112.60
3	C	216	GLY	O-C-N	6.59	130.15	123.88
3	C	226	GLY	N-CA-C	-6.56	103.18	112.37
2	F	105	LEU	CA-C-O	-6.55	113.76	120.71
2	F	65	VAL	CA-CB-CG1	6.53	121.50	110.40
3	G	223	SER	CA-CB-OG	-6.51	98.07	111.10
3	G	156	GLN	OE1-CD-NE2	-6.51	116.09	122.60
2	B	20	GLU	CG-CD-OE1	6.50	133.34	118.40
3	G	211	GLY	CA-C-O	6.50	128.58	121.63
2	B	121	VAL	CA-C-O	-6.49	113.81	121.80
2	B	132	ALA	N-CA-C	-6.49	100.70	110.24
3	G	190	SER	CA-C-O	-6.49	114.49	121.56
2	B	48	ASN	CB-CA-C	-6.48	96.37	111.09
3	C	165	ASN	O-C-N	6.47	129.80	122.22
3	G	234	LEU	CA-C-O	-6.47	111.78	118.90
2	B	23	VAL	N-CA-C	-6.45	103.08	108.63
1	E	7	GLN	CB-CG-CD	6.45	123.56	112.60
3	C	165	ASN	CA-CB-CG	-6.43	106.17	112.60
3	C	159	SER	O-C-N	-6.42	115.71	123.16
2	B	98	THR	CA-C-O	6.40	126.18	119.14
3	C	151	THR	CA-CB-OG1	-6.39	100.02	109.60
2	F	141	TRP	CA-C-O	-6.38	112.42	119.95
2	F	53	VAL	CA-C-O	-6.36	113.74	120.48
3	G	221	SER	N-CA-CB	-6.36	100.23	109.83
3	G	178	ASP	N-CA-CB	-6.35	98.92	109.72
2	F	23	VAL	N-CA-C	-6.33	103.19	108.63
3	C	157	GLN	CG-CD-NE2	6.31	125.86	116.40
2	B	123	LEU	N-CA-CB	-6.30	99.64	110.10
3	G	177	LYS	CA-CB-CG	6.30	126.69	114.10
3	G	204	ASN	OD1-CG-ND2	-6.30	116.30	122.60
2	F	32	SER	CA-C-O	-6.28	113.92	120.70
3	C	200	VAL	O-C-N	-6.27	116.46	122.98
2	F	105	LEU	O-C-N	6.26	131.16	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	90	LYS	N-CA-CB	-6.26	99.66	110.17
2	B	93	LYS	CA-CB-CG	6.25	126.59	114.10
2	B	40	HIS	O-C-N	6.20	131.56	123.07
2	F	141	TRP	CB-CA-C	-6.19	101.05	111.02
3	C	231	VAL	O-C-N	6.19	127.87	121.87
2	B	48	ASN	O-C-N	6.17	130.20	123.10
2	B	27	TRP	CA-C-O	6.17	128.92	121.02
2	B	116	GLN	N-CA-CB	6.17	120.45	110.40
2	F	53	VAL	CA-CB-CG1	6.17	120.89	110.40
2	B	18	ASN	N-CA-C	6.17	120.75	113.23
2	B	109	SER	CA-CB-OG	-6.17	98.77	111.10
2	F	103	ILE	O-C-N	6.16	130.24	123.09
3	G	204	ASN	O-C-N	6.16	129.97	122.58
2	F	92	SER	O-C-N	6.16	130.62	122.43
2	F	39	PHE	O-C-N	6.13	130.69	122.96
2	F	129	ASP	CA-CB-CG	-6.13	106.47	112.60
2	B	102	ASP	CA-CB-CG	6.13	118.73	112.60
2	F	101	ASN	OD1-CG-ND2	6.12	128.72	122.60
2	B	63	SER	N-CA-CB	-6.12	101.41	110.53
2	B	130	PHE	CB-CA-C	6.12	120.59	111.17
2	B	145	ARG	NE-CZ-NH2	6.12	124.70	119.20
2	F	91	ASN	OD1-CG-ND2	-6.11	116.49	122.60
2	B	27	TRP	O-C-N	-6.11	115.91	121.34
2	B	43	GLY	N-CA-C	-6.10	102.03	112.64
2	F	104	THR	CA-C-O	-6.09	114.00	121.06
2	F	116	GLN	O-C-N	6.09	129.34	122.22
2	F	115	SER	N-CA-CB	-6.08	101.49	110.97
2	F	101	ASN	CA-CB-CG	-6.06	106.54	112.60
2	B	135	THR	N-CA-CB	6.05	119.84	110.21
2	B	62	THR	CA-CB-OG1	-6.05	100.53	109.60
2	B	32	SER	N-CA-CB	-6.05	100.52	110.68
3	C	186	SER	O-C-N	6.05	129.44	122.25
3	C	150	ASN	CB-CG-ND2	-6.04	107.34	116.40
2	F	109	SER	CA-CB-OG	-6.02	99.06	111.10
3	G	239	GLN	CA-C-N	6.02	128.34	120.28
3	G	239	GLN	C-N-CA	6.02	128.34	120.28
2	B	128	ASP	CB-CA-C	6.01	120.59	109.54
2	B	42	CYS	CA-C-O	-6.00	114.86	121.28
3	G	156	GLN	O-C-N	5.99	130.71	123.16
3	C	170	LYS	N-CA-C	-5.98	104.09	111.33
3	G	170	LYS	CA-C-N	5.96	128.76	120.29
3	G	170	LYS	C-N-CA	5.96	128.76	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	104	THR	O-C-N	5.94	130.36	123.41
3	C	187	GLY	CA-C-N	5.93	130.27	122.51
3	C	187	GLY	C-N-CA	5.93	130.27	122.51
2	F	18	ASN	CB-CG-ND2	5.92	125.28	116.40
3	G	195	SER	N-CA-C	5.92	123.40	110.80
3	C	244	ALA	N-CA-C	5.91	120.65	113.38
2	B	34	GLN	CG-CD-NE2	-5.89	107.56	116.40
3	G	199	LEU	O-C-N	5.88	130.88	123.12
2	F	100	ASN	OD1-CG-ND2	5.88	128.48	122.60
3	G	199	LEU	CA-C-N	-5.87	112.82	122.67
3	G	199	LEU	C-N-CA	-5.87	112.82	122.67
3	G	182	CYS	O-C-N	5.83	130.62	123.10
3	C	202	LYS	CB-CG-CD	5.82	124.69	111.30
3	C	189	SER	N-CA-CB	-5.82	101.11	110.77
3	C	167	ASN	CB-CG-ND2	-5.81	107.68	116.40
3	C	173	GLY	CA-C-N	5.81	131.79	120.99
3	C	173	GLY	C-N-CA	5.81	131.79	120.99
2	F	63	SER	CB-CA-C	5.80	119.75	109.65
2	B	30	GLN	CG-CD-NE2	5.78	125.07	116.40
3	C	149	ALA	O-C-N	5.78	132.24	123.00
2	F	119	SER	O-C-N	5.77	129.06	123.29
3	G	199	LEU	N-CA-CB	5.77	119.76	110.65
2	F	128	ASP	CB-CG-OD1	5.75	131.63	118.40
2	F	133	GLY	O-C-N	5.75	128.77	122.56
2	B	128	ASP	N-CA-CB	5.75	118.45	110.17
2	F	46	LEU	CA-C-O	-5.74	113.83	120.49
3	G	244	ALA	N-CA-C	5.73	119.53	112.54
3	G	155	LEU	CA-C-N	5.73	132.10	122.87
3	G	155	LEU	C-N-CA	5.73	132.10	122.87
3	C	245	ASN	N-CA-C	5.64	126.79	111.00
2	F	92	SER	CA-CB-OG	-5.62	99.85	111.10
2	F	99	ILE	CA-CB-CG2	5.62	120.06	110.50
2	F	131	ALA	O-C-N	5.62	129.31	122.96
2	F	63	SER	N-CA-C	-5.60	106.49	113.38
2	F	129	ASP	N-CA-C	5.60	117.99	108.02
3	G	243	ALA	CA-C-O	-5.59	114.95	120.82
3	C	192	MET	CA-CB-CG	-5.58	102.93	114.10
2	F	60	VAL	CA-C-O	5.57	127.49	121.36
2	F	130	PHE	CB-CA-C	5.57	119.21	110.19
2	B	18	ASN	O-C-N	5.54	130.96	122.03
2	F	72	ASP	CA-C-O	5.54	126.42	120.38
3	C	190	SER	N-CA-CB	5.53	118.27	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	39	PHE	CA-C-N	5.53	130.05	121.26
2	B	39	PHE	C-N-CA	5.53	130.05	121.26
3	C	150	ASN	OD1-CG-ND2	5.52	128.12	122.60
2	B	61	THR	CA-CB-OG1	-5.52	101.32	109.60
3	C	175	LYS	CA-CB-CG	-5.50	103.10	114.10
3	G	229	ALA	N-CA-CB	-5.50	101.28	109.69
3	C	208	THR	O-C-N	5.49	130.36	123.23
2	F	17	VAL	CA-C-O	-5.48	114.70	120.57
2	B	130	PHE	N-CA-C	-5.48	96.24	107.70
3	G	208	THR	CA-CB-OG1	-5.47	101.39	109.60
2	B	70	GLU	CG-CD-OE1	5.46	130.96	118.40
3	C	215	TRP	CA-CB-CG	5.45	123.95	113.60
1	E	4	PRO	CB-CA-C	5.45	118.09	110.95
2	B	16	ILE	CA-CB-CG2	5.43	119.74	110.50
3	G	214	SER	O-C-N	5.43	128.98	121.92
3	C	164	SER	CB-CA-C	-5.42	99.48	109.46
3	C	220	CYS	CA-C-O	-5.41	114.10	120.81
3	G	178	ASP	CA-CB-CG	-5.41	107.19	112.60
3	G	169	LYS	N-CA-C	-5.40	105.95	112.54
2	B	116	GLN	CA-CB-CG	5.39	124.89	114.10
2	F	53	VAL	CG1-CB-CG2	-5.39	98.94	110.80
2	F	81	GLN	CA-C-O	-5.37	114.55	120.30
3	G	227	VAL	CA-C-N	-5.37	114.38	122.81
3	G	227	VAL	C-N-CA	-5.37	114.38	122.81
3	C	153	ASP	CB-CA-C	5.36	121.18	109.99
3	C	183	ALA	CA-C-O	-5.35	114.99	120.99
3	G	219	THR	CA-CB-OG1	-5.35	101.57	109.60
2	B	128	ASP	OD1-CG-OD2	-5.34	110.07	122.90
2	F	144	THR	O-C-N	-5.34	115.42	122.42
3	G	165	ASN	CB-CA-C	5.34	120.51	110.63
3	C	211	GLY	CA-C-O	5.33	127.34	121.63
3	C	169	LYS	CA-C-O	-5.33	113.84	119.97
2	B	91	ASN	N-CA-CB	-5.33	101.91	109.85
3	C	217	SER	O-C-N	5.32	129.44	123.06
2	B	97	LEU	N-CA-CB	-5.31	102.71	110.47
3	G	208	THR	CA-C-O	-5.31	114.97	120.70
2	B	94	TYR	CA-CB-CG	-5.30	104.35	113.90
1	E	7	GLN	CA-CB-CG	-5.29	103.51	114.10
1	A	5	ALA	N-CA-CB	5.29	117.98	110.16
2	B	83	LEU	N-CA-C	5.29	117.86	109.24
2	F	66	VAL	CB-CA-C	-5.28	104.57	110.96
2	B	40	HIS	CB-CA-C	-5.28	102.72	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	96	SER	CA-CB-OG	-5.28	100.55	111.10
2	F	107	LYS	CG-CD-CE	-5.27	99.17	111.30
2	B	144	THR	CA-CB-OG1	-5.27	101.69	109.60
3	G	150	ASN	CA-CB-CG	5.27	117.87	112.60
2	B	37	THR	CA-C-O	5.26	128.04	120.51
2	B	48	ASN	OD1-CG-ND2	5.26	127.86	122.60
3	C	214	SER	O-C-N	5.26	128.11	121.95
2	B	42	CYS	CA-C-N	-5.26	116.41	122.77
2	B	42	CYS	C-N-CA	-5.26	116.41	122.77
3	G	204	ASN	CA-C-O	-5.25	115.50	121.65
3	C	199	LEU	N-CA-C	-5.25	98.67	108.02
2	B	93	LYS	CA-C-N	5.25	128.55	121.05
2	B	93	LYS	C-N-CA	5.25	128.55	121.05
3	C	192	MET	N-CA-C	5.24	118.07	110.42
3	C	210	VAL	CA-C-N	-5.24	115.96	121.35
3	C	210	VAL	C-N-CA	-5.24	115.96	121.35
2	B	39	PHE	CB-CA-C	5.23	121.58	110.07
2	B	91	ASN	CA-C-O	-5.21	114.82	120.81
2	B	115	SER	O-C-N	5.20	129.51	122.59
3	C	229	ALA	O-C-N	5.20	129.33	122.93
2	B	35	ASP	O-C-N	5.20	128.55	121.74
2	F	117	THR	CA-C-O	-5.20	113.22	119.15
2	F	89	PHE	CA-C-N	5.20	129.31	122.30
2	F	89	PHE	C-N-CA	5.20	129.31	122.30
2	B	112	ALA	CA-C-O	-5.18	115.86	121.87
3	C	182	CYS	CA-CB-SG	-5.18	102.49	114.40
3	G	240	GLN	N-CA-C	-5.17	105.64	111.28
2	B	33	LEU	O-C-N	5.17	129.11	123.27
3	C	164	SER	CA-CB-OG	-5.16	100.79	111.10
2	B	20	GLU	CB-CG-CD	-5.15	103.85	112.60
2	F	102	ASP	CA-CB-CG	5.13	117.73	112.60
2	B	41	PHE	CA-C-O	5.13	124.59	118.69
3	C	232	THR	CB-CA-C	5.13	120.41	110.46
2	B	32	SER	CB-CA-C	5.13	119.09	109.71
2	F	127	SER	CA-CB-OG	-5.12	100.86	111.10
2	F	107	LYS	CD-CE-NZ	-5.12	95.53	111.90
2	B	83	LEU	N-CA-CB	-5.11	102.10	110.43
1	E	5	ALA	CB-CA-C	5.11	119.53	110.85
3	G	153	ASP	OD1-CG-OD2	5.10	135.13	122.90
2	F	36	LYS	CB-CG-CD	5.09	123.02	111.30
2	B	70	GLU	CG-CD-OE2	-5.09	106.69	118.40
3	C	178	ASP	O-C-N	5.09	128.17	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	185	ALA	CA-C-N	5.09	130.20	122.37
3	G	185	ALA	C-N-CA	5.09	130.20	122.37
3	G	151	THR	CA-C-O	5.08	123.08	119.32
3	G	174	THR	CA-CB-CG2	5.08	119.14	110.50
2	B	125	SER	CA-CB-OG	-5.08	100.94	111.10
3	G	192	MET	CB-CA-C	5.08	116.05	109.80
2	B	111	ALA	CA-C-N	5.07	130.20	120.97
2	B	111	ALA	C-N-CA	5.07	130.20	120.97
3	C	228	TYR	CB-CG-CD2	-5.07	113.19	120.80
2	B	120	ALA	N-CA-C	5.07	118.33	110.17
3	G	175	LYS	O-C-N	5.06	128.14	122.22
2	F	52	VAL	CA-C-N	-5.05	116.93	123.19
2	F	52	VAL	C-N-CA	-5.05	116.93	123.19
2	F	20	GLU	CG-CD-OE1	5.04	129.99	118.40
3	C	225	PRO	CA-C-N	5.04	125.69	120.60
3	C	225	PRO	C-N-CA	5.04	125.69	120.60
2	F	39	PHE	N-CA-CB	5.03	119.77	111.62
1	E	5	ALA	N-CA-C	-5.02	105.89	111.36
2	B	103	ILE	O-C-N	-5.02	117.28	123.00
2	B	109	SER	N-CA-CB	-5.01	102.77	110.44
2	B	22	ALA	O-C-N	-5.01	117.14	122.85
2	F	138	THR	CA-C-N	5.01	130.45	122.59
2	F	138	THR	C-N-CA	5.01	130.45	122.59
3	G	183	ALA	O-C-N	5.01	128.78	123.42
3	C	170	LYS	CB-CG-CD	5.00	122.81	111.30
2	B	29	TRP	CB-CG-CD1	-5.00	119.40	126.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	A	54	0	55	9	0
1	E	54	0	56	9	4
2	B	980	0	951	79	5
2	F	980	0	951	85	0
3	C	702	0	698	57	1
3	G	702	0	698	39	0
4	A	9	0	0	5	0
4	B	75	0	0	27	0
4	C	57	0	0	22	0
4	E	3	0	0	0	0
4	F	59	0	0	30	0
4	G	44	0	0	19	0
All	All	3719	0	3409	252	5

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 37.

All (252) 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:183:ALA:HB1	4:G:720:HOH:O	1.26	1.34
2:B:110:THR:HB	4:B:715:HOH:O	1.31	1.25
3:C:232:THR:HG23	4:C:681:HOH:O	1.40	1.19
3:C:235:VAL:HG22	4:C:627:HOH:O	1.44	1.16
3:C:221:SER:HB2	4:C:701:HOH:O	1.49	1.11
1:A:1:CYS:HB3	4:A:683:HOH:O	1.53	1.07
2:F:101:ASN:ND2	4:F:724:HOH:O	1.86	1.07
2:F:119:SER:CB	4:F:723:HOH:O	2.03	1.06
2:F:119:SER:HB2	4:F:723:HOH:O	1.55	1.06
2:F:146:TYR:CE1	3:G:192:MET:HE1	1.90	1.06
2:F:36:LYS:NZ	2:F:63:SER:O	1.90	1.05
2:B:143:LEU:HD23	3:C:151:THR:HG22	1.39	1.05
2:B:103:ILE:HD13	2:B:104:THR:N	1.71	1.03
2:F:146:TYR:HE1	3:G:192:MET:HE1	1.18	1.03
2:F:100:ASN:ND2	4:F:724:HOH:O	1.93	1.01
2:F:53:VAL:HG23	2:F:105:LEU:HD23	1.40	1.00
3:C:239:GLN:NE2	4:C:627:HOH:O	1.94	0.96
3:C:154:ARG:NE	4:C:719:HOH:O	1.98	0.95
1:A:1:CYS:SG	1:A:1:CYS:O	2.25	0.94
2:B:87:LYS:NZ	4:B:727:HOH:O	2.02	0.91
2:B:53:VAL:HG23	2:B:103:ILE:HD11	1.51	0.91
3:C:181:ILE:HD11	3:C:199:LEU:CD2	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:168:CYS:HB2	4:G:717:HOH:O	1.69	0.91
2:B:88:VAL:HG12	2:B:90:LYS:HD2	1.53	0.90
2:F:51:TRP:CZ2	2:F:107:LYS:HE2	2.06	0.90
2:B:84:LYS:HD2	4:B:656:HOH:O	1.70	0.90
2:B:84:LYS:CB	4:B:656:HOH:O	2.19	0.90
2:B:103:ILE:HD13	2:B:104:THR:H	1.32	0.90
3:C:181:ILE:HD11	3:C:199:LEU:HD23	1.53	0.88
2:F:53:VAL:HG23	2:F:105:LEU:CD2	2.03	0.88
2:B:116:GLN:C	4:B:707:HOH:O	2.16	0.88
2:F:58:CYS:HB2	4:F:613:HOH:O	1.72	0.87
3:G:163:LEU:HB3	4:G:717:HOH:O	1.75	0.87
2:F:93:LYS:HE3	4:F:601:HOH:O	1.74	0.87
2:F:91:ASN:ND2	2:F:93:LYS:H	1.71	0.86
2:B:84:LYS:HD3	4:B:742:HOH:O	1.76	0.86
1:E:7:GLN:NE2	1:E:7:GLN:H	1.71	0.86
2:F:146:TYR:CZ	4:F:732:HOH:O	2.27	0.85
3:C:204:ASN:OD1	4:C:566:HOH:O	1.95	0.85
3:C:153:ASP:OD1	4:C:690:HOH:O	1.94	0.84
3:G:155:LEU:O	4:G:589:HOH:O	1.92	0.84
2:B:70:GLU:OE2	2:B:141:TRP:CH2	2.31	0.84
3:C:181:ILE:HG13	4:C:621:HOH:O	1.76	0.83
2:F:47:ILE:C	2:F:48:ASN:HD22	1.86	0.83
2:F:91:ASN:C	2:F:91:ASN:HD22	1.87	0.83
2:F:100:ASN:CG	4:F:724:HOH:O	2.22	0.82
3:C:221:SER:CB	4:C:701:HOH:O	2.13	0.82
4:C:690:HOH:O	2:F:37:THR:HG22	1.82	0.80
2:F:48:ASN:ND2	4:F:679:HOH:O	2.14	0.80
2:F:90:LYS:HB2	4:F:686:HOH:O	1.81	0.80
1:A:1:CYS:N	4:A:677:HOH:O	2.02	0.80
2:F:63:SER:HB3	4:F:629:HOH:O	1.83	0.79
3:C:181:ILE:HD13	3:C:228:TYR:HB2	1.62	0.78
3:C:219:THR:HG22	4:C:701:HOH:O	1.83	0.78
2:B:95:ASN:HB3	2:B:98:THR:HG22	1.66	0.77
3:C:181:ILE:CB	4:C:621:HOH:O	2.33	0.77
1:A:8:PRO:HB3	4:B:702:HOH:O	1.84	0.77
2:B:116:GLN:O	4:B:707:HOH:O	2.02	0.77
4:B:730:HOH:O	3:C:155:LEU:HD11	1.85	0.77
2:B:84:LYS:HB3	4:B:656:HOH:O	1.83	0.77
2:F:110:THR:OG1	4:F:696:HOH:O	2.02	0.76
3:C:181:ILE:HB	4:C:621:HOH:O	1.86	0.75
2:B:84:LYS:CD	4:B:656:HOH:O	2.29	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:SER:N	2:B:128:ASP:OD1	2.20	0.75
2:B:70:GLU:OE2	2:B:141:TRP:HH2	1.68	0.75
1:E:7:GLN:HG2	1:E:7:GLN:O	1.88	0.74
3:C:235:VAL:CG2	4:C:627:HOH:O	2.16	0.74
2:F:146:TYR:HE1	3:G:192:MET:CE	1.99	0.74
2:B:22:ALA:HA	3:C:157:GLN:NE2	2.04	0.73
4:B:619:HOH:O	3:C:195:SER:HB2	1.89	0.73
2:F:49:GLU:HG2	2:F:112:ALA:O	1.90	0.72
2:B:35:ASP:CG	2:B:37:THR:HG23	2.14	0.72
2:B:18:ASN:HB3	3:C:188:VAL:HG12	1.69	0.72
2:F:84:LYS:N	2:F:84:LYS:HD2	2.04	0.72
2:B:103:ILE:CD1	2:B:104:THR:N	2.53	0.71
4:B:622:HOH:O	3:G:219:THR:HG23	1.90	0.71
2:F:91:ASN:HD22	2:F:93:LYS:H	1.37	0.71
3:C:170:LYS:O	4:C:722:HOH:O	2.08	0.71
2:B:143:LEU:HD23	3:C:151:THR:CG2	2.19	0.70
1:E:7:GLN:H	1:E:7:GLN:CD	1.97	0.70
1:A:9:VAL:N	4:A:590:HOH:O	2.23	0.70
3:G:161:PRO:O	4:G:720:HOH:O	2.08	0.70
4:B:622:HOH:O	3:G:219:THR:CG2	2.40	0.70
2:F:60:VAL:HG23	4:F:613:HOH:O	1.92	0.70
2:F:55:ALA:O	4:F:613:HOH:O	2.09	0.70
3:C:164:SER:HB2	3:C:167:ASN:OD1	1.92	0.69
2:B:36:LYS:O	2:B:37:THR:C	2.36	0.69
2:B:30:GLN:OE1	4:B:730:HOH:O	2.11	0.69
2:F:21:GLU:OE1	3:G:154:ARG:HD2	1.94	0.68
2:B:129:ASP:HB2	4:B:628:HOH:O	1.93	0.67
3:C:154:ARG:CZ	4:C:719:HOH:O	2.38	0.67
3:C:165:ASN:O	3:C:169:LYS:HG3	1.95	0.67
3:C:181:ILE:CD1	3:C:199:LEU:HD23	2.25	0.67
1:E:7:GLN:CD	1:E:7:GLN:N	2.52	0.66
2:B:35:ASP:OD2	2:B:37:THR:HG23	1.96	0.66
2:B:21:GLU:OE2	3:C:154:ARG:HD2	1.96	0.65
4:B:730:HOH:O	3:C:155:LEU:HD21	1.95	0.65
2:F:35:ASP:OD2	2:F:35:ASP:N	2.23	0.65
2:B:87:LYS:CD	4:B:727:HOH:O	2.45	0.65
2:F:67:VAL:HG12	2:F:70:GLU:HG3	1.77	0.65
2:F:22:ALA:O	4:F:716:HOH:O	2.14	0.65
2:F:125:SER:HB3	2:F:128:ASP:OD2	1.97	0.65
2:B:136:CYS:HB3	3:C:200:VAL:O	1.96	0.65
2:F:40:HIS:CE1	2:F:42:CYS:O	2.51	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:THR:HG22	2:B:100:ASN:H	1.62	0.63
2:F:71:PHE:CZ	4:F:716:HOH:O	2.49	0.63
3:G:163:LEU:HD23	4:G:717:HOH:O	1.98	0.63
3:G:184:GLY:N	4:G:720:HOH:O	2.32	0.62
2:B:95:ASN:HB3	2:B:98:THR:CG2	2.29	0.62
3:C:164:SER:CB	3:C:167:ASN:OD1	2.47	0.62
1:A:1:CYS:HB2	4:A:605:HOH:O	1.99	0.62
2:F:16:ILE:N	3:G:194:ASP:OD1	2.33	0.62
1:A:8:PRO:HG3	2:B:26:SER:O	2.00	0.62
2:B:39:PHE:CG	2:B:40:HIS:N	2.65	0.61
2:F:134:THR:HB	3:G:162:LEU:HD12	1.81	0.61
2:F:21:GLU:CG	4:G:589:HOH:O	2.49	0.61
2:F:21:GLU:HG3	4:G:589:HOH:O	1.99	0.60
1:A:4:PRO:HG2	1:A:8:PRO:HD3	1.83	0.60
2:F:146:TYR:OH	4:F:732:HOH:O	2.15	0.60
2:F:90:LYS:CB	4:F:686:HOH:O	2.45	0.60
2:F:63:SER:CB	4:F:629:HOH:O	2.47	0.59
3:C:232:THR:HB	4:C:520:HOH:O	2.02	0.59
2:B:145:ARG:HD3	3:C:150:ASN:OD1	2.03	0.58
2:F:99:ILE:HD13	2:F:99:ILE:N	2.17	0.58
1:E:7:GLN:NE2	1:E:7:GLN:N	2.49	0.58
1:E:7:GLN:H	1:E:7:GLN:HE21	1.52	0.58
2:B:90:LYS:HD3	2:B:90:LYS:H	1.68	0.58
2:F:40:HIS:HE1	2:F:42:CYS:O	1.87	0.57
2:F:70:GLU:HB2	4:F:557:HOH:O	2.04	0.57
2:B:30:GLN:CG	4:B:730:HOH:O	2.53	0.57
2:B:35:ASP:OD2	2:B:35:ASP:C	2.48	0.57
3:C:165:ASN:ND2	4:C:504:HOH:O	2.38	0.57
2:F:91:ASN:ND2	2:F:91:ASN:C	2.57	0.56
3:C:181:ILE:CG1	4:C:621:HOH:O	2.38	0.56
2:F:101:ASN:CG	4:F:724:HOH:O	2.33	0.56
2:F:24:PRO:HD3	4:F:716:HOH:O	2.04	0.56
4:B:516:HOH:O	3:C:197:GLY:HA3	2.05	0.56
2:F:91:ASN:HD22	2:F:92:SER:N	2.04	0.56
2:B:90:LYS:HE3	4:B:646:HOH:O	2.05	0.55
2:F:36:LYS:CB	2:F:36:LYS:HZ2	2.18	0.55
3:G:167:ASN:O	3:G:170:LYS:HB2	2.06	0.55
3:G:232:THR:HB	4:G:524:HOH:O	2.06	0.55
2:F:98:THR:HG23	4:G:665:HOH:O	2.07	0.55
2:F:125:SER:N	2:F:128:ASP:OD2	2.40	0.54
2:B:35:ASP:OD1	2:B:37:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:TRP:NE1	4:B:702:HOH:O	2.41	0.53
3:C:181:ILE:HG22	3:C:230:ARG:HA	1.90	0.53
3:C:221:SER:N	4:C:701:HOH:O	2.40	0.53
2:F:67:VAL:CG1	2:F:70:GLU:HG3	2.38	0.53
2:B:64:ASP:OD1	3:G:149:ALA:N	2.42	0.52
1:E:7:GLN:O	1:E:7:GLN:CG	2.56	0.52
3:C:153:ASP:OD2	2:F:37:THR:HG21	2.09	0.52
3:C:181:ILE:HG22	3:C:230:ARG:CA	2.39	0.52
2:B:30:GLN:HG2	4:B:730:HOH:O	2.08	0.52
2:B:93:LYS:HB3	2:B:101:ASN:ND2	2.24	0.52
2:B:87:LYS:HD3	4:B:727:HOH:O	2.09	0.52
2:B:91:ASN:OD1	2:B:93:LYS:HB2	2.10	0.52
2:B:96:SER:HB2	2:F:145:ARG:HH12	1.74	0.51
3:G:169:LYS:HG2	3:G:173:GLY:O	2.11	0.51
3:C:187:GLY:C	3:C:222:THR:HB	2.35	0.51
3:C:221:SER:OG	3:C:223:SER:HB2	2.11	0.51
3:G:160:LEU:HD12	4:G:720:HOH:O	2.11	0.51
3:G:165:ASN:ND2	4:G:522:HOH:O	2.42	0.51
3:G:235:VAL:HA	3:G:238:VAL:HB	1.93	0.51
2:F:22:ALA:N	4:G:589:HOH:O	2.44	0.51
2:F:28:PRO:HG3	4:F:723:HOH:O	2.11	0.50
2:B:27:TRP:CZ2	2:B:137:VAL:HG11	2.46	0.50
2:B:49:GLU:O	2:B:111:ALA:HA	2.11	0.50
3:G:236:ASN:O	3:G:240:GLN:HG3	2.12	0.50
2:B:17:VAL:O	2:B:18:ASN:HB2	2.11	0.49
2:F:30:GLN:HG3	2:F:31:VAL:N	2.24	0.49
2:B:98:THR:HG23	2:B:100:ASN:HB2	1.94	0.49
2:B:47:ILE:O	2:B:48:ASN:ND2	2.46	0.49
2:B:53:VAL:HG23	2:B:103:ILE:CD1	2.35	0.48
2:F:60:VAL:HG12	2:F:61:THR:N	2.28	0.48
2:F:72:ASP:OD2	3:G:153:ASP:HB3	2.13	0.48
2:F:35:ASP:OD2	2:F:39:PHE:O	2.32	0.48
3:C:181:ILE:CG2	3:C:230:ARG:HA	2.44	0.48
2:B:24:PRO:HB3	2:B:71:PHE:CG	2.48	0.48
2:B:33:LEU:HD11	2:B:54:THR:HG21	1.96	0.47
3:G:212:ILE:HB	3:G:229:ALA:HB3	1.96	0.47
2:B:88:VAL:CG1	2:B:90:LYS:HD2	2.36	0.47
2:F:21:GLU:OE1	3:G:154:ARG:NH2	2.45	0.47
3:G:164:SER:OG	3:G:167:ASN:OD1	2.32	0.47
2:B:90:LYS:H	2:B:90:LYS:CD	2.27	0.47
3:G:160:LEU:CD1	4:G:720:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LYS:C	2:B:38:GLY:N	2.67	0.47
3:G:163:LEU:CB	4:G:717:HOH:O	2.46	0.47
2:F:87:LYS:HE2	2:F:89:PHE:CZ	2.49	0.47
2:F:49:GLU:OE2	4:F:675:HOH:O	2.21	0.47
2:F:33:LEU:HD12	2:F:33:LEU:N	2.30	0.47
3:G:183:ALA:CB	4:G:720:HOH:O	2.12	0.47
2:B:41:PHE:O	2:B:42:CYS:SG	2.73	0.46
3:C:218:SER:CB	3:G:216:GLY:O	2.63	0.46
2:F:75:SER:O	2:F:75:SER:OG	2.23	0.46
2:B:84:LYS:CG	4:B:656:HOH:O	2.48	0.46
2:B:89:PHE:HB2	2:B:105:LEU:HB2	1.98	0.46
3:C:230:ARG:HG2	3:C:232:THR:HG22	1.97	0.46
2:B:144:THR:C	2:B:145:ARG:HG3	2.41	0.46
2:F:16:ILE:O	2:F:144:THR:HA	2.15	0.46
3:C:164:SER:OG	3:C:167:ASN:OD1	2.31	0.46
2:F:125:SER:CB	2:F:128:ASP:OD2	2.64	0.46
2:B:114:PHE:HA	2:B:118:VAL:O	2.17	0.45
2:F:130:PHE:CE2	3:G:203:LYS:HD2	2.51	0.45
2:B:90:LYS:CD	2:B:90:LYS:N	2.79	0.45
3:C:181:ILE:O	3:C:181:ILE:HG12	2.05	0.45
3:C:216:GLY:O	3:G:218:SER:HB2	2.17	0.45
2:F:16:ILE:HA	3:G:189:SER:O	2.17	0.45
3:C:235:VAL:O	3:C:236:ASN:C	2.60	0.45
2:F:53:VAL:HG23	2:F:105:LEU:HD21	1.96	0.45
3:G:187:GLY:C	3:G:222:THR:HB	2.41	0.45
2:B:48:ASN:HD22	2:B:48:ASN:HA	1.28	0.45
3:C:191:CYS:O	3:C:192:MET:C	2.59	0.44
3:C:181:ILE:HD13	3:C:228:TYR:CB	2.41	0.44
2:B:95:ASN:CG	2:B:98:THR:HB	2.43	0.44
3:C:149:ALA:N	4:C:611:HOH:O	2.50	0.44
2:F:125:SER:O	2:F:128:ASP:OD2	2.35	0.44
2:B:62:THR:O	4:B:573:HOH:O	2.21	0.44
2:F:47:ILE:HB	4:F:679:HOH:O	2.17	0.44
2:B:16:ILE:HA	3:C:189:SER:O	2.17	0.43
2:F:90:LYS:CA	4:F:686:HOH:O	2.66	0.43
2:F:61:THR:HB	4:F:737:HOH:O	2.18	0.43
2:F:67:VAL:HG12	2:F:70:GLU:CG	2.48	0.43
3:C:160:LEU:N	3:C:160:LEU:HD23	2.32	0.43
2:B:16:ILE:HD13	2:B:16:ILE:HG21	1.81	0.43
2:B:103:ILE:CD1	2:B:103:ILE:C	2.92	0.43
2:F:110:THR:OG1	4:F:664:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:PHE:CE1	4:F:716:HOH:O	2.69	0.43
2:B:39:PHE:CE2	2:B:40:HIS:HB3	2.53	0.43
2:F:145:ARG:NH1	2:F:145:ARG:CG	2.81	0.43
2:F:28:PRO:CG	4:F:723:HOH:O	2.67	0.43
2:B:53:VAL:CG2	2:B:103:ILE:HD11	2.36	0.42
2:F:33:LEU:N	2:F:33:LEU:CD1	2.82	0.42
3:G:230:ARG:HG2	3:G:232:THR:HG22	2.00	0.42
2:B:32:SER:HB2	2:B:141:TRP:CZ3	2.55	0.42
3:G:162:LEU:C	3:G:163:LEU:HD12	2.44	0.42
2:B:24:PRO:HG3	2:B:71:PHE:CD2	2.55	0.42
1:E:1:CYS:C	2:F:122:CYS:SG	3.03	0.42
2:B:98:THR:CG2	2:B:100:ASN:H	2.31	0.41
2:B:82:LYS:CG	4:B:645:HOH:O	2.68	0.41
3:G:183:ALA:C	4:G:720:HOH:O	2.64	0.41
3:C:236:ASN:O	3:C:240:GLN:HG3	2.21	0.41
3:C:219:THR:O	3:C:220:CYS:HB2	2.19	0.41
2:B:99:ILE:HG22	2:B:99:ILE:O	2.20	0.41
3:C:209:LEU:HA	3:C:209:LEU:HD12	1.92	0.41
2:B:52:VAL:HB	2:B:106:LEU:HB2	2.03	0.41
2:B:123:LEU:HG	4:C:627:HOH:O	2.20	0.40
3:G:160:LEU:CG	4:G:720:HOH:O	2.69	0.40
1:A:1:CYS:CB	4:A:683:HOH:O	2.32	0.40
1:E:8:PRO:HA	2:F:26:SER:HB2	2.02	0.40
2:F:41:PHE:O	2:F:42:CYS:SG	2.79	0.40
2:F:125:SER:H	2:F:128:ASP:CG	2.29	0.40

All (5) 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:B:116:GLN:NE2	1:E:7:GLN:OE1[2_746]	1.47	0.73
2:B:116:GLN:CG	1:E:7:GLN:OE1[2_746]	1.55	0.65
2:B:116:GLN:CD	1:E:7:GLN:OE1[2_746]	1.90	0.30
2:B:116:GLN:NE2	1:E:7:GLN:CD[2_746]	2.11	0.09
2:B:79:LYS:CD	3:C:170:LYS:NZ[1_655]	2.17	0.03

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	7/13 (54%)	6 (86%)	0	1 (14%)	0	0
1	E	7/13 (54%)	7 (100%)	0	0	100	100
2	B	129/131 (98%)	124 (96%)	4 (3%)	1 (1%)	16	4
2	F	129/131 (98%)	123 (95%)	4 (3%)	2 (2%)	7	0
3	C	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
3	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
All	All	462/482 (96%)	442 (96%)	16 (4%)	4 (1%)	14	3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	GLY
2	F	99	ILE
2	F	77	SER
2	B	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	A	6/10 (60%)	5 (83%)	1 (17%)	2	0
1	E	6/10 (60%)	5 (83%)	1 (17%)	2	0
2	B	109/109 (100%)	91 (84%)	18 (16%)	2	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	109/109 (100%)	90 (83%)	19 (17%)	2	0
3	C	77/77 (100%)	69 (90%)	8 (10%)	7	0
3	G	77/77 (100%)	71 (92%)	6 (8%)	11	1
All	All	384/392 (98%)	331 (86%)	53 (14%)	3	0

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
2	B	18	ASN
2	B	20	GLU
2	B	36	LYS
2	B	37	THR
2	B	42	CYS
2	B	62	THR
2	B	70	GLU
2	B	80	ILE
2	B	90	LYS
2	B	92	SER
2	B	97	LEU
2	B	98	THR
2	B	103	ILE
2	B	109	SER
2	B	116	GLN
2	B	123	LEU
2	B	128	ASP
2	B	145	ARG
3	C	164	SER
3	C	166	THR
3	C	178	ASP
3	C	181	ILE
3	C	192	MET
3	C	219	THR
3	C	232	THR
3	C	234	LEU
1	E	7	GLN
2	F	32	SER
2	F	33	LEU
2	F	35	ASP
2	F	36	LYS
2	F	48	ASN

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Mol	Chain	Res	Type
2	F	53	VAL
2	F	65	VAL
2	F	70	GLU
2	F	82	LYS
2	F	83	LEU
2	F	84	LYS
2	F	91	ASN
2	F	92	SER
2	F	104	THR
2	F	109	SER
2	F	110	THR
2	F	115	SER
2	F	128	ASP
2	F	145	ARG
3	G	164	SER
3	G	165	ASN
3	G	166	THR
3	G	195	SER
3	G	219	THR
3	G	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	48	ASN
2	B	101	ASN
3	C	165	ASN
3	C	240	GLN
1	E	7	GLN
2	F	34	GLN
2	F	48	ASN
2	F	91	ASN
3	G	165	ASN
3	G	240	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.