



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:57 AM UTC

PDB ID : 1LTO / pdb_00001lto
Title : Human alpha1-tryptase
Authors : Marquardt, U.; Zettl, F.; Huber, R.; Bode, W.; Sommerhoff, C.P.
Deposited on : 2002-05-20
Resolution : 2.20 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

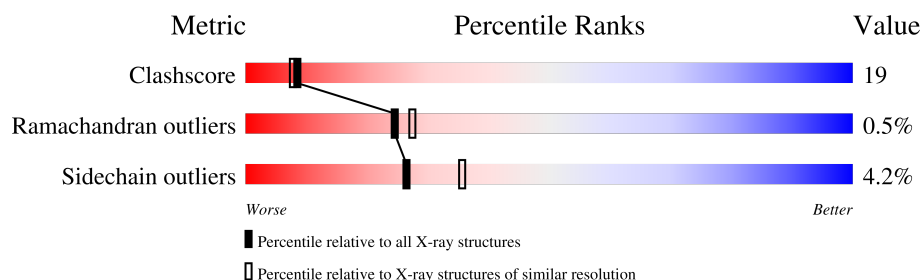
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	245	 64% 30% . .
1	B	245	 67% 29% . .
1	C	245	 66% 30% . .
1	D	245	 67% 29% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8351 atoms, of which 8 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 tryptase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	243	Total	C	H	N	O	S	66	0	0
			1937	1239	2	338	345	13			
1	B	243	Total	C	H	N	O	S	42	0	0
			1937	1239	2	338	345	13			
1	C	243	Total	C	H	N	O	S	72	0	0
			1937	1239	2	338	345	13			
1	D	243	Total	C	H	N	O	S	76	0	0
			1937	1239	2	338	345	13			

- Molecule 2 is water.

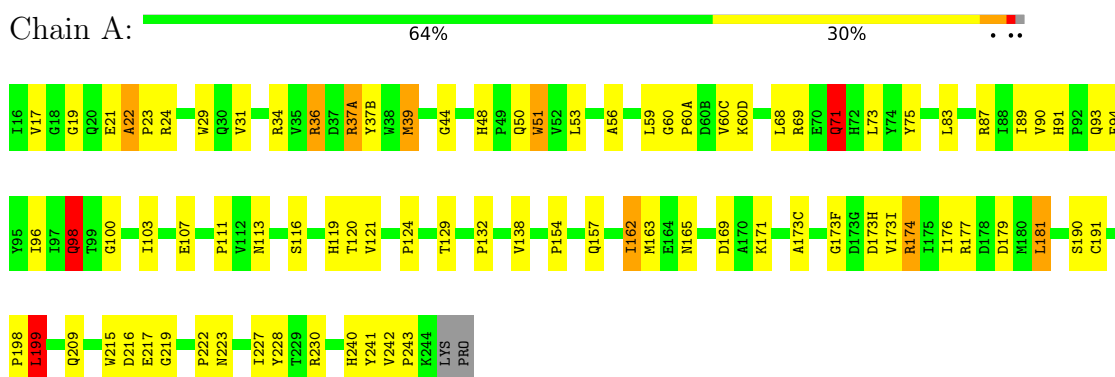
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	153	Total	O	0	0
			153	153		
2	B	220	Total	O	0	0
			220	220		
2	C	96	Total	O	0	0
			96	96		
2	D	134	Total	O	0	0
			134	134		

3 Residue-property plots [i](#)

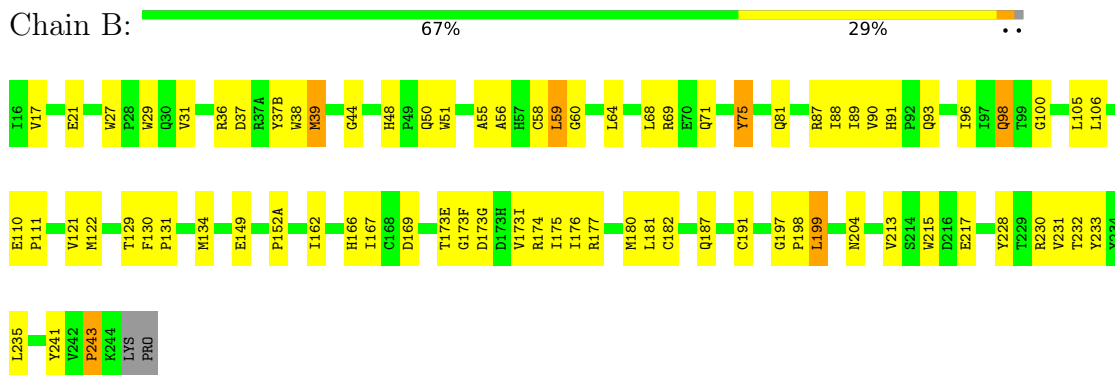
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

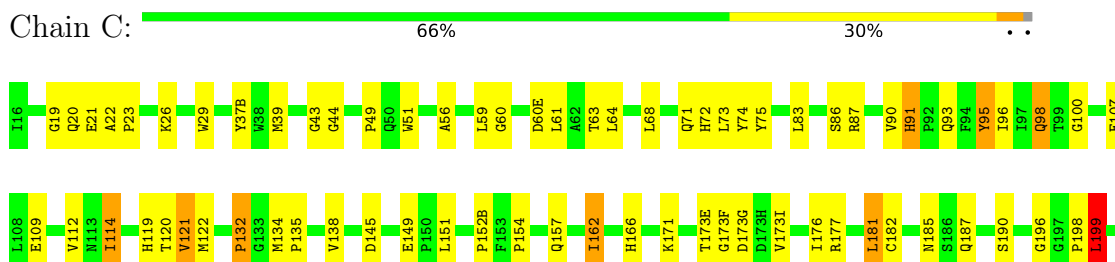
• Molecule 1: alpha tryptase I



• Molecule 1: alpha tryptase I

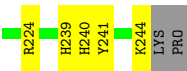
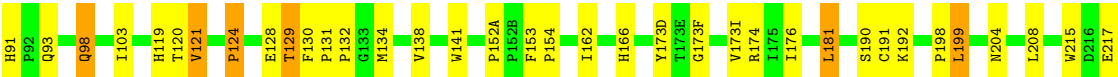


• Molecule 1: alpha tryptase I





● Molecule 1: alpha tryptase I



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.44Å 110.69Å 130.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.94 – 2.20	Depositor
% Data completeness (in resolution range)	94.7 (23.94-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8351	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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	A	0.60	0/1998	1.06	13/2735 (0.5%)
1	B	0.72	0/1998	1.06	8/2735 (0.3%)
1	C	0.53	0/1998	1.02	12/2735 (0.4%)
1	D	0.55	0/1998	1.07	8/2735 (0.3%)
All	All	0.61	0/7992	1.05	41/10940 (0.4%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	129	THR	N-CA-C	-11.60	93.29	110.46
1	C	176	ILE	CB-CG1-CD1	8.24	131.10	113.80
1	A	242	VAL	N-CA-C	8.23	116.08	107.76
1	A	199	LEU	N-CA-C	-7.51	94.87	108.02
1	D	130	PHE	CA-C-N	6.74	124.58	119.66
1	D	130	PHE	C-N-CA	6.74	124.58	119.66
1	C	95	TYR	N-CA-C	-6.61	103.26	112.12
1	D	190	SER	N-CA-C	-6.52	102.12	110.53
1	A	37(A)	ARG	N-CA-C	-6.49	104.62	112.54
1	B	75	TYR	N-CA-C	6.47	119.33	111.82
1	A	22	ALA	CA-C-N	5.96	125.90	119.76
1	A	22	ALA	C-N-CA	5.96	125.90	119.76
1	B	199	LEU	N-CA-C	-5.87	97.75	108.02
1	B	152(A)	PRO	N-CA-C	-5.60	104.58	110.58
1	A	138	VAL	CB-CA-C	-5.58	102.32	110.81
1	A	94	PHE	N-CA-C	5.57	118.62	109.76
1	B	231	VAL	N-CA-C	5.55	116.28	110.62
1	D	124	PRO	CA-C-N	5.54	125.30	119.76
1	D	124	PRO	C-N-CA	5.54	125.30	119.76
1	A	190	SER	N-CA-C	-5.54	102.56	110.59
1	C	151	LEU	CA-C-N	-5.48	114.73	120.38
1	C	151	LEU	C-N-CA	-5.48	114.73	120.38
1	C	91	HIS	CA-C-N	5.42	125.76	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	HIS	C-N-CA	5.42	125.76	119.47
1	C	199	LEU	N-CA-C	-5.39	98.59	108.02
1	A	173(I)	VAL	N-CA-C	5.39	116.47	108.23
1	D	199	LEU	N-CA-C	-5.37	98.49	107.99
1	C	121	VAL	N-CA-C	-5.36	100.76	108.48
1	B	198	PRO	N-CA-C	5.34	121.83	112.01
1	C	43	GLY	N-CA-C	-5.29	105.32	112.57
1	C	114	ILE	N-CA-C	5.26	115.88	108.36
1	C	190	SER	N-CA-C	-5.25	102.75	110.52
1	C	64	LEU	N-CA-C	5.23	117.43	108.90
1	D	121	VAL	N-CA-C	-5.21	100.97	108.89
1	A	39	MET	N-CA-C	5.21	118.42	110.20
1	A	51	TRP	N-CA-C	5.18	117.34	108.90
1	B	39	MET	N-CA-C	5.15	118.00	109.46
1	A	71	GLN	N-CA-C	-5.10	105.80	111.36
1	A	98	GLN	N-CA-C	5.10	118.99	112.87
1	B	51	TRP	N-CA-C	5.09	117.74	109.24
1	B	81	GLN	N-CA-C	-5.01	98.43	107.60

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	1935	2	1876	75	0
1	B	1935	2	1876	81	0
1	C	1935	2	1876	63	0
1	D	1935	2	1876	67	0
2	A	153	0	0	12	0
2	B	220	0	0	19	0
2	C	96	0	0	8	0
2	D	134	0	0	10	0
All	All	8343	8	7504	278	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 19.

All (278) 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)
1:B:169:ASP:HB2	1:B:176:ILE:CG1	1.67	1.24
1:A:98:GLN:H	1:A:98:GLN:NE2	1.50	1.09
1:A:60:GLY:HA3	2:A:315:HOH:O	1.55	1.04
1:B:98:GLN:H	1:B:98:GLN:NE2	1.62	0.96
1:D:91:HIS:HD2	1:D:93:GLN:H	1.15	0.93
1:A:169:ASP:HB2	1:A:176:ILE:CG2	1.99	0.93
1:B:169:ASP:CB	1:B:176:ILE:CG1	2.46	0.93
1:C:98:GLN:H	1:C:98:GLN:NE2	1.68	0.89
1:C:166:HIS:HB3	2:C:294:HOH:O	1.73	0.87
1:B:130:PHE:HA	1:B:134:MET:CE	2.08	0.83
1:A:100:GLY:HA3	1:A:177:ARG:NH2	1.94	0.82
1:A:98:GLN:H	1:A:98:GLN:HE21	1.28	0.82
1:C:60:GLY:HA3	2:C:300:HOH:O	1.79	0.81
1:D:98:GLN:H	1:D:98:GLN:NE2	1.79	0.81
1:A:75:TYR:HB2	1:B:75:TYR:CE2	2.15	0.81
1:B:50:GLN:NE2	1:B:111:PRO:HG3	1.96	0.81
1:C:91:HIS:HD2	1:C:93:GLN:H	1.27	0.80
1:B:169:ASP:HB2	1:B:176:ILE:HG13	1.62	0.79
1:B:60:GLY:HA3	2:B:311:HOH:O	1.84	0.76
1:B:98:GLN:H	1:B:98:GLN:HE21	1.31	0.75
1:C:145:ASP:HB3	1:C:149:GLU:HG3	1.67	0.74
1:B:169:ASP:CB	1:B:176:ILE:HG12	2.18	0.73
1:B:130:PHE:HA	1:B:134:MET:HE3	1.71	0.72
1:A:169:ASP:HB2	1:A:176:ILE:HG22	1.70	0.72
1:B:91:HIS:HD2	1:B:93:GLN:H	1.37	0.72
1:B:173(F):GLY:O	1:B:173(I):VAL:HG12	1.89	0.72
1:B:39:MET:HE1	2:B:387:HOH:O	1.90	0.71
1:D:91:HIS:CD2	1:D:93:GLN:H	2.05	0.71
1:A:169:ASP:CB	1:A:176:ILE:HG22	2.20	0.71
1:B:166:HIS:HB3	2:B:359:HOH:O	1.91	0.70
1:B:167:ILE:HD11	2:B:366:HOH:O	1.91	0.69
1:A:171:LYS:HG2	1:A:223:ASN:HD22	1.58	0.69
1:B:131:PRO:HD2	1:B:134:MET:HE2	1.75	0.68
1:D:61:LEU:H	1:D:61:LEU:HD12	1.59	0.68
1:C:173(F):GLY:O	1:C:173(I):VAL:HG12	1.94	0.68
1:D:68:LEU:HD21	1:D:83:LEU:HD11	1.76	0.68
1:D:68:LEU:HD21	1:D:83:LEU:CD1	2.23	0.68
1:B:173(E):THR:HG22	1:B:173(I):VAL:HG13	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:NE2	1:A:98:GLN:N	2.35	0.67
1:B:98:GLN:NE2	1:B:98:GLN:N	2.41	0.66
1:B:173(E):THR:HG22	1:B:173(I):VAL:CG1	2.26	0.66
1:C:138:VAL:HG21	1:C:228:TYR:OH	1.97	0.65
1:A:24:ARG:HG2	1:A:71:GLN:HG3	1.79	0.65
1:C:98:GLN:H	1:C:98:GLN:HE21	1.41	0.64
1:C:181:LEU:C	1:C:181:LEU:HD23	2.22	0.64
1:C:56:ALA:HB1	1:C:90:VAL:HG13	1.79	0.64
1:A:177:ARG:HD2	2:A:329:HOH:O	1.98	0.64
1:B:204:ASN:HB3	2:B:378:HOH:O	1.98	0.63
1:B:129:THR:O	1:B:230:ARG:NH1	2.32	0.63
1:C:211:GLY:HA2	1:C:231:VAL:HG23	1.80	0.63
1:C:171:LYS:HG2	1:C:223:ASN:HD22	1.64	0.63
1:D:98:GLN:H	1:D:98:GLN:HE21	1.45	0.62
1:A:96:ILE:HD13	1:D:98:GLN:HB2	1.82	0.62
1:A:181:LEU:C	1:A:181:LEU:HD23	2.24	0.62
1:B:31:VAL:HG22	1:B:44:GLY:C	2.25	0.62
1:A:75:TYR:HB2	1:B:75:TYR:HE2	1.59	0.61
1:B:91:HIS:CD2	1:B:93:GLN:H	2.17	0.61
1:A:60(A):PRO:HA	2:A:315:HOH:O	2.00	0.60
1:C:114:ILE:HG23	1:C:119:HIS:HB3	1.82	0.60
1:A:39:MET:HE2	2:A:377:HOH:O	2.01	0.60
1:B:48:HIS:NE2	1:B:243:PRO:HG2	2.15	0.60
1:D:181:LEU:C	1:D:181:LEU:HD23	2.26	0.60
1:C:173(E):THR:HG22	1:C:173(I):VAL:HG13	1.83	0.60
1:D:46:LEU:O	1:D:120:THR:HA	2.01	0.59
1:D:192:LYS:HE3	1:D:217:GLU:OE2	2.02	0.59
1:C:68:LEU:HD21	1:C:83:LEU:HD12	1.84	0.59
1:C:232:THR:HG23	2:C:263:HOH:O	2.02	0.59
1:A:129:THR:O	1:A:230:ARG:NH1	2.35	0.59
1:A:169:ASP:CB	1:A:176:ILE:CG2	2.76	0.59
1:B:50:GLN:HE21	1:B:111:PRO:HG3	1.67	0.59
1:B:64:LEU:CD2	1:B:88:ILE:HD11	2.32	0.58
1:D:53:LEU:HD11	1:D:103:ILE:HD11	1.84	0.58
1:A:215:TRP:HB3	1:A:227:ILE:HB	1.84	0.58
1:A:100:GLY:HA3	1:A:177:ARG:HH22	1.66	0.58
1:B:100:GLY:HA3	1:B:177:ARG:HH21	1.69	0.58
1:C:49:PRO:O	1:C:112:VAL:HG22	2.04	0.58
1:C:86:SER:HB3	1:C:109:GLU:HA	1.86	0.57
1:D:215:TRP:NE1	2:D:295:HOH:O	2.31	0.57
1:D:215:TRP:CH2	1:D:217:GLU:HB2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:HIS:HD2	2:B:399:HOH:O	1.86	0.57
1:D:128:GLU:OE2	1:D:129:THR:O	2.21	0.57
1:C:19:GLY:HA3	1:C:157:GLN:O	2.03	0.57
1:C:122:MET:HE2	1:C:208:LEU:HD21	1.86	0.57
1:A:50:GLN:NE2	1:A:111:PRO:HG3	2.19	0.57
1:B:166:HIS:HE1	2:B:434:HOH:O	1.88	0.57
1:A:191:CYS:HA	1:A:216:ASP:O	2.04	0.57
1:C:51:TRP:CH2	1:C:107:GLU:HB2	2.39	0.57
1:D:91:HIS:CD2	1:D:93:GLN:HB2	2.40	0.57
1:D:124:PRO:CB	1:D:208:LEU:HD13	2.35	0.57
1:B:96:ILE:HG12	1:B:98:GLN:NE2	2.20	0.56
1:D:166:HIS:HD2	2:D:288:HOH:O	1.88	0.56
1:A:37(B):TYR:OH	1:A:39:MET:HE3	2.06	0.56
1:D:68:LEU:HD23	2:D:356:HOH:O	2.04	0.56
1:D:98:GLN:NE2	1:D:98:GLN:N	2.53	0.56
1:B:98:GLN:HB2	1:C:96:ILE:HD13	1.88	0.56
1:D:240:HIS:O	1:D:240:HIS:ND1	2.39	0.56
1:B:105:LEU:C	1:B:106:LEU:HD12	2.31	0.56
1:D:29:TRP:CD2	1:D:121:VAL:HB	2.41	0.56
1:C:162:ILE:HG12	1:C:181:LEU:HD21	1.88	0.55
1:C:145:ASP:HB3	1:C:149:GLU:CG	2.36	0.55
1:D:124:PRO:HB3	1:D:208:LEU:HD13	1.87	0.55
1:A:98:GLN:H	1:A:98:GLN:CD	2.14	0.55
1:D:48:HIS:HA	1:D:120:THR:HG21	1.88	0.55
1:C:173(E):THR:HG22	1:C:173(I):VAL:CG1	2.37	0.55
1:A:59:LEU:O	1:A:60(D):LYS:HD3	2.06	0.55
1:A:177:ARG:NH2	1:A:179:ASP:OD1	2.39	0.55
1:B:130:PHE:HA	1:B:134:MET:HE2	1.85	0.55
1:A:91:HIS:CD2	1:A:93:GLN:H	2.24	0.55
1:B:96:ILE:HG12	1:B:98:GLN:HE22	1.72	0.55
1:B:131:PRO:HD2	1:B:134:MET:CE	2.37	0.54
1:B:71:GLN:NE2	2:B:424:HOH:O	2.40	0.54
1:C:132:PRO:C	1:C:134:MET:H	2.15	0.54
1:C:72:HIS:HB3	1:C:152(B):PRO:O	2.08	0.54
1:A:199:LEU:HG	1:A:228:TYR:CE2	2.43	0.54
1:D:48:HIS:CD2	1:D:49:PRO:HD2	2.42	0.54
1:B:100:GLY:HA3	1:B:177:ARG:NH2	2.23	0.54
1:C:91:HIS:CD2	1:C:93:GLN:H	2.17	0.54
1:D:21:GLU:HG3	1:D:154:PRO:HB2	1.90	0.54
1:C:181:LEU:HD23	1:C:182:CYS:N	2.24	0.53
1:D:61:LEU:HD23	1:D:85:VAL:O	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:VAL:HG23	1:B:191:CYS:HB2	1.90	0.53
1:D:24:ARG:HG2	1:D:71:GLN:CG	2.37	0.53
1:D:68:LEU:O	1:D:69:ARG:C	2.51	0.53
1:D:173(F):GLY:O	1:D:173(I):VAL:HG13	2.08	0.53
1:A:132:PRO:HA	1:A:162:ILE:O	2.09	0.53
1:C:68:LEU:CD2	1:C:83:LEU:HD12	2.37	0.53
1:A:29:TRP:CD2	1:A:121:VAL:HB	2.44	0.53
1:B:29:TRP:CG	1:B:121:VAL:HB	2.44	0.53
1:D:60(E):ASP:OD2	1:D:62:ALA:HB3	2.09	0.52
1:B:181:LEU:HD23	1:B:181:LEU:C	2.34	0.52
1:D:73:LEU:HG	1:D:141:TRP:CD1	2.45	0.52
1:A:21:GLU:HG3	2:A:372:HOH:O	2.09	0.52
1:C:29:TRP:CD2	1:C:121:VAL:HB	2.45	0.52
1:C:173(F):GLY:O	1:C:173(I):VAL:CG1	2.58	0.52
1:B:173(F):GLY:O	1:B:173(I):VAL:CG1	2.57	0.52
1:A:174:ARG:NH1	2:A:276:HOH:O	2.43	0.51
1:C:215:TRP:HB3	1:C:227:ILE:HB	1.91	0.51
1:C:135:PRO:HA	2:C:316:HOH:O	2.09	0.51
1:D:48:HIS:CG	1:D:49:PRO:HD2	2.45	0.51
1:A:173(F):GLY:C	1:A:173(H):ASP:N	2.66	0.51
1:B:21:GLU:CD	2:B:316:HOH:O	2.52	0.51
1:B:21:GLU:OE2	2:B:354:HOH:O	2.18	0.51
1:B:174:ARG:HD3	2:B:428:HOH:O	2.10	0.51
1:C:37(B):TYR:OH	1:C:39:MET:HE3	2.11	0.51
1:C:91:HIS:CD2	1:C:93:GLN:HB2	2.45	0.50
1:D:17:VAL:HG23	1:D:191:CYS:HB2	1.93	0.50
1:D:68:LEU:CD2	1:D:83:LEU:HD11	2.41	0.50
1:D:204:ASN:HA	2:D:354:HOH:O	2.10	0.50
1:A:171:LYS:HG2	1:A:223:ASN:ND2	2.25	0.50
1:C:222:PRO:O	1:C:223:ASN:HB2	2.12	0.50
1:A:17:VAL:HG23	1:A:191:CYS:HB2	1.94	0.50
1:A:37(A):ARG:HD3	1:B:149:GLU:OE1	2.12	0.49
1:A:173(F):GLY:C	1:A:173(H):ASP:H	2.19	0.49
1:C:51:TRP:CZ3	1:C:107:GLU:HB2	2.47	0.49
1:C:173(G):ASP:HB2	2:C:339:HOH:O	2.12	0.49
1:A:91:HIS:HD2	1:A:93:GLN:H	1.57	0.49
1:C:171:LYS:HG2	1:C:223:ASN:ND2	2.27	0.49
1:B:122:MET:HG3	2:B:408:HOH:O	2.13	0.49
1:D:28:PRO:HG3	1:D:119:HIS:CE1	2.47	0.49
1:D:239:HIS:CE1	2:D:302:HOH:O	2.64	0.49
1:D:131:PRO:HD2	1:D:134:MET:HE2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:TRP:O	1:B:69:ARG:HD3	2.13	0.49
1:A:177:ARG:HH22	1:A:179:ASP:CG	2.20	0.48
1:C:51:TRP:CG	1:C:242:VAL:HG22	2.48	0.48
1:D:29:TRP:CG	1:D:121:VAL:HB	2.49	0.48
1:C:73:LEU:O	1:C:74:TYR:HB2	2.13	0.48
1:D:68:LEU:HD21	1:D:83:LEU:HD12	1.95	0.48
1:D:166:HIS:CD2	2:D:288:HOH:O	2.65	0.48
1:D:174:ARG:HD2	1:D:176:ILE:O	2.14	0.47
1:B:87:ARG:NE	2:B:427:HOH:O	2.41	0.47
1:D:31:VAL:HG22	1:D:44:GLY:C	2.39	0.47
1:A:165:ASN:O	1:A:176:ILE:HG21	2.13	0.47
1:B:59:LEU:HD21	1:B:106:LEU:HD11	1.96	0.47
1:D:37(B):TYR:OH	1:D:39:MET:HE3	2.14	0.47
1:A:154:PRO:HG3	2:A:391:HOH:O	2.13	0.47
1:A:68:LEU:HD12	2:A:266:HOH:O	2.14	0.47
1:A:71:GLN:NE2	2:A:372:HOH:O	2.33	0.47
1:B:174:ARG:NE	2:B:465:HOH:O	2.47	0.47
1:C:75:TYR:CE2	1:D:75:TYR:HB2	2.49	0.47
1:A:19:GLY:HA3	1:A:157:GLN:O	2.15	0.47
1:A:89:ILE:HD13	1:A:241:TYR:CD1	2.50	0.47
1:B:215:TRP:CH2	1:B:217:GLU:HB2	2.49	0.46
1:A:87:ARG:HD3	1:A:107:GLU:OE2	2.15	0.46
1:C:21:GLU:HG3	2:C:341:HOH:O	2.15	0.46
1:B:169:ASP:OD1	1:B:176:ILE:HG12	2.16	0.46
1:D:24:ARG:HG2	1:D:71:GLN:HG3	1.98	0.46
1:B:87:ARG:NH2	2:B:427:HOH:O	2.32	0.46
1:C:68:LEU:HD21	1:C:83:LEU:CD1	2.45	0.45
1:A:60(A):PRO:O	2:A:328:HOH:O	2.20	0.45
1:B:177:ARG:HD3	1:B:180:MET:HE3	1.99	0.45
1:B:169:ASP:CA	1:B:176:ILE:HG12	2.45	0.45
1:B:173(G):ASP:OD1	2:B:353:HOH:O	2.21	0.45
1:D:80:ASP:O	1:D:81:GLN:HG3	2.16	0.45
1:A:98:GLN:HE21	1:A:98:GLN:N	2.03	0.45
1:A:31:VAL:HG22	1:A:44:GLY:C	2.41	0.45
1:C:181:LEU:C	1:C:181:LEU:CD2	2.89	0.45
1:C:185:ASN:OD1	1:C:187:GLN:N	2.37	0.45
1:D:48:HIS:HB3	1:D:51:TRP:HB2	1.98	0.45
1:A:60(C):VAL:HA	1:D:173(D):TYR:CE2	2.52	0.45
1:A:24:ARG:HG2	1:A:71:GLN:CG	2.45	0.45
1:A:169:ASP:HB2	1:A:176:ILE:HG21	1.90	0.45
1:B:181:LEU:HD23	1:B:182:CYS:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LYS:NZ	2:C:276:HOH:O	2.47	0.45
1:C:120:THR:HG23	2:C:319:HOH:O	2.17	0.45
1:B:169:ASP:CA	1:B:176:ILE:CG1	2.89	0.45
1:D:119:HIS:HB2	2:D:297:HOH:O	2.16	0.45
1:D:152(A):PRO:HA	1:D:153:PHE:N	2.32	0.44
1:A:219:GLY:HA3	2:A:364:HOH:O	2.18	0.44
1:B:48:HIS:CD2	1:B:243:PRO:HG2	2.52	0.44
1:B:64:LEU:HD23	1:B:88:ILE:HD11	1.99	0.44
1:D:60(A):PRO:HA	2:D:347:HOH:O	2.16	0.44
1:A:91:HIS:HD2	1:A:93:GLN:HB2	1.83	0.44
1:A:56:ALA:HB1	1:A:90:VAL:HG13	1.99	0.44
1:A:240:HIS:O	1:A:240:HIS:ND1	2.50	0.44
1:B:197:GLY:HA3	2:B:247:HOH:O	2.17	0.44
1:C:44:GLY:HA2	1:C:196:GLY:O	2.17	0.44
1:B:56:ALA:HB1	1:B:90:VAL:HG13	2.00	0.44
1:D:204:ASN:N	2:D:330:HOH:O	2.50	0.44
1:A:132:PRO:HG3	1:A:163:MET:HA	1.99	0.43
1:B:37(B):TYR:OH	1:B:39:MET:HE3	2.18	0.43
1:B:213:VAL:HG22	1:B:228:TYR:CE2	2.53	0.43
1:C:51:TRP:CD2	1:C:242:VAL:HG22	2.53	0.43
1:A:29:TRP:CG	1:A:121:VAL:HB	2.54	0.43
1:D:68:LEU:CD2	1:D:83:LEU:CD1	2.96	0.43
1:D:131:PRO:HA	1:D:132:PRO:HD3	1.86	0.43
1:A:68:LEU:CD2	1:A:83:LEU:HD12	2.49	0.43
1:B:233:TYR:O	1:B:233:TYR:CD1	2.72	0.43
1:A:53:LEU:HD11	1:A:103:ILE:HD11	1.99	0.43
1:A:91:HIS:CD2	1:A:93:GLN:HB2	2.54	0.43
1:A:48:HIS:HB3	1:A:51:TRP:HB2	2.00	0.43
1:B:29:TRP:CD2	1:B:121:VAL:HB	2.53	0.43
1:B:130:PHE:CD1	1:B:134:MET:HE3	2.54	0.43
1:D:61:LEU:HD12	1:D:61:LEU:N	2.32	0.43
1:B:232:THR:HA	1:B:235:LEU:HG	2.00	0.43
1:D:174:ARG:NH1	1:D:176:ILE:O	2.51	0.42
1:B:36:ARG:HA	1:B:36:ARG:HD3	1.77	0.42
1:B:89:ILE:HD13	1:B:241:TYR:CD1	2.54	0.42
1:B:175:ILE:HG23	1:C:95:TYR:CZ	2.54	0.42
1:C:60(E):ASP:HB3	1:C:63:THR:HG23	2.00	0.42
1:C:71:GLN:O	1:C:154:PRO:HA	2.18	0.42
1:D:59:LEU:O	1:D:60(D):LYS:HE3	2.19	0.42
1:B:173(E):THR:CG2	1:B:173(I):VAL:CG1	2.97	0.42
1:D:70:GLU:HG2	1:D:72:HIS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:PRO:HB3	1:D:208:LEU:HB3	2.01	0.42
1:A:22:ALA:HA	1:A:23:PRO:HD3	1.80	0.42
1:C:87:ARG:HD3	1:C:107:GLU:OE1	2.19	0.42
1:B:36:ARG:HD2	1:B:37:ASP:O	2.19	0.42
1:A:21:GLU:HB2	2:A:290:HOH:O	2.19	0.42
1:B:55:ALA:O	1:B:58:CYS:HB2	2.20	0.42
1:C:59:LEU:N	1:C:59:LEU:HD22	2.35	0.42
1:A:222:PRO:O	1:A:223:ASN:HB2	2.19	0.41
1:D:91:HIS:HD2	1:D:93:GLN:N	1.98	0.41
1:A:68:LEU:O	1:A:69:ARG:C	2.62	0.41
1:B:169:ASP:HA	1:B:176:ILE:HG12	2.03	0.41
1:C:29:TRP:CG	1:C:121:VAL:HB	2.55	0.41
1:D:38:TRP:HZ3	1:D:63:THR:O	2.01	0.41
1:A:199:LEU:HB2	1:A:228:TYR:CD2	2.55	0.41
1:C:22:ALA:HA	1:C:23:PRO:HD3	1.91	0.41
1:D:38:TRP:CG	1:D:82:LEU:HD11	2.55	0.41
1:A:165:ASN:OD1	1:A:230:ARG:NH2	2.54	0.41
1:B:149:GLU:HG3	2:B:426:HOH:O	2.20	0.41
1:D:35:VAL:HG22	1:D:36:ARG:N	2.36	0.41
1:A:34:ARG:HH21	1:A:73:LEU:HD22	1.85	0.41
1:A:36:ARG:HH11	1:A:37(B):TYR:HA	1.85	0.41
1:A:215:TRP:CH2	1:A:217:GLU:HB2	2.56	0.41
1:B:87:ARG:NH2	2:B:390:HOH:O	2.54	0.41
1:C:56:ALA:CB	1:C:90:VAL:HG13	2.48	0.41
1:C:132:PRO:C	1:C:134:MET:N	2.79	0.41
1:D:38:TRP:CG	1:D:82:LEU:CD1	3.03	0.41
1:D:89:ILE:HD13	1:D:241:TYR:CD1	2.56	0.41
1:C:73:LEU:O	1:C:74:TYR:CB	2.68	0.41
1:C:138:VAL:HG22	1:C:199:LEU:HG	2.03	0.40
1:A:119:HIS:HD2	1:A:120:THR:O	2.04	0.40
1:B:91:HIS:HD2	1:B:93:GLN:N	2.13	0.40
1:A:173(C):ALA:HB1	2:D:326:HOH:O	2.22	0.40
1:C:100:GLY:HA3	1:C:177:ARG:HH21	1.85	0.40
1:A:124:PRO:HD3	1:A:209:GLN:O	2.22	0.40
1:B:36:ARG:HB2	1:B:38:TRP:CH2	2.56	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	A	241/245 (98%)	223 (92%)	17 (7%)	1 (0%)	30	34
1	B	241/245 (98%)	226 (94%)	14 (6%)	1 (0%)	30	34
1	C	241/245 (98%)	221 (92%)	19 (8%)	1 (0%)	30	34
1	D	241/245 (98%)	219 (91%)	20 (8%)	2 (1%)	16	16
All	All	964/980 (98%)	889 (92%)	70 (7%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	75	TYR
1	A	243	PRO
1	B	243	PRO
1	D	81	GLN
1	C	132	PRO

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	212/214 (99%)	202 (95%)	10 (5%)	23	31
1	B	212/214 (99%)	205 (97%)	7 (3%)	33	45
1	C	212/214 (99%)	204 (96%)	8 (4%)	29	40
1	D	212/214 (99%)	201 (95%)	11 (5%)	21	26
All	All	848/856 (99%)	812 (96%)	36 (4%)	26	36

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	71	GLN
1	A	98	GLN
1	A	113	ASN
1	A	116	SER
1	A	162	ILE
1	A	174	ARG
1	A	181	LEU
1	A	198	PRO
1	A	199	LEU
1	B	59	LEU
1	B	68	LEU
1	B	98	GLN
1	B	110	GLU
1	B	162	ILE
1	B	187	GLN
1	B	199	LEU
1	C	20	GLN
1	C	61	LEU
1	C	98	GLN
1	C	162	ILE
1	C	181	LEU
1	C	198	PRO
1	C	199	LEU
1	C	244	LYS
1	D	20	GLN
1	D	27	TRP
1	D	59	LEU
1	D	98	GLN
1	D	138	VAL
1	D	162	ILE
1	D	181	LEU
1	D	198	PRO
1	D	199	LEU
1	D	224	ARG
1	D	244	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	91	HIS
1	A	93	GLN
1	A	98	GLN
1	A	119	HIS
1	A	223	ASN
1	B	50	GLN
1	B	91	HIS
1	B	98	GLN
1	B	119	HIS
1	B	166	HIS
1	B	221(A)	GLN
1	B	223	ASN
1	C	50	GLN
1	C	72	HIS
1	C	81	GLN
1	C	91	HIS
1	C	98	GLN
1	C	119	HIS
1	C	223	ASN
1	D	20	GLN
1	D	91	HIS
1	D	98	GLN
1	D	146	ASN
1	D	166	HIS
1	D	221(A)	GLN
1	D	223	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.