



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:28 PM UTC

PDB ID : 1K86 / pdb_00001k86
Title : Crystal structure of caspase-7
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Deposited on : 2001-10-23
Resolution : 2.60 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

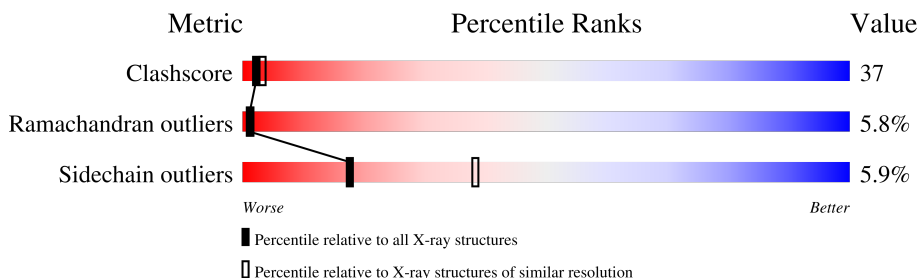
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	253	
1	B	253	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3755 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 caspase-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1853	1177	316	345	15			
1	B	232	Total	C	N	O	S	0	0	0
			1853	1177	316	345	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ALA	ASP	engineered mutation	UNP P55210
B	169	ALA	ASP	engineered mutation	UNP P55210

- Molecule 2 is water.

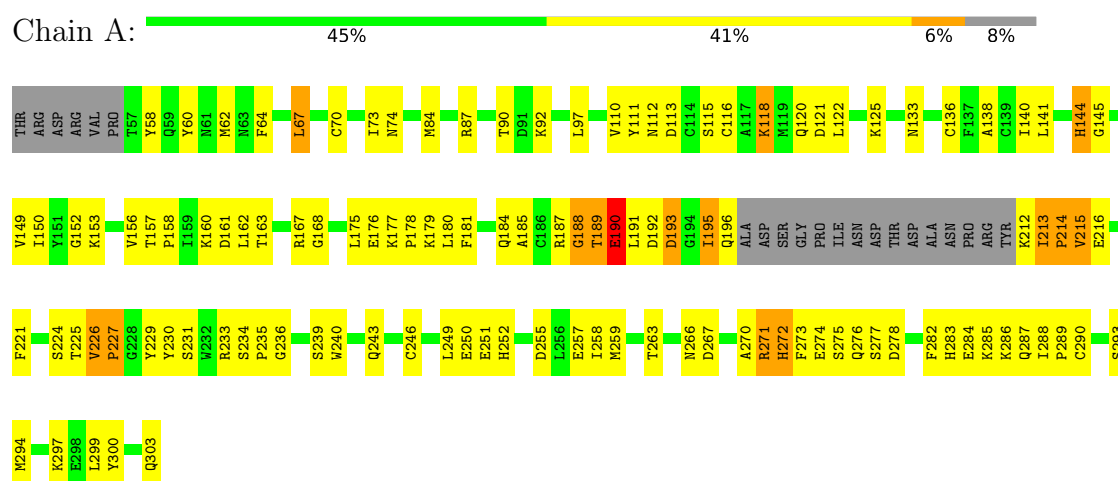
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	14	Total	O	0	0
			14	14		
2	B	35	Total	O	0	0
			35	35		

3 Residue-property plots

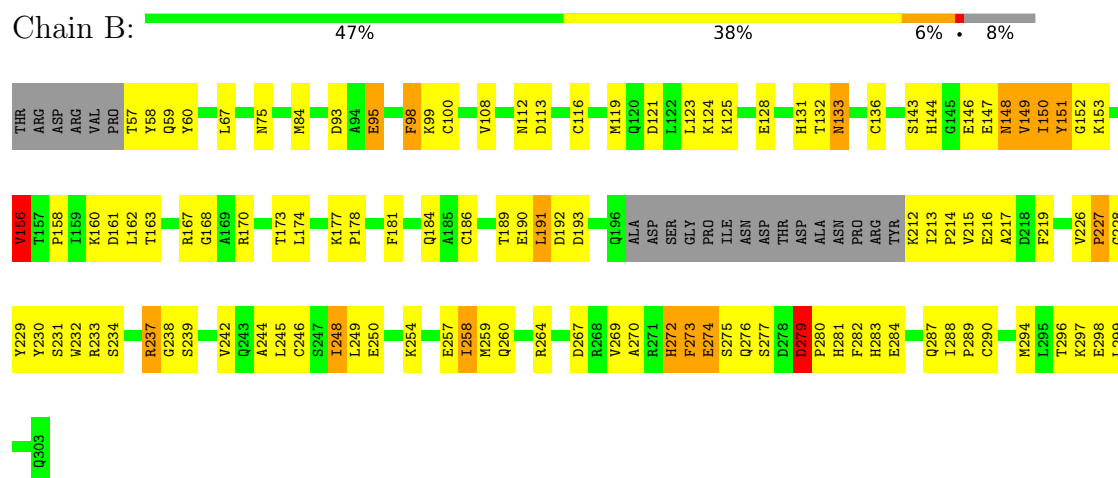
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: caspase-7



• Molecule 1: caspase-7



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.90Å 88.90Å 186.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3755	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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	0.76	6/1892 (0.3%)	1.79	27/2546 (1.1%)
1	B	0.44	0/1892	1.02	10/2546 (0.4%)
All	All	0.62	6/3784 (0.2%)	1.46	37/5092 (0.7%)

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	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	272	HIS	N-CA	-11.10	1.31	1.46
1	A	213	ILE	N-CA	-10.75	1.33	1.46
1	A	271	ARG	CA-C	-8.61	1.41	1.53
1	A	215	VAL	CA-CB	7.72	1.62	1.53
1	A	189	THR	CA-C	-5.94	1.45	1.52
1	A	272	HIS	CA-CB	-5.91	1.43	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	GLY	CA-C-O	-47.45	79.63	120.91
1	A	188	GLY	O-C-N	-36.01	95.88	123.61
1	A	215	VAL	N-CA-C	-20.65	77.52	106.85
1	A	213	ILE	C-N-CD	-17.56	81.96	120.60
1	A	213	ILE	N-CA-C	-13.72	79.25	108.88
1	A	213	ILE	CA-C-N	12.50	156.99	127.00
1	A	213	ILE	C-N-CA	12.50	156.99	127.00
1	A	271	ARG	N-CA-C	-12.45	94.75	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ILE	N-CA-CB	-9.78	97.52	111.21
1	A	188	GLY	CA-C-N	-9.64	109.40	122.99
1	A	188	GLY	C-N-CA	-9.64	109.40	122.99
1	B	189	THR	N-CA-C	8.76	129.45	110.80
1	A	190	GLU	N-CA-C	-8.25	93.23	110.80
1	A	214	PRO	N-CA-C	-8.22	90.74	112.10
1	B	279	ASP	CA-C-N	8.14	128.23	119.28
1	B	279	ASP	C-N-CA	8.14	128.23	119.28
1	A	152	GLY	N-CA-C	-7.75	99.25	112.51
1	B	191	LEU	N-CA-C	6.75	120.45	109.59
1	A	214	PRO	CA-CB-CG	-6.71	91.25	104.00
1	B	58	TYR	N-CA-C	-6.71	104.23	112.88
1	A	58	TYR	N-CA-C	6.69	125.04	110.80
1	A	189	THR	N-CA-C	6.68	119.78	108.90
1	A	272	HIS	CB-CA-C	6.67	123.70	110.42
1	B	217	ALA	N-CA-C	6.62	118.84	110.24
1	B	151	TYR	N-CA-C	6.50	120.47	110.20
1	A	214	PRO	CA-N-CD	-6.48	102.42	111.50
1	A	271	ARG	N-CA-CB	6.47	119.05	110.25
1	B	152	GLY	N-CA-C	-6.11	102.93	112.58
1	B	108	VAL	N-CA-C	5.95	117.30	109.21
1	A	144	HIS	N-CA-C	-5.70	102.09	110.52
1	A	67	LEU	N-CA-C	-5.59	105.27	111.36
1	A	188	GLY	N-CA-C	-5.53	101.33	110.95
1	A	271	ARG	CA-C-O	5.33	127.60	122.01
1	A	110	VAL	N-CA-C	5.25	115.66	107.99
1	A	293	SER	N-CA-C	5.23	117.43	108.90
1	A	92	LYS	N-CA-C	-5.22	105.67	111.36
1	B	156	VAL	N-CA-C	5.08	115.43	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	GLY	Mainchain

5.2 Too-close contacts [i](#)

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	1853	0	1818	160	0
1	B	1853	0	1818	126	0
2	A	14	0	0	0	0
2	B	35	0	0	1	0
All	All	3755	0	3636	269	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 37.

All (269) 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:A:213:ILE:CG1	1:A:214:PRO:HD3	1.80	1.11
1:A:195:ILE:HG13	1:A:196:GLN:H	1.17	1.06
1:A:213:ILE:HG13	1:A:214:PRO:HD3	1.06	1.02
1:A:214:PRO:HD2	1:A:221:PHE:HZ	1.23	0.99
1:A:214:PRO:HD2	1:A:221:PHE:CZ	1.98	0.98
1:A:160:LYS:HA	1:A:213:ILE:HG12	1.45	0.97
1:A:215:VAL:HG12	1:B:226:VAL:HB	1.48	0.95
1:A:259:MET:HE2	1:B:259:MET:HE2	1.49	0.95
1:A:213:ILE:HG13	1:A:214:PRO:CD	1.96	0.95
1:B:258:ILE:HD13	1:B:258:ILE:N	1.83	0.94
1:B:272:HIS:ND1	1:B:273:PHE:N	2.20	0.89
1:B:133:ASN:H	1:B:133:ASN:HD22	1.25	0.83
1:B:258:ILE:CD1	1:B:299:LEU:HB3	2.11	0.81
1:B:258:ILE:HD13	1:B:258:ILE:H	1.42	0.80
1:A:215:VAL:HG21	1:B:229:TYR:CE1	2.15	0.80
1:B:237:ARG:HD2	1:B:237:ARG:H	1.46	0.80
1:A:192:ASP:HB2	1:A:287:GLN:HE22	1.44	0.79
1:B:131:HIS:H	1:B:173:THR:HG21	1.45	0.79
1:B:226:VAL:HG23	1:B:288:ILE:O	1.82	0.79
1:A:191:LEU:HD12	1:A:191:LEU:H	1.48	0.78
1:B:131:HIS:N	1:B:173:THR:HG21	1.98	0.78
1:A:225:THR:HG22	1:A:226:VAL:N	1.99	0.78
1:B:258:ILE:CD1	1:B:258:ILE:H	1.96	0.78
1:B:234:SER:HB3	1:B:237:ARG:CD	2.15	0.77
1:A:191:LEU:HD22	1:A:285:LYS:HG3	1.67	0.77
1:B:84:MET:HE3	1:B:144:HIS:HB3	1.66	0.77
1:B:296:THR:O	1:B:297:LYS:HG2	1.85	0.76
1:A:275:SER:HB3	1:A:285:LYS:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:ILE:HD12	1:B:299:LEU:HB3	1.69	0.74
1:B:272:HIS:CG	1:B:273:PHE:H	2.04	0.74
1:A:120:GLN:NE2	1:A:162:LEU:HD23	2.04	0.73
1:B:258:ILE:N	1:B:258:ILE:CD1	2.51	0.73
1:A:195:ILE:HG13	1:A:196:GLN:N	1.98	0.73
1:A:274:GLU:HA	1:A:286:LYS:NZ	2.05	0.71
1:B:237:ARG:HD2	1:B:237:ARG:N	2.05	0.71
1:A:191:LEU:CD2	1:A:285:LYS:HG3	2.21	0.70
1:B:133:ASN:H	1:B:133:ASN:ND2	1.90	0.69
1:A:192:ASP:H	1:A:285:LYS:HB3	1.57	0.69
1:A:149:VAL:HG22	1:A:156:VAL:HG22	1.73	0.68
1:B:233:ARG:HA	1:B:239:SER:HA	1.75	0.68
1:A:272:HIS:O	1:A:273:PHE:C	2.33	0.67
1:B:279:ASP:OD1	1:B:280:PRO:HD2	1.94	0.67
1:B:226:VAL:HG23	1:B:288:ILE:HG23	1.76	0.66
1:A:257:GLU:OE2	1:A:258:ILE:HG22	1.95	0.65
1:A:271:ARG:HG3	1:A:272:HIS:HB2	1.77	0.65
1:B:269:VAL:HG21	1:B:289:PRO:CD	2.28	0.64
1:A:118:LYS:O	1:A:122:LEU:HB2	1.98	0.64
1:B:228:GLY:C	1:B:229:TYR:HD1	2.04	0.64
1:A:184:GLN:O	1:A:184:GLN:HG3	1.97	0.64
1:A:191:LEU:HD12	1:A:191:LEU:N	2.13	0.64
1:B:136:CYS:HB3	1:B:178:PRO:HG2	1.80	0.64
1:A:189:THR:O	1:A:190:GLU:HB2	1.98	0.63
1:B:269:VAL:HG21	1:B:289:PRO:HD3	1.80	0.62
1:B:258:ILE:HD11	1:B:299:LEU:HB3	1.81	0.62
1:A:274:GLU:HA	1:A:286:LYS:CD	2.30	0.61
1:B:133:ASN:HD22	1:B:133:ASN:N	1.90	0.61
1:A:163:THR:HB	1:A:214:PRO:HG2	1.81	0.61
1:B:167:ARG:HB3	1:B:216:GLU:OE2	2.00	0.61
1:A:275:SER:O	1:A:284:GLU:HA	2.02	0.60
1:A:160:LYS:HA	1:A:213:ILE:CG1	2.25	0.60
1:A:225:THR:O	1:A:226:VAL:HB	2.01	0.59
1:B:234:SER:HB3	1:B:237:ARG:HD2	1.84	0.59
1:A:213:ILE:CB	1:A:214:PRO:HD3	2.26	0.59
1:B:84:MET:HE3	1:B:144:HIS:CB	2.33	0.59
1:A:62:MET:HB2	1:A:303:GLN:HA	1.84	0.59
1:A:233:ARG:HG3	1:A:234:SER:N	2.18	0.58
1:A:231:SER:HA	1:A:287:GLN:HG3	1.86	0.58
1:A:120:GLN:HE21	1:A:157:THR:HG21	1.68	0.58
1:A:276:GLN:HG2	1:A:277:SER:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ALA:O	1:B:248:ILE:HG12	2.04	0.58
1:B:186:CYS:SG	1:B:231:SER:HB3	2.43	0.58
1:A:192:ASP:CB	1:A:287:GLN:HE22	2.15	0.58
1:B:226:VAL:CG2	1:B:288:ILE:HG23	2.33	0.58
1:A:62:MET:HB3	1:A:303:GLN:HG2	1.85	0.58
1:B:163:THR:HG22	1:B:181:PHE:CE2	2.39	0.57
1:B:269:VAL:HG21	1:B:289:PRO:CG	2.34	0.57
1:A:215:VAL:O	1:A:216:GLU:HG2	2.04	0.57
1:A:233:ARG:CB	1:A:239:SER:HA	2.35	0.57
1:B:146:GLU:O	1:B:147:GLU:C	2.47	0.57
1:A:64:PHE:HB3	1:A:133:ASN:O	2.04	0.57
1:A:167:ARG:HG3	1:A:216:GLU:CG	2.35	0.57
1:A:274:GLU:HA	1:A:286:LYS:HD3	1.86	0.57
1:A:229:TYR:HE1	1:B:215:VAL:O	1.86	0.57
1:B:131:HIS:H	1:B:173:THR:CG2	2.16	0.57
1:A:97:LEU:HD13	1:A:140:ILE:HG21	1.86	0.57
1:A:239:SER:O	1:A:243:GLN:HG3	2.05	0.56
1:A:150:ILE:HD11	1:A:162:LEU:HD11	1.86	0.56
1:A:60:TYR:CD1	1:A:178:PRO:HD3	2.40	0.56
1:A:160:LYS:CA	1:A:213:ILE:HG12	2.28	0.56
1:A:233:ARG:HB2	1:A:239:SER:HA	1.87	0.56
1:A:145:GLY:HA3	1:A:185:ALA:HB1	1.88	0.55
1:A:227:PRO:O	1:B:212:LYS:HD2	2.06	0.55
1:B:232:TRP:CD1	1:B:275:SER:HG	2.25	0.55
1:A:225:THR:HG22	1:A:226:VAL:H	1.70	0.55
1:A:62:MET:CB	1:A:303:GLN:HA	2.37	0.54
1:A:215:VAL:HG21	1:B:229:TYR:HE1	1.70	0.54
1:A:271:ARG:HG3	1:A:272:HIS:N	2.23	0.54
1:A:229:TYR:CE1	1:B:215:VAL:O	2.61	0.54
1:A:167:ARG:HG3	1:A:216:GLU:HG3	1.90	0.54
1:A:213:ILE:CG1	1:A:214:PRO:CD	2.70	0.54
1:A:163:THR:HG22	1:A:181:PHE:CE2	2.43	0.54
1:A:226:VAL:HG11	1:B:215:VAL:HB	1.88	0.54
1:A:212:LYS:NZ	1:B:226:VAL:HG13	2.23	0.54
1:B:234:SER:HB2	1:B:238:GLY:O	2.09	0.53
1:A:163:THR:CB	1:A:214:PRO:HG2	2.39	0.53
1:A:294:MET:SD	1:B:290:CYS:HB2	2.48	0.53
1:B:191:LEU:HG	1:B:281:HIS:HB3	1.90	0.53
1:A:226:VAL:HG12	1:A:229:TYR:HB2	1.89	0.53
1:A:192:ASP:HB2	1:A:287:GLN:NE2	2.17	0.53
1:A:229:TYR:CZ	1:B:215:VAL:HG23	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:SER:H	1:A:286:LYS:HZ2	1.57	0.52
1:B:184:GLN:HE22	1:B:231:SER:CB	2.22	0.52
1:A:226:VAL:HG23	1:A:290:CYS:HB2	1.90	0.52
1:A:167:ARG:HD3	1:A:214:PRO:HB3	1.92	0.52
1:A:259:MET:HE2	1:B:259:MET:CE	2.31	0.52
1:A:270:ALA:C	1:A:271:ARG:O	2.47	0.52
1:B:113:ASP:HB3	1:B:153:LYS:HE2	1.90	0.52
1:A:234:SER:C	1:A:236:GLY:H	2.18	0.52
1:B:124:LYS:O	1:B:128:GLU:HG3	2.10	0.52
1:A:229:TYR:CD1	1:A:287:GLN:OE1	2.63	0.52
1:A:87:ARG:O	1:A:90:THR:HG22	2.11	0.51
1:B:277:SER:HB3	1:B:282:PHE:O	2.10	0.51
1:B:174:LEU:HD23	1:B:177:LYS:HD2	1.92	0.51
1:A:111:TYR:CG	1:A:122:LEU:HD21	2.46	0.51
1:B:160:LYS:HA	1:B:214:PRO:HD3	1.93	0.51
1:A:167:ARG:NH2	1:A:213:ILE:HD11	2.26	0.50
1:A:270:ALA:HB2	1:A:288:ILE:CD1	2.41	0.50
1:B:163:THR:OG1	1:B:214:PRO:HG2	2.12	0.50
1:A:276:GLN:HA	1:A:284:GLU:H	1.76	0.50
1:A:74:ASN:C	1:A:74:ASN:ND2	2.70	0.50
1:B:93:ASP:HB3	1:B:242:VAL:HG11	1.94	0.50
1:B:228:GLY:C	1:B:229:TYR:CD1	2.89	0.50
1:B:59:GLN:C	1:B:297:LYS:HE3	2.37	0.49
1:B:237:ARG:CD	1:B:237:ARG:N	2.72	0.49
1:B:275:SER:O	1:B:277:SER:N	2.45	0.49
1:A:74:ASN:C	1:A:74:ASN:HD22	2.18	0.49
1:A:191:LEU:HB2	1:A:285:LYS:CD	2.43	0.49
1:B:132:THR:N	1:B:173:THR:CG2	2.75	0.49
1:A:225:THR:HA	1:A:231:SER:HB3	1.94	0.49
1:B:184:GLN:HE22	1:B:231:SER:HB3	1.78	0.49
1:A:191:LEU:HB2	1:A:285:LYS:HD2	1.95	0.49
1:B:277:SER:HB3	1:B:283:HIS:HA	1.95	0.49
1:A:60:TYR:CD2	1:A:297:LYS:HB2	2.48	0.49
1:A:149:VAL:HG23	1:A:157:THR:C	2.38	0.49
1:B:230:TYR:CD1	1:B:230:TYR:C	2.90	0.49
1:B:84:MET:HE2	1:B:151:TYR:CZ	2.48	0.49
1:B:136:CYS:CB	1:B:178:PRO:HG2	2.41	0.49
1:B:274:GLU:HB3	1:B:284:GLU:OE2	2.13	0.49
1:A:230:TYR:C	1:A:230:TYR:CD1	2.92	0.48
1:A:249:LEU:C	1:A:251:GLU:H	2.21	0.48
1:A:276:GLN:HG2	1:A:277:SER:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:HA	1:A:138:ALA:O	2.12	0.48
1:A:274:GLU:HA	1:A:286:LYS:HZ2	1.77	0.48
1:B:112:ASN:HB3	2:B:6:HOH:O	2.12	0.48
1:A:191:LEU:HD11	1:A:282:PHE:HD1	1.78	0.48
1:B:131:HIS:N	1:B:173:THR:CG2	2.73	0.48
1:A:62:MET:HE2	1:A:300:TYR:O	2.13	0.48
1:B:269:VAL:CG2	1:B:289:PRO:HD3	2.44	0.48
1:B:274:GLU:HB3	1:B:284:GLU:HG2	1.94	0.48
1:A:160:LYS:HZ3	1:A:160:LYS:HB3	1.79	0.47
1:B:296:THR:C	1:B:297:LYS:HG2	2.39	0.47
1:A:240:TRP:CZ3	1:A:273:PHE:HB3	2.49	0.47
1:B:234:SER:CB	1:B:237:ARG:HD3	2.44	0.47
1:A:116:CYS:HB3	1:A:157:THR:OG1	2.14	0.47
1:A:191:LEU:HD22	1:A:285:LYS:HE3	1.95	0.47
1:A:272:HIS:O	1:A:273:PHE:O	2.32	0.47
1:B:84:MET:HE3	1:B:144:HIS:CG	2.49	0.47
1:A:160:LYS:NZ	1:A:160:LYS:H	2.13	0.47
1:B:219:PHE:O	1:B:294:MET:HB2	2.15	0.47
1:A:168:GLY:N	1:A:216:GLU:HG3	2.30	0.47
1:A:274:GLU:O	1:A:274:GLU:HG2	2.13	0.47
1:A:175:LEU:O	1:A:176:GLU:HB2	2.14	0.46
1:B:191:LEU:HG	1:B:281:HIS:CB	2.45	0.46
1:A:168:GLY:H	1:A:216:GLU:HG3	1.81	0.46
1:B:167:ARG:O	1:B:168:GLY:C	2.57	0.46
1:B:95:GLU:O	1:B:99:LYS:HG3	2.14	0.46
1:B:260:GLN:O	1:B:264:ARG:HG3	2.15	0.46
1:A:84:MET:HB3	1:A:144:HIS:CD2	2.51	0.46
1:B:59:GLN:CB	1:B:298:GLU:HB2	2.46	0.46
1:A:115:SER:HA	1:A:153:LYS:HG2	1.97	0.46
1:A:121:ASP:OD2	1:A:125:LYS:HE3	2.15	0.46
1:A:226:VAL:HG13	1:B:215:VAL:HG11	1.96	0.46
1:B:213:ILE:HB	1:B:214:PRO:HD2	1.98	0.46
1:A:167:ARG:HG3	1:A:216:GLU:HG2	1.98	0.46
1:A:184:GLN:HA	1:A:224:SER:HB3	1.99	0.45
1:A:240:TRP:CE3	1:A:273:PHE:HB3	2.51	0.45
1:B:267:ASP:O	1:B:270:ALA:HB3	2.16	0.45
1:A:270:ALA:HB2	1:A:288:ILE:HD13	1.97	0.45
1:B:163:THR:OG1	1:B:214:PRO:CD	2.63	0.45
1:A:251:GLU:HG2	1:A:252:HIS:CD2	2.52	0.45
1:B:232:TRP:HE3	1:B:233:ARG:N	2.14	0.45
1:A:193:ASP:N	1:A:285:LYS:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:O	1:B:249:LEU:HB2	2.17	0.45
1:B:59:GLN:HB3	1:B:298:GLU:HB2	1.97	0.45
1:B:277:SER:CB	1:B:282:PHE:O	2.65	0.45
1:A:225:THR:CG2	1:A:226:VAL:N	2.68	0.45
1:B:212:LYS:O	1:B:213:ILE:HG23	2.16	0.45
1:A:118:LYS:HB2	1:A:118:LYS:NZ	2.32	0.45
1:B:98:PHE:CD1	1:B:98:PHE:C	2.93	0.45
1:B:272:HIS:CG	1:B:273:PHE:N	2.77	0.45
1:A:278:ASP:OD1	1:A:278:ASP:O	2.34	0.44
1:A:215:VAL:HG21	1:B:229:TYR:CZ	2.51	0.44
1:A:226:VAL:HG22	1:A:227:PRO:HD2	2.00	0.44
1:B:226:VAL:HG22	1:B:290:CYS:HB3	2.00	0.44
1:A:267:ASP:HB2	1:B:296:THR:O	2.17	0.44
1:B:192:ASP:HB3	1:B:193:ASP:H	1.66	0.44
1:A:136:CYS:CB	1:A:178:PRO:HG2	2.48	0.44
1:B:149:VAL:HG13	1:B:156:VAL:HG22	2.00	0.44
1:B:230:TYR:HE1	1:B:232:TRP:HA	1.82	0.44
1:A:177:LYS:O	1:A:179:LYS:HE2	2.18	0.43
1:B:143:SER:OG	1:B:144:HIS:N	2.51	0.43
1:A:158:PRO:HG2	1:A:161:ASP:OD2	2.18	0.43
1:A:225:THR:O	1:A:226:VAL:CB	2.66	0.43
1:A:191:LEU:HD21	1:A:282:PHE:HB3	1.99	0.43
1:A:226:VAL:HG11	1:B:215:VAL:CB	2.48	0.43
1:B:132:THR:N	1:B:173:THR:HG22	2.34	0.43
1:A:233:ARG:HB3	1:A:239:SER:HA	2.01	0.43
1:B:75:ASN:HB2	1:B:143:SER:HB2	2.01	0.43
1:A:213:ILE:HG23	1:A:214:PRO:HD3	2.00	0.43
1:B:148:ASN:HD22	1:B:148:ASN:C	2.27	0.43
1:B:257:GLU:CD	1:B:258:ILE:HD13	2.44	0.43
1:B:272:HIS:O	1:B:273:PHE:HB2	2.19	0.43
1:A:287:GLN:OE1	1:A:287:GLN:HA	2.18	0.42
1:B:116:CYS:HA	1:B:119:MET:HE2	2.01	0.42
1:A:149:VAL:HG21	1:A:156:VAL:HG13	2.01	0.42
1:A:257:GLU:OE1	1:A:259:MET:HB2	2.19	0.42
1:A:263:THR:O	1:A:266:ASN:HB2	2.19	0.42
1:A:271:ARG:CG	1:A:272:HIS:N	2.73	0.42
1:A:252:HIS:HA	1:A:255:ASP:OD1	2.19	0.42
1:B:158:PRO:HG2	1:B:161:ASP:HB2	2.00	0.42
1:A:178:PRO:HG3	1:A:299:LEU:HD13	2.02	0.42
1:B:121:ASP:OD1	1:B:125:LYS:HE3	2.20	0.42
1:B:229:TYR:CD1	1:B:229:TYR:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASN:O	1:A:113:ASP:C	2.63	0.42
1:B:273:PHE:O	1:B:274:GLU:HB2	2.19	0.42
1:A:136:CYS:HB3	1:A:178:PRO:HG2	2.01	0.42
1:A:226:VAL:HG11	1:A:229:TYR:CD1	2.55	0.42
1:B:246:CYS:O	1:B:250:GLU:HG2	2.19	0.42
1:A:84:MET:HE2	1:A:144:HIS:HB3	2.01	0.41
1:A:121:ASP:CG	1:A:125:LYS:HE3	2.45	0.41
1:A:187:ARG:HG3	1:A:230:TYR:CE2	2.55	0.41
1:A:191:LEU:H	1:A:191:LEU:CD1	2.25	0.41
1:A:191:LEU:HD22	1:A:282:PHE:HA	2.02	0.41
1:A:136:CYS:HB2	1:A:178:PRO:O	2.21	0.41
1:A:214:PRO:O	1:A:294:MET:HE3	2.21	0.41
1:B:213:ILE:HD12	1:B:213:ILE:O	2.20	0.41
1:B:229:TYR:HD1	1:B:229:TYR:N	2.17	0.41
1:A:271:ARG:O	1:A:272:HIS:C	2.64	0.41
1:B:254:LYS:N	1:B:254:LYS:HD2	2.36	0.41
1:A:163:THR:HG22	1:A:181:PHE:CZ	2.54	0.41
1:B:84:MET:HE2	1:B:151:TYR:CE1	2.55	0.41
1:A:192:ASP:CB	1:A:287:GLN:NE2	2.80	0.41
1:A:215:VAL:HG11	1:B:229:TYR:CD1	2.55	0.41
1:B:100:CYS:SG	1:B:249:LEU:HD23	2.61	0.41
1:B:226:VAL:O	1:B:227:PRO:C	2.64	0.41
1:A:121:ASP:OD1	1:A:125:LYS:HE3	2.21	0.41
1:A:246:CYS:O	1:A:250:GLU:HB2	2.20	0.41
1:A:213:ILE:CG2	1:A:214:PRO:HD3	2.51	0.40
1:A:266:ASN:OD1	1:A:289:PRO:HB2	2.22	0.40
1:A:283:HIS:CE1	1:A:284:GLU:HG2	2.55	0.40
1:A:184:GLN:HA	1:A:224:SER:CB	2.51	0.40
1:A:195:ILE:HG23	1:A:196:GLN:N	2.36	0.40
1:B:150:ILE:HG12	1:B:151:TYR:N	2.36	0.40
1:B:60:TYR:CD1	1:B:178:PRO:HD3	2.56	0.40
1:B:84:MET:HB3	1:B:144:HIS:CD2	2.56	0.40
1:A:73:ILE:HD12	1:A:141:LEU:CD2	2.52	0.40
1:B:163:THR:OG1	1:B:214:PRO:CG	2.70	0.40
1:A:180:LEU:HD13	1:A:180:LEU:N	2.37	0.40
1:B:123:LEU:HD12	1:B:162:LEU:HD22	2.02	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	102/253 (40%)	78 (76%)	18 (18%)	6 (6%)	1	1
1	B	105/253 (42%)	88 (84%)	11 (10%)	6 (6%)	1	1
All	All	207/506 (41%)	166 (80%)	29 (14%)	12 (6%)	1	1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	GLU
1	B	190	GLU
1	B	276	GLN
1	A	193	ASP
1	B	272	HIS
1	B	227	PRO
1	B	273	PHE
1	A	226	VAL
1	A	227	PRO
1	A	235	PRO
1	B	274	GLU
1	A	195	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	119/221 (54%)	117 (98%)	2 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	171/221 (77%)	156 (91%)	15 (9%)	9	21
All	All	290/442 (66%)	273 (94%)	17 (6%)	18	38

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	118	LYS
1	B	57	THR
1	B	67	LEU
1	B	95	GLU
1	B	98	PHE
1	B	133	ASN
1	B	148	ASN
1	B	149	VAL
1	B	150	ILE
1	B	156	VAL
1	B	170	ARG
1	B	237	ARG
1	B	248	ILE
1	B	258	ILE
1	B	279	ASP
1	B	287	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	120	GLN
1	A	276	GLN
1	A	281	HIS
1	A	287	GLN
1	B	59	GLN
1	B	74	ASN
1	B	88	ASN
1	B	112	ASN
1	B	133	ASN
1	B	148	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

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.