



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:39 AM UTC

PDB ID : 1FC9 / pdb_00001fc9
Title : PHOTOSYSTEM II D1 C-TERMINAL PROCESSING PROTEASE
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Deposited on : 2000-07-18
Resolution : 1.90 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

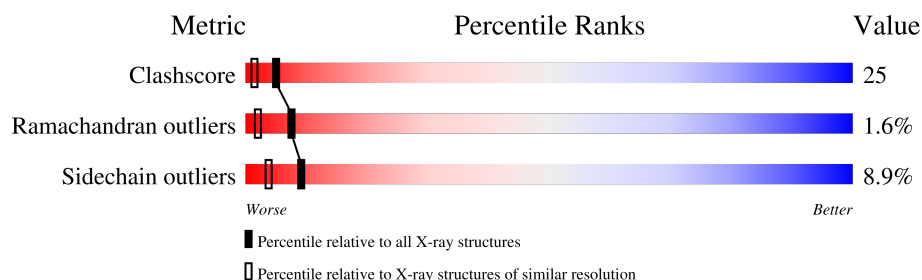
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	388	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3065 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 PHOTOSYSTEM II D1 PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2853	1786	505	558	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	MET	-	initiating methionine	UNP O04073

- Molecule 2 is water.

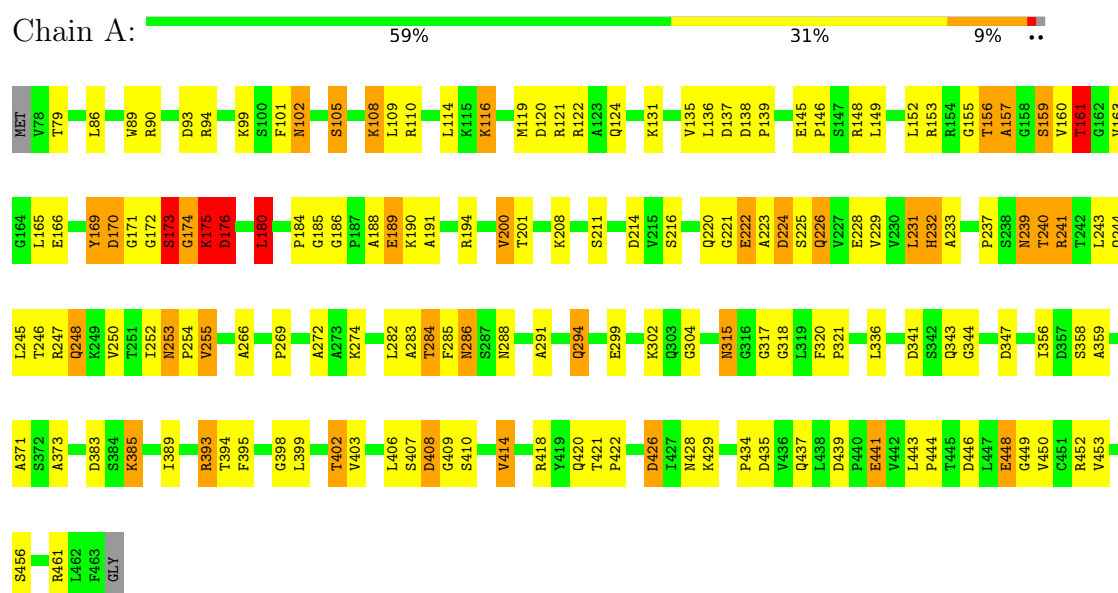
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	212	Total	O	0	0
			212	212		

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: PHOTOSYSTEM II D1 PROTEASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.60Å 63.10Å 60.70Å 90.00° 119.80° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.90)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.191 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3065	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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	1.29	3/2894 (0.1%)	1.82	55/3938 (1.4%)

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	A	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	414	VAL	C-O	-6.33	1.17	1.24
1	A	170	ASP	N-CA	5.92	1.53	1.46
1	A	200	VAL	CA-CB	-5.30	1.48	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ASP	CA-CB-CG	-17.43	95.17	112.60
1	A	174	GLY	N-CA-C	-9.64	100.43	112.77
1	A	269	PRO	N-CA-CB	9.22	108.01	103.22
1	A	173	SER	N-CA-C	9.08	124.96	108.17
1	A	407	SER	CA-C-N	8.53	131.71	120.28
1	A	407	SER	C-N-CA	8.53	131.71	120.28
1	A	176	ASP	N-CA-C	8.51	128.92	110.80
1	A	222	GLU	N-CA-CB	8.36	122.98	109.69
1	A	356	ILE	CB-CA-C	-7.96	103.66	111.30
1	A	409	GLY	N-CA-C	-7.87	104.69	114.92
1	A	356	ILE	N-CA-C	-7.81	105.58	111.90
1	A	269	PRO	O-C-N	7.74	124.79	121.15
1	A	105	SER	N-CA-CB	7.54	121.58	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	LYS	CA-C-N	6.99	134.90	121.54
1	A	175	LYS	C-N-CA	6.99	134.90	121.54
1	A	159	SER	N-CA-C	-6.98	104.38	113.17
1	A	239	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	222	GLU	CB-CA-C	6.81	120.66	109.70
1	A	224	ASP	N-CA-C	6.68	121.20	113.38
1	A	408	ASP	CB-CA-C	-6.66	99.73	110.79
1	A	269	PRO	CB-CA-C	-6.50	105.06	111.17
1	A	184	PRO	N-CA-CB	6.42	109.99	103.25
1	A	170	ASP	N-CA-C	6.26	119.35	109.96
1	A	441	GLU	CB-CG-CD	-6.26	101.96	112.60
1	A	184	PRO	CB-CA-C	6.14	121.69	111.56
1	A	255	VAL	N-CA-C	6.09	117.47	108.45
1	A	448	GLU	N-CA-CB	6.06	119.03	109.82
1	A	169	TYR	CA-C-O	-5.98	114.37	121.66
1	A	131	LYS	CA-C-O	5.88	126.79	120.55
1	A	407	SER	O-C-N	5.87	128.90	122.20
1	A	402	THR	CA-C-N	-5.82	115.60	122.93
1	A	402	THR	C-N-CA	-5.82	115.60	122.93
1	A	116	LYS	N-CA-C	5.67	120.48	113.50
1	A	200	VAL	CB-CA-C	-5.65	104.48	111.94
1	A	102	ASN	CA-CB-CG	5.63	118.23	112.60
1	A	395	PHE	N-CA-C	5.62	117.85	111.11
1	A	359	ALA	N-CA-C	5.55	120.54	113.55
1	A	456	SER	CA-C-N	5.50	128.41	120.38
1	A	456	SER	C-N-CA	5.50	128.41	120.38
1	A	347	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	120	ASP	N-CA-CB	5.47	119.04	110.46
1	A	161	THR	N-CA-CB	-5.43	102.09	111.55
1	A	121	ARG	CA-CB-CG	5.42	124.95	114.10
1	A	226	GLN	N-CA-C	5.42	118.54	110.14
1	A	160	VAL	N-CA-CB	5.38	116.92	110.31
1	A	174	GLY	O-C-N	5.27	127.30	122.19
1	A	138	ASP	CA-C-O	5.21	124.52	119.62
1	A	406	LEU	N-CA-CB	5.19	118.65	110.56
1	A	232	HIS	CA-CB-CG	5.17	118.97	113.80
1	A	371	ALA	N-CA-C	5.16	117.04	109.24
1	A	180	LEU	N-CA-C	-5.07	103.80	111.56
1	A	408	ASP	CB-CG-OD2	-5.07	106.75	118.40
1	A	344	GLY	N-CA-C	-5.05	103.82	110.29
1	A	119	MET	CA-C-N	-5.03	112.71	122.06
1	A	119	MET	C-N-CA	-5.03	112.71	122.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	222	GLU	CA

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	2853	0	2893	143	0
2	A	212	0	0	12	1
All	All	3065	0	2893	143	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (143) 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:161:THR:HG21	1:A:223:ALA:HA	1.23	1.12
1:A:385:LYS:HA	1:A:385:LYS:HE2	1.30	1.10
1:A:434:PRO:HG2	1:A:437:GLN:HE22	1.20	1.04
1:A:232:HIS:HB3	1:A:240:THR:HG22	1.48	0.95
1:A:434:PRO:HG2	1:A:437:GLN:NE2	1.85	0.92
1:A:175:LYS:HD3	1:A:208:LYS:HD2	1.52	0.91
1:A:408:ASP:HB3	1:A:410:SER:H	1.33	0.90
1:A:228:GLU:HB2	1:A:244:GLN:NE2	1.87	0.90
1:A:285:PHE:HB2	1:A:317:GLY:O	1.79	0.82
1:A:393:ARG:HD3	1:A:394:THR:O	1.81	0.80
1:A:255:VAL:HG22	1:A:282:LEU:HD22	1.64	0.79
1:A:229:VAL:HG12	1:A:231:LEU:HD13	1.67	0.76
1:A:175:LYS:CD	1:A:208:LYS:HD2	2.15	0.76
1:A:241:ARG:HG3	1:A:241:ARG:HH11	1.53	0.74
1:A:247:ARG:C	1:A:248:GLN:HG3	2.11	0.74
1:A:175:LYS:HB2	1:A:208:LYS:HD2	1.70	0.73
1:A:286:ASN:HD22	1:A:288:ASN:H	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:GLY:H	1:A:428:ASN:HD22	1.38	0.72
1:A:228:GLU:HB2	1:A:244:GLN:HE22	1.53	0.72
1:A:175:LYS:HD3	1:A:208:LYS:CD	2.19	0.71
1:A:175:LYS:HG2	1:A:208:LYS:HZ2	1.54	0.71
1:A:266:ALA:HB1	1:A:461:ARG:HG2	1.71	0.71
1:A:175:LYS:HG2	1:A:208:LYS:NZ	2.06	0.70
1:A:224:ASP:HA	1:A:247:ARG:O	1.90	0.70
1:A:149:LEU:O	1:A:153:ARG:HG3	1.91	0.70
1:A:286:ASN:ND2	1:A:288:ASN:H	1.91	0.69
1:A:161:THR:CG2	1:A:223:ALA:HA	2.13	0.68
1:A:241:ARG:NH1	1:A:243:LEU:HD21	2.09	0.68
1:A:94:ARG:NH1	2:A:637:HOH:O	2.26	0.67
1:A:336:LEU:O	1:A:422:PRO:HG3	1.95	0.66
1:A:116:LYS:NZ	2:A:534:HOH:O	2.29	0.65
1:A:402:THR:HG22	1:A:403:VAL:N	2.10	0.65
1:A:389:ILE:O	1:A:435:ASP:N	2.28	0.65
1:A:315:ASN:C	1:A:315:ASN:HD22	2.05	0.65
1:A:299:GLU:O	1:A:302:LYS:HB3	1.98	0.63
1:A:175:LYS:HD3	1:A:208:LYS:CE	2.30	0.62
1:A:174:GLY:O	1:A:175:LYS:HG3	2.00	0.61
1:A:232:HIS:HD2	1:A:233:ALA:O	1.83	0.61
1:A:255:VAL:HG22	1:A:282:LEU:CD2	2.30	0.60
1:A:152:LEU:HD23	2:A:574:HOH:O	2.01	0.60
1:A:161:THR:HG21	1:A:223:ALA:CA	2.14	0.59
1:A:166:GLU:CD	1:A:180:LEU:HD13	2.27	0.59
1:A:418:ARG:HD2	1:A:426:ASP:OD1	2.02	0.59
1:A:175:LYS:CB	1:A:208:LYS:HD2	2.32	0.59
1:A:439:ASP:OD1	1:A:441:GLU:HB2	2.03	0.58
1:A:274:LYS:HE2	1:A:304:GLY:O	2.03	0.58
1:A:248:GLN:O	1:A:250:VAL:HG23	2.04	0.57
1:A:286:ASN:HD22	1:A:286:ASN:C	2.13	0.57
1:A:385:LYS:HA	1:A:385:LYS:CE	2.19	0.56
1:A:146:PRO:HD3	1:A:410:SER:HB3	1.86	0.56
1:A:226:GLN:HG2	1:A:245:LEU:O	2.05	0.56
1:A:148:ARG:O	1:A:152:LEU:HD13	2.06	0.55
1:A:185:GLY:N	1:A:189:GLU:OE1	2.38	0.55
1:A:246:THR:O	1:A:248:GLN:OE1	2.25	0.54
1:A:320:PHE:HB3	1:A:321:PRO:HD3	1.89	0.54
1:A:175:LYS:CD	1:A:208:LYS:HZ3	2.21	0.53
1:A:225:SER:OG	1:A:247:ARG:HD2	2.07	0.53
1:A:402:THR:HG22	1:A:403:VAL:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:HG3	1:A:241:ARG:NH1	2.24	0.52
1:A:194:ARG:NH2	2:A:622:HOH:O	2.42	0.52
1:A:283:ALA:C	1:A:284:THR:HG22	2.35	0.52
1:A:408:ASP:HB3	1:A:410:SER:N	2.16	0.51
1:A:101:PHE:O	1:A:102:ASN:HB3	2.09	0.51
1:A:266:ALA:HA	1:A:461:ARG:HE	1.75	0.51
1:A:229:VAL:HG12	1:A:231:LEU:CD1	2.39	0.51
1:A:434:PRO:O	1:A:437:GLN:OE1	2.29	0.51
1:A:175:LYS:CG	1:A:208:LYS:HD2	2.41	0.50
1:A:216:SER:O	1:A:220:GLN:HG3	2.10	0.50
1:A:226:GLN:HG2	1:A:245:LEU:C	2.37	0.50
1:A:286:ASN:HB2	2:A:606:HOH:O	2.12	0.50
1:A:315:ASN:HD22	1:A:317:GLY:H	1.60	0.50
1:A:446:ASP:O	1:A:450:VAL:HG23	2.11	0.50
1:A:163:VAL:HB	1:A:245:LEU:HD13	1.94	0.49
1:A:93:ASP:O	1:A:99:LYS:NZ	2.42	0.49
1:A:266:ALA:O	1:A:461:ARG:HA	2.12	0.49
1:A:286:ASN:HD21	1:A:288:ASN:HB2	1.77	0.48
1:A:421:THR:HB	1:A:422:PRO:CD	2.43	0.48
1:A:175:LYS:CB	1:A:208:LYS:HG3	2.44	0.48
1:A:232:HIS:CB	1:A:240:THR:HG22	2.33	0.48
1:A:145:GLU:HG3	2:A:513:HOH:O	2.13	0.48
1:A:169:TYR:HA	1:A:176:ASP:O	2.14	0.47
1:A:266:ALA:HB1	1:A:461:ARG:CG	2.41	0.47
1:A:315:ASN:ND2	1:A:317:GLY:H	2.12	0.47
1:A:246:THR:HG22	1:A:248:GLN:HG3	1.96	0.47
1:A:86:LEU:HD21	1:A:114:LEU:HD11	1.95	0.47
1:A:105:SER:HB3	1:A:108:LYS:HB2	1.96	0.47
1:A:159:SER:O	1:A:161:THR:HG22	2.14	0.47
1:A:200:VAL:HG12	1:A:201:THR:HG23	1.96	0.47
1:A:443:LEU:HD12	1:A:453:VAL:HB	1.95	0.47
1:A:266:ALA:CB	1:A:461:ARG:NE	2.79	0.46
1:A:232:HIS:CG	1:A:237:PRO:HA	2.50	0.46
1:A:266:ALA:O	1:A:461:ARG:HG2	2.14	0.46
1:A:139:PRO:HB2	1:A:169:TYR:CZ	2.51	0.46
1:A:161:THR:HG23	1:A:221:GLY:O	2.15	0.46
1:A:246:THR:HG22	1:A:248:GLN:CG	2.46	0.46
1:A:336:LEU:C	1:A:422:PRO:HG3	2.40	0.46
1:A:402:THR:CG2	1:A:403:VAL:N	2.79	0.45
1:A:254:PRO:HA	1:A:284:THR:HG23	1.99	0.45
1:A:399:LEU:HD23	1:A:418:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:CB	1:A:208:LYS:CG	2.95	0.45
1:A:266:ALA:HB1	1:A:461:ARG:NE	2.31	0.45
1:A:139:PRO:HB2	1:A:169:TYR:CE1	2.52	0.45
1:A:173:SER:OG	1:A:175:LYS:O	2.35	0.45
1:A:266:ALA:HB2	1:A:461:ARG:NH2	2.32	0.45
1:A:186:GLY:O	1:A:190:LYS:N	2.34	0.44
1:A:420:GLN:NE2	1:A:426:ASP:OD2	2.46	0.44
1:A:317:GLY:O	1:A:373:ALA:HB3	2.17	0.44
1:A:291:ALA:O	1:A:294:GLN:NE2	2.51	0.44
1:A:341:ASP:OD1	1:A:343:GLN:N	2.45	0.44
1:A:79:THR:HB	2:A:502:HOH:O	2.19	0.43
1:A:254:PRO:HG3	1:A:288:ASN:HB2	2.00	0.43
1:A:175:LYS:HB2	1:A:208:LYS:HG3	2.01	0.43
1:A:253:ASN:ND2	1:A:255:VAL:H	2.17	0.43
1:A:191:ALA:HB1	1:A:243:LEU:HD22	2.00	0.43
1:A:175:LYS:CG	1:A:208:LYS:NZ	2.78	0.43
1:A:421:THR:HG21	2:A:490:HOH:O	2.18	0.42
1:A:136:LEU:O	1:A:137:ASP:HB2	2.19	0.42
1:A:149:LEU:HD11	1:A:153:ARG:HE	1.84	0.42
1:A:248:GLN:HE21	1:A:248:GLN:HB2	1.38	0.42
1:A:444:PRO:HG2	1:A:449:GLY:C	2.45	0.42
1:A:156:THR:O	1:A:157:ALA:HB2	2.19	0.42
1:A:302:LYS:HB2	1:A:302:LYS:HE2	1.77	0.42
1:A:429:LYS:NZ	2:A:605:HOH:O	2.52	0.42
1:A:89:TRP:NE1	1:A:110:ARG:HB2	2.35	0.42
1:A:443:LEU:CD1	1:A:453:VAL:HB	2.50	0.42
1:A:358:SER:HB2	2:A:557:HOH:O	2.18	0.41
1:A:86:LEU:O	1:A:90:ARG:HB2	2.19	0.41
1:A:341:ASP:OD1	1:A:343:GLN:HB3	2.20	0.41
1:A:153:ARG:C	1:A:155:GLY:N	2.77	0.41
1:A:175:LYS:CD	1:A:208:LYS:NZ	2.82	0.41
1:A:165:LEU:HG	1:A:188:ALA:CB	2.51	0.41
1:A:170:ASP:O	1:A:172:GLY:N	2.53	0.41
1:A:175:LYS:CE	1:A:208:LYS:HZ3	2.34	0.41
1:A:232:HIS:HE1	2:A:503:HOH:O	2.02	0.41
1:A:266:ALA:CB	1:A:461:ARG:CZ	2.99	0.41
1:A:247:ARG:O	1:A:248:GLN:HG3	2.20	0.41
1:A:253:ASN:ND2	1:A:253:ASN:C	2.79	0.41
1:A:449:GLY:HA2	1:A:452:ARG:CZ	2.51	0.41
1:A:272:ALA:HA	2:A:533:HOH:O	2.20	0.41
1:A:320:PHE:N	1:A:321:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ASP:OD2	1:A:421:THR:HB	2.21	0.40
1:A:175:LYS:HB3	1:A:208:LYS:HG3	2.03	0.40
1:A:211:SER:HG	1:A:214:ASP:H	1.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:623:HOH:O	2:A:648:HOH:O[1_556]	2.19	0.01

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	384/388 (99%)	360 (94%)	18 (5%)	6 (2%)	7 2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LYS
1	A	176	ASP
1	A	239	ASN
1	A	157	ALA
1	A	318	GLY
1	A	171	GLY

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	302/303 (100%)	275 (91%)	27 (9%)	9 4

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	109	LEU
1	A	122	ARG
1	A	124	GLN
1	A	135	VAL
1	A	156	THR
1	A	161	THR
1	A	173	SER
1	A	175	LYS
1	A	180	LEU
1	A	189	GLU
1	A	222	GLU
1	A	231	LEU
1	A	240	THR
1	A	241	ARG
1	A	248	GLN
1	A	252	ILE
1	A	253	ASN
1	A	284	THR
1	A	286	ASN
1	A	294	GLN
1	A	315	ASN
1	A	385	LYS
1	A	393	ARG
1	A	414	VAL
1	A	426	ASP
1	A	448	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	239	ASN
1	A	244	GLN

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Mol	Chain	Res	Type
1	A	253	ASN
1	A	262	ASN
1	A	286	ASN
1	A	315	ASN
1	A	428	ASN
1	A	437	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.