



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:26 am GMT

PDB ID : 1FC9  
Title : PHOTOSYSTEM II D1 C-TERMINAL PROCESSING PROTEASE  
Authors : Liao, D.I.; Qian, J.; Chisholm, D.A.; Jordan, D.B.; Diner, B.A.  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

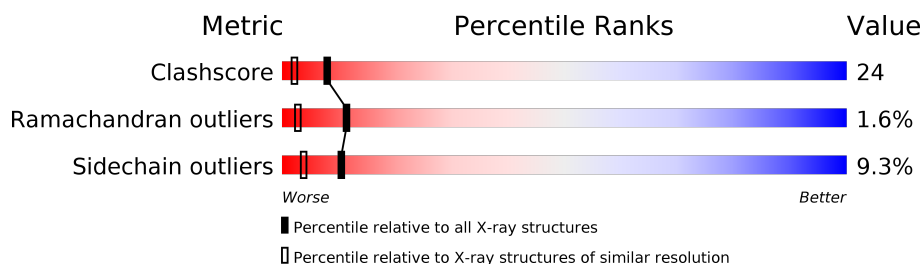
# 1 Overall quality at a glance

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	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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.

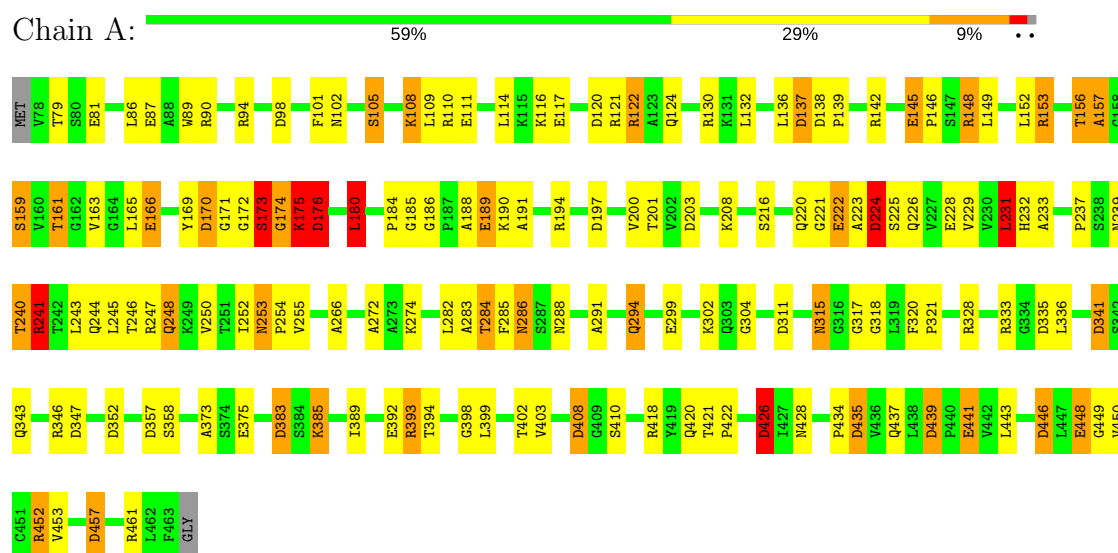
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	212	Total	O	0	0
			212	212		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	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 V. 5-E	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 <sup>2</sup> )	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	1.02	11/2894 (0.4%)	1.60	65/3938 (1.7%)

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	1	0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	GLU	CD-OE2	7.96	1.34	1.25
1	A	166	GLU	CD-OE2	7.66	1.34	1.25
1	A	145	GLU	CD-OE2	7.45	1.33	1.25
1	A	441	GLU	CD-OE2	7.36	1.33	1.25
1	A	111	GLU	CD-OE2	7.13	1.33	1.25
1	A	222	GLU	CD-OE2	6.92	1.33	1.25
1	A	375	GLU	CD-OE2	6.12	1.32	1.25
1	A	81	GLU	CD-OE2	6.07	1.32	1.25
1	A	87	GLU	CD-OE2	5.41	1.31	1.25
1	A	392	GLU	CD-OE2	5.35	1.31	1.25
1	A	117	GLU	CD-OE2	5.25	1.31	1.25

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ASP	CB-CG-OD2	-12.84	106.75	118.30
1	A	408	ASP	CB-CG-OD1	10.95	128.15	118.30
1	A	341	ASP	CB-CG-OD2	-10.52	108.83	118.30
1	A	439	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	A	357	ASP	CB-CG-OD2	-8.92	110.27	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASP	CB-CG-OD1	8.75	126.17	118.30
1	A	203	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	A	408	ASP	CA-CB-CG	-8.28	95.17	113.40
1	A	341	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	241	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	120	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	452	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	105	SER	N-CA-CB	7.39	121.58	110.50
1	A	153	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	A	446	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	383	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	A	439	ASP	CB-CG-OD1	7.20	124.78	118.30
1	A	452	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	311	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	357	ASP	CB-CG-OD1	6.94	124.54	118.30
1	A	148	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	222	GLU	N-CA-CB	6.88	122.98	110.60
1	A	346	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	176	ASP	N-CA-C	6.64	128.92	111.00
1	A	98	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	311	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	A	457	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	333	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	121	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	224	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	352	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	138	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	435	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	122	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	137	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	A	197	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	138	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	335	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	335	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	426	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	435	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	137	ASP	CB-CG-OD1	5.91	123.61	118.30
1	A	457	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	241	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	383	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	184	PRO	N-CA-CB	5.58	109.99	103.30
1	A	446	ASP	CB-CG-OD1	5.51	123.26	118.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	130	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	180	LEU	CB-CG-CD2	5.49	120.33	111.00
1	A	231	LEU	CB-CG-CD2	5.42	120.22	111.00
1	A	197	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	132	LEU	CB-CG-CD1	5.38	120.14	111.00
1	A	408	ASP	CB-CA-C	-5.33	99.73	110.40
1	A	170	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	A	175	LYS	C-N-CA	5.28	134.90	121.70
1	A	347	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	121	ARG	CA-CB-CG	5.25	124.95	113.40
1	A	173	SER	N-CA-C	5.17	124.96	111.00
1	A	222	GLU	CB-CA-C	5.13	120.66	110.40
1	A	426	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	121	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	174	GLY	N-CA-C	-5.07	100.43	113.10
1	A	328	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	142	ARG	NE-CZ-NH2	-5.03	117.79	120.30

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 [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	2853	0	2893	137	0
2	A	212	0	0	11	1
All	All	3065	0	2893	137	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 24.

All (137) 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:HH11	1:A:241:ARG:HG3	1.53	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
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:247:ARG:C	1:A:248:GLN:HG3	2.11	0.69
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:402:THR:HG22	1:A:403:VAL:N	2.10	0.67
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:389:ILE:O	1:A:435:ASP:N	2.28	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:315:ASN:HD22	1:A:315:ASN:C	2.05	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:418:ARG:HD2	1:A:426:ASP:OD1	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:LYS:HA	1:A:385:LYS:CE	2.19	0.56
1:A:226:GLN:HG2	1:A:245:LEU:O	2.05	0.56
1:A:146:PRO:HD3	1:A:410:SER:HB3	1.86	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:166:GLU:CD	1:A:180:LEU:HD13	2.27	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
1:A:241:ARG:NH1	1:A:241:ARG:HG3	2.24	0.52
1:A:286:ASN:HD22	1:A:286:ASN:C	2.13	0.52
1:A:194:ARG:NH2	2:A:622:HOH:O	2.42	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: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: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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:HD21	1:A:114:LEU:HD11	1.95	0.47
1:A:200:VAL:HG12	1:A:201:THR:HG23	1.96	0.47
1:A:283:ALA:C	1:A:284:THR:HG22	2.35	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:226:GLN:HG2	1:A:245:LEU:C	2.37	0.45
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
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:254:PRO:HG3	1:A:288:ASN:HB2	2.00	0.43
1:A:79:THR:HB	2:A:502:HOH:O	2.19	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:156:THR:O	1:A:157:ALA:HB2	2.19	0.42
1:A:302:LYS:HE2	1:A:302:LYS:HB2	1.77	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:CD	1:A:208:LYS:NZ	2.82	0.41
1:A:170:ASP:O	1:A:172:GLY:N	2.53	0.41
1:A:165:LEU:HG	1:A:188:ALA:CB	2.51	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:336:LEU:C	1:A:422:PRO:HG3	2.40	0.41
1:A:449:GLY:HA2	1:A:452:ARG:CZ	2.51	0.41
1:A:116:LYS:NZ	2:A:534:HOH:O	2.29	0.41
1:A:247:ARG:O	1:A:248:GLN:HG3	2.20	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
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

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%)	<b>11</b> <b>3</b>

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LYS
1	A	176	ASP

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	239	ASN
1	A	157	ALA
1	A	318	GLY
1	A	171	GLY

### 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	302/303 (100%)	274 (91%)	28 (9%)	10 4

All (28) 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	156	THR
1	A	159	SER
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	224	ASP
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	315	ASN
1	A	385	LYS
1	A	393	ARG
1	A	426	ASP
1	A	448	GLU
1	A	457	ASP

Some 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	232	HIS
1	A	244	GLN
1	A	248	GLN
1	A	253	ASN
1	A	286	ASN
1	A	315	ASN
1	A	428	ASN
1	A	437	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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.