



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 06:24 AM EST

PDB ID : 1Q2L  
Title : Crystal Structure of pitrilysin  
Authors : Maskos, K.; Jozic, D.; Fernandez-Catalan, C.  
Deposited on : 2003-07-25  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

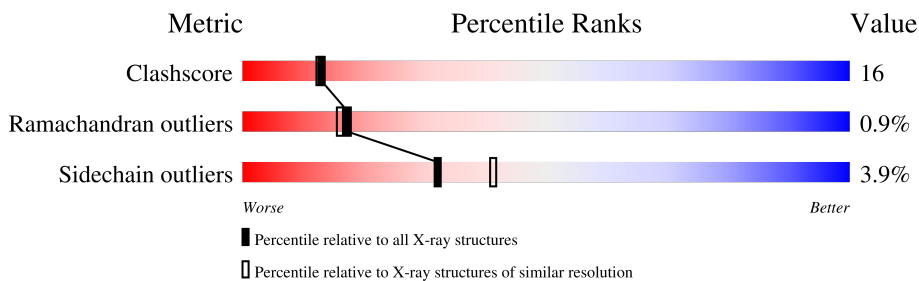
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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  $\geq 3$ , 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	939	 71% 27%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8967 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 Protease III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	937	7369	4666	1261	1411	31	92	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Pt	0	0
			6	6		

- Molecule 4 is water.

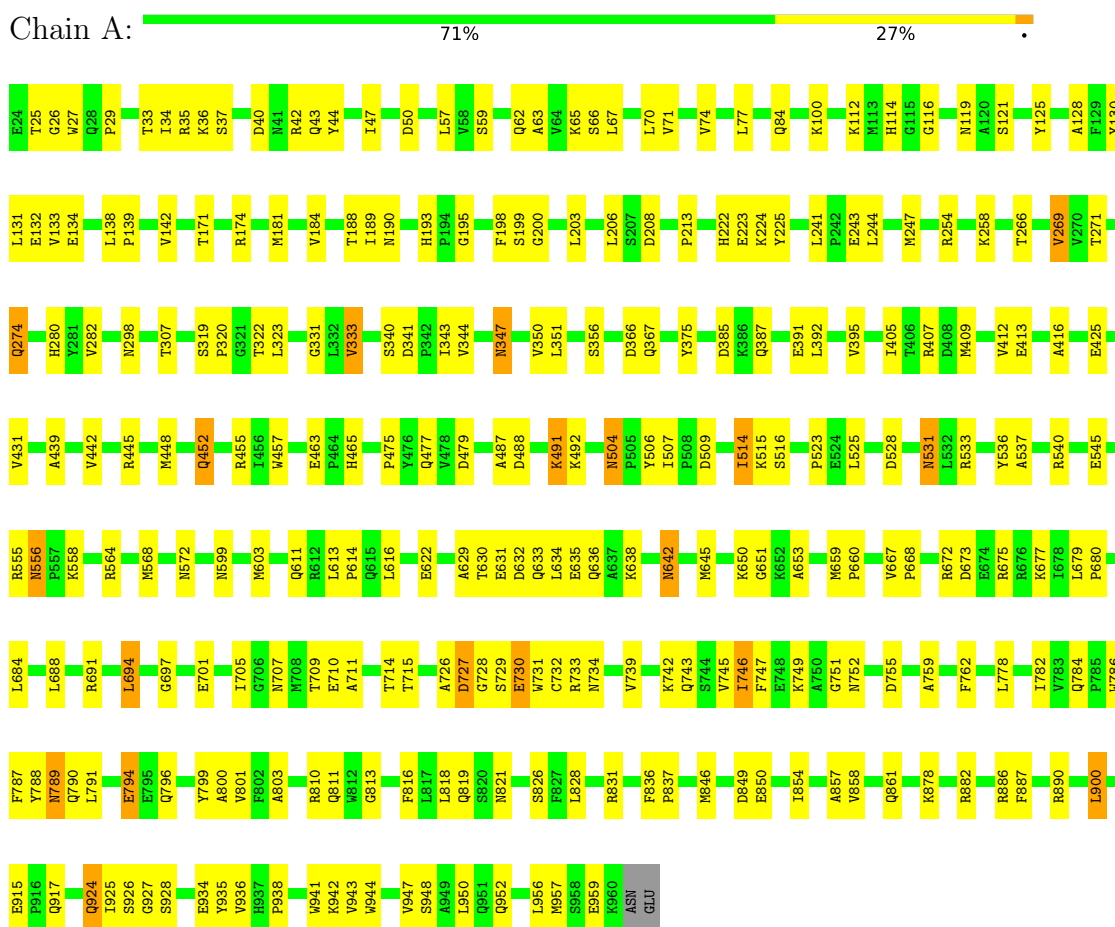
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1591	Total	O	2	0
			1591	1591		

### 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: Protease III



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	115.20Å 115.20Å 178.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.85, REFMAC	Depositor
R, $R_{free}$	0.210 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8967	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PT

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	0.34	0/7527	0.58	0/10202

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	7369	0	7281	237	0
2	A	1	0	0	0	0
3	A	6	0	0	0	0
4	A	1591	0	0	59	1
All	All	8967	0	7281	237	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 16.

All (237) 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:188:THR:HG23	1:A:455:ARG:HH22	1.27	0.97
1:A:739:VAL:H	1:A:811:GLN:HE22	1.14	0.96
1:A:514:ILE:H	1:A:707:ASN:HD21	1.16	0.91
1:A:100:LYS:HG2	4:A:3138:HOH:O	1.71	0.88
1:A:936:VAL:HG12	1:A:938:PRO:HD3	1.59	0.84
1:A:509:ASP:H	1:A:611:GLN:HE22	1.26	0.84
1:A:84:GLN:HE21	1:A:198:PHE:H	1.29	0.81
1:A:796:GLN:HE22	1:A:831:ARG:HG3	1.45	0.80
1:A:116:GLY:HA2	4:A:3314:HOH:O	1.84	0.77
1:A:959:GLU:HA	4:A:3243:HOH:O	1.85	0.77
1:A:514:ILE:H	1:A:707:ASN:ND2	1.83	0.76
1:A:672:ARG:HG3	4:A:3019:HOH:O	1.87	0.73
1:A:322:THR:HG22	4:A:2231:HOH:O	1.88	0.73
1:A:84:GLN:NE2	1:A:198:PHE:H	1.87	0.73
1:A:778:LEU:HD12	1:A:900:LEU:HD23	1.69	0.72
1:A:651:GLY:HA2	1:A:752:ASN:HD21	1.54	0.72
1:A:193:HIS:HD2	1:A:195:GLY:H	1.38	0.72
1:A:659:MET:HB3	1:A:660:PRO:HD3	1.71	0.72
1:A:439:ALA:O	1:A:442:VAL:HG22	1.90	0.71
1:A:810:ARG:NH2	4:A:3243:HOH:O	2.25	0.69
1:A:516:SER:HA	4:A:3468:HOH:O	1.92	0.68
1:A:271:THR:H	1:A:274:GLN:HE21	1.40	0.68
1:A:298:ASN:HD21	1:A:343:ILE:HG22	1.58	0.68
1:A:67:LEU:HB2	1:A:412:VAL:HG11	1.76	0.68
1:A:739:VAL:H	1:A:811:GLN:NE2	1.88	0.68
1:A:786:TRP:O	1:A:789:ASN:HB3	1.94	0.68
1:A:193:HIS:CD2	1:A:195:GLY:H	2.12	0.67
1:A:271:THR:H	1:A:274:GLN:NE2	1.92	0.67
1:A:171:THR:O	1:A:174:ARG:HG2	1.94	0.67
1:A:282:VAL:HB	1:A:475:PRO:HG2	1.76	0.67
1:A:367:GLN:HE21	1:A:492:LYS:HD3	1.61	0.66
1:A:200:GLY:N	4:A:3322:HOH:O	1.99	0.65
1:A:322:THR:HG22	1:A:323:LEU:N	2.11	0.65
1:A:347:ASN:H	1:A:347:ASN:HD22	1.42	0.65
1:A:672:ARG:NH1	1:A:675:ARG:HH12	1.95	0.65
1:A:836:PHE:HB2	1:A:837:PRO:HD3	1.78	0.65
1:A:794:GLU:HB3	1:A:796:GLN:HG3	1.77	0.65
1:A:784:GLN:HA	1:A:803:ALA:HB3	1.78	0.64
1:A:751:GLY:H	1:A:927:GLY:H	1.44	0.64
1:A:710:GLU:O	1:A:714:THR:HG23	1.98	0.64
1:A:784:GLN:NE2	1:A:803:ALA:H	1.96	0.64
1:A:697:GLY:HA2	1:A:728:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASN:ND2	1:A:558:LYS:HG2	2.14	0.62
1:A:298:ASN:ND2	1:A:343:ILE:HG22	2.13	0.62
1:A:465:HIS:HA	1:A:477:GLN:HB2	1.82	0.61
1:A:645:MET:HE2	1:A:672:ARG:HD3	1.83	0.61
1:A:100:LYS:O	4:A:3138:HOH:O	2.16	0.61
1:A:442:VAL:HG21	4:A:2943:HOH:O	2.00	0.61
1:A:181:MET:HA	1:A:184:VAL:HG22	1.83	0.60
1:A:307:THR:HG23	1:A:442:VAL:HG12	1.83	0.60
1:A:514:ILE:HG23	1:A:515:LYS:N	2.15	0.60
1:A:533:ARG:HG3	4:A:3374:HOH:O	2.01	0.59
1:A:531:ASN:H	1:A:531:ASN:HD22	1.50	0.59
1:A:659:MET:HG3	4:A:2348:HOH:O	2.02	0.59
1:A:452:GLN:NE2	1:A:452:GLN:H	2.00	0.59
1:A:523:PRO:HA	1:A:537:ALA:HB2	1.83	0.58
1:A:555:ARG:HD3	4:A:3323:HOH:O	2.02	0.58
1:A:188:THR:CG2	1:A:455:ARG:HH22	2.11	0.58
1:A:322:THR:HG22	1:A:323:LEU:H	1.66	0.58
1:A:243:GLU:HG2	4:A:3331:HOH:O	2.04	0.58
1:A:613:LEU:HB3	1:A:614:PRO:HD3	1.85	0.58
1:A:504:ASN:ND2	1:A:506:TYR:H	2.01	0.58
1:A:340:SER:HB3	1:A:351:LEU:HD13	1.86	0.57
1:A:746:ILE:HG23	1:A:943:VAL:HA	1.86	0.57
1:A:448:MET:HG2	4:A:2792:HOH:O	2.03	0.57
1:A:555:ARG:HG3	1:A:701:GLU:OE2	2.05	0.57
1:A:63:ALA:HA	4:A:3045:HOH:O	2.04	0.57
1:A:487:ALA:O	1:A:491:LYS:HD2	2.05	0.57
1:A:514:ILE:N	1:A:707:ASN:HD21	1.96	0.56
1:A:956:LEU:HD11	4:A:2984:HOH:O	2.05	0.56
1:A:347:ASN:HD22	1:A:347:ASN:N	2.04	0.56
1:A:942:LYS:HE2	4:A:2729:HOH:O	2.05	0.56
1:A:42:ARG:HB2	1:A:44:TYR:CE1	2.40	0.56
1:A:199:SER:CA	4:A:3322:HOH:O	2.54	0.56
1:A:504:ASN:HD22	1:A:506:TYR:H	1.53	0.55
1:A:746:ILE:HD12	1:A:747:PHE:N	2.21	0.55
1:A:709:THR:HA	4:A:3468:HOH:O	2.06	0.55
1:A:697:GLY:HA2	1:A:728:GLY:CA	2.37	0.55
1:A:509:ASP:H	1:A:611:GLN:NE2	1.98	0.55
1:A:431:VAL:HG22	4:A:3271:HOH:O	2.07	0.55
1:A:924:GLN:HE22	1:A:936:VAL:H	1.54	0.55
1:A:514:ILE:HG13	1:A:709:THR:HG23	1.89	0.54
1:A:74:VAL:HG21	1:A:225:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HE2	4:A:3536:HOH:O	2.05	0.54
1:A:343:ILE:HD12	1:A:344:VAL:N	2.23	0.53
1:A:762:PHE:O	1:A:813:GLY:HA3	2.07	0.53
1:A:392:LEU:O	1:A:395:VAL:HG22	2.08	0.53
1:A:743:GLN:HA	4:A:2360:HOH:O	2.07	0.53
1:A:732:CYS:HB2	4:A:3129:HOH:O	2.09	0.53
1:A:114:HIS:O	1:A:134:GLU:HG3	2.09	0.53
1:A:193:HIS:HE1	1:A:347:ASN:HD21	1.55	0.53
1:A:755:ASP:HA	1:A:821:ASN:HA	1.91	0.53
1:A:800:ALA:HB3	4:A:3389:HOH:O	2.07	0.53
1:A:934:GLU:HG2	1:A:935:TYR:N	2.24	0.53
1:A:728:GLY:C	1:A:730:GLU:H	2.12	0.53
1:A:488:ASP:OD1	1:A:492:LYS:HE2	2.10	0.52
1:A:65:LYS:NZ	4:A:3314:HOH:O	2.42	0.52
1:A:119:ASN:HB3	1:A:130:TYR:CE1	2.45	0.52
1:A:742:LYS:HB3	4:A:3506:HOH:O	2.09	0.52
1:A:280:HIS:HD2	1:A:463:GLU:OE2	1.93	0.52
1:A:540:ARG:NE	4:A:3207:HOH:O	2.42	0.51
1:A:826:SER:HA	1:A:936:VAL:HG22	1.92	0.51
1:A:857:ALA:O	1:A:861:GLN:HG3	2.09	0.51
1:A:385:ASP:OD2	1:A:387:GLN:HG3	2.11	0.51
1:A:603:MET:HE1	4:A:3373:HOH:O	2.10	0.51
1:A:34:ILE:N	1:A:34:ILE:HD12	2.26	0.51
1:A:133:VAL:HG22	1:A:134:GLU:N	2.26	0.51
1:A:915:GLU:HG2	4:A:3340:HOH:O	2.09	0.51
1:A:366:ASP:N	4:A:3324:HOH:O	2.44	0.51
1:A:223:GLU:HG2	4:A:2052:HOH:O	2.11	0.51
1:A:673:ASP:O	1:A:677:LYS:HD3	2.10	0.51
1:A:445:ARG:O	1:A:448:MET:HG3	2.11	0.51
1:A:139:PRO:HG3	1:A:247:MET:CE	2.41	0.50
1:A:630:THR:C	1:A:632:ASP:H	2.15	0.50
1:A:726:ALA:O	1:A:727:ASP:HB2	2.11	0.50
1:A:184:VAL:HG23	1:A:457:TRP:HH2	1.77	0.50
1:A:223:GLU:HA	1:A:258:LYS:NZ	2.27	0.49
1:A:630:THR:O	1:A:631:GLU:HB3	2.11	0.49
1:A:850:GLU:O	1:A:854:ILE:HG12	2.12	0.49
1:A:956:LEU:HD12	1:A:956:LEU:N	2.26	0.49
1:A:280:HIS:HE1	1:A:479:ASP:OD1	1.95	0.49
1:A:224:LYS:HE3	1:A:225:TYR:OH	2.12	0.49
1:A:199:SER:HA	4:A:3322:HOH:O	2.12	0.49
1:A:878:LYS:NZ	1:A:878:LYS:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:HIS:HD2	4:A:2113:HOH:O	1.95	0.49
1:A:694:LEU:HD22	4:A:2026:HOH:O	2.13	0.49
1:A:556:ASN:HD21	1:A:558:LYS:HG2	1.77	0.49
1:A:878:LYS:HB3	1:A:878:LYS:HZ3	1.78	0.49
1:A:341:ASP:OD2	1:A:344:VAL:HB	2.13	0.48
1:A:778:LEU:HD23	1:A:858:VAL:HG21	1.95	0.48
1:A:810:ARG:NH1	4:A:3243:HOH:O	2.46	0.48
1:A:782:ILE:HD13	1:A:846:MET:HE1	1.94	0.48
1:A:269:VAL:HG22	4:A:2165:HOH:O	2.14	0.48
1:A:791:LEU:HB3	1:A:801:VAL:HG21	1.96	0.48
1:A:491:LYS:HE3	1:A:491:LYS:N	2.29	0.47
1:A:778:LEU:HD22	1:A:854:ILE:HG22	1.96	0.47
1:A:131:LEU:HD12	1:A:131:LEU:C	2.35	0.47
1:A:525:LEU:HG	1:A:528:ASP:HB2	1.96	0.47
1:A:184:VAL:O	1:A:188:THR:HG22	2.14	0.47
1:A:189:ILE:HG23	1:A:190:ASN:N	2.30	0.47
1:A:788:TYR:CE2	1:A:791:LEU:HD21	2.50	0.47
1:A:208:ASP:OD1	1:A:213:PRO:HA	2.15	0.47
1:A:319:SER:OG	1:A:320:PRO:HD2	2.15	0.46
1:A:634:LEU:HD11	1:A:638:LYS:HE3	1.97	0.46
1:A:27:TRP:HZ2	4:A:3442:HOH:O	1.98	0.46
1:A:651:GLY:HA2	1:A:752:ASN:ND2	2.27	0.46
1:A:684:LEU:O	1:A:688:LEU:HD13	2.15	0.46
1:A:746:ILE:HD13	1:A:924:GLN:OE1	2.16	0.46
1:A:40:ASP:HA	4:A:3235:HOH:O	2.14	0.46
1:A:514:ILE:CG2	1:A:515:LYS:N	2.79	0.46
1:A:789:ASN:HB2	4:A:2884:HOH:O	2.16	0.46
1:A:43:GLN:HB3	1:A:241:LEU:HD11	1.97	0.46
1:A:572:ASN:HD21	1:A:691:ARG:HD3	1.81	0.46
1:A:745:VAL:HG13	1:A:944:TRP:CD1	2.51	0.46
1:A:199:SER:O	4:A:2670:HOH:O	2.20	0.46
1:A:43:GLN:HB2	1:A:59:SER:HB3	1.98	0.45
1:A:25:THR:HB	4:A:2573:HOH:O	2.17	0.45
1:A:790:GLN:NE2	4:A:3222:HOH:O	2.49	0.45
1:A:26:GLY:HA2	1:A:50:ASP:OD2	2.17	0.45
1:A:37:SER:HB2	4:A:3345:HOH:O	2.16	0.45
1:A:653:ALA:HB3	1:A:819:GLN:HG3	1.98	0.45
1:A:322:THR:CG2	1:A:323:LEU:N	2.80	0.45
1:A:810:ARG:CZ	4:A:3243:HOH:O	2.63	0.45
1:A:938:PRO:HG2	1:A:941:TRP:CG	2.51	0.45
1:A:133:VAL:HG22	1:A:134:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:HG22	1:A:356:SER:O	2.17	0.45
1:A:697:GLY:HA2	1:A:728:GLY:N	2.32	0.45
1:A:787:PHE:C	1:A:789:ASN:H	2.20	0.45
1:A:926:SER:HB2	1:A:935:TYR:CE1	2.52	0.45
1:A:531:ASN:HD22	1:A:531:ASN:N	2.11	0.45
1:A:347:ASN:H	1:A:347:ASN:ND2	2.14	0.44
1:A:558:LYS:HD2	4:A:3576:HOH:O	2.17	0.44
1:A:392:LEU:HA	1:A:395:VAL:HG22	1.97	0.44
1:A:138:LEU:O	1:A:142:VAL:HG23	2.18	0.44
1:A:749:LYS:O	1:A:925:ILE:HA	2.18	0.44
1:A:331:GLY:HA2	4:A:2958:HOH:O	2.17	0.44
1:A:504:ASN:HD22	1:A:504:ASN:C	2.19	0.44
1:A:514:ILE:CG1	1:A:709:THR:HG23	2.47	0.44
1:A:667:VAL:HA	1:A:668:PRO:HA	1.88	0.44
1:A:70:LEU:HD13	1:A:70:LEU:C	2.37	0.44
1:A:711:ALA:O	1:A:715:THR:HG23	2.17	0.44
1:A:886:ARG:NH1	4:A:3293:HOH:O	2.50	0.44
1:A:787:PHE:C	1:A:789:ASN:N	2.71	0.44
1:A:224:LYS:HE3	1:A:225:TYR:CZ	2.53	0.43
1:A:556:ASN:HD21	1:A:558:LYS:CG	2.31	0.43
1:A:739:VAL:N	1:A:811:GLN:HE22	1.97	0.43
1:A:745:VAL:HG11	1:A:950:LEU:HD22	2.00	0.43
1:A:536:TYR:CG	1:A:537:ALA:N	2.86	0.43
1:A:130:TYR:HD1	1:A:409:MET:HG2	1.83	0.43
1:A:71:VAL:HG22	1:A:128:ALA:HB2	2.00	0.43
1:A:36:LYS:HD2	1:A:40:ASP:HB3	2.00	0.43
1:A:35:ARG:HG2	1:A:425:GLU:O	2.19	0.43
1:A:727:ASP:HA	4:A:2930:HOH:O	2.19	0.43
1:A:948:SER:O	1:A:952:GLN:HG3	2.19	0.43
1:A:125:TYR:CZ	1:A:343:ILE:HD13	2.53	0.43
1:A:266:THR:HA	4:A:3427:HOH:O	2.19	0.43
1:A:540:ARG:CZ	4:A:3207:HOH:O	2.65	0.43
1:A:745:VAL:HG13	1:A:944:TRP:HD1	1.83	0.43
1:A:184:VAL:CG2	1:A:457:TRP:HH2	2.31	0.42
1:A:350:VAL:HG12	1:A:351:LEU:N	2.34	0.42
1:A:66:SER:HB3	1:A:138:LEU:HG	2.00	0.42
1:A:121:SER:HB2	4:A:2652:HOH:O	2.18	0.42
1:A:139:PRO:HG3	1:A:247:MET:HE2	2.01	0.42
1:A:629:ALA:HA	1:A:633:GLN:NE2	2.34	0.42
1:A:57:LEU:HD22	1:A:244:LEU:HB3	2.00	0.42
1:A:27:TRP:CZ3	1:A:29:PRO:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:PRO:HA	1:A:947:VAL:HG21	2.01	0.42
1:A:132:GLU:HG3	4:A:3314:HOH:O	2.19	0.42
1:A:890:ARG:HG3	1:A:890:ARG:HH11	1.83	0.42
1:A:62:GLN:HG3	4:A:3132:HOH:O	2.20	0.42
1:A:71:VAL:HG23	1:A:416:ALA:HB1	2.02	0.42
1:A:322:THR:HG23	1:A:375:TYR:OH	2.19	0.42
1:A:679:LEU:HB3	1:A:680:PRO:HD3	2.02	0.42
1:A:47:ILE:HD13	1:A:57:LEU:HD11	2.02	0.41
1:A:537:ALA:O	1:A:705:ILE:HA	2.20	0.41
1:A:796:GLN:NE2	1:A:831:ARG:HG3	2.24	0.41
1:A:545:GLU:HG3	4:A:3202:HOH:O	2.20	0.41
1:A:642:ASN:HD22	1:A:642:ASN:HA	1.64	0.41
1:A:633:GLN:HA	1:A:636:GLN:OE1	2.20	0.41
1:A:488:ASP:OD2	1:A:492:LYS:HE2	2.21	0.41
1:A:759:ALA:HA	1:A:816:PHE:O	2.21	0.41
1:A:890:ARG:HG3	1:A:890:ARG:NH1	2.35	0.41
1:A:488:ASP:CG	1:A:492:LYS:HE2	2.41	0.41
1:A:810:ARG:HD2	1:A:882:ARG:HH21	1.86	0.41
1:A:84:GLN:HB3	1:A:198:PHE:O	2.20	0.41
1:A:555:ARG:HH12	1:A:734:ASN:HD21	1.69	0.41
1:A:564:ARG:O	1:A:568:MET:HG3	2.21	0.41
1:A:616:LEU:C	1:A:616:LEU:HD13	2.41	0.41
1:A:784:GLN:HE22	1:A:803:ALA:H	1.65	0.41
1:A:343:ILE:HD12	1:A:343:ILE:C	2.41	0.41
1:A:254:ARG:HD3	4:A:2063:HOH:O	2.21	0.40
1:A:391:GLU:HG2	1:A:507:ILE:CD1	2.51	0.40
1:A:62:GLN:HA	4:A:3545:HOH:O	2.20	0.40
1:A:139:PRO:HG3	1:A:247:MET:HE1	2.02	0.40
1:A:934:GLU:HA	4:A:2576:HOH:O	2.20	0.40
1:A:818:LEU:C	1:A:818:LEU:HD23	2.41	0.40
1:A:650:LYS:HA	4:A:3304:HOH:O	2.21	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)
4:A:2306:HOH:O	4:A:2306:HOH:O[4_555]	1.51	0.69

## 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	935/939 (100%)	881 (94%)	46 (5%)	8 (1%)	17 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	727	ASP
1	A	730	GLU
1	A	928	SER
1	A	33	THR
1	A	731	TRP
1	A	405	ILE
1	A	729	SER
1	A	887	PHE

### 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	788/794 (99%)	757 (96%)	31 (4%)	32 41

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	203	LEU
1	A	206	LEU

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Mol	Chain	Res	Type
1	A	269	VAL
1	A	274	GLN
1	A	333	VAL
1	A	347	ASN
1	A	407	ARG
1	A	413	GLU
1	A	452	GLN
1	A	491	LYS
1	A	504	ASN
1	A	514	ILE
1	A	531	ASN
1	A	556	ASN
1	A	599	ASN
1	A	622	GLU
1	A	635	GLU
1	A	642	ASN
1	A	694	LEU
1	A	733	ARG
1	A	746	ILE
1	A	789	ASN
1	A	794	GLU
1	A	799	TYR
1	A	828	LEU
1	A	849	ASP
1	A	900	LEU
1	A	917	GLN
1	A	924	GLN
1	A	957	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	84	GLN
1	A	135	ASN
1	A	164	ASN
1	A	193	HIS
1	A	216	GLN
1	A	222	HIS
1	A	274	GLN
1	A	280	HIS
1	A	330	GLN

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Mol	Chain	Res	Type
1	A	345	ASN
1	A	347	ASN
1	A	367	GLN
1	A	452	GLN
1	A	453	ASN
1	A	465	HIS
1	A	484	GLN
1	A	504	ASN
1	A	531	ASN
1	A	556	ASN
1	A	565	ASN
1	A	572	ASN
1	A	582	GLN
1	A	585	ASN
1	A	599	ASN
1	A	607	ASN
1	A	611	GLN
1	A	618	GLN
1	A	633	GLN
1	A	642	ASN
1	A	662	GLN
1	A	707	ASN
1	A	712	GLN
1	A	723	GLN
1	A	784	GLN
1	A	796	GLN
1	A	811	GLN
1	A	861	GLN
1	A	924	GLN
1	A	937	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.