



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 1SRP / pdb_00001srp
Title : STRUCTURAL ANALYSIS OF SERRATIA PROTEASE
Authors : Hamada, K.; Hiramatsu, H.; Katsuya, Y.; Hata, Y.; Katsube, Y.
Deposited on : 1994-11-02
Resolution : 2.00 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

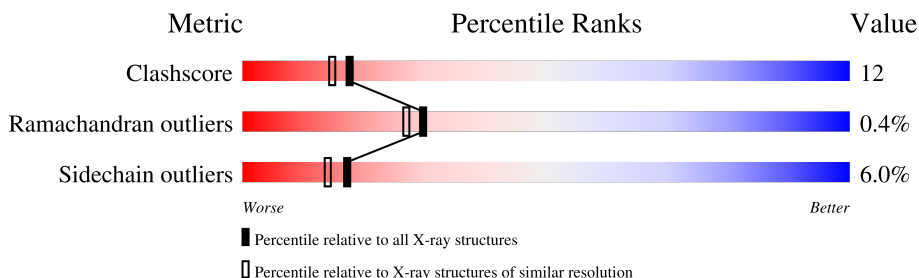
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	471	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3780 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 SERRALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3560	2227	609	723	1			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	200	ARG	ASN	conflict	UNP P07268
A	250	LEU	PRO	conflict	UNP P07268
A	412	GLN	ASN	conflict	UNP P07268
A	426	ALA	THR	conflict	UNP P07268
A	438	ASN	SER	conflict	UNP P07268

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Ca	0	0
			7	7		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

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

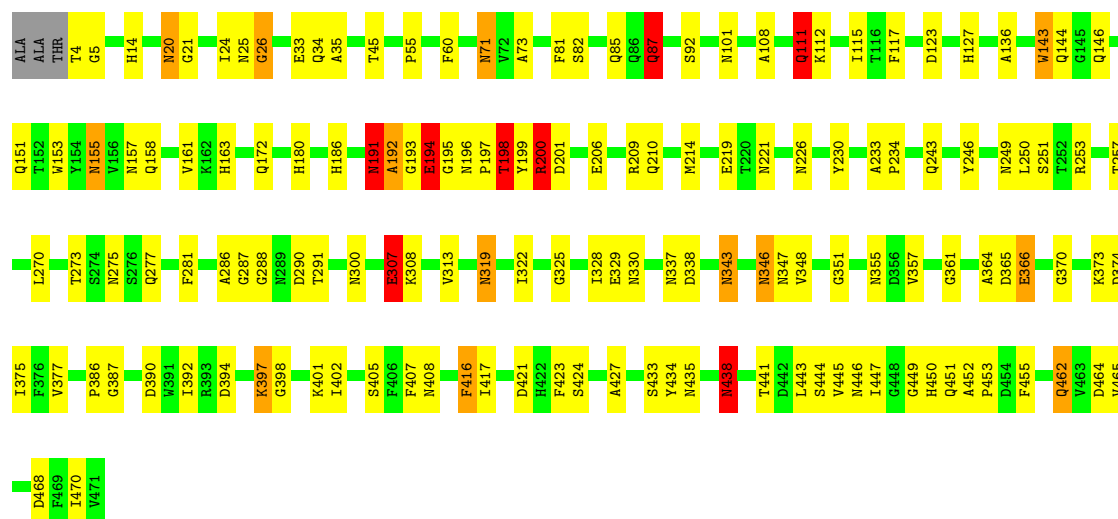
3 Residue-property plots

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: SERRALYSIN

Chain A:  68% 27% . . .



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	109.14Å 150.89Å 42.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	78.6 (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.193 , 0.184	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3780	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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, CA

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	1.07	1/3645 (0.0%)	2.02	98/4952 (2.0%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	GLY	N-CA	5.03	1.52	1.45

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ALA	O-C-N	9.58	127.84	121.71
1	A	200	ARG	CD-NE-CZ	-9.18	111.54	124.40
1	A	416	PHE	CA-CB-CG	-7.49	106.31	113.80
1	A	394	ASP	N-CA-CB	-7.48	102.81	111.79
1	A	210	GLN	OE1-CD-NE2	-7.36	115.24	122.60
1	A	387	GLY	N-CA-C	-7.34	105.20	113.79
1	A	329	GLU	N-CA-C	7.17	122.42	112.45
1	A	346	ASN	CA-CB-CG	7.14	119.74	112.60
1	A	35	ALA	CA-C-N	7.09	127.85	119.98
1	A	35	ALA	C-N-CA	7.09	127.85	119.98
1	A	5	GLY	N-CA-C	-6.97	104.42	112.50
1	A	441	THR	CA-CB-OG1	-6.93	99.21	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	GLU	CA-C-O	-6.86	113.65	121.19
1	A	365	ASP	CA-C-O	-6.85	113.30	121.66
1	A	25	ASN	N-CA-C	-6.82	103.44	112.72
1	A	186	HIS	N-CA-C	-6.79	100.71	110.08
1	A	375	ILE	O-C-N	6.74	130.48	123.20
1	A	117	PHE	CA-C-O	-6.71	113.11	120.36
1	A	470	ILE	N-CA-CB	6.71	120.35	111.90
1	A	194	GLU	CA-CB-CG	6.54	127.17	114.10
1	A	386	PRO	CA-C-N	-6.53	115.67	123.44
1	A	386	PRO	C-N-CA	-6.53	115.67	123.44
1	A	281	PHE	CA-CB-CG	6.39	120.19	113.80
1	A	136	ALA	O-C-N	6.39	130.25	123.42
1	A	307	GLU	CB-CA-C	-6.35	99.19	109.72
1	A	198	THR	N-CA-CB	-6.33	100.68	111.69
1	A	451	GLN	CB-CG-CD	6.30	123.32	112.60
1	A	161	VAL	CA-C-O	6.30	127.53	120.85
1	A	468	ASP	N-CA-C	6.09	120.41	112.92
1	A	287	GLY	CA-C-O	-6.08	115.67	121.87
1	A	33	GLU	CB-CG-CD	-6.06	102.30	112.60
1	A	308	LYS	CA-CB-CG	-6.02	102.06	114.10
1	A	351	GLY	CA-C-O	-6.01	114.29	120.66
1	A	338	ASP	N-CA-C	5.97	118.92	110.14
1	A	427	ALA	CA-C-O	-5.94	115.09	121.56
1	A	416	PHE	CB-CA-C	5.92	122.21	110.42
1	A	290	ASP	O-C-N	5.89	130.84	123.19
1	A	405	SER	N-CA-C	5.85	119.95	112.34
1	A	402	ILE	N-CA-CB	5.82	118.80	111.46
1	A	407	PHE	N-CA-C	5.80	117.28	111.07
1	A	111	GLN	N-CA-C	5.79	118.02	110.43
1	A	92	SER	CA-C-O	-5.72	114.81	120.70
1	A	214	MET	CA-C-O	5.70	126.37	119.31
1	A	464	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	286	ALA	CA-C-O	-5.68	112.41	119.28
1	A	291	THR	N-CA-C	5.67	118.35	108.76
1	A	392	ILE	N-CA-C	-5.67	99.06	107.51
1	A	45	THR	CA-C-O	-5.64	115.19	121.51
1	A	288	GLY	CA-C-O	-5.62	116.77	122.56
1	A	307	GLU	CG-CD-OE2	-5.59	105.54	118.40
1	A	180	HIS	CA-C-O	-5.58	114.96	120.82
1	A	243	GLN	N-CA-C	-5.57	105.36	111.82
1	A	14	HIS	CA-CB-CG	-5.53	108.27	113.80
1	A	433	SER	N-CA-CB	5.53	119.25	110.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	GLN	CA-CB-CG	5.51	125.13	114.10
1	A	398	GLY	N-CA-C	-5.50	108.13	115.40
1	A	198	THR	CA-CB-CG2	5.47	119.80	110.50
1	A	219	GLU	CB-CG-CD	5.42	121.81	112.60
1	A	221	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	A	221	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	226	ASN	O-C-N	5.40	129.35	122.39
1	A	433	SER	CB-CA-C	-5.39	102.48	110.62
1	A	438	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	A	401	LYS	O-C-N	5.38	129.51	123.27
1	A	377	VAL	O-C-N	5.37	128.62	123.14
1	A	444	SER	CA-C-N	-5.36	115.50	122.94
1	A	444	SER	C-N-CA	-5.36	115.50	122.94
1	A	230	TYR	CA-CB-CG	-5.34	104.28	113.90
1	A	357	VAL	CA-C-O	-5.33	114.85	120.39
1	A	455	PHE	CA-CB-CG	5.32	119.12	113.80
1	A	155	ASN	CA-C-O	-5.32	115.24	120.98
1	A	26	GLY	N-CA-C	-5.31	107.91	115.30
1	A	199	TYR	N-CA-C	-5.28	105.64	111.71
1	A	163	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	441	THR	CA-CB-CG2	5.27	119.45	110.50
1	A	392	ILE	N-CA-CB	5.21	117.92	111.41
1	A	191	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	322	ILE	CA-C-O	-5.20	114.94	120.39
1	A	180	HIS	N-CA-CB	5.19	117.54	110.01
1	A	366	GLU	CA-C-O	-5.16	114.98	120.40
1	A	87	GLN	O-C-N	5.15	127.59	122.08
1	A	444	SER	O-C-N	5.15	129.42	123.30
1	A	374	ASP	CA-CB-CG	-5.14	107.46	112.60
1	A	180	HIS	O-C-N	5.14	127.36	122.07
1	A	243	GLN	OE1-CD-NE2	5.13	127.73	122.60
1	A	361	GLY	CA-C-O	-5.12	114.34	122.28
1	A	421	ASP	CB-CA-C	5.11	119.93	109.55
1	A	34	GLN	CB-CG-CD	-5.11	103.92	112.60
1	A	375	ILE	CA-C-O	-5.08	114.98	120.36
1	A	270	LEU	O-C-N	5.08	128.38	122.24
1	A	246	TYR	CA-C-O	-5.07	113.60	119.59
1	A	424	SER	N-CA-C	-5.06	107.05	114.39
1	A	206	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	390	ASP	N-CA-C	-5.03	103.76	110.55
1	A	370	GLY	N-CA-C	-5.02	103.49	112.22
1	A	275	ASN	CA-C-O	5.01	125.81	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	THR	CA-CB-CG2	5.00	119.01	110.50
1	A	328	ILE	N-CA-C	-5.00	101.21	108.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	ARG	Sidechain

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	3560	0	3277	85	0
2	A	7	0	0	0	0
3	A	1	0	0	0	0
4	A	212	0	0	1	0
All	All	3780	0	3277	85	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 12.

All (85) 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:198:THR:HG22	1:A:200:ARG:HB2	1.30	1.12
1:A:408:ASN:HD21	1:A:417:ILE:H	1.11	0.95
1:A:198:THR:CG2	1:A:200:ARG:HB2	1.96	0.95
1:A:20:ASN:ND2	1:A:21:GLY:N	2.20	0.89
1:A:20:ASN:ND2	1:A:21:GLY:H	1.74	0.86
1:A:123:ASP:OD1	1:A:127:HIS:HD2	1.58	0.85
1:A:337:ASN:ND2	1:A:355:ASN:H	1.75	0.84
1:A:337:ASN:HD22	1:A:355:ASN:H	1.27	0.83
1:A:198:THR:HG22	1:A:200:ARG:H	1.46	0.80
1:A:198:THR:HG22	1:A:200:ARG:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:H	1:A:319:ASN:HD21	1.27	0.79
1:A:20:ASN:HD22	1:A:21:GLY:N	1.80	0.79
1:A:151:GLN:HE21	1:A:153:TRP:HE1	1.31	0.78
1:A:82:SER:H	1:A:85:GLN:HE21	1.31	0.77
1:A:143:TRP:HA	1:A:143:TRP:CE3	2.20	0.76
1:A:191:ASN:C	1:A:191:ASN:HD22	1.92	0.75
1:A:438:ASN:HD22	1:A:438:ASN:C	1.95	0.74
1:A:330:ASN:HD22	1:A:348:VAL:H	1.37	0.71
1:A:108:ALA:HB3	1:A:111:GLN:CG	2.21	0.71
1:A:108:ALA:HB3	1:A:111:GLN:CD	2.16	0.70
1:A:194:GLU:OE1	1:A:195:GLY:N	2.24	0.70
1:A:143:TRP:HA	1:A:143:TRP:HE3	1.53	0.70
1:A:20:ASN:CG	1:A:21:GLY:H	1.97	0.69
1:A:172:GLN:HE22	1:A:209:ARG:HE	1.41	0.68
1:A:319:ASN:HD22	1:A:319:ASN:H	1.41	0.67
1:A:198:THR:HG22	1:A:200:ARG:N	2.09	0.66
1:A:108:ALA:HB3	1:A:111:GLN:HG2	1.76	0.66
1:A:194:GLU:CD	1:A:195:GLY:H	2.05	0.64
1:A:197:PRO:HA	1:A:201:ASP:OD2	1.97	0.64
1:A:71:ASN:HD22	1:A:71:ASN:C	2.06	0.64
1:A:355:ASN:ND2	1:A:373:LYS:H	1.96	0.64
1:A:249:ASN:C	1:A:249:ASN:HD22	2.07	0.63
1:A:20:ASN:HD22	1:A:20:ASN:C	2.02	0.61
1:A:155:ASN:HD22	1:A:155:ASN:C	2.09	0.61
1:A:155:ASN:HD22	1:A:157:ASN:H	1.48	0.61
1:A:172:GLN:NE2	1:A:209:ARG:HE	1.98	0.61
1:A:155:ASN:ND2	1:A:157:ASN:H	2.00	0.59
1:A:446:ASN:HD21	1:A:450:HIS:H	1.51	0.59
1:A:355:ASN:HD22	1:A:373:LYS:H	1.52	0.58
1:A:300:ASN:ND2	1:A:337:ASN:H	2.01	0.58
1:A:249:ASN:ND2	1:A:251:SER:H	2.02	0.57
1:A:191:ASN:C	1:A:191:ASN:ND2	2.61	0.57
1:A:319:ASN:H	1:A:319:ASN:ND2	2.03	0.56
1:A:346:ASN:ND2	1:A:364:ALA:H	2.03	0.56
1:A:307:GLU:CD	1:A:325:GLY:H	2.12	0.56
1:A:435:ASN:HB3	1:A:438:ASN:HD21	1.71	0.56
1:A:446:ASN:ND2	1:A:449:GLY:H	2.04	0.56
1:A:198:THR:CG2	1:A:200:ARG:H	2.15	0.56
1:A:337:ASN:HD22	1:A:355:ASN:N	2.01	0.55
1:A:195:GLY:C	1:A:197:PRO:HD3	2.32	0.55
1:A:123:ASP:OD1	1:A:127:HIS:CD2	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:C	1:A:26:GLY:H	2.16	0.54
1:A:249:ASN:HD22	1:A:251:SER:H	1.56	0.54
1:A:434:TYR:CZ	1:A:462:GLN:HG2	2.43	0.54
1:A:172:GLN:NE2	4:A:625:HOH:O	2.40	0.53
1:A:273:THR:H	1:A:277:GLN:NE2	2.08	0.51
1:A:249:ASN:HD21	1:A:251:SER:HB2	1.75	0.51
1:A:172:GLN:HE22	1:A:209:ARG:NE	2.07	0.50
1:A:343:ASN:C	1:A:343:ASN:HD22	2.20	0.50
1:A:82:SER:H	1:A:85:GLN:NE2	2.05	0.50
1:A:60:PHE:HA	1:A:115:ILE:O	2.11	0.50
1:A:194:GLU:CG	1:A:195:GLY:H	2.23	0.50
1:A:397:LYS:HB3	1:A:462:GLN:O	2.12	0.50
1:A:423:PHE:CE2	1:A:453:PRO:HG3	2.46	0.49
1:A:408:ASN:ND2	1:A:416:PHE:HB3	2.28	0.49
1:A:343:ASN:ND2	1:A:347:ASN:HD21	2.11	0.48
1:A:445:VAL:HG12	1:A:447:ILE:HG13	1.95	0.48
1:A:253:ARG:HD2	1:A:257:THR:HG21	1.96	0.47
1:A:191:ASN:HD22	1:A:192:ALA:N	2.13	0.47
1:A:158:GLN:HE21	1:A:158:GLN:HA	1.80	0.46
1:A:155:ASN:HD21	1:A:157:ASN:HB2	1.80	0.46
1:A:438:ASN:C	1:A:438:ASN:ND2	2.67	0.45
1:A:200:ARG:HB3	1:A:200:ARG:CZ	2.47	0.44
1:A:111:GLN:HG2	1:A:111:GLN:H	1.36	0.44
1:A:55:PRO:HB3	1:A:101:ASN:HB3	2.00	0.44
1:A:71:ASN:ND2	1:A:73:ALA:H	2.16	0.44
1:A:143:TRP:CE3	1:A:143:TRP:CA	2.98	0.44
1:A:343:ASN:HD21	1:A:347:ASN:HD21	1.67	0.42
1:A:24:ILE:C	1:A:26:GLY:N	2.77	0.42
1:A:233:ALA:HB1	1:A:234:PRO:HD2	2.01	0.42
1:A:435:ASN:HB3	1:A:438:ASN:ND2	2.36	0.41
1:A:191:ASN:O	1:A:192:ALA:O	2.37	0.41
1:A:191:ASN:O	1:A:192:ALA:C	2.64	0.41
1:A:87:GLN:HE21	1:A:87:GLN:HB3	1.41	0.41
1:A:71:ASN:C	1:A:71:ASN:ND2	2.73	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	466/471 (99%)	449 (96%)	15 (3%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLY
1	A	192	ALA

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	365/366 (100%)	343 (94%)	22 (6%)	17	14

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	71	ASN
1	A	81	PHE
1	A	87	GLN
1	A	111	GLN
1	A	112	LYS
1	A	143	TRP
1	A	144	GLN
1	A	146	GLN

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Mol	Chain	Res	Type
1	A	191	ASN
1	A	194	GLU
1	A	196	ASN
1	A	198	THR
1	A	250	LEU
1	A	307	GLU
1	A	319	ASN
1	A	343	ASN
1	A	366	GLU
1	A	397	LYS
1	A	438	ASN
1	A	443	LEU
1	A	465	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	23	GLN
1	A	34	GLN
1	A	47	ASN
1	A	54	GLN
1	A	71	ASN
1	A	85	GLN
1	A	86	GLN
1	A	87	GLN
1	A	101	ASN
1	A	119	ASN
1	A	122	GLN
1	A	127	HIS
1	A	140	ASN
1	A	144	GLN
1	A	151	GLN
1	A	155	ASN
1	A	157	ASN
1	A	158	GLN
1	A	172	GLN
1	A	191	ASN
1	A	196	ASN
1	A	244	HIS
1	A	249	ASN
1	A	277	GLN

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Mol	Chain	Res	Type
1	A	300	ASN
1	A	304	ASN
1	A	319	ASN
1	A	330	ASN
1	A	337	ASN
1	A	343	ASN
1	A	346	ASN
1	A	355	ASN
1	A	408	ASN
1	A	422	HIS
1	A	438	ASN
1	A	439	ASN
1	A	446	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](#)

Of 8 ligands modelled in this entry, 8 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

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.