



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:05 AM UTC

PDB ID : 1UCU / pdb_00001ucu
Title : R-type straight flagellar filament made of full-length flagellin
Authors : Yonekura, K.; Maki-Yonekura, S.; Namba, K.
Deposited on : 2003-04-22
Resolution : 4.00 Å(reported)
Based on initial model : 1IO1

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

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
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

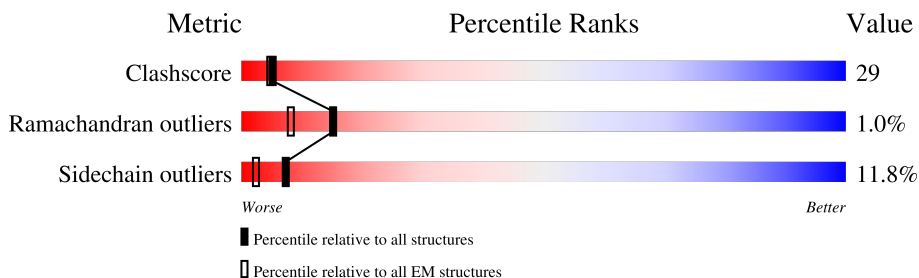
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	494	51% 37% 9% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3617 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 phase 1 Flagellin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	494	Total	C	N	O	S	0	0
			3617	2191	640	784	2		

There is a discrepancy between the modelled and reference sequences:

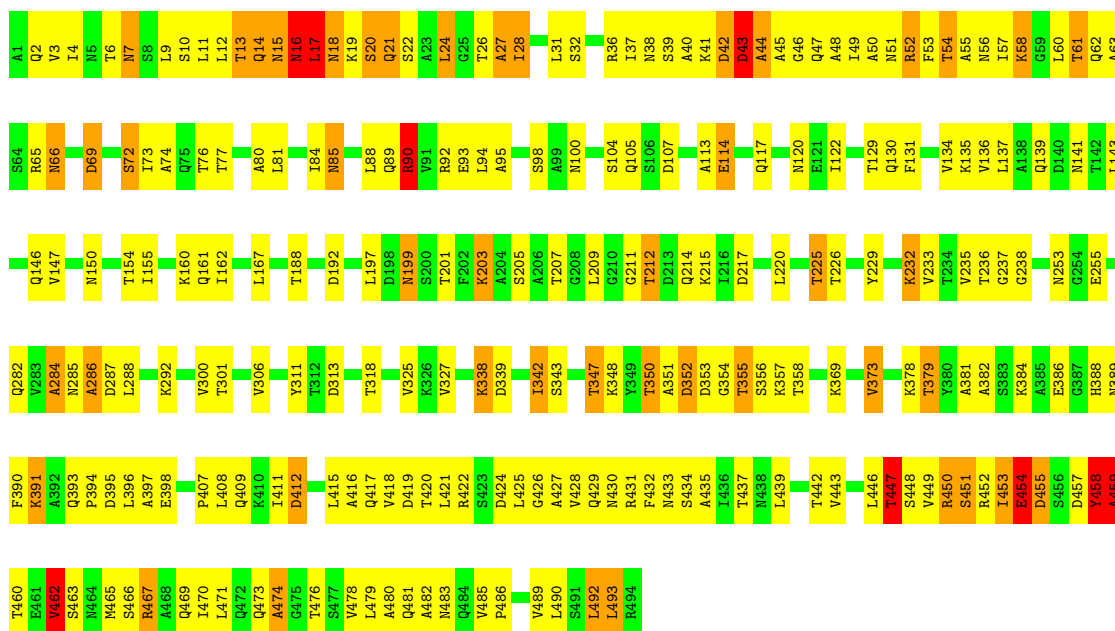
Chain	Residue	Modelled	Actual	Comment	Reference
A	449	VAL	ALA	SEE REMARK 999	UNP P06179

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.

- Molecule 1: phase 1 Flagellin

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	1.00Å 1.00Å 1.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-4.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	FEX-PLOR, FX-PLOR	Depositor
R, R_{free}	0.300 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3617	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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	0.87	11/3640 (0.3%)	1.38	68/4941 (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	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	THR	CB-CG2	9.10	1.82	1.52
1	A	211	GLY	CA-C	-7.29	1.44	1.52
1	A	66	ASN	CA-C	-6.99	1.43	1.52
1	A	238	GLY	N-CA	6.72	1.54	1.45
1	A	236	THR	CA-CB	-6.32	1.42	1.53
1	A	235	VAL	CA-CB	-6.12	1.45	1.53
1	A	237	GLY	CA-C	-5.92	1.43	1.51
1	A	462	VAL	CA-CB	5.81	1.61	1.54
1	A	212	THR	N-CA	-5.61	1.39	1.46
1	A	100	ASN	CA-C	-5.41	1.45	1.52
1	A	458	TYR	C-N	5.26	1.41	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	TYR	O-C-N	-13.02	113.34	123.11
1	A	284	ALA	N-CA-C	-9.63	95.28	109.15
1	A	211	GLY	N-CA-C	-9.54	95.62	112.22
1	A	40	ALA	N-CA-C	-9.01	102.30	113.20
1	A	301	THR	N-CA-C	8.81	122.15	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ASN	OD1-CG-ND2	8.53	131.13	122.60
1	A	66	ASN	CB-CG-OD1	-8.26	104.28	120.80
1	A	453	ILE	N-CA-C	-7.88	103.57	110.74
1	A	22	SER	N-CA-C	-7.64	102.96	111.82
1	A	21	GLN	N-CA-C	-7.55	102.71	112.23
1	A	467	ARG	N-CA-C	-7.31	103.31	111.28
1	A	18	ASN	N-CA-C	-7.22	103.45	111.82
1	A	459	ALA	N-CA-C	7.16	126.04	110.80
1	A	458	TYR	CB-CA-C	7.00	125.45	114.87
1	A	85	ASN	N-CA-C	-6.97	103.62	111.07
1	A	69	ASP	N-CA-C	-6.94	103.64	111.07
1	A	449	VAL	N-CA-C	6.89	117.68	110.72
1	A	480	ALA	N-CA-C	-6.74	103.08	112.45
1	A	43	ASP	N-CA-C	-6.68	96.58	110.80
1	A	54	THR	CA-CB-CG2	6.67	121.84	110.50
1	A	20	SER	N-CA-C	-6.64	104.65	112.89
1	A	17	LEU	N-CA-C	-6.62	104.69	112.89
1	A	209	LEU	N-CA-C	-6.59	105.39	113.50
1	A	474	ALA	N-CA-C	-6.57	104.20	111.36
1	A	238	GLY	N-CA-C	6.42	121.68	112.82
1	A	452	ARG	N-CA-C	6.36	118.29	111.36
1	A	481	GLN	N-CA-C	-6.36	104.27	111.14
1	A	61	THR	N-CA-C	-6.34	103.90	111.69
1	A	58	LYS	N-CA-C	-6.32	104.47	111.36
1	A	381	ALA	N-CA-C	-6.26	101.21	110.48
1	A	454	GLU	N-CA-C	-6.26	97.46	110.80
1	A	16	ASN	N-CA-C	-6.11	105.08	112.54
1	A	150	ASN	N-CA-C	6.08	119.08	110.14
1	A	54	THR	N-CA-CB	6.06	119.68	110.28
1	A	90	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	A	188	THR	N-CA-C	6.05	119.74	110.36
1	A	39	SER	N-CA-C	5.99	119.95	111.92
1	A	447	THR	N-CA-C	-5.98	104.76	111.28
1	A	205	SER	N-CA-C	-5.92	106.09	113.38
1	A	54	THR	CA-CB-OG1	5.91	118.47	109.60
1	A	232	LYS	N-CA-C	-5.90	100.38	109.76
1	A	19	LYS	N-CA-C	-5.87	104.83	112.23
1	A	433	ASN	CA-C-N	5.81	128.06	120.28
1	A	433	ASN	C-N-CA	5.81	128.06	120.28
1	A	74	ALA	N-CA-C	-5.75	104.65	111.03
1	A	43	ASP	CA-C-N	5.73	128.23	120.38
1	A	43	ASP	C-N-CA	5.73	128.23	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GLN	N-CA-C	-5.72	105.18	111.82
1	A	44	ALA	N-CA-C	-5.71	104.42	111.33
1	A	27	ALA	N-CA-C	-5.71	104.97	111.14
1	A	355	THR	N-CA-C	5.59	122.71	110.80
1	A	15	ASN	N-CA-C	-5.55	106.00	112.89
1	A	114	GLU	CA-CB-CG	5.50	125.10	114.10
1	A	452	ARG	CG-CD-NE	-5.49	99.93	112.00
1	A	353	ASP	N-CA-C	-5.42	99.26	110.80
1	A	14	GLN	N-CA-C	-5.38	105.58	111.82
1	A	24	LEU	N-CA-C	-5.36	105.52	111.36
1	A	457	ASP	N-CA-C	5.33	118.09	109.40
1	A	203	LYS	N-CA-C	5.26	119.19	112.34
1	A	136	VAL	N-CA-C	5.25	120.27	109.34
1	A	347	THR	N-CA-C	5.22	120.65	113.97
1	A	52	ARG	N-CA-C	-5.17	105.82	111.82
1	A	54	THR	OG1-CB-CG2	5.17	119.63	109.30
1	A	114	GLU	CB-CG-CD	5.16	121.37	112.60
1	A	12	LEU	N-CA-C	-5.15	105.85	111.82
1	A	13	THR	N-CA-C	-5.11	105.90	111.82
1	A	7	ASN	N-CA-C	-5.09	105.81	111.36
1	A	233	VAL	N-CA-C	5.01	115.18	107.77

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	54	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	ASN	Sidechain
1	A	90	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	3617	0	3580	207	0
All	All	3617	0	3580	207	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 29.

All (207) 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:212:THR:CG2	1:A:212:THR:CB	1.82	1.54
1:A:450:ARG:HD2	1:A:454:GLU:HG2	1.21	1.11
1:A:424:ASP:O	1:A:428:VAL:HG23	1.53	1.07
1:A:53:PHE:HA	1:A:56:ASN:HD22	1.17	1.05
1:A:427:ALA:O	1:A:431:ARG:HG3	1.63	0.99
1:A:94:LEU:HD11	1:A:114:GLU:HG3	1.41	0.99
1:A:162:ILE:HD11	1:A:421:LEU:HD11	1.47	0.96
1:A:450:ARG:HD2	1:A:454:GLU:CG	1.98	0.94
1:A:450:ARG:O	1:A:454:GLU:HG3	1.68	0.92
1:A:347:THR:HG21	1:A:382:ALA:HB1	1.50	0.91
1:A:49:ILE:HG12	1:A:52:ARG:NH1	1.92	0.85
1:A:53:PHE:HA	1:A:56:ASN:ND2	1.91	0.85
1:A:47:GLN:HA	1:A:453:ILE:HD13	1.60	0.84
1:A:217:ASP:HB2	1:A:232:LYS:HD3	1.57	0.84
1:A:57:ILE:HA	1:A:60:LEU:HB2	1.58	0.84
1:A:160:LYS:HG3	1:A:421:LEU:HD22	1.62	0.82
1:A:81:LEU:HD23	1:A:84:ILE:HD12	1.62	0.82
1:A:450:ARG:CD	1:A:454:GLU:HG2	2.08	0.81
1:A:458:TYR:O	1:A:462:VAL:HB	1.80	0.80
1:A:49:ILE:HG12	1:A:52:ARG:HH11	1.47	0.80
1:A:92:ARG:HH21	1:A:412:ASP:HA	1.46	0.80
1:A:425:LEU:O	1:A:428:VAL:HB	1.82	0.78
1:A:3:VAL:HA	1:A:6:THR:HG22	1.63	0.78
1:A:41:LYS:HG3	1:A:47:GLN:HB3	1.67	0.77
1:A:451:SER:HA	1:A:454:GLU:OE2	1.85	0.77
1:A:14:GLN:HA	1:A:479:LEU:HD13	1.67	0.76
1:A:85:ASN:HB2	1:A:422:ARG:HH22	1.50	0.76
1:A:42:ASP:C	1:A:44:ALA:N	2.44	0.76
1:A:338:LYS:HD3	1:A:339:ASP:H	1.50	0.75
1:A:41:LYS:HE2	1:A:453:ILE:HG23	1.68	0.75
1:A:450:ARG:C	1:A:454:GLU:HG3	2.10	0.75
1:A:458:TYR:C	1:A:462:VAL:HB	2.11	0.75
1:A:42:ASP:C	1:A:44:ALA:H	1.94	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:CZ	1:A:415:LEU:HD12	2.18	0.74
1:A:407:PRO:O	1:A:411:ILE:HG13	1.89	0.73
1:A:94:LEU:CD1	1:A:114:GLU:HG3	2.19	0.72
1:A:225:THR:HG22	1:A:226:THR:HG23	1.73	0.71
1:A:88:LEU:HG	1:A:122:ILE:HD11	1.73	0.70
1:A:396:LEU:HD12	1:A:397:ALA:H	1.57	0.69
1:A:55:ALA:HA	1:A:58:LYS:HD2	1.75	0.69
1:A:60:LEU:HD13	1:A:443:VAL:HG22	1.75	0.68
1:A:354:GLY:HA2	1:A:391:LYS:NZ	2.07	0.68
1:A:41:LYS:HG3	1:A:47:GLN:CB	2.25	0.66
1:A:489:VAL:O	1:A:492:LEU:HG	1.96	0.66
1:A:162:ILE:HD11	1:A:421:LEU:CD1	2.24	0.64
1:A:77:THR:CG2	1:A:425:LEU:HD13	2.27	0.63
1:A:50:ALA:HB2	1:A:453:ILE:HD12	1.79	0.63
1:A:352:ASP:HB3	1:A:357:LYS:HZ2	1.63	0.63
1:A:88:LEU:HG	1:A:122:ILE:CD1	2.29	0.63
1:A:451:SER:HA	1:A:454:GLU:CD	2.24	0.62
1:A:73:ILE:HG12	1:A:131:PHE:CD2	2.35	0.62
1:A:352:ASP:HA	1:A:390:PHE:HB2	1.81	0.62
1:A:17:LEU:HB2	1:A:479:LEU:HD12	1.82	0.62
1:A:90:ARG:O	1:A:93:GLU:HB2	1.99	0.62
1:A:427:ALA:HB1	1:A:431:ARG:NH2	2.15	0.61
1:A:450:ARG:NH1	1:A:454:GLU:OE1	2.33	0.61
1:A:85:ASN:HD22	1:A:422:ARG:NH1	1.99	0.61
1:A:50:ALA:HA	1:A:53:PHE:HD1	1.66	0.60
1:A:89:GLN:O	1:A:92:ARG:HB2	2.01	0.60
1:A:418:VAL:HG12	1:A:422:ARG:NE	2.17	0.60
1:A:17:LEU:HD13	1:A:20:SER:HB2	1.81	0.60
1:A:197:LEU:HD13	1:A:220:LEU:HD22	1.82	0.60
1:A:192:ASP:HB3	1:A:282:GLN:HE22	1.67	0.60
1:A:80:ALA:CB	1:A:129:THR:HG21	2.31	0.60
1:A:451:SER:O	1:A:454:GLU:O	2.20	0.59
1:A:44:ALA:O	1:A:48:ALA:N	2.33	0.59
1:A:60:LEU:HA	1:A:63:ALA:HB3	1.84	0.59
1:A:77:THR:HG22	1:A:425:LEU:HD13	1.85	0.58
1:A:443:VAL:O	1:A:447:THR:HG23	2.03	0.58
1:A:352:ASP:HB3	1:A:357:LYS:NZ	2.18	0.58
1:A:463:SER:O	1:A:467:ARG:HB3	2.04	0.58
1:A:31:LEU:HD13	1:A:469:GLN:NE2	2.18	0.58
1:A:479:LEU:HA	1:A:482:ALA:HB3	1.86	0.58
1:A:81:LEU:O	1:A:422:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLN:OE1	1:A:453:ILE:HG23	2.04	0.58
1:A:325:VAL:HG22	1:A:342:ILE:HD11	1.86	0.58
1:A:41:LYS:HE2	1:A:453:ILE:CG2	2.32	0.57
1:A:439:LEU:O	1:A:443:VAL:HG23	2.03	0.57
1:A:42:ASP:O	1:A:44:ALA:N	2.29	0.57
1:A:418:VAL:O	1:A:422:ARG:HG3	2.05	0.57
1:A:417:GLN:O	1:A:421:LEU:HG	2.04	0.57
1:A:288:LEU:HB2	1:A:292:LYS:HG3	1.88	0.56
1:A:458:TYR:O	1:A:462:VAL:CB	2.51	0.56
1:A:85:ASN:HB2	1:A:422:ARG:NH2	2.21	0.56
1:A:160:LYS:HG3	1:A:421:LEU:CD2	2.34	0.56
1:A:43:ASP:O	1:A:46:GLY:N	2.39	0.56
1:A:450:ARG:CZ	1:A:454:GLU:OE1	2.54	0.55
1:A:85:ASN:HB2	1:A:422:ARG:HH12	1.72	0.55
1:A:474:ALA:O	1:A:478:VAL:HG23	2.07	0.55
1:A:45:ALA:O	1:A:49:ILE:HG13	2.07	0.55
1:A:253:ASN:OD1	1:A:255:GLU:HG3	2.07	0.55
1:A:300:VAL:CG1	1:A:327:VAL:HG11	2.37	0.55
1:A:73:ILE:HG12	1:A:131:PHE:CG	2.41	0.54
1:A:429:GLN:O	1:A:432:PHE:HB2	2.07	0.54
1:A:458:TYR:O	1:A:462:VAL:N	2.38	0.54
1:A:354:GLY:HA2	1:A:391:LYS:HZ1	1.72	0.54
1:A:428:VAL:HG12	1:A:432:PHE:CE1	2.42	0.54
1:A:453:ILE:O	1:A:455:ASP:N	2.41	0.54
1:A:285:ASN:O	1:A:287:ASP:N	2.41	0.54
1:A:378:LYS:HB3	1:A:398:GLU:HG2	1.90	0.53
1:A:300:VAL:HG12	1:A:327:VAL:HG11	1.89	0.53
1:A:311:TYR:CE2	1:A:369:LYS:HB3	2.44	0.53
1:A:354:GLY:HA2	1:A:391:LYS:HZ2	1.74	0.52
1:A:462:VAL:O	1:A:466:SER:N	2.41	0.52
1:A:284:ALA:O	1:A:285:ASN:C	2.53	0.52
1:A:13:THR:HA	1:A:16:ASN:HB2	1.91	0.52
1:A:443:VAL:O	1:A:447:THR:CG2	2.58	0.52
1:A:427:ALA:CB	1:A:431:ARG:NH2	2.73	0.51
1:A:73:ILE:HA	1:A:76:THR:OG1	2.11	0.51
1:A:389:ASN:OD1	1:A:391:LYS:HB3	2.10	0.51
1:A:7:ASN:O	1:A:11:LEU:HG	2.11	0.51
1:A:85:ASN:O	1:A:89:GLN:HG3	2.10	0.51
1:A:217:ASP:CB	1:A:232:LYS:HD3	2.37	0.50
1:A:61:THR:O	1:A:65:ARG:HG3	2.11	0.50
1:A:467:ARG:O	1:A:471:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:HA	1:A:154:THR:HG22	1.93	0.50
1:A:396:LEU:HD12	1:A:397:ALA:N	2.25	0.50
1:A:347:THR:CG2	1:A:382:ALA:HB1	2.34	0.50
1:A:442:THR:O	1:A:446:LEU:HG	2.12	0.49
1:A:379:THR:O	1:A:398:GLU:HB3	2.12	0.49
1:A:379:THR:HG23	1:A:398:GLU:OE1	2.12	0.49
1:A:486:PRO:O	1:A:490:LEU:HG	2.13	0.49
1:A:137:LEU:HD22	1:A:162:ILE:HB	1.94	0.49
1:A:427:ALA:HB3	1:A:431:ARG:NH1	2.28	0.49
1:A:199:ASN:HD22	1:A:199:ASN:N	2.11	0.48
1:A:306:VAL:HG22	1:A:342:ILE:HD13	1.94	0.48
1:A:52:ARG:O	1:A:56:ASN:ND2	2.45	0.48
1:A:72:SER:O	1:A:76:THR:HG23	2.13	0.48
1:A:9:LEU:HD13	1:A:9:LEU:HA	1.50	0.48
1:A:338:LYS:HD3	1:A:339:ASP:N	2.22	0.48
1:A:470:ILE:HA	1:A:473:GLN:HB2	1.94	0.47
1:A:80:ALA:HB2	1:A:129:THR:HG21	1.95	0.47
1:A:155:ILE:HD11	1:A:435:ALA:CB	2.44	0.47
1:A:15:ASN:O	1:A:18:ASN:HB2	2.14	0.47
1:A:85:ASN:ND2	1:A:422:ARG:NH1	2.63	0.47
1:A:105:GLN:HG3	1:A:313:ASP:HB2	1.96	0.47
1:A:50:ALA:HA	1:A:53:PHE:CD1	2.47	0.47
1:A:73:ILE:CG1	1:A:131:PHE:CD2	2.98	0.47
1:A:92:ARG:NH2	1:A:412:ASP:CG	2.73	0.46
1:A:160:LYS:CG	1:A:421:LEU:HD22	2.42	0.46
1:A:459:ALA:O	1:A:460:THR:C	2.58	0.46
1:A:141:ASN:HD21	1:A:143:LEU:CD1	2.28	0.46
1:A:485:VAL:N	1:A:486:PRO:HD2	2.29	0.46
1:A:120:ASN:HD21	1:A:384:LYS:HE3	1.81	0.46
1:A:418:VAL:HG11	1:A:422:ARG:NH2	2.30	0.46
1:A:426:GLY:O	1:A:429:GLN:HB2	2.16	0.46
1:A:373:VAL:O	1:A:379:THR:HA	2.16	0.46
1:A:6:THR:O	1:A:9:LEU:HB2	2.15	0.46
1:A:3:VAL:O	1:A:7:ASN:HB2	2.16	0.45
1:A:416:ALA:O	1:A:420:THR:HG22	2.17	0.45
1:A:139:GLN:HA	1:A:161:GLN:HB2	1.98	0.45
1:A:351:ALA:HB2	1:A:391:LYS:HZ3	1.81	0.45
1:A:284:ALA:O	1:A:286:ALA:N	2.50	0.45
1:A:493:LEU:H	1:A:493:LEU:HD23	1.82	0.45
1:A:60:LEU:HA	1:A:63:ALA:CB	2.47	0.45
1:A:69:ASP:O	1:A:73:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:THR:CG2	1:A:212:THR:HB	2.22	0.45
1:A:356:SER:O	1:A:357:LYS:HG3	2.17	0.45
1:A:473:GLN:O	1:A:476:THR:HG22	2.16	0.45
1:A:17:LEU:CB	1:A:479:LEU:HD12	2.46	0.44
1:A:21:GLN:HA	1:A:24:LEU:HD12	1.99	0.44
1:A:113:ALA:O	1:A:117:GLN:HG2	2.17	0.44
1:A:284:ALA:C	1:A:286:ALA:N	2.72	0.44
1:A:147:VAL:O	1:A:439:LEU:HD13	2.18	0.44
1:A:338:LYS:CD	1:A:339:ASP:H	2.24	0.44
1:A:388:HIS:HE1	1:A:393:GLN:O	2.01	0.44
1:A:429:GLN:HB2	1:A:430:ASN:H	1.62	0.44
1:A:18:ASN:O	1:A:21:GLN:HB3	2.18	0.43
1:A:88:LEU:HD11	1:A:167:LEU:HD13	2.01	0.43
1:A:155:ILE:HD12	1:A:432:PHE:CD2	2.54	0.43
1:A:465:MET:O	1:A:469:GLN:HG3	2.18	0.43
1:A:27:ALA:O	1:A:31:LEU:HD12	2.18	0.43
1:A:427:ALA:CB	1:A:431:ARG:CZ	2.97	0.43
1:A:462:VAL:O	1:A:466:SER:HB2	2.18	0.42
1:A:458:TYR:CA	1:A:462:VAL:HB	2.48	0.42
1:A:11:LEU:HD21	1:A:486:PRO:CB	2.50	0.42
1:A:201:THR:HG21	1:A:255:GLU:OE2	2.19	0.42
1:A:17:LEU:CG	1:A:479:LEU:HD12	2.50	0.42
1:A:94:LEU:HD11	1:A:114:GLU:CG	2.30	0.42
1:A:48:ALA:HA	1:A:51:ASN:HD22	1.84	0.42
1:A:351:ALA:HA	1:A:355:THR:O	2.19	0.42
1:A:95:ALA:HB3	1:A:408:LEU:HD21	2.01	0.42
1:A:350:THR:O	1:A:389:ASN:HA	2.19	0.42
1:A:104:SER:O	1:A:107:ASP:HB2	2.19	0.42
1:A:81:LEU:HD22	1:A:418:VAL:HG13	2.00	0.42
1:A:459:ALA:HA	1:A:462:VAL:HG12	2.01	0.42
1:A:354:GLY:C	1:A:355:THR:HG23	2.46	0.41
1:A:447:THR:OG1	1:A:448:SER:N	2.51	0.41
1:A:57:ILE:O	1:A:61:THR:N	2.54	0.41
1:A:203:LYS:HE3	1:A:203:LYS:HB2	1.89	0.41
1:A:37:ILE:HG22	1:A:37:ILE:O	2.21	0.41
1:A:427:ALA:HB1	1:A:431:ARG:CZ	2.51	0.41
1:A:130:GLN:HB3	1:A:135:LYS:HD3	2.03	0.41
1:A:28:ILE:O	1:A:32:SER:HB2	2.21	0.41
1:A:77:THR:CG2	1:A:425:LEU:CD1	2.97	0.41
1:A:418:VAL:HG11	1:A:422:ARG:HH21	1.86	0.41
1:A:85:ASN:HB2	1:A:422:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ARG:HG3	1:A:411:ILE:HG21	2.02	0.41
1:A:130:GLN:HA	1:A:134:VAL:O	2.21	0.41
1:A:451:SER:HA	1:A:454:GLU:HG3	2.03	0.41
1:A:47:GLN:HA	1:A:453:ILE:CD1	2.39	0.40
1:A:60:LEU:HD21	1:A:439:LEU:HB3	2.03	0.40
1:A:458:TYR:O	1:A:459:ALA:C	2.64	0.40
1:A:418:VAL:HG12	1:A:422:ARG:HE	1.83	0.40
1:A:49:ILE:HG21	1:A:49:ILE:HD13	1.74	0.40
1:A:105:GLN:HE21	1:A:105:GLN:HB3	1.72	0.40
1:A:351:ALA:HB2	1:A:391:LYS:NZ	2.37	0.40

There are no symmetry-related clashes.

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 PDB entries followed by that with respect to all EM entries.

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	492/494 (100%)	460 (94%)	27 (6%)	5 (1%)	12	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	ALA
1	A	352	ASP
1	A	395	ASP
1	A	459	ALA
1	A	394	PRO

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 PDB entries followed by that with respect to all EM

entries.

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	391/391 (100%)	345 (88%)	46 (12%)	5 21

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	4	ILE
1	A	10	SER
1	A	16	ASN
1	A	17	LEU
1	A	26	THR
1	A	28	ILE
1	A	36	ARG
1	A	38	ASN
1	A	42	ASP
1	A	43	ASP
1	A	54	THR
1	A	72	SER
1	A	98	SER
1	A	199	ASN
1	A	207	THR
1	A	214	GLN
1	A	215	LYS
1	A	225	THR
1	A	229	TYR
1	A	318	THR
1	A	338	LYS
1	A	342	ILE
1	A	343	SER
1	A	348	LYS
1	A	350	THR
1	A	358	THR
1	A	373	VAL
1	A	379	THR
1	A	386	GLU
1	A	391	LYS
1	A	409	GLN
1	A	412	ASP
1	A	419	ASP

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Mol	Chain	Res	Type
1	A	434	SER
1	A	437	THR
1	A	447	THR
1	A	450	ARG
1	A	451	SER
1	A	454	GLU
1	A	455	ASP
1	A	458	TYR
1	A	462	VAL
1	A	483	ASN
1	A	492	LEU
1	A	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	7	ASN
1	A	51	ASN
1	A	56	ASN
1	A	85	ASN
1	A	87	ASN
1	A	89	GLN
1	A	120	ASN
1	A	141	ASN
1	A	165	GLN
1	A	282	GLN
1	A	388	HIS
1	A	409	GLN
1	A	417	GLN
1	A	469	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 [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.