



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2026 – 05:28 pm BST

PDB ID : 9SJ6 / pdb_00009sj6
Title : Structure of the Clostridioides difficile CspB protease
Authors : Alcorlo, M.; Hermoso, J.
Deposited on : 2025-08-30
Resolution : 1.94 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

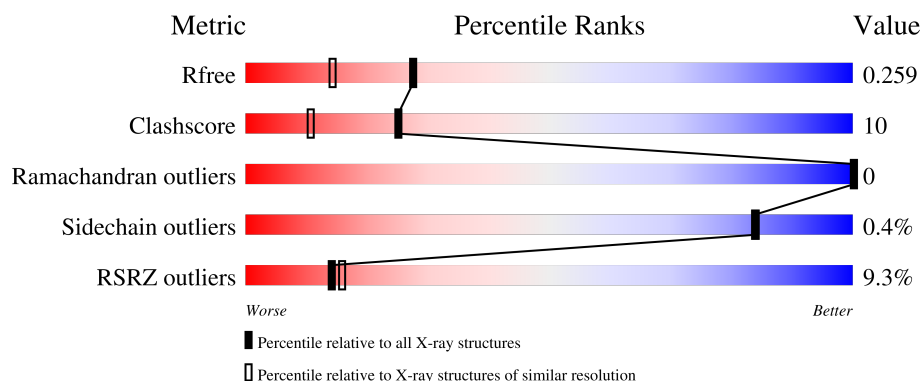
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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))
R_{free}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	65	<div> <div>9%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
1	B	65	<div> <div>3%</div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
2	C	492	<div> <div>7%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
2	D	492	<div> <div>11%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8535 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 Subtilisin-like serine germination related protease.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	61	Total	C	N	O	0	0	0
			497	321	72	104			
1	B	61	Total	C	N	O	0	0	0
			497	321	72	104			

- Molecule 2 is a protein called Subtilisin-like serine germination related protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	470	Total	C	N	O	S	0	0	0
			3637	2297	622	709	9			
2	D	470	Total	C	N	O	S	0	0	0
			3639	2297	622	711	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	65	MET	-	initiating methionine	UNP A0AB74Q767
C	549	LEU	-	expression tag	UNP A0AB74Q767
C	550	GLU	-	expression tag	UNP A0AB74Q767
C	551	HIS	-	expression tag	UNP A0AB74Q767
C	552	HIS	-	expression tag	UNP A0AB74Q767
C	553	HIS	-	expression tag	UNP A0AB74Q767
C	554	HIS	-	expression tag	UNP A0AB74Q767
C	555	HIS	-	expression tag	UNP A0AB74Q767
C	556	HIS	-	expression tag	UNP A0AB74Q767
D	65	MET	-	initiating methionine	UNP A0AB74Q767
D	549	LEU	-	expression tag	UNP A0AB74Q767
D	550	GLU	-	expression tag	UNP A0AB74Q767
D	551	HIS	-	expression tag	UNP A0AB74Q767
D	552	HIS	-	expression tag	UNP A0AB74Q767
D	553	HIS	-	expression tag	UNP A0AB74Q767
D	554	HIS	-	expression tag	UNP A0AB74Q767

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Chain	Residue	Modelled	Actual	Comment	Reference
D	555	HIS	-	expression tag	UNP A0AB74Q767
D	556	HIS	-	expression tag	UNP A0AB74Q767

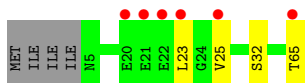
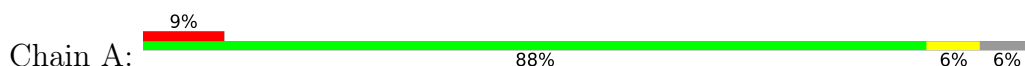
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	26	Total 26	O 26	0	0
3	C	132	Total 132	O 132	0	0
3	D	87	Total 87	O 87	0	0

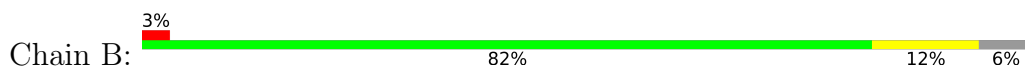
3 Residue-property plots [i](#)

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 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.

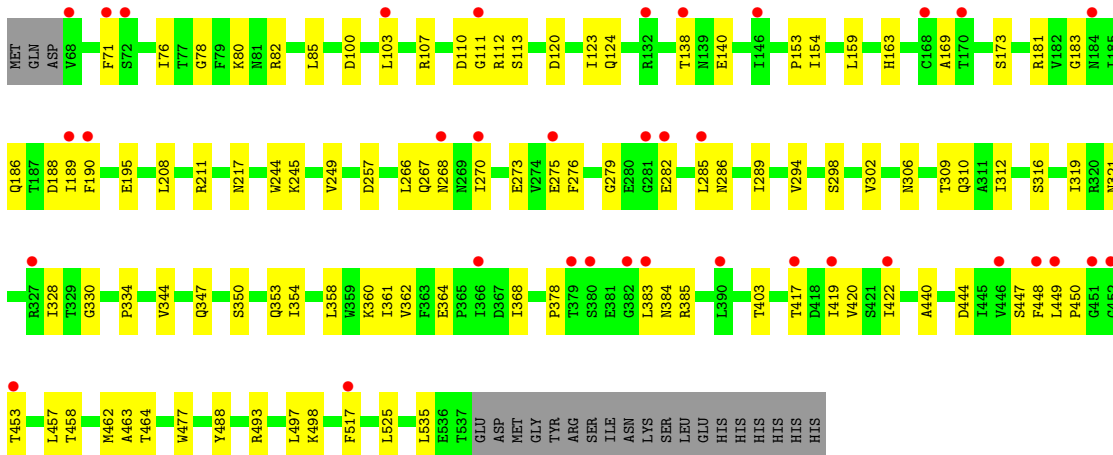
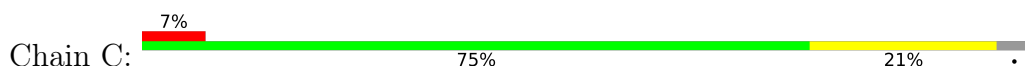
- Molecule 1: Subtilisin-like serine germination related protease



- Molecule 1: Subtilisin-like serine germination related protease

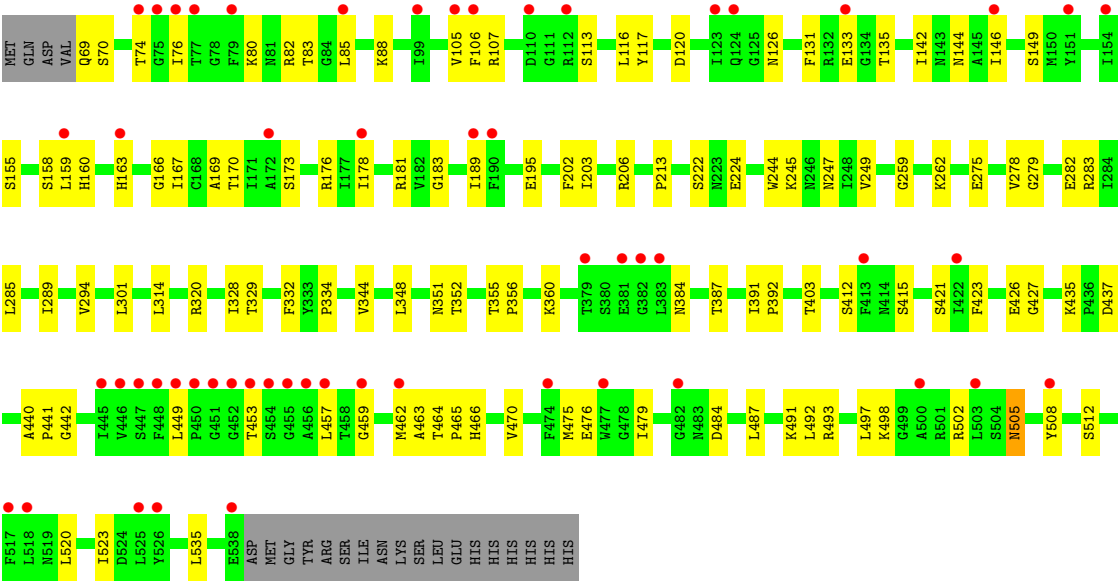


- Molecule 2: Subtilisin-like serine germination related protease



- Molecule 2: Subtilisin-like serine germination related protease





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	101.91Å 115.73Å 201.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 1.94 49.40 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.40-1.94) 99.9 (49.40-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.218 , 0.258 0.220 , 0.259	Depositor DCC
R_{free} test set	4531 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8535	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.42	0/504	0.66	0/684
1	B	0.43	0/504	0.65	0/684
2	C	0.36	0/3708	0.59	0/5043
2	D	0.34	1/3710 (0.0%)	0.56	0/5045
All	All	0.36	1/8426 (0.0%)	0.59	0/11456

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	352	THR	CA-C	5.72	1.57	1.52

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	497	0	492	3	0
1	B	497	0	492	5	0
2	C	3637	0	3595	82	0
2	D	3639	0	3592	76	0
3	A	20	0	0	0	0
3	B	26	0	0	0	0
3	C	132	0	0	3	0
3	D	87	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8535	0	8171	159	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 10.

All (159) 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)
2:C:159:LEU:HD11	2:C:449:LEU:HD22	1.55	0.89
2:D:116:LEU:HD21	2:D:176:ARG:HB3	1.55	0.87
2:D:159:LEU:HD23	2:D:160:HIS:H	1.45	0.81
2:C:159:LEU:CD1	2:C:449:LEU:HD22	2.13	0.77
2:C:100:ASP:HA	2:C:154:ILE:HD13	1.67	0.75
2:C:289:ILE:HB	2:C:344:VAL:HB	1.68	0.75
2:D:475:MET:HG2	2:D:479:ILE:HD12	1.74	0.70
2:C:310:GLN:HE21	2:C:321:ASN:HD21	1.40	0.69
2:C:310:GLN:NE2	2:C:321:ASN:HD21	1.92	0.67
2:D:262:LYS:HE3	2:D:391:ILE:HG23	1.76	0.67
2:D:449:LEU:HB2	2:D:453:THR:HG23	1.76	0.66
2:C:123:ILE:HD13	2:C:153:PRO:HG2	1.77	0.66
2:C:244:TRP:CG	2:C:245:LYS:H	2.13	0.66
2:D:457:LEU:HB3	2:D:462:MET:HE2	1.78	0.65
2:C:286:ASN:OD1	2:C:347:GLN:HG3	1.95	0.65
2:D:320:ARG:HG2	2:D:329:THR:HG22	1.79	0.65
2:D:244:TRP:CG	2:D:245:LYS:H	2.15	0.65
2:D:83:THR:HB	2:D:85:LEU:HG	1.80	0.64
2:D:502:ARG:HG2	2:D:508:TYR:CD2	2.33	0.63
2:D:159:LEU:HD23	2:D:160:HIS:N	2.14	0.62
2:D:169:ALA:O	2:D:173:SER:HA	1.99	0.62
1:A:65:THR:HG23	2:D:189:ILE:HD12	1.81	0.62
2:C:159:LEU:HD12	2:C:450:PRO:HD3	1.81	0.61
1:A:32:SER:HB2	1:B:32:SER:HB2	1.82	0.61
2:C:312:ILE:HD13	2:C:330:GLY:HA3	1.83	0.61
2:C:309:THR:HG21	2:C:328:ILE:HG21	1.83	0.61
2:C:249:VAL:HG12	2:C:464:THR:HG23	1.82	0.61
2:D:166:GLY:O	2:D:170:THR:HG23	2.00	0.61
2:C:535:LEU:HD23	2:D:334:PRO:HG2	1.83	0.61
2:D:283:ARG:NH1	2:D:351:ASN:O	2.34	0.60
2:C:159:LEU:HD12	2:C:450:PRO:CD	2.32	0.60
1:A:23:LEU:HB2	1:A:25:VAL:HG22	1.84	0.60
2:C:334:PRO:HG2	2:D:535:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:78:GLY:O	2:C:82:ARG:HG3	2.03	0.58
2:C:107:ARG:HG2	2:C:112:ARG:O	2.03	0.58
2:D:116:LEU:CD2	2:D:176:ARG:HB3	2.30	0.58
1:B:23:LEU:HD11	1:B:51:TYR:OH	2.04	0.57
2:C:123:ILE:HG12	2:C:186:GLN:HE21	1.70	0.57
2:D:88:LYS:O	2:D:476:GLU:HG3	2.06	0.56
2:D:449:LEU:HB2	2:D:453:THR:CG2	2.35	0.56
2:D:222:SER:OG	2:D:224:GLU:HG3	2.06	0.56
2:C:183:GLY:HA2	2:C:195:GLU:OE1	2.06	0.55
2:D:278:VAL:HG13	2:D:356:PRO:HA	1.88	0.55
1:B:44:ASP:CG	1:B:47:ILE:HD12	2.32	0.55
2:D:421:SER:HB3	2:D:423:PHE:CE1	2.42	0.55
2:C:163:HIS:CD2	2:C:457:LEU:HD12	2.42	0.54
2:C:266:LEU:HB2	2:C:368:ILE:HD12	1.89	0.54
2:C:159:LEU:HD11	2:C:449:LEU:CD2	2.34	0.54
2:D:178:ILE:HG21	2:D:203:ILE:HG12	1.89	0.54
2:D:131:PHE:HB3	2:D:133:GLU:OE2	2.08	0.54
2:C:306:ASN:ND2	3:C:608:HOH:O	2.41	0.54
2:D:213:PRO:HB2	2:D:475:MET:SD	2.48	0.53
2:D:289:ILE:HB	2:D:344:VAL:HB	1.91	0.53
2:C:270:ILE:HD12	2:C:270:ILE:O	2.09	0.53
2:D:279:GLY:HA3	2:D:384:ASN:OD1	2.08	0.53
2:C:159:LEU:CD1	2:C:450:PRO:HD2	2.38	0.53
2:C:107:ARG:HD3	2:C:111:GLY:O	2.08	0.53
2:C:163:HIS:ND1	2:C:447:SER:HB3	2.24	0.53
2:D:76:ILE:O	2:D:80:LYS:HG3	2.08	0.52
2:C:302:VAL:HB	2:C:360:LYS:HB2	1.92	0.52
1:B:6:TYR:CE1	1:B:42:GLU:HG3	2.46	0.51
2:C:85:LEU:HD11	2:C:477:TRP:HB2	1.91	0.51
2:D:423:PHE:CE2	2:D:459:GLY:HA2	2.46	0.51
2:C:188:ASP:OD1	2:C:189:ILE:N	2.44	0.51
2:C:316:SER:HB2	2:C:319:ILE:HD11	1.93	0.51
2:D:505:ASN:OD1	2:D:505:ASN:N	2.28	0.51
2:D:470:VAL:HG22	2:D:520:LEU:HD11	1.93	0.50
2:D:282:GLU:OE1	2:D:387:THR:OG1	2.25	0.50
2:C:107:ARG:HG2	2:C:112:ARG:C	2.37	0.50
2:C:169:ALA:O	2:C:173:SER:HA	2.11	0.50
2:D:142:ILE:O	2:D:146:ILE:HG13	2.12	0.50
2:C:163:HIS:CE1	2:C:447:SER:HB3	2.47	0.50
2:D:440:ALA:HB3	2:D:463:ALA:HB1	1.93	0.49
2:D:183:GLY:HA2	2:D:195:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:GLN:HB2	2:C:270:ILE:CG1	2.43	0.49
2:C:378:PRO:HD2	2:C:383:LEU:HD11	1.93	0.49
2:C:110:ASP:HB2	2:C:112:ARG:HG2	1.94	0.49
2:C:124:GLN:HA	2:C:124:GLN:OE1	2.12	0.49
2:D:328:ILE:HG12	2:D:348:LEU:CD2	2.43	0.49
2:C:462:MET:HE2	2:C:462:MET:H	1.77	0.49
2:D:247:ASN:ND2	2:D:492:LEU:HD23	2.28	0.49
2:D:275:GLU:HG3	2:D:360:LYS:HG2	1.94	0.49
2:D:441:PRO:HB2	2:D:466:HIS:CE1	2.48	0.49
2:C:384:ASN:OD1	2:C:385:ARG:N	2.46	0.48
2:C:208:LEU:O	2:C:211:ARG:HD3	2.13	0.48
2:D:105:VAL:HG13	2:D:106:PHE:CD1	2.49	0.48
2:D:163:HIS:O	2:D:167:ILE:HG13	2.14	0.48
2:D:487:LEU:HA	2:D:491:LYS:HD2	1.95	0.48
2:D:74:THR:OG1	2:D:76:ILE:HG13	2.13	0.48
2:C:417:THR:HB	2:C:419:ILE:HD12	1.95	0.48
2:D:437:ASP:HB3	2:D:497:LEU:HD21	1.95	0.48
1:B:64:GLN:NE2	2:C:190:PHE:HE2	2.12	0.47
2:D:178:ILE:CG2	2:D:203:ILE:HG12	2.44	0.47
2:D:426:GLU:HG2	2:D:512:SER:HA	1.95	0.47
2:C:294:VAL:HG23	2:D:498:LYS:HA	1.97	0.47
2:C:353:GLN:HG3	3:C:602:HOH:O	2.14	0.47
2:C:493:ARG:O	2:C:497:LEU:HG	2.15	0.47
2:D:155:SER:O	2:D:158:SER:OG	2.29	0.46
2:C:159:LEU:HD13	2:C:450:PRO:HD2	1.97	0.46
2:C:268:ASN:OD1	2:C:368:ILE:HB	2.15	0.46
2:D:285:LEU:HD12	2:D:285:LEU:HA	1.75	0.46
2:D:502:ARG:HG2	2:D:508:TYR:CE2	2.50	0.46
2:D:328:ILE:HG12	2:D:348:LEU:HD23	1.97	0.46
2:C:282:GLU:O	2:C:354:ILE:HG13	2.14	0.46
2:C:285:LEU:HD12	2:C:285:LEU:HA	1.86	0.46
2:C:120:ASP:HA	2:C:181:ARG:HB3	1.98	0.45
2:C:159:LEU:HD11	2:C:449:LEU:HD13	1.99	0.45
2:C:188:ASP:CG	2:C:190:PHE:HB2	2.42	0.45
2:D:120:ASP:HA	2:D:181:ARG:HB3	1.99	0.45
2:C:244:TRP:CG	2:C:245:LYS:N	2.80	0.45
2:C:189:ILE:HD12	2:C:190:PHE:N	2.32	0.45
2:D:117:TYR:HD1	2:D:178:ILE:HD11	1.82	0.45
2:C:279:GLY:HA3	2:C:384:ASN:ND2	2.33	0.44
2:D:82:ARG:NH2	2:D:523:ILE:O	2.50	0.44
2:D:244:TRP:CG	2:D:245:LYS:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:ASN:OD1	2:C:464:THR:HG22	2.18	0.44
2:C:245:LYS:HG2	2:C:488:TYR:CZ	2.53	0.43
2:C:417:THR:CB	2:C:419:ILE:HD12	2.47	0.43
2:C:103:LEU:HD23	2:C:448:PHE:HB3	1.99	0.43
2:C:113:SER:OG	3:C:601:HOH:O	2.21	0.43
2:C:449:LEU:HB2	2:C:453:THR:HG23	2.00	0.43
2:D:249:VAL:HG12	2:D:464:THR:HG23	1.99	0.43
2:D:314:LEU:HG	2:D:332:PHE:CD1	2.52	0.43
2:C:71:PHE:N	2:C:71:PHE:CD1	2.87	0.43
2:C:138:THR:HG22	2:C:140:GLU:H	1.84	0.43
2:D:126:ASN:H	2:D:135:THR:HG23	1.83	0.43
2:C:458:THR:C	2:C:462:MET:HE3	2.44	0.43
2:D:301:LEU:HD13	2:D:348:LEU:HD21	2.01	0.43
2:C:275:GLU:HB3	2:C:358:LEU:HD11	2.01	0.43
2:C:273:GLU:HG2	2:C:362:VAL:HG22	2.01	0.43
2:C:498:LYS:HA	2:D:294:VAL:HG23	2.01	0.43
2:C:159:LEU:CD1	2:C:450:PRO:CD	2.96	0.42
2:D:69:GLN:NE2	2:D:415:SER:O	2.52	0.42
2:D:484:ASP:HB3	2:D:487:LEU:HB2	2.01	0.42
2:D:282:GLU:OE2	2:D:384:ASN:N	2.29	0.42
2:C:477:TRP:NE1	2:C:525:LEU:HD13	2.35	0.42
2:C:276:PHE:HE1	2:C:361:ILE:HG13	1.84	0.42
2:C:85:LEU:CD1	2:C:477:TRP:HB2	2.50	0.42
2:C:298:SER:OG	2:C:364:GLU:HB2	2.20	0.41
2:C:440:ALA:HB3	2:C:463:ALA:HB1	2.02	0.41
2:D:259:GLY:HA2	2:D:392:PRO:HB3	2.01	0.41
2:C:76:ILE:O	2:C:80:LYS:HG3	2.21	0.41
2:D:144:ASN:HB3	2:D:149:SER:HB2	2.03	0.41
2:D:69:GLN:HG3	2:D:70:SER:N	2.35	0.41
2:D:107:ARG:HG2	2:D:113:SER:HA	2.01	0.41
2:D:107:ARG:HH11	2:D:146:ILE:HG21	1.85	0.41
2:D:493:ARG:O	2:D:497:LEU:HG	2.20	0.41
2:C:159:LEU:HD12	2:C:449:LEU:HD22	1.98	0.41
2:C:257:ASP:HB3	2:C:422:ILE:HG13	2.03	0.41
2:D:275:GLU:CG	2:D:360:LYS:HG2	2.50	0.41
2:C:350:SER:OG	2:C:353:GLN:N	2.54	0.41
2:C:419:ILE:HG22	2:C:420:VAL:O	2.21	0.41
2:C:517:PHE:CD1	2:C:517:PHE:N	2.89	0.41
2:D:355:THR:H	2:D:355:THR:HG23	1.59	0.40
2:D:412:SER:OG	2:D:442:GLY:HA3	2.21	0.40
2:C:189:ILE:H	2:C:189:ILE:HG13	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:167:ILE:HB	2:D:465:PRO:HB2	2.02	0.40
2:D:202:PHE:O	2:D:206:ARG:HG2	2.22	0.40
2:D:427:GLY:HA3	2:D:435:LYS:O	2.21	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 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	59/65 (91%)	59 (100%)	0	0	100	100
1	B	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
2	C	468/492 (95%)	454 (97%)	14 (3%)	0	100	100
2	D	468/492 (95%)	455 (97%)	13 (3%)	0	100	100
All	All	1054/1114 (95%)	1026 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	58/62 (94%)	58 (100%)	0	100	100
1	B	58/62 (94%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	407/428 (95%)	405 (100%)	2 (0%)	81	82
2	D	407/428 (95%)	405 (100%)	2 (0%)	81	82
All	All	930/980 (95%)	926 (100%)	4 (0%)	84	84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	403	THR
2	C	444	ASP
2	D	403	THR
2	D	505	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	B	64	GLN
2	C	126	ASN
2	C	163	HIS
2	C	186	GLN
2	C	307	ASN
2	C	310	GLN
2	C	506	GLN
2	D	217	ASN
2	D	247	ASN
2	D	300	HIS
2	D	307	ASN
2	D	351	ASN
2	D	466	HIS

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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	61/65 (93%)	0.59	6 (9%) 13 14	28, 46, 84, 100	0
1	B	61/65 (93%)	0.26	2 (3%) 49 55	27, 38, 66, 72	0
2	C	470/492 (95%)	0.81	36 (7%) 19 22	27, 60, 88, 113	0
2	D	470/492 (95%)	0.98	55 (11%) 9 10	29, 66, 97, 118	0
All	All	1062/1114 (95%)	0.84	99 (9%) 14 16	27, 61, 94, 118	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	68	VAL	6.4
2	D	159	LEU	4.1
2	D	446	VAL	4.0
2	C	382	GLY	3.9
2	D	190	PHE	3.9
2	C	270	ILE	3.7
2	D	462	MET	3.6
2	D	455	GLY	3.6
2	C	383	LEU	3.6
2	D	451	GLY	3.5
2	D	452	GLY	3.5
2	C	190	PHE	3.5
2	C	446	VAL	3.4
2	C	452	GLY	3.4
2	C	453	THR	3.4
2	D	448	PHE	3.3
2	C	451	GLY	3.3
1	B	65	THR	3.2
2	D	449	LEU	3.2
2	D	447	SER	3.2
2	D	457	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	170	THR	3.1
2	D	79	PHE	3.1
2	D	189	ILE	3.1
2	D	151	TYR	3.0
1	A	21	GLU	3.0
2	D	382	GLY	2.9
2	D	456	ALA	2.9
2	C	379	THR	2.9
2	D	163	HIS	2.9
2	C	380	SER	2.8
2	C	146	ILE	2.8
2	D	85	LEU	2.8
2	C	366	ILE	2.8
2	D	77	THR	2.7
1	A	22	GLU	2.7
2	D	76	ILE	2.7
2	D	154	ILE	2.7
2	D	477	TRP	2.6
2	D	508	TYR	2.6
2	D	453	THR	2.6
2	D	538	GLU	2.6
2	D	133	GLU	2.6
2	D	74	THR	2.6
2	D	482	GLY	2.6
2	D	450	PRO	2.5
2	D	383	LEU	2.5
2	C	422	ILE	2.5
2	D	105	VAL	2.5
1	A	23	LEU	2.5
2	C	449	LEU	2.5
2	C	517	PHE	2.4
2	C	419	ILE	2.4
2	D	517	PHE	2.3
2	C	103	LEU	2.3
2	C	71	PHE	2.3
2	D	459	GLY	2.3
1	A	20	GLU	2.3
2	D	503	LEU	2.3
2	D	75	GLY	2.3
2	D	146	ILE	2.3
2	D	422	ILE	2.3
2	C	72	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	448	PHE	2.2
2	D	381	GLU	2.2
2	D	474	PHE	2.2
2	C	268	ASN	2.2
2	C	132	ARG	2.2
2	C	168	CYS	2.2
2	D	454	SER	2.2
2	C	281	GLY	2.2
2	D	178	ILE	2.2
2	C	327	ARG	2.2
2	D	525	LEU	2.2
2	D	172	ALA	2.2
1	B	5	ASN	2.1
2	D	413	PHE	2.1
2	D	526	TYR	2.1
2	D	110	ASP	2.1
2	C	111	GLY	2.1
2	D	518	LEU	2.1
1	A	65	THR	2.1
2	D	379	THR	2.1
2	C	390	LEU	2.1
2	D	500	ALA	2.1
2	D	106	PHE	2.1
2	C	189	ILE	2.1
2	D	99	ILE	2.1
2	D	123	ILE	2.1
1	A	25	VAL	2.1
2	C	184	ASN	2.0
2	D	124	GLN	2.0
2	C	285	LEU	2.0
2	C	275	GLU	2.0
2	C	282	GLU	2.0
2	D	445	ILE	2.0
2	C	138	THR	2.0
2	C	417	THR	2.0
2	D	112	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.