



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:40 PM UTC

PDB ID : 4IM4 / pdb_00004im4
Title : Multifunctional cellulase, xylanase, mannanase
Authors : Bianchetti, C.M.; Takasuka, T.E.; Fox, B.G.
Deposited on : 2013-01-02
Resolution : 2.42 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

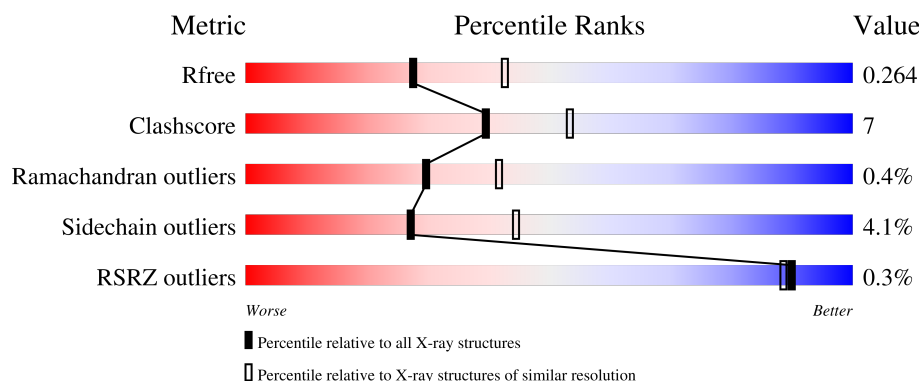
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	336	% 82% 15% .
1	B	336	86% 13% .
1	C	336	% 78% 21% .
1	D	336	88% 12% .
1	E	336	80% 18% .

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Mol	Chain	Length	Quality of chain
1	F	336	 85%15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17521 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 Endoglucanase E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2702	1715	469	508	10			
1	B	336	Total	C	N	O	S	0	1	0
			2702	1715	469	508	10			
1	C	336	Total	C	N	O	S	0	2	0
			2720	1731	469	510	10			
1	D	336	Total	C	N	O	S	0	0	0
			2694	1710	466	508	10			
1	E	336	Total	C	N	O	S	0	0	0
			2694	1710	466	508	10			
1	F	336	Total	C	N	O	S	0	1	0
			2697	1712	466	509	10			

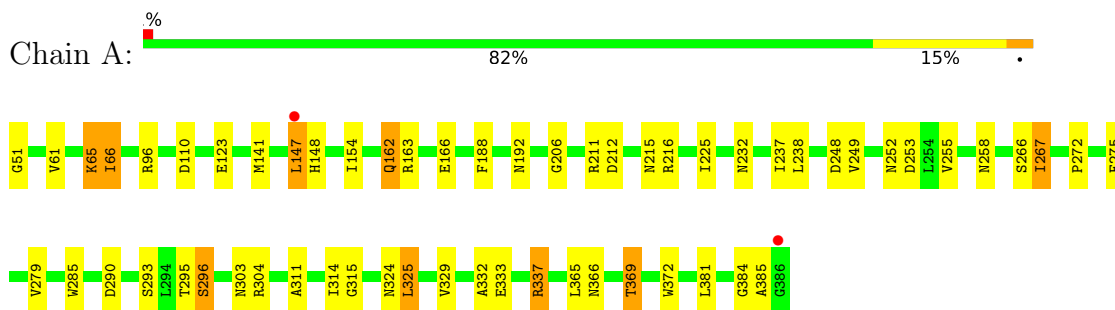
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	248	Total	O	0	0
			248	248		
2	B	205	Total	O	0	0
			205	205		
2	C	228	Total	O	0	0
			228	228		
2	D	205	Total	O	0	0
			205	205		
2	E	208	Total	O	0	0
			208	208		
2	F	218	Total	O	0	0
			218	218		

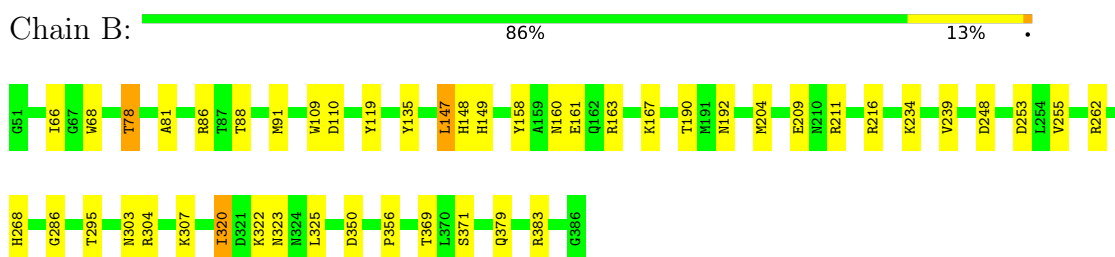
3 Residue-property plots

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 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.

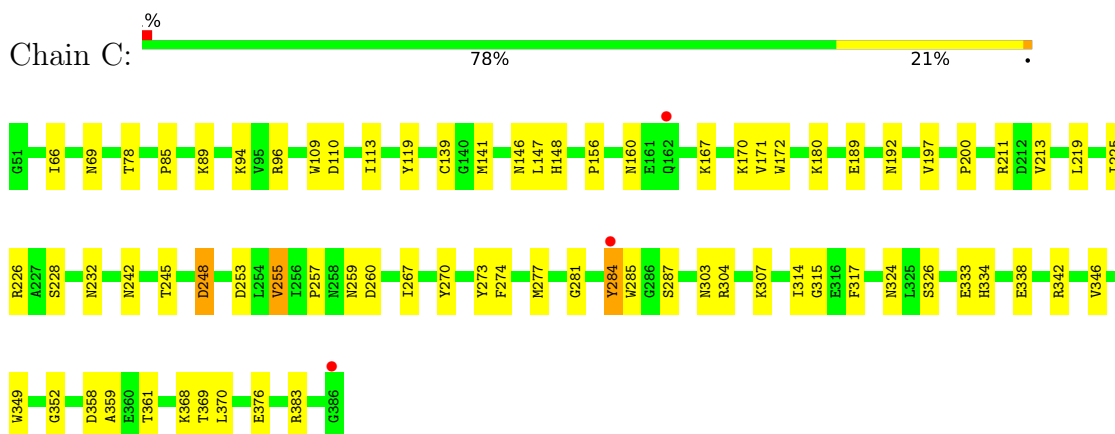
• Molecule 1: Endoglucanase E



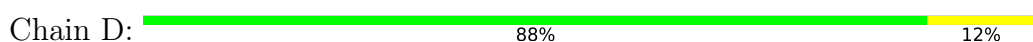
• Molecule 1: Endoglucanase E

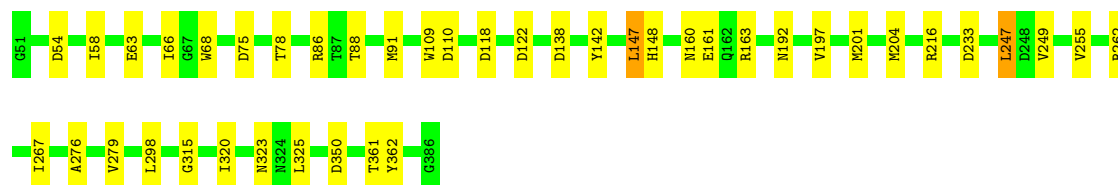


• Molecule 1: Endoglucanase E

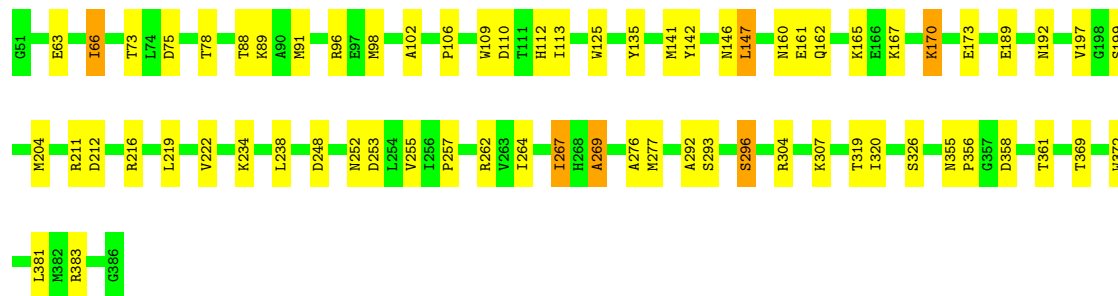
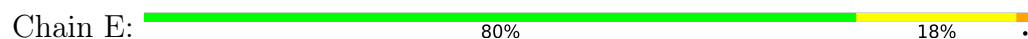


• Molecule 1: Endoglucanase E

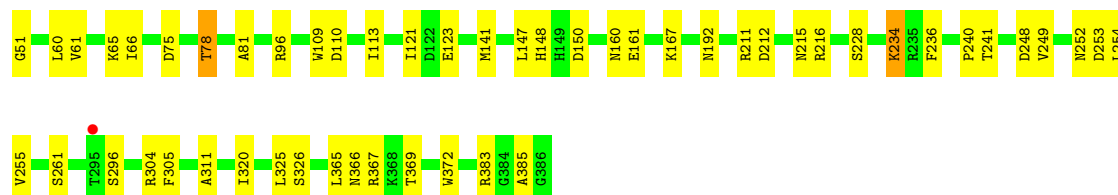
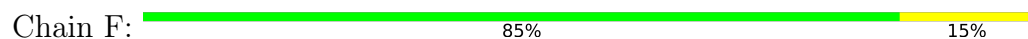




• Molecule 1: Endoglucanase E



• Molecule 1: Endoglucanase E



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.41Å 111.70Å 120.37Å 90.00° 97.29° 90.00°	Depositor
Resolution (Å)	47.35 – 2.42 47.35 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.35-2.42) 91.2 (47.35-2.42)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.209 , 0.264 0.211 , 0.264	Depositor DCC
R_{free} test set	1994 reflections (2.15%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17521	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1293e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.59	0/2773	0.86	0/3775
1	B	0.53	0/2773	0.82	1/3775 (0.0%)
1	C	0.54	0/2799	0.87	1/3811 (0.0%)
1	D	0.52	0/2762	0.84	0/3761
1	E	0.56	0/2762	0.87	1/3761 (0.0%)
1	F	0.53	0/2768	0.87	0/3769
All	All	0.55	0/16637	0.86	3/22652 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	ALA	N-CA-C	5.62	116.60	107.32
1	C	273	TYR	N-CA-C	5.11	117.25	111.11
1	B	135	TYR	N-CA-C	-5.09	105.73	111.28

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	2702	0	2610	37	0
1	B	2702	0	2610	25	0
1	C	2720	0	2628	49	0
1	D	2694	0	2597	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2694	0	2597	46	0
1	F	2697	0	2602	31	0
2	A	248	0	0	13	0
2	B	205	0	0	7	0
2	C	228	0	0	20	0
2	D	205	0	0	9	0
2	E	208	0	0	16	0
2	F	218	0	0	9	0
All	All	17521	0	15644	213	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 7.

All (213) 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:A:593:HOH:O	1:E:204:MET:SD	1.91	1.25
1:E:304:ARG:NH2	2:E:567:HOH:O	1.95	0.99
1:D:118:ASP:OD1	2:D:567:HOH:O	1.82	0.95
1:C:285:TRP:O	2:C:610:HOH:O	1.89	0.91
1:E:369:THR:OG1	2:E:444:HOH:O	1.87	0.88
1:E:253:ASP:OD1	2:E:585:HOH:O	1.93	0.86
1:D:54:ASP:OD1	2:D:404:HOH:O	1.92	0.86
1:D:233:ASP:OD1	2:D:559:HOH:O	1.94	0.86
1:F:121:ILE:O	2:F:468:HOH:O	1.94	0.85
1:D:138:ASP:OD2	2:D:495:HOH:O	1.96	0.83
1:F:147:LEU:HD21	1:F:150:ASP:HB2	1.60	0.83
1:A:248:ASP:OD2	2:A:561:HOH:O	1.96	0.83
1:F:211:ARG:NH1	1:F:253:ASP:OD2	2.13	0.82
1:A:381:LEU:HA	2:A:634:HOH:O	1.80	0.81
1:A:332:ALA:O	2:A:634:HOH:O	2.00	0.80
1:F:261:SER:O	2:F:472:HOH:O	2.00	0.79
1:E:211:ARG:NH2	2:E:523:HOH:O	2.15	0.79
1:A:51:GLY:N	2:A:412:HOH:O	2.15	0.79
1:A:211:ARG:NH1	1:A:253:ASP:OD2	2.17	0.77
1:C:228:SER:O	2:C:493:HOH:O	2.01	0.76
1:C:139:CYS:SG	2:C:570:HOH:O	2.43	0.76
1:D:58:ILE:O	2:D:432:HOH:O	2.03	0.76
1:C:200:PRO:O	2:C:508:HOH:O	2.04	0.75
1:A:304:ARG:HH21	1:D:204:MET:HE1	1.54	0.73
1:F:51:GLY:N	2:F:582:HOH:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:VAL:O	2:C:434:HOH:O	2.07	0.72
1:B:286:GLY:O	2:B:437:HOH:O	2.08	0.71
1:A:65:LYS:HD3	1:A:385:ALA:HB1	1.73	0.71
1:F:212:ASP:OD2	1:F:216:ARG:NH2	2.23	0.71
1:F:192:ASN:HB3	2:F:418:HOH:O	1.92	0.70
1:C:109:TRP:CD1	1:C:147:LEU:HG	2.28	0.67
1:C:94:LYS:HE3	1:C:370:LEU:HB3	1.76	0.67
1:A:296:SER:OG	2:A:622:HOH:O	2.02	0.67
1:A:304:ARG:NH2	1:D:204:MET:HE1	2.10	0.67
1:E:383:ARG:NH2	2:E:408:HOH:O	2.28	0.66
1:E:296:SER:OG	2:E:462:HOH:O	2.14	0.65
1:F:215:ASN:HA	2:F:501:HOH:O	1.96	0.64
1:B:356:PRO:O	2:B:521:HOH:O	2.15	0.64
1:F:228:SER:O	2:F:602:HOH:O	2.15	0.63
1:F:252:ASN:OD1	1:F:304:ARG:NH2	2.27	0.63
1:B:383:ARG:NH1	2:B:592:HOH:O	2.30	0.63
1:C:383:ARG:NH2	2:C:435:HOH:O	2.31	0.63
1:F:161:GLU:OE1	1:F:216:ARG:NH1	2.33	0.62
1:C:119:TYR:OH	2:C:487:HOH:O	1.90	0.62
1:E:248:ASP:OD2	1:E:304:ARG:NH1	2.33	0.62
1:F:234:LYS:HB2	1:F:234:LYS:HZ2	1.64	0.61
1:D:86:ARG:NH1	2:D:460:HOH:O	2.33	0.61
1:C:94:LYS:NZ	2:C:613:HOH:O	2.25	0.61
1:E:358:ASP:OD1	2:E:570:HOH:O	2.16	0.61
1:F:147:LEU:C	1:F:147:LEU:HD23	2.27	0.60
1:E:326:SER:HB3	2:E:471:HOH:O	2.03	0.59
1:C:146:ASN:HB3	1:C:189:GLU:HB3	1.83	0.59
1:C:89:LYS:HG3	2:C:570:HOH:O	2.01	0.59
1:D:262:ARG:NH2	2:D:501:HOH:O	2.31	0.59
1:C:304:ARG:NH2	2:C:585:HOH:O	2.36	0.58
1:D:247:LEU:HD12	1:D:249:VAL:HG22	1.86	0.57
1:A:324:ASN:OD1	2:A:447:HOH:O	2.17	0.57
1:C:148:HIS:HA	1:C:192:ASN:HB2	1.87	0.57
1:E:63:GLU:OE2	1:E:142:TYR:OH	2.22	0.57
1:F:167:LYS:NZ	2:F:436:HOH:O	2.29	0.57
1:F:147:LEU:CD2	1:F:150:ASP:HB2	2.34	0.56
1:A:325:LEU:HD22	1:A:329:VAL:HG23	1.87	0.56
1:C:352:GLY:HA2	2:C:527:HOH:O	2.05	0.56
1:E:170:LYS:NZ	1:E:173:GLU:OE2	2.38	0.56
1:B:86:ARG:NH1	2:B:429:HOH:O	2.34	0.56
1:B:160:ASN:HA	1:B:163[B]:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:THR:HA	1:E:356:PRO:O	2.06	0.55
1:D:320:ILE:HD11	1:D:362:TYR:CE2	2.42	0.55
1:F:65:LYS:HD3	1:F:385:ALA:HB1	1.88	0.55
1:E:212:ASP:OD2	1:E:216:ARG:NH2	2.39	0.55
1:E:96:ARG:HB2	1:E:141:MET:HE2	1.89	0.55
1:C:248:ASP:OD2	1:C:304:ARG:NH1	2.40	0.54
1:E:66:ILE:HD11	1:E:381:LEU:HD13	1.90	0.54
1:D:315:GLY:HA3	2:D:523:HOH:O	2.07	0.54
1:C:147:LEU:HD21	1:C:171:VAL:HG11	1.89	0.53
1:B:158:TYR:CE2	1:B:209:GLU:HG3	2.44	0.53
1:A:303:ASN:ND2	2:A:642:HOH:O	2.31	0.53
1:A:148:HIS:HA	1:A:192:ASN:HB2	1.89	0.53
1:A:258:ASN:HA	2:A:429:HOH:O	2.09	0.53
1:A:315:GLY:HA3	2:A:542:HOH:O	2.08	0.52
1:E:167:LYS:NZ	2:E:518:HOH:O	2.17	0.52
1:A:96:ARG:HB2	1:A:141:MET:HE2	1.92	0.51
1:D:122:ASP:OD1	2:D:497:HOH:O	2.19	0.51
1:A:215:ASN:HA	2:A:433:HOH:O	2.10	0.51
1:B:234:LYS:HB3	1:B:262:ARG:HH21	1.74	0.51
1:D:161:GLU:OE2	1:D:216:ARG:HD2	2.10	0.51
1:C:113:ILE:HG21	1:C:167:LYS:HE3	1.93	0.51
1:C:303:ASN:HA	1:C:307:LYS:HD3	1.93	0.51
1:C:96:ARG:HB2	1:C:141:MET:HE2	1.92	0.50
1:E:248:ASP:OD1	2:E:458:HOH:O	2.19	0.50
1:C:284[A]:TYR:OH	1:C:287:SER:HB3	2.10	0.50
1:A:212:ASP:CG	1:A:216:ARG:HH22	2.20	0.50
1:B:119:TYR:CE1	1:B:167:LYS:HD2	2.47	0.50
1:C:211:ARG:NH1	1:C:253:ASP:OD2	2.43	0.50
1:A:267:ILE:O	1:A:314:ILE:HA	2.12	0.50
1:B:204:MET:O	2:B:431:HOH:O	2.19	0.50
1:E:267:ILE:HD11	1:E:269:ALA:HB2	1.94	0.50
1:A:333:GLU:OE2	1:A:337[A]:ARG:NH2	2.45	0.50
1:E:211:ARG:NH1	1:E:253:ASP:OD2	2.45	0.49
1:A:66:ILE:HD11	1:A:381:LEU:HD13	1.94	0.49
1:D:109:TRP:CD1	1:D:147:LEU:HG	2.47	0.49
1:D:320:ILE:HD12	1:D:361:THR:N	2.29	0.48
1:E:146:ASN:HB3	1:E:189:GLU:HB3	1.94	0.48
1:F:366:ASN:CG	1:F:369:THR:HG22	2.39	0.48
1:C:334:HIS:HE1	2:C:628:HOH:O	1.97	0.48
1:D:320:ILE:HD11	1:D:362:TYR:CZ	2.49	0.47
1:B:248:ASP:OD2	1:B:304:ARG:NH1	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:ARG:HB2	1:F:141:MET:HE2	1.96	0.47
1:B:161:GLU:OE2	1:B:216:ARG:HD2	2.15	0.47
1:A:248:ASP:OD1	1:A:249:VAL:N	2.48	0.47
1:D:88:THR:HG23	1:D:91:MET:HE3	1.96	0.47
1:F:383:ARG:NH2	2:F:502:HOH:O	2.08	0.47
1:F:304:ARG:HD3	1:F:305:PHE:CZ	2.50	0.47
1:D:68:TRP:NE1	1:D:350:ASP:OD2	2.44	0.47
1:D:109:TRP:HD1	1:D:147:LEU:HG	1.79	0.47
1:C:361:THR:HB	2:C:492:HOH:O	2.15	0.46
1:F:248:ASP:OD1	1:F:249:VAL:N	2.48	0.46
1:B:320:ILE:HD11	1:B:322:LYS:HE3	1.97	0.46
1:B:379:GLN:OE1	2:B:456:HOH:O	2.20	0.46
1:C:180:LYS:NZ	2:C:545:HOH:O	2.19	0.46
1:D:75:ASP:OD1	1:D:75:ASP:N	2.46	0.46
1:E:109:TRP:CD1	1:E:147:LEU:HG	2.51	0.46
1:E:219:LEU:HA	1:E:257:PRO:HB3	1.98	0.46
1:A:147:LEU:HD11	1:A:154:ILE:HD11	1.97	0.46
1:A:238:LEU:HB3	1:A:266:SER:HB2	1.98	0.45
1:C:270:TYR:HB2	1:C:277:MET:SD	2.56	0.45
1:C:274:PHE:O	1:C:281:GLY:HA3	2.16	0.45
1:D:148:HIS:HA	1:D:192:ASN:HB2	1.98	0.45
1:A:61:VAL:HG21	1:A:311:ALA:HB1	1.98	0.45
1:E:252:ASN:HA	1:E:304:ARG:NH2	2.31	0.45
1:B:148:HIS:HA	1:B:192:ASN:HB2	1.98	0.45
1:E:113:ILE:HG21	1:E:167:LYS:HE3	1.99	0.45
1:A:162:GLN:HG3	1:A:163:ARG:N	2.32	0.45
1:B:78:THR:HG22	1:B:81:ALA:N	2.31	0.45
1:C:304:ARG:NE	2:C:585:HOH:O	2.50	0.45
1:E:73:THR:HB	2:E:410:HOH:O	2.16	0.45
1:E:106:PRO:HD2	2:E:409:HOH:O	2.16	0.45
1:C:242:ASN:O	1:C:245:THR:HG22	2.17	0.44
1:E:89:LYS:HB2	1:E:135:TYR:CD1	2.52	0.44
1:E:102:ALA:HB2	1:E:142:TYR:HB2	1.98	0.44
1:B:149:HIS:NE2	2:B:501:HOH:O	2.03	0.44
1:F:148:HIS:HA	1:F:192:ASN:HB2	2.00	0.44
1:F:161:GLU:CD	1:F:216:ARG:HH11	2.26	0.44
1:A:272:PRO:HG2	1:A:275:PHE:HB3	1.99	0.44
1:E:292:ALA:O	1:E:296:SER:HB3	2.17	0.44
1:F:367:ARG:HG3	2:F:428:HOH:O	2.18	0.44
1:A:381:LEU:HD23	2:A:634:HOH:O	2.17	0.44
1:C:324:ASN:N	1:C:324:ASN:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:SER:HB3	2:C:566:HOH:O	2.17	0.44
1:E:222:VAL:HG21	1:E:257:PRO:HG2	2.00	0.44
1:F:241:THR:HB	1:F:254:LEU:HD13	2.00	0.44
1:B:211:ARG:NE	1:B:253:ASP:OD2	2.41	0.43
1:C:219:LEU:HA	1:C:257:PRO:HB3	2.00	0.43
1:B:234:LYS:HB3	1:B:262:ARG:NH2	2.32	0.43
1:E:234:LYS:HB3	1:E:262:ARG:NH2	2.33	0.43
1:D:276:ALA:O	1:D:320:ILE:HG12	2.18	0.43
1:A:188:PHE:O	1:A:237:ILE:HA	2.18	0.43
1:E:234:LYS:HE2	2:E:551:HOH:O	2.17	0.43
1:B:192:ASN:OD1	1:B:268:HIS:HE1	2.01	0.43
1:C:315:GLY:HA3	2:C:401:HOH:O	2.19	0.43
1:D:63:GLU:OE2	1:D:142:TYR:OH	2.35	0.43
1:E:96:ARG:NH1	2:E:564:HOH:O	2.50	0.43
1:B:68:TRP:NE1	1:B:350:ASP:OD2	2.46	0.42
1:F:61:VAL:HG21	1:F:311:ALA:HB1	2.01	0.42
1:C:226:ARG:HH21	1:C:260:ASP:CG	2.27	0.42
1:C:314:ILE:HB	1:C:346:VAL:HG12	2.01	0.42
1:F:161:GLU:OE2	1:F:216:ARG:HD2	2.19	0.42
1:C:96:ARG:NH1	2:C:432:HOH:O	2.52	0.42
1:B:88:THR:HG23	1:B:91:MET:HE3	2.00	0.42
1:E:199:SER:OG	2:E:429:HOH:O	2.07	0.42
1:B:109:TRP:CD1	1:B:147:LEU:HG	2.55	0.42
1:A:365:LEU:HB2	1:A:372:TRP:CZ3	2.54	0.42
1:A:366:ASN:CG	1:A:369:THR:HG22	2.44	0.42
1:F:60:LEU:HD13	1:F:236:PHE:CE1	2.55	0.42
1:C:147:LEU:HD13	1:C:172:TRP:NE1	2.34	0.42
1:C:225:ILE:O	1:C:232:ASN:HB3	2.19	0.42
1:A:147:LEU:HD21	1:A:154:ILE:CD1	2.49	0.42
1:D:201:MET:SD	1:D:204:MET:HE3	2.59	0.42
1:E:75:ASP:OD1	1:E:75:ASP:N	2.47	0.42
1:E:98:MET:HG3	1:E:372:TRP:CE2	2.55	0.42
1:F:109:TRP:O	1:F:113:ILE:HG13	2.20	0.42
1:A:252:ASN:OD1	1:A:304:ARG:NH2	2.38	0.42
1:B:303:ASN:HA	1:B:307:LYS:HD3	2.02	0.42
1:E:88:THR:HG23	1:E:91:MET:HE3	2.01	0.42
1:F:365:LEU:HB2	1:F:372:TRP:CZ3	2.54	0.42
1:B:190:THR:HG21	1:B:239:VAL:HG12	2.02	0.41
1:E:161:GLU:OE2	1:E:216:ARG:HD2	2.19	0.41
1:C:304:ARG:CZ	2:C:585:HOH:O	2.66	0.41
1:C:333:GLU:OE1	1:C:383:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:THR:HB	1:F:81:ALA:HB2	2.03	0.41
1:A:337[B]:ARG:HD2	1:A:384:GLY:O	2.20	0.41
1:C:358:ASP:OD1	1:C:359:ALA:N	2.49	0.41
1:C:85:PRO:HB3	1:C:368:LYS:HZ3	1.85	0.41
1:C:94:LYS:NZ	2:C:574:HOH:O	2.11	0.41
1:C:156:PRO:HA	1:C:213:VAL:HG11	2.03	0.41
1:C:338:GLU:O	1:C:342:ARG:NH1	2.50	0.41
1:C:85:PRO:HB3	1:C:368:LYS:NZ	2.35	0.41
1:C:317:PHE:CE1	1:C:346:VAL:HB	2.56	0.41
1:E:112:HIS:CD2	1:E:125:TRP:CE2	3.09	0.41
1:E:165:LYS:HB2	1:E:165:LYS:HE3	1.92	0.41
1:E:277:MET:HE2	1:E:277:MET:HB3	1.93	0.41
1:A:285:TRP:NE1	1:A:290:ASP:HB3	2.36	0.40
1:C:69:ASN:HB2	1:C:349:TRP:HA	2.03	0.40
1:E:276:ALA:CB	1:E:319:THR:HG22	2.51	0.40
1:C:376:GLU:H	1:C:376:GLU:CD	2.29	0.40
1:A:225:ILE:O	1:A:232:ASN:HB3	2.22	0.40
1:D:298:LEU:HD23	1:D:298:LEU:HA	1.87	0.40
1:A:206:GLY:HA2	2:A:514:HOH:O	2.19	0.40
1:E:192:ASN:HB3	2:E:428:HOH:O	2.20	0.40
1:D:320:ILE:HD12	1:D:320:ILE:HG23	1.88	0.40
1:D:320:ILE:HD12	1:D:361:THR:H	1.85	0.40
1:E:238:LEU:HA	1:E:264:ILE:O	2.22	0.40
1:E:355:ASN:O	1:E:361:THR:HG21	2.22	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	335/336 (100%)	320 (96%)	13 (4%)	2 (1%)	21 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	335/336 (100%)	320 (96%)	14 (4%)	1 (0%)	36	49
1	C	337/336 (100%)	322 (96%)	14 (4%)	1 (0%)	36	49
1	D	334/336 (99%)	319 (96%)	14 (4%)	1 (0%)	36	49
1	E	334/336 (99%)	320 (96%)	13 (4%)	1 (0%)	36	49
1	F	335/336 (100%)	320 (96%)	13 (4%)	2 (1%)	21	30
All	All	2010/2016 (100%)	1921 (96%)	81 (4%)	8 (0%)	30	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	B	110	ASP
1	C	110	ASP
1	D	110	ASP
1	E	110	ASP
1	F	110	ASP
1	A	65	LYS
1	F	240	PRO

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	285/284 (100%)	270 (95%)	15 (5%)	20	34
1	B	285/284 (100%)	276 (97%)	9 (3%)	34	54
1	C	287/284 (101%)	274 (96%)	13 (4%)	24	40
1	D	284/284 (100%)	272 (96%)	12 (4%)	26	43
1	E	284/284 (100%)	271 (95%)	13 (5%)	24	39
1	F	285/284 (100%)	274 (96%)	11 (4%)	28	46
All	All	1710/1704 (100%)	1637 (96%)	73 (4%)	27	42

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ILE
1	A	123	GLU
1	A	147	LEU
1	A	162	GLN
1	A	166	GLU
1	A	255	VAL
1	A	267	ILE
1	A	279	VAL
1	A	293	SER
1	A	295	THR
1	A	296	SER
1	A	325	LEU
1	A	337[A]	ARG
1	A	337[B]	ARG
1	A	369	THR
1	B	66	ILE
1	B	78	THR
1	B	147	LEU
1	B	255	VAL
1	B	295	THR
1	B	320	ILE
1	B	323	ASN
1	B	325	LEU
1	B	371	SER
1	C	66	ILE
1	C	78	THR
1	C	160	ASN
1	C	170	LYS
1	C	197	VAL
1	C	248	ASP
1	C	255	VAL
1	C	259	ASN
1	C	267	ILE
1	C	284[A]	TYR
1	C	284[B]	TYR
1	C	284[C]	TYR
1	C	369	THR
1	D	66	ILE
1	D	78	THR
1	D	147	LEU
1	D	160	ASN
1	D	163	ARG
1	D	197	VAL

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Mol	Chain	Res	Type
1	D	247	LEU
1	D	255	VAL
1	D	267	ILE
1	D	279	VAL
1	D	323	ASN
1	D	325	LEU
1	E	66	ILE
1	E	78	THR
1	E	147	LEU
1	E	160	ASN
1	E	162	GLN
1	E	170	LYS
1	E	197	VAL
1	E	255	VAL
1	E	267	ILE
1	E	293	SER
1	E	296	SER
1	E	307	LYS
1	E	320	ILE
1	F	66	ILE
1	F	75	ASP
1	F	78	THR
1	F	123	GLU
1	F	160	ASN
1	F	234	LYS
1	F	255	VAL
1	F	296	SER
1	F	320	ILE
1	F	325	LEU
1	F	326	SER

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	268	HIS
1	A	323	ASN
1	B	160	ASN
1	B	185	HIS
1	B	252	ASN
1	B	258	ASN
1	C	112	HIS
1	C	323	ASN

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Mol	Chain	Res	Type
1	C	334	HIS
1	D	185	HIS
1	D	308	ASN
1	E	151	ASN
1	E	160	ASN
1	F	151	ASN
1	F	242	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	336/336 (100%)	-0.08	2 (0%) 85 84	6, 12, 22, 40	1 (0%)
1	B	336/336 (100%)	-0.17	0 100 100	6, 13, 25, 34	1 (0%)
1	C	336/336 (100%)	0.06	3 (0%) 81 79	5, 14, 24, 40	2 (0%)
1	D	336/336 (100%)	-0.08	0 100 100	7, 14, 28, 39	0
1	E	336/336 (100%)	-0.05	0 100 100	6, 12, 22, 35	0
1	F	336/336 (100%)	0.05	1 (0%) 90 88	8, 14, 26, 34	1 (0%)
All	All	2016/2016 (100%)	-0.04	6 (0%) 90 88	5, 13, 25, 40	5 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	284[A]	TYR	6.5
1	C	162	GLN	2.7
1	A	147	LEU	2.4
1	A	386	GLY	2.2
1	C	386	GLY	2.1
1	F	295	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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.