Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:41 PM GMT

PDB ID	:	4PMU
Title	:	Crystal structure of a novel reducing-end xylose-releasing exo-oligoxylanase (XynA) belonging to GH10 family (space group P1211)
Authors	:	Santos, C.R.; Martins, V.P.M.; Zanphorlin, L.M.; Ruller, R.; Murakami, M.T.
Deposited on	:	2014-05-22
Resolution	:	2.86 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

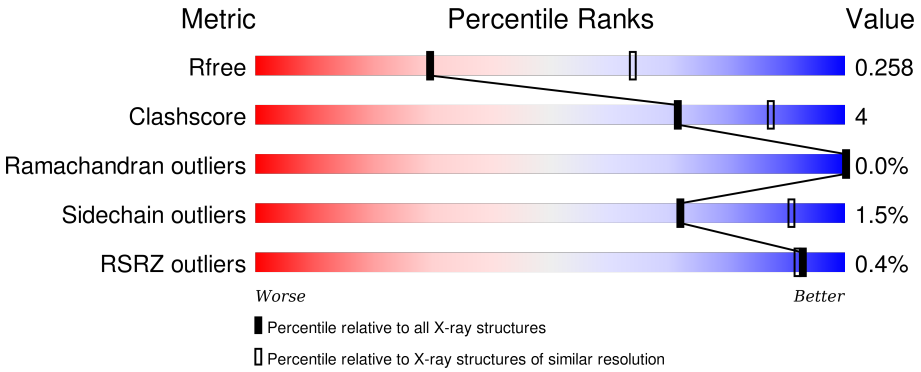
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.86 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	356	88% 11%
1	B	356	% 87% 13%
1	C	356	% 88% 12%
1	D	356	88% 12%
1	E	356	89% 11%

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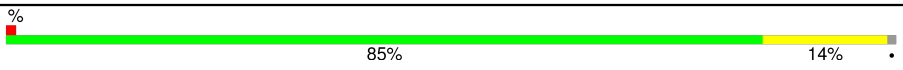
Mol	Chain	Length	Quality of chain
1	F	356	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16928 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 Endo-1,4-beta-xylanase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2805	1780	505	511	9			
1	B	356	Total	C	N	O	S	0	0	0
			2812	1784	506	513	9			
1	C	356	Total	C	N	O	S	0	0	0
			2812	1784	506	513	9			
1	D	355	Total	C	N	O	S	0	0	0
			2805	1780	505	511	9			
1	E	355	Total	C	N	O	S	0	0	0
			2805	1780	505	511	9			
1	F	354	Total	C	N	O	S	0	0	0
			2798	1776	504	509	9			

- Molecule 2 is water.

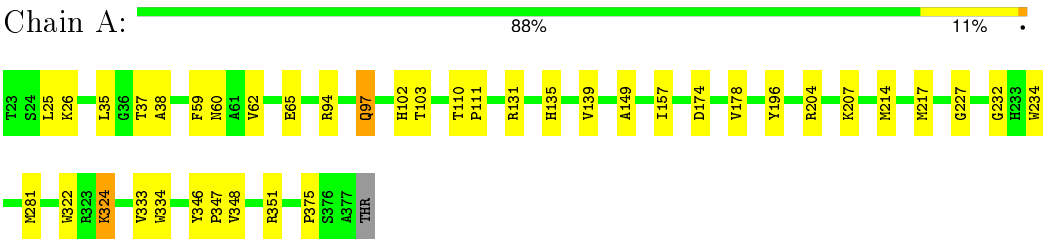
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	17	Total	O	0	0
			17	17		
2	C	19	Total	O	0	0
			19	19		
2	D	17	Total	O	0	0
			17	17		
2	E	21	Total	O	0	0
			21	21		
2	F	8	Total	O	0	0
			8	8		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

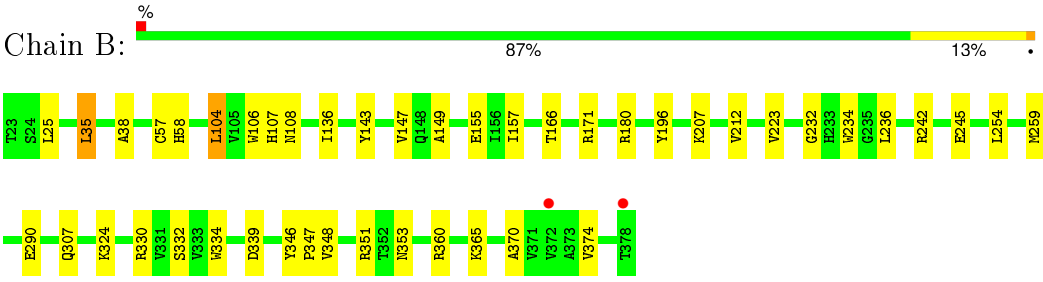
- Molecule 1: Endo-1,4-beta-xylanase A

Chain A:



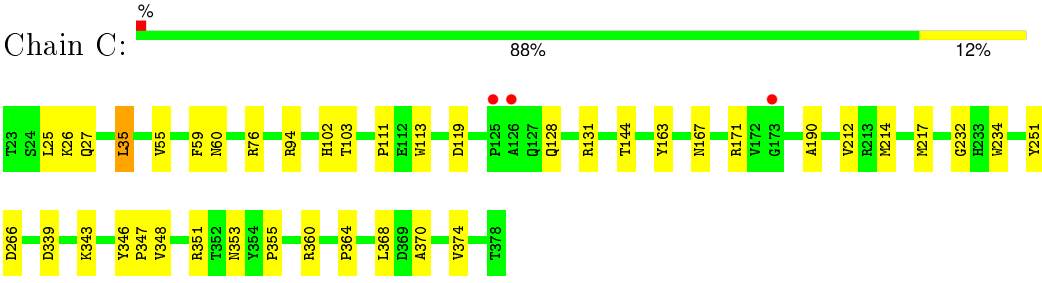
- Molecule 1: Endo-1,4-beta-xylanase A

Chain B:



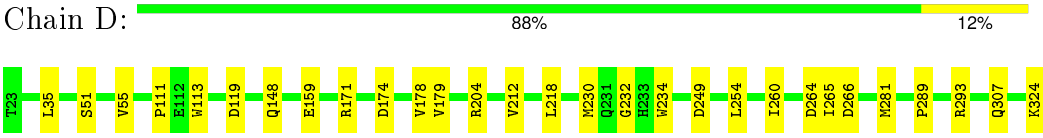
- Molecule 1: Endo-1,4-beta-xylanase A

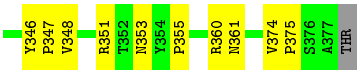
Chain C:



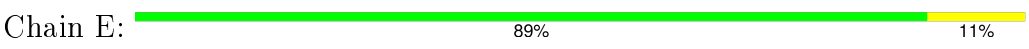
- Molecule 1: Endo-1,4-beta-xylanase A

Chain D:

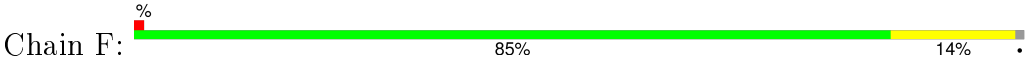


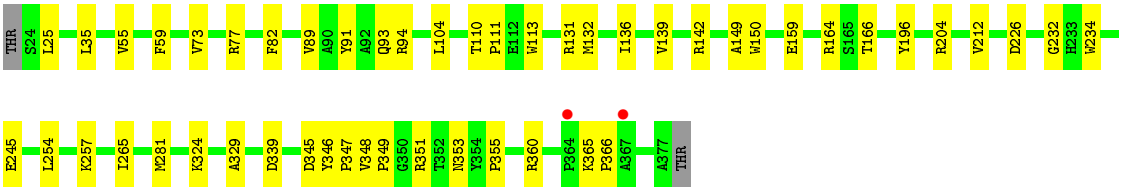


• Molecule 1: Endo-1,4-beta-xylanase A



• Molecule 1: Endo-1,4-beta-xylanase A





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.02Å 100.74Å 134.20Å 90.00° 95.15° 90.00°	Depositor
Resolution (Å)	41.15 – 2.86 41.15 – 2.86	Depositor EDS
% Data completeness (in resolution range)	97.2 (41.15-2.86) 97.2 (41.15-2.86)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.211 , 0.261 0.209 , 0.258	Depositor DCC
R_{free} test set	2651 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	46.2	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 16.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 52253 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16928	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.30	0/2875	0.49	0/3911
1	B	0.30	0/2882	0.49	0/3921
1	C	0.30	0/2882	0.48	0/3921
1	D	0.30	0/2875	0.49	0/3911
1	E	0.30	0/2875	0.48	0/3911
1	F	0.30	0/2868	0.48	0/3901
All	All	0.30	0/17257	0.48	0/23476

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

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	2805	0	2733	24	0
1	B	2812	0	2740	25	0
1	C	2812	0	2740	23	0
1	D	2805	0	2733	21	0
1	E	2805	0	2733	23	0
1	F	2798	0	2726	28	0
2	A	9	0	0	0	0
2	B	17	0	0	0	0
2	C	19	0	0	0	0
2	D	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	21	0	0	1	0
2	F	8	0	0	0	0
All	All	16928	0	16405	142	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 4.

All (142) 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:C:348:VAL:HB	1:C:351:ARG:HD2	1.30	1.13
1:A:348:VAL:HB	1:A:351:ARG:HD2	1.26	1.09
1:D:348:VAL:HB	1:D:351:ARG:HD2	1.37	1.06
1:E:348:VAL:HB	1:E:351:ARG:HD2	1.51	0.93
1:F:348:VAL:HB	1:F:351:ARG:HD2	1.51	0.89
1:B:348:VAL:HB	1:B:351:ARG:HD2	1.63	0.79
1:C:364:PRO:HB3	1:C:368:LEU:HD23	1.69	0.74
1:F:25:LEU:HB3	1:F:35:LEU:HD23	1.68	0.73
1:C:339:ASP:HB3	1:C:360:ARG:HG2	1.72	0.71
1:B:339:ASP:HB3	1:B:360:ARG:HG2	1.73	0.70
1:C:25:LEU:HB3	1:C:35:LEU:HD22	1.75	0.67
1:A:149:ALA:HB1	1:A:196:TYR:CE2	2.30	0.67
1:A:25:LEU:HB3	1:A:35:LEU:HD22	1.77	0.66
1:B:281:MET:HB3	1:B:348:VAL:HG22	1.76	0.66
1:B:348:VAL:HB	1:B:351:ARG:CD	2.27	0.65
1:E:348:VAL:HB	1:E:351:ARG:CD	2.25	0.64
1:F:232:GLY:HA2	1:F:234:TRP:CE2	2.34	0.63
1:C:353:ASN:O	1:C:360:ARG:NH2	2.33	0.62
1:B:353:ASN:O	1:B:360:ARG:NH2	2.33	0.62
1:C:348:VAL:CB	1:C:351:ARG:HD2	2.19	0.62
1:B:245:GLU:HG3	1:B:324:LYS:HD2	1.82	0.61
1:A:62:VAL:HG13	1:A:97:GLN:HG2	1.83	0.61
1:E:212:VAL:HG13	1:E:254:LEU:HD21	1.82	0.60
1:A:232:GLY:HA2	1:A:234:TRP:CE2	2.37	0.59
1:E:232:GLY:HA2	1:E:234:TRP:CE2	2.39	0.58
1:C:266:ASP:OD2	1:C:343:LYS:HE2	2.02	0.58
1:D:361:ASN:HD21	1:E:299:ARG:H	1.52	0.57
1:F:281:MET:HB3	1:F:348:VAL:HG22	1.85	0.57
1:F:212:VAL:HG13	1:F:254:LEU:HD21	1.88	0.56
1:D:339:ASP:HB3	1:D:360:ARG:HG2	1.87	0.56
1:F:353:ASN:O	1:F:360:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLY:HA2	1:B:234:TRP:CE2	2.41	0.56
1:A:245:GLU:HG3	1:A:324:LYS:HZ3	1.70	0.55
1:D:346:TYR:CD1	1:D:347:PRO:HA	2.42	0.55
1:C:76:ARG:HH11	1:C:113:TRP:HB3	1.72	0.55
1:D:174:ASP:O	1:D:178:VAL:HG23	2.06	0.55
1:A:135:HIS:O	1:A:139:VAL:HG23	2.06	0.55
1:F:91:TYR:O	1:F:94:ARG:HG2	2.07	0.55
1:D:353:ASN:O	1:D:360:ARG:NH2	2.40	0.55
1:E:339:ASP:HB3	1:E:360:ARG:HG2	1.89	0.55
1:C:265:ILE:O	1:C:355:PRO:HA	2.08	0.53
1:E:353:ASN:O	1:E:360:ARG:NH2	2.41	0.53
1:F:149:ALA:HB1	1:F:196:TYR:CE2	2.44	0.53
1:F:82:PHE:HB3	1:F:142:ARG:NH2	2.24	0.53
1:E:265:ILE:O	1:E:355:PRO:HA	2.09	0.52
1:D:289:PRO:O	1:D:293:ARG:HG2	2.10	0.52
1:F:164:ARG:HB2	1:F:166:THR:HG23	1.90	0.52
1:C:232:GLY:HA2	1:C:234:TRP:CE2	2.45	0.52
1:E:281:MET:HB2	1:E:347:PRO:HB2	1.91	0.51
1:A:214:MET:O	1:A:217:MET:HG3	2.11	0.51
1:D:212:VAL:HG13	1:D:254:LEU:HD21	1.92	0.51
1:C:144:THR:HG22	1:C:190:ALA:HA	1.93	0.51
1:B:307:GLN:HE22	1:B:365:LYS:HD2	1.76	0.50
1:B:25:LEU:HB3	1:B:35:LEU:HD22	1.94	0.50
1:F:348:VAL:CB	1:F:351:ARG:HD2	2.35	0.50
1:A:346:TYR:CD1	1:A:347:PRO:HA	2.47	0.49
1:A:59:PHE:O	1:A:97:GLN:NE2	2.45	0.49
1:E:149:ALA:HB1	1:E:196:TYR:CE2	2.47	0.49
1:B:106:TRP:CZ2	1:B:108:ASN:HB2	2.47	0.49
1:C:212:VAL:HG13	1:C:254:LEU:HD21	1.95	0.49
1:E:214:MET:O	1:E:217:MET:HG3	2.13	0.48
1:A:174:ASP:O	1:A:178:VAL:HG23	2.13	0.48
1:B:212:VAL:HG13	1:B:254:LEU:HD21	1.95	0.48
1:D:374:VAL:HB	1:D:375:PRO:HD3	1.95	0.48
1:E:174:ASP:O	1:E:178:VAL:HG23	2.14	0.48
1:D:51:SER:O	1:D:55:VAL:HG23	2.13	0.48
1:D:281:MET:HB3	1:D:348:VAL:HG22	1.96	0.47
1:C:348:VAL:HB	1:C:351:ARG:CD	2.22	0.47
1:D:264:ASP:HB2	1:D:355:PRO:HB2	1.95	0.47
1:F:257:LYS:HD2	1:F:329:ALA:HB2	1.96	0.47
1:E:208:ARG:HD2	1:E:247:ALA:HA	1.95	0.47
1:E:226:ASP:O	1:E:257:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:VAL:HA	1:C:59:PHE:HD2	1.80	0.47
1:E:179:VAL:HG12	1:E:218:LEU:HD21	1.95	0.47
1:F:348:VAL:HB	1:F:351:ARG:CD	2.34	0.47
1:A:38:ALA:HB2	1:A:334:TRP:CE3	2.49	0.47
1:D:346:TYR:CG	1:D:347:PRO:HA	2.50	0.47
1:F:265:ILE:O	1:F:355:PRO:HA	2.16	0.46
1:E:25:LEU:HB3	1:E:35:LEU:HD22	1.98	0.46
1:C:102:HIS:HA	1:C:103:THR:HA	1.79	0.46
1:F:346:TYR:CG	1:F:347:PRO:HA	2.51	0.46
1:B:106:TRP:CE2	1:B:108:ASN:HB2	2.51	0.46
1:F:345:ASP:HA	1:F:349:PRO:HA	1.98	0.46
1:D:232:GLY:HA2	1:D:234:TRP:CE2	2.51	0.45
1:E:73:VAL:HG11	1:E:139:VAL:HG22	1.98	0.45
1:D:249:ASP:OD1	1:D:324:LYS:NZ	2.49	0.45
1:A:245:GLU:HG3	1:A:324:LYS:NZ	2.31	0.45
1:F:89:VAL:O	1:F:93:GLN:HG2	2.16	0.45
1:B:143:TYR:HB3	1:B:147:VAL:HG23	1.97	0.45
1:B:25:LEU:HD12	1:B:58:HIS:HB3	1.98	0.45
1:A:281:MET:HB2	1:A:347:PRO:HB2	1.99	0.45
1:A:322:TRP:CE2	1:A:375:PRO:HA	2.52	0.44
1:A:204:ARG:NH2	1:B:290:GLU:OE1	2.50	0.44
1:E:102:HIS:HA	1:E:103:THR:HA	1.76	0.44
1:C:131:ARG:HA	1:C:131:ARG:HD2	1.77	0.44
1:C:111:PRO:HB2	1:C:113:TRP:CD1	2.52	0.44
1:C:346:TYR:CG	1:C:347:PRO:HA	2.53	0.44
1:B:38:ALA:HB2	1:B:334:TRP:CE3	2.53	0.44
1:A:227:GLY:HA2	1:A:256:VAL:HB	1.99	0.44
1:F:159:GLU:OE1	1:F:204:ARG:NH1	2.51	0.44
1:D:111:PRO:HB2	1:D:113:TRP:CD1	2.53	0.44
1:E:157:ILE:O	1:E:207:LYS:HE3	2.18	0.43
1:F:73:VAL:HG11	1:F:139:VAL:HG22	2.00	0.43
1:A:102:HIS:HA	1:A:103:THR:HA	1.79	0.43
1:F:55:VAL:HA	1:F:59:PHE:HD2	1.83	0.43
1:A:346:TYR:CG	1:A:347:PRO:HA	2.53	0.43
1:A:62:VAL:HG22	1:A:97:GLN:HB3	2.00	0.43
1:F:245:GLU:HG3	1:F:324:LYS:HZ3	1.84	0.43
1:C:163:TYR:OH	1:C:214:MET:HG3	2.19	0.43
1:B:346:TYR:CG	1:B:347:PRO:HA	2.54	0.43
1:F:110:THR:HA	1:F:111:PRO:HD3	1.92	0.42
1:C:251:TYR:HA	1:C:254:LEU:HD12	2.02	0.42
1:F:104:LEU:HG	1:F:150:TRP:CE3	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ARG:HG2	1:B:223:VAL:HG21	2.01	0.42
1:F:77:ARG:HG3	1:F:113:TRP:CE3	2.54	0.42
1:E:224:ARG:HB2	2:E:409:HOH:O	2.19	0.42
1:A:157:ILE:O	1:A:207:LYS:HE3	2.19	0.42
1:B:157:ILE:O	1:B:207:LYS:HE3	2.20	0.42
1:F:132:MET:O	1:F:136:ILE:HG12	2.20	0.42
1:F:131:ARG:HA	1:F:131:ARG:HD2	1.92	0.42
1:B:107:HIS:HB3	1:B:166:THR:HB	2.00	0.42
1:E:348:VAL:CB	1:E:351:ARG:HD2	2.36	0.42
1:E:25:LEU:HB2	1:E:58:HIS:HB3	2.01	0.42
1:A:37:THR:HA	1:A:333:VAL:O	2.20	0.42
1:B:370:ALA:O	1:B:374:VAL:HG23	2.20	0.41
1:D:266:ASP:OD2	1:D:343:LYS:HE3	2.20	0.41
1:C:370:ALA:O	1:C:374:VAL:HG23	2.20	0.41
1:B:149:ALA:HB1	1:B:196:TYR:CE2	2.55	0.41
1:C:26:LYS:HB2	1:C:60:ASN:ND2	2.35	0.41
1:E:36:GLY:HA3	1:E:61:ALA:HB3	2.01	0.41
1:F:365:LYS:HB3	1:F:366:PRO:HD2	2.01	0.41
1:D:159:GLU:OE1	1:D:204:ARG:NH1	2.53	0.41
1:D:179:VAL:HG12	1:D:218:LEU:HD21	2.03	0.41
1:B:104:LEU:HG	1:B:136:ILE:HG12	2.01	0.41
1:D:230:MET:O	1:D:260:ILE:HA	2.21	0.41
1:B:236:LEU:HD21	1:B:267:VAL:HG12	2.02	0.41
1:F:346:TYR:CD1	1:F:347:PRO:HA	2.55	0.41
1:A:26:LYS:HB2	1:A:60:ASN:ND2	2.36	0.41
1:B:259:MET:HG2	1:B:330:ARG:HB3	2.03	0.40
1:A:110:THR:HA	1:A:111:PRO:HD3	1.91	0.40
1:D:265:ILE:O	1:D:355:PRO:HA	2.21	0.40
1:C:128:GLN:HG2	1:C:171:ARG:HB3	2.02	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	353/356 (99%)	339 (96%)	14 (4%)	0	100	100
1	B	354/356 (99%)	342 (97%)	11 (3%)	1 (0%)	46	76
1	C	354/356 (99%)	341 (96%)	13 (4%)	0	100	100
1	D	353/356 (99%)	341 (97%)	12 (3%)	0	100	100
1	E	353/356 (99%)	341 (97%)	12 (3%)	0	100	100
1	F	352/356 (99%)	338 (96%)	14 (4%)	0	100	100
All	All	2119/2136 (99%)	2042 (96%)	76 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155	GLU

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	284/285 (100%)	279 (98%)	5 (2%)	66	89
1	B	285/285 (100%)	279 (98%)	6 (2%)	61	86
1	C	285/285 (100%)	279 (98%)	6 (2%)	61	86
1	D	284/285 (100%)	279 (98%)	5 (2%)	66	89
1	E	284/285 (100%)	283 (100%)	1 (0%)	93	98
1	F	283/285 (99%)	281 (99%)	2 (1%)	88	96
All	All	1705/1710 (100%)	1680 (98%)	25 (2%)	72	91

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	94	ARG
1	A	97	GLN
1	A	131	ARG

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Mol	Chain	Res	Type
1	A	324	LYS
1	B	35	LEU
1	B	57	CYS
1	B	104	LEU
1	B	171	ARG
1	B	242	ARG
1	B	332	SER
1	C	27	GLN
1	C	35	LEU
1	C	94	ARG
1	C	119	ASP
1	C	167	ASN
1	C	217	MET
1	D	35	LEU
1	D	119	ASP
1	D	148	GLN
1	D	171	ARG
1	D	307	GLN
1	E	96	ARG
1	F	226	ASP
1	F	339	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	93	GLN
1	A	97	GLN
1	B	181	ASN
1	C	31	GLN
1	D	307	GLN
1	D	361	ASN
1	E	275	GLN
1	F	361	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 carbohydrates 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

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, 95^{th} 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	355/356 (99%)	-0.41	0 100 100	34, 48, 60, 71	0
1	B	356/356 (100%)	-0.49	2 (0%) 90 89	30, 39, 54, 74	1 (0%)
1	C	356/356 (100%)	-0.42	3 (0%) 87 86	31, 46, 63, 85	2 (0%)
1	D	355/356 (99%)	-0.53	0 100 100	30, 40, 50, 57	0
1	E	355/356 (99%)	-0.53	1 (0%) 94 93	33, 43, 57, 75	0
1	F	354/356 (99%)	-0.41	2 (0%) 90 89	36, 54, 80, 98	0
All	All	2131/2136 (99%)	-0.47	8 (0%) 93 92	30, 44, 66, 98	3 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	126	ALA	3.3
1	F	364	PRO	2.5
1	C	125	PRO	2.4
1	B	372	VAL	2.4
1	B	378	THR	2.3
1	E	27	GLN	2.2
1	F	367	ALA	2.2
1	C	173	GLY	2.1

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.