Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2016 – 11:32 PM EDT

PDB ID	:	5BYW
Title	:	Crystal structure of engineered trifunctional CtCEL5E
Authors	:	Lin, W.L.; Liang, P.H.; Ho, M.C.
Deposited on	:	2015-06-11
Resolution	:	2.60 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 ⓘ) were used in the production of this report:

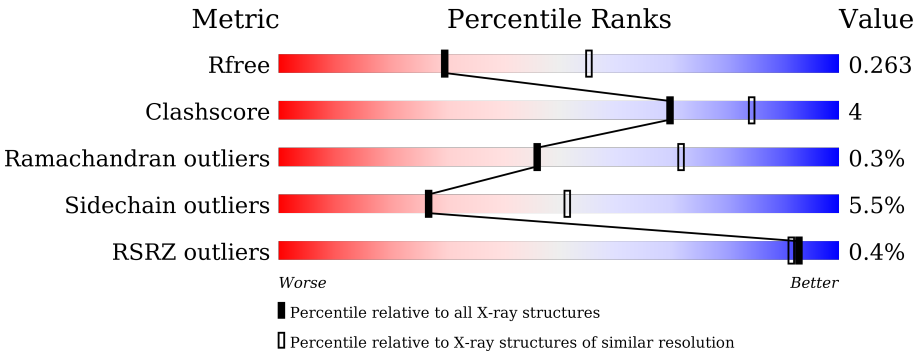
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	414	66% 9% • 23%
1	B	414	68% 7% • 24%
1	C	414	% 63% 11% • 23%
1	D	414	65% 9% • 23%
1	E	414	68% 8% • 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13396 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 H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2639	1688	442	498	11			
1	B	316	Total	C	N	O	S	0	0	0
			2623	1679	439	494	11			
1	C	318	Total	C	N	O	S	0	0	0
			2634	1685	441	497	11			
1	D	320	Total	C	N	O	S	0	0	0
			2648	1694	444	499	11			
1	E	323	Total	C	N	O	S	0	0	0
			2676	1714	446	505	11			

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P16218
A	2	GLY	-	expression tag	UNP P16218
A	3	SER	-	expression tag	UNP P16218
A	4	SER	-	expression tag	UNP P16218
A	5	HIS	-	expression tag	UNP P16218
A	6	HIS	-	expression tag	UNP P16218
A	7	HIS	-	expression tag	UNP P16218
A	8	HIS	-	expression tag	UNP P16218
A	9	HIS	-	expression tag	UNP P16218
A	10	HIS	-	expression tag	UNP P16218
A	11	SER	-	expression tag	UNP P16218
A	12	SER	-	expression tag	UNP P16218
A	13	GLY	-	expression tag	UNP P16218
A	14	LEU	-	expression tag	UNP P16218
A	15	VAL	-	expression tag	UNP P16218
A	16	PRO	-	expression tag	UNP P16218
A	17	ARG	-	expression tag	UNP P16218
A	18	GLY	-	expression tag	UNP P16218
A	19	SER	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	HIS	-	expression tag	UNP P16218
A	21	MET	-	expression tag	UNP P16218
A	22	ALA	-	expression tag	UNP P16218
A	23	SER	-	expression tag	UNP P16218
A	24	MET	-	expression tag	UNP P16218
A	25	THR	-	expression tag	UNP P16218
A	26	GLY	-	expression tag	UNP P16218
A	27	GLY	-	expression tag	UNP P16218
A	28	GLN	-	expression tag	UNP P16218
A	29	GLN	-	expression tag	UNP P16218
A	30	MET	-	expression tag	UNP P16218
A	31	GLY	-	expression tag	UNP P16218
A	32	ARG	-	expression tag	UNP P16218
A	33	ILE	-	expression tag	UNP P16218
A	34	GLU	-	expression tag	UNP P16218
A	35	GLY	-	expression tag	UNP P16218
A	36	ARG	-	expression tag	UNP P16218
A	37	GLU	-	expression tag	UNP P16218
A	38	PHE	-	expression tag	UNP P16218
A	267	ALA	PHE	engineered mutation	UNP P16218
A	273	PHE	TYR	engineered mutation	UNP P16218
A	278	GLN	-	insertion	UNP P16218
A	279	GLY	-	insertion	UNP P16218
A	280	ALA	-	insertion	UNP P16218
A	281	GLU	-	insertion	UNP P16218
A	282	TRP	-	insertion	UNP P16218
A	283	VAL	-	insertion	UNP P16218
A	284	GLU	-	insertion	UNP P16218
A	285	GLY	-	insertion	UNP P16218
A	286	SER	-	insertion	UNP P16218
A	287	GLU	-	insertion	UNP P16218
A	288	LYS	-	insertion	UNP P16218
A	289	TRP	LYS	engineered mutation	UNP P16218
A	290	LEU	TRP	engineered mutation	UNP P16218
A	291	GLY	ARG	engineered mutation	UNP P16218
A	292	ARG	GLY	engineered mutation	UNP P16218
A	293	LYS	THR	engineered mutation	UNP P16218
B	1	MET	-	initiating methionine	UNP P16218
B	2	GLY	-	expression tag	UNP P16218
B	3	SER	-	expression tag	UNP P16218
B	4	SER	-	expression tag	UNP P16218
B	5	HIS	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP P16218
B	7	HIS	-	expression tag	UNP P16218
B	8	HIS	-	expression tag	UNP P16218
B	9	HIS	-	expression tag	UNP P16218
B	10	HIS	-	expression tag	UNP P16218
B	11	SER	-	expression tag	UNP P16218
B	12	SER	-	expression tag	UNP P16218
B	13	GLY	-	expression tag	UNP P16218
B	14	LEU	-	expression tag	UNP P16218
B	15	VAL	-	expression tag	UNP P16218
B	16	PRO	-	expression tag	UNP P16218
B	17	ARG	-	expression tag	UNP P16218
B	18	GLY	-	expression tag	UNP P16218
B	19	SER	-	expression tag	UNP P16218
B	20	HIS	-	expression tag	UNP P16218
B	21	MET	-	expression tag	UNP P16218
B	22	ALA	-	expression tag	UNP P16218
B	23	SER	-	expression tag	UNP P16218
B	24	MET	-	expression tag	UNP P16218
B	25	THR	-	expression tag	UNP P16218
B	26	GLY	-	expression tag	UNP P16218
B	27	GLY	-	expression tag	UNP P16218
B	28	GLN	-	expression tag	UNP P16218
B	29	GLN	-	expression tag	UNP P16218
B	30	MET	-	expression tag	UNP P16218
B	31	GLY	-	expression tag	UNP P16218
B	32	ARG	-	expression tag	UNP P16218
B	33	ILE	-	expression tag	UNP P16218
B	34	GLU	-	expression tag	UNP P16218
B	35	GLY	-	expression tag	UNP P16218
B	36	ARG	-	expression tag	UNP P16218
B	37	GLU	-	expression tag	UNP P16218
B	38	PHE	-	expression tag	UNP P16218
B	267	ALA	PHE	engineered mutation	UNP P16218
B	273	PHE	TYR	engineered mutation	UNP P16218
B	278	GLN	-	insertion	UNP P16218
B	279	GLY	-	insertion	UNP P16218
B	280	ALA	-	insertion	UNP P16218
B	281	GLU	-	insertion	UNP P16218
B	282	TRP	-	insertion	UNP P16218
B	283	VAL	-	insertion	UNP P16218
B	284	GLU	-	insertion	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
B	285	GLY	-	insertion	UNP P16218
B	286	SER	-	insertion	UNP P16218
B	287	GLU	-	insertion	UNP P16218
B	288	LYS	-	insertion	UNP P16218
B	289	TRP	LYS	engineered mutation	UNP P16218
B	290	LEU	TRP	engineered mutation	UNP P16218
B	291	GLY	ARG	engineered mutation	UNP P16218
B	292	ARG	GLY	engineered mutation	UNP P16218
B	293	LYS	THR	engineered mutation	UNP P16218
C	1	MET	-	initiating methionine	UNP P16218
C	2	GLY	-	expression tag	UNP P16218
C	3	SER	-	expression tag	UNP P16218
C	4	SER	-	expression tag	UNP P16218
C	5	HIS	-	expression tag	UNP P16218
C	6	HIS	-	expression tag	UNP P16218
C	7	HIS	-	expression tag	UNP P16218
C	8	HIS	-	expression tag	UNP P16218
C	9	HIS	-	expression tag	UNP P16218
C	10	HIS	-	expression tag	UNP P16218
C	11	SER	-	expression tag	UNP P16218
C	12	SER	-	expression tag	UNP P16218
C	13	GLY	-	expression tag	UNP P16218
C	14	LEU	-	expression tag	UNP P16218
C	15	VAL	-	expression tag	UNP P16218
C	16	PRO	-	expression tag	UNP P16218
C	17	ARG	-	expression tag	UNP P16218
C	18	GLY	-	expression tag	UNP P16218
C	19	SER	-	expression tag	UNP P16218
C	20	HIS	-	expression tag	UNP P16218
C	21	MET	-	expression tag	UNP P16218
C	22	ALA	-	expression tag	UNP P16218
C	23	SER	-	expression tag	UNP P16218
C	24	MET	-	expression tag	UNP P16218
C	25	THR	-	expression tag	UNP P16218
C	26	GLY	-	expression tag	UNP P16218
C	27	GLY	-	expression tag	UNP P16218
C	28	GLN	-	expression tag	UNP P16218
C	29	GLN	-	expression tag	UNP P16218
C	30	MET	-	expression tag	UNP P16218
C	31	GLY	-	expression tag	UNP P16218
C	32	ARG	-	expression tag	UNP P16218
C	33	ILE	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
C	34	GLU	-	expression tag	UNP P16218
C	35	GLY	-	expression tag	UNP P16218
C	36	ARG	-	expression tag	UNP P16218
C	37	GLU	-	expression tag	UNP P16218
C	38	PHE	-	expression tag	UNP P16218
C	267	ALA	PHE	engineered mutation	UNP P16218
C	273	PHE	TYR	engineered mutation	UNP P16218
C	278	GLN	-	insertion	UNP P16218
C	279	GLY	-	insertion	UNP P16218
C	280	ALA	-	insertion	UNP P16218
C	281	GLU	-	insertion	UNP P16218
C	282	TRP	-	insertion	UNP P16218
C	283	VAL	-	insertion	UNP P16218
C	284	GLU	-	insertion	UNP P16218
C	285	GLY	-	insertion	UNP P16218
C	286	SER	-	insertion	UNP P16218
C	287	GLU	-	insertion	UNP P16218
C	288	LYS	-	insertion	UNP P16218
C	289	TRP	LYS	engineered mutation	UNP P16218
C	290	LEU	TRP	engineered mutation	UNP P16218
C	291	GLY	ARG	engineered mutation	UNP P16218
C	292	ARG	GLY	engineered mutation	UNP P16218
C	293	LYS	THR	engineered mutation	UNP P16218
D	1	MET	-	initiating methionine	UNP P16218
D	2	GLY	-	expression tag	UNP P16218
D	3	SER	-	expression tag	UNP P16218
D	4	SER	-	expression tag	UNP P16218
D	5	HIS	-	expression tag	UNP P16218
D	6	HIS	-	expression tag	UNP P16218
D	7	HIS	-	expression tag	UNP P16218
D	8	HIS	-	expression tag	UNP P16218
D	9	HIS	-	expression tag	UNP P16218
D	10	HIS	-	expression tag	UNP P16218
D	11	SER	-	expression tag	UNP P16218
D	12	SER	-	expression tag	UNP P16218
D	13	GLY	-	expression tag	UNP P16218
D	14	LEU	-	expression tag	UNP P16218
D	15	VAL	-	expression tag	UNP P16218
D	16	PRO	-	expression tag	UNP P16218
D	17	ARG	-	expression tag	UNP P16218
D	18	GLY	-	expression tag	UNP P16218
D	19	SER	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	HIS	-	expression tag	UNP P16218
D	21	MET	-	expression tag	UNP P16218
D	22	ALA	-	expression tag	UNP P16218
D	23	SER	-	expression tag	UNP P16218
D	24	MET	-	expression tag	UNP P16218
D	25	THR	-	expression tag	UNP P16218
D	26	GLY	-	expression tag	UNP P16218
D	27	GLY	-	expression tag	UNP P16218
D	28	GLN	-	expression tag	UNP P16218
D	29	GLN	-	expression tag	UNP P16218
D	30	MET	-	expression tag	UNP P16218
D	31	GLY	-	expression tag	UNP P16218
D	32	ARG	-	expression tag	UNP P16218
D	33	ILE	-	expression tag	UNP P16218
D	34	GLU	-	expression tag	UNP P16218
D	35	GLY	-	expression tag	UNP P16218
D	36	ARG	-	expression tag	UNP P16218
D	37	GLU	-	expression tag	UNP P16218
D	38	PHE	-	expression tag	UNP P16218
D	267	ALA	PHE	engineered mutation	UNP P16218
D	273	PHE	TYR	engineered mutation	UNP P16218
D	278	GLN	-	insertion	UNP P16218
D	279	GLY	-	insertion	UNP P16218
D	280	ALA	-	insertion	UNP P16218
D	281	GLU	-	insertion	UNP P16218
D	282	TRP	-	insertion	UNP P16218
D	283	VAL	-	insertion	UNP P16218
D	284	GLU	-	insertion	UNP P16218
D	285	GLY	-	insertion	UNP P16218
D	286	SER	-	insertion	UNP P16218
D	287	GLU	-	insertion	UNP P16218
D	288	LYS	-	insertion	UNP P16218
D	289	TRP	LYS	engineered mutation	UNP P16218
D	290	LEU	TRP	engineered mutation	UNP P16218
D	291	GLY	ARG	engineered mutation	UNP P16218
D	292	ARG	GLY	engineered mutation	UNP P16218
D	293	LYS	THR	engineered mutation	UNP P16218
E	1	MET	-	initiating methionine	UNP P16218
E	2	GLY	-	expression tag	UNP P16218
E	3	SER	-	expression tag	UNP P16218
E	4	SER	-	expression tag	UNP P16218
E	5	HIS	-	expression tag	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	HIS	-	expression tag	UNP P16218
E	7	HIS	-	expression tag	UNP P16218
E	8	HIS	-	expression tag	UNP P16218
E	9	HIS	-	expression tag	UNP P16218
E	10	HIS	-	expression tag	UNP P16218
E	11	SER	-	expression tag	UNP P16218
E	12	SER	-	expression tag	UNP P16218
E	13	GLY	-	expression tag	UNP P16218
E	14	LEU	-	expression tag	UNP P16218
E	15	VAL	-	expression tag	UNP P16218
E	16	PRO	-	expression tag	UNP P16218
E	17	ARG	-	expression tag	UNP P16218
E	18	GLY	-	expression tag	UNP P16218
E	19	SER	-	expression tag	UNP P16218
E	20	HIS	-	expression tag	UNP P16218
E	21	MET	-	expression tag	UNP P16218
E	22	ALA	-	expression tag	UNP P16218
E	23	SER	-	expression tag	UNP P16218
E	24	MET	-	expression tag	UNP P16218
E	25	THR	-	expression tag	UNP P16218
E	26	GLY	-	expression tag	UNP P16218
E	27	GLY	-	expression tag	UNP P16218
E	28	GLN	-	expression tag	UNP P16218
E	29	GLN	-	expression tag	UNP P16218
E	30	MET	-	expression tag	UNP P16218
E	31	GLY	-	expression tag	UNP P16218
E	32	ARG	-	expression tag	UNP P16218
E	33	ILE	-	expression tag	UNP P16218
E	34	GLU	-	expression tag	UNP P16218
E	35	GLY	-	expression tag	UNP P16218
E	36	ARG	-	expression tag	UNP P16218
E	37	GLU	-	expression tag	UNP P16218
E	38	PHE	-	expression tag	UNP P16218
E	267	ALA	PHE	engineered mutation	UNP P16218
E	273	PHE	TYR	engineered mutation	UNP P16218
E	278	GLN	-	insertion	UNP P16218
E	279	GLY	-	insertion	UNP P16218
E	280	ALA	-	insertion	UNP P16218
E	281	GLU	-	insertion	UNP P16218
E	282	TRP	-	insertion	UNP P16218
E	283	VAL	-	insertion	UNP P16218
E	284	GLU	-	insertion	UNP P16218

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Chain	Residue	Modelled	Actual	Comment	Reference
E	285	GLY	-	insertion	UNP P16218
E	286	SER	-	insertion	UNP P16218
E	287	GLU	-	insertion	UNP P16218
E	288	LYS	-	insertion	UNP P16218
E	289	TRP	LYS	engineered mutation	UNP P16218
E	290	LEU	TRP	engineered mutation	UNP P16218
E	291	GLY	ARG	engineered mutation	UNP P16218
E	292	ARG	GLY	engineered mutation	UNP P16218
E	293	LYS	THR	engineered mutation	UNP P16218

- Molecule 2 is water.

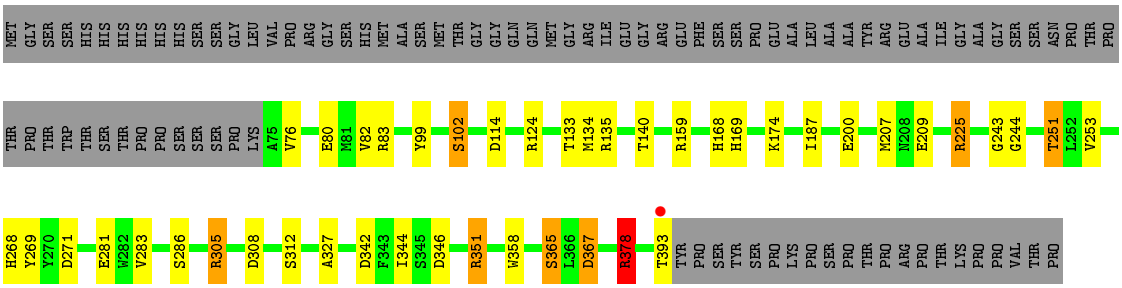
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	36	Total O 36 36	0	0
2	B	54	Total O 54 54	0	0
2	C	19	Total O 19 19	0	0
2	D	23	Total O 23 23	0	0
2	E	44	Total O 44 44	0	0

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.

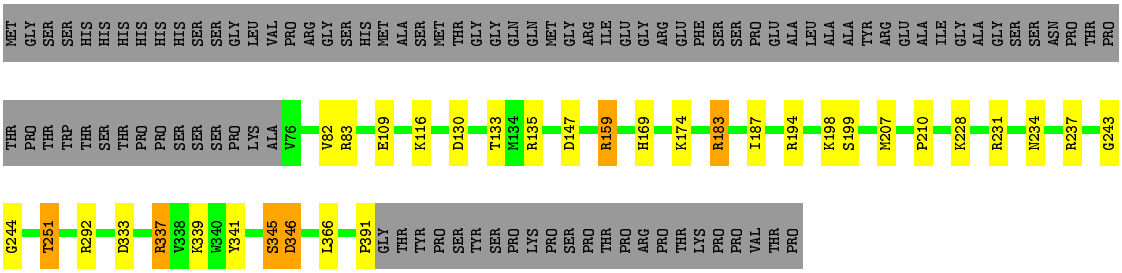
- Molecule 1: Endoglucanase H

Chain A:



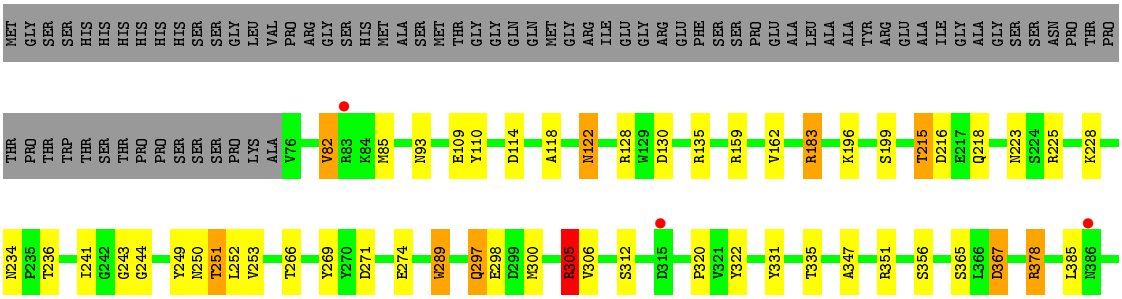
- Molecule 1: Endoglucanase H

Chain B:



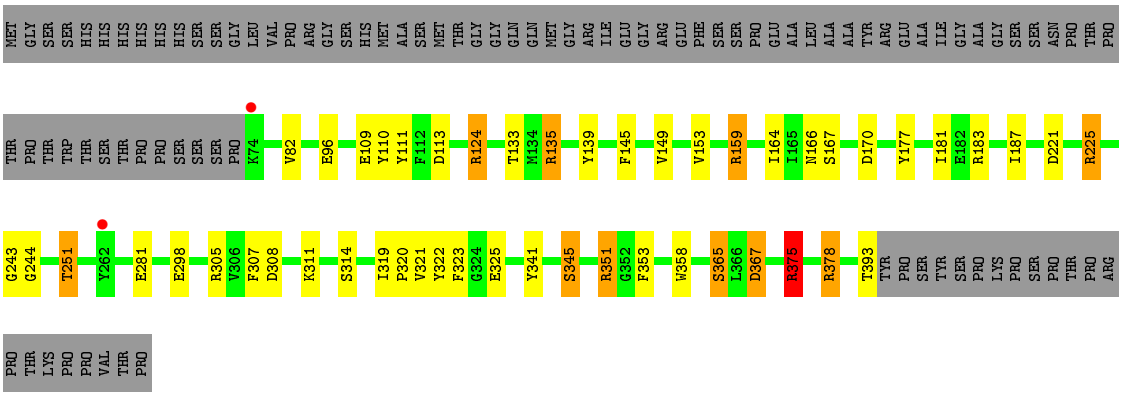
- Molecule 1: Endoglucanase H

Chain C:



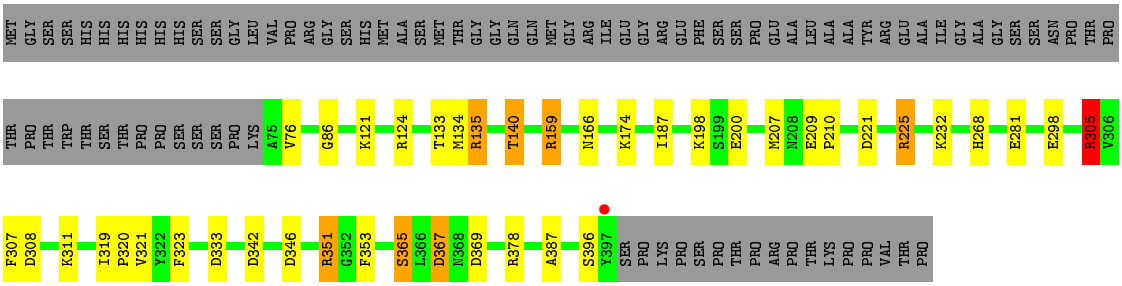
• Molecule 1: Endoglucanase H

Chain D:



• Molecule 1: Endoglucanase H

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	222.32Å 222.32Å 207.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.60) 100.0 (19.99-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.209 , 0.260 0.214 , 0.263	Depositor DCC
R_{free} test set	4549 reflections (5.17%)	DCC
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13396	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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	0.61	0/2714	0.85	11/3683 (0.3%)
1	B	0.64	0/2698	0.86	4/3661 (0.1%)
1	C	0.60	0/2709	0.84	2/3676 (0.1%)
1	D	0.61	0/2723	0.87	5/3694 (0.1%)
1	E	0.59	0/2754	0.84	6/3739 (0.2%)
All	All	0.61	0/13598	0.85	28/18453 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	346	ASP	CB-CG-OD1	10.26	127.53	118.30
1	B	346	ASP	CB-CG-OD2	-9.91	109.38	118.30
1	C	305	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	378	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	D	375	ARG	CG-CD-NE	7.17	126.86	111.80
1	E	124	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	346	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	346	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	E	305	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	124	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	E	159	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	375	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	135	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	305	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	159	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	E	369	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	124	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	124	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	337	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	375	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	378	ARG	CG-CD-NE	5.51	123.37	111.80
1	A	159	ARG	NE-CZ-NH1	5.43	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	124	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	342	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	378	ARG	CD-NE-CZ	5.33	131.06	123.60
1	E	346	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	C	128	ARG	CG-CD-NE	5.21	122.74	111.80
1	A	225	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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	2639	0	2486	22	0
1	B	2623	0	2471	21	0
1	C	2634	0	2481	28	0
1	D	2648	0	2499	25	0
1	E	2676	0	2516	20	0
2	A	36	0	0	0	0
2	B	54	0	0	1	0
2	C	19	0	0	0	0
2	D	23	0	0	0	0
2	E	44	0	0	1	0
All	All	13396	0	12453	115	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 (115) 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:134:MET:HE2	1:A:140:THR:HB	1.67	0.77
1:A:133:THR:HG21	1:A:187:ILE:CD1	2.17	0.74
1:D:113:ASP:OD1	1:D:159:ARG:NH2	2.23	0.71
1:B:133:THR:HG21	1:B:187:ILE:CD1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LYS:HG2	1:B:207:MET:HE3	1.75	0.67
1:E:133:THR:HG21	1:E:187:ILE:CD1	2.26	0.66
1:D:133:THR:HG21	1:D:187:ILE:HD11	1.77	0.65
1:C:392:GLY:O	1:C:393:THR:HG23	1.95	0.65
1:A:308:ASP:OD1	1:A:351:ARG:NH1	2.31	0.62
1:D:111:TYR:CZ	1:D:375:ARG:HD3	2.35	0.61
1:E:134:MET:SD	1:E:140:THR:HG23	2.41	0.61
1:B:169:HIS:HD2	2:B:515:HOH:O	1.83	0.61
1:C:122:ASN:ND2	1:C:356:SER:OG	2.28	0.60
1:B:231:ARG:NH2	1:B:237:ARG:O	2.35	0.60
1:B:133:THR:HG21	1:B:187:ILE:HD11	1.84	0.59
1:D:133:THR:HG21	1:D:187:ILE:CD1	2.33	0.58
1:A:243:GLY:HA3	1:A:251:THR:HG23	1.85	0.57
1:C:365:SER:HB2	1:C:367:ASP:HB2	1.86	0.57
1:D:341:TYR:O	1:D:345:SER:HB2	2.04	0.57
1:B:147:ASP:OD1	1:B:194:ARG:NH2	2.38	0.57
1:C:243:GLY:C	1:C:251:THR:HG21	2.25	0.56
1:B:243:GLY:HA3	1:B:251:THR:HG23	1.86	0.56
1:C:269:TYR:CE1	1:C:271:ASP:HB2	2.39	0.56
1:A:244:GLY:O	1:A:251:THR:HG21	2.05	0.56
1:B:244:GLY:N	1:B:251:THR:HG21	2.21	0.55
1:A:114:ASP:OD1	1:A:378:ARG:NH1	2.40	0.55
1:B:341:TYR:O	1:B:345:SER:OG	2.25	0.55
1:A:244:GLY:N	1:A:251:THR:HG21	2.23	0.54
1:B:109:GLU:HG2	1:B:159:ARG:HH22	1.73	0.54
1:A:76:VAL:HG21	1:A:200:GLU:HG3	1.89	0.54
1:A:134:MET:CE	1:A:140:THR:HB	2.35	0.53
1:A:133:THR:HG21	1:A:187:ILE:HD11	1.89	0.53
1:C:109:GLU:OE1	1:C:159:ARG:NH2	2.42	0.53
1:C:266:THR:HG22	1:C:322:TYR:O	2.09	0.53
1:D:243:GLY:HA3	1:D:251:THR:HG23	1.91	0.53
1:E:133:THR:HG21	1:E:187:ILE:HD11	1.90	0.53
1:B:130:ASP:OD1	1:B:183:ARG:NH2	2.39	0.53
1:E:221:ASP:O	1:E:225:ARG:HG3	2.09	0.52
1:A:174:LYS:HG2	1:A:207:MET:HE1	1.91	0.51
1:B:135:ARG:HD3	2:E:502:HOH:O	2.10	0.51
1:A:243:GLY:C	1:A:251:THR:HG21	2.30	0.51
1:C:215:THR:HG22	1:C:218:GLN:H	1.75	0.51
1:C:244:GLY:O	1:C:251:THR:HG21	2.11	0.50
1:E:174:LYS:HD3	1:E:210:PRO:HA	1.94	0.50
1:D:96:GLU:OE2	1:D:358:TRP:HH2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ASP:OD2	1:B:391:PRO:HA	2.12	0.49
1:D:308:ASP:OD1	1:D:351:ARG:NH1	2.45	0.49
1:C:297:GLN:HA	1:C:297:GLN:NE2	2.26	0.49
1:D:221:ASP:O	1:D:225:ARG:HG3	2.13	0.49
1:C:274:GLU:HG2	1:C:289:TRP:CD2	2.48	0.49
1:C:243:GLY:HA3	1:C:251:THR:HG23	1.95	0.49
1:B:198:LYS:O	1:B:237:ARG:NH2	2.47	0.48
1:E:207:MET:HE1	1:E:210:PRO:HB3	1.95	0.48
1:E:342:ASP:HB2	1:E:387:ALA:HB1	1.95	0.48
1:A:168:HIS:O	1:A:169:HIS:HB2	2.13	0.48
1:A:114:ASP:OD2	1:A:378:ARG:HG3	2.13	0.48
1:D:139:TYR:CD1	1:D:183:ARG:HG3	2.48	0.48
1:E:209:GLU:OE2	1:E:268:HIS:HD2	1.97	0.48
1:A:80:GLU:O	1:A:83:ARG:HB2	2.14	0.48
1:E:307:PHE:CZ	1:E:323:PHE:HE2	2.32	0.48
1:C:114:ASP:OD2	1:C:378:ARG:HG3	2.14	0.48
1:C:130:ASP:OD1	1:C:183:ARG:NH2	2.46	0.48
1:E:207:MET:CE	1:E:210:PRO:HB3	2.44	0.48
1:C:249:TYR:CE2	1:C:306:VAL:HG13	2.50	0.47
1:C:82:VAL:HG21	1:C:320:PRO:HB2	1.96	0.47
1:B:243:GLY:C	1:B:251:THR:HG21	2.35	0.47
1:E:365:SER:HB2	1:E:367:ASP:HB2	1.96	0.47
1:B:243:GLY:HA3	1:B:251:THR:CG2	2.44	0.47
1:D:164:ILE:HD13	1:D:322:TYR:OH	2.15	0.47
1:D:124:ARG:NH2	1:D:325:GLU:OE2	2.48	0.46
1:B:133:THR:O	1:E:135:ARG:NH2	2.39	0.46
1:D:145:PHE:O	1:D:149:VAL:HG23	2.14	0.46
1:C:196:LYS:HA	1:C:234:ASN:OD1	2.15	0.46
1:A:243:GLY:HA3	1:A:251:THR:CG2	2.44	0.45
1:D:109:GLU:OE1	1:D:159:ARG:NH1	2.49	0.45
1:C:274:GLU:HG2	1:C:289:TRP:CE2	2.50	0.45
1:D:307:PHE:CZ	1:D:323:PHE:HE2	2.34	0.45
1:D:167:SER:OG	1:D:170:ASP:OD2	2.32	0.45
1:A:209:GLU:OE2	1:A:268:HIS:HD2	2.00	0.45
1:D:110:TYR:CE1	1:D:378:ARG:HD2	2.52	0.45
1:D:177:TYR:CZ	1:D:181:ILE:HD13	2.52	0.44
1:E:166:ASN:C	1:E:166:ASN:OD1	2.55	0.44
1:A:99:TYR:O	1:A:102:SER:OG	2.34	0.44
1:D:321:VAL:HB	1:D:353:PHE:CD1	2.52	0.44
1:B:244:GLY:O	1:B:251:THR:HG21	2.17	0.44
1:C:347:ALA:O	1:C:351:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:TYR:CD1	1:C:378:ARG:HD2	2.53	0.43
1:D:244:GLY:O	1:D:251:THR:HG21	2.17	0.43
1:D:149:VAL:O	1:D:153:VAL:HG23	2.18	0.43
1:C:223:ASN:ND2	1:C:241:ILE:HG22	2.34	0.42
1:C:305:ARG:HB2	1:C:305:ARG:HH11	1.83	0.42
1:C:85:MET:HG2	1:C:162:VAL:HG11	2.00	0.42
1:A:327:ALA:HB2	1:A:358:TRP:HB3	2.01	0.42
1:E:207:MET:CE	1:E:210:PRO:HG3	2.50	0.42
1:C:251:THR:HG22	1:C:252:LEU:N	2.35	0.42
1:A:269:TYR:CZ	1:A:271:ASP:HB2	2.54	0.42
1:C:243:GLY:C	1:C:251:THR:CG2	2.88	0.42
1:C:305:ARG:CB	1:C:305:ARG:HH11	2.33	0.42
1:A:283:VAL:O	1:A:286:SER:OG	2.38	0.41
1:B:207:MET:HE1	1:B:210:PRO:HB3	2.01	0.41
1:C:110:TYR:CE1	1:C:378:ARG:HD2	2.55	0.41
1:E:159:ARG:HG3	1:E:159:ARG:HH11	1.84	0.41
1:B:116:LYS:HD2	1:B:159:ARG:HB3	2.02	0.41
1:E:321:VAL:HB	1:E:353:PHE:CD1	2.55	0.41
1:E:308:ASP:OD1	1:E:351:ARG:NH1	2.53	0.41
1:B:234:ASN:OD1	1:B:237:ARG:NH1	2.51	0.41
1:D:166:ASN:OD1	1:D:166:ASN:C	2.59	0.41
1:E:319:ILE:HA	1:E:320:PRO:HD3	1.95	0.41
1:E:305:ARG:HG2	1:E:305:ARG:HH11	1.86	0.41
1:A:365:SER:HB2	1:A:367:ASP:HB2	2.03	0.41
1:D:314:SER:OG	1:D:319:ILE:O	2.32	0.41
1:C:118:ALA:HB1	1:C:385:LEU:HD21	2.03	0.40
1:D:365:SER:HB2	1:D:367:ASP:HB2	2.03	0.40
1:E:76:VAL:HG23	1:E:200:GLU:HG3	2.03	0.40
1:D:82:VAL:HG21	1:D:320:PRO:HB2	2.03	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	317/414 (77%)	300 (95%)	16 (5%)	1 (0%)	46	72
1	B	314/414 (76%)	302 (96%)	12 (4%)	0	100	100
1	C	316/414 (76%)	292 (92%)	23 (7%)	1 (0%)	46	72
1	D	318/414 (77%)	289 (91%)	28 (9%)	1 (0%)	46	72
1	E	321/414 (78%)	301 (94%)	18 (6%)	2 (1%)	30	56
All	All	1586/2070 (77%)	1484 (94%)	97 (6%)	5 (0%)	46	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ASP
1	C	367	ASP
1	D	367	ASP
1	E	86	GLY
1	E	367	ASP

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	281/361 (78%)	267 (95%)	14 (5%)	30	56
1	B	280/361 (78%)	268 (96%)	12 (4%)	35	64
1	C	281/361 (78%)	258 (92%)	23 (8%)	14	27
1	D	282/361 (78%)	268 (95%)	14 (5%)	30	56
1	E	285/361 (79%)	270 (95%)	15 (5%)	28	53
All	All	1409/1805 (78%)	1331 (94%)	78 (6%)	27	51

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	102	SER
1	A	135	ARG

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Mol	Chain	Res	Type
1	A	225	ARG
1	A	251	THR
1	A	253	VAL
1	A	281	GLU
1	A	305	ARG
1	A	312	SER
1	A	344	ILE
1	A	351	ARG
1	A	365	SER
1	A	378	ARG
1	A	393	THR
1	B	82	VAL
1	B	83	ARG
1	B	183	ARG
1	B	199	SER
1	B	228	LYS
1	B	251	THR
1	B	292	ARG
1	B	333	ASP
1	B	337	ARG
1	B	339	LYS
1	B	345	SER
1	B	366	LEU
1	C	82	VAL
1	C	93	ASN
1	C	122	ASN
1	C	135	ARG
1	C	183	ARG
1	C	199	SER
1	C	215	THR
1	C	216	ASP
1	C	225	ARG
1	C	228	LYS
1	C	236	THR
1	C	250	ASN
1	C	251	THR
1	C	253	VAL
1	C	289	TRP
1	C	297	GLN
1	C	298	GLU
1	C	300	MET
1	C	305	ARG

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Mol	Chain	Res	Type
1	C	312	SER
1	C	331	TYR
1	C	335	THR
1	C	378	ARG
1	D	135	ARG
1	D	159	ARG
1	D	225	ARG
1	D	251	THR
1	D	281	GLU
1	D	298	GLU
1	D	305	ARG
1	D	311	LYS
1	D	345	SER
1	D	351	ARG
1	D	365	SER
1	D	375	ARG
1	D	378	ARG
1	D	393	THR
1	E	121	LYS
1	E	135	ARG
1	E	140	THR
1	E	198	LYS
1	E	225	ARG
1	E	232	LYS
1	E	281	GLU
1	E	298	GLU
1	E	305	ARG
1	E	311	LYS
1	E	333	ASP
1	E	351	ARG
1	E	365	SER
1	E	378	ARG
1	E	396	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	B	132	HIS
1	B	169	HIS
1	C	93	ASN
1	C	122	ASN

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Mol	Chain	Res	Type
1	C	223	ASN
1	C	297	GLN
1	D	151	GLN
1	D	169	HIS
1	D	208	ASN
1	D	213	ASN
1	E	169	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

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	319/414 (77%)	-0.61	1 (0%) 94 93	31, 45, 61, 79	0
1	B	316/414 (76%)	-0.71	0 100 100	30, 38, 54, 70	0
1	C	318/414 (76%)	-0.31	3 (0%) 85 83	36, 55, 74, 89	0
1	D	320/414 (77%)	-0.30	2 (0%) 90 88	35, 55, 76, 93	0
1	E	323/414 (78%)	-0.52	1 (0%) 94 93	33, 48, 68, 105	0
All	All	1596/2070 (77%)	-0.49	7 (0%) 93 91	30, 48, 71, 105	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	397	TYR	4.2
1	D	74	LYS	3.2
1	A	393	THR	2.6
1	C	386	ASN	2.6
1	C	315	ASP	2.4
1	C	83	ARG	2.1
1	D	262	TYR	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.