Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2024 – 10:03 PM EST

PDB ID	:	4DEV
Title	:	An Acetyl Xylan Esterase (Est2A) from the Rumen Bacterium Butyrivibrio proteoclasticus.
Authors	:	Till, M.; Arcus, V.L.
Deposited on	:	2012-01-22
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

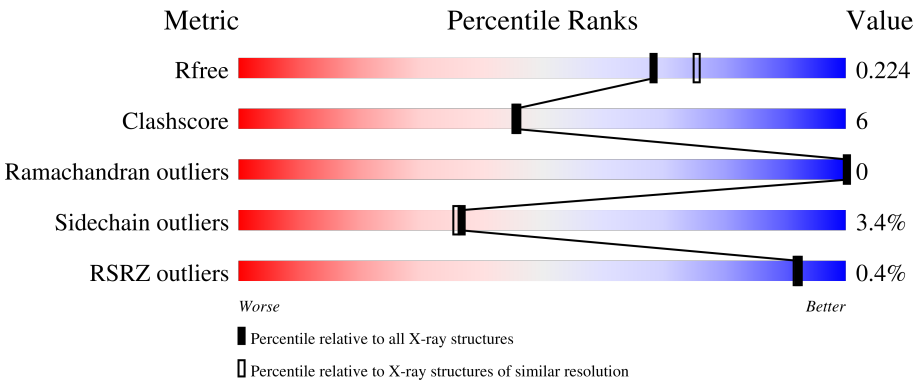
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	408	78% 12% • 9%
1	B	408	80% 10% • 9%
1	C	408	80% 10% • 9%
1	D	408	.% 80% 10% • 9%
1	E	408	76% 14% • 9%

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Mol	Chain	Length	Quality of chain
1	F	408	80% 10% • 9%
1	G	408	78% 12% • 9%
1	H	408	% 80% 11% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACY	A	402	-	-	X	-
2	ACY	B	401	-	-	X	-
3	PEG	D	403	-	-	X	-
3	PEG	E	404	-	-	-	X
3	PEG	E	405	-	-	X	-
3	PEG	G	404	-	-	X	-
5	GOL	C	403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25485 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 Acetyl-xylan esterase Est2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	372	2951	1869	498	568	16	0	0	0
1	B	372	2951	1869	498	568	16	8	0	0
1	C	372	2951	1869	498	568	16	0	0	0
1	D	373	2958	1874	499	569	16	4	0	0
1	E	372	2951	1869	498	568	16	4	0	0
1	F	373	2958	1874	499	569	16	4	0	0
1	G	373	2958	1874	499	569	16	0	0	0
1	H	373	2958	1874	499	569	16	4	0	0

There are 264 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	expression tag	UNP E0RVY7
A	-30	SER	-	expression tag	UNP E0RVY7
A	-29	TYR	-	expression tag	UNP E0RVY7
A	-28	TYR	-	expression tag	UNP E0RVY7
A	-27	HIS	-	expression tag	UNP E0RVY7
A	-26	HIS	-	expression tag	UNP E0RVY7
A	-25	HIS	-	expression tag	UNP E0RVY7
A	-24	HIS	-	expression tag	UNP E0RVY7
A	-23	HIS	-	expression tag	UNP E0RVY7
A	-22	HIS	-	expression tag	UNP E0RVY7
A	-21	LEU	-	expression tag	UNP E0RVY7
A	-20	GLU	-	expression tag	UNP E0RVY7
A	-19	SER	-	expression tag	UNP E0RVY7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	THR	-	expression tag	UNP E0RVY7
A	-17	SER	-	expression tag	UNP E0RVY7
A	-16	LEU	-	expression tag	UNP E0RVY7
A	-15	TYR	-	expression tag	UNP E0RVY7
A	-14	LYS	-	expression tag	UNP E0RVY7
A	-13	LYS	-	expression tag	UNP E0RVY7
A	-12	ALA	-	expression tag	UNP E0RVY7
A	-11	GLY	-	expression tag	UNP E0RVY7
A	-10	PHE	-	expression tag	UNP E0RVY7
A	-9	GLU	-	expression tag	UNP E0RVY7
A	-8	ASN	-	expression tag	UNP E0RVY7
A	-7	LEU	-	expression tag	UNP E0RVY7
A	-6	TYR	-	expression tag	UNP E0RVY7
A	-5	PHE	-	expression tag	UNP E0RVY7
A	-4	GLN	-	expression tag	UNP E0RVY7
A	-3	GLY	-	expression tag	UNP E0RVY7
A	-2	SER	-	expression tag	UNP E0RVY7
A	-1	GLY	-	expression tag	UNP E0RVY7
A	0	ALA	-	expression tag	UNP E0RVY7
A	351	ALA	HIS	engineered mutation	UNP E0RVY7
B	-31	MET	-	expression tag	UNP E0RVY7
B	-30	SER	-	expression tag	UNP E0RVY7
B	-29	TYR	-	expression tag	UNP E0RVY7
B	-28	TYR	-	expression tag	UNP E0RVY7
B	-27	HIS	-	expression tag	UNP E0RVY7
B	-26	HIS	-	expression tag	UNP E0RVY7
B	-25	HIS	-	expression tag	UNP E0RVY7
B	-24	HIS	-	expression tag	UNP E0RVY7
B	-23	HIS	-	expression tag	UNP E0RVY7
B	-22	HIS	-	expression tag	UNP E0RVY7
B	-21	LEU	-	expression tag	UNP E0RVY7
B	-20	GLU	-	expression tag	UNP E0RVY7
B	-19	SER	-	expression tag	UNP E0RVY7
B	-18	THR	-	expression tag	UNP E0RVY7
B	-17	SER	-	expression tag	UNP E0RVY7
B	-16	LEU	-	expression tag	UNP E0RVY7
B	-15	TYR	-	expression tag	UNP E0RVY7
B	-14	LYS	-	expression tag	UNP E0RVY7
B	-13	LYS	-	expression tag	UNP E0RVY7
B	-12	ALA	-	expression tag	UNP E0RVY7
B	-11	GLY	-	expression tag	UNP E0RVY7
B	-10	PHE	-	expression tag	UNP E0RVY7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	GLU	-	expression tag	UNP E0RVY7
B	-8	ASN	-	expression tag	UNP E0RVY7
B	-7	LEU	-	expression tag	UNP E0RVY7
B	-6	TYR	-	expression tag	UNP E0RVY7
B	-5	PHE	-	expression tag	UNP E0RVY7
B	-4	GLN	-	expression tag	UNP E0RVY7
B	-3	GLY	-	expression tag	UNP E0RVY7
B	-2	SER	-	expression tag	UNP E0RVY7
B	-1	GLY	-	expression tag	UNP E0RVY7
B	0	ALA	-	expression tag	UNP E0RVY7
B	351	ALA	HIS	engineered mutation	UNP E0RVY7
C	-31	MET	-	expression tag	UNP E0RVY7
C	-30	SER	-	expression tag	UNP E0RVY7
C	-29	TYR	-	expression tag	UNP E0RVY7
C	-28	TYR	-	expression tag	UNP E0RVY7
C	-27	HIS	-	expression tag	UNP E0RVY7
C	-26	HIS	-	expression tag	UNP E0RVY7
C	-25	HIS	-	expression tag	UNP E0RVY7
C	-24	HIS	-	expression tag	UNP E0RVY7
C	-23	HIS	-	expression tag	UNP E0RVY7
C	-22	HIS	-	expression tag	UNP E0RVY7
C	-21	LEU	-	expression tag	UNP E0RVY7
C	-20	GLU	-	expression tag	UNP E0RVY7
C	-19	SER	-	expression tag	UNP E0RVY7
C	-18	THR	-	expression tag	UNP E0RVY7
C	-17	SER	-	expression tag	UNP E0RVY7
C	-16	LEU	-	expression tag	UNP E0RVY7
C	-15	TYR	-	expression tag	UNP E0RVY7
C	-14	LYS	-	expression tag	UNP E0RVY7
C	-13	LYS	-	expression tag	UNP E0RVY7
C	-12	ALA	-	expression tag	UNP E0RVY7
C	-11	GLY	-	expression tag	UNP E0RVY7
C	-10	PHE	-	expression tag	UNP E0RVY7
C	-9	GLU	-	expression tag	UNP E0RVY7
C	-8	ASN	-	expression tag	UNP E0RVY7
C	-7	LEU	-	expression tag	UNP E0RVY7
C	-6	TYR	-	expression tag	UNP E0RVY7
C	-5	PHE	-	expression tag	UNP E0RVY7
C	-4	GLN	-	expression tag	UNP E0RVY7
C	-3	GLY	-	expression tag	UNP E0RVY7
C	-2	SER	-	expression tag	UNP E0RVY7
C	-1	GLY	-	expression tag	UNP E0RVY7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	ALA	-	expression tag	UNP E0RVY7
C	351	ALA	HIS	engineered mutation	UNP E0RVY7
D	-31	MET	-	expression tag	UNP E0RVY7
D	-30	SER	-	expression tag	UNP E0RVY7
D	-29	TYR	-	expression tag	UNP E0RVY7
D	-28	TYR	-	expression tag	UNP E0RVY7
D	-27	HIS	-	expression tag	UNP E0RVY7
D	-26	HIS	-	expression tag	UNP E0RVY7
D	-25	HIS	-	expression tag	UNP E0RVY7
D	-24	HIS	-	expression tag	UNP E0RVY7
D	-23	HIS	-	expression tag	UNP E0RVY7
D	-22	HIS	-	expression tag	UNP E0RVY7
D	-21	LEU	-	expression tag	UNP E0RVY7
D	-20	GLU	-	expression tag	UNP E0RVY7
D	-19	SER	-	expression tag	UNP E0RVY7
D	-18	THR	-	expression tag	UNP E0RVY7
D	-17	SER	-	expression tag	UNP E0RVY7
D	-16	LEU	-	expression tag	UNP E0RVY7
D	-15	TYR	-	expression tag	UNP E0RVY7
D	-14	LYS	-	expression tag	UNP E0RVY7
D	-13	LYS	-	expression tag	UNP E0RVY7
D	-12	ALA	-	expression tag	UNP E0RVY7
D	-11	GLY	-	expression tag	UNP E0RVY7
D	-10	PHE	-	expression tag	UNP E0RVY7
D	-9	GLU	-	expression tag	UNP E0RVY7
D	-8	ASN	-	expression tag	UNP E0RVY7
D	-7	LEU	-	expression tag	UNP E0RVY7
D	-6	TYR	-	expression tag	UNP E0RVY7
D	-5	PHE	-	expression tag	UNP E0RVY7
D	-4	GLN	-	expression tag	UNP E0RVY7
D	-3	GLY	-	expression tag	UNP E0RVY7
D	-2	SER	-	expression tag	UNP E0RVY7
D	-1	GLY	-	expression tag	UNP E0RVY7
D	0	ALA	-	expression tag	UNP E0RVY7
D	351	ALA	HIS	engineered mutation	UNP E0RVY7
E	-31	MET	-	expression tag	UNP E0RVY7
E	-30	SER	-	expression tag	UNP E0RVY7
E	-29	TYR	-	expression tag	UNP E0RVY7
E	-28	TYR	-	expression tag	UNP E0RVY7
E	-27	HIS	-	expression tag	UNP E0RVY7
E	-26	HIS	-	expression tag	UNP E0RVY7
E	-25	HIS	-	expression tag	UNP E0RVY7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-24	HIS	-	expression tag	UNP E0RVY7
E	-23	HIS	-	expression tag	UNP E0RVY7
E	-22	HIS	-	expression tag	UNP E0RVY7
E	-21	LEU	-	expression tag	UNP E0RVY7
E	-20	GLU	-	expression tag	UNP E0RVY7
E	-19	SER	-	expression tag	UNP E0RVY7
E	-18	THR	-	expression tag	UNP E0RVY7
E	-17	SER	-	expression tag	UNP E0RVY7
E	-16	LEU	-	expression tag	UNP E0RVY7
E	-15	TYR	-	expression tag	UNP E0RVY7
E	-14	LYS	-	expression tag	UNP E0RVY7
E	-13	LYS	-	expression tag	UNP E0RVY7
E	-12	ALA	-	expression tag	UNP E0RVY7
E	-11	GLY	-	expression tag	UNP E0RVY7
E	-10	PHE	-	expression tag	UNP E0RVY7
E	-9	GLU	-	expression tag	UNP E0RVY7
E	-8	ASN	-	expression tag	UNP E0RVY7
E	-7	LEU	-	expression tag	UNP E0RVY7
E	-6	TYR	-	expression tag	UNP E0RVY7
E	-5	PHE	-	expression tag	UNP E0RVY7
E	-4	GLN	-	expression tag	UNP E0RVY7
E	-3	GLY	-	expression tag	UNP E0RVY7
E	-2	SER	-	expression tag	UNP E0RVY7
E	-1	GLY	-	expression tag	UNP E0RVY7
E	0	ALA	-	expression tag	UNP E0RVY7
E	351	ALA	HIS	engineered mutation	UNP E0RVY7
F	-31	MET	-	expression tag	UNP E0RVY7
F	-30	SER	-	expression tag	UNP E0RVY7
F	-29	TYR	-	expression tag	UNP E0RVY7
F	-28	TYR	-	expression tag	UNP E0RVY7
F	-27	HIS	-	expression tag	UNP E0RVY7
F	-26	HIS	-	expression tag	UNP E0RVY7
F	-25	HIS	-	expression tag	UNP E0RVY7
F	-24	HIS	-	expression tag	UNP E0RVY7
F	-23	HIS	-	expression tag	UNP E0RVY7
F	-22	HIS	-	expression tag	UNP E0RVY7
F	-21	LEU	-	expression tag	UNP E0RVY7
F	-20	GLU	-	expression tag	UNP E0RVY7
F	-19	SER	-	expression tag	UNP E0RVY7
F	-18	THR	-	expression tag	UNP E0RVY7
F	-17	SER	-	expression tag	UNP E0RVY7
F	-16	LEU	-	expression tag	UNP E0RVY7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-15	TYR	-	expression tag	UNP E0RVY7
F	-14	LYS	-	expression tag	UNP E0RVY7
F	-13	LYS	-	expression tag	UNP E0RVY7
F	-12	ALA	-	expression tag	UNP E0RVY7
F	-11	GLY	-	expression tag	UNP E0RVY7
F	-10	PHE	-	expression tag	UNP E0RVY7
F	-9	GLU	-	expression tag	UNP E0RVY7
F	-8	ASN	-	expression tag	UNP E0RVY7
F	-7	LEU	-	expression tag	UNP E0RVY7
F	-6	TYR	-	expression tag	UNP E0RVY7
F	-5	PHE	-	expression tag	UNP E0RVY7
F	-4	GLN	-	expression tag	UNP E0RVY7
F	-3	GLY	-	expression tag	UNP E0RVY7
F	-2	SER	-	expression tag	UNP E0RVY7
F	-1	GLY	-	expression tag	UNP E0RVY7
F	0	ALA	-	expression tag	UNP E0RVY7
F	351	ALA	HIS	engineered mutation	UNP E0RVY7
G	-31	MET	-	expression tag	UNP E0RVY7
G	-30	SER	-	expression tag	UNP E0RVY7
G	-29	TYR	-	expression tag	UNP E0RVY7
G	-28	TYR	-	expression tag	UNP E0RVY7
G	-27	HIS	-	expression tag	UNP E0RVY7
G	-26	HIS	-	expression tag	UNP E0RVY7
G	-25	HIS	-	expression tag	UNP E0RVY7
G	-24	HIS	-	expression tag	UNP E0RVY7
G	-23	HIS	-	expression tag	UNP E0RVY7
G	-22	HIS	-	expression tag	UNP E0RVY7
G	-21	LEU	-	expression tag	UNP E0RVY7
G	-20	GLU	-	expression tag	UNP E0RVY7
G	-19	SER	-	expression tag	UNP E0RVY7
G	-18	THR	-	expression tag	UNP E0RVY7
G	-17	SER	-	expression tag	UNP E0RVY7
G	-16	LEU	-	expression tag	UNP E0RVY7
G	-15	TYR	-	expression tag	UNP E0RVY7
G	-14	LYS	-	expression tag	UNP E0RVY7
G	-13	LYS	-	expression tag	UNP E0RVY7
G	-12	ALA	-	expression tag	UNP E0RVY7
G	-11	GLY	-	expression tag	UNP E0RVY7
G	-10	PHE	-	expression tag	UNP E0RVY7
G	-9	GLU	-	expression tag	UNP E0RVY7
G	-8	ASN	-	expression tag	UNP E0RVY7
G	-7	LEU	-	expression tag	UNP E0RVY7

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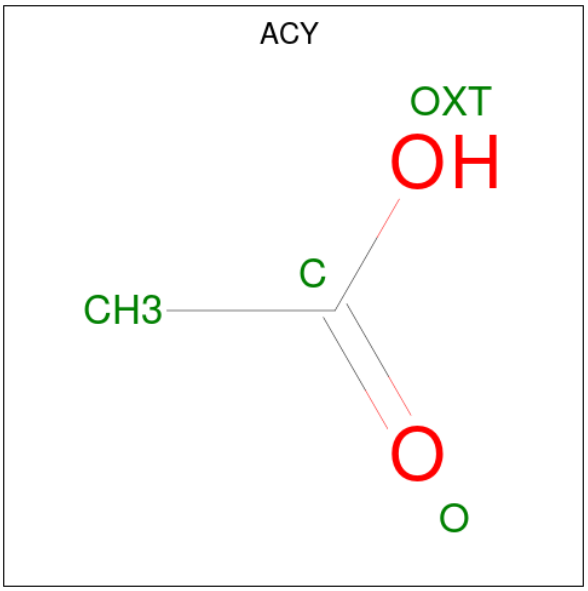
Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	TYR	-	expression tag	UNP E0RVY7
G	-5	PHE	-	expression tag	UNP E0RVY7
G	-4	GLN	-	expression tag	UNP E0RVY7
G	-3	GLY	-	expression tag	UNP E0RVY7
G	-2	SER	-	expression tag	UNP E0RVY7
G	-1	GLY	-	expression tag	UNP E0RVY7
G	0	ALA	-	expression tag	UNP E0RVY7
G	351	ALA	HIS	engineered mutation	UNP E0RVY7
H	-31	MET	-	expression tag	UNP E0RVY7
H	-30	SER	-	expression tag	UNP E0RVY7
H	-29	TYR	-	expression tag	UNP E0RVY7
H	-28	TYR	-	expression tag	UNP E0RVY7
H	-27	HIS	-	expression tag	UNP E0RVY7
H	-26	HIS	-	expression tag	UNP E0RVY7
H	-25	HIS	-	expression tag	UNP E0RVY7
H	-24	HIS	-	expression tag	UNP E0RVY7
H	-23	HIS	-	expression tag	UNP E0RVY7
H	-22	HIS	-	expression tag	UNP E0RVY7
H	-21	LEU	-	expression tag	UNP E0RVY7
H	-20	GLU	-	expression tag	UNP E0RVY7
H	-19	SER	-	expression tag	UNP E0RVY7
H	-18	THR	-	expression tag	UNP E0RVY7
H	-17	SER	-	expression tag	UNP E0RVY7
H	-16	LEU	-	expression tag	UNP E0RVY7
H	-15	TYR	-	expression tag	UNP E0RVY7
H	-14	LYS	-	expression tag	UNP E0RVY7
H	-13	LYS	-	expression tag	UNP E0RVY7
H	-12	ALA	-	expression tag	UNP E0RVY7
H	-11	GLY	-	expression tag	UNP E0RVY7
H	-10	PHE	-	expression tag	UNP E0RVY7
H	-9	GLU	-	expression tag	UNP E0RVY7
H	-8	ASN	-	expression tag	UNP E0RVY7
H	-7	LEU	-	expression tag	UNP E0RVY7
H	-6	TYR	-	expression tag	UNP E0RVY7
H	-5	PHE	-	expression tag	UNP E0RVY7
H	-4	GLN	-	expression tag	UNP E0RVY7
H	-3	GLY	-	expression tag	UNP E0RVY7
H	-2	SER	-	expression tag	UNP E0RVY7
H	-1	GLY	-	expression tag	UNP E0RVY7
H	0	ALA	-	expression tag	UNP E0RVY7
H	351	ALA	HIS	engineered mutation	UNP E0RVY7

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	E	1	4	2	2	0	0
			Total	C	O		
2	E	1	4	2	2	0	0
			Total	C	O		
2	E	1	4	2	2	0	0
			Total	C	O		
2	F	1	4	2	2	0	0

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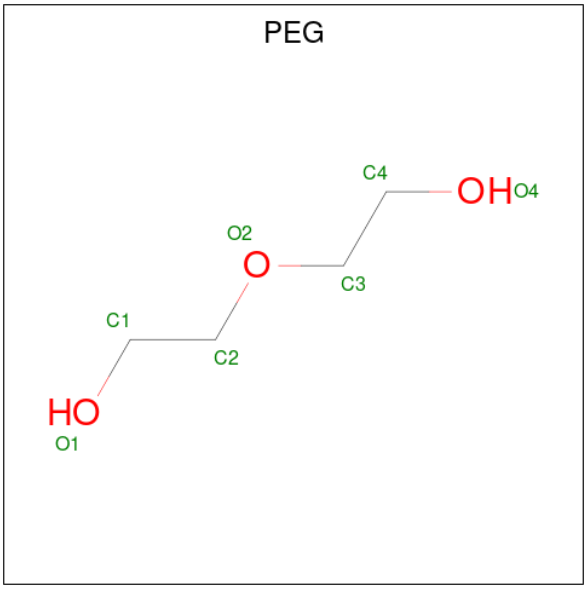
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	F	1	4	2	2		0	0
			Total	C	O			
2	F	1	4	2	2		0	0
			Total	C	O			
2	G	1	4	2	2		0	0
			Total	C	O			
2	G	1	4	2	2		0	0
			Total	C	O			
2	H	1	4	2	2		0	0
			Total	C	O			
2	H	1	4	2	2		0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	7	4	3		0	0
			Total	C	O			
3	D	1	7	4	3		0	0
			Total	C	O			
3	E	1	7	4	3		0	0
			Total	C	O			
3	E	1	7	4	3		0	0
			Total	C	O			
3	G	1	7	4	3		0	0

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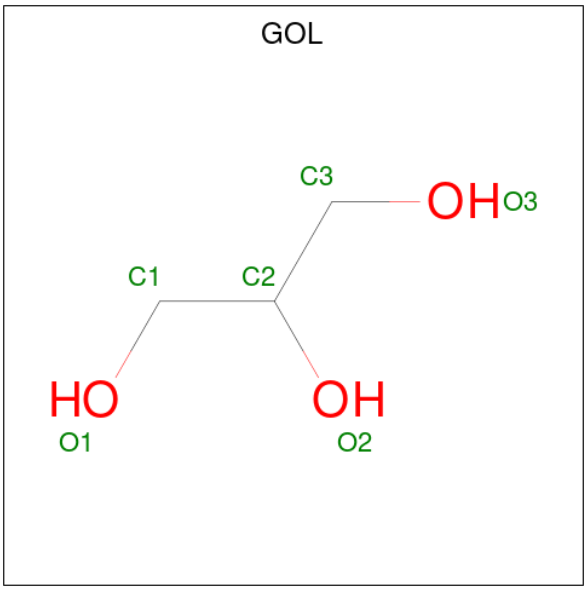
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 7 4 3	0	0
3	H	1	Total C O 7 4 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	231	Total O 231 231	0	0
6	B	233	Total O 233 233	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	C	240	240	240	0	0
			Total	O		
6	D	200	200	200	0	0
			Total	O		
6	E	228	228	228	0	0
			Total	O		
6	F	210	210	210	0	0
			Total	O		
6	G	197	197	197	0	0
			Total	O		
6	H	168	168	168	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: Acetyl-xylan esterase Est2A

Chain A: 78% 12% • 9%

MET SER TYR TYR HIS HIS HIS HIS HIS HIS LEU GLU SER THR SER LEU TYR LYS LYS ALA GLY PHE GLU ASN LEU TYR PHE GLN GLY SER GLY ALA MET SER VAL L4 I9 S10 S13 K25 Q28 V39 V42 V43 L48 W49 L52 L78 H82

C85 L86 Q105 N108 F120 K121 Q127 L136 E147 W158 Y162 M163 Y181 H182 L183 Q186 G187 G188 W189 D196 N197 D198 V199 K215 G216 E217 G243 T244 V247 N257 P258 D259 M266 N269 T270 D271 G272 T273 L280 S305

L313 N314 E331 F336 Q337 M343 H349 K371 F375 GLU

• Molecule 1: Acetyl-xylan esterase Est2A

Chain B: 80% 10% • 9%

MET SER TYR TYR HIS HIS HIS HIS HIS HIS LEU GLU SER THR SER LEU TYR LYS LYS ALA GLY PHE GLU ASN LEU TYR PHE GLN GLY SER GLY ALA MET SER VAL L4 I9 S13 V39 V42 L48 W49 L52 L78 H82 C85 Q105 F120 K121

Q127 D141 S142 E147 D157 W158 Y162 M163 L183 Q186 G187 G188 N197 D198 V199 W233 N245 D246 V247 N257 P258 D259 M266 L280 S305 D312 L313 N314 E331 F336 Q337 M343 H349 K371 W374 F375 GLU

• Molecule 1: Acetyl-xylan esterase Est2A

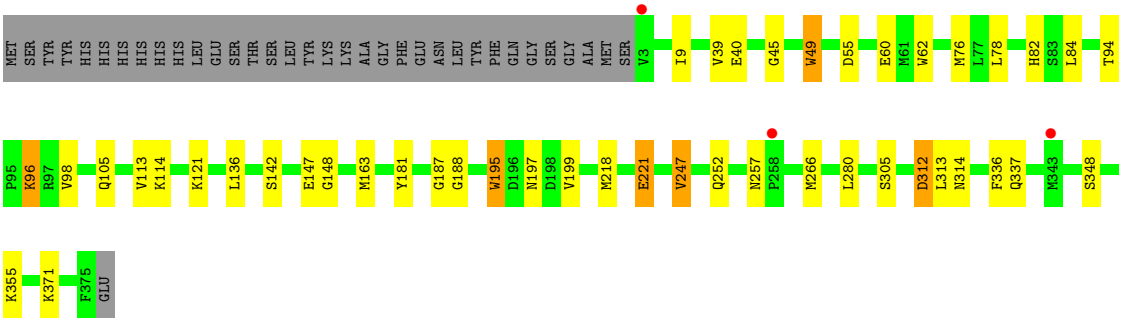
Chain C: 80% 10% • 9%

MET SER TYR TYR HIS HIS HIS HIS HIS HIS LEU GLU SER THR SER LEU TYR LYS LYS ALA GLY PHE GLU ASN LEU TYR PHE GLN GLY SER GLY ALA MET SER VAL L4 I9 G21 F34 N35 V39 I50 D51 L52 W62 F71 M76 L77 L78 H82 S83

L84 Q105 N108 L136 W158 Y162 Y181 H182 L183 Q186 G187 G188 N197 K215 G216 E217 W233 V247 N257 P258 D259 M266 T273 R274 L280 W304 S305 D312 L313 F336 Q337 H349 K371 W374 F375 GLU

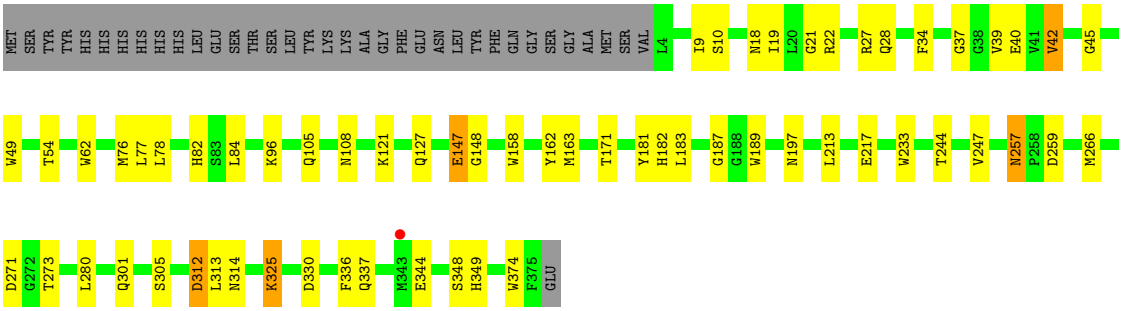
• Molecule 1: Acetyl-xylan esterase Est2A

Chain D: % 80% 10% • 9%



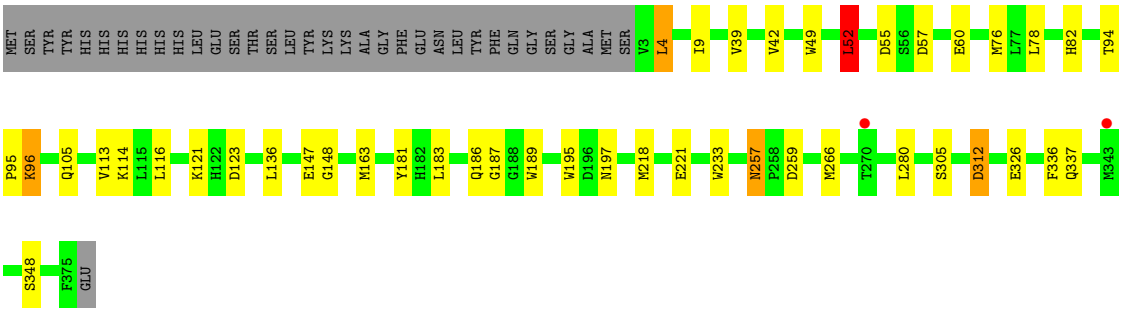
- Molecule 1: Acetyl-xylan esterase Est2A

Chain E: 76% 14% • 9%



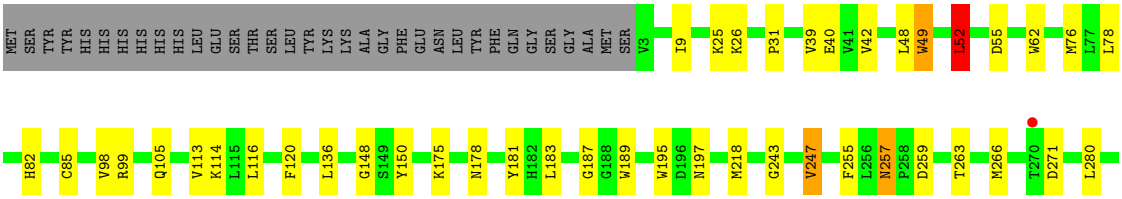
- Molecule 1: Acetyl-xylan esterase Est2A

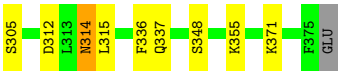
Chain F: 80% 10% • 9%



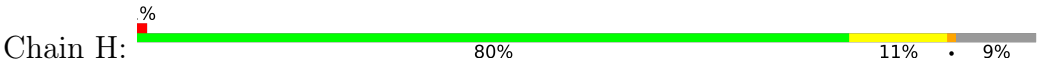
- Molecule 1: Acetyl-xylan esterase Est2A

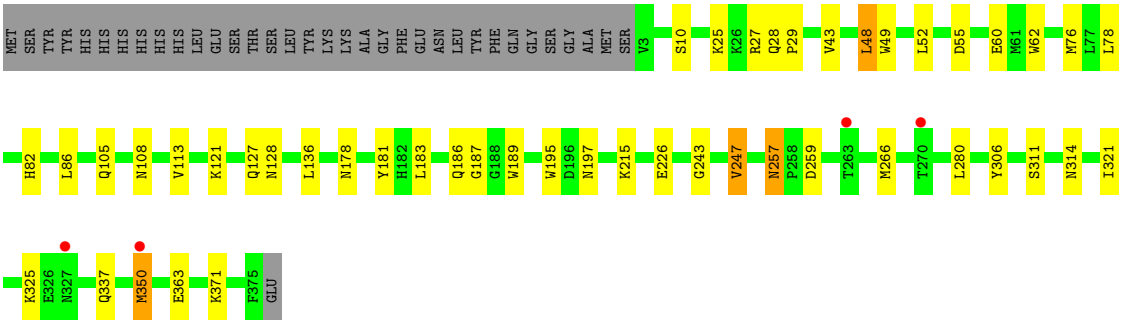
Chain G: 78% 12% • 9%





• Molecule 1: Acetyl-xylan esterase Est2A





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	90.11Å 95.79Å 98.79Å 89.96° 99.74° 92.50°	Depositor
Resolution (Å)	97.36 – 2.00 71.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (97.36-2.00) 98.2 (71.92-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.190 , 0.224 0.190 , 0.224	Depositor DCC
R_{free} test set	10845 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.067 for -h,k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25485	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, CL, PEG, GOL

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	0.50	2/3019 (0.1%)	0.55	0/4086
1	B	0.50	3/3019 (0.1%)	0.55	1/4086 (0.0%)
1	C	0.51	5/3019 (0.2%)	0.56	1/4086 (0.0%)
1	D	0.49	3/3026 (0.1%)	0.55	0/4096
1	E	0.50	4/3019 (0.1%)	0.55	0/4086
1	F	0.50	3/3026 (0.1%)	0.55	1/4096 (0.0%)
1	G	0.50	3/3026 (0.1%)	0.56	1/4096 (0.0%)
1	H	0.49	3/3026 (0.1%)	0.55	0/4096
All	All	0.50	26/24180 (0.1%)	0.55	4/32728 (0.0%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	195	TRP	CD2-CE2	5.27	1.47	1.41
1	D	49	TRP	CD2-CE2	5.23	1.47	1.41
1	E	158	TRP	CD2-CE2	5.22	1.47	1.41
1	G	189	TRP	CD2-CE2	5.20	1.47	1.41
1	C	158	TRP	CD2-CE2	5.18	1.47	1.41
1	E	233	TRP	CD2-CE2	5.14	1.47	1.41
1	C	233	TRP	CD2-CE2	5.13	1.47	1.41
1	C	374	TRP	CD2-CE2	5.13	1.47	1.41
1	F	233	TRP	CD2-CE2	5.12	1.47	1.41
1	C	62	TRP	CD2-CE2	5.11	1.47	1.41
1	A	158	TRP	CD2-CE2	5.11	1.47	1.41
1	A	189	TRP	CD2-CE2	5.11	1.47	1.41
1	H	189	TRP	CD2-CE2	5.10	1.47	1.41
1	H	195	TRP	CD2-CE2	5.10	1.47	1.41
1	E	374	TRP	CD2-CE2	5.09	1.47	1.41
1	B	158	TRP	CD2-CE2	5.08	1.47	1.41
1	D	195	TRP	CD2-CE2	5.08	1.47	1.41
1	E	189	TRP	CD2-CE2	5.07	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	374	TRP	CD2-CE2	5.06	1.47	1.41
1	F	195	TRP	CD2-CE2	5.05	1.47	1.41
1	G	49	TRP	CD2-CE2	5.05	1.47	1.41
1	D	62	TRP	CD2-CE2	5.04	1.47	1.41
1	H	62	TRP	CD2-CE2	5.03	1.47	1.41
1	C	304	TRP	CD2-CE2	5.03	1.47	1.41
1	B	233	TRP	CD2-CE2	5.02	1.47	1.41
1	F	189	TRP	CD2-CE2	5.01	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	52	LEU	CA-CB-CG	5.76	128.55	115.30
1	F	52	LEU	CA-CB-CG	5.70	128.41	115.30
1	C	52	LEU	CA-CB-CG	5.62	128.23	115.30
1	B	52	LEU	CA-CB-CG	5.23	127.33	115.30

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	2951	0	2853	51	0
1	B	2951	0	2853	42	0
1	C	2951	0	2853	44	0
1	D	2958	0	2862	31	0
1	E	2951	0	2853	49	0
1	F	2958	0	2862	31	0
1	G	2958	0	2862	37	0
1	H	2958	0	2862	28	0
2	A	8	0	6	3	0
2	B	8	0	6	16	0
2	C	8	0	6	1	0
2	D	16	0	12	1	0
2	E	12	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	12	0	9	0	0
2	G	8	0	6	0	0
2	H	8	0	6	0	0
3	A	7	0	10	1	0
3	D	7	0	10	4	0
3	E	14	0	20	14	0
3	G	14	0	20	8	0
3	H	7	0	10	0	0
4	A	1	0	0	0	0
5	C	6	0	8	12	0
5	G	6	0	8	3	0
6	A	231	0	0	4	0
6	B	233	0	0	1	0
6	C	240	0	0	1	0
6	D	200	0	0	2	0
6	E	228	0	0	3	0
6	F	210	0	0	2	0
6	G	197	0	0	2	0
6	H	168	0	0	0	0
All	All	25485	0	23006	301	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 6.

All (301) 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:76:MET:CE	1:G:85:CYS:HB3	1.65	1.27
1:C:21:GLY:HA2	5:C:403:GOL:H31	1.20	1.16
1:B:85:CYS:HB3	1:D:76:MET:HE1	1.28	1.11
1:C:76:MET:HE1	1:G:85:CYS:HB3	1.34	1.10
1:C:182:HIS:HA	5:C:403:GOL:H32	1.26	1.10
1:E:34:PHE:HB2	3:E:405:PEG:H21	1.32	1.03
1:C:76:MET:HE2	1:G:85:CYS:HB3	1.37	1.02
1:A:85:CYS:HB3	1:F:76:MET:HE1	1.40	1.01
1:E:247:VAL:HG12	1:E:313:LEU:HD13	1.46	0.98
1:A:314:ASN:HD21	1:A:337:GLN:NE2	1.64	0.95
1:C:21:GLY:CA	5:C:403:GOL:H31	2.00	0.91
1:B:141:ASP:HB2	2:B:401:ACY:H1	1.51	0.90
1:E:9:ILE:HD11	1:E:39:VAL:HG11	1.54	0.90
1:A:314:ASN:HD21	1:A:337:GLN:HE21	0.90	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:ASN:HD22	3:G:404:PEG:H32	1.36	0.89
1:A:52:LEU:C	1:A:52:LEU:HD23	1.93	0.88
1:D:94:THR:HB	3:D:403:PEG:H11	1.54	0.88
1:B:9:ILE:HD11	1:B:39:VAL:HG11	1.56	0.87
1:G:150:TYR:HA	5:G:405:GOL:H12	1.54	0.87
1:C:21:GLY:HA2	5:C:403:GOL:C3	2.03	0.86
1:B:245:ASN:HD21	2:B:401:ACY:H3	1.40	0.86
1:B:188:GLY:H	2:B:401:ACY:H3	1.41	0.85
1:E:22:ARG:H	3:E:405:PEG:H11	1.41	0.85
1:G:175:LYS:HA	3:G:404:PEG:H11	1.55	0.85
1:B:245:ASN:HD21	2:B:401:ACY:CH3	1.91	0.83
1:D:105:GLN:HE22	1:D:187:GLY:H	1.22	0.83
1:A:52:LEU:C	1:A:52:LEU:CD2	2.47	0.83
1:A:314:ASN:ND2	1:A:337:GLN:HE21	1.75	0.83
1:C:76:MET:HE1	1:G:85:CYS:CB	2.07	0.82
1:F:105:GLN:HE22	1:F:187:GLY:H	1.27	0.82
1:B:105:GLN:HE22	1:B:187:GLY:H	1.28	0.81
1:E:34:PHE:CB	3:E:405:PEG:H21	2.10	0.81
1:C:183:LEU:H	5:C:403:GOL:H11	1.46	0.81
1:E:105:GLN:HE22	1:E:187:GLY:H	1.28	0.80
1:C:105:GLN:HE22	1:C:187:GLY:H	1.29	0.80
1:A:52:LEU:CD2	1:A:52:LEU:O	2.30	0.80
1:C:9:ILE:HD11	1:C:39:VAL:HG11	1.62	0.80
1:G:105:GLN:HE22	1:G:187:GLY:H	1.28	0.80
1:A:105:GLN:HE22	1:A:187:GLY:H	1.30	0.79
1:A:247:VAL:CG1	1:A:313:LEU:HB2	2.13	0.79
1:A:52:LEU:HD23	1:A:52:LEU:O	1.83	0.78
1:C:183:LEU:N	5:C:403:GOL:H11	1.99	0.78
1:D:60:GLU:HG3	1:D:76:MET:HG3	1.66	0.78
1:A:52:LEU:HD21	1:A:82:HIS:HB2	1.66	0.78
1:B:188:GLY:H	2:B:401:ACY:CH3	1.98	0.77
1:D:314:ASN:HD22	1:D:337:GLN:HE22	1.32	0.76
1:C:76:MET:CE	1:G:85:CYS:CB	2.57	0.75
1:C:182:HIS:HA	5:C:403:GOL:C3	2.15	0.74
1:E:314:ASN:HD22	1:E:337:GLN:HE22	1.37	0.73
1:F:60:GLU:HG3	1:F:76:MET:HG3	1.70	0.73
1:E:247:VAL:CG1	1:E:313:LEU:HB2	2.18	0.73
1:A:269:ASN:HD22	1:A:273:THR:HG23	1.54	0.72
1:A:247:VAL:HG12	1:A:313:LEU:HD13	1.71	0.72
1:A:13:SER:H	2:A:402:ACY:H2	1.54	0.71
1:H:105:GLN:HE22	1:H:187:GLY:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:ARG:HH22	3:G:404:PEG:H12	1.57	0.69
1:E:21:GLY:HA2	3:E:405:PEG:H41	1.74	0.69
1:B:147:GLU:OE2	1:B:158:TRP:HZ3	1.75	0.68
1:F:147:GLU:HG2	1:F:163:MET:HG3	1.76	0.67
1:D:78:LEU:O	1:D:82:HIS:HE1	1.77	0.67
1:E:314:ASN:HD22	1:E:337:GLN:NE2	1.92	0.67
1:C:78:LEU:O	1:C:82:HIS:HE1	1.77	0.67
2:A:402:ACY:H1	1:H:127:GLN:HE22	1.59	0.67
1:D:312:ASP:HB2	6:D:696:HOH:O	1.95	0.66
1:B:142:SER:H	2:B:401:ACY:CH3	2.09	0.65
1:A:247:VAL:HG11	1:A:313:LEU:HB2	1.78	0.65
1:B:142:SER:H	2:B:401:ACY:H2	1.62	0.65
1:B:312:ASP:HB2	6:B:503:HOH:O	1.97	0.64
1:H:314:ASN:HD21	1:H:337:GLN:HE22	1.45	0.64
1:A:52:LEU:CD2	1:A:82:HIS:HB2	2.28	0.64
1:D:247:VAL:HG13	1:D:313:LEU:HD13	1.78	0.64
1:E:247:VAL:HG11	1:E:313:LEU:HB2	1.79	0.64
1:F:78:LEU:O	1:F:82:HIS:HE1	1.79	0.63
1:G:78:LEU:O	1:G:82:HIS:HE1	1.82	0.63
1:F:218:MET:O	1:F:221:GLU:HG3	1.99	0.63
1:B:52:LEU:CD2	1:B:82:HIS:HB2	2.29	0.63
1:E:22:ARG:N	3:E:405:PEG:H11	2.14	0.62
1:G:197:ASN:ND2	1:G:266:MET:H	1.97	0.62
1:H:350:MET:CE	1:H:350:MET:HA	2.30	0.62
1:G:178:ASN:HA	3:G:404:PEG:H32	1.82	0.62
1:A:52:LEU:O	1:A:52:LEU:HD22	2.00	0.61
1:B:141:ASP:HB2	2:B:401:ACY:CH3	2.27	0.61
1:D:9:ILE:HD11	1:D:39:VAL:HG11	1.82	0.61
1:H:78:LEU:O	1:H:82:HIS:HE1	1.84	0.61
1:D:78:LEU:O	1:D:82:HIS:CE1	2.54	0.61
1:A:271:ASP:HB3	1:A:273:THR:HG22	1.82	0.61
1:A:85:CYS:HB3	1:F:76:MET:CE	2.24	0.61
1:B:42:VAL:HG22	1:B:127:GLN:HB2	1.82	0.60
1:F:9:ILE:HD11	1:F:39:VAL:HG11	1.83	0.60
1:A:197:ASN:ND2	1:A:266:MET:H	1.98	0.60
1:E:197:ASN:ND2	1:E:266:MET:H	1.99	0.60
1:C:162:TYR:CD2	1:C:349:HIS:HE1	2.19	0.60
1:E:247:VAL:CG1	1:E:313:LEU:HD13	2.28	0.59
1:B:142:SER:HB3	2:B:401:ACY:H2	1.85	0.59
1:B:147:GLU:HG2	1:B:163:MET:HG3	1.85	0.59
1:C:197:ASN:ND2	1:C:266:MET:H	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:CYS:CB	1:D:76:MET:HE1	2.18	0.58
1:F:52:LEU:HD22	1:F:82:HIS:HB2	1.86	0.58
1:F:197:ASN:ND2	1:F:266:MET:H	2.03	0.57
2:A:402:ACY:CH3	1:H:127:GLN:HE22	2.16	0.57
1:B:78:LEU:O	1:B:82:HIS:CE1	2.57	0.57
1:B:147:GLU:OE2	1:B:158:TRP:CZ3	2.57	0.57
1:H:78:LEU:O	1:H:82:HIS:CE1	2.58	0.57
1:A:9:ILE:HD11	1:A:39:VAL:HG11	1.86	0.57
1:B:314:ASN:OD1	1:B:337:GLN:NE2	2.38	0.56
1:F:78:LEU:O	1:F:82:HIS:CE1	2.58	0.56
1:H:197:ASN:ND2	1:H:266:MET:H	2.03	0.56
1:A:42:VAL:HG22	1:A:127:GLN:HB2	1.86	0.56
1:A:78:LEU:O	1:A:82:HIS:CE1	2.58	0.56
1:E:37:GLY:N	3:E:405:PEG:H32	2.21	0.56
1:E:181:TYR:O	3:E:405:PEG:H42	2.06	0.56
1:G:99:ARG:NH2	3:G:404:PEG:H12	2.20	0.56
1:A:197:ASN:HD21	1:A:266:MET:H	1.53	0.56
1:E:42:VAL:HG22	1:E:127:GLN:HB2	1.87	0.56
1:C:9:ILE:CD1	1:C:39:VAL:HG11	2.34	0.55
1:C:247:VAL:CG2	1:C:313:LEU:HB2	2.36	0.55
1:A:217:GLU:HG3	6:A:719:HOH:O	2.06	0.55
1:G:48:LEU:HD23	1:G:49:TRP:N	2.22	0.55
1:C:76:MET:HE2	1:G:85:CYS:CB	2.25	0.55
1:F:337:GLN:NE2	1:G:337:GLN:H	2.05	0.55
1:B:188:GLY:N	2:B:401:ACY:H3	2.18	0.55
1:E:54:THR:HG22	1:E:82:HIS:HE1	1.72	0.55
1:F:60:GLU:CG	1:F:76:MET:HG3	2.36	0.54
1:A:269:ASN:HD22	1:A:273:THR:CG2	2.20	0.54
1:G:78:LEU:O	1:G:82:HIS:CE1	2.60	0.54
1:A:197:ASN:HD21	1:A:266:MET:HB2	1.71	0.54
3:A:403:PEG:H21	6:A:656:HOH:O	2.07	0.54
1:B:48:LEU:HD21	1:B:120:PHE:CD2	2.42	0.53
1:H:60:GLU:HG3	1:H:76:MET:HG3	1.90	0.53
1:B:197:ASN:ND2	1:B:266:MET:H	2.06	0.53
1:E:54:THR:HG22	1:E:82:HIS:CE1	2.44	0.53
1:E:78:LEU:O	1:E:82:HIS:CE1	2.61	0.53
1:A:49:TRP:HB2	1:A:121:LYS:HB2	1.90	0.53
1:A:305:SER:HA	1:A:336:PHE:O	2.09	0.53
1:B:141:ASP:CB	2:B:401:ACY:H1	2.32	0.52
1:B:162:TYR:CD2	1:B:349:HIS:HE1	2.28	0.52
1:G:9:ILE:HD11	1:G:39:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:O	1:A:82:HIS:HE1	1.91	0.52
1:D:314:ASN:HD22	1:D:337:GLN:NE2	2.04	0.51
1:A:48:LEU:HD21	1:A:120:PHE:CD2	2.46	0.51
1:C:305:SER:HA	1:C:336:PHE:O	2.11	0.51
1:H:243:GLY:O	1:H:247:VAL:HG12	2.09	0.51
1:H:321:ILE:O	1:H:325:LYS:HB2	2.10	0.51
1:F:55:ASP:O	1:F:113:VAL:HA	2.11	0.50
1:C:62:TRP:CE2	1:C:76:MET:HB3	2.46	0.50
1:C:257:ASN:ND2	1:C:259:ASP:H	2.09	0.50
1:H:350:MET:HE3	1:H:350:MET:H	1.77	0.50
1:G:305:SER:HA	1:G:336:PHE:O	2.12	0.50
1:A:243:GLY:O	1:A:247:VAL:HG13	2.11	0.50
1:A:48:LEU:HD23	1:A:49:TRP:N	2.26	0.50
1:A:244:THR:O	1:A:247:VAL:HG22	2.12	0.50
1:E:77:LEU:HD21	1:E:84:LEU:HD11	1.92	0.50
1:F:4:LEU:HD12	1:F:123:ASP:HB3	1.92	0.50
5:G:405:GOL:C3	6:G:691:HOH:O	2.60	0.50
1:C:108:ASN:HD21	1:C:215:LYS:NZ	2.10	0.50
1:F:312:ASP:HB2	6:F:573:HOH:O	2.11	0.50
1:G:243:GLY:O	1:G:247:VAL:HG12	2.12	0.50
1:C:188:GLY:HA3	2:C:402:ACY:H1	1.94	0.50
1:E:21:GLY:HA2	3:E:405:PEG:H11	1.94	0.50
1:D:96:LYS:HE3	3:D:403:PEG:C1	2.42	0.49
1:G:55:ASP:O	1:G:113:VAL:HA	2.12	0.49
1:G:99:ARG:HH22	3:G:404:PEG:C1	2.23	0.49
1:A:247:VAL:HG12	1:A:313:LEU:HB2	1.93	0.49
1:C:183:LEU:H	5:C:403:GOL:C1	2.20	0.49
1:H:55:ASP:O	1:H:113:VAL:HA	2.13	0.49
1:H:48:LEU:HD13	1:H:86:LEU:HD12	1.95	0.49
1:G:114:LYS:HD3	1:G:218:MET:SD	2.52	0.49
1:B:13:SER:H	2:B:402:ACY:H1	1.76	0.49
1:D:305:SER:HA	1:D:336:PHE:O	2.12	0.49
1:H:257:ASN:ND2	1:H:259:ASP:H	2.10	0.49
1:E:21:GLY:CA	3:E:405:PEG:H22	2.42	0.48
1:B:48:LEU:HD21	1:B:120:PHE:HD2	1.78	0.48
1:D:60:GLU:CG	1:D:76:MET:HG3	2.40	0.48
1:E:162:TYR:CD2	1:E:349:HIS:HE1	2.31	0.48
1:D:197:ASN:ND2	1:D:266:MET:H	2.12	0.48
1:G:314:ASN:HD22	1:G:315:LEU:H	1.61	0.48
1:B:78:LEU:O	1:B:82:HIS:HE1	1.96	0.48
3:G:404:PEG:H31	6:G:604:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TRP:HB2	1:D:121:LYS:HB2	1.94	0.48
1:E:49:TRP:HB2	1:E:121:LYS:HB2	1.96	0.48
1:B:245:ASN:ND2	2:B:401:ACY:H3	2.19	0.48
1:D:96:LYS:HE3	3:D:403:PEG:H12	1.96	0.48
1:C:197:ASN:HD21	1:C:266:MET:H	1.62	0.47
1:E:45:GLY:O	1:E:96:LYS:NZ	2.41	0.47
1:G:197:ASN:HD21	1:G:266:MET:H	1.61	0.47
1:F:257:ASN:ND2	1:F:259:ASP:H	2.12	0.47
1:E:21:GLY:HA3	3:E:405:PEG:H22	1.96	0.47
1:E:171:THR:HB	2:E:402:ACY:H2	1.96	0.47
1:E:147:GLU:HG2	1:E:163:MET:HG2	1.95	0.47
1:E:197:ASN:HD21	1:E:266:MET:H	1.60	0.47
1:H:49:TRP:HB2	1:H:121:LYS:HB2	1.96	0.47
1:C:21:GLY:CA	5:C:403:GOL:C3	2.79	0.47
1:C:34:PHE:CB	5:C:403:GOL:H12	2.44	0.47
1:E:257:ASN:ND2	1:E:259:ASP:H	2.13	0.47
1:G:99:ARG:HH12	3:G:404:PEG:H21	1.80	0.47
1:B:257:ASN:ND2	1:B:259:ASP:H	2.11	0.47
1:D:221:GLU:HG3	6:D:513:HOH:O	2.15	0.46
1:E:182:HIS:HA	3:E:405:PEG:H42	1.97	0.46
1:C:52:LEU:HD11	1:C:84:LEU:HD12	1.96	0.46
1:G:52:LEU:HB2	1:G:116:LEU:O	2.15	0.46
1:A:48:LEU:HD21	1:A:120:PHE:HD2	1.79	0.46
1:H:350:MET:HA	1:H:350:MET:HE3	1.97	0.46
1:B:49:TRP:HB2	1:B:121:LYS:HB2	1.98	0.46
1:D:105:GLN:HG2	1:D:163:MET:SD	2.56	0.46
1:C:312:ASP:HB2	6:C:542:HOH:O	2.16	0.46
1:B:197:ASN:HD21	1:B:266:MET:H	1.64	0.46
1:G:62:TRP:CE2	1:G:76:MET:HB3	2.51	0.45
1:E:18:ASN:HB2	1:E:40:GLU:HB3	1.98	0.45
1:F:136:LEU:O	1:F:181:TYR:HA	2.16	0.45
1:A:147:GLU:HG2	1:A:163:MET:HG3	1.98	0.45
1:B:142:SER:CB	2:B:401:ACY:H2	2.45	0.45
1:E:325:LYS:HB2	1:E:330:ASP:O	2.16	0.45
1:E:312:ASP:HB2	6:E:511:HOH:O	2.16	0.45
1:F:337:GLN:HE22	1:G:337:GLN:H	1.62	0.45
1:H:10:SER:H	1:H:28:GLN:NE2	2.15	0.45
1:D:114:LYS:HD3	1:D:218:MET:SD	2.57	0.45
1:H:136:LEU:O	1:H:181:TYR:HA	2.16	0.45
6:A:519:HOH:O	1:F:96:LYS:CE	2.65	0.44
1:B:48:LEU:HD23	1:B:49:TRP:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:GLU:HG3	1:H:76:MET:CG	2.47	0.44
1:A:331:GLU:HG3	1:C:273:THR:HG21	1.99	0.44
1:B:331:GLU:HG3	1:E:273:THR:HG21	1.99	0.44
1:C:78:LEU:O	1:C:82:HIS:CE1	2.66	0.44
1:E:21:GLY:CA	3:E:405:PEG:H41	2.44	0.44
1:A:337:GLN:H	1:C:337:GLN:NE2	2.15	0.44
1:D:105:GLN:HE22	1:D:187:GLY:N	2.01	0.44
1:A:136:LEU:O	1:A:181:TYR:HA	2.17	0.44
1:B:157:ASP:OD2	3:D:403:PEG:H21	2.16	0.44
1:C:162:TYR:CD2	1:C:349:HIS:CE1	3.04	0.44
1:A:196:ASP:O	1:A:197:ASN:HB2	2.17	0.44
1:D:148:GLY:HA2	1:D:348:SER:OG	2.17	0.44
1:D:188:GLY:HA3	2:D:404:ACY:H3	1.99	0.44
1:D:136:LEU:O	1:D:181:TYR:HA	2.18	0.44
1:E:247:VAL:CG2	6:E:710:HOH:O	2.66	0.44
1:G:257:ASN:ND2	1:G:259:ASP:H	2.16	0.44
1:H:43:VAL:HG21	1:H:48:LEU:HG	2.00	0.44
1:E:10:SER:H	1:E:28:GLN:NE2	2.17	0.43
1:H:197:ASN:HD21	1:H:266:MET:H	1.66	0.43
1:E:301:GLN:NE2	6:E:538:HOH:O	2.48	0.43
1:D:142:SER:HB2	1:D:147:GLU:HB2	2.01	0.43
1:E:21:GLY:HA2	3:E:405:PEG:C1	2.48	0.43
1:F:197:ASN:HD21	1:F:266:MET:H	1.65	0.43
1:H:257:ASN:C	1:H:257:ASN:HD22	2.21	0.43
1:D:40:GLU:HA	1:D:98:VAL:O	2.19	0.43
1:C:257:ASN:C	1:C:257:ASN:HD22	2.21	0.43
1:D:55:ASP:O	1:D:113:VAL:HA	2.18	0.43
1:B:142:SER:H	2:B:401:ACY:H1	1.83	0.43
1:B:257:ASN:C	1:B:257:ASN:HD22	2.21	0.42
1:G:314:ASN:HD22	1:G:315:LEU:N	2.17	0.42
1:A:9:ILE:CD1	1:A:39:VAL:HG11	2.49	0.42
1:E:182:HIS:HA	3:E:405:PEG:C4	2.49	0.42
1:F:49:TRP:HB2	1:F:121:LYS:HB2	2.01	0.42
1:G:136:LEU:O	1:G:181:TYR:HA	2.19	0.42
1:C:247:VAL:HG22	1:C:313:LEU:HD13	2.01	0.42
1:E:305:SER:HA	1:E:336:PHE:O	2.19	0.42
1:C:105:GLN:HE22	1:C:187:GLY:N	2.08	0.42
1:H:28:GLN:HA	1:H:29:PRO:HA	1.96	0.42
1:E:62:TRP:CE2	1:E:76:MET:HB3	2.55	0.42
1:A:181:TYR:HD1	1:A:183:LEU:HD13	1.83	0.42
1:B:247:VAL:CG2	1:B:313:LEU:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ARG:NH2	1:C:312:ASP:OD2	2.52	0.42
1:D:147:GLU:HG2	1:D:163:MET:CG	2.49	0.42
1:E:19:ILE:HD12	1:E:27:ARG:HH21	1.84	0.42
1:E:257:ASN:C	1:E:257:ASN:HD22	2.23	0.42
1:A:162:TYR:CD2	1:A:349:HIS:HE1	2.37	0.42
1:B:245:ASN:HD21	2:B:401:ACY:H1	1.80	0.42
1:C:50:ILE:HG23	1:C:52:LEU:HD12	2.01	0.42
1:D:45:GLY:O	1:D:96:LYS:NZ	2.51	0.42
1:F:305:SER:HA	1:F:336:PHE:O	2.20	0.42
6:A:519:HOH:O	1:F:96:LYS:HE2	2.20	0.41
1:C:136:LEU:O	1:C:181:TYR:HA	2.20	0.41
1:C:35:ASN:O	5:C:403:GOL:O2	2.34	0.41
1:F:52:LEU:HB2	1:F:116:LEU:O	2.20	0.41
1:F:57:ASP:HB3	6:F:698:HOH:O	2.19	0.41
1:F:114:LYS:HD3	1:F:218:MET:SD	2.60	0.41
1:H:60:GLU:CG	1:H:76:MET:HG3	2.50	0.41
1:A:4:LEU:HD23	1:A:121:LYS:HB3	2.02	0.41
1:A:257:ASN:ND2	1:A:259:ASP:H	2.17	0.41
1:C:21:GLY:HA2	5:C:403:GOL:C2	2.48	0.41
1:A:314:ASN:ND2	1:A:337:GLN:NE2	2.48	0.41
1:D:195:TRP:O	1:D:252:GLN:HG3	2.20	0.41
1:H:306:TYR:CE2	1:H:311:SER:HA	2.56	0.41
1:C:71:PHE:O	5:G:405:GOL:H11	2.20	0.41
1:F:257:ASN:C	1:F:257:ASN:HD22	2.24	0.41
1:G:255:PHE:O	1:G:263:THR:HA	2.20	0.41
1:A:10:SER:H	1:A:28:GLN:NE2	2.18	0.41
1:A:43:VAL:HG21	1:A:48:LEU:HD12	2.02	0.41
1:E:108:ASN:HD22	1:E:213:LEU:HA	1.85	0.41
1:G:40:GLU:HA	1:G:98:VAL:O	2.21	0.41
1:H:25:LYS:HD2	1:H:226:GLU:OE1	2.21	0.41
1:H:108:ASN:HD21	1:H:215:LYS:NZ	2.19	0.41
1:F:60:GLU:HG3	1:F:76:MET:CG	2.44	0.41
1:F:148:GLY:HA2	1:F:348:SER:OG	2.21	0.41
1:E:244:THR:O	1:E:247:VAL:HG22	2.21	0.40
1:G:48:LEU:HD21	1:G:120:PHE:HD2	1.86	0.40
1:G:148:GLY:HA2	1:G:348:SER:OG	2.21	0.40
1:E:148:GLY:HA2	1:E:348:SER:OG	2.21	0.40
1:B:305:SER:HA	1:B:336:PHE:O	2.20	0.40
1:F:94:THR:HA	1:F:95:PRO:HD3	1.97	0.40
1:A:48:LEU:HD22	1:A:86:LEU:HD12	2.03	0.40
1:A:108:ASN:HD21	1:A:215:LYS:NZ	2.18	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	370/408 (91%)	360 (97%)	10 (3%)	0	100	100
1	B	370/408 (91%)	360 (97%)	10 (3%)	0	100	100
1	C	370/408 (91%)	362 (98%)	8 (2%)	0	100	100
1	D	371/408 (91%)	362 (98%)	9 (2%)	0	100	100
1	E	370/408 (91%)	359 (97%)	11 (3%)	0	100	100
1	F	371/408 (91%)	362 (98%)	9 (2%)	0	100	100
1	G	371/408 (91%)	364 (98%)	7 (2%)	0	100	100
1	H	371/408 (91%)	363 (98%)	8 (2%)	0	100	100
All	All	2964/3264 (91%)	2892 (98%)	72 (2%)	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	320/351 (91%)	308 (96%)	12 (4%)	33	31
1	B	320/351 (91%)	311 (97%)	9 (3%)	43	44
1	C	320/351 (91%)	312 (98%)	8 (2%)	47	49
1	D	321/351 (92%)	311 (97%)	10 (3%)	40	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	320/351 (91%)	310 (97%)	10 (3%)	40	40
1	F	321/351 (92%)	311 (97%)	10 (3%)	40	40
1	G	321/351 (92%)	307 (96%)	14 (4%)	28	25
1	H	321/351 (92%)	308 (96%)	13 (4%)	31	29
All	All	2564/2808 (91%)	2478 (97%)	86 (3%)	37	36

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	42	VAL
1	A	52	LEU
1	A	183	LEU
1	A	186	GLN
1	A	199	VAL
1	A	257	ASN
1	A	266	MET
1	A	271	ASP
1	A	280	LEU
1	A	343	MET
1	A	371	LYS
1	B	52	LEU
1	B	147	GLU
1	B	183	LEU
1	B	186	GLN
1	B	199	VAL
1	B	257	ASN
1	B	280	LEU
1	B	312	ASP
1	B	371	LYS
1	C	52	LEU
1	C	183	LEU
1	C	186	GLN
1	C	217	GLU
1	C	257	ASN
1	C	280	LEU
1	C	312	ASP
1	C	371	LYS
1	D	84	LEU
1	D	96	LYS
1	D	199	VAL

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Mol	Chain	Res	Type
1	D	221	GLU
1	D	247	VAL
1	D	257	ASN
1	D	280	LEU
1	D	312	ASP
1	D	355	LYS
1	D	371	LYS
1	E	42	VAL
1	E	147	GLU
1	E	183	LEU
1	E	217	GLU
1	E	257	ASN
1	E	271	ASP
1	E	280	LEU
1	E	312	ASP
1	E	325	LYS
1	E	344	GLU
1	F	4	LEU
1	F	42	VAL
1	F	52	LEU
1	F	96	LYS
1	F	183	LEU
1	F	186	GLN
1	F	257	ASN
1	F	280	LEU
1	F	312	ASP
1	F	326	GLU
1	G	25	LYS
1	G	26	LYS
1	G	31	PRO
1	G	42	VAL
1	G	52	LEU
1	G	183	LEU
1	G	247	VAL
1	G	257	ASN
1	G	271	ASP
1	G	280	LEU
1	G	312	ASP
1	G	314	ASN
1	G	355	LYS
1	G	371	LYS
1	H	27	ARG

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Mol	Chain	Res	Type
1	H	48	LEU
1	H	52	LEU
1	H	128	ASN
1	H	178	ASN
1	H	183	LEU
1	H	186	GLN
1	H	247	VAL
1	H	257	ASN
1	H	280	LEU
1	H	350	MET
1	H	363	GLU
1	H	371	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	18	ASN
1	A	28	GLN
1	A	82	HIS
1	A	105	GLN
1	A	108	ASN
1	A	128	ASN
1	A	197	ASN
1	A	252	GLN
1	A	257	ASN
1	A	269	ASN
1	A	297	ASN
1	A	301	GLN
1	A	337	GLN
1	A	358	GLN
1	A	370	ASN
1	B	11	ASN
1	B	18	ASN
1	B	28	GLN
1	B	82	HIS
1	B	105	GLN
1	B	108	ASN
1	B	128	ASN
1	B	197	ASN
1	B	245	ASN
1	B	252	GLN

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Mol	Chain	Res	Type
1	B	257	ASN
1	B	297	ASN
1	B	301	GLN
1	B	314	ASN
1	B	337	GLN
1	C	11	ASN
1	C	18	ASN
1	C	28	GLN
1	C	82	HIS
1	C	105	GLN
1	C	108	ASN
1	C	128	ASN
1	C	197	ASN
1	C	257	ASN
1	C	297	ASN
1	C	301	GLN
1	C	314	ASN
1	C	337	GLN
1	C	359	ASN
1	D	11	ASN
1	D	18	ASN
1	D	28	GLN
1	D	82	HIS
1	D	105	GLN
1	D	108	ASN
1	D	128	ASN
1	D	197	ASN
1	D	252	GLN
1	D	257	ASN
1	D	297	ASN
1	D	301	GLN
1	D	337	GLN
1	D	359	ASN
1	E	11	ASN
1	E	18	ASN
1	E	28	GLN
1	E	82	HIS
1	E	105	GLN
1	E	108	ASN
1	E	128	ASN
1	E	197	ASN
1	E	252	GLN

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Mol	Chain	Res	Type
1	E	257	ASN
1	E	297	ASN
1	E	301	GLN
1	E	337	GLN
1	E	359	ASN
1	F	11	ASN
1	F	18	ASN
1	F	28	GLN
1	F	82	HIS
1	F	105	GLN
1	F	108	ASN
1	F	128	ASN
1	F	197	ASN
1	F	257	ASN
1	F	297	ASN
1	F	301	GLN
1	F	314	ASN
1	F	337	GLN
1	F	359	ASN
1	G	11	ASN
1	G	18	ASN
1	G	28	GLN
1	G	82	HIS
1	G	105	GLN
1	G	108	ASN
1	G	128	ASN
1	G	178	ASN
1	G	197	ASN
1	G	252	GLN
1	G	257	ASN
1	G	297	ASN
1	G	301	GLN
1	G	314	ASN
1	G	337	GLN
1	G	345	ASN
1	G	370	ASN
1	H	11	ASN
1	H	18	ASN
1	H	28	GLN
1	H	82	HIS
1	H	105	GLN
1	H	108	ASN

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Mol	Chain	Res	Type
1	H	127	GLN
1	H	128	ASN
1	H	197	ASN
1	H	252	GLN
1	H	257	ASN
1	H	297	ASN
1	H	301	GLN
1	H	314	ASN
1	H	327	ASN
1	H	359	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 1 is monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PEG	G	404	-	6,6,6	0.43	0	5,5,5	0.25	0
2	ACY	F	401	-	3,3,3	0.80	0	3,3,3	0.65	0
2	ACY	B	401	-	3,3,3	0.57	0	3,3,3	1.06	0
2	ACY	D	404	-	3,3,3	0.79	0	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ACY	A	402	-	3,3,3	0.77	0	3,3,3	0.78	0
5	GOL	G	405	-	5,5,5	0.28	0	5,5,5	0.63	0
3	PEG	A	403	-	6,6,6	0.42	0	5,5,5	0.42	0
2	ACY	F	403	-	3,3,3	0.79	0	3,3,3	0.69	0
3	PEG	E	404	-	6,6,6	0.43	0	5,5,5	0.37	0
3	PEG	G	403	-	6,6,6	0.52	0	5,5,5	0.31	0
2	ACY	G	401	-	3,3,3	0.79	0	3,3,3	0.66	0
2	ACY	H	402	-	3,3,3	0.83	0	3,3,3	0.59	0
3	PEG	D	403	-	6,6,6	0.44	0	5,5,5	0.23	0
2	ACY	C	402	-	3,3,3	0.68	0	3,3,3	1.08	0
2	ACY	D	405	-	3,3,3	0.73	0	3,3,3	0.79	0
2	ACY	H	401	-	3,3,3	0.71	0	3,3,3	0.74	0
2	ACY	D	401	-	3,3,3	0.68	0	3,3,3	0.84	0
3	PEG	H	403	-	6,6,6	0.44	0	5,5,5	0.34	0
2	ACY	E	402	-	3,3,3	0.81	0	3,3,3	0.58	0
2	ACY	C	401	-	3,3,3	0.81	0	3,3,3	0.69	0
3	PEG	E	405	-	6,6,6	0.35	0	5,5,5	0.31	0
2	ACY	G	402	-	3,3,3	0.83	0	3,3,3	0.68	0
2	ACY	A	401	-	3,3,3	0.68	0	3,3,3	0.80	0
2	ACY	E	401	-	3,3,3	0.65	0	3,3,3	0.87	0
2	ACY	F	402	-	3,3,3	0.81	0	3,3,3	0.63	0
5	GOL	C	403	-	5,5,5	0.56	0	5,5,5	1.06	0
2	ACY	E	403	-	3,3,3	0.78	0	3,3,3	0.72	0
2	ACY	D	402	-	3,3,3	0.78	0	3,3,3	0.69	0
2	ACY	B	402	-	3,3,3	0.75	0	3,3,3	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	D	403	-	-	4/4/4/4	-
5	GOL	G	405	-	-	4/4/4/4	-
3	PEG	A	403	-	-	1/4/4/4	-
3	PEG	G	404	-	-	2/4/4/4	-
3	PEG	H	403	-	-	1/4/4/4	-
3	PEG	E	404	-	-	2/4/4/4	-
5	GOL	C	403	-	-	0/4/4/4	-
3	PEG	G	403	-	-	3/4/4/4	-
3	PEG	E	405	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	405	GOL	C1-C2-C3-O3
3	D	403	PEG	C1-C2-O2-C3
3	D	403	PEG	O1-C1-C2-O2
3	G	404	PEG	O1-C1-C2-O2
3	E	404	PEG	O2-C3-C4-O4
3	G	403	PEG	O1-C1-C2-O2
3	H	403	PEG	O1-C1-C2-O2
5	G	405	GOL	O1-C1-C2-C3
3	E	405	PEG	O1-C1-C2-O2
5	G	405	GOL	O2-C2-C3-O3
3	A	403	PEG	O2-C3-C4-O4
3	E	405	PEG	C1-C2-O2-C3
3	D	403	PEG	C4-C3-O2-C2
3	E	404	PEG	C1-C2-O2-C3
3	E	405	PEG	O2-C3-C4-O4
3	G	404	PEG	O2-C3-C4-O4
3	G	403	PEG	C4-C3-O2-C2
5	G	405	GOL	O1-C1-C2-O2
3	G	403	PEG	C1-C2-O2-C3
3	E	405	PEG	C4-C3-O2-C2
3	D	403	PEG	O2-C3-C4-O4

There are no ring outliers.

12 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	404	PEG	8	0
2	B	401	ACY	15	0
2	D	404	ACY	1	0
2	A	402	ACY	3	0
5	G	405	GOL	3	0
3	A	403	PEG	1	0
3	D	403	PEG	4	0
2	C	402	ACY	1	0
2	E	402	ACY	1	0
3	E	405	PEG	14	0
5	C	403	GOL	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	402	ACY	1	0

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 (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	372/408 (91%)	-0.32	0	100	100	14, 21, 33, 43	0
1	B	372/408 (91%)	-0.30	1 (0%)	94	93	14, 20, 32, 46	2 (0%)
1	C	372/408 (91%)	-0.28	0	100	100	13, 19, 32, 41	0
1	D	373/408 (91%)	-0.17	3 (0%)	86	85	13, 24, 40, 52	1 (0%)
1	E	372/408 (91%)	-0.31	1 (0%)	94	93	15, 22, 34, 43	1 (0%)
1	F	373/408 (91%)	-0.24	2 (0%)	91	90	14, 23, 38, 52	1 (0%)
1	G	373/408 (91%)	-0.14	1 (0%)	94	93	13, 23, 42, 55	0
1	H	373/408 (91%)	-0.06	4 (1%)	80	79	16, 28, 46, 58	1 (0%)
All	All	2980/3264 (91%)	-0.23	12 (0%)	92	92	13, 22, 38, 58	6 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	270	THR	3.5
1	D	343	MET	2.9
1	F	270	THR	2.8
1	H	327	ASN	2.5
1	D	3	VAL	2.5
1	G	270	THR	2.4
1	H	263	THR	2.3
1	H	350	MET	2.3
1	E	343	MET	2.1
1	B	343	MET	2.1
1	D	258	PRO	2.0
1	F	343	MET	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACY	C	402	4/4	0.51	0.24	32,33,35,36	0
2	ACY	E	403	4/4	0.58	0.28	46,49,50,50	0
3	PEG	G	403	7/7	0.68	0.39	37,42,43,43	0
2	ACY	F	403	4/4	0.72	0.18	36,36,37,37	0
2	ACY	D	404	4/4	0.72	0.18	41,41,43,45	0
3	PEG	E	404	7/7	0.74	0.42	45,48,49,49	0
2	ACY	A	402	4/4	0.78	0.18	36,39,39,41	0
2	ACY	H	402	4/4	0.78	0.17	42,43,43,44	0
3	PEG	H	403	7/7	0.78	0.22	50,50,52,52	0
2	ACY	G	402	4/4	0.80	0.15	37,37,39,40	0
2	ACY	B	402	4/4	0.81	0.15	32,35,36,37	0
3	PEG	G	404	7/7	0.81	0.27	26,29,36,36	0
2	ACY	B	401	4/4	0.81	0.17	17,19,19,20	0
2	ACY	D	402	4/4	0.82	0.14	37,37,38,40	0
2	ACY	E	402	4/4	0.82	0.19	36,38,38,38	0
5	GOL	G	405	6/6	0.83	0.21	21,25,26,28	0
2	ACY	H	401	4/4	0.84	0.17	29,30,31,31	0
2	ACY	D	405	4/4	0.85	0.15	29,30,31,33	0
3	PEG	A	403	7/7	0.86	0.27	38,40,42,42	0
5	GOL	C	403	6/6	0.86	0.28	18,18,19,19	0
2	ACY	F	402	4/4	0.86	0.13	36,38,39,39	0
3	PEG	D	403	7/7	0.87	0.23	25,26,28,29	0
2	ACY	F	401	4/4	0.89	0.17	26,27,27,29	0
2	ACY	A	401	4/4	0.92	0.13	22,22,23,26	0
3	PEG	E	405	7/7	0.93	0.29	19,20,22,22	0
2	ACY	E	401	4/4	0.94	0.13	23,24,24,26	0
2	ACY	D	401	4/4	0.94	0.09	24,25,25,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACY	G	401	4/4	0.95	0.11	23,23,23,24	0
2	ACY	C	401	4/4	0.97	0.09	18,18,19,19	0
4	CL	A	404	1/1	0.99	0.11	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.